Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:12 PM UTC

PDB ID	:	1RWT / pdb_00001rwt
Title	:	Crystal Structure of Spinach Major Light-harvesting complex at 2.72 Angstrom Resolution
Authors	:	Liu, Z.; Yan, H.; Wang, K.; Kuang, T.; Zhang, J.; Gui, L.; An, X.; Chang, W.
Deposited on	:	2003-12-17
Resolution	:	2.72 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

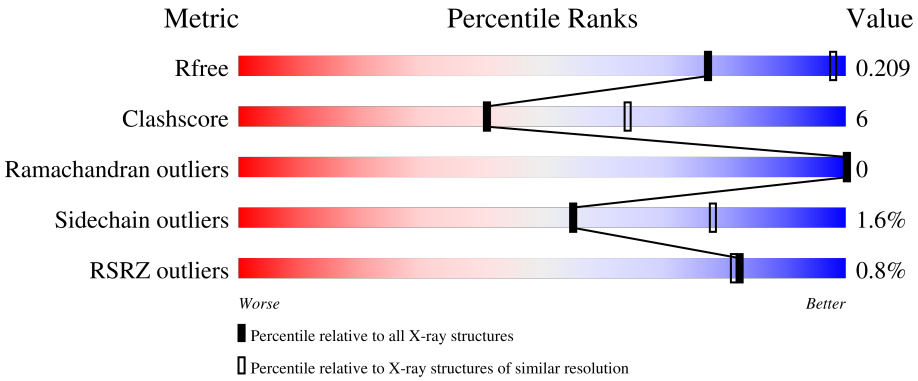
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	232	73% 21% 6%
1	B	232	69% 24% 6%
1	C	232	75% 19% 6%
1	D	232	77% 17% 6%
1	E	232	74% 19% 6%

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Mol	Chain	Length	Quality of chain
1	F	232	72% 22% 6%
1	G	232	75% 18% 6%
1	H	232	74% 20% 6%
1	I	232	75% 19% 6%
1	J	232	81% 12% 6%

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
10	CLA	A	602	X	-	-	-
10	CLA	A	603	X	-	-	-
10	CLA	A	604	X	-	-	-
10	CLA	A	610	X	-	-	-
10	CLA	A	611	X	-	-	-
10	CLA	A	612	X	-	-	-
10	CLA	A	613	X	-	-	-
10	CLA	A	614	X	-	-	-
10	CLA	B	602	X	-	-	-
10	CLA	B	603	X	-	-	-
10	CLA	B	604	X	-	-	-
10	CLA	B	610	X	-	-	-
10	CLA	B	611	X	-	-	-
10	CLA	B	612	X	-	-	-
10	CLA	B	613	X	-	-	-
10	CLA	B	614	X	-	-	-
10	CLA	C	602	X	-	-	-
10	CLA	C	603	X	-	-	-
10	CLA	C	604	X	-	-	-
10	CLA	C	610	X	-	-	-
10	CLA	C	611	X	-	-	-
10	CLA	C	612	X	-	-	-
10	CLA	C	613	X	-	-	-
10	CLA	C	614	X	-	-	-
10	CLA	D	602	X	-	-	-
10	CLA	D	603	X	-	-	-
10	CLA	D	604	X	-	-	-
10	CLA	D	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	D	611	X	-	-	-
10	CLA	D	612	X	-	-	-
10	CLA	D	613	X	-	-	-
10	CLA	D	614	X	-	-	-
10	CLA	E	602	X	-	-	-
10	CLA	E	603	X	-	-	-
10	CLA	E	604	X	-	-	-
10	CLA	E	610	X	-	-	-
10	CLA	E	611	X	-	-	-
10	CLA	E	612	X	-	-	-
10	CLA	E	613	X	-	-	-
10	CLA	E	614	X	-	-	-
10	CLA	F	602	X	-	-	-
10	CLA	F	603	X	-	-	-
10	CLA	F	604	X	-	-	-
10	CLA	F	610	X	-	-	-
10	CLA	F	611	X	-	-	-
10	CLA	F	612	X	-	-	-
10	CLA	F	613	X	-	-	-
10	CLA	F	614	X	-	-	-
10	CLA	G	602	X	-	-	-
10	CLA	G	603	X	-	-	-
10	CLA	G	604	X	-	-	-
10	CLA	G	610	X	-	-	-
10	CLA	G	611	X	-	-	-
10	CLA	G	612	X	-	-	-
10	CLA	G	613	X	-	-	-
10	CLA	G	614	X	-	-	-
10	CLA	H	602	X	-	-	-
10	CLA	H	603	X	-	-	-
10	CLA	H	604	X	-	-	-
10	CLA	H	610	X	-	-	-
10	CLA	H	611	X	-	-	-
10	CLA	H	612	X	-	-	-
10	CLA	H	613	X	-	-	-
10	CLA	H	614	X	-	-	-
10	CLA	I	602	X	-	-	-
10	CLA	I	603	X	-	-	-
10	CLA	I	604	X	-	-	-
10	CLA	I	610	X	-	-	-
10	CLA	I	611	X	-	-	-
10	CLA	I	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	I	613	X	-	-	-
10	CLA	I	614	X	-	-	-
10	CLA	J	602	X	-	-	-
10	CLA	J	603	X	-	-	-
10	CLA	J	604	X	-	-	-
10	CLA	J	610	X	-	-	-
10	CLA	J	611	X	-	-	-
10	CLA	J	612	X	-	-	-
10	CLA	J	613	X	-	-	-
10	CLA	J	614	X	-	-	-
3	NA	A	634	-	-	-	X
8	DGD	A	632	X	-	-	-
8	DGD	B	1632	X	-	-	-
8	DGD	B	2632	X	-	-	-
8	DGD	D	3632	X	-	-	-
8	DGD	D	5632	X	-	-	-
8	DGD	E	4632	X	-	-	-
8	DGD	G	9632	X	-	-	-
8	DGD	H	6632	X	-	-	-
8	DGD	H	7632	X	-	-	-
8	DGD	I	8632	X	-	-	-
9	CHL	A	601	X	-	-	-
9	CHL	A	605	X	-	-	-
9	CHL	A	606	X	-	-	-
9	CHL	A	607	X	-	-	-
9	CHL	A	608	X	-	-	-
9	CHL	A	609	X	-	-	-
9	CHL	B	601	X	-	-	-
9	CHL	B	605	X	-	-	-
9	CHL	B	606	X	-	-	-
9	CHL	B	607	X	-	-	-
9	CHL	B	608	X	-	-	-
9	CHL	B	609	X	-	-	-
9	CHL	C	601	X	-	-	-
9	CHL	C	605	X	-	-	-
9	CHL	C	606	X	-	-	-
9	CHL	C	607	X	-	-	-
9	CHL	C	608	X	-	-	-
9	CHL	C	609	X	-	-	-
9	CHL	D	601	X	-	-	-
9	CHL	D	605	X	-	-	-
9	CHL	D	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CHL	D	607	X	-	-	-
9	CHL	D	608	X	-	-	-
9	CHL	D	609	X	-	-	-
9	CHL	E	601	X	-	-	-
9	CHL	E	605	X	-	-	-
9	CHL	E	606	X	-	-	-
9	CHL	E	607	X	-	-	-
9	CHL	E	608	X	-	-	-
9	CHL	E	609	X	-	-	-
9	CHL	F	601	X	-	-	-
9	CHL	F	605	X	-	-	-
9	CHL	F	606	X	-	-	-
9	CHL	F	607	X	-	-	-
9	CHL	F	608	X	-	-	-
9	CHL	F	609	X	-	-	-
9	CHL	G	601	X	-	-	-
9	CHL	G	605	X	-	-	-
9	CHL	G	606	X	-	-	-
9	CHL	G	607	X	-	-	-
9	CHL	G	608	X	-	-	-
9	CHL	G	609	X	-	-	-
9	CHL	H	601	X	-	-	-
9	CHL	H	605	X	-	-	-
9	CHL	H	606	X	-	-	-
9	CHL	H	607	X	-	-	-
9	CHL	H	608	X	-	-	-
9	CHL	H	609	X	-	-	-
9	CHL	I	601	X	-	-	-
9	CHL	I	605	X	-	-	-
9	CHL	I	606	X	-	-	-
9	CHL	I	607	X	-	-	-
9	CHL	I	608	X	-	-	-
9	CHL	I	609	X	-	-	-
9	CHL	J	601	X	-	-	-
9	CHL	J	605	X	-	-	-
9	CHL	J	606	X	-	-	-
9	CHL	J	607	X	-	-	-
9	CHL	J	608	X	-	-	-
9	CHL	J	609	X	-	-	-

2 Entry composition (i)

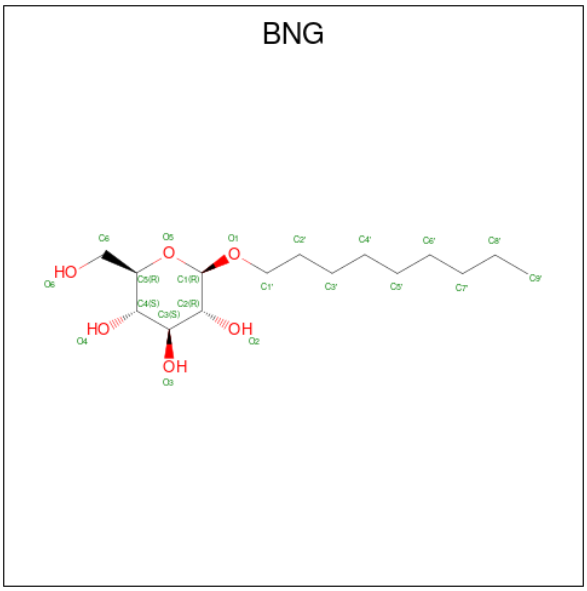
There are 11 unique types of molecules in this entry. The entry contains 29039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll A-B binding protein, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	B	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	C	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	D	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	E	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	F	219	Total	C	N	O	S	0	0	0
			1670	1085	272	306	7			
1	G	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	H	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	I	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	J	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			

- Molecule 2 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: $C_{15}H_{30}O_6$).



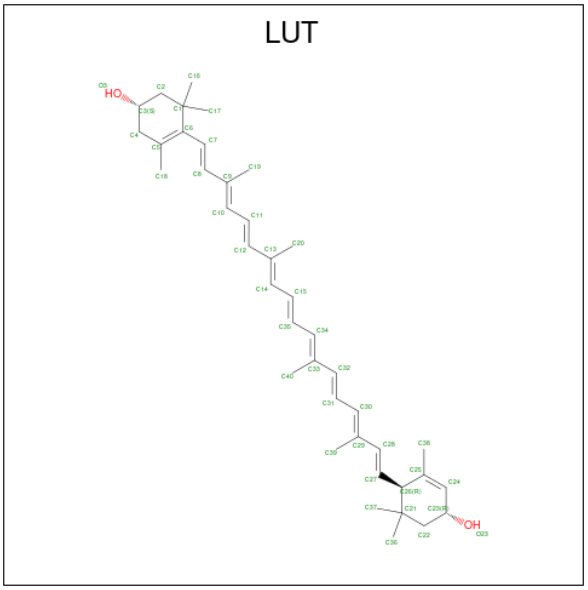
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	C	1	Total C O 21 15 6	0	0
2	D	1	Total C O 21 15 6	0	0
2	E	1	Total C O 21 15 6	0	0
2	F	1	Total C O 21 15 6	0	0
2	G	1	Total C O 21 15 6	0	0
2	H	1	Total C O 21 15 6	0	0
2	I	1	Total C O 21 15 6	0	0
2	J	1	Total C O 21 15 6	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

- Molecule 4 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
4	A	1	Total C O 42 40 2	0	0
4	A	1	Total C O 42 40 2	0	0
4	B	1	Total C O 42 40 2	0	0
4	B	1	Total C O 42 40 2	0	0
4	C	1	Total C O 42 40 2	0	0
4	C	1	Total C O 42 40 2	0	0
4	D	1	Total C O 42 40 2	0	0
4	D	1	Total C O 42 40 2	0	0
4	E	1	Total C O 42 40 2	0	0
4	E	1	Total C O 42 40 2	0	0
4	F	1	Total C O 42 40 2	0	0
4	F	1	Total C O 42 40 2	0	0
4	G	1	Total C O 42 40 2	0	0

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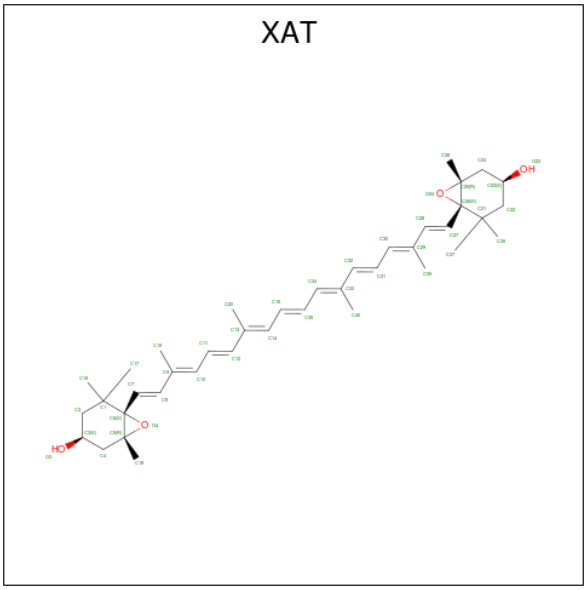
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 42 40 2	0	0
4	H	1	Total C O 42 40 2	0	0
4	H	1	Total C O 42 40 2	0	0
4	I	1	Total C O 42 40 2	0	0
4	I	1	Total C O 42 40 2	0	0
4	J	1	Total C O 42 40 2	0	0
4	J	1	Total C O 42 40 2	0	0

- Molecule 5 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
5	A	1	Total C O 44 40 4	0	0
5	B	1	Total C O 44 40 4	0	0
5	B	1	Total C O 44 40 4	0	0
5	C	1	Total C O 44 40 4	0	0

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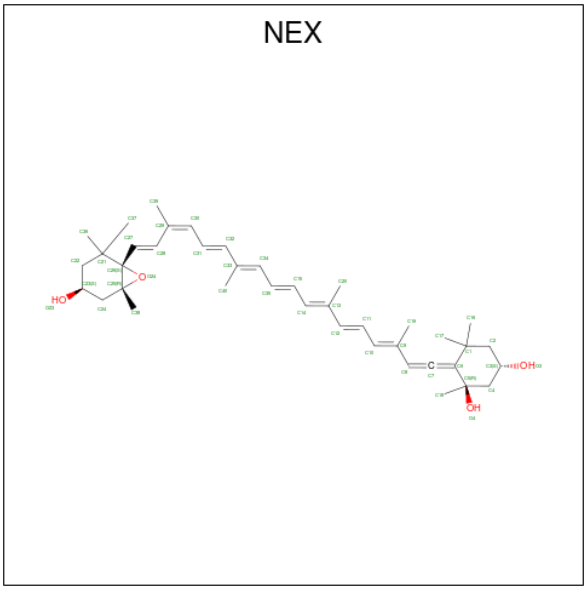
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 44 40 4	0	0
5	E	1	Total C O 44 40 4	0	0
5	F	1	Total C O 44 40 4	0	0
5	H	1	Total C O 44 40 4	0	0
5	I	1	Total C O 44 40 4	0	0
5	J	1	Total C O 44 40 4	0	0

- Molecule 6 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 44 40 4	0	0
6	B	1	Total C O 44 40 4	0	0
6	C	1	Total C O 44 40 4	0	0
6	D	1	Total C O 44 40 4	0	0

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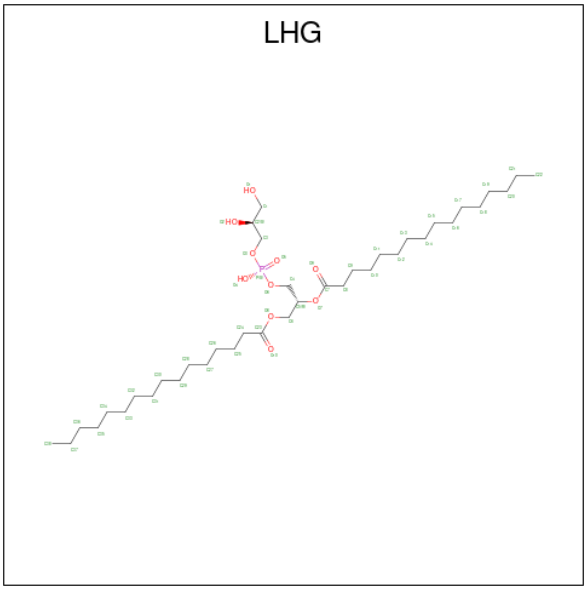
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 44 40 4	0	0
6	F	1	Total C O 44 40 4	0	0
6	G	1	Total C O 44 40 4	0	0
6	H	1	Total C O 44 40 4	0	0
6	I	1	Total C O 44 40 4	0	0
6	J	1	Total C O 44 40 4	0	0

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O P 49 38 10 1	0	0
7	B	1	Total C O P 49 38 10 1	0	0
7	C	1	Total C O P 49 38 10 1	0	0
7	D	1	Total C O P 49 38 10 1	0	0
7	E	1	Total C O P 49 38 10 1	0	0

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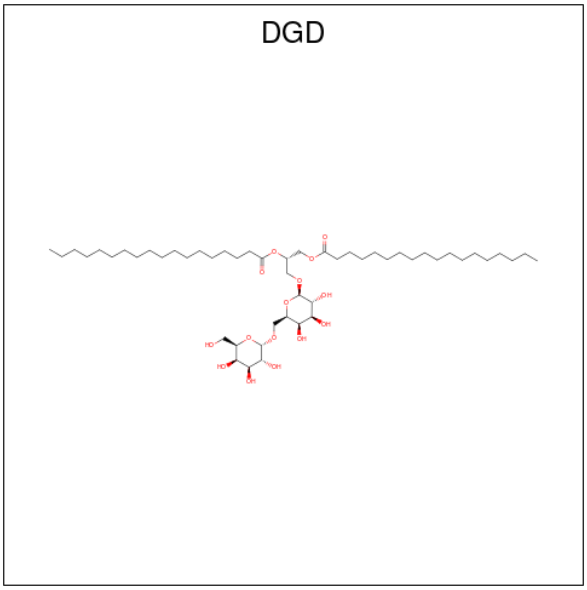
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	O	P	0	0
			49	38	10	1		
7	G	1	Total	C	O	P	0	0
			49	38	10	1		
7	H	1	Total	C	O	P	0	0
			49	38	10	1		
7	I	1	Total	C	O	P	0	0
			49	38	10	1		
7	J	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 8 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			66	51	15		
8	B	1	Total	C	O	0	0
			66	51	15		
8	B	1	Total	C	O	0	0
			66	51	15		
8	D	1	Total	C	O	0	0
			66	51	15		
8	D	1	Total	C	O	0	0
			66	51	15		
8	E	1	Total	C	O	0	0
			66	51	15		

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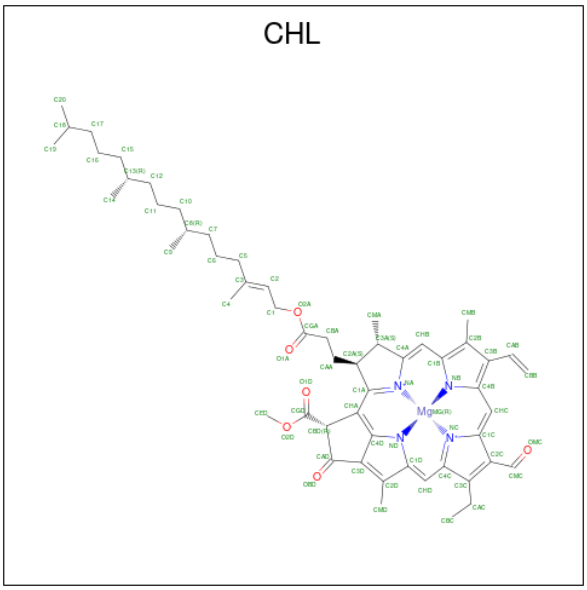
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total C O 66 51 15	0	0
8	H	1	Total C O 66 51 15	0	0
8	H	1	Total C O 66 51 15	0	0
8	I	1	Total C O 66 51 15	0	0

- Molecule 9 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C Mg N O 66 55 1 4 6	0	0
9	A	1	Total C Mg N O 48 37 1 4 6	0	0
9	A	1	Total C Mg N O 51 40 1 4 6	0	0
9	A	1	Total C Mg N O 66 55 1 4 6	0	0
9	A	1	Total C Mg N O 66 55 1 4 6	0	0
9	A	1	Total C Mg N O 66 55 1 4 6	0	0
9	B	1	Total C Mg N O 66 55 1 4 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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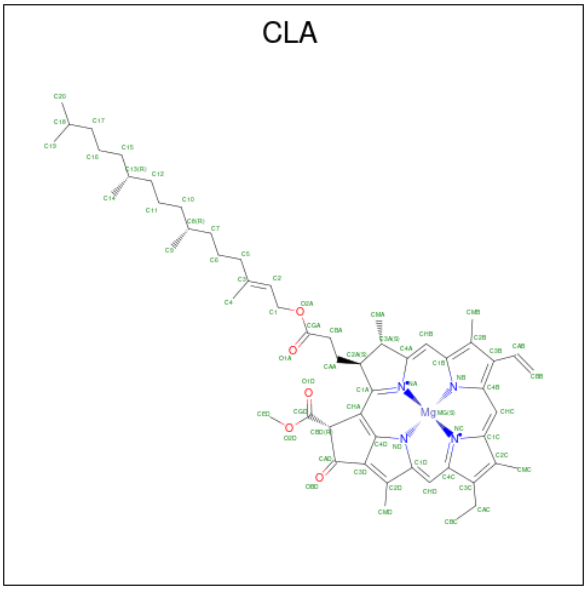
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	I	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	60	Total	O	0	0
			60	60		
11	B	78	Total	O	0	0
			78	78		
11	C	69	Total	O	0	0
			69	69		

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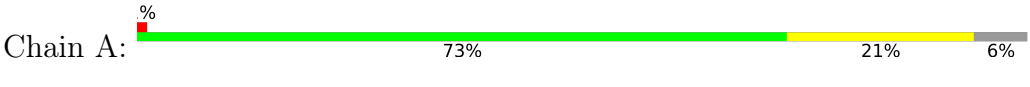
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	77	Total O 77 77	0	0
11	E	67	Total O 67 67	0	0
11	F	73	Total O 73 73	0	0
11	G	71	Total O 71 71	0	0
11	H	70	Total O 70 70	0	0
11	I	68	Total O 68 68	0	0
11	J	66	Total O 66 66	0	0

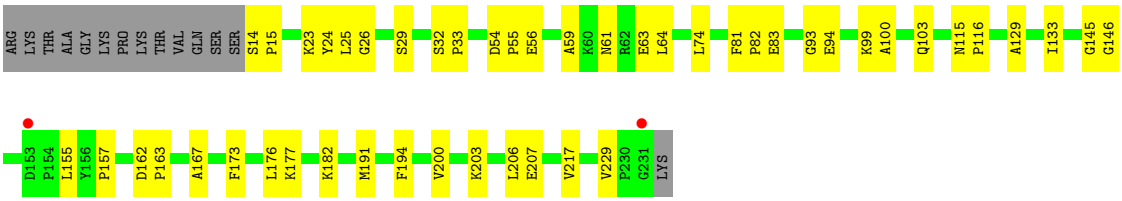
3 Residue-property plots (i)

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, chloroplast

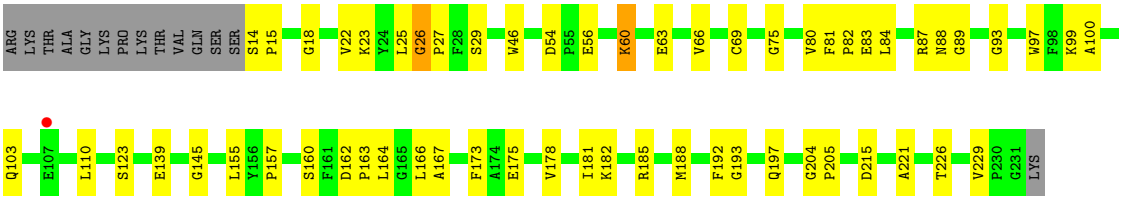
Chain A:





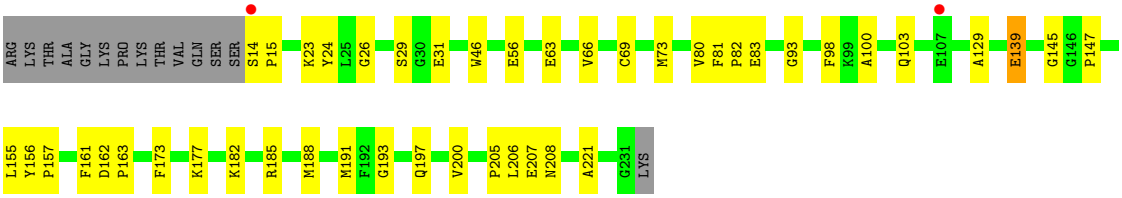
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain B:



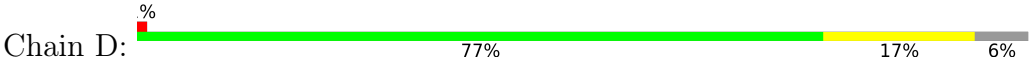
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

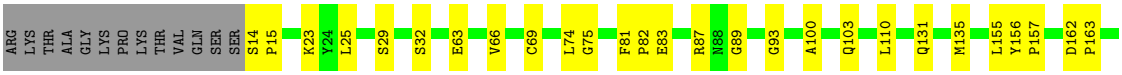
Chain C:



• Molecule 1: Chlorophyll A-B binding protein, chloroplast

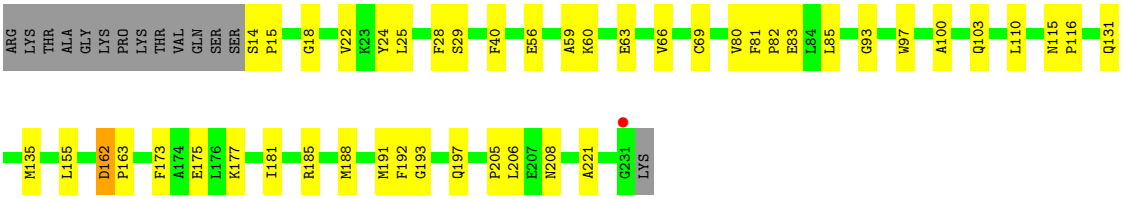
Chain D:





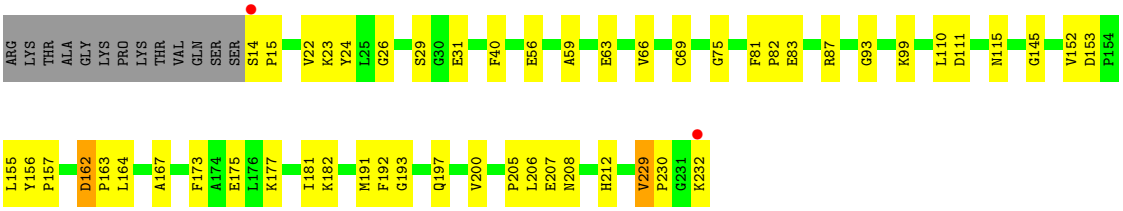
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain E:



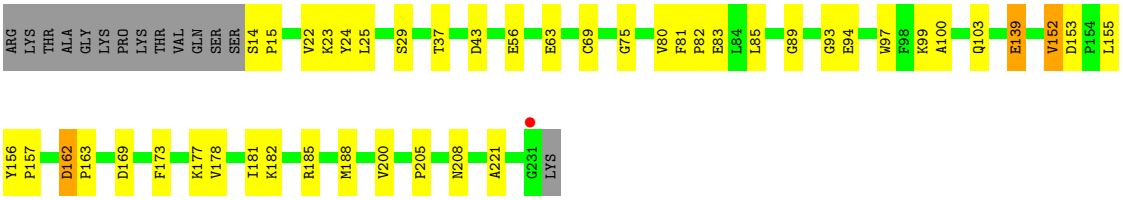
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain F:



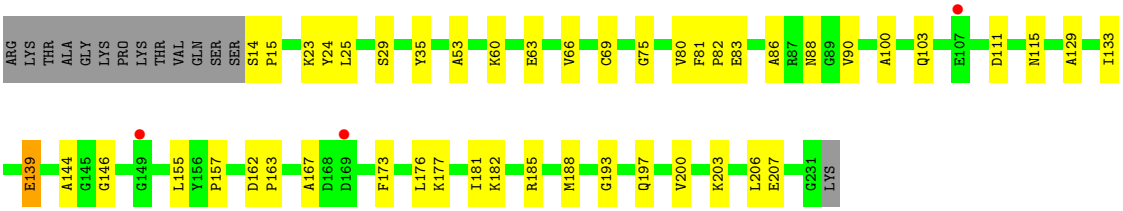
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain G:



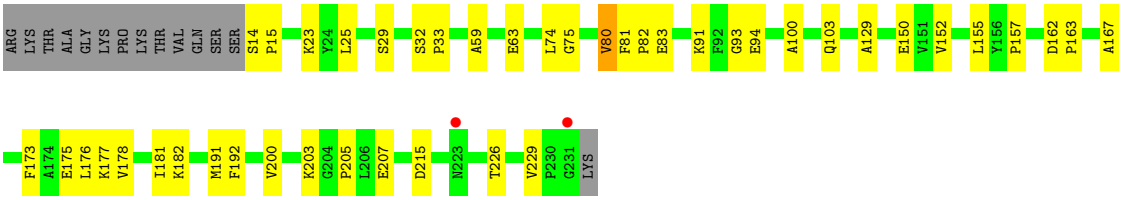
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain H:



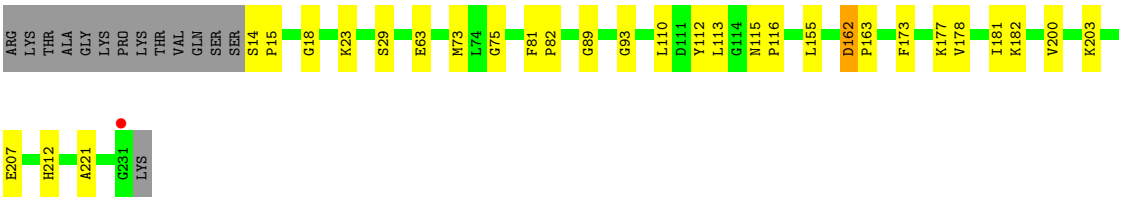
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain I:



• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	261.79Å 261.79Å 660.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.72 10.00 – 2.72	Depositor EDS
% Data completeness (in resolution range)	83.0 (10.00-2.72) 81.2 (10.00-2.72)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.04 (at 2.72Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.221 0.183 , 0.209	Depositor DCC
R_{free} test set	9326 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 73.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.008 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.005 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	29039	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BNG, XAT, LHG, CLA, DGD, NA, CHL, NEX, LUT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/1713	0.98	10/2333 (0.4%)
1	B	0.41	0/1713	0.99	15/2333 (0.6%)
1	C	0.42	0/1713	1.02	11/2333 (0.5%)
1	D	0.41	0/1713	0.99	8/2333 (0.3%)
1	E	0.42	0/1713	0.99	11/2333 (0.5%)
1	F	0.42	0/1722	1.01	13/2344 (0.6%)
1	G	0.41	0/1713	1.02	14/2333 (0.6%)
1	H	0.42	0/1713	0.97	6/2333 (0.3%)
1	I	0.40	0/1713	0.96	7/2333 (0.3%)
1	J	0.41	0/1713	0.97	7/2333 (0.3%)
All	All	0.41	0/17139	0.99	102/23341 (0.4%)

There are no bond length outliers.

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	93	GLY	N-CA-C	-7.45	103.79	112.73
1	C	93	GLY	N-CA-C	-7.16	104.14	112.73
1	F	93	GLY	N-CA-C	-7.00	104.02	112.49
1	B	145	GLY	N-CA-C	-6.88	104.58	112.29
1	G	156	TYR	CA-C-N	6.65	126.16	119.24
1	G	156	TYR	C-N-CA	6.65	126.16	119.24
1	G	93	GLY	N-CA-C	-6.54	104.88	112.73
1	F	26	GLY	CA-C-N	6.47	126.40	119.28
1	F	26	GLY	C-N-CA	6.47	126.40	119.28
1	B	192	PHE	N-CA-C	-6.45	104.25	111.28
1	C	156	TYR	CA-C-N	6.28	125.77	119.24
1	C	156	TYR	C-N-CA	6.28	125.77	119.24
1	B	80	VAL	N-CA-C	6.19	116.97	110.72
1	B	215	ASP	CA-C-N	6.16	125.64	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ASP	C-N-CA	6.16	125.64	119.24
1	J	93	GLY	N-CA-C	-6.14	105.36	112.73
1	G	97	TRP	N-CA-C	6.09	118.42	111.11
1	A	200	VAL	N-CA-C	6.08	117.62	111.00
1	H	200	VAL	N-CA-C	6.05	116.69	110.82
1	F	192	PHE	N-CA-C	-6.01	104.73	111.28
1	E	192	PHE	N-CA-C	-5.98	104.76	111.28
1	I	93	GLY	N-CA-C	-5.94	105.17	112.77
1	F	200	VAL	N-CA-C	5.92	117.46	111.00
1	B	97	TRP	N-CA-C	5.91	118.47	111.33
1	I	200	VAL	N-CA-C	5.90	116.68	110.72
1	E	24	TYR	N-CA-C	5.89	119.57	112.38
1	F	156	TYR	CA-C-N	5.86	125.34	119.24
1	F	156	TYR	C-N-CA	5.86	125.34	119.24
1	F	145	GLY	N-CA-C	-5.84	105.75	112.29
1	D	156	TYR	CA-C-N	5.83	125.52	119.05
1	D	156	TYR	C-N-CA	5.83	125.52	119.05
1	G	162	ASP	CA-C-N	5.81	125.28	119.24
1	G	162	ASP	C-N-CA	5.81	125.28	119.24
1	J	162	ASP	CA-C-N	5.80	125.27	119.24
1	J	162	ASP	C-N-CA	5.80	125.27	119.24
1	A	24	TYR	N-CA-C	5.72	119.36	112.38
1	G	200	VAL	N-CA-C	5.70	116.35	110.82
1	B	204	GLY	CA-C-N	5.70	125.17	119.24
1	B	204	GLY	C-N-CA	5.70	125.17	119.24
1	B	18	GLY	CA-C-N	5.69	125.37	119.56
1	B	18	GLY	C-N-CA	5.69	125.37	119.56
1	I	215	ASP	CA-C-N	5.68	125.15	119.24
1	I	215	ASP	C-N-CA	5.68	125.15	119.24
1	E	80	VAL	N-CA-C	5.68	116.46	110.72
1	C	26	GLY	CA-C-N	5.67	125.34	119.56
1	C	26	GLY	C-N-CA	5.67	125.34	119.56
1	H	80	VAL	N-CA-C	5.66	117.16	111.00
1	A	26	GLY	CA-C-N	5.62	125.47	119.28
1	A	26	GLY	C-N-CA	5.62	125.47	119.28
1	C	145	GLY	N-CA-C	-5.62	105.60	112.68
1	E	18	GLY	CA-C-N	5.60	125.27	119.56
1	E	18	GLY	C-N-CA	5.60	125.27	119.56
1	D	89	GLY	N-CA-C	5.58	120.32	113.79
1	G	169	ASP	CA-C-N	5.57	125.04	119.24
1	G	169	ASP	C-N-CA	5.57	125.04	119.24
1	E	162	ASP	CA-C-N	5.57	125.03	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	162	ASP	C-N-CA	5.57	125.03	119.24
1	D	93	GLY	N-CA-C	-5.57	106.05	112.73
1	A	93	GLY	N-CA-C	-5.53	105.96	113.37
1	B	93	GLY	N-CA-C	-5.53	105.70	112.77
1	D	200	VAL	N-CA-C	5.51	116.16	110.82
1	G	139	GLU	N-CA-C	-5.50	105.36	111.36
1	F	24	TYR	N-CA-C	5.50	119.09	112.38
1	H	139	GLU	N-CA-C	-5.49	105.30	111.28
1	B	26	GLY	CA-C-N	5.48	125.31	119.28
1	B	26	GLY	C-N-CA	5.48	125.31	119.28
1	B	89	GLY	N-CA-C	5.46	122.02	114.92
1	C	200	VAL	N-CA-C	5.46	116.95	111.00
1	G	37	THR	N-CA-C	5.44	119.55	113.02
1	I	192	PHE	N-CA-C	-5.41	105.38	111.28
1	H	146	GLY	CA-C-N	5.39	124.84	119.24
1	H	146	GLY	C-N-CA	5.39	124.84	119.24
1	I	80	VAL	N-CA-C	5.38	117.29	111.58
1	A	217	VAL	N-CA-C	5.37	116.15	110.72
1	J	18	GLY	CA-C-N	5.37	125.04	119.56
1	J	18	GLY	C-N-CA	5.37	125.04	119.56
1	A	145	GLY	N-CA-C	-5.36	106.28	112.29
1	E	97	TRP	N-CA-C	5.36	117.82	111.33
1	F	162	ASP	CA-C-N	5.35	124.80	119.24
1	F	162	ASP	C-N-CA	5.35	124.80	119.24
1	C	80	VAL	N-CA-C	5.33	116.81	111.00
1	H	24	TYR	N-CA-C	5.30	118.84	112.38
1	E	40	PHE	CA-C-N	5.26	125.51	119.83
1	E	40	PHE	C-N-CA	5.26	125.51	119.83
1	G	89	GLY	N-CA-C	5.26	121.00	114.37
1	C	24	TYR	N-CA-C	5.24	119.16	112.87
1	I	74	LEU	N-CA-C	-5.15	105.67	111.28
1	B	123	SER	N-CA-C	5.13	116.77	108.41
1	A	146	GLY	CA-C-N	5.13	125.42	119.47
1	A	146	GLY	C-N-CA	5.13	125.42	119.47
1	D	192	PHE	N-CA-C	-5.11	105.71	111.28
1	F	40	PHE	CA-C-N	5.08	124.99	119.76
1	F	40	PHE	C-N-CA	5.08	124.99	119.76
1	G	24	TYR	N-CA-C	5.08	118.58	112.38
1	C	207	GLU	N-CA-C	-5.06	105.95	111.82
1	D	215	ASP	CA-C-N	5.05	124.49	119.24
1	D	215	ASP	C-N-CA	5.05	124.49	119.24
1	A	74	LEU	N-CA-C	-5.04	105.87	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	80	VAL	N-CA-C	5.03	116.49	111.00
1	J	89	GLY	N-CA-C	5.03	120.79	114.25
1	C	139	GLU	N-CA-C	-5.02	105.89	111.36
1	J	200	VAL	N-CA-C	5.00	116.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1661	0	1592	29	0
1	B	1661	0	1592	36	0
1	C	1661	0	1592	30	0
1	D	1661	0	1592	23	0
1	E	1661	0	1592	27	0
1	F	1670	0	1605	30	0
1	G	1661	0	1592	29	0
1	H	1661	0	1592	32	0
1	I	1661	0	1592	28	0
1	J	1661	0	1592	17	0
2	A	21	0	30	0	0
2	B	21	0	30	0	0
2	C	21	0	30	0	0
2	D	21	0	30	1	0
2	E	21	0	30	0	0
2	F	21	0	30	0	0
2	G	21	0	30	0	0
2	H	21	0	30	0	0
2	I	21	0	30	0	0
2	J	21	0	30	0	0
3	A	1	0	0	0	0
4	A	84	0	112	4	0
4	B	84	0	112	4	0
4	C	84	0	112	2	0
4	D	84	0	112	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	84	0	112	3	0
4	F	84	0	112	3	0
4	G	84	0	112	1	0
4	H	84	0	112	2	0
4	I	84	0	112	4	0
4	J	84	0	112	1	0
5	A	44	0	56	0	0
5	B	88	0	112	1	0
5	C	44	0	56	0	0
5	D	44	0	56	0	0
5	E	44	0	56	2	0
5	F	44	0	56	1	0
5	H	44	0	56	1	0
5	I	44	0	56	1	0
5	J	44	0	56	1	0
6	A	44	0	56	0	0
6	B	44	0	56	0	0
6	C	44	0	56	0	0
6	D	44	0	56	0	0
6	E	44	0	56	0	0
6	F	44	0	56	0	0
6	G	44	0	56	1	0
6	H	44	0	56	0	0
6	I	44	0	56	0	0
6	J	44	0	56	0	0
7	A	49	0	74	2	0
7	B	49	0	74	3	0
7	C	49	0	74	1	0
7	D	49	0	74	1	0
7	E	49	0	74	1	0
7	F	49	0	74	3	0
7	G	49	0	74	2	0
7	H	49	0	74	2	0
7	I	49	0	74	3	0
7	J	49	0	74	0	0
8	A	66	0	96	1	0
8	B	132	0	192	0	0
8	D	132	0	192	1	0
8	E	66	0	96	0	0
8	G	66	0	96	0	0
8	H	132	0	192	1	0
8	I	66	0	96	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	363	0	349	4	0
9	B	363	0	349	6	0
9	C	363	0	350	5	0
9	D	363	0	349	2	0
9	E	363	0	350	2	0
9	F	363	0	350	5	0
9	G	363	0	349	8	0
9	H	363	0	350	3	0
9	I	363	0	350	4	0
9	J	363	0	350	2	0
10	A	501	0	534	9	0
10	B	501	0	532	11	0
10	C	501	0	533	12	0
10	D	501	0	532	6	0
10	E	501	0	534	7	0
10	F	501	0	534	5	0
10	G	501	0	532	8	0
10	H	501	0	534	12	0
10	I	501	0	532	7	0
10	J	501	0	533	10	0
11	A	60	0	0	1	0
11	B	78	0	0	1	0
11	C	69	0	0	0	0
11	D	77	0	0	2	0
11	E	67	0	0	0	0
11	F	73	0	0	0	0
11	G	71	0	0	1	0
11	H	70	0	0	0	0
11	I	68	0	0	1	0
11	J	66	0	0	0	0
All	All	29039	0	28999	372	0

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

All (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:SER:HB2	1:I:15:PRO:HD2	1.56	0.85
1:F:152:VAL:HG23	1:F:153:ASP:H	1.44	0.82
1:B:14:SER:HB2	1:B:15:PRO:HD2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:SER:HB2	1:H:15:PRO:HD2	1.64	0.78
1:E:60:LYS:HA	1:E:60:LYS:HE2	1.66	0.77
1:B:99:LYS:HE2	1:F:232:LYS:HE3	1.68	0.76
6:G:6623:NEX:H403	9:G:606:CHL:HBA1	1.67	0.75
4:A:621:LUT:H32	10:A:602:CLA:HBB1	1.68	0.74
1:D:83:GLU:O	1:D:87:ARG:HG3	1.87	0.73
1:I:173:PHE:CZ	1:I:177:LYS:HE3	2.24	0.73
1:C:14:SER:HB2	1:C:15:PRO:HD2	1.70	0.72
1:A:167:ALA:HB1	1:A:173:PHE:CD1	2.26	0.71
1:G:81:PHE:HB3	1:G:82:PRO:HD3	1.72	0.71
1:B:83:GLU:O	1:B:87:ARG:HG2	1.92	0.70
1:F:81:PHE:HB3	1:F:82:PRO:HD3	1.74	0.69
10:E:602:CLA:H92	10:H:603:CLA:H52	1.75	0.69
1:I:81:PHE:HB3	1:I:82:PRO:HD3	1.75	0.69
1:G:14:SER:HB2	1:G:15:PRO:HD2	1.77	0.67
1:E:14:SER:HB2	1:E:15:PRO:HD2	1.77	0.67
4:B:1620:LUT:H32	10:B:610:CLA:HBB1	1.77	0.66
1:J:162:ASP:N	1:J:163:PRO:HD3	2.11	0.66
1:B:60:LYS:HE3	1:B:60:LYS:HA	1.78	0.65
1:G:173:PHE:CZ	1:G:177:LYS:HE3	2.31	0.65
1:C:83:GLU:HG2	1:C:206:LEU:HD12	1.79	0.65
10:C:603:CLA:H52	10:H:602:CLA:H92	1.80	0.64
7:B:1630:LHG:H152	9:B:601:CHL:H41	1.80	0.64
1:G:162:ASP:N	1:G:163:PRO:HD3	2.13	0.63
1:I:14:SER:HB2	1:I:15:PRO:CD	2.29	0.63
1:F:162:ASP:N	1:F:163:PRO:HD3	2.14	0.63
1:J:81:PHE:HB3	1:J:82:PRO:HD3	1.79	0.63
10:B:603:CLA:H52	10:F:602:CLA:H92	1.81	0.62
1:A:162:ASP:N	1:A:163:PRO:HD3	2.14	0.62
1:A:81:PHE:HB3	1:A:82:PRO:HD3	1.82	0.62
1:E:81:PHE:HB3	1:E:82:PRO:HD3	1.80	0.62
1:F:191:MET:HE2	4:F:5621:LUT:H10	1.80	0.62
1:B:81:PHE:HB3	1:B:82:PRO:HD3	1.81	0.62
1:D:14:SER:HB2	1:D:15:PRO:HD2	1.81	0.61
1:A:25:LEU:HB2	1:A:29:SER:HA	1.82	0.61
1:C:162:ASP:N	1:C:163:PRO:HD3	2.15	0.61
1:H:25:LEU:HB2	1:H:29:SER:HA	1.83	0.60
1:F:63:GLU:HA	1:F:155:LEU:HD11	1.83	0.60
1:B:205:PRO:HG3	11:B:5623:HOH:O	2.00	0.60
9:B:606:CHL:HBA2	9:B:606:CHL:HBD	1.83	0.60
1:A:100:ALA:O	1:A:103:GLN:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:ALA:O	1:F:63:GLU:HG3	2.02	0.60
1:A:173:PHE:CZ	1:A:177:LYS:HE3	2.37	0.59
1:B:63:GLU:HA	1:B:155:LEU:HD11	1.83	0.59
1:C:23:LYS:HB2	1:C:29:SER:OG	2.02	0.59
10:C:602:CLA:H92	10:E:603:CLA:H52	1.85	0.59
1:C:81:PHE:HB3	1:C:82:PRO:HD3	1.83	0.59
1:E:162:ASP:N	1:E:163:PRO:HD3	2.17	0.59
1:D:83:GLU:OE1	1:D:205:PRO:HD2	2.01	0.59
1:J:182:LYS:HE2	10:J:611:CLA:O1D	2.01	0.59
1:J:14:SER:HB2	1:J:15:PRO:HD2	1.85	0.59
1:B:69:CYS:SG	1:B:188:MET:HE2	2.44	0.58
1:B:193:GLY:O	1:B:197:GLN:HG3	2.03	0.58
1:H:81:PHE:HB3	1:H:82:PRO:HD3	1.84	0.58
1:F:173:PHE:CZ	1:F:177:LYS:HE3	2.39	0.58
1:H:185:ARG:HA	1:H:188:MET:HE3	1.84	0.58
1:E:173:PHE:CZ	1:E:177:LYS:HE3	2.39	0.58
1:I:63:GLU:HA	1:I:155:LEU:HD11	1.86	0.58
1:I:203:LYS:HD3	1:I:207:GLU:OE2	2.04	0.58
1:F:75:GLY:HA2	4:F:5621:LUT:H181	1.86	0.57
1:H:162:ASP:N	1:H:163:PRO:HD3	2.18	0.57
1:D:25:LEU:HB2	1:D:29:SER:HA	1.84	0.57
1:F:182:LYS:HE2	10:F:611:CLA:O1D	2.05	0.57
1:A:83:GLU:HG2	1:A:206:LEU:HD12	1.87	0.57
1:E:173:PHE:CE1	1:E:177:LYS:HE3	2.40	0.57
1:I:162:ASP:N	1:I:163:PRO:HD3	2.19	0.57
1:D:23:LYS:HB2	1:D:29:SER:OG	2.05	0.57
10:I:611:CLA:HBA2	10:I:612:CLA:OBD	2.05	0.57
1:A:63:GLU:HA	1:A:155:LEU:HD11	1.86	0.56
1:E:63:GLU:HA	1:E:155:LEU:HD21	1.85	0.56
1:G:100:ALA:O	1:G:103:GLN:HG3	2.05	0.56
7:C:2630:LHG:H212	10:E:603:CLA:H191	1.88	0.56
1:H:14:SER:HB2	1:H:15:PRO:CD	2.36	0.56
10:C:611:CLA:HBA1	10:C:612:CLA:OBD	2.05	0.56
1:C:185:ARG:HA	1:C:188:MET:HE3	1.88	0.55
1:H:173:PHE:CZ	1:H:177:LYS:HE3	2.40	0.55
1:F:83:GLU:HG2	1:F:206:LEU:HD12	1.89	0.55
7:G:6630:LHG:HC62	7:G:6630:LHG:H262	1.89	0.55
1:H:75:GLY:HA2	4:H:7621:LUT:H181	1.88	0.55
1:D:173:PHE:CZ	1:D:177:LYS:HE3	2.42	0.55
1:D:75:GLY:HA2	4:D:3621:LUT:H181	1.88	0.55
10:G:604:CLA:HMB1	10:G:604:CLA:HBB1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:LYS:HD3	1:H:207:GLU:OE2	2.06	0.55
1:I:191:MET:HE2	4:I:8621:LUT:H10	1.88	0.55
1:I:23:LYS:HB2	1:I:29:SER:OG	2.07	0.55
1:J:63:GLU:HA	1:J:155:LEU:HD11	1.87	0.55
1:E:100:ALA:O	1:E:103:GLN:HG3	2.06	0.54
1:F:66:VAL:O	1:F:69:CYS:HB2	2.07	0.54
1:A:94:GLU:HG2	1:A:99:LYS:HB3	1.89	0.54
1:I:59:ALA:O	1:I:63:GLU:HG3	2.08	0.54
1:D:205:PRO:HG3	11:D:8623:HOH:O	2.07	0.54
1:B:182:LYS:HE2	10:B:611:CLA:O1D	2.09	0.53
10:E:611:CLA:HBA1	10:E:612:CLA:OBD	2.09	0.53
1:A:182:LYS:HE2	10:A:611:CLA:O1D	2.08	0.53
1:D:205:PRO:O	1:D:208:ASN:HB2	2.08	0.53
1:I:100:ALA:O	1:I:103:GLN:HG3	2.08	0.53
1:J:75:GLY:HA2	4:J:9621:LUT:H181	1.91	0.53
10:B:602:CLA:H93	10:B:603:CLA:HMA3	1.90	0.52
1:C:147:PRO:HB2	9:C:608:CHL:HBB2	1.91	0.52
1:D:81:PHE:HB3	1:D:82:PRO:HD3	1.90	0.52
1:H:167:ALA:HB1	1:H:173:PHE:CD1	2.44	0.52
1:I:25:LEU:HB2	1:I:29:SER:HA	1.91	0.52
10:G:611:CLA:HBA1	10:G:612:CLA:OBD	2.09	0.52
1:B:162:ASP:N	1:B:163:PRO:CD	2.72	0.52
1:C:191:MET:HE2	4:C:2621:LUT:H10	1.92	0.52
1:E:83:GLU:OE1	1:E:205:PRO:HD2	2.09	0.52
1:G:25:LEU:HB2	1:G:29:SER:HA	1.92	0.52
1:J:23:LYS:HB2	1:J:29:SER:OG	2.10	0.52
1:B:14:SER:HB2	1:B:15:PRO:CD	2.38	0.51
1:F:193:GLY:O	1:F:197:GLN:HG3	2.09	0.51
1:F:205:PRO:O	1:F:208:ASN:HB2	2.10	0.51
1:B:100:ALA:O	1:B:103:GLN:HG3	2.10	0.51
1:C:193:GLY:O	1:C:197:GLN:HG3	2.10	0.51
10:D:611:CLA:HBA1	10:D:612:CLA:OBD	2.10	0.51
1:H:69:CYS:SG	1:H:188:MET:HE2	2.51	0.51
9:I:601:CHL:HHC	9:I:601:CHL:HBB1	1.92	0.51
1:E:28:PHE:O	1:H:144:ALA:HB2	2.11	0.51
1:I:167:ALA:HB1	1:I:173:PHE:CD1	2.47	0.50
1:A:64:LEU:HD13	10:A:603:CLA:HBA2	1.92	0.50
1:B:75:GLY:HA2	4:B:1621:LUT:H181	1.92	0.50
7:I:8630:LHG:H152	9:I:601:CHL:H41	1.93	0.50
1:B:54:ASP:OD1	1:B:56:GLU:N	2.44	0.50
8:D:5632:DGD:HD2	11:D:8628:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LYS:HE2	10:C:611:CLA:O1D	2.12	0.50
1:H:203:LYS:HD3	1:H:207:GLU:CD	2.36	0.50
10:A:603:CLA:HBB1	10:A:603:CLA:HHC	1.94	0.50
10:A:611:CLA:HBA1	10:A:612:CLA:OBD	2.12	0.49
1:E:110:LEU:C	1:E:110:LEU:HD23	2.38	0.49
1:C:14:SER:HB2	1:C:15:PRO:CD	2.42	0.49
7:I:8630:LHG:HC62	7:I:8630:LHG:H262	1.93	0.49
1:A:14:SER:HB2	1:A:15:PRO:HD2	1.95	0.49
7:A:630:LHG:H262	7:A:630:LHG:HC62	1.94	0.49
10:D:602:CLA:H92	10:J:603:CLA:H52	1.95	0.49
1:E:191:MET:HE2	4:E:4621:LUT:H10	1.93	0.49
1:C:205:PRO:O	1:C:208:ASN:HB2	2.13	0.49
1:D:178:VAL:O	1:D:181:ILE:HG22	2.12	0.49
1:G:83:GLU:OE1	1:G:205:PRO:HD2	2.13	0.49
10:H:611:CLA:HBA1	10:H:612:CLA:OBD	2.13	0.49
1:B:25:LEU:HB2	1:B:29:SER:HA	1.95	0.48
10:B:603:CLA:HHC	10:B:603:CLA:HBB1	1.94	0.48
1:E:193:GLY:O	1:E:197:GLN:HG3	2.13	0.48
1:I:182:LYS:HE2	10:I:611:CLA:O1D	2.13	0.48
1:E:205:PRO:O	1:E:208:ASN:HB2	2.13	0.48
1:H:176:LEU:HD13	10:H:610:CLA:O1A	2.13	0.48
1:J:203:LYS:HD3	1:J:207:GLU:OE2	2.13	0.48
1:A:176:LEU:HD13	10:A:610:CLA:O1A	2.12	0.48
4:E:4620:LUT:H32	10:E:610:CLA:HBB1	1.95	0.48
1:C:147:PRO:HB2	9:C:608:CHL:CBB	2.44	0.48
1:G:75:GLY:HA2	4:G:6621:LUT:H181	1.95	0.48
1:J:110:LEU:C	1:J:110:LEU:HD23	2.39	0.48
1:H:23:LYS:HB2	1:H:29:SER:OG	2.14	0.48
1:H:182:LYS:HE2	10:H:611:CLA:O1D	2.14	0.48
7:A:630:LHG:H152	9:A:601:CHL:H41	1.95	0.48
1:B:23:LYS:HB2	1:B:29:SER:OG	2.14	0.48
10:C:604:CLA:HBB1	10:C:604:CLA:HMB3	1.96	0.48
1:H:129:ALA:O	1:H:133:ILE:HG12	2.13	0.47
1:A:129:ALA:HB1	8:I:8632:DGD:HAE2	1.95	0.47
10:H:603:CLA:HHC	10:H:603:CLA:HBB1	1.96	0.47
10:H:612:CLA:HHC	10:H:612:CLA:HBB1	1.94	0.47
10:B:603:CLA:H201	7:F:5630:LHG:H212	1.96	0.47
10:I:603:CLA:HHC	10:I:603:CLA:HBB1	1.96	0.47
1:A:203:LYS:HD3	1:A:207:GLU:OE2	2.14	0.47
1:E:83:GLU:HG2	1:E:206:LEU:HD12	1.95	0.47
1:F:23:LYS:HB2	1:F:29:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:ALA:C	1:H:88:ASN:H	2.22	0.47
10:I:603:CLA:H52	10:J:602:CLA:H92	1.97	0.47
9:A:601:CHL:HHC	9:A:601:CHL:HBB1	1.96	0.47
1:D:162:ASP:N	1:D:163:PRO:CD	2.77	0.47
10:F:603:CLA:H52	10:G:602:CLA:H92	1.96	0.47
1:H:63:GLU:HA	1:H:155:LEU:HD21	1.95	0.47
1:H:193:GLY:O	1:H:197:GLN:HG3	2.15	0.47
10:H:611:CLA:HHC	10:H:611:CLA:HBB1	1.95	0.47
1:D:100:ALA:O	1:D:103:GLN:HG3	2.14	0.47
1:E:69:CYS:SG	1:E:188:MET:HE2	2.54	0.47
8:A:632:DGD:HAE2	1:I:129:ALA:HB1	1.95	0.46
1:E:221:ALA:CB	5:H:4622:XAT:H193	2.45	0.46
1:F:229:VAL:HA	1:F:230:PRO:HD3	1.85	0.46
1:J:178:VAL:O	1:J:182:LYS:HG3	2.15	0.46
1:B:164:LEU:HD12	4:B:1620:LUT:H222	1.97	0.46
10:A:611:CLA:HHC	10:A:611:CLA:HBB1	1.96	0.46
1:E:25:LEU:HB2	1:E:29:SER:HA	1.97	0.46
1:F:155:LEU:C	1:F:157:PRO:HD3	2.40	0.46
1:B:110:LEU:HD23	1:B:110:LEU:C	2.41	0.46
9:D:601:CHL:HHB	9:J:609:CHL:HMB2	1.97	0.46
1:F:14:SER:HB2	1:F:15:PRO:CD	2.45	0.46
7:F:5630:LHG:H152	9:F:601:CHL:H41	1.98	0.46
10:G:611:CLA:HHC	10:G:611:CLA:HBB1	1.96	0.46
1:I:173:PHE:CE1	1:I:177:LYS:HE3	2.49	0.46
1:A:162:ASP:N	1:A:163:PRO:CD	2.79	0.46
1:C:221:ALA:CB	5:E:2622:XAT:H193	2.46	0.46
9:I:606:CHL:HBD	9:I:606:CHL:HBA1	1.98	0.46
1:C:14:SER:CB	1:C:15:PRO:HD2	2.43	0.46
1:D:63:GLU:HA	1:D:155:LEU:HD11	1.97	0.46
1:B:229:VAL:HG21	9:G:607:CHL:HED1	1.98	0.45
10:H:613:CLA:HBB1	10:H:613:CLA:HMB3	1.98	0.45
1:B:155:LEU:C	1:B:157:PRO:HD3	2.42	0.45
1:A:59:ALA:O	1:A:63:GLU:HG3	2.16	0.45
1:A:157:PRO:HD2	10:A:610:CLA:OBD	2.16	0.45
1:C:155:LEU:C	1:C:157:PRO:HD3	2.41	0.45
10:B:611:CLA:HBA1	10:B:612:CLA:OBD	2.17	0.45
9:D:601:CHL:HHC	9:D:601:CHL:HBB1	1.98	0.45
1:F:162:ASP:N	1:F:163:PRO:CD	2.80	0.45
1:J:173:PHE:CZ	1:J:177:LYS:HE3	2.52	0.45
1:B:178:VAL:O	1:B:181:ILE:HG22	2.17	0.45
1:G:69:CYS:SG	1:G:188:MET:HE2	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:MET:HE2	4:A:621:LUT:H10	1.98	0.45
1:C:100:ALA:O	1:C:103:GLN:HG3	2.17	0.45
1:I:75:GLY:HA2	4:I:8621:LUT:H181	1.98	0.45
1:J:162:ASP:N	1:J:163:PRO:CD	2.79	0.45
9:A:605:CHL:HHC	9:A:605:CHL:HBB1	1.99	0.45
1:C:63:GLU:HA	1:C:155:LEU:HD21	1.99	0.45
9:H:605:CHL:HHC	9:H:605:CHL:HBB1	1.98	0.45
1:A:163:PRO:HD2	4:A:620:LUT:H23	1.99	0.44
1:B:46:TRP:CE3	4:B:1621:LUT:H383	2.52	0.44
7:B:1630:LHG:HC62	7:B:1630:LHG:H262	1.99	0.44
1:E:163:PRO:HD2	4:E:4620:LUT:H23	1.97	0.44
7:E:4630:LHG:H212	10:H:603:CLA:H191	1.99	0.44
10:E:603:CLA:HHC	10:E:603:CLA:HBB1	1.98	0.44
1:B:84:LEU:O	1:B:88:ASN:ND2	2.49	0.44
1:C:46:TRP:CE3	4:C:2621:LUT:H383	2.51	0.44
1:D:131:GLN:O	1:D:135:MET:HB2	2.17	0.44
1:D:167:ALA:HB1	1:D:173:PHE:CD1	2.53	0.44
1:J:212:HIS:CG	10:J:613:CLA:HAA2	2.52	0.44
1:G:162:ASP:N	1:G:163:PRO:CD	2.79	0.44
1:I:157:PRO:HD2	10:I:610:CLA:OBD	2.17	0.44
1:I:176:LEU:HD13	10:I:610:CLA:O1A	2.17	0.44
9:B:601:CHL:HHC	9:B:601:CHL:HBB1	1.99	0.44
9:H:601:CHL:HHC	9:H:601:CHL:HBB1	1.98	0.44
1:D:110:LEU:C	1:D:110:LEU:HD23	2.43	0.44
2:D:3633:BNG:H1'1	10:D:611:CLA:O1A	2.17	0.44
1:F:66:VAL:HG22	1:F:181:ILE:HD11	1.99	0.44
1:I:94:GLU:HG3	11:I:9626:HOH:O	2.17	0.44
1:A:94:GLU:HG3	11:A:638:HOH:O	2.18	0.44
1:D:74:LEU:HB3	10:D:604:CLA:HAB	2.00	0.44
1:H:157:PRO:HD2	10:H:610:CLA:OBD	2.17	0.44
1:B:26:GLY:HA3	1:B:27:PRO:HD3	1.86	0.44
1:B:167:ALA:HB1	1:B:173:PHE:CD1	2.52	0.44
1:B:182:LYS:NZ	7:B:1630:LHG:O5	2.51	0.44
1:F:22:VAL:HB	9:F:601:CHL:CBC	2.48	0.44
1:G:182:LYS:HE2	10:G:611:CLA:O1D	2.18	0.44
1:H:173:PHE:CE2	1:H:177:LYS:HE3	2.53	0.44
10:I:602:CLA:H93	10:I:603:CLA:HMA1	1.99	0.44
9:I:605:CHL:HHC	9:I:605:CHL:HBB1	1.99	0.44
10:B:612:CLA:HHC	10:B:612:CLA:HBB1	1.99	0.43
1:F:152:VAL:HG23	1:F:153:ASP:N	2.22	0.43
1:H:139:GLU:OE2	1:H:139:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:7630:LHG:HC62	7:H:7630:LHG:H262	1.99	0.43
1:I:32:SER:HB2	1:I:33:PRO:CD	2.48	0.43
10:J:603:CLA:HHC	10:J:603:CLA:HBB1	2.00	0.43
10:J:614:CLA:HHC	10:J:614:CLA:HBB1	1.99	0.43
10:B:611:CLA:HHC	10:B:611:CLA:HBB1	1.99	0.43
1:C:221:ALA:HB1	5:E:2622:XAT:H193	2.01	0.43
1:I:163:PRO:HD2	4:I:8620:LUT:H23	1.99	0.43
1:I:226:THR:O	1:I:229:VAL:HG23	2.18	0.43
10:J:611:CLA:HBA1	10:J:612:CLA:OBD	2.18	0.43
1:B:160:SER:O	1:B:163:PRO:HD3	2.17	0.43
1:H:139:GLU:HG3	9:H:609:CHL:C4B	2.49	0.43
7:I:8630:LHG:H282	7:I:8630:LHG:HC92	2.00	0.43
7:F:5630:LHG:HC62	7:F:5630:LHG:H262	2.00	0.43
10:F:603:CLA:HBB1	10:F:603:CLA:HHC	2.00	0.43
1:C:173:PHE:CZ	1:C:177:LYS:HE3	2.53	0.43
10:C:603:CLA:H192	7:H:7630:LHG:H212	1.99	0.43
10:J:611:CLA:HHC	10:J:611:CLA:HBB1	2.01	0.43
10:J:612:CLA:HHC	10:J:612:CLA:HBB1	2.00	0.43
1:C:66:VAL:O	1:C:69:CYS:HB2	2.18	0.43
1:E:131:GLN:O	1:E:135:MET:HB2	2.18	0.43
10:E:612:CLA:HHC	10:E:612:CLA:HBB1	2.00	0.43
1:G:23:LYS:HE2	11:G:9702:HOH:O	2.18	0.43
1:G:205:PRO:O	1:G:208:ASN:HB2	2.19	0.43
1:F:229:VAL:CG2	1:F:232:LYS:HD2	2.48	0.43
1:G:63:GLU:HA	1:G:155:LEU:HD11	2.01	0.43
5:I:9622:XAT:H193	1:J:221:ALA:CB	2.49	0.43
10:C:603:CLA:HHC	10:C:603:CLA:HBB1	2.00	0.43
10:G:612:CLA:HHC	10:G:612:CLA:HBB1	2.01	0.43
1:B:185:ARG:HA	1:B:188:MET:HE3	2.01	0.43
9:C:601:CHL:HHC	9:C:601:CHL:HBB1	2.00	0.43
1:G:23:LYS:HB2	1:G:29:SER:OG	2.19	0.43
1:G:155:LEU:C	1:G:157:PRO:HD3	2.43	0.43
1:H:100:ALA:O	1:H:103:GLN:HG3	2.19	0.43
9:B:605:CHL:HHC	9:B:605:CHL:HBB1	2.00	0.42
1:F:164:LEU:HD12	4:F:5620:LUT:H222	2.01	0.42
1:C:162:ASP:N	1:C:163:PRO:CD	2.81	0.42
1:D:69:CYS:SG	1:D:188:MET:HE2	2.59	0.42
1:D:173:PHE:CE1	1:D:177:LYS:HE3	2.55	0.42
4:H:7621:LUT:H382	10:H:602:CLA:HBA1	2.01	0.42
1:C:139:GLU:HG3	9:C:609:CHL:NB	2.35	0.42
1:J:112:TYR:O	1:J:113:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:ARG:NH2	1:F:207:GLU:HA	2.34	0.42
1:G:63:GLU:HA	1:G:155:LEU:HD21	2.01	0.42
1:G:22:VAL:HB	9:G:601:CHL:HBC1	2.01	0.42
10:C:611:CLA:HHC	10:C:611:CLA:HBB1	2.00	0.42
9:F:601:CHL:HHC	9:F:601:CHL:HBB1	2.01	0.42
1:J:73:MET:SD	10:J:610:CLA:HBB1	2.60	0.42
1:C:129:ALA:HB1	8:H:6632:DGD:HAE2	2.01	0.42
7:D:3630:LHG:HC62	7:D:3630:LHG:H262	2.01	0.42
1:G:173:PHE:CE1	1:G:177:LYS:HE3	2.55	0.42
9:J:605:CHL:HHC	9:J:605:CHL:HBB1	2.01	0.42
10:A:612:CLA:HHC	10:A:612:CLA:HBB1	2.01	0.42
1:D:155:LEU:C	1:D:157:PRO:HD3	2.45	0.42
1:I:178:VAL:O	1:I:182:LYS:HG3	2.20	0.42
1:A:23:LYS:HB2	1:A:29:SER:OG	2.20	0.41
1:C:161:PHE:C	1:C:163:PRO:HD3	2.44	0.41
1:G:178:VAL:O	1:G:182:LYS:HG3	2.19	0.41
1:I:83:GLU:OE1	1:I:205:PRO:HD2	2.20	0.41
1:D:66:VAL:O	1:D:69:CYS:HB2	2.20	0.41
9:E:605:CHL:HHC	9:E:605:CHL:HBB1	2.02	0.41
1:G:22:VAL:HB	9:G:601:CHL:CBC	2.50	0.41
1:G:94:GLU:HG2	1:G:99:LYS:HB3	2.02	0.41
1:H:83:GLU:HG2	1:H:206:LEU:HD12	2.03	0.41
1:H:111:ASP:HB3	1:H:115:ASN:O	2.20	0.41
1:B:66:VAL:O	1:B:69:CYS:HB2	2.20	0.41
7:G:6630:LHG:H152	9:G:601:CHL:H41	2.01	0.41
1:H:66:VAL:O	1:H:69:CYS:HB2	2.20	0.41
1:H:162:ASP:N	1:H:163:PRO:CD	2.82	0.41
1:A:61:ASN:HA	1:A:64:LEU:HD12	2.01	0.41
1:B:221:ALA:CB	5:B:1622:XAT:H193	2.50	0.41
1:C:173:PHE:CE1	1:C:177:LYS:HE3	2.56	0.41
4:D:3620:LUT:H3	10:D:613:CLA:HMA2	2.02	0.41
1:E:81:PHE:CE2	1:E:85:LEU:HD11	2.55	0.41
1:F:110:LEU:C	1:F:110:LEU:HD23	2.46	0.41
1:C:14:SER:CB	1:C:15:PRO:CD	2.98	0.41
1:E:115:ASN:HA	1:E:116:PRO:HD3	1.92	0.41
1:I:155:LEU:C	1:I:157:PRO:HD3	2.46	0.41
1:A:54:ASP:HA	1:A:55:PRO:HD3	1.94	0.41
1:A:83:GLU:CD	1:A:206:LEU:HB2	2.46	0.41
1:A:115:ASN:HA	1:A:116:PRO:HD3	1.89	0.41
1:A:194:PHE:HE2	4:A:620:LUT:H41	1.85	0.41
1:B:166:LEU:HD12	10:B:610:CLA:CGA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:602:CLA:H92	10:G:603:CLA:H52	2.02	0.41
1:H:35:TYR:CE2	1:H:53:ALA:HA	2.56	0.41
1:H:86:ALA:HA	1:H:90:VAL:O	2.20	0.41
1:F:83:GLU:OE1	1:F:205:PRO:HD2	2.21	0.41
1:G:25:LEU:HD23	1:G:25:LEU:HA	1.90	0.41
10:G:603:CLA:HHC	10:G:603:CLA:HBB1	2.02	0.41
9:A:608:CHL:HHC	9:A:608:CHL:HBB1	2.03	0.41
1:E:162:ASP:N	1:E:163:PRO:CD	2.84	0.41
1:G:185:ARG:HA	1:G:188:MET:HE3	2.02	0.41
1:A:32:SER:HB2	1:A:33:PRO:CD	2.51	0.41
1:B:178:VAL:O	1:B:182:LYS:HG3	2.21	0.41
1:D:221:ALA:CB	5:J:3622:XAT:H193	2.51	0.41
1:G:43:ASP:OD1	1:G:43:ASP:C	2.64	0.41
1:G:81:PHE:CE2	1:G:85:LEU:HD11	2.56	0.41
1:G:139:GLU:HG3	9:G:609:CHL:NB	2.36	0.41
1:A:129:ALA:O	1:A:133:ILE:HG12	2.21	0.41
1:H:23:LYS:HB2	1:H:29:SER:CB	2.51	0.40
1:B:139:GLU:HG3	9:B:609:CHL:C4B	2.51	0.40
10:D:612:CLA:HHC	10:D:612:CLA:HBB1	2.02	0.40
1:E:22:VAL:HB	9:E:601:CHL:CBC	2.51	0.40
1:E:59:ALA:O	1:E:63:GLU:HG3	2.22	0.40
1:E:185:ARG:HA	1:E:188:MET:HE3	2.04	0.40
1:F:212:HIS:CG	10:F:613:CLA:HAA2	2.56	0.40
1:I:163:PRO:HD2	4:I:8620:LUT:C23	2.51	0.40
1:J:115:ASN:HA	1:J:116:PRO:HD3	1.90	0.40
1:B:22:VAL:HB	9:B:601:CHL:CBC	2.52	0.40
1:B:226:THR:O	1:B:229:VAL:HG23	2.21	0.40
1:C:98:PHE:HB2	9:C:607:CHL:HMA1	2.04	0.40
10:C:612:CLA:HHC	10:C:612:CLA:HBB1	2.04	0.40
1:E:66:VAL:O	1:E:69:CYS:HB2	2.22	0.40
9:F:609:CHL:HMB2	9:G:601:CHL:HHB	2.03	0.40
1:G:152:VAL:HB	1:G:153:ASP:H	1.69	0.40
10:C:614:CLA:HHC	10:C:614:CLA:HBB1	2.04	0.40
1:F:111:ASP:HB3	1:F:115:ASN:O	2.22	0.40
9:G:608:CHL:HBA1	9:G:608:CHL:H151	2.01	0.40
1:I:150:GLU:OE2	1:I:150:GLU:HA	2.21	0.40
1:C:73:MET:SD	10:C:610:CLA:HBB1	2.62	0.40
10:C:613:CLA:HBB1	10:C:613:CLA:HMB1	2.04	0.40
1:F:167:ALA:HB1	1:F:173:PHE:CD1	2.56	0.40
9:F:608:CHL:HHC	9:F:608:CHL:HBB1	2.02	0.40
5:F:6622:XAT:H193	1:G:221:ALA:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/232 (93%)	207 (96%)	9 (4%)	0	100	100
1	B	216/232 (93%)	210 (97%)	6 (3%)	0	100	100
1	C	216/232 (93%)	209 (97%)	7 (3%)	0	100	100
1	D	216/232 (93%)	208 (96%)	8 (4%)	0	100	100
1	E	216/232 (93%)	208 (96%)	8 (4%)	0	100	100
1	F	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	G	216/232 (93%)	209 (97%)	7 (3%)	0	100	100
1	H	216/232 (93%)	206 (95%)	10 (5%)	0	100	100
1	I	216/232 (93%)	209 (97%)	7 (3%)	0	100	100
1	J	216/232 (93%)	207 (96%)	9 (4%)	0	100	100
All	All	2161/2320 (93%)	2084 (96%)	77 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	168/180 (93%)	166 (99%)	2 (1%)	63	82
1	B	168/180 (93%)	166 (99%)	2 (1%)	63	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	168/180 (93%)	166 (99%)	2 (1%)	63	82
1	D	168/180 (93%)	166 (99%)	2 (1%)	63	82
1	E	168/180 (93%)	165 (98%)	3 (2%)	51	76
1	F	169/180 (94%)	164 (97%)	5 (3%)	36	64
1	G	168/180 (93%)	165 (98%)	3 (2%)	51	76
1	H	168/180 (93%)	166 (99%)	2 (1%)	63	82
1	I	168/180 (93%)	163 (97%)	5 (3%)	36	64
1	J	168/180 (93%)	167 (99%)	1 (1%)	78	90
All	All	1681/1800 (93%)	1654 (98%)	27 (2%)	55	78

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	229	VAL
1	B	60	LYS
1	B	175	GLU
1	C	31	GLU
1	C	56	GLU
1	D	32	SER
1	D	175	GLU
1	E	56	GLU
1	E	175	GLU
1	E	181	ILE
1	F	31	GLU
1	F	56	GLU
1	F	99	LYS
1	F	175	GLU
1	F	229	VAL
1	G	56	GLU
1	G	152	VAL
1	G	181	ILE
1	H	60	LYS
1	H	181	ILE
1	I	80	VAL
1	I	91	LYS
1	I	152	VAL
1	I	175	GLU
1	I	181	ILE

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Mol	Chain	Res	Type
1	J	181	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	223	ASN
1	B	223	ASN
1	C	88	ASN
1	C	183	ASN
1	C	218	ASN
1	D	88	ASN
1	D	219	ASN
1	D	223	ASN
1	E	223	ASN
1	F	88	ASN
1	F	223	ASN
1	G	88	ASN
1	G	219	ASN
1	G	223	ASN
1	H	223	ASN
1	I	219	ASN
1	I	223	ASN
1	J	219	ASN
1	J	223	ASN

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 (i)

Of 211 ligands modelled in this entry, 1 is monoatomic - leaving 210 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	$\#\|Z\| > 2$
10	CLA	H	611	7	69,73,73	1.32	7 (10%)	82,113,113	1.81	14 (17%)
9	CHL	F	608	11	60,74,74	1.90	13 (21%)	58,114,114	2.67	23 (39%)
10	CLA	E	610	1	69,73,73	1.42	8 (11%)	82,113,113	1.60	12 (14%)
9	CHL	G	609	1	60,74,74	1.93	15 (25%)	58,114,114	2.48	20 (34%)
10	CLA	D	604	11	66,70,73	1.35	7 (10%)	78,109,113	2.10	15 (19%)
2	BNG	E	4633	-	21,21,21	0.52	0	26,26,26	0.76	1 (3%)
10	CLA	A	613	1	69,73,73	1.35	10 (14%)	82,113,113	1.62	12 (14%)
10	CLA	C	602	1	69,73,73	1.36	7 (10%)	82,113,113	1.90	18 (21%)
6	NEX	F	5623	-	40,46,46	1.64	3 (7%)	50,70,70	1.03	4 (8%)
10	CLA	I	603	1	69,73,73	1.37	7 (10%)	82,113,113	1.60	12 (14%)
10	CLA	A	602	1	69,73,73	1.31	7 (10%)	82,113,113	1.88	19 (23%)
4	LUT	C	2620	-	42,43,43	0.93	3 (7%)	51,60,60	1.32	5 (9%)
10	CLA	B	610	1	69,73,73	1.34	6 (8%)	82,113,113	1.59	10 (12%)
5	XAT	D	8622	-	41,47,47	0.71	1 (2%)	54,74,74	1.24	6 (11%)
10	CLA	F	613	1	69,73,73	1.37	8 (11%)	82,113,113	1.71	9 (10%)
10	CLA	C	612	1	69,73,73	1.32	7 (10%)	82,113,113	1.66	12 (14%)
9	CHL	C	608	11	60,74,74	1.93	16 (26%)	58,114,114	2.66	22 (37%)
10	CLA	D	612	1	69,73,73	1.39	7 (10%)	82,113,113	1.73	14 (17%)
10	CLA	E	602	1	69,73,73	1.36	8 (11%)	82,113,113	1.86	17 (20%)
8	DGD	E	4632	-	67,67,67	0.96	1 (1%)	81,81,81	1.03	8 (9%)
10	CLA	J	610	1	69,73,73	1.34	6 (8%)	82,113,113	1.63	14 (17%)
10	CLA	E	612	1	69,73,73	1.44	7 (10%)	82,113,113	1.61	12 (14%)
10	CLA	H	612	1	69,73,73	1.42	9 (13%)	82,113,113	1.68	15 (18%)
10	CLA	H	603	1	69,73,73	1.37	8 (11%)	82,113,113	1.66	11 (13%)
6	NEX	B	1623	-	40,46,46	1.56	2 (5%)	50,70,70	0.95	3 (6%)
9	CHL	I	606	11	45,59,74	2.17	13 (28%)	40,96,114	2.97	19 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BNG	H	7633	-	21,21,21	0.51	0	26,26,26	0.80	1 (3%)
6	NEX	G	6623	-	40,46,46	1.67	3 (7%)	50,70,70	1.07	4 (8%)
10	CLA	C	603	1	69,73,73	1.37	8 (11%)	82,113,113	1.75	13 (15%)
9	CHL	F	609	1	60,74,74	1.90	14 (23%)	58,114,114	2.54	25 (43%)
4	LUT	A	620	-	42,43,43	0.95	4 (9%)	51,60,60	1.46	7 (13%)
10	CLA	F	611	7	69,73,73	1.32	6 (8%)	82,113,113	1.75	14 (17%)
6	NEX	H	7623	-	40,46,46	1.67	3 (7%)	50,70,70	1.01	4 (8%)
10	CLA	G	604	11	66,70,73	1.30	8 (12%)	78,109,113	1.95	17 (21%)
10	CLA	I	604	11	66,70,73	1.33	8 (12%)	78,109,113	2.03	16 (20%)
10	CLA	J	613	1	69,73,73	1.36	9 (13%)	82,113,113	1.65	13 (15%)
7	LHG	F	5630	10	48,48,48	1.04	3 (6%)	51,54,54	1.33	5 (9%)
10	CLA	B	612	1	69,73,73	1.42	8 (11%)	82,113,113	1.62	11 (13%)
4	LUT	H	7620	-	42,43,43	0.89	1 (2%)	51,60,60	1.44	5 (9%)
9	CHL	I	601	1	60,74,74	1.75	12 (20%)	58,114,114	2.51	20 (34%)
10	CLA	H	610	1	69,73,73	1.39	8 (11%)	82,113,113	1.65	14 (17%)
10	CLA	I	602	1	69,73,73	1.36	10 (14%)	82,113,113	2.06	21 (25%)
10	CLA	H	604	11	66,70,73	1.29	8 (12%)	78,109,113	2.03	18 (23%)
2	BNG	A	633	-	21,21,21	0.55	0	26,26,26	0.80	1 (3%)
10	CLA	E	604	11	66,70,73	1.34	10 (15%)	78,109,113	1.90	13 (16%)
10	CLA	D	610	1	69,73,73	1.41	6 (8%)	82,113,113	1.67	12 (14%)
8	DGD	B	2632	-	67,67,67	0.91	1 (1%)	81,81,81	1.03	8 (9%)
9	CHL	E	601	1	60,74,74	1.99	14 (23%)	58,114,114	2.56	21 (36%)
10	CLA	H	602	1	69,73,73	1.41	9 (13%)	82,113,113	1.91	21 (25%)
10	CLA	F	612	1	69,73,73	1.49	8 (11%)	82,113,113	1.69	15 (18%)
7	LHG	J	9630	10	48,48,48	0.99	3 (6%)	51,54,54	1.35	5 (9%)
9	CHL	G	605	1	42,56,74	2.28	12 (28%)	36,92,114	2.82	18 (50%)
10	CLA	G	610	1	69,73,73	1.32	8 (11%)	82,113,113	1.66	12 (14%)
10	CLA	J	603	1	69,73,73	1.46	9 (13%)	82,113,113	1.77	14 (17%)
9	CHL	J	605	1	42,56,74	2.24	12 (28%)	36,92,114	2.98	18 (50%)
5	XAT	F	6622	-	41,47,47	0.66	0	54,74,74	1.20	5 (9%)
8	DGD	A	632	-	67,67,67	0.94	2 (2%)	81,81,81	0.95	6 (7%)
10	CLA	D	611	7	69,73,73	1.30	6 (8%)	82,113,113	1.85	16 (19%)
8	DGD	H	6632	-	67,67,67	0.85	1 (1%)	81,81,81	0.99	7 (8%)
6	NEX	A	623	-	40,46,46	1.72	3 (7%)	50,70,70	1.02	4 (8%)
5	XAT	C	7622	-	41,47,47	0.77	1 (2%)	54,74,74	1.26	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LUT	J	9621	-	42,43,43	1.04	4 (9%)	51,60,60	1.35	6 (11%)
10	CLA	B	604	11	66,70,73	1.33	7 (10%)	78,109,113	2.13	19 (24%)
7	LHG	D	3630	10	48,48,48	0.87	3 (6%)	51,54,54	1.27	5 (9%)
9	CHL	B	601	1	60,74,74	1.80	12 (20%)	58,114,114	2.49	21 (36%)
9	CHL	C	607	11	60,74,74	1.87	14 (23%)	58,114,114	2.78	23 (39%)
9	CHL	D	606	11	45,59,74	2.28	13 (28%)	40,96,114	3.21	24 (60%)
6	NEX	C	2623	-	40,46,46	1.71	3 (7%)	50,70,70	0.96	2 (4%)
9	CHL	G	607	11	60,74,74	1.85	11 (18%)	58,114,114	2.68	24 (41%)
9	CHL	I	608	11	60,74,74	1.85	11 (18%)	58,114,114	2.48	21 (36%)
10	CLA	A	603	1	69,73,73	1.38	8 (11%)	82,113,113	1.75	14 (17%)
10	CLA	D	613	1	69,73,73	1.42	10 (14%)	82,113,113	1.81	13 (15%)
9	CHL	C	606	11	45,59,74	2.31	13 (28%)	40,96,114	3.22	22 (55%)
10	CLA	C	614	1	53,57,73	1.45	6 (11%)	61,93,113	2.00	13 (21%)
10	CLA	D	614	1	53,57,73	1.45	5 (9%)	61,93,113	1.88	10 (16%)
9	CHL	G	606	11	45,59,74	2.31	15 (33%)	40,96,114	2.97	18 (45%)
6	NEX	I	8623	-	40,46,46	1.74	3 (7%)	50,70,70	0.95	3 (6%)
9	CHL	H	606	11	45,59,74	2.22	14 (31%)	40,96,114	2.98	18 (45%)
8	DGD	G	9632	-	67,67,67	1.05	2 (2%)	81,81,81	1.05	8 (9%)
10	CLA	A	614	1	53,57,73	1.42	5 (9%)	61,93,113	1.92	10 (16%)
10	CLA	E	603	1	69,73,73	1.42	9 (13%)	82,113,113	1.66	13 (15%)
10	CLA	E	614	1	53,57,73	1.49	5 (9%)	61,93,113	1.99	11 (18%)
10	CLA	H	613	1	69,73,73	1.31	6 (8%)	82,113,113	1.82	15 (18%)
9	CHL	G	601	1	60,74,74	1.89	14 (23%)	58,114,114	2.59	18 (31%)
9	CHL	A	605	1	42,56,74	2.31	12 (28%)	36,92,114	2.87	18 (50%)
10	CLA	B	611	7	69,73,73	1.33	6 (8%)	82,113,113	1.88	17 (20%)
9	CHL	E	608	11	60,74,74	1.92	14 (23%)	58,114,114	2.55	21 (36%)
2	BNG	D	3633	-	21,21,21	0.50	0	26,26,26	0.85	1 (3%)
9	CHL	A	601	1	60,74,74	1.81	11 (18%)	58,114,114	2.58	19 (32%)
9	CHL	B	606	11	45,59,74	2.26	13 (28%)	40,96,114	2.94	20 (50%)
10	CLA	B	613	1	69,73,73	1.35	8 (11%)	82,113,113	1.78	12 (14%)
9	CHL	E	606	11	45,59,74	2.25	15 (33%)	40,96,114	3.13	22 (55%)
9	CHL	H	609	1	60,74,74	1.86	12 (20%)	58,114,114	2.48	19 (32%)
10	CLA	B	614	1	53,57,73	1.47	6 (11%)	61,93,113	1.98	10 (16%)
10	CLA	E	613	1	69,73,73	1.38	7 (10%)	82,113,113	1.74	16 (19%)
10	CLA	A	611	7	69,73,73	1.35	6 (8%)	82,113,113	1.86	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	CLA	J	611	7	69,73,73	1.27	6 (8%)	82,113,113	1.82	14 (17%)
8	DGD	D	5632	-	67,67,67	0.94	1 (1%)	81,81,81	1.07	9 (11%)
6	NEX	J	9623	-	40,46,46	1.71	3 (7%)	50,70,70	1.00	3 (6%)
7	LHG	C	2630	10	48,48,48	0.96	3 (6%)	51,54,54	1.36	5 (9%)
9	CHL	J	606	11	45,59,74	2.35	14 (31%)	40,96,114	2.97	18 (45%)
10	CLA	F	602	1	69,73,73	1.35	10 (14%)	82,113,113	1.94	18 (21%)
9	CHL	B	608	11	60,74,74	1.95	12 (20%)	58,114,114	2.64	25 (43%)
7	LHG	H	7630	10	48,48,48	0.94	3 (6%)	51,54,54	1.34	6 (11%)
2	BNG	J	9633	-	21,21,21	0.51	0	26,26,26	0.81	1 (3%)
10	CLA	I	611	7	69,73,73	1.38	5 (7%)	82,113,113	1.74	17 (20%)
10	CLA	J	612	1	69,73,73	1.36	7 (10%)	82,113,113	1.71	17 (20%)
9	CHL	J	608	11	60,74,74	1.98	16 (26%)	58,114,114	2.44	19 (32%)
9	CHL	A	608	11	60,74,74	1.94	14 (23%)	58,114,114	2.63	22 (37%)
10	CLA	I	613	1	69,73,73	1.32	8 (11%)	82,113,113	1.77	11 (13%)
7	LHG	I	8630	10	48,48,48	1.04	3 (6%)	51,54,54	1.39	5 (9%)
10	CLA	C	604	11	66,70,73	1.31	8 (12%)	78,109,113	2.04	13 (16%)
5	XAT	A	622	-	41,47,47	0.61	0	54,74,74	1.17	3 (5%)
6	NEX	E	4623	-	40,46,46	1.72	2 (5%)	50,70,70	0.92	3 (6%)
10	CLA	I	614	1	53,57,73	1.43	6 (11%)	61,93,113	1.92	9 (14%)
10	CLA	D	603	1	69,73,73	1.31	6 (8%)	82,113,113	1.63	13 (15%)
9	CHL	A	609	1	60,74,74	1.98	13 (21%)	58,114,114	2.55	20 (34%)
2	BNG	I	8633	-	21,21,21	0.53	0	26,26,26	0.77	1 (3%)
10	CLA	F	604	11	66,70,73	1.28	8 (12%)	78,109,113	2.02	21 (26%)
9	CHL	I	607	11	60,74,74	1.94	13 (21%)	58,114,114	2.66	24 (41%)
4	LUT	C	2621	-	42,43,43	1.22	5 (11%)	51,60,60	1.25	6 (11%)
9	CHL	D	607	11	60,74,74	1.96	12 (20%)	58,114,114	2.62	22 (37%)
10	CLA	J	604	11	66,70,73	1.35	8 (12%)	78,109,113	2.05	17 (21%)
5	XAT	H	4622	-	41,47,47	0.73	0	54,74,74	1.33	5 (9%)
9	CHL	H	607	11	60,74,74	1.90	13 (21%)	58,114,114	2.66	23 (39%)
5	XAT	B	1622	-	41,47,47	0.67	0	54,74,74	1.35	4 (7%)
9	CHL	J	601	1	60,74,74	1.92	15 (25%)	58,114,114	2.46	18 (31%)
9	CHL	D	608	11	60,74,74	1.79	15 (25%)	58,114,114	2.55	19 (32%)
9	CHL	E	605	1	42,56,74	2.16	13 (30%)	36,92,114	2.95	18 (50%)
9	CHL	D	609	1	60,74,74	1.83	11 (18%)	58,114,114	2.56	21 (36%)
9	CHL	I	609	1	60,74,74	1.94	14 (23%)	58,114,114	2.58	18 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	DGD	D	3632	-	67,67,67	0.96	2 (2%)	81,81,81	0.98	8 (9%)
10	CLA	H	614	1	53,57,73	1.43	5 (9%)	61,93,113	1.98	11 (18%)
9	CHL	D	605	1	42,56,74	2.26	13 (30%)	36,92,114	2.98	18 (50%)
9	CHL	C	609	1	60,74,74	1.90	12 (20%)	58,114,114	2.47	19 (32%)
2	BNG	F	5633	-	21,21,21	0.54	0	26,26,26	0.81	1 (3%)
8	DGD	I	8632	-	67,67,67	0.91	1 (1%)	81,81,81	0.98	8 (9%)
4	LUT	D	3620	-	42,43,43	0.92	3 (7%)	51,60,60	1.43	6 (11%)
4	LUT	E	4621	-	42,43,43	1.09	4 (9%)	51,60,60	1.20	5 (9%)
10	CLA	B	603	1	69,73,73	1.38	8 (11%)	82,113,113	1.74	13 (15%)
10	CLA	I	612	1	69,73,73	1.39	6 (8%)	82,113,113	1.67	11 (13%)
9	CHL	H	601	1	60,74,74	1.88	13 (21%)	58,114,114	2.54	21 (36%)
9	CHL	J	609	1	60,74,74	2.00	11 (18%)	58,114,114	2.48	20 (34%)
10	CLA	G	603	1	69,73,73	1.36	8 (11%)	82,113,113	1.79	12 (14%)
10	CLA	C	610	1	69,73,73	1.44	9 (13%)	82,113,113	1.57	11 (13%)
10	CLA	I	610	1	69,73,73	1.40	8 (11%)	82,113,113	1.55	11 (13%)
10	CLA	D	602	1	69,73,73	1.40	9 (13%)	82,113,113	1.90	17 (20%)
8	DGD	B	1632	-	67,67,67	0.95	2 (2%)	81,81,81	1.02	8 (9%)
9	CHL	D	601	1	60,74,74	1.87	12 (20%)	58,114,114	2.60	22 (37%)
9	CHL	B	609	1	60,74,74	1.99	14 (23%)	58,114,114	2.48	20 (34%)
10	CLA	G	612	1	69,73,73	1.37	7 (10%)	82,113,113	1.73	12 (14%)
10	CLA	G	614	1	53,57,73	1.48	6 (11%)	61,93,113	1.89	10 (16%)
5	XAT	E	2622	-	41,47,47	0.71	0	54,74,74	1.20	6 (11%)
9	CHL	B	605	1	42,56,74	2.29	12 (28%)	36,92,114	2.93	16 (44%)
9	CHL	J	607	11	60,74,74	1.84	11 (18%)	58,114,114	2.60	22 (37%)
4	LUT	G	6620	-	42,43,43	0.96	4 (9%)	51,60,60	1.42	6 (11%)
10	CLA	F	603	1	69,73,73	1.45	8 (11%)	82,113,113	1.72	15 (18%)
10	CLA	G	602	1	69,73,73	1.35	10 (14%)	82,113,113	1.94	21 (25%)
5	XAT	J	3622	-	41,47,47	0.72	0	54,74,74	1.19	4 (7%)
10	CLA	J	614	1	53,57,73	1.40	4 (7%)	61,93,113	1.84	10 (16%)
4	LUT	A	621	-	42,43,43	1.17	4 (9%)	51,60,60	1.39	7 (13%)
4	LUT	E	4620	-	42,43,43	1.04	4 (9%)	51,60,60	1.50	5 (9%)
9	CHL	B	607	11	60,74,74	1.89	15 (25%)	58,114,114	2.74	25 (43%)
10	CLA	C	611	7	69,73,73	1.28	6 (8%)	82,113,113	1.83	12 (14%)
4	LUT	F	5620	-	42,43,43	0.88	3 (7%)	51,60,60	1.33	6 (11%)
4	LUT	I	8621	-	42,43,43	0.97	4 (9%)	51,60,60	1.34	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CHL	F	605	1	42,56,74	2.21	11 (26%)	36,92,114	2.95	18 (50%)
2	BNG	C	2633	-	21,21,21	0.53	0	26,26,26	0.80	1 (3%)
9	CHL	A	606	11	45,59,74	2.31	12 (26%)	40,96,114	3.08	22 (55%)
9	CHL	F	607	11	60,74,74	1.97	10 (16%)	58,114,114	2.79	26 (44%)
9	CHL	H	608	11	60,74,74	1.93	12 (20%)	58,114,114	2.58	21 (36%)
10	CLA	E	611	7	69,73,73	1.37	6 (8%)	82,113,113	1.81	14 (17%)
9	CHL	E	609	1	60,74,74	1.90	12 (20%)	58,114,114	2.51	16 (27%)
10	CLA	B	602	1	69,73,73	1.37	9 (13%)	82,113,113	1.99	17 (20%)
9	CHL	F	606	11	45,59,74	2.32	15 (33%)	40,96,114	3.06	21 (52%)
10	CLA	C	613	1	69,73,73	1.33	10 (14%)	82,113,113	1.73	10 (12%)
10	CLA	F	614	1	53,57,73	1.45	5 (9%)	61,93,113	1.85	9 (14%)
10	CLA	G	611	7	69,73,73	1.31	7 (10%)	82,113,113	1.85	14 (17%)
4	LUT	B	1621	-	42,43,43	1.05	4 (9%)	51,60,60	1.18	3 (5%)
10	CLA	J	602	1	69,73,73	1.30	9 (13%)	82,113,113	2.01	19 (23%)
5	XAT	I	9622	-	41,47,47	0.75	1 (2%)	54,74,74	1.22	3 (5%)
10	CLA	A	612	1	69,73,73	1.42	6 (8%)	82,113,113	1.66	13 (15%)
9	CHL	C	605	1	42,56,74	2.25	13 (30%)	36,92,114	2.98	18 (50%)
4	LUT	H	7621	-	42,43,43	0.99	4 (9%)	51,60,60	1.29	5 (9%)
9	CHL	I	605	1	42,56,74	2.31	12 (28%)	36,92,114	2.86	18 (50%)
4	LUT	F	5621	-	42,43,43	1.05	4 (9%)	51,60,60	1.38	7 (13%)
10	CLA	F	610	1	69,73,73	1.43	8 (11%)	82,113,113	1.56	9 (10%)
9	CHL	A	607	11	60,74,74	1.85	12 (20%)	58,114,114	2.72	22 (37%)
7	LHG	A	630	10	48,48,48	0.93	3 (6%)	51,54,54	1.43	5 (9%)
8	DGD	H	7632	-	67,67,67	0.94	2 (2%)	81,81,81	0.98	8 (9%)
4	LUT	I	8620	-	42,43,43	0.88	4 (9%)	51,60,60	1.40	6 (11%)
9	CHL	F	601	1	60,74,74	1.82	13 (21%)	58,114,114	2.54	18 (31%)
7	LHG	B	1630	10	48,48,48	1.04	3 (6%)	51,54,54	1.34	5 (9%)
6	NEX	D	3623	-	40,46,46	1.73	3 (7%)	50,70,70	0.95	3 (6%)
2	BNG	B	1633	-	21,21,21	0.49	0	26,26,26	0.82	1 (3%)
7	LHG	G	6630	10	48,48,48	1.00	3 (6%)	51,54,54	1.41	5 (9%)
4	LUT	D	3621	-	42,43,43	1.09	4 (9%)	51,60,60	1.30	8 (15%)
4	LUT	J	9620	-	42,43,43	1.01	4 (9%)	51,60,60	1.49	4 (7%)
5	XAT	B	5622	-	41,47,47	0.72	0	54,74,74	1.20	5 (9%)
9	CHL	G	608	11	60,74,74	1.97	14 (23%)	58,114,114	2.47	19 (32%)
10	CLA	A	610	1	69,73,73	1.36	7 (10%)	82,113,113	1.62	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BNG	G	6633	-	21,21,21	0.53	0	26,26,26	0.81	1 (3%)
9	CHL	H	605	1	42,56,74	2.31	13 (30%)	36,92,114	2.79	17 (47%)
4	LUT	G	6621	-	42,43,43	0.96	3 (7%)	51,60,60	1.21	6 (11%)
10	CLA	A	604	11	66,70,73	1.37	8 (12%)	78,109,113	1.93	13 (16%)
10	CLA	G	613	1	69,73,73	1.33	8 (11%)	82,113,113	1.80	12 (14%)
7	LHG	E	4630	10	48,48,48	0.92	3 (6%)	51,54,54	1.34	5 (9%)
9	CHL	E	607	11	60,74,74	1.84	13 (21%)	58,114,114	2.79	24 (41%)
9	CHL	C	601	1	60,74,74	1.83	11 (18%)	58,114,114	2.47	18 (31%)
4	LUT	B	1620	-	42,43,43	0.96	4 (9%)	51,60,60	1.35	7 (13%)

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
10	CLA	H	611	7	1/1/15/20	16/39/115/115	-
9	CHL	F	608	11	4/4/20/26	17/39/137/137	-
10	CLA	E	610	1	1/1/15/20	3/39/115/115	-
9	CHL	G	609	1	5/5/20/26	17/39/137/137	-
10	CLA	D	604	11	1/1/14/20	13/36/112/115	-
2	BNG	E	4633	-	-	10/12/32/32	0/1/1/1
10	CLA	A	613	1	1/1/15/20	8/39/115/115	-
10	CLA	C	602	1	2/2/15/20	15/39/115/115	-
10	CLA	I	603	1	2/2/15/20	16/39/115/115	-
6	NEX	F	5623	-	-	2/27/83/83	0/3/3/3
10	CLA	A	602	1	2/2/15/20	16/39/115/115	-
10	CLA	F	613	1	1/1/15/20	7/39/115/115	-
10	CLA	B	610	1	1/1/15/20	3/39/115/115	-
4	LUT	C	2620	-	-	0/29/67/67	0/2/2/2
5	XAT	D	8622	-	-	1/31/93/93	0/4/4/4
10	CLA	C	612	1	1/1/15/20	10/39/115/115	-
9	CHL	C	608	11	4/4/20/26	16/39/137/137	-
10	CLA	D	612	1	1/1/15/20	13/39/115/115	-
10	CLA	E	602	1	2/2/15/20	14/39/115/115	-
8	DGD	E	4632	-	2/2/13/13	24/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	J	610	1	1/1/15/20	5/39/115/115	-
10	CLA	E	612	1	1/1/15/20	14/39/115/115	-
10	CLA	H	612	1	1/1/15/20	13/39/115/115	-
10	CLA	H	603	1	2/2/15/20	13/39/115/115	-
6	NEX	B	1623	-	-	3/27/83/83	0/3/3/3
9	CHL	I	606	11	3/3/17/26	6/21/119/137	-
2	BNG	H	7633	-	-	10/12/32/32	0/1/1/1
6	NEX	G	6623	-	-	2/27/83/83	0/3/3/3
10	CLA	C	603	1	2/2/15/20	15/39/115/115	-
9	CHL	F	609	1	5/5/20/26	17/39/137/137	-
4	LUT	A	620	-	-	0/29/67/67	0/2/2/2
10	CLA	F	611	7	1/1/15/20	19/39/115/115	-
6	NEX	H	7623	-	-	3/27/83/83	0/3/3/3
10	CLA	G	604	11	1/1/14/20	11/36/112/115	-
10	CLA	I	604	11	1/1/14/20	10/36/112/115	-
10	CLA	J	613	1	1/1/15/20	14/39/115/115	-
10	CLA	B	612	1	1/1/15/20	14/39/115/115	-
7	LHG	F	5630	10	-	31/53/53/53	-
10	CLA	H	610	1	2/2/15/20	9/39/115/115	-
9	CHL	I	601	1	4/4/20/26	12/39/137/137	-
10	CLA	I	602	1	2/2/15/20	13/39/115/115	-
4	LUT	H	7620	-	-	0/29/67/67	0/2/2/2
10	CLA	H	604	11	1/1/14/20	16/36/112/115	-
2	BNG	A	633	-	-	11/12/32/32	0/1/1/1
10	CLA	E	604	11	1/1/14/20	5/36/112/115	-
10	CLA	D	610	1	1/1/15/20	9/39/115/115	-
8	DGD	B	2632	-	2/2/13/13	29/55/95/95	0/2/2/2
9	CHL	E	601	1	4/4/20/26	9/39/137/137	-
10	CLA	H	602	1	2/2/15/20	18/39/115/115	-
10	CLA	F	612	1	1/1/15/20	16/39/115/115	-
7	LHG	J	9630	10	-	29/53/53/53	-
9	CHL	G	605	1	3/3/16/26	6/18/116/137	-
10	CLA	G	610	1	1/1/15/20	7/39/115/115	-
10	CLA	J	603	1	2/2/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CHL	J	605	1	3/3/16/26	10/18/116/137	-
5	XAT	F	6622	-	-	1/31/93/93	0/4/4/4
8	DGD	A	632	-	2/2/13/13	27/55/95/95	0/2/2/2
10	CLA	D	611	7	1/1/15/20	18/39/115/115	-
8	DGD	H	6632	-	2/2/13/13	33/55/95/95	0/2/2/2
6	NEX	A	623	-	-	3/27/83/83	0/3/3/3
5	XAT	C	7622	-	-	0/31/93/93	0/4/4/4
4	LUT	J	9621	-	-	1/29/67/67	0/2/2/2
10	CLA	B	604	11	1/1/14/20	9/36/112/115	-
7	LHG	D	3630	10	-	31/53/53/53	-
9	CHL	B	601	1	4/4/20/26	9/39/137/137	-
9	CHL	C	607	11	3/3/20/26	14/39/137/137	-
9	CHL	D	606	11	3/3/17/26	7/21/119/137	-
9	CHL	I	608	11	4/4/20/26	17/39/137/137	-
9	CHL	G	607	11	3/3/20/26	14/39/137/137	-
10	CLA	D	613	1	1/1/15/20	9/39/115/115	-
10	CLA	A	603	1	2/2/15/20	18/39/115/115	-
10	CLA	D	614	1	1/1/11/20	5/20/96/115	-
9	CHL	C	606	11	3/3/17/26	8/21/119/137	-
10	CLA	C	614	1	1/1/11/20	5/20/96/115	-
6	NEX	C	2623	-	-	2/27/83/83	0/3/3/3
9	CHL	G	606	11	3/3/17/26	5/21/119/137	-
9	CHL	H	606	11	3/3/17/26	5/21/119/137	-
10	CLA	A	614	1	1/1/11/20	6/20/96/115	-
8	DGD	G	9632	-	2/2/13/13	28/55/95/95	0/2/2/2
10	CLA	E	603	1	2/2/15/20	13/39/115/115	-
10	CLA	E	614	1	1/1/11/20	6/20/96/115	-
10	CLA	H	613	1	1/1/15/20	14/39/115/115	-
6	NEX	I	8623	-	-	2/27/83/83	0/3/3/3
9	CHL	G	601	1	4/4/20/26	10/39/137/137	-
9	CHL	A	605	1	3/3/16/26	8/18/116/137	-
10	CLA	B	611	7	1/1/15/20	19/39/115/115	-
9	CHL	E	608	11	4/4/20/26	17/39/137/137	-
2	BNG	D	3633	-	-	10/12/32/32	0/1/1/1
9	CHL	A	601	1	5/5/20/26	12/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CHL	B	606	11	3/3/17/26	7/21/119/137	-
10	CLA	B	613	1	1/1/15/20	7/39/115/115	-
9	CHL	E	606	11	3/3/17/26	5/21/119/137	-
9	CHL	H	609	1	5/5/20/26	14/39/137/137	-
10	CLA	B	614	1	1/1/11/20	4/20/96/115	-
10	CLA	E	613	1	1/1/15/20	13/39/115/115	-
10	CLA	A	611	7	1/1/15/20	19/39/115/115	-
10	CLA	J	611	7	1/1/15/20	17/39/115/115	-
8	DGD	D	5632	-	2/2/13/13	27/55/95/95	0/2/2/2
6	NEX	J	9623	-	-	2/27/83/83	0/3/3/3
9	CHL	J	606	11	3/3/17/26	6/21/119/137	-
10	CLA	F	602	1	2/2/15/20	16/39/115/115	-
7	LHG	C	2630	10	-	33/53/53/53	-
9	CHL	B	608	11	4/4/20/26	21/39/137/137	-
7	LHG	H	7630	10	-	32/53/53/53	-
2	BNG	J	9633	-	-	10/12/32/32	0/1/1/1
10	CLA	I	611	7	1/1/15/20	19/39/115/115	-
10	CLA	J	612	1	1/1/15/20	15/39/115/115	-
9	CHL	J	608	11	4/4/20/26	18/39/137/137	-
9	CHL	A	608	11	4/4/20/26	18/39/137/137	-
10	CLA	I	613	1	1/1/15/20	10/39/115/115	-
7	LHG	I	8630	10	-	37/53/53/53	-
10	CLA	C	604	11	1/1/14/20	15/36/112/115	-
5	XAT	A	622	-	-	0/31/93/93	0/4/4/4
6	NEX	E	4623	-	-	3/27/83/83	0/3/3/3
10	CLA	I	614	1	1/1/11/20	8/20/96/115	-
10	CLA	D	603	1	2/2/15/20	17/39/115/115	-
9	CHL	A	609	1	5/5/20/26	19/39/137/137	-
2	BNG	I	8633	-	-	9/12/32/32	0/1/1/1
10	CLA	F	604	11	1/1/14/20	14/36/112/115	-
9	CHL	I	607	11	3/3/20/26	12/39/137/137	-
9	CHL	D	607	11	3/3/20/26	14/39/137/137	-
4	LUT	C	2621	-	-	1/29/67/67	0/2/2/2
10	CLA	J	604	11	1/1/14/20	8/36/112/115	-
5	XAT	H	4622	-	-	1/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CHL	H	607	11	3/3/20/26	12/39/137/137	-
5	XAT	B	1622	-	-	1/31/93/93	0/4/4/4
9	CHL	J	601	1	4/4/20/26	13/39/137/137	-
9	CHL	D	608	11	4/4/20/26	15/39/137/137	-
9	CHL	E	605	1	3/3/16/26	10/18/116/137	-
9	CHL	D	609	1	5/5/20/26	16/39/137/137	-
9	CHL	I	609	1	5/5/20/26	16/39/137/137	-
8	DGD	D	3632	-	2/2/13/13	28/55/95/95	0/2/2/2
10	CLA	H	614	1	1/1/11/20	5/20/96/115	-
9	CHL	D	605	1	3/3/16/26	9/18/116/137	-
9	CHL	C	609	1	5/5/20/26	13/39/137/137	-
2	BNG	F	5633	-	-	9/12/32/32	0/1/1/1
8	DGD	I	8632	-	2/2/13/13	27/55/95/95	0/2/2/2
4	LUT	D	3620	-	-	0/29/67/67	0/2/2/2
4	LUT	E	4621	-	-	1/29/67/67	0/2/2/2
10	CLA	B	603	1	2/2/15/20	13/39/115/115	-
10	CLA	I	612	1	1/1/15/20	14/39/115/115	-
9	CHL	H	601	1	4/4/20/26	6/39/137/137	-
9	CHL	J	609	1	5/5/20/26	20/39/137/137	-
10	CLA	G	603	1	2/2/15/20	14/39/115/115	-
10	CLA	C	610	1	1/1/15/20	4/39/115/115	-
10	CLA	I	610	1	2/2/15/20	8/39/115/115	-
10	CLA	D	602	1	2/2/15/20	16/39/115/115	-
8	DGD	B	1632	-	2/2/13/13	30/55/95/95	0/2/2/2
9	CHL	D	601	1	4/4/20/26	13/39/137/137	-
9	CHL	B	609	1	5/5/20/26	16/39/137/137	-
10	CLA	G	612	1	1/1/15/20	12/39/115/115	-
10	CLA	G	614	1	1/1/11/20	5/20/96/115	-
5	XAT	E	2622	-	-	1/31/93/93	0/4/4/4
9	CHL	B	605	1	3/3/16/26	7/18/116/137	-
9	CHL	J	607	11	3/3/20/26	11/39/137/137	-
10	CLA	F	603	1	2/2/15/20	15/39/115/115	-
10	CLA	G	602	1	2/2/15/20	15/39/115/115	-
4	LUT	G	6620	-	-	0/29/67/67	0/2/2/2
10	CLA	J	614	1	1/1/11/20	5/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	XAT	J	3622	-	-	0/31/93/93	0/4/4/4
4	LUT	A	621	-	-	1/29/67/67	0/2/2/2
4	LUT	E	4620	-	-	0/29/67/67	0/2/2/2
9	CHL	B	607	11	3/3/20/26	14/39/137/137	-
10	CLA	C	611	7	1/1/15/20	16/39/115/115	-
4	LUT	F	5620	-	-	0/29/67/67	0/2/2/2
4	LUT	I	8621	-	-	1/29/67/67	0/2/2/2
9	CHL	F	605	1	3/3/16/26	6/18/116/137	-
2	BNG	C	2633	-	-	9/12/32/32	0/1/1/1
9	CHL	A	606	11	3/3/17/26	5/21/119/137	-
9	CHL	F	607	11	3/3/20/26	16/39/137/137	-
9	CHL	H	608	11	4/4/20/26	21/39/137/137	-
10	CLA	E	611	7	1/1/15/20	16/39/115/115	-
9	CHL	E	609	1	5/5/20/26	17/39/137/137	-
10	CLA	B	602	1	2/2/15/20	18/39/115/115	-
9	CHL	F	606	11	3/3/17/26	7/21/119/137	-
10	CLA	C	613	1	1/1/15/20	9/39/115/115	-
10	CLA	F	614	1	1/1/11/20	4/20/96/115	-
10	CLA	G	611	7	1/1/15/20	17/39/115/115	-
10	CLA	J	602	1	2/2/15/20	14/39/115/115	-
4	LUT	B	1621	-	-	2/29/67/67	0/2/2/2
5	XAT	I	9622	-	-	0/31/93/93	0/4/4/4
10	CLA	A	612	1	1/1/15/20	14/39/115/115	-
9	CHL	C	605	1	3/3/16/26	8/18/116/137	-
4	LUT	H	7621	-	-	1/29/67/67	0/2/2/2
9	CHL	I	605	1	3/3/16/26	10/18/116/137	-
4	LUT	F	5621	-	-	1/29/67/67	0/2/2/2
10	CLA	F	610	1	1/1/15/20	6/39/115/115	-
9	CHL	A	607	11	3/3/20/26	13/39/137/137	-
7	LHG	A	630	10	-	39/53/53/53	-
8	DGD	H	7632	-	2/2/13/13	30/55/95/95	0/2/2/2
4	LUT	I	8620	-	-	0/29/67/67	0/2/2/2
9	CHL	F	601	1	4/4/20/26	13/39/137/137	-
7	LHG	B	1630	10	-	34/53/53/53	-
6	NEX	D	3623	-	-	2/27/83/83	0/3/3/3
2	BNG	B	1633	-	-	11/12/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LHG	G	6630	10	-	38/53/53/53	-
9	CHL	G	608	11	4/4/20/26	17/39/137/137	-
4	LUT	D	3621	-	-	1/29/67/67	0/2/2/2
4	LUT	J	9620	-	-	1/29/67/67	0/2/2/2
5	XAT	B	5622	-	-	1/31/93/93	0/4/4/4
10	CLA	A	610	1	1/1/15/20	4/39/115/115	-
2	BNG	G	6633	-	-	9/12/32/32	0/1/1/1
9	CHL	H	605	1	3/3/16/26	8/18/116/137	-
4	LUT	G	6621	-	-	0/29/67/67	0/2/2/2
10	CLA	A	604	11	1/1/14/20	10/36/112/115	-
10	CLA	G	613	1	1/1/15/20	11/39/115/115	-
9	CHL	E	607	11	3/3/20/26	13/39/137/137	-
7	LHG	E	4630	10	-	33/53/53/53	-
9	CHL	C	601	1	4/4/20/26	14/39/137/137	-
4	LUT	B	1620	-	-	0/29/67/67	0/2/2/2

All (1517) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	8623	NEX	C7-C6	9.03	1.41	1.30
6	E	4623	NEX	C7-C6	8.95	1.41	1.30
6	D	3623	NEX	C7-C6	8.92	1.41	1.30
6	J	9623	NEX	C7-C6	8.69	1.40	1.30
6	C	2623	NEX	C7-C6	8.65	1.40	1.30
6	A	623	NEX	C7-C6	8.64	1.40	1.30
6	H	7623	NEX	C7-C6	8.61	1.40	1.30
6	G	6623	NEX	C7-C6	8.47	1.40	1.30
6	F	5623	NEX	C7-C6	8.36	1.40	1.30
6	B	1623	NEX	C7-C6	8.06	1.40	1.30
10	F	612	CLA	MG-NA	7.23	2.23	2.06
8	G	9632	DGD	O2G-C1B	7.12	1.54	1.34
10	A	612	CLA	MG-NA	6.66	2.22	2.06
8	E	4632	DGD	O2G-C1B	6.63	1.53	1.34
10	E	612	CLA	MG-NA	6.60	2.22	2.06
10	I	612	CLA	MG-NA	6.57	2.21	2.06
9	G	606	CHL	O2A-CGA	6.55	1.52	1.33
10	J	612	CLA	MG-NA	6.35	2.21	2.06
9	C	606	CHL	O2A-CGA	6.34	1.51	1.33
9	D	606	CHL	O2A-CGA	6.34	1.51	1.33
10	H	612	CLA	MG-NA	6.34	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	5632	DGD	O2G-C1B	6.32	1.52	1.34
8	D	3632	DGD	O2G-C1B	6.28	1.52	1.34
8	H	7632	DGD	O2G-C1B	6.27	1.52	1.34
9	D	601	CHL	C1D-C2D	6.25	1.46	1.39
9	A	606	CHL	O2A-CGA	6.25	1.51	1.33
9	C	601	CHL	C1D-C2D	6.23	1.46	1.39
8	B	1632	DGD	O2G-C1B	6.22	1.51	1.34
9	F	606	CHL	C1B-C2B	6.22	1.46	1.39
9	F	606	CHL	O2A-CGA	6.21	1.51	1.33
9	G	607	CHL	C1B-C2B	6.20	1.46	1.39
9	B	607	CHL	C1B-C2B	6.19	1.46	1.39
9	I	605	CHL	C1D-C2D	6.19	1.46	1.39
10	H	603	CLA	MG-NA	6.18	2.21	2.06
8	B	2632	DGD	O2G-C1B	6.18	1.51	1.34
9	F	609	CHL	C1D-C2D	6.17	1.46	1.39
9	J	608	CHL	C1D-C2D	6.16	1.46	1.39
9	B	609	CHL	C1D-C2D	6.15	1.46	1.39
9	C	609	CHL	C1D-C2D	6.13	1.46	1.39
9	J	606	CHL	O2A-CGA	6.13	1.51	1.33
8	A	632	DGD	O2G-C1B	6.11	1.51	1.34
9	D	607	CHL	C1B-C2B	6.09	1.46	1.39
10	F	603	CLA	MG-NA	6.06	2.20	2.06
9	G	601	CHL	C1D-C2D	6.06	1.46	1.39
9	J	606	CHL	C1B-C2B	6.05	1.46	1.39
9	G	608	CHL	C1D-C2D	6.04	1.46	1.39
8	I	8632	DGD	O2G-C1B	6.02	1.51	1.34
10	C	603	CLA	MG-NA	6.02	2.20	2.06
10	I	603	CLA	MG-NA	6.01	2.20	2.06
9	A	609	CHL	C3B-C4B	6.00	1.47	1.41
9	F	601	CHL	C1D-C2D	6.00	1.46	1.39
9	D	609	CHL	C1D-C2D	6.00	1.46	1.39
9	E	608	CHL	C1D-C2D	6.00	1.46	1.39
9	J	607	CHL	C1B-C2B	6.00	1.46	1.39
9	J	609	CHL	C1D-C2D	5.98	1.46	1.39
9	I	609	CHL	C3B-C4B	5.97	1.47	1.41
9	C	606	CHL	C1B-C2B	5.96	1.46	1.39
9	G	605	CHL	C1D-C2D	5.96	1.46	1.39
9	E	606	CHL	C1B-C2B	5.96	1.46	1.39
9	J	608	CHL	C3B-C4B	5.96	1.47	1.41
9	D	606	CHL	C1D-C2D	5.96	1.46	1.39
10	C	614	CLA	MG-NA	5.93	2.20	2.06
9	I	606	CHL	O2A-CGA	5.91	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	609	CHL	C1D-C2D	5.91	1.46	1.39
9	B	608	CHL	C3B-C4B	5.91	1.47	1.41
9	F	607	CHL	C1B-C2B	5.90	1.46	1.39
9	A	608	CHL	C1D-C2D	5.89	1.46	1.39
9	F	605	CHL	C3B-C4B	5.89	1.47	1.41
9	D	605	CHL	C1D-C2D	5.89	1.46	1.39
9	H	606	CHL	C1B-C2B	5.86	1.46	1.39
9	D	607	CHL	C1D-C2D	5.85	1.46	1.39
10	G	612	CLA	MG-NA	5.84	2.20	2.06
9	A	605	CHL	C3B-C4B	5.84	1.47	1.41
9	A	609	CHL	C1D-C2D	5.83	1.46	1.39
10	I	611	CLA	MG-NA	5.83	2.20	2.06
10	B	612	CLA	MG-NA	5.80	2.20	2.06
9	A	605	CHL	C1D-C2D	5.80	1.46	1.39
10	B	614	CLA	MG-NA	5.79	2.20	2.06
9	E	609	CHL	C1D-C2D	5.79	1.46	1.39
9	C	608	CHL	C1D-C2D	5.79	1.46	1.39
10	E	613	CLA	MG-NA	5.78	2.20	2.06
9	G	606	CHL	C1B-C2B	5.77	1.46	1.39
9	E	601	CHL	C3B-C4B	5.76	1.47	1.41
9	J	607	CHL	C1D-C2D	5.74	1.46	1.39
10	E	614	CLA	MG-NA	5.74	2.19	2.06
9	J	605	CHL	C3B-C4B	5.73	1.47	1.41
9	A	606	CHL	C1B-C2B	5.73	1.46	1.39
10	C	612	CLA	MG-NA	5.73	2.19	2.06
9	D	605	CHL	C3B-C4B	5.72	1.47	1.41
9	J	606	CHL	C1D-C2D	5.71	1.46	1.39
9	F	601	CHL	C3B-C4B	5.71	1.47	1.41
9	B	606	CHL	C1B-C2B	5.71	1.46	1.39
10	G	614	CLA	MG-NA	5.70	2.19	2.06
9	E	609	CHL	C3B-C4B	5.70	1.46	1.41
9	E	608	CHL	C3B-C4B	5.70	1.46	1.41
9	C	605	CHL	C1D-C2D	5.70	1.46	1.39
10	D	612	CLA	MG-NA	5.70	2.19	2.06
9	E	601	CHL	C1D-C2D	5.70	1.46	1.39
9	E	606	CHL	C1D-C2D	5.70	1.46	1.39
9	C	609	CHL	C3B-C4B	5.69	1.46	1.41
9	H	601	CHL	C1D-C2D	5.69	1.46	1.39
10	H	614	CLA	MG-NA	5.69	2.19	2.06
9	F	608	CHL	C1D-C2D	5.67	1.46	1.39
9	I	608	CHL	C1D-C2D	5.66	1.46	1.39
9	B	605	CHL	C1D-C2D	5.64	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	607	CHL	C1D-C2D	5.64	1.45	1.39
9	F	605	CHL	C1D-C2D	5.63	1.45	1.39
9	D	608	CHL	C1D-C2D	5.62	1.45	1.39
9	E	605	CHL	C1D-C2D	5.62	1.45	1.39
10	J	603	CLA	MG-NA	5.61	2.19	2.06
9	C	607	CHL	C1B-C2B	5.61	1.45	1.39
9	C	601	CHL	C3B-C4B	5.61	1.46	1.41
9	A	607	CHL	C1B-C2B	5.60	1.45	1.39
9	I	609	CHL	C1D-C2D	5.60	1.45	1.39
10	D	614	CLA	MG-NA	5.59	2.19	2.06
9	J	601	CHL	C3B-C4B	5.58	1.46	1.41
10	D	603	CLA	MG-NA	5.58	2.19	2.06
9	J	609	CHL	C3A-C2A	-5.58	1.49	1.54
9	A	601	CHL	C1D-C2D	5.57	1.45	1.39
9	B	606	CHL	C1D-C2D	5.56	1.45	1.39
9	H	605	CHL	C1D-C2D	5.55	1.45	1.39
9	J	605	CHL	C1D-C2D	5.54	1.45	1.39
9	C	608	CHL	C3B-C4B	5.54	1.46	1.41
9	G	605	CHL	C3B-C4B	5.54	1.46	1.41
9	D	606	CHL	C1B-C2B	5.53	1.45	1.39
9	H	609	CHL	C1D-C2D	5.53	1.45	1.39
9	A	608	CHL	C3B-C4B	5.53	1.46	1.41
9	J	609	CHL	C3B-C4B	5.53	1.46	1.41
9	B	608	CHL	C1D-C2D	5.53	1.45	1.39
9	G	609	CHL	C3B-C4B	5.52	1.46	1.41
9	B	609	CHL	C3B-C4B	5.51	1.46	1.41
10	A	603	CLA	MG-NA	5.51	2.19	2.06
8	H	6632	DGD	O2G-C1B	5.49	1.49	1.34
9	I	607	CHL	C1B-C2B	5.49	1.45	1.39
9	H	608	CHL	C1D-C2D	5.48	1.45	1.39
9	I	606	CHL	C1B-C2B	5.48	1.45	1.39
9	I	606	CHL	C1D-C2D	5.48	1.45	1.39
10	B	603	CLA	MG-NA	5.47	2.19	2.06
9	H	608	CHL	C3B-C4B	5.47	1.46	1.41
9	B	601	CHL	C1D-C2D	5.46	1.45	1.39
9	G	606	CHL	C1D-C2D	5.45	1.45	1.39
9	A	609	CHL	C3A-C2A	-5.44	1.50	1.54
9	C	606	CHL	C1D-C2D	5.44	1.45	1.39
9	H	607	CHL	C1B-C2B	5.42	1.45	1.39
9	A	606	CHL	C1D-C2D	5.42	1.45	1.39
10	D	610	CLA	MG-NA	5.41	2.19	2.06
10	E	603	CLA	MG-NA	5.41	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	608	CHL	C3B-C4B	5.39	1.46	1.41
9	H	609	CHL	C3B-C4B	5.37	1.46	1.41
10	D	611	CLA	MG-NA	5.37	2.19	2.06
10	J	610	CLA	O2A-CGA	5.36	1.49	1.33
9	H	605	CHL	C1B-C2B	5.36	1.45	1.39
9	B	605	CHL	CBD-CGD	5.36	1.59	1.52
9	G	601	CHL	C3B-C4B	5.36	1.46	1.41
9	H	601	CHL	C1B-C2B	5.35	1.45	1.39
9	I	607	CHL	C1D-C2D	5.35	1.45	1.39
10	F	614	CLA	MG-NA	5.35	2.19	2.06
9	H	605	CHL	O2A-CGA	5.35	1.48	1.33
9	I	608	CHL	C3B-C4B	5.34	1.46	1.41
9	C	605	CHL	C3B-C4B	5.34	1.46	1.41
10	G	611	CLA	MG-NA	5.33	2.18	2.06
9	F	607	CHL	C1A-CHA	5.31	1.46	1.40
9	H	606	CHL	C1D-C2D	5.31	1.45	1.39
10	G	603	CLA	MG-NA	5.31	2.18	2.06
10	H	610	CLA	O2D-CGD	5.30	1.46	1.33
10	B	611	CLA	MG-NA	5.30	2.18	2.06
10	J	611	CLA	MG-NA	5.30	2.18	2.06
10	E	611	CLA	MG-NA	5.30	2.18	2.06
9	I	605	CHL	C3B-C4B	5.30	1.46	1.41
10	H	602	CLA	MG-NA	5.30	2.18	2.06
10	I	610	CLA	O2D-CGD	5.30	1.46	1.33
9	C	607	CHL	C1D-C2D	5.29	1.45	1.39
9	H	601	CHL	C3B-C4B	5.29	1.46	1.41
10	A	614	CLA	MG-NA	5.28	2.18	2.06
9	E	605	CHL	C3B-C4B	5.28	1.46	1.41
9	F	609	CHL	C3B-C4B	5.28	1.46	1.41
10	H	602	CLA	O2D-CGD	5.27	1.46	1.33
9	J	605	CHL	C1B-C2B	5.27	1.45	1.39
9	F	606	CHL	C1D-C2D	5.27	1.45	1.39
9	F	607	CHL	C1D-C2D	5.27	1.45	1.39
9	A	601	CHL	C1B-C2B	5.26	1.45	1.39
9	I	607	CHL	O2D-CGD	5.24	1.46	1.33
10	F	610	CLA	O2A-CGA	5.24	1.48	1.33
9	A	607	CHL	C1D-C2D	5.23	1.45	1.39
9	H	608	CHL	C3A-C2A	-5.22	1.50	1.54
9	D	601	CHL	C1B-C2B	5.22	1.45	1.39
9	G	607	CHL	C1D-C2D	5.22	1.45	1.39
9	D	601	CHL	C3B-C4B	5.21	1.46	1.41
9	D	609	CHL	C3B-C4B	5.21	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	607	CHL	O2D-CGD	5.21	1.46	1.33
9	H	605	CHL	C3B-C4B	5.21	1.46	1.41
9	J	601	CHL	C1D-C2D	5.20	1.45	1.39
9	J	601	CHL	C1B-C2B	5.19	1.45	1.39
10	F	611	CLA	MG-NA	5.19	2.18	2.06
9	C	605	CHL	C1B-C2B	5.18	1.45	1.39
10	C	602	CLA	MG-NA	5.18	2.18	2.06
10	C	611	CLA	MG-NA	5.17	2.18	2.06
9	B	606	CHL	O2A-CGA	5.16	1.48	1.33
9	J	608	CHL	C1B-C2B	5.16	1.45	1.39
10	J	613	CLA	MG-NA	5.15	2.18	2.06
9	B	605	CHL	C1B-C2B	5.13	1.45	1.39
9	G	608	CHL	C3A-C2A	-5.12	1.50	1.54
9	B	601	CHL	C1B-C2B	5.12	1.45	1.39
9	A	605	CHL	C1B-C2B	5.12	1.45	1.39
9	G	608	CHL	C3B-C4B	5.11	1.46	1.41
10	A	604	CLA	O2A-CGA	5.11	1.48	1.33
9	E	601	CHL	C1B-C2B	5.10	1.45	1.39
9	B	601	CHL	C3B-C4B	5.09	1.46	1.41
9	G	605	CHL	C1B-C2B	5.08	1.45	1.39
9	B	605	CHL	C3B-C4B	5.08	1.46	1.41
10	H	613	CLA	O2D-CGD	5.08	1.45	1.33
10	A	611	CLA	MG-NA	5.07	2.18	2.06
9	I	601	CHL	C1D-C2D	5.06	1.45	1.39
10	H	611	CLA	MG-NA	5.06	2.18	2.06
9	A	601	CHL	C3B-C4B	5.04	1.46	1.41
9	F	601	CHL	C1B-C2B	5.04	1.45	1.39
9	A	608	CHL	C1B-C2B	5.03	1.45	1.39
10	E	610	CLA	O2D-CGD	5.02	1.45	1.33
10	E	610	CLA	O2A-CGA	5.02	1.48	1.33
9	I	601	CHL	C1B-C2B	5.01	1.45	1.39
9	B	606	CHL	C3B-C4B	5.00	1.46	1.41
9	A	605	CHL	O2A-CGA	5.00	1.47	1.33
9	A	607	CHL	C1A-CHA	4.99	1.45	1.40
9	I	605	CHL	O2A-CGA	4.99	1.47	1.33
10	E	604	CLA	O2D-CGD	4.99	1.45	1.33
9	H	607	CHL	C1D-C2D	4.98	1.45	1.39
10	D	610	CLA	O2D-CGD	4.98	1.45	1.33
9	B	607	CHL	C1D-C2D	4.98	1.45	1.39
10	F	613	CLA	O2D-CGD	4.97	1.45	1.33
10	B	602	CLA	MG-NA	4.97	2.18	2.06
10	C	610	CLA	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	608	CHL	C3B-C4B	4.96	1.46	1.41
10	I	614	CLA	MG-NA	4.96	2.18	2.06
10	E	602	CLA	MG-NA	4.95	2.18	2.06
9	I	605	CHL	C1B-C2B	4.95	1.45	1.39
10	J	614	CLA	MG-NA	4.93	2.18	2.06
9	D	605	CHL	O2D-CGD	4.93	1.45	1.33
10	D	610	CLA	O2A-CGA	4.93	1.47	1.33
10	C	610	CLA	O2A-CGA	4.93	1.47	1.33
10	I	613	CLA	MG-NA	4.92	2.18	2.06
10	A	610	CLA	O2A-CGA	4.92	1.47	1.33
9	I	609	CHL	O2A-CGA	4.91	1.47	1.33
10	B	613	CLA	O2D-CGD	4.90	1.45	1.33
9	E	606	CHL	O2A-CGA	4.90	1.47	1.33
9	H	609	CHL	C3A-C2A	-4.90	1.50	1.54
10	B	610	CLA	O2A-CGA	4.89	1.47	1.33
9	E	608	CHL	O2D-CGD	4.89	1.45	1.33
9	E	608	CHL	C1B-C2B	4.88	1.45	1.39
10	A	602	CLA	O2D-CGD	4.88	1.45	1.33
9	D	605	CHL	C1B-C2B	4.88	1.45	1.39
10	I	602	CLA	MG-NA	4.88	2.17	2.06
9	B	608	CHL	C1B-C2B	4.87	1.45	1.39
10	F	613	CLA	MG-NA	4.87	2.17	2.06
9	H	606	CHL	O2A-CGA	4.86	1.47	1.33
9	C	605	CHL	O2A-CGA	4.86	1.47	1.33
9	G	609	CHL	C1B-C2B	4.86	1.45	1.39
9	E	601	CHL	O2A-CGA	4.85	1.47	1.33
9	J	609	CHL	C1B-C2B	4.85	1.45	1.39
9	F	605	CHL	O2D-CGD	4.85	1.45	1.33
10	H	613	CLA	MG-NA	4.83	2.17	2.06
10	C	613	CLA	MG-NA	4.83	2.17	2.06
9	F	605	CHL	O2A-CGA	4.82	1.47	1.33
9	D	607	CHL	C1A-CHA	4.80	1.45	1.40
9	E	605	CHL	C1B-C2B	4.80	1.45	1.39
7	B	1630	LHG	O8-C23	4.79	1.47	1.33
9	B	609	CHL	C1B-C2B	4.79	1.45	1.39
9	E	607	CHL	C1B-C2B	4.79	1.45	1.39
10	E	610	CLA	MG-NA	4.79	2.17	2.06
9	G	601	CHL	C1B-C2B	4.79	1.45	1.39
10	G	613	CLA	MG-NA	4.78	2.17	2.06
9	C	608	CHL	C1B-C2B	4.78	1.45	1.39
9	A	606	CHL	C1A-CHA	4.77	1.45	1.40
10	D	613	CLA	MG-NA	4.77	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	612	CLA	O2D-CGD	4.77	1.45	1.33
9	B	609	CHL	C3A-C2A	-4.77	1.50	1.54
9	I	608	CHL	C1B-C2B	4.77	1.45	1.39
9	C	607	CHL	O2D-CGD	4.77	1.44	1.33
10	F	610	CLA	MG-NA	4.76	2.17	2.06
10	D	613	CLA	O2D-CGD	4.76	1.44	1.33
9	B	608	CHL	C3A-C2A	-4.75	1.50	1.54
10	A	610	CLA	O2D-CGD	4.75	1.44	1.33
10	G	610	CLA	O2D-CGD	4.74	1.44	1.33
10	I	610	CLA	O2A-CGA	4.74	1.47	1.33
9	A	606	CHL	C3B-C4B	4.73	1.46	1.41
9	H	607	CHL	C3B-C4B	4.73	1.46	1.41
10	E	613	CLA	O2D-CGD	4.72	1.44	1.33
10	F	602	CLA	MG-NA	4.72	2.17	2.06
10	D	613	CLA	O2A-CGA	4.72	1.47	1.33
10	J	604	CLA	O2D-CGD	4.72	1.44	1.33
10	D	602	CLA	MG-NA	4.72	2.17	2.06
10	A	613	CLA	MG-NA	4.71	2.17	2.06
9	H	607	CHL	O2D-CGD	4.71	1.44	1.33
6	D	3623	NEX	C7-C8	4.71	1.39	1.31
9	D	605	CHL	O2A-CGA	4.70	1.47	1.33
10	D	604	CLA	O2A-CGA	4.70	1.47	1.33
9	F	609	CHL	C3A-C2A	-4.70	1.50	1.54
9	D	606	CHL	C3B-C4B	4.69	1.46	1.41
10	J	603	CLA	O2A-CGA	4.69	1.47	1.33
10	H	610	CLA	O2A-CGA	4.68	1.47	1.33
9	E	609	CHL	C3A-C2A	-4.67	1.50	1.54
9	I	601	CHL	C3B-C4B	4.67	1.45	1.41
9	C	601	CHL	C1B-C2B	4.66	1.44	1.39
9	F	608	CHL	C1B-C2B	4.65	1.44	1.39
9	F	605	CHL	C1B-C2B	4.64	1.44	1.39
7	I	8630	LHG	O8-C23	4.64	1.46	1.33
9	E	601	CHL	CBD-CGD	4.64	1.58	1.52
10	G	610	CLA	O2A-CGA	4.64	1.46	1.33
9	A	605	CHL	C3A-C2A	-4.63	1.50	1.54
10	B	602	CLA	O2D-CGD	4.62	1.44	1.33
9	J	608	CHL	C3A-C2A	-4.61	1.50	1.54
10	E	602	CLA	O2D-CGD	4.60	1.44	1.33
10	G	604	CLA	MG-NA	4.59	2.17	2.06
9	E	609	CHL	C1B-C2B	4.59	1.44	1.39
10	A	602	CLA	MG-NA	4.56	2.17	2.06
10	I	611	CLA	O2A-CGA	4.56	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	602	CLA	MG-NA	4.56	2.17	2.06
6	A	623	NEX	C7-C8	4.56	1.39	1.31
9	D	607	CHL	CBD-CGD	4.56	1.58	1.52
10	B	610	CLA	MG-NA	4.56	2.17	2.06
10	D	602	CLA	O2D-CGD	4.55	1.44	1.33
9	A	609	CHL	C1B-C2B	4.55	1.44	1.39
9	H	608	CHL	C1B-C2B	4.55	1.44	1.39
9	G	608	CHL	O2A-CGA	4.55	1.46	1.33
10	A	614	CLA	O2A-CGA	4.55	1.46	1.33
10	C	610	CLA	MG-NA	4.55	2.17	2.06
9	C	606	CHL	C3B-C4B	4.54	1.45	1.41
10	F	610	CLA	O2D-CGD	4.54	1.44	1.33
10	G	602	CLA	MG-NA	4.53	2.17	2.06
9	F	609	CHL	C1B-C2B	4.53	1.44	1.39
10	H	611	CLA	O2D-CGD	4.52	1.44	1.33
9	F	609	CHL	O2A-CGA	4.52	1.46	1.33
9	H	609	CHL	C1B-C2B	4.52	1.44	1.39
9	J	605	CHL	O2A-CGA	4.52	1.46	1.33
9	G	606	CHL	C3B-C4B	4.51	1.45	1.41
9	G	608	CHL	C1B-C2B	4.49	1.44	1.39
10	J	602	CLA	O2D-CGD	4.48	1.44	1.33
10	C	602	CLA	O2D-CGD	4.48	1.44	1.33
10	I	614	CLA	O2A-CGA	4.48	1.46	1.33
9	J	609	CHL	O2A-CGA	4.47	1.46	1.33
10	G	602	CLA	O2D-CGD	4.47	1.44	1.33
10	I	610	CLA	MG-NA	4.45	2.16	2.06
10	C	604	CLA	O2A-CGA	4.43	1.46	1.33
9	G	607	CHL	C1A-CHA	4.43	1.45	1.40
9	G	605	CHL	O2D-CGD	4.43	1.44	1.33
10	B	610	CLA	O2D-CGD	4.42	1.44	1.33
9	A	609	CHL	O2A-CGA	4.42	1.46	1.33
10	J	613	CLA	O2D-CGD	4.42	1.44	1.33
9	C	608	CHL	C3A-C2A	-4.42	1.50	1.54
10	B	604	CLA	O2A-CGA	4.41	1.46	1.33
10	H	604	CLA	MG-NA	4.41	2.16	2.06
9	A	605	CHL	O2D-CGD	4.41	1.44	1.33
10	E	602	CLA	O2A-CGA	4.40	1.46	1.33
9	H	605	CHL	C3A-C2A	-4.39	1.50	1.54
9	J	608	CHL	O2A-CGA	4.38	1.46	1.33
9	F	606	CHL	C3B-C4B	4.37	1.45	1.41
9	D	608	CHL	C1B-C2B	4.37	1.44	1.39
10	B	613	CLA	MG-NA	4.37	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	4623	NEX	C7-C8	4.36	1.39	1.31
10	I	604	CLA	O2D-CGD	4.36	1.43	1.33
10	B	603	CLA	O2A-CGA	4.35	1.46	1.33
10	A	604	CLA	MG-NA	4.35	2.16	2.06
9	B	601	CHL	O2A-CGA	4.35	1.46	1.33
10	J	604	CLA	MG-NA	4.34	2.16	2.06
10	H	614	CLA	O2A-CGA	4.33	1.46	1.33
10	I	602	CLA	O2D-CGD	4.33	1.43	1.33
6	I	8623	NEX	C7-C8	4.33	1.38	1.31
9	D	609	CHL	O2A-CGA	4.33	1.46	1.33
10	I	604	CLA	MG-NA	4.32	2.16	2.06
9	I	607	CHL	C1A-CHA	4.32	1.44	1.40
6	J	9623	NEX	C7-C8	4.32	1.38	1.31
9	C	606	CHL	C3A-C2A	-4.31	1.51	1.54
9	I	609	CHL	C3A-C2A	-4.30	1.51	1.54
10	C	603	CLA	O2A-CGA	4.30	1.45	1.33
9	I	606	CHL	C3B-C4B	4.30	1.45	1.41
9	I	609	CHL	C1B-C2B	4.29	1.44	1.39
9	E	601	CHL	O2D-CGD	4.29	1.43	1.33
10	F	602	CLA	O2D-CGD	4.29	1.43	1.33
9	E	606	CHL	C3B-C4B	4.29	1.45	1.41
9	G	605	CHL	O2A-CGA	4.29	1.45	1.33
7	F	5630	LHG	O7-C7	4.29	1.46	1.34
9	D	609	CHL	C1B-C2B	4.28	1.44	1.39
10	J	614	CLA	O2A-CGA	4.28	1.45	1.33
9	C	609	CHL	C1B-C2B	4.28	1.44	1.39
10	F	604	CLA	MG-NA	4.27	2.16	2.06
9	I	605	CHL	C3A-C2A	-4.27	1.51	1.54
10	B	604	CLA	O2D-CGD	4.27	1.43	1.33
9	H	601	CHL	O2A-CGA	4.27	1.45	1.33
7	G	6630	LHG	O8-C23	4.27	1.45	1.33
10	G	614	CLA	O2A-CGA	4.26	1.45	1.33
10	E	611	CLA	O2D-CGD	4.26	1.43	1.33
9	H	605	CHL	O2D-CGD	4.26	1.43	1.33
9	G	605	CHL	CBD-CGD	4.26	1.57	1.52
9	B	609	CHL	O2A-CGA	4.26	1.45	1.33
9	I	607	CHL	C3B-C4B	4.25	1.45	1.41
9	E	608	CHL	C3A-C2A	-4.25	1.51	1.54
9	B	605	CHL	O2A-CGA	4.25	1.45	1.33
10	A	603	CLA	O2D-CGD	4.24	1.43	1.33
9	J	606	CHL	C3B-C4B	4.23	1.45	1.41
9	H	608	CHL	O2A-CGA	4.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	606	CHL	O2D-CGD	4.22	1.43	1.33
6	H	7623	NEX	C7-C8	4.22	1.38	1.31
10	J	610	CLA	MG-NA	4.22	2.16	2.06
10	F	614	CLA	O2D-CGD	4.21	1.43	1.33
10	B	612	CLA	O2D-CGD	4.21	1.43	1.33
6	F	5623	NEX	C7-C8	4.21	1.38	1.31
10	F	611	CLA	O2D-CGD	4.21	1.43	1.33
10	E	614	CLA	O2A-CGA	4.21	1.45	1.33
9	A	608	CHL	O2D-CGD	4.21	1.43	1.33
10	D	604	CLA	MG-NA	4.20	2.16	2.06
9	A	608	CHL	C3A-C2A	-4.20	1.51	1.54
9	F	606	CHL	C1A-CHA	4.20	1.44	1.40
9	J	606	CHL	C1A-CHA	4.20	1.44	1.40
9	F	608	CHL	O2A-CGA	4.19	1.45	1.33
7	J	9630	LHG	O7-C7	4.19	1.46	1.34
9	A	607	CHL	C3B-C4B	4.19	1.45	1.41
10	B	614	CLA	O2A-CGA	4.19	1.45	1.33
10	D	604	CLA	O2D-CGD	4.19	1.43	1.33
10	D	602	CLA	O2A-CGA	4.17	1.45	1.33
10	J	603	CLA	O2D-CGD	4.16	1.43	1.33
10	C	614	CLA	O2D-CGD	4.16	1.43	1.33
10	F	614	CLA	O2A-CGA	4.16	1.45	1.33
10	J	610	CLA	O2D-CGD	4.16	1.43	1.33
10	A	610	CLA	MG-NA	4.16	2.16	2.06
10	E	603	CLA	MG-ND	-4.16	1.97	2.05
9	E	606	CHL	O2D-CGD	4.15	1.43	1.33
9	C	605	CHL	O2D-CGD	4.15	1.43	1.33
6	C	2623	NEX	C7-C8	4.15	1.38	1.31
9	E	607	CHL	C3B-C4B	4.14	1.45	1.41
9	H	609	CHL	O2A-CGA	4.14	1.45	1.33
9	B	608	CHL	O2D-CGD	4.14	1.43	1.33
10	G	611	CLA	O2A-CGA	4.13	1.45	1.33
9	D	606	CHL	C3A-C2A	-4.13	1.51	1.54
10	H	604	CLA	O2A-CGA	4.12	1.45	1.33
6	G	6623	NEX	C7-C8	4.11	1.38	1.31
10	G	613	CLA	O2D-CGD	4.11	1.43	1.33
9	J	607	CHL	O2D-CGD	4.11	1.43	1.33
7	C	2630	LHG	O8-C23	4.11	1.45	1.33
10	A	611	CLA	O2A-CGA	4.10	1.45	1.33
9	E	605	CHL	O2D-CGD	4.09	1.43	1.33
9	G	609	CHL	C3A-C2A	-4.09	1.51	1.54
10	I	613	CLA	O2D-CGD	4.09	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	601	CHL	O2D-CGD	4.08	1.43	1.33
9	E	609	CHL	O2A-CGA	4.08	1.45	1.33
9	C	607	CHL	C1A-CHA	4.08	1.44	1.40
10	D	603	CLA	O2A-CGA	4.07	1.45	1.33
9	C	608	CHL	O2A-CGA	4.07	1.45	1.33
10	A	604	CLA	O2D-CGD	4.07	1.43	1.33
10	B	611	CLA	O2A-CGA	4.07	1.45	1.33
9	D	601	CHL	O2A-CGA	4.06	1.45	1.33
9	G	609	CHL	CBD-CGD	4.06	1.57	1.52
9	A	609	CHL	CBD-CGD	4.06	1.57	1.52
10	F	603	CLA	O2A-CGA	4.06	1.45	1.33
10	B	611	CLA	O2D-CGD	4.05	1.43	1.33
9	B	607	CHL	C1A-CHA	4.05	1.44	1.40
9	I	607	CHL	O2A-CGA	4.05	1.45	1.33
10	H	604	CLA	O2D-CGD	4.05	1.43	1.33
10	E	603	CLA	O2A-CGA	4.05	1.45	1.33
10	J	604	CLA	O2A-CGA	4.05	1.45	1.33
10	F	612	CLA	O2D-CGD	4.04	1.43	1.33
10	A	612	CLA	O2D-CGD	4.04	1.43	1.33
9	G	608	CHL	O2D-CGD	4.04	1.43	1.33
9	C	605	CHL	C3A-C2A	-4.04	1.51	1.54
9	E	601	CHL	C3A-C2A	-4.04	1.51	1.54
9	B	606	CHL	C3A-C2A	-4.04	1.51	1.54
10	H	612	CLA	O2A-CGA	4.04	1.45	1.33
9	E	607	CHL	O2D-CGD	4.04	1.43	1.33
10	D	614	CLA	O2D-CGD	4.03	1.43	1.33
10	G	612	CLA	O2D-CGD	4.03	1.43	1.33
10	E	611	CLA	O2A-CGA	4.01	1.45	1.33
9	I	608	CHL	O2A-CGA	4.01	1.45	1.33
9	C	606	CHL	O2D-CGD	4.01	1.43	1.33
10	D	611	CLA	O2D-CGD	4.01	1.43	1.33
9	H	606	CHL	C3B-C4B	4.01	1.45	1.41
10	C	613	CLA	O2D-CGD	4.01	1.43	1.33
9	J	601	CHL	O2A-CGA	4.00	1.45	1.33
10	F	611	CLA	O2A-CGA	4.00	1.45	1.33
10	A	611	CLA	O2D-CGD	4.00	1.43	1.33
10	A	602	CLA	O2A-CGA	3.99	1.45	1.33
10	I	604	CLA	O2A-CGA	3.99	1.45	1.33
10	B	604	CLA	MG-NA	3.99	2.15	2.06
9	G	607	CHL	O2D-CGD	3.99	1.43	1.33
10	D	612	CLA	O2D-CGD	3.98	1.43	1.33
10	I	603	CLA	O2A-CGA	3.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	612	CLA	O2A-CGA	3.98	1.44	1.33
9	I	609	CHL	O2D-CGD	3.97	1.43	1.33
9	C	609	CHL	C3A-C2A	-3.97	1.51	1.54
9	D	601	CHL	O2D-CGD	3.96	1.43	1.33
10	F	603	CLA	O2D-CGD	3.95	1.43	1.33
10	J	614	CLA	O2D-CGD	3.95	1.43	1.33
10	G	614	CLA	O2D-CGD	3.95	1.42	1.33
9	B	605	CHL	O2D-CGD	3.94	1.42	1.33
10	A	613	CLA	O2D-CGD	3.94	1.42	1.33
9	A	601	CHL	O2A-CGA	3.94	1.44	1.33
10	E	604	CLA	MG-NA	3.93	2.15	2.06
9	H	607	CHL	O2A-CGA	3.93	1.44	1.33
9	C	609	CHL	O2A-CGA	3.93	1.44	1.33
9	C	609	CHL	CBD-CGD	3.92	1.57	1.52
9	J	605	CHL	O2D-CGD	3.91	1.42	1.33
10	B	612	CLA	O2A-CGA	3.91	1.44	1.33
9	D	607	CHL	C3B-C4B	3.91	1.45	1.41
10	C	604	CLA	O2D-CGD	3.91	1.42	1.33
9	I	608	CHL	C3A-C2A	-3.91	1.51	1.54
9	I	601	CHL	O2A-CGA	3.90	1.44	1.33
10	D	611	CLA	O2A-CGA	3.90	1.44	1.33
9	F	607	CHL	O2A-CGA	3.90	1.44	1.33
10	J	611	CLA	O2D-CGD	3.89	1.42	1.33
10	E	612	CLA	O2A-CGA	3.89	1.44	1.33
9	G	605	CHL	C3A-C2A	-3.89	1.51	1.54
10	B	613	CLA	O2A-CGA	3.89	1.44	1.33
9	A	608	CHL	O2A-CGA	3.88	1.44	1.33
9	G	606	CHL	O2D-CGD	3.88	1.42	1.33
9	B	607	CHL	O2D-CGD	3.86	1.42	1.33
10	J	613	CLA	O2A-CGA	3.86	1.44	1.33
9	B	605	CHL	C3A-C2A	-3.86	1.51	1.54
10	J	612	CLA	O2D-CGD	3.86	1.42	1.33
10	F	612	CLA	O2A-CGA	3.85	1.44	1.33
10	G	603	CLA	O2D-CGD	3.85	1.42	1.33
10	I	613	CLA	O2A-CGA	3.85	1.44	1.33
10	I	611	CLA	O2D-CGD	3.85	1.42	1.33
9	A	607	CHL	O2A-CGA	3.85	1.44	1.33
9	E	607	CHL	C1A-CHA	3.85	1.44	1.40
9	G	601	CHL	O2A-CGA	3.84	1.44	1.33
10	C	602	CLA	O2A-CGA	3.84	1.44	1.33
9	G	607	CHL	O2A-CGA	3.83	1.44	1.33
7	F	5630	LHG	O8-C23	3.83	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	603	CLA	O2D-CGD	3.82	1.42	1.33
10	G	603	CLA	O2A-CGA	3.81	1.44	1.33
9	I	605	CHL	CBD-CGD	3.81	1.57	1.52
9	B	608	CHL	CBD-CGD	3.81	1.57	1.52
10	H	610	CLA	MG-NA	3.80	2.15	2.06
10	D	614	CLA	O2A-CGA	3.80	1.44	1.33
10	G	610	CLA	MG-NA	3.80	2.15	2.06
10	G	604	CLA	O2D-CGD	3.79	1.42	1.33
9	D	609	CHL	O2D-CGD	3.79	1.42	1.33
9	D	608	CHL	O2A-CGA	3.78	1.44	1.33
9	H	601	CHL	C3A-C2A	-3.78	1.51	1.54
9	J	607	CHL	C3B-C4B	3.77	1.45	1.41
9	E	605	CHL	O2A-CGA	3.77	1.44	1.33
10	C	612	CLA	O2D-CGD	3.77	1.42	1.33
7	A	630	LHG	O8-C23	3.76	1.44	1.33
10	I	614	CLA	O2D-CGD	3.75	1.42	1.33
10	A	603	CLA	O2A-CGA	3.75	1.44	1.33
9	C	609	CHL	O2D-CGD	3.75	1.42	1.33
10	C	611	CLA	O2D-CGD	3.75	1.42	1.33
10	I	612	CLA	O2D-CED	-3.75	1.36	1.45
9	B	609	CHL	O2D-CGD	3.74	1.42	1.33
9	B	606	CHL	C1A-CHA	3.74	1.44	1.40
9	D	609	CHL	C3A-C2A	-3.73	1.51	1.54
10	E	613	CLA	O2A-CGA	3.73	1.44	1.33
9	F	608	CHL	C3A-C2A	-3.73	1.51	1.54
9	G	601	CHL	C3A-C2A	-3.71	1.51	1.54
9	B	601	CHL	C3A-C2A	-3.71	1.51	1.54
9	A	606	CHL	C3A-C2A	-3.71	1.51	1.54
9	H	607	CHL	CBD-CGD	3.70	1.57	1.52
9	G	601	CHL	O2D-CED	-3.70	1.37	1.45
4	C	2621	LUT	C23-C24	3.70	1.55	1.50
9	E	607	CHL	O2A-CGA	3.70	1.44	1.33
10	F	613	CLA	O2A-CGA	3.70	1.44	1.33
10	A	613	CLA	O2A-CGA	3.68	1.44	1.33
9	E	606	CHL	CBD-CGD	3.68	1.57	1.52
10	H	603	CLA	O2A-CGA	3.67	1.44	1.33
9	I	607	CHL	CMB-C2B	3.67	1.58	1.51
9	B	606	CHL	O2D-CGD	3.67	1.42	1.33
9	H	608	CHL	O2D-CED	-3.66	1.37	1.45
9	I	605	CHL	O2D-CGD	3.65	1.42	1.33
9	F	606	CHL	O2D-CGD	3.65	1.42	1.33
9	J	609	CHL	O2D-CGD	3.65	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	607	CHL	C3B-C4B	3.65	1.44	1.41
10	E	614	CLA	O2D-CGD	3.65	1.42	1.33
9	J	606	CHL	O2D-CGD	3.64	1.42	1.33
9	G	607	CHL	C3B-C4B	3.64	1.44	1.41
10	E	603	CLA	O2D-CGD	3.63	1.42	1.33
9	H	601	CHL	O2D-CGD	3.63	1.42	1.33
9	G	609	CHL	O2A-CGA	3.63	1.43	1.33
9	C	607	CHL	O2A-CGA	3.63	1.43	1.33
9	F	608	CHL	O2D-CGD	3.63	1.42	1.33
10	F	603	CLA	O2D-CED	-3.63	1.37	1.45
9	A	607	CHL	O2D-CGD	3.62	1.42	1.33
9	E	605	CHL	C1A-CHA	3.62	1.44	1.40
10	H	611	CLA	O2A-CGA	3.61	1.43	1.33
10	G	613	CLA	O2A-CGA	3.61	1.43	1.33
9	B	607	CHL	O2A-CGA	3.60	1.43	1.33
10	B	602	CLA	O2A-CGA	3.60	1.43	1.33
10	A	612	CLA	O2D-CED	-3.60	1.37	1.45
6	B	1623	NEX	C7-C8	3.60	1.37	1.31
9	B	607	CHL	C3B-C4B	3.60	1.44	1.41
9	J	609	CHL	CBD-CGD	3.60	1.57	1.52
9	C	608	CHL	O2D-CGD	3.59	1.42	1.33
9	J	601	CHL	C3A-C2A	-3.59	1.51	1.54
10	G	611	CLA	O2D-CGD	3.59	1.42	1.33
9	D	605	CHL	C3A-C2A	-3.59	1.51	1.54
9	B	601	CHL	O2D-CGD	3.58	1.42	1.33
7	H	7630	LHG	O8-C23	3.57	1.43	1.33
9	H	607	CHL	C1A-CHA	3.57	1.44	1.40
9	J	605	CHL	C3A-C2A	-3.57	1.51	1.54
9	A	601	CHL	O2D-CGD	3.57	1.42	1.33
10	F	604	CLA	O2A-CGA	3.57	1.43	1.33
4	A	621	LUT	C1-C6	3.57	1.58	1.53
9	J	601	CHL	O2D-CGD	3.56	1.42	1.33
9	F	605	CHL	C3A-C2A	-3.55	1.51	1.54
10	C	611	CLA	O2A-CGA	3.55	1.43	1.33
9	F	607	CHL	CBD-CGD	3.54	1.57	1.52
10	J	611	CLA	O2A-CGA	3.54	1.43	1.33
9	F	607	CHL	C3B-C4B	3.54	1.44	1.41
10	H	602	CLA	O2A-CGA	3.53	1.43	1.33
9	I	606	CHL	C3A-C2A	-3.53	1.51	1.54
9	F	608	CHL	CBD-CGD	3.53	1.57	1.52
9	G	609	CHL	O2D-CGD	3.53	1.41	1.33
10	B	614	CLA	O2D-CGD	3.51	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	601	CHL	O2A-CGA	3.51	1.43	1.33
9	F	601	CHL	C3A-C2A	-3.50	1.51	1.54
9	J	606	CHL	CBD-CGD	3.50	1.57	1.52
10	C	614	CLA	O2A-CGA	3.50	1.43	1.33
10	C	604	CLA	O2D-CED	-3.49	1.37	1.45
9	G	608	CHL	O2D-CED	-3.49	1.37	1.45
9	E	608	CHL	O2A-CGA	3.49	1.43	1.33
7	E	4630	LHG	O8-C23	3.49	1.43	1.33
9	H	606	CHL	C1A-CHA	3.48	1.44	1.40
9	J	601	CHL	C1A-CHA	3.48	1.44	1.40
10	F	603	CLA	MG-ND	-3.47	1.98	2.05
9	A	609	CHL	O2D-CGD	3.47	1.41	1.33
10	I	602	CLA	O2A-CGA	3.46	1.43	1.33
9	D	606	CHL	O2D-CGD	3.46	1.41	1.33
9	E	605	CHL	C3A-C2A	-3.46	1.51	1.54
10	G	604	CLA	O2A-CGA	3.46	1.43	1.33
10	C	604	CLA	MG-NA	3.46	2.14	2.06
9	H	605	CHL	CBD-CGD	3.46	1.56	1.52
9	I	608	CHL	O2D-CED	-3.45	1.37	1.45
9	I	601	CHL	O2D-CGD	3.44	1.41	1.33
10	I	612	CLA	O2A-CGA	3.44	1.43	1.33
9	A	601	CHL	CBD-CGD	3.44	1.56	1.52
10	E	604	CLA	O2A-CGA	3.43	1.43	1.33
9	I	608	CHL	O2D-CGD	3.43	1.41	1.33
10	G	612	CLA	O2A-CGA	3.42	1.43	1.33
9	J	607	CHL	CMB-C2B	3.42	1.58	1.51
10	H	612	CLA	O2D-CGD	3.41	1.41	1.33
10	F	602	CLA	O2A-CGA	3.40	1.43	1.33
10	I	612	CLA	O2D-CGD	3.40	1.41	1.33
9	H	608	CHL	CBD-CGD	3.40	1.56	1.52
9	A	605	CHL	CBD-CGD	3.38	1.56	1.52
10	D	613	CLA	CMB-C2B	3.38	1.57	1.50
9	C	607	CHL	CBD-CGD	3.38	1.56	1.52
9	E	606	CHL	C1A-CHA	3.38	1.43	1.40
9	D	607	CHL	O2D-CGD	3.37	1.41	1.33
7	H	7630	LHG	O7-C7	3.36	1.43	1.34
9	B	608	CHL	O2A-CGA	3.36	1.43	1.33
9	J	607	CHL	C1A-CHA	3.36	1.43	1.40
9	G	601	CHL	O2D-CGD	3.36	1.41	1.33
10	I	603	CLA	O2D-CGD	3.35	1.41	1.33
10	F	604	CLA	O2D-CGD	3.35	1.41	1.33
9	D	601	CHL	C3A-C2A	-3.34	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	612	CLA	O2D-CED	-3.34	1.37	1.45
10	G	612	CLA	O2D-CED	-3.34	1.37	1.45
9	B	601	CHL	C1A-CHA	3.33	1.43	1.40
10	B	603	CLA	O2D-CGD	3.33	1.41	1.33
10	J	603	CLA	CMB-C2B	3.33	1.57	1.50
9	G	606	CHL	CBD-CGD	3.33	1.56	1.52
9	I	605	CHL	C1A-CHA	3.32	1.43	1.40
10	A	603	CLA	MG-ND	-3.32	1.99	2.05
10	A	614	CLA	O2D-CGD	3.31	1.41	1.33
9	F	607	CHL	CMB-C2B	3.30	1.58	1.51
9	D	608	CHL	O2D-CGD	3.30	1.41	1.33
10	J	612	CLA	O2A-CGA	3.30	1.43	1.33
9	I	606	CHL	O2D-CGD	3.30	1.41	1.33
4	J	9621	LUT	C1-C6	3.30	1.58	1.53
10	G	603	CLA	CMB-C2B	3.29	1.57	1.50
10	B	603	CLA	O2D-CED	-3.28	1.38	1.45
9	D	605	CHL	CBD-CGD	3.28	1.56	1.52
9	C	605	CHL	CBD-CGD	3.27	1.56	1.52
10	C	603	CLA	MG-ND	-3.27	1.99	2.05
10	E	611	CLA	O2D-CED	-3.27	1.38	1.45
10	F	612	CLA	O2D-CED	-3.27	1.38	1.45
9	B	607	CHL	CBD-CGD	3.26	1.56	1.52
9	E	605	CHL	CBD-CGD	3.26	1.56	1.52
9	J	608	CHL	O2D-CED	-3.26	1.38	1.45
9	I	601	CHL	C3A-C2A	-3.25	1.51	1.54
10	D	612	CLA	CMB-C2B	3.25	1.57	1.50
10	D	603	CLA	MG-ND	-3.25	1.99	2.05
9	I	606	CHL	C1A-CHA	3.24	1.43	1.40
10	C	612	CLA	O2D-CED	-3.24	1.38	1.45
9	E	609	CHL	CBD-CGD	3.24	1.56	1.52
9	H	606	CHL	CBD-CGD	3.23	1.56	1.52
9	D	608	CHL	C3A-C2A	-3.23	1.51	1.54
10	F	612	CLA	C2-C3	3.22	1.40	1.33
9	D	607	CHL	CMB-C2B	3.21	1.58	1.51
9	A	607	CHL	CBD-CGD	3.21	1.56	1.52
9	J	607	CHL	MG-ND	-3.21	1.99	2.05
10	G	602	CLA	C1-C2	-3.21	1.40	1.49
10	I	602	CLA	C1-C2	-3.20	1.40	1.49
10	B	612	CLA	CMB-C2B	3.20	1.57	1.50
9	B	608	CHL	O2D-CED	-3.20	1.38	1.45
10	H	612	CLA	C2-C3	3.20	1.40	1.33
9	J	605	CHL	C1A-CHA	3.19	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	608	CHL	O2D-CED	-3.19	1.38	1.45
9	A	608	CHL	O2D-CED	-3.19	1.38	1.45
10	I	604	CLA	O2D-CED	-3.19	1.38	1.45
10	C	612	CLA	O2A-CGA	3.19	1.42	1.33
10	G	613	CLA	C2-C3	3.19	1.40	1.33
9	F	609	CHL	CBD-CGD	3.18	1.56	1.52
10	F	604	CLA	O2D-CED	-3.18	1.38	1.45
10	D	602	CLA	C1-C2	-3.18	1.40	1.49
10	H	612	CLA	O2D-CED	-3.17	1.38	1.45
9	G	601	CHL	CBD-CGD	3.17	1.56	1.52
9	G	607	CHL	CMB-C2B	3.17	1.57	1.51
10	B	612	CLA	C2-C3	3.17	1.40	1.33
10	A	612	CLA	O2A-CGA	3.16	1.42	1.33
9	C	601	CHL	C3A-C2A	-3.15	1.52	1.54
9	A	606	CHL	O2D-CGD	3.15	1.41	1.33
9	B	606	CHL	O2D-CED	-3.15	1.38	1.45
4	E	4621	LUT	C23-C24	3.15	1.54	1.50
9	F	608	CHL	O2D-CED	-3.14	1.38	1.45
7	I	8630	LHG	O7-C7	3.14	1.43	1.34
9	D	606	CHL	C1A-CHA	3.13	1.43	1.40
9	D	601	CHL	CBD-CGD	3.12	1.56	1.52
10	J	602	CLA	O2A-CGA	3.12	1.42	1.33
10	J	603	CLA	MG-ND	-3.12	1.99	2.05
7	G	6630	LHG	O7-C7	3.11	1.43	1.34
9	J	606	CHL	C3A-C2A	-3.11	1.52	1.54
9	B	608	CHL	C2-C3	3.11	1.40	1.33
10	J	612	CLA	C2-C3	3.10	1.40	1.33
9	H	608	CHL	O2D-CGD	3.10	1.40	1.33
7	D	3630	LHG	O8-C23	3.10	1.42	1.33
9	F	606	CHL	C3A-C2A	-3.10	1.52	1.54
9	G	606	CHL	C1A-CHA	3.10	1.43	1.40
9	B	609	CHL	C1A-CHA	3.09	1.43	1.40
10	D	603	CLA	O2D-CGD	3.09	1.40	1.33
7	C	2630	LHG	O7-C7	3.09	1.43	1.34
10	H	602	CLA	O2D-CED	-3.09	1.38	1.45
10	G	602	CLA	O2D-CED	-3.09	1.38	1.45
9	J	605	CHL	CBD-CGD	3.09	1.56	1.52
10	C	602	CLA	C1-C2	-3.08	1.40	1.49
10	G	612	CLA	C2-C3	3.07	1.40	1.33
10	C	613	CLA	O2A-CGA	3.07	1.42	1.33
9	F	601	CHL	O2D-CGD	3.07	1.40	1.33
9	I	605	CHL	O2D-CED	-3.07	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	606	CHL	CHA-CBD	3.07	1.55	1.51
10	G	602	CLA	O2A-CGA	3.07	1.42	1.33
9	A	606	CHL	CMB-C2B	3.07	1.57	1.51
7	J	9630	LHG	O8-C23	3.07	1.42	1.33
9	G	608	CHL	CBD-CGD	3.07	1.56	1.52
9	C	609	CHL	O2D-CED	-3.06	1.38	1.45
10	B	610	CLA	CMB-C2B	3.06	1.57	1.50
9	F	606	CHL	CMB-C2B	3.06	1.57	1.51
10	D	604	CLA	O2D-CED	-3.06	1.38	1.45
9	D	609	CHL	O2D-CED	-3.05	1.38	1.45
7	B	1630	LHG	C26-C25	-3.05	1.36	1.51
10	I	612	CLA	C2-C3	3.05	1.40	1.33
9	J	606	CHL	CMB-C2B	3.04	1.57	1.51
10	F	613	CLA	C2-C3	3.04	1.40	1.33
10	H	610	CLA	O2D-CED	-3.04	1.38	1.45
10	D	612	CLA	C2-C3	3.03	1.40	1.33
7	I	8630	LHG	C26-C25	-3.03	1.36	1.51
9	E	606	CHL	CMB-C2B	3.03	1.57	1.51
9	H	609	CHL	CBD-CGD	3.03	1.56	1.52
9	H	609	CHL	O2D-CGD	3.03	1.40	1.33
10	C	603	CLA	O2D-CGD	3.03	1.40	1.33
10	H	613	CLA	C2-C3	3.02	1.40	1.33
7	J	9630	LHG	C26-C25	-3.02	1.36	1.51
10	H	611	CLA	C2-C3	3.02	1.40	1.33
10	H	613	CLA	O2A-CGA	3.02	1.42	1.33
10	D	604	CLA	C2-C3	3.02	1.40	1.33
9	B	607	CHL	O2D-CED	-3.01	1.38	1.45
10	J	603	CLA	O2D-CED	-3.01	1.38	1.45
10	E	612	CLA	C2-C3	3.01	1.40	1.33
9	B	607	CHL	C2-C3	3.01	1.40	1.33
10	C	611	CLA	C2-C3	3.00	1.40	1.33
9	G	609	CHL	O2D-CED	-3.00	1.38	1.45
9	H	607	CHL	MG-ND	-3.00	1.99	2.05
10	A	613	CLA	C2-C3	3.00	1.40	1.33
10	F	603	CLA	C2-C3	3.00	1.40	1.33
9	C	605	CHL	O2D-CED	-3.00	1.38	1.45
10	B	604	CLA	O2D-CED	-3.00	1.38	1.45
9	F	608	CHL	C2-C3	3.00	1.40	1.33
10	E	604	CLA	O2D-CED	-3.00	1.38	1.45
9	I	608	CHL	C2-C3	2.99	1.39	1.33
10	I	612	CLA	CMB-C2B	2.99	1.56	1.50
9	B	609	CHL	O2D-CED	-2.99	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	608	CHL	O2D-CGD	2.99	1.40	1.33
4	D	3621	LUT	C23-C24	2.99	1.54	1.50
10	A	603	CLA	O2D-CED	-2.99	1.38	1.45
9	B	609	CHL	CBD-CGD	2.98	1.56	1.52
10	H	604	CLA	C2-C3	2.98	1.39	1.33
9	D	601	CHL	C1A-CHA	2.98	1.43	1.40
9	I	607	CHL	MG-ND	-2.98	1.99	2.05
7	D	3630	LHG	C26-C25	-2.98	1.37	1.51
9	J	609	CHL	O2D-CED	-2.98	1.38	1.45
10	G	610	CLA	C2-C3	2.98	1.39	1.33
10	F	610	CLA	C2-C3	2.97	1.39	1.33
10	A	604	CLA	O2D-CED	-2.97	1.38	1.45
10	J	613	CLA	C2-C3	2.97	1.39	1.33
7	A	630	LHG	O7-C7	2.97	1.42	1.34
10	I	613	CLA	C2-C3	2.97	1.39	1.33
9	C	601	CHL	O2A-CGA	2.97	1.42	1.33
9	H	608	CHL	C2-C3	2.96	1.39	1.33
10	G	611	CLA	C2-C3	2.95	1.39	1.33
10	J	614	CLA	CMB-C2B	2.95	1.56	1.50
10	A	611	CLA	C2-C3	2.95	1.39	1.33
10	B	613	CLA	C2-C3	2.95	1.39	1.33
10	J	611	CLA	C2-C3	2.95	1.39	1.33
10	B	604	CLA	C2-C3	2.95	1.39	1.33
10	E	610	CLA	O2D-CED	-2.94	1.38	1.45
9	D	607	CHL	CHA-CBD	2.94	1.55	1.51
10	J	612	CLA	O2D-CED	-2.94	1.38	1.45
4	J	9620	LUT	C5-C6	2.94	1.39	1.34
10	B	614	CLA	CMB-C2B	2.94	1.56	1.50
10	A	604	CLA	C2-C3	2.94	1.39	1.33
10	E	610	CLA	C2-C3	2.94	1.39	1.33
7	G	6630	LHG	C26-C25	-2.94	1.37	1.51
10	A	612	CLA	C2-C3	2.94	1.39	1.33
7	E	4630	LHG	C26-C25	-2.94	1.37	1.51
10	C	614	CLA	CMB-C2B	2.93	1.56	1.50
9	H	601	CHL	C1A-CHA	2.93	1.43	1.40
10	J	610	CLA	C2-C3	2.93	1.39	1.33
10	E	611	CLA	C2-C3	2.93	1.39	1.33
4	G	6621	LUT	C23-C24	2.93	1.54	1.50
10	G	604	CLA	C2-C3	2.93	1.39	1.33
10	D	611	CLA	C2-C3	2.93	1.39	1.33
9	J	608	CHL	C2-C3	2.92	1.39	1.33
10	I	604	CLA	C2-C3	2.92	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	602	CLA	O2D-CED	-2.92	1.38	1.45
9	J	607	CHL	O2A-CGA	2.92	1.41	1.33
9	H	609	CHL	C2-C3	2.92	1.39	1.33
9	G	605	CHL	CMB-C2B	2.92	1.57	1.51
9	H	607	CHL	C2-C3	2.92	1.39	1.33
9	A	608	CHL	C2-C3	2.92	1.39	1.33
9	F	607	CHL	C2-C3	2.92	1.39	1.33
10	E	613	CLA	C2-C3	2.92	1.39	1.33
4	E	4620	LUT	C23-C24	2.91	1.54	1.50
10	I	603	CLA	CMB-C2B	2.91	1.56	1.50
10	B	611	CLA	C2-C3	2.91	1.39	1.33
10	E	614	CLA	CMB-C2B	2.91	1.56	1.50
9	A	601	CHL	C3A-C2A	-2.91	1.52	1.54
9	D	608	CHL	O2D-CED	-2.90	1.38	1.45
10	C	610	CLA	C2-C3	2.90	1.39	1.33
10	D	613	CLA	C2-C3	2.90	1.39	1.33
4	G	6620	LUT	C5-C6	2.90	1.39	1.34
9	A	601	CHL	O2D-CED	-2.90	1.38	1.45
9	H	601	CHL	C2-C3	2.90	1.39	1.33
9	E	609	CHL	C2-C3	2.89	1.39	1.33
9	B	605	CHL	C1A-CHA	2.89	1.43	1.40
9	B	607	CHL	CHA-CBD	2.89	1.55	1.51
7	B	1630	LHG	O7-C7	2.89	1.42	1.34
9	B	609	CHL	C2-C3	2.89	1.39	1.33
10	E	603	CLA	O2D-CED	-2.89	1.38	1.45
10	H	610	CLA	C2-C3	2.89	1.39	1.33
10	I	611	CLA	CMB-C2B	2.89	1.56	1.50
9	A	609	CHL	O2D-CED	-2.89	1.38	1.45
10	J	603	CLA	C2-C3	2.89	1.39	1.33
9	C	606	CHL	CMB-C2B	2.89	1.57	1.51
10	F	604	CLA	C2-C3	2.89	1.39	1.33
10	D	610	CLA	C2-C3	2.89	1.39	1.33
10	C	604	CLA	C2-C3	2.89	1.39	1.33
9	E	608	CHL	C2-C3	2.89	1.39	1.33
9	I	607	CHL	C2-C3	2.88	1.39	1.33
4	A	621	LUT	C23-C24	2.88	1.54	1.50
9	G	607	CHL	C2-C3	2.88	1.39	1.33
10	C	612	CLA	C2-C3	2.88	1.39	1.33
9	A	601	CHL	C1A-CHA	2.87	1.43	1.40
4	B	1620	LUT	C23-C24	2.87	1.54	1.50
10	J	604	CLA	O2D-CED	-2.87	1.38	1.45
9	F	606	CHL	C2-C3	2.87	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	613	CLA	CMB-C2B	2.87	1.56	1.50
9	A	609	CHL	C3B-C2B	-2.86	1.36	1.40
10	G	613	CLA	O2D-CED	-2.86	1.38	1.45
9	A	607	CHL	C2-C3	2.86	1.39	1.33
9	H	605	CHL	C1A-CHA	2.86	1.43	1.40
9	C	606	CHL	CHA-CBD	2.85	1.55	1.51
9	E	601	CHL	C2-C3	2.85	1.39	1.33
10	D	603	CLA	O2D-CED	-2.85	1.38	1.45
10	J	613	CLA	O2D-CED	-2.85	1.38	1.45
9	H	607	CHL	O2D-CED	-2.85	1.38	1.45
10	G	613	CLA	CMB-C2B	2.85	1.56	1.50
10	J	602	CLA	O2D-CED	-2.84	1.39	1.45
9	I	601	CHL	C1A-CHA	2.84	1.43	1.40
10	G	614	CLA	CMB-C2B	2.84	1.56	1.50
9	J	601	CHL	C2-C3	2.84	1.39	1.33
10	D	604	CLA	MG-ND	-2.84	2.00	2.05
10	E	602	CLA	C2-C3	2.84	1.39	1.33
9	J	601	CHL	O2D-CED	-2.84	1.39	1.45
10	F	611	CLA	C2-C3	2.83	1.39	1.33
10	G	604	CLA	O2D-CED	-2.83	1.39	1.45
10	I	611	CLA	C2-C3	2.83	1.39	1.33
9	H	606	CHL	MG-ND	-2.83	2.00	2.05
9	A	608	CHL	CBD-CGD	2.83	1.56	1.52
9	D	607	CHL	C2-C3	2.83	1.39	1.33
10	E	612	CLA	CMB-C2B	2.82	1.56	1.50
9	G	609	CHL	C2-C3	2.82	1.39	1.33
4	C	2621	LUT	C1-C6	2.82	1.57	1.53
9	F	609	CHL	C2-C3	2.82	1.39	1.33
9	F	608	CHL	C1A-CHA	2.82	1.43	1.40
10	E	603	CLA	C2-C3	2.82	1.39	1.33
4	F	5621	LUT	C23-C24	2.82	1.54	1.50
9	J	607	CHL	C2-C3	2.81	1.39	1.33
10	J	602	CLA	C1-C2	-2.81	1.41	1.49
9	C	607	CHL	C2-C3	2.81	1.39	1.33
9	C	609	CHL	C2-C3	2.81	1.39	1.33
9	D	607	CHL	O2D-CED	-2.81	1.39	1.45
9	I	609	CHL	C2-C3	2.81	1.39	1.33
10	E	604	CLA	C2-C3	2.81	1.39	1.33
10	C	603	CLA	C2-C3	2.81	1.39	1.33
7	F	5630	LHG	C26-C25	-2.81	1.37	1.51
10	J	604	CLA	C2-C3	2.81	1.39	1.33
9	G	601	CHL	C2-C3	2.80	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	603	CLA	O2D-CED	-2.80	1.39	1.45
7	C	2630	LHG	C26-C25	-2.80	1.37	1.51
9	F	609	CHL	O2D-CED	-2.80	1.39	1.45
9	G	606	CHL	C2-C3	2.80	1.40	1.32
4	E	4620	LUT	C5-C6	2.80	1.39	1.34
10	B	603	CLA	CMB-C2B	2.80	1.56	1.50
10	B	612	CLA	O2D-CED	-2.80	1.39	1.45
4	C	2621	LUT	C24-C25	2.80	1.36	1.33
10	G	603	CLA	MG-ND	-2.80	2.00	2.05
4	H	7621	LUT	C23-C24	2.80	1.54	1.50
10	H	603	CLA	C2-C3	2.79	1.39	1.33
10	I	613	CLA	O2D-CED	-2.79	1.39	1.45
9	E	607	CHL	CBD-CGD	2.79	1.56	1.52
10	B	603	CLA	MG-ND	-2.79	2.00	2.05
9	C	606	CHL	C2-C3	2.79	1.40	1.32
10	I	603	CLA	C2-C3	2.79	1.39	1.33
10	A	613	CLA	CMB-C2B	2.79	1.56	1.50
9	F	605	CHL	C1A-CHA	2.79	1.43	1.40
9	E	609	CHL	O2D-CGD	2.79	1.40	1.33
9	G	601	CHL	C1A-CHA	2.79	1.43	1.40
10	A	611	CLA	O2D-CED	-2.78	1.39	1.45
9	G	608	CHL	C2-C3	2.78	1.39	1.33
9	I	607	CHL	CBD-CGD	2.78	1.56	1.52
9	C	608	CHL	CBD-CGD	2.78	1.56	1.52
4	A	621	LUT	C24-C25	2.78	1.36	1.33
9	D	609	CHL	C2-C3	2.78	1.39	1.33
10	A	603	CLA	CMB-C2B	2.78	1.56	1.50
8	B	1632	DGD	O1G-C1A	2.77	1.41	1.33
10	H	613	CLA	CMB-C2B	2.77	1.56	1.50
9	A	606	CHL	C2-C3	2.77	1.40	1.32
9	E	607	CHL	CMB-C2B	2.77	1.57	1.51
7	D	3630	LHG	O7-C7	2.77	1.42	1.34
10	B	611	CLA	CMB-C2B	2.77	1.56	1.50
10	E	603	CLA	CMB-C2B	2.77	1.56	1.50
9	H	606	CHL	C3A-C2A	-2.76	1.52	1.54
9	E	609	CHL	C1-C2	-2.76	1.41	1.49
10	J	610	CLA	CMB-C2B	2.76	1.56	1.50
9	J	605	CHL	O2D-CED	-2.76	1.39	1.45
9	F	601	CHL	O2D-CED	-2.75	1.39	1.45
9	D	606	CHL	CMB-C2B	2.75	1.57	1.51
10	C	613	CLA	C2-C3	2.75	1.39	1.33
7	E	4630	LHG	O7-C7	2.75	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	608	CHL	O2D-CED	-2.75	1.39	1.45
10	B	603	CLA	C2-C3	2.75	1.39	1.33
9	I	609	CHL	C3B-C2B	-2.75	1.36	1.40
10	I	610	CLA	C2-C3	2.75	1.39	1.33
9	J	609	CHL	C3B-C2B	-2.75	1.36	1.40
9	I	601	CHL	O2D-CED	-2.74	1.39	1.45
10	H	602	CLA	C1-C2	-2.74	1.41	1.49
10	F	602	CLA	CMB-C2B	2.74	1.56	1.50
9	E	607	CHL	C2-C3	2.74	1.39	1.33
9	H	601	CHL	O2D-CED	-2.74	1.39	1.45
9	J	601	CHL	CBD-CGD	2.74	1.56	1.52
10	D	603	CLA	C2-C3	2.73	1.39	1.33
9	A	607	CHL	CHA-CBD	2.73	1.54	1.51
9	A	608	CHL	C3B-C2B	-2.73	1.36	1.40
9	B	601	CHL	C2-C3	2.73	1.39	1.33
10	G	603	CLA	C2-C3	2.73	1.39	1.33
10	I	610	CLA	CMB-C2B	2.73	1.56	1.50
4	E	4621	LUT	C24-C25	2.73	1.36	1.33
9	J	606	CHL	CHA-CBD	2.73	1.54	1.51
9	C	601	CHL	C2-C3	2.73	1.39	1.33
9	H	606	CHL	C2-C3	2.72	1.40	1.32
10	H	610	CLA	CMB-C2B	2.72	1.56	1.50
10	I	602	CLA	CMB-C2B	2.72	1.56	1.50
10	A	610	CLA	CMB-C2B	2.72	1.56	1.50
7	A	630	LHG	C26-C25	-2.72	1.38	1.51
10	A	610	CLA	C2-C3	2.72	1.39	1.33
10	A	602	CLA	O2D-CED	-2.72	1.39	1.45
9	A	606	CHL	CBD-CGD	2.72	1.56	1.52
9	D	608	CHL	C2-C3	2.72	1.39	1.33
9	I	601	CHL	C2-C3	2.71	1.39	1.33
9	G	605	CHL	MG-ND	-2.71	2.00	2.05
9	C	609	CHL	C3B-C2B	-2.71	1.36	1.40
9	D	601	CHL	C2-C3	2.71	1.39	1.33
9	F	609	CHL	O2D-CGD	2.71	1.39	1.33
9	D	606	CHL	C2-C3	2.71	1.40	1.32
9	A	601	CHL	C2-C3	2.70	1.39	1.33
9	F	606	CHL	CHA-CBD	2.70	1.54	1.51
7	H	7630	LHG	C26-C25	-2.70	1.38	1.51
4	E	4621	LUT	C1-C6	2.70	1.57	1.53
10	I	602	CLA	O2D-CED	-2.70	1.39	1.45
10	C	611	CLA	O2D-CED	-2.70	1.39	1.45
10	B	610	CLA	C2-C3	2.70	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	602	CLA	O2D-CED	-2.69	1.39	1.45
9	H	605	CHL	CMB-C2B	2.69	1.57	1.51
10	C	613	CLA	CMC-C2C	2.69	1.56	1.50
10	H	612	CLA	CMB-C2B	2.69	1.56	1.50
9	J	609	CHL	C2-C3	2.69	1.39	1.33
9	C	607	CHL	CHA-CBD	2.69	1.54	1.51
10	E	610	CLA	CMB-C2B	2.69	1.56	1.50
9	D	607	CHL	O2A-CGA	2.68	1.41	1.33
9	E	609	CHL	O2D-CED	-2.68	1.39	1.45
9	E	606	CHL	C2-C3	2.68	1.40	1.32
9	I	606	CHL	C2-C3	2.68	1.40	1.32
9	D	608	CHL	CBD-CGD	2.68	1.55	1.52
10	B	602	CLA	C1-C2	-2.68	1.41	1.49
9	F	601	CHL	C2-C3	2.68	1.39	1.33
9	E	609	CHL	C3B-C2B	-2.68	1.36	1.40
10	C	610	CLA	O2D-CED	-2.67	1.39	1.45
10	A	602	CLA	C2-C3	2.67	1.39	1.33
10	F	602	CLA	C1-C2	-2.67	1.41	1.49
9	D	609	CHL	C3B-C2B	-2.67	1.36	1.40
10	B	602	CLA	CMB-C2B	2.67	1.56	1.50
10	A	603	CLA	C2-C3	2.66	1.39	1.33
9	C	608	CHL	C2-C3	2.66	1.39	1.33
9	J	606	CHL	C2-C3	2.66	1.40	1.32
9	D	605	CHL	O2D-CED	-2.66	1.39	1.45
10	H	603	CLA	O2D-CED	-2.66	1.39	1.45
10	C	611	CLA	CMB-C2B	2.66	1.56	1.50
10	J	602	CLA	CMB-C2B	2.65	1.56	1.50
9	B	606	CHL	C2-C3	2.65	1.40	1.32
9	J	607	CHL	CBD-CGD	2.65	1.55	1.52
9	E	606	CHL	C3A-C2A	-2.65	1.52	1.54
9	E	607	CHL	O2D-CED	-2.64	1.39	1.45
10	C	602	CLA	C2-C3	2.64	1.39	1.33
9	E	609	CHL	CMB-C2B	2.64	1.56	1.51
9	C	606	CHL	CBD-CGD	2.63	1.55	1.52
9	F	607	CHL	CHA-CBD	2.63	1.54	1.51
9	I	607	CHL	O2D-CED	-2.63	1.39	1.45
4	C	2620	LUT	C23-C24	2.63	1.54	1.50
10	E	611	CLA	CMB-C2B	2.63	1.56	1.50
9	C	608	CHL	C1-C2	-2.62	1.41	1.49
9	A	609	CHL	C2-C3	2.62	1.39	1.33
9	B	606	CHL	CMB-C2B	2.62	1.56	1.51
9	J	609	CHL	C1-C2	-2.62	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4620	LUT	C24-C25	2.61	1.36	1.33
9	A	606	CHL	CHA-CBD	2.61	1.54	1.51
9	G	605	CHL	O2D-CED	-2.61	1.39	1.45
9	J	608	CHL	C3B-C2B	-2.61	1.36	1.40
9	H	606	CHL	CMB-C2B	2.61	1.56	1.51
9	I	608	CHL	C3B-C2B	-2.61	1.36	1.40
9	E	606	CHL	O2D-CED	-2.61	1.39	1.45
10	H	604	CLA	O2D-CED	-2.61	1.39	1.45
10	A	604	CLA	MG-ND	-2.61	2.00	2.05
9	E	608	CHL	MG-ND	-2.61	2.00	2.05
10	G	604	CLA	C4-C3	2.61	1.57	1.50
9	D	608	CHL	C1A-CHA	2.60	1.43	1.40
9	B	606	CHL	CBD-CGD	2.60	1.55	1.52
9	E	607	CHL	CHA-CBD	2.60	1.54	1.51
9	H	606	CHL	O2D-CED	-2.60	1.39	1.45
9	E	601	CHL	CMB-C2B	2.59	1.56	1.51
10	E	602	CLA	CMB-C2B	2.59	1.56	1.50
9	H	609	CHL	C1A-CHA	2.59	1.42	1.40
4	B	1621	LUT	C23-C24	2.58	1.54	1.50
9	E	601	CHL	C1A-CHA	2.58	1.42	1.40
10	B	613	CLA	CMB-C2B	2.58	1.56	1.50
9	C	601	CHL	O2D-CED	-2.58	1.39	1.45
9	I	605	CHL	CMB-C2B	2.58	1.56	1.51
10	I	614	CLA	CMB-C2B	2.58	1.56	1.50
9	I	609	CHL	CBD-CGD	2.57	1.55	1.52
10	D	613	CLA	O2D-CED	-2.57	1.39	1.45
8	G	9632	DGD	O1G-C1A	2.57	1.40	1.33
9	D	606	CHL	CHA-CBD	2.57	1.54	1.51
10	D	614	CLA	CMB-C2B	2.57	1.56	1.50
9	F	609	CHL	C3B-C2B	-2.57	1.36	1.40
9	H	609	CHL	O2D-CED	-2.57	1.39	1.45
9	I	606	CHL	O2D-CED	-2.57	1.39	1.45
4	G	6621	LUT	C24-C25	2.56	1.36	1.33
9	I	607	CHL	CHA-CBD	2.56	1.54	1.51
9	F	608	CHL	MG-ND	-2.55	2.00	2.05
9	I	601	CHL	CBD-CGD	2.55	1.55	1.52
9	D	608	CHL	C3B-C2B	-2.55	1.36	1.40
10	A	611	CLA	CMB-C2B	2.55	1.56	1.50
4	I	8621	LUT	C1-C6	2.54	1.57	1.53
10	B	602	CLA	C2-C3	2.54	1.38	1.33
9	G	607	CHL	CHA-CBD	2.54	1.54	1.51
10	C	603	CLA	CMB-C2B	2.54	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	614	CLA	CMB-C2B	2.54	1.56	1.50
9	J	601	CHL	CHA-CBD	2.54	1.54	1.51
10	A	612	CLA	CMB-C2B	2.53	1.56	1.50
10	F	613	CLA	CMB-C2B	2.53	1.56	1.50
10	D	602	CLA	CMC-C2C	2.53	1.56	1.50
10	E	602	CLA	CMC-C2C	2.53	1.56	1.50
10	D	602	CLA	MG-ND	-2.53	2.00	2.05
9	C	608	CHL	C1A-CHA	2.53	1.42	1.40
9	G	609	CHL	C3B-C2B	-2.52	1.37	1.40
4	D	3621	LUT	C24-C25	2.52	1.36	1.33
4	I	8620	LUT	C23-C24	2.52	1.53	1.50
9	J	608	CHL	MG-ND	-2.52	2.00	2.05
9	G	608	CHL	MG-ND	-2.52	2.00	2.05
10	G	602	CLA	CMB-C2B	2.52	1.55	1.50
9	A	608	CHL	MG-ND	-2.52	2.00	2.05
10	G	612	CLA	CMB-C2B	2.51	1.55	1.50
10	H	603	CLA	CMB-C2B	2.51	1.55	1.50
9	I	608	CHL	CBD-CGD	2.51	1.55	1.52
9	J	605	CHL	CHA-CBD	2.51	1.54	1.51
10	B	603	CLA	CMC-C2C	2.50	1.55	1.50
10	D	613	CLA	CMC-C2C	2.50	1.55	1.50
10	B	613	CLA	C5-C3	2.50	1.56	1.51
10	D	610	CLA	O2D-CED	-2.50	1.39	1.45
9	H	601	CHL	CBD-CGD	2.50	1.55	1.52
9	G	607	CHL	O2D-CED	-2.49	1.39	1.45
9	A	607	CHL	O2D-CED	-2.49	1.39	1.45
9	J	608	CHL	CBD-CGD	2.49	1.55	1.52
9	E	607	CHL	MG-ND	-2.49	2.00	2.05
9	B	609	CHL	C1-C2	-2.49	1.42	1.49
9	G	608	CHL	C3B-C2B	-2.49	1.37	1.40
9	H	608	CHL	CMB-C2B	2.49	1.56	1.51
9	H	608	CHL	C3B-C2B	-2.48	1.37	1.40
10	D	602	CLA	C2-C3	2.48	1.38	1.33
4	D	3620	LUT	C5-C6	2.48	1.38	1.34
10	A	613	CLA	CMC-C2C	2.48	1.55	1.50
9	C	607	CHL	CMB-C2B	2.48	1.56	1.51
9	H	606	CHL	CHA-CBD	2.48	1.54	1.51
9	H	608	CHL	MG-ND	-2.48	2.00	2.05
9	C	608	CHL	C3B-C2B	-2.48	1.37	1.40
9	F	608	CHL	C3B-C2B	-2.48	1.37	1.40
9	F	601	CHL	CBD-CGD	2.47	1.55	1.52
10	I	604	CLA	C4-C3	2.47	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	608	CHL	CMB-C2B	2.46	1.56	1.51
4	F	5621	LUT	C24-C25	2.46	1.36	1.33
9	B	609	CHL	C3B-C2B	-2.46	1.37	1.40
4	B	1621	LUT	C24-C25	2.46	1.36	1.33
4	F	5621	LUT	C5-C6	2.46	1.38	1.34
10	D	602	CLA	CMB-C2B	2.46	1.55	1.50
10	E	613	CLA	CMB-C2B	2.46	1.55	1.50
9	D	609	CHL	C4-C3	2.46	1.56	1.50
9	D	605	CHL	CMB-C2B	2.46	1.56	1.51
10	H	604	CLA	MG-ND	-2.45	2.00	2.05
9	F	605	CHL	CBD-CGD	2.45	1.55	1.52
10	B	611	CLA	O2D-CED	-2.45	1.39	1.45
10	B	610	CLA	O2D-CED	-2.45	1.39	1.45
10	G	613	CLA	CMC-C2C	2.45	1.55	1.50
9	E	601	CHL	MG-ND	-2.45	2.00	2.05
10	G	603	CLA	O2D-CED	-2.45	1.39	1.45
4	B	1621	LUT	C5-C6	2.44	1.38	1.34
10	G	610	CLA	CMB-C2B	2.44	1.55	1.50
9	A	605	CHL	O2D-CED	-2.44	1.39	1.45
4	A	620	LUT	C23-C24	2.44	1.53	1.50
10	G	604	CLA	CMC-C2C	2.44	1.55	1.50
9	H	601	CHL	MG-ND	-2.44	2.01	2.05
9	B	605	CHL	CHA-CBD	2.44	1.54	1.51
9	J	601	CHL	CMB-C2B	2.43	1.56	1.51
9	B	607	CHL	CHB-C4A	2.43	1.41	1.38
10	F	602	CLA	CMC-C2C	2.43	1.55	1.50
9	C	605	CHL	CMB-C2B	2.43	1.56	1.51
4	E	4620	LUT	C1-C6	2.43	1.56	1.53
9	E	608	CHL	C3B-C2B	-2.43	1.37	1.40
9	B	607	CHL	C3A-C2A	-2.43	1.52	1.54
9	G	609	CHL	C1A-CHA	2.43	1.42	1.40
9	B	607	CHL	CMB-C2B	2.43	1.56	1.51
10	B	612	CLA	CBD-CGD	2.43	1.59	1.52
10	G	602	CLA	C2-C3	2.43	1.38	1.33
4	J	9621	LUT	C23-C24	2.43	1.53	1.50
10	F	613	CLA	O2D-CED	-2.42	1.39	1.45
10	J	613	CLA	CMB-C2B	2.42	1.55	1.50
9	B	605	CHL	C3B-C2B	-2.42	1.37	1.40
9	B	605	CHL	CMB-C2B	2.42	1.56	1.51
9	B	608	CHL	C3B-C2B	-2.42	1.37	1.40
10	F	603	CLA	CBD-CGD	2.42	1.59	1.52
9	F	606	CHL	CBD-CGD	2.42	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	610	CLA	O2D-CED	-2.42	1.39	1.45
10	J	611	CLA	O2D-CED	-2.42	1.39	1.45
9	C	609	CHL	C4-C3	2.42	1.56	1.50
10	I	613	CLA	CMB-C2B	2.42	1.55	1.50
10	B	614	CLA	O2D-CED	-2.42	1.39	1.45
10	F	602	CLA	C2-C3	2.42	1.38	1.33
10	H	602	CLA	C2-C3	2.42	1.38	1.33
10	C	613	CLA	C1-C2	-2.41	1.42	1.49
4	B	1620	LUT	C5-C6	2.41	1.38	1.34
9	J	601	CHL	C3B-C2B	-2.41	1.37	1.40
4	J	9621	LUT	C24-C25	2.41	1.36	1.33
10	F	611	CLA	CMB-C2B	2.41	1.55	1.50
9	E	607	CHL	C3A-C2A	-2.41	1.52	1.54
9	I	609	CHL	CHA-CBD	2.41	1.54	1.51
10	J	611	CLA	CMB-C2B	2.41	1.55	1.50
10	F	610	CLA	O2D-CED	-2.41	1.39	1.45
10	C	610	CLA	CBD-CGD	2.41	1.59	1.52
9	A	605	CHL	C3B-C2B	-2.40	1.37	1.40
9	C	607	CHL	O2D-CED	-2.40	1.39	1.45
4	D	3621	LUT	C5-C6	2.40	1.38	1.34
4	G	6620	LUT	C23-C24	2.40	1.53	1.50
9	B	609	CHL	C4-C3	2.39	1.56	1.50
10	F	612	CLA	CMB-C2B	2.39	1.55	1.50
9	H	607	CHL	CMB-C2B	2.39	1.56	1.51
10	I	602	CLA	C2-C3	2.39	1.38	1.33
4	J	9620	LUT	C26-C27	2.39	1.54	1.50
10	C	613	CLA	MG-ND	-2.39	2.01	2.05
10	D	610	CLA	CMB-C2B	2.38	1.55	1.50
4	F	5620	LUT	C5-C6	2.38	1.38	1.34
10	G	610	CLA	O2D-CED	-2.38	1.40	1.45
9	I	606	CHL	CHA-CBD	2.38	1.54	1.51
10	G	611	CLA	O2D-CED	-2.38	1.40	1.45
9	C	605	CHL	MG-ND	-2.38	2.01	2.05
9	C	605	CHL	C1A-CHA	2.38	1.42	1.40
10	F	610	CLA	CMB-C2B	2.38	1.55	1.50
9	J	601	CHL	C4-C3	2.38	1.56	1.50
9	D	605	CHL	MG-ND	-2.37	2.01	2.05
9	E	608	CHL	CMB-C2B	2.37	1.56	1.51
10	J	602	CLA	C2-C3	2.37	1.38	1.33
4	D	3620	LUT	C23-C24	2.36	1.53	1.50
9	E	605	CHL	O2D-CED	-2.36	1.40	1.45
9	I	601	CHL	CMB-C2B	2.36	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	608	CHL	CMB-C2B	2.36	1.56	1.51
4	B	1621	LUT	C1-C6	2.36	1.56	1.53
9	C	606	CHL	C1A-CHA	2.35	1.42	1.40
9	E	601	CHL	O2D-CED	-2.35	1.40	1.45
4	B	1620	LUT	C24-C25	2.35	1.36	1.33
9	E	606	CHL	CHA-CBD	2.35	1.54	1.51
8	A	632	DGD	O1G-C1A	2.35	1.40	1.33
9	E	601	CHL	C3B-C2B	-2.35	1.37	1.40
4	H	7621	LUT	C1-C6	2.35	1.56	1.53
10	J	604	CLA	MG-ND	-2.35	2.01	2.05
9	H	601	CHL	C3B-C2B	-2.35	1.37	1.40
9	G	606	CHL	C3A-C2A	-2.35	1.52	1.54
9	A	605	CHL	C1A-CHA	2.35	1.42	1.40
10	H	612	CLA	MG-ND	-2.34	2.01	2.05
10	F	613	CLA	C1-C2	-2.34	1.42	1.49
4	A	621	LUT	C5-C6	2.34	1.38	1.34
10	F	604	CLA	C5-C3	2.34	1.56	1.51
9	H	609	CHL	C3B-C2B	-2.34	1.37	1.40
4	H	7621	LUT	C24-C25	2.34	1.36	1.33
4	F	5621	LUT	C1-C6	2.33	1.56	1.53
9	A	608	CHL	CAC-C3C	2.33	1.56	1.51
8	D	3632	DGD	O1G-C1A	2.33	1.40	1.33
9	J	605	CHL	CMB-C2B	2.33	1.56	1.51
10	G	613	CLA	C5-C3	2.33	1.56	1.51
10	G	610	CLA	CAC-C3C	2.33	1.57	1.51
10	A	613	CLA	C1-C2	-2.33	1.42	1.49
10	E	612	CLA	O2D-CED	-2.33	1.40	1.45
9	J	605	CHL	C3B-C2B	-2.33	1.37	1.40
9	C	601	CHL	C3B-C2B	-2.33	1.37	1.40
9	F	605	CHL	CAC-C3C	2.32	1.56	1.51
10	D	611	CLA	CMB-C2B	2.32	1.55	1.50
10	E	604	CLA	C4-C3	2.32	1.56	1.50
9	G	601	CHL	MG-ND	-2.32	2.01	2.05
9	D	609	CHL	CBD-CGD	2.32	1.55	1.52
10	E	604	CLA	C1-C2	-2.32	1.42	1.49
9	D	601	CHL	C3B-C2B	-2.31	1.37	1.40
4	A	620	LUT	C5-C6	2.31	1.38	1.34
9	D	605	CHL	C1A-CHA	2.31	1.42	1.40
9	C	601	CHL	C1A-CHA	2.31	1.42	1.40
9	D	607	CHL	C4-C3	2.31	1.56	1.50
10	E	613	CLA	CMC-C2C	2.31	1.55	1.50
9	E	606	CHL	CAC-C3C	2.31	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5620	LUT	C23-C24	2.31	1.53	1.50
9	C	607	CHL	MG-ND	-2.30	2.01	2.05
4	I	8621	LUT	C23-C24	2.30	1.53	1.50
9	A	605	CHL	CHA-CBD	2.30	1.54	1.51
10	F	610	CLA	C4-C3	2.30	1.56	1.50
10	C	614	CLA	O2D-CED	-2.30	1.40	1.45
4	I	8621	LUT	C5-C6	2.30	1.38	1.34
6	I	8623	NEX	C1-C6	2.30	1.58	1.54
10	B	604	CLA	MG-ND	-2.29	2.01	2.05
4	H	7620	LUT	C5-C6	2.29	1.38	1.34
9	D	601	CHL	CMB-C2B	2.29	1.56	1.51
10	I	610	CLA	C4-C3	2.29	1.56	1.50
9	E	605	CHL	CHA-CBD	2.29	1.54	1.51
9	H	607	CHL	CAC-C3C	2.29	1.56	1.51
6	C	2623	NEX	C1-C6	2.29	1.58	1.54
8	H	7632	DGD	O1G-C1A	2.29	1.40	1.33
9	J	601	CHL	C1-C2	-2.29	1.42	1.49
10	G	602	CLA	C4-C3	2.29	1.56	1.50
9	B	608	CHL	MG-ND	-2.28	2.01	2.05
9	E	601	CHL	CHA-CBD	2.28	1.54	1.51
4	E	4621	LUT	C26-C27	2.28	1.53	1.50
9	I	606	CHL	C4-C3	2.28	1.56	1.50
10	B	613	CLA	O2D-CED	-2.28	1.40	1.45
9	E	608	CHL	C1A-CHA	2.28	1.42	1.40
10	I	613	CLA	C1-C2	-2.28	1.42	1.49
10	G	611	CLA	CMB-C2B	2.27	1.55	1.50
4	F	5620	LUT	C1-C6	2.27	1.56	1.53
10	C	612	CLA	CMB-C2B	2.27	1.55	1.50
9	B	601	CHL	C3B-C2B	-2.27	1.37	1.40
9	G	606	CHL	C4-C3	2.27	1.56	1.50
4	D	3621	LUT	C26-C27	2.27	1.53	1.50
10	H	603	CLA	MG-ND	-2.27	2.01	2.05
9	I	609	CHL	MG-ND	-2.26	2.01	2.05
9	F	606	CHL	C5-C3	2.26	1.56	1.50
9	I	609	CHL	O2D-CED	-2.26	1.40	1.45
10	I	614	CLA	O2D-CED	-2.26	1.40	1.45
9	D	606	CHL	O2D-CED	-2.26	1.40	1.45
9	A	609	CHL	CAC-C3C	2.26	1.56	1.51
9	J	606	CHL	C4-C3	2.26	1.56	1.50
10	A	613	CLA	C4-C3	2.26	1.56	1.50
10	H	604	CLA	C4-C3	2.26	1.56	1.50
9	H	605	CHL	O2D-CED	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	602	CLA	O2D-CED	-2.25	1.40	1.45
4	C	2620	LUT	C1-C6	2.25	1.56	1.53
9	B	607	CHL	MG-ND	-2.25	2.01	2.05
10	D	613	CLA	C1-C2	-2.25	1.42	1.49
10	C	610	CLA	CMB-C2B	2.25	1.55	1.50
9	G	605	CHL	C3B-C2B	-2.25	1.37	1.40
10	G	604	CLA	C5-C3	2.25	1.55	1.51
9	E	605	CHL	CMB-C2B	2.25	1.56	1.51
10	E	603	CLA	CAC-C3C	2.25	1.56	1.51
10	I	603	CLA	MG-ND	-2.25	2.01	2.05
10	F	611	CLA	O2D-CED	-2.24	1.40	1.45
9	G	609	CHL	CAC-C3C	2.24	1.56	1.51
10	C	613	CLA	CBD-CGD	2.24	1.59	1.52
9	G	606	CHL	CMB-C2B	2.24	1.56	1.51
9	C	608	CHL	MG-ND	-2.24	2.01	2.05
9	G	609	CHL	C4-C3	2.24	1.56	1.50
10	F	602	CLA	MG-ND	-2.24	2.01	2.05
10	H	614	CLA	O2D-CGD	2.23	1.38	1.33
9	I	606	CHL	CBD-CGD	2.23	1.55	1.52
9	G	606	CHL	C5-C3	2.23	1.56	1.50
9	D	606	CHL	C5-C3	2.23	1.56	1.50
10	B	602	CLA	C4-C3	2.23	1.56	1.50
9	J	608	CHL	CMB-C2B	2.23	1.56	1.51
6	J	9623	NEX	C1-C6	2.23	1.58	1.54
10	G	614	CLA	CAC-C3C	2.23	1.56	1.51
9	G	601	CHL	C3B-C2B	-2.23	1.37	1.40
9	C	605	CHL	C3B-C2B	-2.22	1.37	1.40
4	I	8621	LUT	C24-C25	2.22	1.35	1.33
9	B	601	CHL	MG-ND	-2.22	2.01	2.05
9	G	601	CHL	CHA-CBD	2.22	1.54	1.51
10	G	603	CLA	CMC-C2C	2.22	1.55	1.50
9	J	606	CHL	C5-C3	2.22	1.56	1.50
10	C	604	CLA	CBD-CGD	2.22	1.59	1.52
10	H	603	CLA	CMD-C2D	2.22	1.55	1.50
4	C	2621	LUT	C26-C27	2.21	1.53	1.50
9	I	608	CHL	C1A-CHA	2.21	1.42	1.40
10	B	613	CLA	C4-C3	2.21	1.56	1.50
10	A	610	CLA	CAC-C3C	2.21	1.56	1.51
9	J	608	CHL	CAC-C3C	2.21	1.56	1.51
10	C	602	CLA	CMB-C2B	2.21	1.55	1.50
9	A	601	CHL	C3B-C2B	-2.21	1.37	1.40
4	I	8620	LUT	C1-C6	2.21	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	611	CLA	CMB-C2B	2.20	1.55	1.50
9	E	606	CHL	C4-C3	2.20	1.56	1.50
10	J	613	CLA	C4-C3	2.20	1.56	1.50
9	I	607	CHL	C3A-C2A	-2.20	1.52	1.54
9	F	605	CHL	C3B-C2B	-2.20	1.37	1.40
10	A	603	CLA	CMC-C2C	2.20	1.55	1.50
10	C	603	CLA	CBD-CGD	2.20	1.59	1.52
10	H	612	CLA	C4-C3	2.20	1.56	1.50
10	H	611	CLA	O2D-CED	-2.20	1.40	1.45
9	A	607	CHL	CMB-C2B	2.20	1.56	1.51
9	H	601	CHL	CHA-CBD	2.19	1.54	1.51
5	C	7622	XAT	C28-C27	2.19	1.37	1.32
10	I	602	CLA	MG-ND	-2.19	2.01	2.05
4	A	620	LUT	C1-C6	2.19	1.56	1.53
9	H	609	CHL	CMB-C2B	2.19	1.56	1.51
10	F	612	CLA	C4-C3	2.19	1.56	1.50
9	A	609	CHL	C1-C2	-2.19	1.43	1.49
10	F	603	CLA	CAC-C3C	2.19	1.56	1.51
9	D	608	CHL	CMB-C2B	2.19	1.56	1.51
10	E	604	CLA	C5-C3	2.19	1.55	1.51
6	A	623	NEX	C1-C6	2.18	1.58	1.54
9	B	607	CHL	CAC-C3C	2.18	1.55	1.51
10	E	614	CLA	CMC-C2C	2.18	1.55	1.50
9	D	606	CHL	C4-C3	2.18	1.56	1.50
9	J	608	CHL	C1A-CHA	2.18	1.42	1.40
10	H	611	CLA	CMD-C2D	2.18	1.55	1.50
9	C	609	CHL	C1-C2	-2.18	1.43	1.49
4	C	2621	LUT	C5-C6	2.18	1.38	1.34
9	C	607	CHL	C3A-C2A	-2.17	1.52	1.54
9	B	601	CHL	CBD-CGD	2.17	1.55	1.52
9	G	609	CHL	C1-C2	-2.17	1.43	1.49
10	E	604	CLA	MG-ND	-2.17	2.01	2.05
9	C	607	CHL	CMD-C2D	2.17	1.55	1.51
10	J	604	CLA	CMC-C2C	2.17	1.55	1.50
5	D	8622	XAT	C28-C27	2.17	1.37	1.32
10	D	604	CLA	C4-C3	2.17	1.56	1.50
4	H	7621	LUT	C5-C6	2.17	1.38	1.34
9	F	601	CHL	C3B-C2B	-2.17	1.37	1.40
9	I	609	CHL	C1-C2	-2.16	1.43	1.49
10	C	604	CLA	C4-C3	2.16	1.56	1.50
10	D	612	CLA	C4-C3	2.16	1.56	1.50
9	H	606	CHL	C4-C3	2.16	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	610	CLA	CMC-C2C	2.16	1.55	1.50
9	C	606	CHL	C5-C3	2.16	1.56	1.50
9	F	609	CHL	C4-C3	2.16	1.56	1.50
10	H	602	CLA	CMB-C2B	2.16	1.55	1.50
9	A	607	CHL	MG-ND	-2.16	2.01	2.05
9	B	608	CHL	CAC-C3C	2.16	1.55	1.51
10	F	614	CLA	CMB-C2B	2.16	1.55	1.50
9	A	606	CHL	C5-C3	2.16	1.56	1.50
10	I	602	CLA	CMC-C2C	2.15	1.55	1.50
10	A	604	CLA	C4-C3	2.15	1.56	1.50
9	B	606	CHL	CHA-CBD	2.15	1.54	1.51
9	G	609	CHL	CHA-CBD	2.15	1.54	1.51
10	I	610	CLA	O2D-CED	-2.15	1.40	1.45
9	B	609	CHL	CMB-C2B	2.15	1.55	1.51
4	J	9620	LUT	C1-C6	2.15	1.56	1.53
4	G	6620	LUT	C1-C6	2.15	1.56	1.53
10	H	604	CLA	CMD-C2D	2.15	1.55	1.50
10	E	610	CLA	CAC-C3C	2.14	1.56	1.51
9	D	608	CHL	CAC-C3C	2.14	1.55	1.51
9	E	608	CHL	CBD-CGD	2.14	1.55	1.52
10	D	614	CLA	CAC-C3C	2.14	1.56	1.51
10	A	613	CLA	O2D-CED	-2.14	1.40	1.45
10	J	612	CLA	C4-C3	2.14	1.55	1.50
9	F	605	CHL	CHA-CBD	2.14	1.54	1.51
9	C	601	CHL	CMB-C2B	2.13	1.55	1.51
9	I	609	CHL	CAC-C3C	2.13	1.55	1.51
9	J	607	CHL	CHA-CBD	2.13	1.54	1.51
9	D	608	CHL	C4-C3	2.13	1.55	1.50
9	E	606	CHL	C5-C3	2.13	1.56	1.50
10	E	602	CLA	C4-C3	2.13	1.55	1.50
10	A	602	CLA	CMB-C2B	2.13	1.55	1.50
10	J	602	CLA	CHC-C1C	2.13	1.42	1.38
10	F	613	CLA	CMC-C2C	2.13	1.55	1.50
10	A	614	CLA	CMC-C2C	2.13	1.55	1.50
10	E	602	CLA	O2D-CED	-2.13	1.40	1.45
9	H	607	CHL	CHA-CBD	2.13	1.54	1.51
10	B	604	CLA	CMD-C2D	2.13	1.55	1.50
10	E	604	CLA	CBB-CAB	2.13	1.40	1.30
9	F	609	CHL	CMB-C2B	2.13	1.55	1.51
9	F	606	CHL	CHB-C4A	2.13	1.41	1.38
9	A	608	CHL	C1A-CHA	2.13	1.42	1.40
10	F	604	CLA	CMD-C2D	2.12	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	606	CHL	C4-C3	2.12	1.56	1.50
10	C	614	CLA	CMC-C2C	2.12	1.55	1.50
4	D	3620	LUT	C24-C25	2.12	1.35	1.33
10	I	602	CLA	CAC-C3C	2.12	1.56	1.51
9	F	608	CHL	CMB-C2B	2.12	1.55	1.51
10	B	612	CLA	C4-C3	2.12	1.55	1.50
10	G	612	CLA	C4-C3	2.12	1.55	1.50
4	J	9621	LUT	C5-C6	2.12	1.38	1.34
9	F	609	CHL	C1-C2	-2.12	1.43	1.49
10	J	613	CLA	CMC-C2C	2.12	1.55	1.50
4	G	6620	LUT	C24-C25	2.12	1.35	1.33
10	G	602	CLA	CHC-C1C	2.12	1.42	1.38
9	F	601	CHL	CHA-CBD	2.12	1.54	1.51
5	I	9622	XAT	C28-C27	2.11	1.37	1.32
10	I	614	CLA	CMC-C2C	2.11	1.55	1.50
9	C	608	CHL	CAC-C3C	2.11	1.55	1.51
9	C	608	CHL	CHA-CBD	2.11	1.54	1.51
9	D	601	CHL	O2D-CED	-2.11	1.40	1.45
9	G	608	CHL	CHA-CBD	2.11	1.54	1.51
10	C	613	CLA	O2D-CED	-2.11	1.40	1.45
9	J	608	CHL	C4-C3	2.11	1.55	1.50
10	G	602	CLA	CAC-C3C	2.11	1.56	1.51
9	F	609	CHL	CHA-CBD	2.10	1.54	1.51
4	I	8620	LUT	C24-C25	2.10	1.35	1.33
10	C	603	CLA	O2D-CED	-2.10	1.40	1.45
9	A	608	CHL	CHA-CBD	2.10	1.54	1.51
9	H	605	CHL	MG-ND	-2.10	2.01	2.05
6	G	6623	NEX	C1-C6	2.10	1.58	1.54
4	G	6621	LUT	C1-C6	2.09	1.56	1.53
9	F	601	CHL	CAC-C3C	2.09	1.55	1.51
9	G	605	CHL	CHA-CBD	2.09	1.54	1.51
10	H	614	CLA	CMB-C2B	2.09	1.55	1.50
10	I	604	CLA	MG-NB	-2.09	2.01	2.05
9	C	605	CHL	CHA-CBD	2.09	1.54	1.51
9	G	601	CHL	CMB-C2B	2.09	1.55	1.51
10	A	602	CLA	CAC-C3C	2.09	1.56	1.51
10	F	612	CLA	MG-ND	-2.08	2.01	2.05
9	G	606	CHL	CAC-C3C	2.08	1.55	1.51
9	F	601	CHL	C1A-CHA	2.08	1.42	1.40
10	H	610	CLA	CAC-C3C	2.08	1.56	1.51
10	J	602	CLA	C4-C3	2.08	1.55	1.50
10	G	611	CLA	CMC-C2C	2.08	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	610	CLA	CMC-C2C	2.08	1.55	1.50
10	H	602	CLA	C4-C3	2.08	1.55	1.50
10	B	602	CLA	MG-ND	-2.08	2.01	2.05
4	C	2620	LUT	C5-C6	2.08	1.38	1.34
9	E	605	CHL	MG-ND	-2.08	2.01	2.05
9	B	601	CHL	CMB-C2B	2.07	1.55	1.51
10	A	604	CLA	C5-C3	2.07	1.55	1.51
10	I	613	CLA	CMC-C2C	2.07	1.55	1.50
9	E	608	CHL	C4-C3	2.07	1.55	1.50
9	I	601	CHL	C3B-C2B	-2.07	1.37	1.40
10	H	602	CLA	CAC-C3C	2.07	1.56	1.51
10	C	612	CLA	C4-C3	2.07	1.55	1.50
4	B	1620	LUT	C1-C6	2.06	1.56	1.53
4	A	620	LUT	C26-C27	2.06	1.53	1.50
9	H	605	CHL	CHA-CBD	2.06	1.54	1.51
9	E	605	CHL	C3B-C2B	-2.06	1.37	1.40
10	J	603	CLA	CMD-C2D	2.06	1.55	1.50
4	I	8620	LUT	C5-C6	2.06	1.38	1.34
9	D	608	CHL	C1-C2	-2.06	1.43	1.49
10	J	612	CLA	CMB-C2B	2.06	1.55	1.50
10	D	613	CLA	C5-C3	2.06	1.55	1.51
4	J	9620	LUT	C23-C24	2.06	1.53	1.50
9	G	607	CHL	MG-ND	-2.05	2.01	2.05
9	I	605	CHL	CHA-CBD	2.05	1.54	1.51
10	D	611	CLA	MG-ND	-2.05	2.01	2.05
10	H	612	CLA	CAC-C3C	2.05	1.56	1.51
10	J	604	CLA	C4-C3	2.05	1.55	1.50
10	E	612	CLA	C4-C3	2.05	1.55	1.50
10	A	613	CLA	C5-C3	2.05	1.55	1.51
6	D	3623	NEX	C1-C6	2.05	1.58	1.54
9	J	606	CHL	CAC-C3C	2.05	1.55	1.51
9	C	606	CHL	C4-C3	2.05	1.55	1.50
10	E	610	CLA	CHC-C1C	2.04	1.42	1.38
9	B	605	CHL	O2D-CED	-2.04	1.40	1.45
10	J	613	CLA	CAC-C3C	2.04	1.56	1.51
10	F	610	CLA	CHC-C1C	2.04	1.42	1.38
10	I	610	CLA	CHC-C1C	2.04	1.42	1.38
9	H	605	CHL	C3B-C2B	-2.04	1.37	1.40
10	F	604	CLA	C4-C3	2.03	1.55	1.50
9	D	605	CHL	C3B-C2B	-2.03	1.37	1.40
10	F	614	CLA	O2D-CED	-2.03	1.40	1.45
9	F	606	CHL	C4-C3	2.03	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	602	CLA	CHC-C1C	2.03	1.42	1.38
6	F	5623	NEX	C1-C6	2.03	1.57	1.54
10	H	614	CLA	CMC-C2C	2.03	1.54	1.50
10	G	610	CLA	C4-C3	2.03	1.55	1.50
6	H	7623	NEX	C1-C6	2.03	1.57	1.54
9	A	605	CHL	CAC-C3C	2.03	1.55	1.51
10	B	614	CLA	CMC-C2C	2.02	1.54	1.50
9	I	605	CHL	C3B-C2B	-2.02	1.37	1.40
10	E	603	CLA	CMC-C2C	2.02	1.54	1.50
10	C	604	CLA	C5-C3	2.02	1.55	1.51
9	A	609	CHL	C4-C3	2.02	1.55	1.50
10	E	613	CLA	O2D-CED	-2.02	1.40	1.45
10	D	613	CLA	CBB-CAB	2.02	1.40	1.30
9	I	606	CHL	CMB-C2B	2.01	1.55	1.51
10	J	603	CLA	CAC-C3C	2.01	1.56	1.51
9	G	608	CHL	CAC-C3C	2.01	1.55	1.51
9	D	605	CHL	CHA-CBD	2.01	1.54	1.51
10	A	610	CLA	C4-C3	2.01	1.55	1.50
9	G	606	CHL	O2D-CED	-2.01	1.40	1.45
9	F	606	CHL	O2D-CED	-2.01	1.40	1.45
10	C	602	CLA	CAC-C3C	2.01	1.56	1.51
10	H	613	CLA	O2D-CED	-2.01	1.40	1.45
10	G	614	CLA	CMC-C2C	2.01	1.54	1.50
10	I	604	CLA	CBB-CAB	2.00	1.40	1.30
9	J	608	CHL	CHA-CBD	2.00	1.54	1.51
10	C	610	CLA	C4-C3	2.00	1.55	1.50

All (2657) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	607	CHL	C1B-CHB-C4A	11.91	128.98	121.32
9	C	607	CHL	C1B-CHB-C4A	11.51	128.73	121.32
9	C	606	CHL	C1B-CHB-C4A	11.51	128.72	121.32
9	F	607	CHL	C1B-CHB-C4A	11.38	128.64	121.32
9	A	607	CHL	C1B-CHB-C4A	11.36	128.63	121.32
9	H	607	CHL	C1B-CHB-C4A	11.35	128.62	121.32
9	G	607	CHL	C1B-CHB-C4A	11.26	128.56	121.32
9	J	601	CHL	C1B-CHB-C4A	11.23	128.55	121.32
9	F	606	CHL	C1B-CHB-C4A	11.20	128.53	121.32
9	D	601	CHL	C1B-CHB-C4A	11.19	128.52	121.32
9	I	607	CHL	C1B-CHB-C4A	11.15	128.49	121.32
9	A	601	CHL	C1B-CHB-C4A	11.08	128.45	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	607	CHL	C1B-CHB-C4A	11.07	128.45	121.32
9	E	601	CHL	C1B-CHB-C4A	11.06	128.44	121.32
9	J	606	CHL	C1B-CHB-C4A	11.01	128.41	121.32
9	G	606	CHL	C1B-CHB-C4A	11.01	128.40	121.32
9	F	601	CHL	C1B-CHB-C4A	10.99	128.39	121.32
9	A	606	CHL	C1B-CHB-C4A	10.96	128.37	121.32
9	D	609	CHL	C1B-CHB-C4A	10.93	128.35	121.32
9	B	601	CHL	C1B-CHB-C4A	10.92	128.35	121.32
9	C	601	CHL	C1B-CHB-C4A	10.89	128.33	121.32
9	D	606	CHL	C1B-CHB-C4A	10.87	128.32	121.32
9	H	606	CHL	C1B-CHB-C4A	10.86	128.31	121.32
9	I	609	CHL	C1B-CHB-C4A	10.84	128.30	121.32
9	B	609	CHL	C1B-CHB-C4A	10.84	128.30	121.32
9	J	607	CHL	C1B-CHB-C4A	10.84	128.30	121.32
9	G	601	CHL	C1B-CHB-C4A	10.83	128.29	121.32
9	D	607	CHL	C1B-CHB-C4A	10.81	128.28	121.32
9	I	601	CHL	C1B-CHB-C4A	10.81	128.27	121.32
9	I	606	CHL	C1B-CHB-C4A	10.81	128.27	121.32
9	H	601	CHL	C1B-CHB-C4A	10.78	128.26	121.32
9	F	608	CHL	C1B-CHB-C4A	10.71	128.21	121.32
9	A	608	CHL	C1B-CHB-C4A	10.66	128.18	121.32
9	B	608	CHL	C1B-CHB-C4A	10.65	128.17	121.32
9	A	609	CHL	C1B-CHB-C4A	10.61	128.15	121.32
9	H	609	CHL	C1B-CHB-C4A	10.59	128.14	121.32
9	C	608	CHL	C1B-CHB-C4A	10.58	128.13	121.32
9	D	608	CHL	C1B-CHB-C4A	10.58	128.13	121.32
9	G	609	CHL	C1B-CHB-C4A	10.53	128.09	121.32
9	I	608	CHL	C1B-CHB-C4A	10.47	128.06	121.32
9	J	605	CHL	C1B-CHB-C4A	10.47	128.06	121.32
9	E	605	CHL	C1B-CHB-C4A	10.46	128.05	121.32
9	E	608	CHL	C1B-CHB-C4A	10.45	128.04	121.32
9	F	605	CHL	C1B-CHB-C4A	10.42	128.02	121.32
9	B	605	CHL	C1B-CHB-C4A	10.38	128.00	121.32
9	F	609	CHL	C1B-CHB-C4A	10.37	127.99	121.32
9	J	608	CHL	C1B-CHB-C4A	10.36	127.99	121.32
9	G	608	CHL	C1B-CHB-C4A	10.35	127.98	121.32
9	C	609	CHL	C1B-CHB-C4A	10.34	127.97	121.32
9	C	605	CHL	C1B-CHB-C4A	10.33	127.97	121.32
9	H	608	CHL	C1B-CHB-C4A	10.32	127.96	121.32
9	D	605	CHL	C1B-CHB-C4A	10.32	127.96	121.32
9	E	609	CHL	C1B-CHB-C4A	10.31	127.95	121.32
9	E	606	CHL	C1B-CHB-C4A	10.24	127.91	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	609	CHL	C1B-CHB-C4A	10.22	127.90	121.32
9	B	606	CHL	C1B-CHB-C4A	10.15	127.85	121.32
9	G	605	CHL	C1B-CHB-C4A	10.08	127.81	121.32
9	H	605	CHL	C1B-CHB-C4A	10.08	127.81	121.32
9	A	605	CHL	C1B-CHB-C4A	9.99	127.75	121.32
9	I	605	CHL	C1B-CHB-C4A	9.98	127.74	121.32
9	C	607	CHL	OMC-CMC-C2C	8.92	140.62	125.12
9	A	607	CHL	OMC-CMC-C2C	8.69	140.22	125.12
9	A	609	CHL	OMC-CMC-C2C	8.59	140.05	125.12
9	C	608	CHL	OMC-CMC-C2C	8.58	140.03	125.12
10	F	613	CLA	C4A-NA-C1A	8.43	110.52	106.68
10	C	613	CLA	C4A-NA-C1A	8.37	110.50	106.68
9	B	607	CHL	OMC-CMC-C2C	8.25	139.45	125.12
10	I	604	CLA	C4A-NA-C1A	8.24	110.44	106.68
10	G	613	CLA	C4A-NA-C1A	8.23	110.44	106.68
9	E	609	CHL	OMC-CMC-C2C	8.23	139.42	125.12
10	E	613	CLA	C4A-NA-C1A	8.20	110.42	106.68
10	D	613	CLA	C4A-NA-C1A	8.20	110.42	106.68
9	E	607	CHL	OMC-CMC-C2C	8.16	139.30	125.12
10	H	613	CLA	C4A-NA-C1A	8.11	110.38	106.68
10	I	613	CLA	C4A-NA-C1A	8.08	110.37	106.68
9	I	609	CHL	OMC-CMC-C2C	7.99	139.01	125.12
10	A	613	CLA	C4A-NA-C1A	7.90	110.28	106.68
10	H	603	CLA	C4A-NA-C1A	7.82	110.25	106.68
10	G	610	CLA	C4A-NA-C1A	7.81	110.24	106.68
10	I	610	CLA	C4A-NA-C1A	7.81	110.24	106.68
10	F	604	CLA	C4A-NA-C1A	7.79	110.23	106.68
10	A	604	CLA	C4A-NA-C1A	7.75	110.22	106.68
10	H	610	CLA	C4A-NA-C1A	7.74	110.21	106.68
10	J	604	CLA	C4A-NA-C1A	7.72	110.20	106.68
10	E	611	CLA	C4A-NA-C1A	7.71	110.19	106.68
10	J	610	CLA	C4A-NA-C1A	7.70	110.19	106.68
10	J	603	CLA	C4A-NA-C1A	7.65	110.17	106.68
10	E	604	CLA	C4A-NA-C1A	7.64	110.17	106.68
10	B	613	CLA	C4A-NA-C1A	7.64	110.16	106.68
10	J	611	CLA	C4A-NA-C1A	7.63	110.16	106.68
10	C	614	CLA	O2D-CGD-CBD	7.61	124.54	111.23
10	G	604	CLA	C4A-NA-C1A	7.57	110.13	106.68
10	F	610	CLA	C4A-NA-C1A	7.52	110.11	106.68
10	C	611	CLA	C4A-NA-C1A	7.51	110.10	106.68
10	B	614	CLA	O2D-CGD-CBD	7.50	124.34	111.23
9	F	607	CHL	OMC-CMC-C2C	7.49	138.13	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	602	CLA	C4A-NA-C1A	7.49	110.09	106.68
10	A	603	CLA	C4A-NA-C1A	7.48	110.09	106.68
10	H	604	CLA	C4A-NA-C1A	7.48	110.09	106.68
10	E	610	CLA	C4A-NA-C1A	7.47	110.09	106.68
10	J	602	CLA	C4A-NA-C1A	7.46	110.08	106.68
9	F	601	CHL	OMC-CMC-C2C	7.45	138.07	125.12
9	D	609	CHL	OMC-CMC-C2C	7.44	138.04	125.12
9	D	607	CHL	OMC-CMC-C2C	7.41	137.99	125.12
10	J	613	CLA	C4A-NA-C1A	7.40	110.06	106.68
10	B	604	CLA	C4A-NA-C1A	7.40	110.06	106.68
10	G	611	CLA	C4A-NA-C1A	7.39	110.05	106.68
9	J	609	CHL	OMC-CMC-C2C	7.38	137.94	125.12
10	B	602	CLA	C4A-NA-C1A	7.38	110.04	106.68
9	D	608	CHL	OMC-CMC-C2C	7.35	137.89	125.12
10	D	604	CLA	C4A-NA-C1A	7.34	110.03	106.68
10	G	603	CLA	C4A-NA-C1A	7.33	110.02	106.68
10	G	614	CLA	C4A-NA-C1A	7.33	110.02	106.68
10	I	603	CLA	C4A-NA-C1A	7.32	110.02	106.68
9	F	608	CHL	OMC-CMC-C2C	7.30	137.80	125.12
10	E	614	CLA	C4A-NA-C1A	7.29	110.01	106.68
10	D	612	CLA	C4A-NA-C1A	7.28	110.00	106.68
10	A	611	CLA	C4A-NA-C1A	7.27	110.00	106.68
10	A	610	CLA	C4A-NA-C1A	7.27	110.00	106.68
10	D	610	CLA	C4A-NA-C1A	7.25	109.99	106.68
10	I	614	CLA	C4A-NA-C1A	7.25	109.99	106.68
10	B	610	CLA	C4A-NA-C1A	7.24	109.98	106.68
10	C	604	CLA	C4A-NA-C1A	7.24	109.98	106.68
10	I	602	CLA	C4A-NA-C1A	7.22	109.97	106.68
10	G	612	CLA	C4A-NA-C1A	7.21	109.97	106.68
10	F	602	CLA	C4A-NA-C1A	7.20	109.97	106.68
10	E	614	CLA	O2D-CGD-CBD	7.19	123.80	111.23
9	H	607	CHL	OMC-CMC-C2C	7.18	137.59	125.12
10	E	612	CLA	C4A-NA-C1A	7.17	109.95	106.68
10	D	611	CLA	C4A-NA-C1A	7.16	109.94	106.68
10	I	612	CLA	C4A-NA-C1A	7.12	109.93	106.68
10	J	612	CLA	C4A-NA-C1A	7.12	109.93	106.68
10	A	602	CLA	C4A-NA-C1A	7.11	109.92	106.68
10	H	614	CLA	O2D-CGD-CBD	7.11	123.66	111.23
10	F	612	CLA	C4A-NA-C1A	7.10	109.92	106.68
10	A	614	CLA	O2D-CGD-CBD	7.09	123.63	111.23
9	G	601	CHL	OMC-CMC-C2C	7.08	137.43	125.12
10	D	603	CLA	C4A-NA-C1A	7.07	109.90	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	602	CLA	C4A-NA-C1A	7.05	109.90	106.68
10	I	614	CLA	O2D-CGD-CBD	7.01	123.49	111.23
9	F	609	CHL	OMC-CMC-C2C	7.01	137.29	125.12
10	F	603	CLA	C4A-NA-C1A	7.00	109.87	106.68
10	E	603	CLA	C4A-NA-C1A	6.99	109.87	106.68
10	J	614	CLA	C4A-NA-C1A	6.99	109.87	106.68
10	H	612	CLA	C4A-NA-C1A	6.98	109.86	106.68
10	B	603	CLA	C4A-NA-C1A	6.97	109.86	106.68
10	A	612	CLA	C4A-NA-C1A	6.97	109.86	106.68
10	C	602	CLA	C4A-NA-C1A	6.96	109.86	106.68
10	C	603	CLA	C4A-NA-C1A	6.96	109.85	106.68
9	G	609	CHL	OMC-CMC-C2C	6.94	137.18	125.12
10	D	614	CLA	C4A-NA-C1A	6.93	109.84	106.68
10	B	612	CLA	C4A-NA-C1A	6.93	109.84	106.68
9	J	607	CHL	OMC-CMC-C2C	6.90	137.11	125.12
10	H	602	CLA	C4A-NA-C1A	6.90	109.83	106.68
10	H	614	CLA	C4A-NA-C1A	6.90	109.83	106.68
10	B	614	CLA	C4A-NA-C1A	6.86	109.81	106.68
10	I	611	CLA	C4A-NA-C1A	6.86	109.81	106.68
10	B	611	CLA	C4A-NA-C1A	6.78	109.77	106.68
9	D	605	CHL	OMC-CMC-C2C	6.77	136.89	125.12
10	A	614	CLA	C4A-NA-C1A	6.74	109.75	106.68
10	G	602	CLA	C4A-NA-C1A	6.74	109.75	106.68
10	H	611	CLA	C4A-NA-C1A	6.73	109.75	106.68
10	J	611	CLA	CAA-C2A-C3A	-6.72	94.83	113.00
10	D	614	CLA	O2D-CGD-CBD	6.70	122.95	111.23
10	C	612	CLA	C4A-NA-C1A	6.69	109.73	106.68
10	C	604	CLA	O2A-CGA-CBA	6.67	132.17	111.83
10	D	604	CLA	O2A-CGA-CBA	6.66	132.14	111.83
10	B	604	CLA	O2A-CGA-CBA	6.66	132.13	111.83
10	F	611	CLA	C4A-NA-C1A	6.64	109.71	106.68
9	E	606	CHL	CBA-CAA-C2A	-6.62	94.28	113.78
9	D	601	CHL	OMC-CMC-C2C	6.60	136.59	125.12
10	C	614	CLA	O1D-CGD-CBD	-6.59	111.51	124.52
10	C	610	CLA	C4A-NA-C1A	6.58	109.68	106.68
10	C	614	CLA	C4A-NA-C1A	6.56	109.67	106.68
9	E	605	CHL	OMC-CMC-C2C	6.54	136.49	125.12
10	F	614	CLA	C4A-NA-C1A	6.50	109.64	106.68
9	J	605	CHL	OMC-CMC-C2C	6.48	136.38	125.12
9	B	609	CHL	OMC-CMC-C2C	6.47	136.36	125.12
9	F	605	CHL	OMC-CMC-C2C	6.41	136.25	125.12
10	G	611	CLA	CBA-CAA-C2A	6.30	132.55	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	614	CLA	O2D-CGD-CBD	6.30	122.25	111.23
9	I	601	CHL	OMC-CMC-C2C	6.30	136.06	125.12
10	B	614	CLA	O1D-CGD-CBD	-6.24	112.20	124.52
9	I	607	CHL	OMC-CMC-C2C	6.23	135.94	125.12
10	C	611	CLA	CAA-C2A-C3A	-6.23	96.16	113.00
4	E	4620	LUT	C18-C5-C6	6.23	131.28	124.48
10	G	614	CLA	O2D-CGD-CBD	6.22	122.11	111.23
5	B	1622	XAT	C24-C23-C22	6.18	122.34	110.79
9	B	605	CHL	OMC-CMC-C2C	6.17	135.83	125.12
9	A	601	CHL	OMC-CMC-C2C	6.15	135.81	125.12
10	J	614	CLA	O2D-CGD-CBD	6.10	121.89	111.23
9	E	601	CHL	OMC-CMC-C2C	6.09	135.71	125.12
9	I	605	CHL	OMC-CMC-C2C	5.98	135.52	125.12
10	D	611	CLA	CBA-CAA-C2A	5.96	131.54	113.79
9	H	608	CHL	OMC-CMC-C2C	5.96	135.48	125.12
10	I	614	CLA	O1D-CGD-CBD	-5.95	112.79	124.52
9	H	606	CHL	CAA-CBA-CGA	5.94	130.08	113.21
10	H	614	CLA	O1D-CGD-CBD	-5.94	112.80	124.52
5	H	4622	XAT	C24-C23-C22	5.94	121.89	110.79
10	E	611	CLA	CBA-CAA-C2A	5.93	131.45	113.79
10	E	614	CLA	O1D-CGD-CBD	-5.93	112.82	124.52
10	E	604	CLA	O2A-CGA-CBA	5.93	129.91	111.83
10	F	611	CLA	CAA-C2A-C3A	-5.92	97.00	113.00
9	C	609	CHL	OMC-CMC-C2C	5.92	135.40	125.12
10	D	604	CLA	CMB-C2B-C1B	-5.90	116.43	125.42
10	G	613	CLA	CMB-C2B-C1B	-5.89	116.45	125.42
10	A	611	CLA	CBA-CAA-C2A	5.89	131.31	113.79
10	C	604	CLA	CMB-C2B-C1B	-5.89	116.46	125.42
10	A	614	CLA	O1D-CGD-CBD	-5.87	112.94	124.52
10	C	611	CLA	CBA-CAA-C2A	5.86	131.22	113.79
5	C	7622	XAT	C24-C23-C22	5.83	121.69	110.79
10	A	604	CLA	CMB-C2B-C1B	-5.81	116.57	125.42
10	J	604	CLA	O2A-CGA-CBA	5.81	129.56	111.83
10	H	611	CLA	CBA-CAA-C2A	5.79	131.02	113.79
10	E	604	CLA	CAA-C2A-C3A	-5.79	97.37	113.00
10	I	613	CLA	CMB-C2B-C1B	-5.78	116.62	125.42
9	D	606	CHL	CBA-CAA-C2A	-5.75	96.84	113.78
10	D	613	CLA	CMB-C2B-C1B	-5.74	116.67	125.42
9	G	605	CHL	OMC-CMC-C2C	5.74	135.10	125.12
10	B	613	CLA	CED-O2D-CGD	5.74	128.93	115.92
9	H	609	CHL	OMC-CMC-C2C	5.72	135.05	125.12
10	D	613	CLA	CBA-CAA-C2A	5.71	130.78	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	604	CLA	O2A-CGA-CBA	5.70	129.22	111.83
9	G	608	CHL	OMC-CMC-C2C	5.69	135.01	125.12
9	A	608	CHL	OMC-CMC-C2C	5.69	135.00	125.12
7	I	8630	LHG	O8-C23-C24	5.67	129.13	111.83
9	I	606	CHL	CBA-CAA-C2A	-5.65	97.12	113.78
10	I	611	CLA	CAA-CBA-CGA	5.64	129.21	113.21
10	H	604	CLA	O2A-CGA-CBA	5.61	128.93	111.83
9	G	601	CHL	CBA-CAA-C2A	5.59	130.25	113.78
10	I	602	CLA	C1-C2-C3	5.58	135.34	126.20
10	C	613	CLA	CMB-C2B-C1B	-5.57	116.93	125.42
10	D	614	CLA	O1D-CGD-CBD	-5.55	113.56	124.52
10	G	612	CLA	C1-C2-C3	5.55	135.29	126.20
9	B	606	CHL	O2A-CGA-CBA	5.54	128.72	111.83
9	H	601	CHL	OMC-CMC-C2C	5.53	134.73	125.12
10	F	604	CLA	CMB-C2B-C1B	-5.52	117.02	125.42
10	B	613	CLA	CMB-C2B-C1B	-5.52	117.02	125.42
10	H	613	CLA	CMB-C2B-C1B	-5.51	117.03	125.42
10	E	604	CLA	CMB-C2B-C1B	-5.49	117.06	125.42
10	I	604	CLA	O2A-CGA-CBA	5.49	128.57	111.83
9	C	605	CHL	OMC-CMC-C2C	5.49	134.66	125.12
9	G	607	CHL	OMC-CMC-C2C	5.48	134.64	125.12
10	F	614	CLA	O1D-CGD-CBD	-5.48	113.72	124.52
9	C	601	CHL	OMC-CMC-C2C	5.46	134.61	125.12
10	J	614	CLA	O1D-CGD-CBD	-5.45	113.76	124.52
9	E	608	CHL	OMC-CMC-C2C	5.44	134.58	125.12
9	A	608	CHL	CED-O2D-CGD	5.44	128.26	115.92
10	D	602	CLA	C1-C2-C3	5.44	135.11	126.20
10	D	604	CLA	CAA-C2A-C3A	-5.42	98.36	113.00
10	B	604	CLA	CMB-C2B-C1B	-5.34	117.29	125.42
10	C	603	CLA	O2D-CGD-CBD	5.33	120.56	111.23
10	H	611	CLA	C1-C2-C3	5.30	134.88	126.20
9	E	608	CHL	CED-O2D-CGD	5.29	127.92	115.92
10	D	611	CLA	C1-C2-C3	5.28	134.85	126.20
10	B	602	CLA	CED-O2D-CGD	5.27	127.87	115.92
5	D	8622	XAT	C24-C23-C22	5.26	120.63	110.79
4	J	9620	LUT	C18-C5-C6	5.25	130.22	124.48
9	B	601	CHL	OMC-CMC-C2C	5.25	134.24	125.12
10	C	604	CLA	CAA-C2A-C3A	-5.25	98.82	113.00
10	B	611	CLA	CAA-C2A-C3A	-5.24	98.83	113.00
10	B	604	CLA	CED-O2D-CGD	5.24	127.79	115.92
10	G	614	CLA	O1D-CGD-CBD	-5.23	114.19	124.52
10	F	613	CLA	CMB-C2B-C1B	-5.23	117.45	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	612	CLA	C1-C2-C3	5.23	134.76	126.20
9	B	608	CHL	OMC-CMC-C2C	5.22	134.20	125.12
10	G	604	CLA	CMB-C2B-C1B	-5.22	117.47	125.42
10	G	604	CLA	O2A-CGA-CBA	5.20	127.70	111.83
9	J	606	CHL	O2A-CGA-CBA	5.19	127.67	111.83
9	D	601	CHL	CBA-CAA-C2A	5.19	129.07	113.78
10	A	611	CLA	C1-C2-C3	5.19	134.70	126.20
10	F	602	CLA	C1-C2-C3	5.18	134.68	126.20
10	H	613	CLA	CED-O2D-CGD	5.16	127.62	115.92
10	I	604	CLA	CMB-C2B-C1B	-5.14	117.59	125.42
10	I	602	CLA	O2D-CGD-CBD	5.13	120.19	111.23
4	I	8620	LUT	C18-C5-C6	5.12	130.07	124.48
5	I	9622	XAT	C24-C23-C22	5.12	120.36	110.79
9	H	609	CHL	C1-C2-C3	5.12	134.58	126.20
9	H	608	CHL	C7-C6-C5	5.12	126.90	113.26
4	A	620	LUT	C18-C5-C6	5.11	130.06	124.48
10	B	602	CLA	C1-C2-C3	5.11	134.58	126.20
5	F	6622	XAT	C24-C23-C22	5.11	120.35	110.79
10	B	611	CLA	CBA-CAA-C2A	5.11	129.00	113.79
7	A	630	LHG	O8-C23-C24	5.07	127.30	111.83
9	C	601	CHL	CED-O2D-CGD	5.07	127.42	115.92
10	C	613	CLA	CED-O2D-CGD	5.07	127.41	115.92
9	F	606	CHL	O2A-CGA-CBA	5.06	127.25	111.83
4	D	3620	LUT	C18-C5-C6	5.05	130.00	124.48
9	I	606	CHL	CMB-C2B-C3B	5.05	134.77	124.68
9	J	606	CHL	CAA-CBA-CGA	5.04	127.53	113.21
10	E	602	CLA	C1-C2-C3	5.04	134.46	126.20
9	G	606	CHL	C1-C2-C3	5.04	134.91	126.76
10	G	612	CLA	O2D-CGD-CBD	5.02	120.00	111.23
10	A	604	CLA	O2A-CGA-CBA	5.02	127.13	111.83
4	C	2620	LUT	C18-C5-C6	5.01	129.96	124.48
9	D	606	CHL	O2A-CGA-CBA	5.01	127.11	111.83
9	J	601	CHL	CED-O2D-CGD	5.01	127.27	115.92
9	I	606	CHL	CAA-CBA-CGA	5.00	127.40	113.21
10	J	604	CLA	CMB-C2B-C1B	-4.99	117.83	125.42
7	E	4630	LHG	O8-C23-C24	4.98	127.03	111.83
7	G	6630	LHG	O8-C23-C24	4.96	126.95	111.83
10	A	603	CLA	O2D-CGD-CBD	4.95	119.88	111.23
9	C	606	CHL	O2D-CGD-CBD	4.94	116.38	110.95
7	C	2630	LHG	O8-C23-C24	4.94	126.90	111.83
5	B	5622	XAT	C24-C23-C22	4.91	119.98	110.79
10	A	613	CLA	CBA-CAA-C2A	4.91	128.39	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	622	XAT	C24-C23-C22	4.90	119.96	110.79
9	E	607	CHL	CMB-C2B-C3B	4.90	134.48	124.68
10	I	604	CLA	CED-O2D-CGD	4.90	127.03	115.92
7	B	1630	LHG	O8-C23-C24	4.90	126.77	111.83
10	B	604	CLA	CAA-C2A-C3A	-4.90	99.77	113.00
9	C	606	CHL	C1-C2-C3	4.89	134.68	126.76
10	H	604	CLA	O2D-CGD-CBD	4.88	119.77	111.23
9	A	606	CHL	CBA-CAA-C2A	-4.88	99.40	113.78
10	J	612	CLA	C1-C2-C3	4.86	134.16	126.20
9	D	606	CHL	CMB-C2B-C3B	4.86	134.40	124.68
9	A	601	CHL	CBA-CAA-C2A	4.86	128.09	113.78
10	C	602	CLA	C1-C2-C3	4.86	134.15	126.20
9	J	601	CHL	CBA-CAA-C2A	4.86	128.08	113.78
9	H	605	CHL	OMC-CMC-C2C	4.84	133.53	125.12
10	H	613	CLA	CBA-CAA-C2A	4.84	128.19	113.79
7	J	9630	LHG	O8-C23-C24	4.84	126.59	111.83
4	G	6620	LUT	C18-C5-C6	4.82	129.74	124.48
9	I	608	CHL	C1-C2-C3	4.81	134.09	126.20
10	J	604	CLA	CAA-C2A-C3A	-4.81	99.99	113.00
7	A	630	LHG	O8-C6-C5	4.81	122.26	108.40
9	A	606	CHL	C3D-C4D-CHA	4.81	115.84	108.54
9	C	608	CHL	CED-O2D-CGD	4.80	126.81	115.92
9	I	601	CHL	C3D-C4D-CHA	4.80	115.84	108.54
10	B	603	CLA	O2D-CGD-CBD	4.79	119.60	111.23
9	H	606	CHL	C1-C2-C3	4.79	134.51	126.76
10	B	612	CLA	C1-C2-C3	4.78	134.02	126.20
7	G	6630	LHG	O8-C6-C5	4.77	122.15	108.40
9	J	608	CHL	OMC-CMC-C2C	4.77	133.41	125.12
9	C	606	CHL	CBA-CAA-C2A	-4.77	99.73	113.78
4	B	1620	LUT	C18-C5-C6	4.77	129.69	124.48
9	B	601	CHL	C3D-C4D-CHA	4.77	115.78	108.54
9	G	601	CHL	CED-O2D-CGD	4.77	126.73	115.92
9	B	605	CHL	C3D-C4D-CHA	4.76	115.78	108.54
9	H	601	CHL	CBA-CAA-C2A	4.76	127.81	113.78
9	I	608	CHL	OMC-CMC-C2C	4.76	133.39	125.12
10	J	613	CLA	CED-O2D-CGD	4.76	126.71	115.92
10	G	602	CLA	C1-C2-C3	4.76	133.99	126.20
4	H	7620	LUT	C38-C25-C24	-4.75	112.12	123.36
9	F	607	CHL	O2A-CGA-CBA	4.75	126.31	111.83
10	B	611	CLA	O2A-CGA-CBA	4.74	126.30	111.83
4	J	9620	LUT	C38-C25-C24	-4.74	112.15	123.36
9	D	606	CHL	C1-C2-C3	4.73	134.42	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	5620	LUT	C18-C5-C6	4.73	129.65	124.48
9	B	608	CHL	C7-C6-C5	4.72	125.85	113.26
10	J	602	CLA	C1-C2-C3	4.72	133.93	126.20
9	J	601	CHL	C3D-C4D-CHA	4.72	115.71	108.54
9	A	601	CHL	C3D-C4D-CHA	4.72	115.71	108.54
10	G	603	CLA	C6-C5-C3	4.72	124.95	113.47
9	E	607	CHL	C7-C6-C5	-4.71	100.72	113.26
9	F	608	CHL	C7-C6-C5	4.70	125.79	113.26
9	J	601	CHL	OMC-CMC-C2C	4.69	133.27	125.12
10	I	602	CLA	O1D-CGD-CBD	-4.69	115.26	124.52
10	H	612	CLA	C1-C2-C3	4.67	133.86	126.20
10	J	610	CLA	O2A-CGA-CBA	4.67	126.08	111.83
5	J	3622	XAT	C24-C23-C22	4.66	119.51	110.79
9	H	605	CHL	C3D-C4D-CHA	4.65	115.61	108.54
10	F	602	CLA	C4-C3-C5	4.65	123.30	115.23
7	H	7630	LHG	O8-C6-C5	4.65	121.80	108.40
9	J	607	CHL	CMB-C2B-C3B	4.65	133.97	124.68
10	G	611	CLA	C1-C2-C3	4.65	133.81	126.20
10	G	604	CLA	CAA-C2A-C3A	-4.65	100.44	113.00
9	C	606	CHL	O2A-CGA-CBA	4.65	126.00	111.83
10	B	602	CLA	C6-C5-C3	4.64	124.78	113.47
9	E	605	CHL	C3D-C4D-CHA	4.64	115.59	108.54
9	I	607	CHL	CMB-C2B-C3B	4.64	133.95	124.68
4	H	7620	LUT	C18-C5-C6	4.63	129.54	124.48
9	G	607	CHL	CMB-C2B-C3B	4.63	133.94	124.68
10	H	610	CLA	O2A-CGA-CBA	4.63	125.95	111.83
10	H	610	CLA	CBA-CAA-C2A	4.63	127.57	113.79
9	E	609	CHL	C3D-C4D-CHA	4.63	115.58	108.54
9	G	601	CHL	C3D-C4D-CHA	4.63	115.58	108.54
9	H	608	CHL	C3D-C4D-CHA	4.61	115.55	108.54
9	J	606	CHL	C3D-C4D-CHA	4.61	115.55	108.54
9	J	605	CHL	C3D-C4D-CHA	4.61	115.55	108.54
10	J	603	CLA	O2D-CGD-CBD	4.61	119.28	111.23
9	E	608	CHL	C3D-C4D-CHA	4.60	115.53	108.54
9	G	609	CHL	C3D-C4D-CHA	4.60	115.53	108.54
9	D	601	CHL	C3D-C4D-CHA	4.60	115.53	108.54
9	G	607	CHL	C3D-C4D-CHA	4.60	115.53	108.54
9	F	607	CHL	C3D-C4D-CHA	4.59	115.52	108.54
9	A	606	CHL	O2A-CGA-CBA	4.59	125.83	111.83
9	F	608	CHL	C3D-C4D-CHA	4.59	115.52	108.54
10	G	613	CLA	C4-C3-C5	-4.58	107.27	115.23
10	B	611	CLA	C1-C2-C3	4.58	133.70	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	605	CHL	C3D-C4D-CHA	4.58	115.50	108.54
10	G	611	CLA	CAA-C2A-C3A	-4.57	100.64	113.00
9	E	606	CHL	C1-C2-C3	4.57	134.16	126.76
9	F	606	CHL	C1-C2-C3	4.57	134.16	126.76
9	B	609	CHL	C3D-C4D-CHA	4.57	115.48	108.54
9	C	609	CHL	C1-C2-C3	4.56	133.67	126.20
10	A	602	CLA	C6-C5-C3	4.56	124.57	113.47
10	B	603	CLA	CBA-CAA-C2A	4.55	127.34	113.79
9	A	608	CHL	C3D-C4D-CHA	4.55	115.46	108.54
9	B	601	CHL	CBA-CAA-C2A	4.55	127.18	113.78
9	F	601	CHL	CBA-CAA-C2A	4.55	127.18	113.78
9	H	601	CHL	C3D-C4D-CHA	4.54	115.44	108.54
10	E	613	CLA	CED-O2D-CGD	4.54	126.22	115.92
10	A	604	CLA	CAA-C2A-C3A	-4.54	100.73	113.00
9	D	607	CHL	C3D-C4D-CHA	4.54	115.44	108.54
10	H	604	CLA	CMB-C2B-C1B	-4.54	118.51	125.42
10	E	603	CLA	CBA-CAA-C2A	4.54	127.29	113.79
10	J	604	CLA	C1-C2-C3	4.53	133.62	126.20
9	J	607	CHL	C3D-C4D-CHA	4.53	115.43	108.54
10	C	612	CLA	O2D-CGD-CBD	4.53	119.15	111.23
9	I	605	CHL	C3D-C4D-CHA	4.53	115.42	108.54
9	G	606	CHL	CAA-CBA-CGA	4.53	126.07	113.21
9	I	608	CHL	C3D-C4D-CHA	4.53	115.42	108.54
10	D	613	CLA	CED-O2D-CGD	4.53	126.18	115.92
7	H	7630	LHG	O8-C23-C24	4.52	125.63	111.83
9	F	609	CHL	C3D-C4D-CHA	4.51	115.40	108.54
9	B	608	CHL	C3D-C4D-CHA	4.51	115.40	108.54
9	E	601	CHL	C3D-C4D-CHA	4.51	115.39	108.54
10	J	611	CLA	C1-C2-C3	4.51	133.58	126.20
9	B	606	CHL	C3D-C4D-CHA	4.51	115.39	108.54
9	F	601	CHL	C3D-C4D-CHA	4.50	115.39	108.54
9	I	609	CHL	C3D-C4D-CHA	4.50	115.39	108.54
9	H	607	CHL	CMB-C2B-C3B	4.50	133.68	124.68
9	B	607	CHL	C3D-C4D-CHA	4.50	115.38	108.54
9	D	608	CHL	C3D-C4D-CHA	4.50	115.38	108.54
10	H	604	CLA	CAA-C2A-C3A	-4.50	100.85	113.00
10	G	613	CLA	CED-O2D-CGD	4.49	126.11	115.92
9	F	605	CHL	C3D-C4D-CHA	4.49	115.37	108.54
9	C	601	CHL	C3D-C4D-CHA	4.49	115.37	108.54
9	C	608	CHL	C3D-C4D-CHA	4.49	115.37	108.54
10	G	610	CLA	CBA-CAA-C2A	4.49	127.16	113.79
9	H	609	CHL	C3D-C4D-CHA	4.49	115.37	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	606	CHL	CMB-C2B-C3B	4.49	133.66	124.68
9	C	606	CHL	C3D-C4D-CHA	4.49	115.36	108.54
9	C	605	CHL	C3D-C4D-CHA	4.49	115.36	108.54
9	D	606	CHL	C3D-C4D-CHA	4.49	115.36	108.54
9	H	607	CHL	C3D-C4D-CHA	4.49	115.36	108.54
10	E	611	CLA	O2A-CGA-CBA	4.48	125.51	111.83
10	E	602	CLA	C6-C5-C3	4.48	124.39	113.47
10	H	603	CLA	CBA-CAA-C2A	4.47	127.09	113.79
9	F	606	CHL	C3D-C4D-CHA	4.47	115.33	108.54
10	F	612	CLA	C1-C2-C3	4.46	133.51	126.20
9	I	601	CHL	CBA-CAA-C2A	4.46	126.92	113.78
9	H	601	CHL	CED-O2D-CGD	4.46	126.03	115.92
9	E	607	CHL	C3D-C4D-CHA	4.45	115.31	108.54
9	H	606	CHL	C3D-C4D-CHA	4.45	115.31	108.54
10	H	604	CLA	C1-C2-C3	4.44	133.48	126.20
10	H	602	CLA	C1-C2-C3	4.44	133.47	126.20
9	A	607	CHL	CMB-C2B-C3B	4.44	133.55	124.68
10	E	602	CLA	O2D-CGD-CBD	4.43	118.97	111.23
9	A	607	CHL	C3D-C4D-CHA	4.42	115.26	108.54
9	C	606	CHL	CMB-C2B-C3B	4.42	133.52	124.68
9	J	605	CHL	O2A-CGA-CBA	4.42	125.31	111.83
10	D	604	CLA	O2D-CGD-CBD	4.42	118.95	111.23
9	J	608	CHL	C3D-C4D-CHA	4.41	115.25	108.54
9	I	606	CHL	C3D-C4D-CHA	4.41	115.25	108.54
9	J	609	CHL	C3D-C4D-CHA	4.41	115.25	108.54
9	D	605	CHL	C3D-C4D-CHA	4.41	115.24	108.54
9	G	606	CHL	C3D-C4D-CHA	4.41	115.24	108.54
10	A	603	CLA	CBA-CAA-C2A	4.41	126.90	113.79
9	C	609	CHL	C3D-C4D-CHA	4.41	115.24	108.54
9	G	608	CHL	C3D-C4D-CHA	4.41	115.24	108.54
9	G	607	CHL	O2A-CGA-CBA	4.39	125.23	111.83
10	I	603	CLA	O2D-CGD-CBD	4.39	118.91	111.23
9	A	609	CHL	C3D-C4D-CHA	4.38	115.19	108.54
10	J	602	CLA	C4-C3-C5	4.37	122.82	115.23
9	D	609	CHL	C3D-C4D-CHA	4.37	115.18	108.54
10	I	613	CLA	CED-O2D-CGD	4.37	125.82	115.92
9	C	607	CHL	C3D-C4D-CHA	4.36	115.17	108.54
4	F	5621	LUT	C38-C25-C24	-4.35	113.06	123.36
10	I	613	CLA	CBA-CAA-C2A	4.35	126.74	113.79
9	I	607	CHL	C3D-C4D-CHA	4.35	115.15	108.54
10	G	612	CLA	O1D-CGD-CBD	-4.35	115.94	124.52
9	G	606	CHL	O2A-CGA-CBA	4.34	125.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	610	CLA	CBA-CAA-C2A	4.33	126.68	113.79
10	B	602	CLA	O2D-CGD-CBD	4.33	118.80	111.23
10	J	611	CLA	CBA-CAA-C2A	4.32	126.66	113.79
9	A	605	CHL	OMC-CMC-C2C	4.32	132.63	125.12
9	B	608	CHL	CED-O2D-CGD	4.32	125.71	115.92
9	C	605	CHL	CED-O2D-CGD	4.32	125.71	115.92
9	E	606	CHL	C3D-C4D-CHA	4.32	115.10	108.54
10	F	611	CLA	C1-C2-C3	4.31	133.26	126.20
4	I	8620	LUT	C38-C25-C24	-4.30	113.18	123.36
9	E	606	CHL	C1C-C2C-CMC	-4.30	119.05	126.80
10	A	610	CLA	CBA-CAA-C2A	4.30	126.58	113.79
9	H	606	CHL	O2A-CGA-CBA	4.30	124.93	111.83
4	B	1621	LUT	C38-C25-C24	-4.29	113.20	123.36
10	E	603	CLA	O2D-CGD-CBD	4.29	118.73	111.23
7	F	5630	LHG	O8-C23-C24	4.29	124.91	111.83
10	G	603	CLA	CED-O2D-CGD	4.29	125.64	115.92
10	J	602	CLA	O2D-CGD-CBD	4.28	118.72	111.23
9	C	607	CHL	O2A-CGA-CBA	4.28	124.89	111.83
7	D	3630	LHG	O8-C6-C5	4.28	120.73	108.40
9	E	609	CHL	C1-C2-C3	4.28	133.21	126.20
10	G	602	CLA	C4-C3-C5	4.28	122.65	115.23
9	G	605	CHL	C3D-C4D-CHA	4.27	115.03	108.54
10	C	611	CLA	C1-C2-C3	4.27	133.19	126.20
10	F	611	CLA	CBA-CAA-C2A	4.27	126.48	113.79
9	I	609	CHL	C1-C2-C3	4.27	133.19	126.20
7	F	5630	LHG	O8-C6-C5	4.26	120.69	108.40
9	F	606	CHL	CAA-CBA-CGA	4.26	125.31	113.21
9	B	607	CHL	C7-C6-C5	-4.26	101.92	113.26
10	C	602	CLA	C6-C5-C3	4.26	123.84	113.47
10	D	610	CLA	O2A-CGA-CBA	4.25	124.81	111.83
10	H	603	CLA	O2D-CGD-CBD	4.24	118.65	111.23
10	A	611	CLA	O2A-CGA-CBA	4.24	124.77	111.83
7	C	2630	LHG	O8-C6-C5	4.24	120.61	108.40
10	D	610	CLA	CBA-CAA-C2A	4.24	126.40	113.79
9	E	606	CHL	CMB-C2B-C3B	4.22	133.12	124.68
5	E	2622	XAT	C24-C23-C22	4.22	118.69	110.79
9	E	606	CHL	O2A-CGA-CBA	4.22	124.71	111.83
9	D	601	CHL	CED-O2D-CGD	4.22	125.49	115.92
9	I	601	CHL	CED-O2D-CGD	4.22	125.48	115.92
10	G	613	CLA	CMB-C2B-C3B	4.22	136.47	126.55
10	I	604	CLA	CAA-CBA-CGA	4.22	125.18	113.21
10	H	611	CLA	O2A-CGA-CBA	4.21	124.68	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	612	CLA	O2D-CGD-CBD	4.21	118.59	111.23
9	C	606	CHL	CAA-CBA-CGA	4.21	125.16	113.21
10	I	602	CLA	C4-C3-C5	4.20	122.52	115.23
10	C	603	CLA	O1D-CGD-CBD	-4.20	116.24	124.52
9	I	605	CHL	O2A-CGA-CBA	4.19	124.62	111.83
10	I	613	CLA	CMB-C2B-C3B	4.18	136.38	126.55
9	G	606	CHL	CMB-C2B-C3B	4.18	133.03	124.68
10	F	613	CLA	CED-O2D-CGD	4.17	125.38	115.92
9	D	606	CHL	C1C-C2C-CMC	-4.17	119.29	126.80
10	H	604	CLA	O1D-CGD-CBD	-4.17	116.30	124.52
9	I	609	CHL	CED-O2D-CGD	4.16	125.36	115.92
9	H	607	CHL	O2A-CGA-CBA	4.16	124.52	111.83
9	E	601	CHL	CBA-CAA-C2A	4.16	126.03	113.78
7	J	9630	LHG	O8-C6-C5	4.15	120.36	108.40
4	J	9621	LUT	C18-C5-C6	4.15	129.01	124.48
10	D	603	CLA	CBA-CAA-C2A	4.15	126.13	113.79
9	G	607	CHL	CBA-CAA-C2A	4.14	125.98	113.78
9	F	607	CHL	C4-C3-C5	-4.14	108.04	115.23
10	A	603	CLA	O1D-CGD-CBD	-4.14	116.35	124.52
10	C	612	CLA	C1-C2-C3	4.13	132.97	126.20
10	A	602	CLA	CMC-C2C-C1C	4.13	131.49	125.03
10	C	604	CLA	CMB-C2B-C3B	4.13	136.26	126.55
10	D	612	CLA	C1-C2-C3	4.13	132.96	126.20
10	E	610	CLA	CBA-CAA-C2A	4.12	126.06	113.79
10	D	613	CLA	CMB-C2B-C3B	4.12	136.24	126.55
9	A	601	CHL	CED-O2D-CGD	4.12	125.26	115.92
9	I	607	CHL	O2A-CGA-CBA	4.12	124.39	111.83
4	A	620	LUT	C38-C25-C24	-4.11	113.62	123.36
4	I	8621	LUT	C38-C25-C24	-4.11	113.63	123.36
4	J	9620	LUT	C18-C5-C4	-4.11	106.86	114.42
10	E	611	CLA	C1-C2-C3	4.11	132.93	126.20
10	G	603	CLA	O2D-CGD-CBD	4.11	118.41	111.23
9	E	606	CHL	CAA-CBA-CGA	4.10	124.86	113.21
10	C	602	CLA	O2D-CGD-CBD	4.10	118.40	111.23
9	F	601	CHL	CED-O2D-CGD	4.10	125.22	115.92
10	D	610	CLA	CED-O2D-CGD	4.10	125.21	115.92
9	C	605	CHL	O2A-CGA-CBA	4.09	124.32	111.83
9	H	605	CHL	O2A-CGA-CBA	4.09	124.31	111.83
10	J	610	CLA	CBA-CAA-C2A	4.09	125.95	113.79
4	E	4621	LUT	C3-C4-C5	4.08	122.35	112.18
9	E	608	CHL	CBA-CAA-C2A	4.08	125.80	113.78
9	A	605	CHL	CED-O2D-CGD	4.08	125.17	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	612	CLA	O2A-CGA-CBA	4.08	124.27	111.83
4	G	6620	LUT	C38-C25-C24	-4.08	113.71	123.36
9	D	608	CHL	CED-O2D-CGD	4.07	125.16	115.92
9	B	606	CHL	CAA-C2A-C3A	-4.07	102.00	113.00
10	J	603	CLA	C6-C5-C3	4.07	123.38	113.47
9	B	606	CHL	C1-C2-C3	4.07	133.35	126.76
10	D	611	CLA	O2A-CGA-CBA	4.07	124.24	111.83
10	G	602	CLA	O2D-CGD-CBD	4.07	118.34	111.23
9	A	608	CHL	CBA-CAA-C2A	4.06	125.75	113.78
10	D	604	CLA	CMB-C2B-C3B	4.06	136.11	126.55
10	A	611	CLA	CAA-C2A-C3A	-4.06	102.02	113.00
9	C	601	CHL	CBA-CAA-C2A	4.06	125.73	113.78
9	A	606	CHL	C1-C2-C3	4.06	133.33	126.76
4	E	4620	LUT	C18-C5-C4	-4.05	106.97	114.42
10	B	610	CLA	O2A-CGA-CBA	4.05	124.17	111.83
10	C	611	CLA	O2A-CGA-CBA	4.04	124.16	111.83
9	B	606	CHL	C1C-C2C-CMC	-4.04	119.52	126.80
10	J	602	CLA	CMC-C2C-C1C	4.04	131.35	125.03
10	I	604	CLA	O2D-CGD-CBD	4.04	118.29	111.23
10	E	610	CLA	O2A-CGA-CBA	4.03	124.14	111.83
9	E	601	CHL	CED-O2D-CGD	4.03	125.06	115.92
10	A	610	CLA	O2A-CGA-CBA	4.03	124.12	111.83
10	H	611	CLA	CAA-C2A-C3A	-4.03	102.11	113.00
10	A	604	CLA	CMB-C2B-C3B	4.03	136.03	126.55
10	J	602	CLA	C6-C5-C3	4.03	123.28	113.47
8	D	5632	DGD	O2G-C1B-C2B	4.03	120.19	111.48
10	J	612	CLA	O2D-CGD-CBD	4.02	118.27	111.23
9	J	606	CHL	CED-O2D-CGD	4.02	125.04	115.92
10	D	612	CLA	C16-C15-C13	4.02	129.33	115.97
10	I	612	CLA	O2A-CGA-CBA	4.02	124.09	111.83
10	I	602	CLA	CED-O2D-CGD	4.02	125.03	115.92
10	C	613	CLA	CMB-C2B-C3B	4.02	136.00	126.55
10	F	611	CLA	CAA-CBA-CGA	4.01	124.60	113.21
9	A	605	CHL	O2A-CGA-CBA	4.01	124.05	111.83
9	H	606	CHL	CMB-C2B-C3B	4.00	132.68	124.68
10	F	603	CLA	O2D-CGD-CBD	4.00	118.22	111.23
9	C	608	CHL	C16-C15-C13	4.00	129.25	115.97
4	J	9620	LUT	C21-C26-C27	4.00	117.42	112.83
9	A	606	CHL	C1C-C2C-CMC	-4.00	119.60	126.80
9	F	606	CHL	C1C-C2C-CMC	-4.00	119.60	126.80
10	D	602	CLA	O2D-CGD-CBD	3.99	118.21	111.23
10	I	612	CLA	O2D-CGD-CBD	3.99	118.20	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	602	CLA	C6-C5-C3	3.99	123.18	113.47
10	D	610	CLA	C1-C2-C3	3.98	132.73	126.20
10	C	604	CLA	CED-O2D-CGD	3.98	124.95	115.92
10	H	613	CLA	CMB-C2B-C3B	3.98	135.92	126.55
4	D	3620	LUT	C38-C25-C24	-3.98	113.94	123.36
10	G	603	CLA	CAA-CBA-CGA	3.98	124.51	113.21
10	B	613	CLA	CMB-C2B-C3B	3.98	135.90	126.55
9	C	609	CHL	CED-O2D-CGD	3.97	124.92	115.92
10	J	603	CLA	CBA-CAA-C2A	3.97	125.61	113.79
9	D	605	CHL	CED-O2D-CGD	3.97	124.92	115.92
9	J	606	CHL	C1C-C2C-CMC	-3.96	119.67	126.80
10	F	610	CLA	O2A-CGA-CBA	3.96	123.90	111.83
9	G	606	CHL	CED-O2D-CGD	3.96	124.89	115.92
9	H	608	CHL	CBA-CAA-C2A	3.95	125.42	113.78
10	C	610	CLA	C14-C13-C15	3.95	125.36	111.27
9	G	609	CHL	C1-C2-C3	3.95	132.67	126.20
10	G	604	CLA	O2D-CGD-CBD	3.94	118.12	111.23
10	J	611	CLA	O2A-CGA-CBA	3.94	123.85	111.83
4	J	9621	LUT	C3-C4-C5	3.94	121.99	112.18
9	F	609	CHL	CAA-CBA-CGA	3.94	124.39	113.21
9	D	606	CHL	CAA-CBA-CGA	3.94	124.39	113.21
9	D	605	CHL	O2A-CGA-CBA	3.94	123.83	111.83
9	E	608	CHL	O2A-CGA-CBA	3.93	123.83	111.83
10	B	613	CLA	CBA-CAA-C2A	3.93	125.48	113.79
9	G	608	CHL	CED-O2D-CGD	3.93	124.82	115.92
9	H	608	CHL	C6-C5-C3	3.93	123.03	113.47
9	J	609	CHL	O2D-CGD-CBD	3.93	115.26	110.95
10	H	610	CLA	CED-O2D-CGD	3.93	124.82	115.92
10	D	612	CLA	O1D-CGD-CBD	-3.93	116.78	124.52
10	B	604	CLA	C1-C2-C3	3.92	132.63	126.20
4	H	7620	LUT	C18-C5-C4	-3.92	107.22	114.42
10	F	604	CLA	O2D-CGD-CBD	3.91	118.07	111.23
9	A	606	CHL	O2D-CGD-CBD	3.91	115.24	110.95
10	I	610	CLA	CBA-CAA-C2A	3.91	125.43	113.79
10	F	604	CLA	CMB-C2B-C3B	3.91	135.74	126.55
7	B	1630	LHG	O8-C6-C5	3.90	119.65	108.40
4	G	6620	LUT	C18-C5-C4	-3.90	107.25	114.42
9	I	606	CHL	C1C-C2C-CMC	-3.90	119.77	126.80
7	E	4630	LHG	O8-C6-C5	3.90	119.64	108.40
9	D	607	CHL	CMB-C2B-C3B	3.90	132.47	124.68
10	F	602	CLA	C5-C3-C2	-3.90	112.42	121.17
10	H	602	CLA	O2D-CGD-CBD	3.89	118.04	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	609	CHL	CED-O2D-CGD	3.89	124.75	115.92
4	F	5620	LUT	C38-C25-C24	-3.89	114.15	123.36
10	E	602	CLA	O1D-CGD-CBD	-3.89	116.85	124.52
10	J	613	CLA	C4-C3-C5	-3.89	108.48	115.23
9	F	606	CHL	CMB-C2B-C3B	3.89	132.45	124.68
9	A	606	CHL	CAA-CBA-CGA	3.88	124.24	113.21
10	H	611	CLA	CED-O2D-CGD	3.88	124.72	115.92
10	I	612	CLA	O1D-CGD-CBD	-3.88	116.86	124.52
4	H	7621	LUT	C38-C25-C24	-3.88	114.18	123.36
10	F	610	CLA	CBA-CAA-C2A	3.88	125.33	113.79
9	C	607	CHL	CMB-C2B-C3B	3.88	132.43	124.68
9	J	608	CHL	CED-O2D-CGD	3.87	124.70	115.92
9	A	608	CHL	O2D-CGD-CBD	3.87	115.20	110.95
9	B	607	CHL	CMB-C2B-C3B	3.87	132.42	124.68
9	J	606	CHL	CMB-C2B-C3B	3.87	132.41	124.68
7	F	5630	LHG	O7-C7-C8	3.87	119.85	111.48
10	A	604	CLA	C1-C2-C3	3.87	132.53	126.20
10	E	612	CLA	C1-C2-C3	3.87	132.53	126.20
10	J	603	CLA	O1D-CGD-CBD	-3.86	116.90	124.52
10	I	602	CLA	C6-C5-C3	3.86	122.87	113.47
9	I	609	CHL	CAA-CBA-CGA	3.86	124.17	113.21
10	D	602	CLA	C6-C5-C3	3.86	122.87	113.47
9	I	609	CHL	CAA-C2A-C3A	-3.86	102.57	113.00
9	H	606	CHL	C1C-C2C-CMC	-3.85	119.86	126.80
10	H	612	CLA	O2A-CGA-CBA	3.85	123.58	111.83
9	J	608	CHL	O2A-CGA-CBA	3.85	123.58	111.83
10	I	604	CLA	CAA-C2A-C3A	-3.84	102.61	113.00
10	E	604	CLA	CMB-C2B-C3B	3.84	135.59	126.55
10	A	613	CLA	CED-O2D-CGD	3.84	124.62	115.92
10	G	602	CLA	CMC-C2C-C1C	3.83	131.02	125.03
4	J	9621	LUT	C38-C25-C24	-3.83	114.29	123.36
10	A	612	CLA	O2D-CGD-CBD	3.83	117.93	111.23
10	A	603	CLA	C6-C5-C3	3.83	122.80	113.47
9	I	607	CHL	C4-C3-C5	-3.83	108.59	115.23
9	A	609	CHL	C1-C2-C3	3.83	132.47	126.20
10	C	604	CLA	O2D-CGD-CBD	3.83	117.92	111.23
10	B	603	CLA	O1D-CGD-CBD	-3.82	116.98	124.52
9	I	608	CHL	CBA-CAA-C2A	3.82	125.03	113.78
9	B	601	CHL	C11-C12-C13	3.82	128.66	115.97
10	A	602	CLA	C1-C2-C3	3.82	132.45	126.20
9	I	606	CHL	O2A-CGA-CBA	3.81	123.46	111.83
10	G	613	CLA	CBA-CAA-C2A	3.81	125.13	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	3630	LHG	O8-C23-C24	3.81	123.45	111.83
4	B	1620	LUT	C38-C25-C24	-3.81	114.35	123.36
10	E	612	CLA	O2D-CGD-CBD	3.81	117.88	111.23
10	B	602	CLA	O1D-CGD-CBD	-3.81	117.01	124.52
9	A	607	CHL	CBA-CAA-C2A	3.80	124.98	113.78
10	A	604	CLA	O2D-CGD-CBD	3.80	117.88	111.23
9	A	608	CHL	C1-C2-C3	3.80	132.43	126.20
10	F	612	CLA	O2D-CGD-CBD	3.80	117.87	111.23
10	B	611	CLA	CED-O2D-CGD	3.79	124.52	115.92
4	D	3620	LUT	C18-C5-C4	-3.79	107.45	114.42
10	G	610	CLA	CED-O2D-CGD	3.79	124.52	115.92
10	G	610	CLA	O2A-CGA-CBA	3.79	123.39	111.83
9	J	606	CHL	C1-C2-C3	3.79	132.89	126.76
9	B	601	CHL	CED-O2D-CGD	3.79	124.51	115.92
9	G	607	CHL	C1C-C2C-CMC	-3.79	119.98	126.80
10	D	603	CLA	CED-O2D-CGD	3.78	124.50	115.92
10	B	604	CLA	CMB-C2B-C3B	3.78	135.45	126.55
9	A	607	CHL	O2A-CGA-CBA	3.78	123.37	111.83
10	F	613	CLA	CMB-C2B-C3B	3.78	135.44	126.55
7	I	8630	LHG	O8-C6-C5	3.78	119.29	108.40
9	B	605	CHL	O2D-CGD-CBD	3.78	115.10	110.95
10	E	611	CLA	CAA-C2A-C3A	-3.78	102.79	113.00
10	A	610	CLA	CED-O2D-CGD	3.77	124.48	115.92
9	F	605	CHL	O2A-CGA-CBA	3.77	123.34	111.83
9	A	606	CHL	CMB-C2B-C3B	3.77	132.22	124.68
4	A	621	LUT	C3-C4-C5	3.77	121.56	112.18
10	D	603	CLA	O2D-CGD-CBD	3.77	117.82	111.23
10	E	613	CLA	C4-C3-C5	-3.77	108.69	115.23
10	J	602	CLA	O2A-CGA-CBA	3.77	123.32	111.83
10	G	602	CLA	CBA-CAA-C2A	3.76	124.98	113.79
4	E	4620	LUT	C38-C25-C24	-3.76	114.47	123.36
4	A	620	LUT	C18-C5-C4	-3.76	107.51	114.42
7	I	8630	LHG	O10-C23-C24	-3.76	109.09	123.78
10	F	604	CLA	CAA-C2A-C3A	-3.75	102.86	113.00
9	E	606	CHL	O2D-CGD-CBD	3.75	115.07	110.95
10	J	602	CLA	C5-C3-C2	-3.75	112.76	121.17
9	F	608	CHL	C1-C2-C3	3.74	132.33	126.20
4	C	2620	LUT	C38-C25-C24	-3.74	114.50	123.36
9	C	605	CHL	O2D-CGD-CBD	3.74	115.06	110.95
4	A	621	LUT	C38-C25-C24	-3.73	114.52	123.36
9	F	605	CHL	O2D-CGD-CBD	3.73	115.05	110.95
10	A	602	CLA	O2D-CGD-CBD	3.73	117.75	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	602	CLA	C4-C3-C5	3.72	121.69	115.23
10	C	604	CLA	O1A-CGA-CBA	-3.72	109.22	123.78
9	C	606	CHL	C1C-C2C-CMC	-3.72	120.09	126.80
10	B	604	CLA	CAA-CBA-CGA	3.72	123.77	113.21
9	B	605	CHL	O2A-CGA-CBA	3.72	123.18	111.83
10	H	613	CLA	C4-C3-C5	-3.72	108.78	115.23
9	B	608	CHL	O2A-CGA-CBA	3.71	123.16	111.83
9	C	607	CHL	OBD-CAD-CBD	-3.71	120.38	125.82
10	G	604	CLA	CMB-C2B-C3B	3.71	135.27	126.55
9	C	609	CHL	CAA-CBA-CGA	3.70	123.72	113.21
10	I	611	CLA	C1-C2-C3	3.70	132.26	126.20
10	I	603	CLA	CBA-CAA-C2A	3.70	124.81	113.79
10	I	602	CLA	C5-C3-C2	-3.70	112.86	121.17
9	H	601	CHL	C1C-C2C-CMC	-3.70	120.14	126.80
10	C	610	CLA	O2A-CGA-CBA	3.70	123.11	111.83
9	B	606	CHL	O2D-CGD-CBD	3.70	115.01	110.95
9	C	607	CHL	CBA-CAA-C2A	3.69	124.66	113.78
4	F	5621	LUT	C3-C4-C5	3.69	121.36	112.18
10	H	612	CLA	O2D-CGD-CBD	3.69	117.68	111.23
10	I	610	CLA	O2A-CGA-CBA	3.69	123.08	111.83
10	C	612	CLA	O1D-CGD-CBD	-3.68	117.25	124.52
10	D	604	CLA	O1A-CGA-CBA	-3.68	109.39	123.78
10	B	604	CLA	O1A-CGA-CBA	-3.68	109.40	123.78
9	B	608	CHL	CBA-CAA-C2A	3.67	124.60	113.78
9	H	608	CHL	CED-O2D-CGD	3.67	124.25	115.92
10	G	611	CLA	O2A-CGA-CBA	3.67	123.03	111.83
10	B	610	CLA	CED-O2D-CGD	3.67	124.24	115.92
9	D	608	CHL	C16-C15-C13	3.67	128.15	115.97
10	A	602	CLA	CED-O2D-CGD	3.66	124.23	115.92
4	G	6621	LUT	C3-C4-C5	3.66	121.30	112.18
10	I	604	CLA	CMB-C2B-C3B	3.66	135.17	126.55
9	B	608	CHL	C6-C5-C3	3.66	122.39	113.47
9	B	607	CHL	O2A-CGA-CBA	3.66	122.99	111.83
10	J	604	CLA	CED-O2D-CGD	3.66	124.21	115.92
10	E	613	CLA	CMB-C2B-C1B	-3.65	119.86	125.42
9	J	607	CHL	C1C-C2C-CMC	-3.65	120.22	126.80
10	F	612	CLA	CED-O2D-CGD	3.65	124.20	115.92
9	F	609	CHL	O2D-CGD-CBD	3.65	114.96	110.95
10	G	603	CLA	O2A-CGA-CBA	3.65	122.96	111.83
4	C	2621	LUT	C3-C4-C5	3.65	121.26	112.18
10	J	602	CLA	C12-C11-C10	-3.65	96.94	113.28
10	D	602	CLA	CBA-CAA-C2A	3.64	124.63	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	610	CLA	CBA-CAA-C2A	3.64	124.62	113.79
10	D	604	CLA	O1D-CGD-CBD	-3.64	117.34	124.52
8	G	9632	DGD	O2G-C1B-C2B	3.63	119.34	111.48
9	C	605	CHL	C1C-C2C-CMC	-3.63	120.25	126.80
9	H	606	CHL	CED-O2D-CGD	3.63	124.15	115.92
10	G	602	CLA	C5-C3-C2	-3.63	113.02	121.17
10	J	610	CLA	CED-O2D-CGD	3.63	124.14	115.92
9	D	606	CHL	O2D-CGD-CBD	3.62	114.92	110.95
10	B	611	CLA	CAA-C2A-C1A	3.62	123.84	111.97
9	J	607	CHL	O2A-CGA-CBA	3.62	122.87	111.83
9	E	605	CHL	O2A-CGA-CBA	3.62	122.87	111.83
10	H	612	CLA	C4-C3-C5	-3.62	108.95	115.23
9	A	606	CHL	CED-O2D-CGD	3.62	124.12	115.92
9	D	606	CHL	OBD-CAD-CBD	-3.62	120.52	125.82
10	B	610	CLA	C14-C13-C15	3.61	124.16	111.27
10	G	602	CLA	C6-C5-C3	3.61	122.27	113.47
8	B	1632	DGD	O2G-C1B-C2B	3.61	119.29	111.48
9	E	609	CHL	CED-O2D-CGD	3.61	124.10	115.92
10	J	604	CLA	O2D-CGD-CBD	3.61	117.53	111.23
10	C	603	CLA	CED-O2D-CGD	3.60	124.09	115.92
10	G	612	CLA	O2A-CGA-CBA	3.60	122.82	111.83
10	B	612	CLA	O2A-CGA-CBA	3.60	122.81	111.83
4	I	8621	LUT	C18-C5-C6	3.60	128.41	124.48
10	J	613	CLA	CBA-CAA-C2A	3.59	124.47	113.79
10	J	604	CLA	CMB-C2B-C3B	3.58	134.97	126.55
10	G	610	CLA	C14-C13-C15	3.58	124.02	111.27
10	J	602	CLA	O1D-CGD-CBD	-3.57	117.47	124.52
10	G	603	CLA	CBA-CAA-C2A	3.57	124.43	113.79
9	F	606	CHL	O2D-CGD-CBD	3.57	114.87	110.95
9	C	609	CHL	CMB-C2B-C3B	3.57	131.82	124.68
10	B	614	CLA	CAA-CBA-CGA	3.57	123.34	113.21
10	C	602	CLA	C14-C13-C15	3.57	123.99	111.27
10	H	602	CLA	C5-C3-C2	-3.57	113.16	121.17
10	J	602	CLA	CBA-CAA-C2A	3.57	124.41	113.79
9	A	608	CHL	C1C-C2C-CMC	-3.56	120.38	126.80
10	I	602	CLA	C14-C13-C15	3.56	123.97	111.27
10	G	611	CLA	CED-O2D-CGD	3.56	124.00	115.92
10	H	602	CLA	C14-C13-C15	3.56	123.97	111.27
9	A	605	CHL	O2D-CGD-CBD	3.56	114.86	110.95
9	B	608	CHL	C1C-C2C-CMC	-3.56	120.39	126.80
10	H	603	CLA	CED-O2D-CGD	3.56	123.99	115.92
8	B	2632	DGD	O2G-C1B-C2B	3.56	119.18	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	603	CLA	C1-C2-C3	3.56	132.02	126.20
9	G	609	CHL	C1C-C2C-CMC	-3.56	120.39	126.80
10	E	604	CLA	CED-O2D-CGD	3.55	123.98	115.92
10	J	604	CLA	CBA-CAA-C2A	3.55	124.36	113.79
10	E	612	CLA	C16-C15-C13	3.54	127.75	115.97
9	B	609	CHL	CED-O2D-CGD	3.54	123.95	115.92
10	C	602	CLA	C4-C3-C5	3.54	121.37	115.23
10	H	602	CLA	C6-C7-C8	-3.54	104.20	115.97
4	A	621	LUT	C18-C5-C6	3.53	128.34	124.48
10	C	612	CLA	O2A-CGA-CBA	3.53	122.61	111.83
9	G	605	CHL	O2A-CGA-CBA	3.53	122.61	111.83
10	I	613	CLA	C4-C3-C5	-3.53	109.10	115.23
10	D	610	CLA	C14-C13-C15	3.53	123.86	111.27
10	F	602	CLA	O2D-CGD-CBD	3.53	117.39	111.23
9	G	606	CHL	C1C-C2C-CMC	-3.53	120.45	126.80
10	F	612	CLA	C16-C15-C13	3.52	127.68	115.97
9	D	605	CHL	OBD-CAD-CBD	-3.52	120.66	125.82
9	C	608	CHL	OBD-CAD-CBD	-3.52	120.66	125.82
10	B	602	CLA	C5-C3-C2	-3.52	113.26	121.17
10	F	604	CLA	CAA-CBA-CGA	3.52	123.20	113.21
4	H	7621	LUT	C18-C5-C4	-3.52	107.95	114.42
9	B	606	CHL	OBD-CAD-CBD	-3.52	120.66	125.82
10	F	602	CLA	CBA-CAA-C2A	3.52	124.26	113.79
10	A	611	CLA	CAA-C2A-C1A	3.52	123.50	111.97
10	H	603	CLA	O1D-CGD-CBD	-3.51	117.59	124.52
9	A	607	CHL	C12-C11-C10	-3.51	97.54	113.28
10	F	613	CLA	CBA-CAA-C2A	3.51	124.24	113.79
10	C	610	CLA	CMC-C2C-C1C	3.51	130.52	125.03
10	I	604	CLA	O1D-CGD-CBD	-3.51	117.60	124.52
4	B	1620	LUT	C18-C5-C4	-3.51	107.97	114.42
9	A	608	CHL	C16-C15-C13	3.51	127.62	115.97
9	D	607	CHL	O2A-CGA-CBA	3.50	122.52	111.83
9	B	609	CHL	C14-C13-C15	3.50	123.76	111.27
10	E	602	CLA	CBA-CAA-C2A	3.50	124.21	113.79
9	J	608	CHL	C1C-C2C-CMC	-3.50	120.49	126.80
10	J	611	CLA	CAA-C2A-C1A	3.50	123.44	111.97
9	F	608	CHL	C6-C5-C3	3.50	121.98	113.47
9	A	605	CHL	C1C-C2C-CMC	-3.50	120.50	126.80
4	D	3621	LUT	C3-C4-C5	3.49	120.86	112.18
9	G	605	CHL	OBD-CAD-CBD	-3.48	120.71	125.82
10	C	602	CLA	O1D-CGD-CBD	-3.48	117.65	124.52
9	G	608	CHL	C1C-C2C-CMC	-3.48	120.53	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	612	CLA	O2A-CGA-CBA	3.48	122.45	111.83
9	I	607	CHL	C12-C11-C10	-3.48	97.70	113.28
10	F	604	CLA	CBA-CAA-C2A	3.47	124.13	113.79
9	D	609	CHL	C14-C13-C15	3.47	123.66	111.27
9	F	607	CHL	CBA-CAA-C2A	3.47	124.00	113.78
9	E	608	CHL	OBD-CAD-CBD	-3.47	120.73	125.82
4	E	4620	LUT	C21-C26-C27	3.47	116.81	112.83
9	H	605	CHL	C1C-C2C-CMC	-3.46	120.56	126.80
10	I	612	CLA	C1-C2-C3	3.46	131.87	126.20
10	J	614	CLA	CAA-CBA-CGA	3.46	123.04	113.21
9	J	608	CHL	OBD-CAD-CBD	-3.46	120.74	125.82
9	F	607	CHL	C4D-CHA-CBD	-3.46	105.48	108.97
9	J	601	CHL	C1C-C2C-CMC	-3.46	120.57	126.80
10	A	613	CLA	C4-C3-C5	-3.46	109.22	115.23
10	E	614	CLA	O2A-CGA-CBA	3.46	122.38	111.83
9	J	608	CHL	CBA-CAA-C2A	3.46	123.96	113.78
10	G	614	CLA	CBA-CAA-C2A	3.45	124.07	113.79
10	D	611	CLA	CAA-CBA-CGA	3.45	123.01	113.21
10	G	611	CLA	CAA-C2A-C1A	3.45	123.28	111.97
9	J	606	CHL	C4D-CHA-CBD	-3.45	105.49	108.97
9	D	601	CHL	C1C-C2C-CMC	-3.44	120.59	126.80
10	I	612	CLA	C4-C3-C5	-3.44	109.25	115.23
10	D	604	CLA	CBA-CAA-C2A	3.44	124.03	113.79
4	H	7621	LUT	C18-C5-C6	3.44	128.24	124.48
10	I	602	CLA	CBA-CAA-C2A	3.44	124.03	113.79
9	F	607	CHL	O2D-CGD-CBD	3.44	114.72	110.95
9	A	601	CHL	C1C-C2C-CMC	-3.44	120.61	126.80
10	G	603	CLA	O1D-CGD-CBD	-3.44	117.74	124.52
10	J	612	CLA	O1D-CGD-CBD	-3.44	117.74	124.52
10	A	602	CLA	C11-C10-C8	-3.43	104.55	115.97
10	J	612	CLA	C16-C15-C13	3.43	127.38	115.97
9	I	607	CHL	OBD-CAD-CBD	-3.43	120.79	125.82
9	B	607	CHL	C4D-CHA-CBD	-3.43	105.51	108.97
9	E	605	CHL	C1C-C2C-CMC	-3.43	120.62	126.80
9	E	606	CHL	OBD-CAD-CBD	-3.43	120.79	125.82
9	I	601	CHL	C1C-CHC-C4B	3.43	128.34	116.07
9	F	606	CHL	C4D-CHA-CBD	-3.43	105.51	108.97
9	E	608	CHL	C1C-C2C-CMC	-3.43	120.63	126.80
7	A	630	LHG	O10-C23-C24	-3.42	110.39	123.78
10	G	604	CLA	O1D-CGD-CBD	-3.42	117.77	124.52
10	A	612	CLA	O1D-CGD-CBD	-3.42	117.77	124.52
9	H	601	CHL	C1C-CHC-C4B	3.42	128.32	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	603	CLA	CBA-CAA-C2A	3.42	123.97	113.79
10	D	602	CLA	C4-C3-C5	3.42	121.16	115.23
9	A	606	CHL	C4D-CHA-CBD	-3.42	105.52	108.97
10	B	612	CLA	O2D-CGD-CBD	3.42	117.21	111.23
9	G	607	CHL	C1C-CHC-C4B	3.41	128.29	116.07
9	B	609	CHL	C1C-C2C-CMC	-3.41	120.65	126.80
9	H	607	CHL	CBA-CAA-C2A	3.41	123.83	113.78
9	I	605	CHL	C1C-C2C-CMC	-3.41	120.65	126.80
10	D	613	CLA	C6-C5-C3	3.41	121.78	113.47
9	F	608	CHL	OBD-CAD-CBD	-3.41	120.82	125.82
9	E	606	CHL	C1C-CHC-C4B	3.41	128.27	116.07
9	F	605	CHL	OBD-CAD-CBD	-3.41	120.82	125.82
10	E	602	CLA	O2A-CGA-CBA	3.41	122.22	111.83
10	A	602	CLA	CBA-CAA-C2A	3.41	123.93	113.79
10	F	612	CLA	O1D-CGD-CBD	-3.41	117.80	124.52
10	D	611	CLA	O2D-CGD-CBD	3.40	117.18	111.23
9	I	607	CHL	C4D-CHA-CBD	-3.40	105.54	108.97
7	A	630	LHG	O7-C7-C8	3.40	118.84	111.48
4	D	3621	LUT	C38-C25-C24	-3.40	115.31	123.36
10	H	602	CLA	O1D-CGD-CBD	-3.40	117.81	124.52
9	A	607	CHL	C4D-CHA-CBD	-3.40	105.54	108.97
10	F	604	CLA	C1-C2-C3	3.40	131.76	126.20
9	J	608	CHL	C16-C15-C13	3.39	127.25	115.97
10	J	603	CLA	C4-C3-C5	-3.39	109.34	115.23
10	D	602	CLA	CED-O2D-CGD	3.39	123.61	115.92
4	I	8621	LUT	C3-C4-C5	3.39	120.62	112.18
9	C	607	CHL	C4D-CHA-CBD	-3.39	105.55	108.97
9	D	601	CHL	C1C-CHC-C4B	3.39	128.19	116.07
10	I	611	CLA	CAA-C2A-C3A	-3.39	103.85	113.00
9	F	609	CHL	C1C-C2C-CMC	-3.38	120.70	126.80
10	C	602	CLA	CBA-CAA-C2A	3.38	123.86	113.79
10	C	602	CLA	C5-C3-C2	-3.38	113.58	121.17
9	I	608	CHL	CED-O2D-CGD	3.38	123.59	115.92
10	D	611	CLA	CAA-C2A-C1A	3.38	123.06	111.97
10	E	602	CLA	CED-O2D-CGD	3.38	123.58	115.92
9	C	605	CHL	OBD-CAD-CBD	-3.38	120.87	125.82
9	E	601	CHL	C1C-CHC-C4B	3.38	128.16	116.07
9	B	607	CHL	C4-C3-C5	-3.38	109.37	115.23
9	A	608	CHL	OBD-CAD-CBD	-3.38	120.87	125.82
10	C	612	CLA	CED-O2D-CGD	3.38	123.58	115.92
9	D	609	CHL	C1C-C2C-CMC	-3.38	120.72	126.80
9	B	601	CHL	C1C-C2C-CMC	-3.37	120.72	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	601	CHL	C1C-C2C-CMC	-3.37	120.72	126.80
9	B	601	CHL	C1C-CHC-C4B	3.37	128.14	116.07
10	E	612	CLA	CED-O2D-CGD	3.37	123.56	115.92
10	F	602	CLA	C12-C11-C10	-3.37	98.17	113.28
10	D	602	CLA	O1D-CGD-CBD	-3.37	117.87	124.52
9	G	607	CHL	C4D-CHA-CBD	-3.37	105.57	108.97
9	J	607	CHL	C1C-CHC-C4B	3.37	128.13	116.07
10	H	602	CLA	CBA-CAA-C2A	3.37	123.81	113.79
9	B	606	CHL	C1C-CHC-C4B	3.36	128.10	116.07
9	G	608	CHL	O2A-CGA-CBA	3.36	122.09	111.83
9	D	606	CHL	C1C-CHC-C4B	3.36	128.10	116.07
4	G	6621	LUT	C38-C25-C24	-3.36	115.41	123.36
9	I	605	CHL	C1C-CHC-C4B	3.36	128.09	116.07
9	J	601	CHL	C1C-CHC-C4B	3.36	128.09	116.07
10	D	604	CLA	CED-O2D-CGD	3.36	123.53	115.92
10	I	603	CLA	C6-C5-C3	3.36	121.64	113.47
10	E	603	CLA	O1D-CGD-CBD	-3.35	117.90	124.52
10	H	602	CLA	C12-C11-C10	-3.35	98.25	113.28
9	D	607	CHL	C4D-CHA-CBD	-3.35	105.59	108.97
9	H	606	CHL	C4D-CHA-CBD	-3.35	105.59	108.97
9	A	601	CHL	C1C-CHC-C4B	3.35	128.06	116.07
9	F	606	CHL	C5-C3-C4	-3.35	106.87	114.59
9	A	607	CHL	OBD-CAD-CBD	-3.35	120.91	125.82
10	C	602	CLA	CMC-C2C-C1C	3.35	130.27	125.03
9	C	608	CHL	C1C-C2C-CMC	-3.35	120.76	126.80
9	C	609	CHL	C1C-C2C-CMC	-3.35	120.77	126.80
9	F	608	CHL	CED-O2D-CGD	3.35	123.51	115.92
9	A	606	CHL	C1C-CHC-C4B	3.35	128.04	116.07
10	I	611	CLA	O2A-CGA-CBA	3.35	122.03	111.83
10	H	602	CLA	C4-C3-C5	3.34	121.03	115.23
9	G	606	CHL	C4D-CHA-CBD	-3.34	105.60	108.97
10	C	604	CLA	C1-C2-C3	3.34	131.67	126.20
9	E	606	CHL	OMC-CMC-C2C	3.34	130.93	125.12
10	F	603	CLA	CAA-CBA-CGA	3.34	122.69	113.21
10	E	612	CLA	O1D-CGD-CBD	-3.34	117.94	124.52
10	E	614	CLA	CBA-CAA-C2A	3.34	123.72	113.79
2	D	3633	BNG	C1'-O1-C1	3.34	119.38	113.68
10	C	610	CLA	CED-O2D-CGD	3.34	123.48	115.92
10	C	603	CLA	C6-C5-C3	3.34	121.59	113.47
9	D	601	CHL	OBD-CAD-CBD	-3.34	120.93	125.82
9	C	601	CHL	C1C-CHC-C4B	3.33	128.00	116.07
10	H	602	CLA	CMC-C2C-C1C	3.33	130.24	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	603	CLA	O1D-CGD-CBD	-3.33	117.95	124.52
9	H	607	CHL	C7-C6-C5	-3.33	104.38	113.26
4	I	8620	LUT	C18-C5-C4	-3.33	108.30	114.42
9	H	607	CHL	OBD-CAD-CBD	-3.33	120.94	125.82
9	H	607	CHL	C4D-CHA-CBD	-3.33	105.61	108.97
9	J	607	CHL	CBA-CAA-C2A	3.33	123.58	113.78
7	G	6630	LHG	O10-C23-C24	-3.33	110.76	123.78
10	J	603	CLA	CED-O2D-CGD	3.33	123.46	115.92
9	D	608	CHL	C1C-C2C-CMC	-3.33	120.81	126.80
10	H	612	CLA	O1D-CGD-CBD	-3.33	117.96	124.52
10	F	602	CLA	CMC-C2C-C1C	3.32	130.23	125.03
9	E	601	CHL	C1C-C2C-CMC	-3.32	120.81	126.80
10	A	611	CLA	CED-O2D-CGD	3.32	123.45	115.92
9	J	609	CHL	C1C-C2C-CMC	-3.32	120.81	126.80
9	A	605	CHL	OBD-CAD-CBD	-3.32	120.95	125.82
9	F	601	CHL	OBD-CAD-CBD	-3.32	120.95	125.82
9	F	607	CHL	C1C-C2C-CMC	-3.32	120.82	126.80
10	F	602	CLA	C11-C10-C8	-3.32	104.93	115.97
4	A	621	LUT	C18-C5-C4	-3.32	108.32	114.42
9	E	606	CHL	C4D-CHA-CBD	-3.32	105.62	108.97
9	D	607	CHL	C7-C6-C5	-3.32	104.42	113.26
10	I	614	CLA	O2A-CGA-CBA	3.32	121.95	111.83
9	E	608	CHL	C1C-CHC-C4B	3.31	127.93	116.07
9	I	607	CHL	C1C-C2C-CMC	-3.31	120.83	126.80
10	F	613	CLA	C4-C3-C5	-3.31	109.48	115.23
9	J	601	CHL	C4D-CHA-CBD	-3.31	105.63	108.97
10	D	614	CLA	O2A-CGA-CBA	3.31	121.93	111.83
9	D	609	CHL	C7-C6-C5	-3.31	104.44	113.26
10	B	602	CLA	C14-C13-C15	3.31	123.07	111.27
9	B	608	CHL	C1C-CHC-C4B	3.31	127.91	116.07
9	I	605	CHL	OBD-CAD-CBD	-3.31	120.97	125.82
10	G	602	CLA	O1D-CGD-CBD	-3.31	118.00	124.52
9	C	605	CHL	C1C-CHC-C4B	3.31	127.90	116.07
4	F	5621	LUT	C18-C5-C6	3.30	128.09	124.48
9	B	609	CHL	C1-C2-C3	3.30	131.61	126.20
10	B	602	CLA	C11-C10-C8	-3.30	104.98	115.97
10	F	611	CLA	O2A-CGA-CBA	3.30	121.91	111.83
10	A	614	CLA	CBA-CAA-C2A	3.30	123.62	113.79
9	D	605	CHL	C1C-C2C-CMC	-3.30	120.85	126.80
9	J	605	CHL	CED-O2D-CGD	3.30	123.40	115.92
9	J	608	CHL	C1-C2-C3	3.30	131.60	126.20
9	F	606	CHL	C1C-CHC-C4B	3.30	127.88	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1621	LUT	C3-C4-C5	3.30	120.39	112.18
9	G	609	CHL	C1C-CHC-C4B	3.30	127.87	116.07
9	A	605	CHL	C1C-CHC-C4B	3.30	127.87	116.07
9	F	607	CHL	CMB-C2B-C3B	3.30	131.27	124.68
4	H	7621	LUT	C1-C2-C3	3.30	120.82	113.59
9	I	601	CHL	C4D-CHA-CBD	-3.29	105.65	108.97
10	J	602	CLA	C11-C10-C8	-3.29	105.02	115.97
9	B	607	CHL	C1C-CHC-C4B	3.29	127.84	116.07
9	H	605	CHL	C1C-CHC-C4B	3.29	127.84	116.07
9	G	601	CHL	C1C-CHC-C4B	3.29	127.84	116.07
10	A	602	CLA	C7-C6-C5	3.29	122.03	113.26
9	H	607	CHL	C1C-CHC-C4B	3.29	127.84	116.07
9	A	609	CHL	C1C-CHC-C4B	3.29	127.83	116.07
9	I	608	CHL	C1C-C2C-CMC	-3.29	120.88	126.80
10	B	602	CLA	CBA-CAA-C2A	3.28	123.56	113.79
9	E	607	CHL	O2A-CGA-CBA	3.28	121.84	111.83
9	G	608	CHL	O2D-CGD-CBD	3.28	114.55	110.95
9	H	606	CHL	C1C-CHC-C4B	3.28	127.81	116.07
9	F	607	CHL	C1C-CHC-C4B	3.28	127.81	116.07
9	C	608	CHL	C1C-CHC-C4B	3.28	127.80	116.07
9	G	609	CHL	CED-O2D-CGD	3.28	123.35	115.92
8	I	8632	DGD	O2G-C1B-C2B	3.28	118.57	111.48
9	D	608	CHL	C1C-CHC-C4B	3.28	127.79	116.07
10	H	612	CLA	C16-C15-C13	3.28	126.86	115.97
9	C	607	CHL	C1C-CHC-C4B	3.28	127.79	116.07
9	H	609	CHL	C1C-CHC-C4B	3.28	127.79	116.07
9	D	607	CHL	C1C-C2C-CMC	-3.28	120.90	126.80
9	H	609	CHL	C1C-C2C-CMC	-3.28	120.90	126.80
9	G	606	CHL	OBD-CAD-CBD	-3.27	121.02	125.82
10	H	602	CLA	C6-C5-C3	3.27	121.44	113.47
9	H	601	CHL	C1-C2-C3	3.27	131.56	126.20
9	F	605	CHL	C1C-CHC-C4B	3.27	127.78	116.07
9	E	607	CHL	C4D-CHA-CBD	-3.27	105.67	108.97
9	I	606	CHL	C1C-CHC-C4B	3.27	127.78	116.07
9	E	607	CHL	C1C-C2C-CMC	-3.27	120.91	126.80
10	A	602	CLA	O1D-CGD-CBD	-3.27	118.07	124.52
10	C	602	CLA	O2A-CGA-CBA	3.27	121.79	111.83
9	A	608	CHL	C1C-CHC-C4B	3.26	127.75	116.07
7	D	3630	LHG	O7-C7-C8	3.26	118.54	111.48
9	B	608	CHL	OBD-CAD-CBD	-3.26	121.04	125.82
9	B	607	CHL	C14-C13-C12	3.26	122.90	111.27
10	J	613	CLA	CMB-C2B-C1B	-3.26	120.46	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	605	CHL	OBD-CAD-CBD	-3.26	121.04	125.82
9	C	606	CHL	C4D-CHA-CBD	-3.26	105.68	108.97
9	F	608	CHL	C1C-CHC-C4B	3.26	127.72	116.07
9	E	609	CHL	C1C-C2C-CMC	-3.26	120.93	126.80
9	B	605	CHL	C1C-CHC-C4B	3.26	127.72	116.07
4	C	2621	LUT	C1-C2-C3	3.26	120.73	113.59
7	B	1630	LHG	O10-C23-C24	-3.25	111.05	123.78
9	E	605	CHL	C1C-CHC-C4B	3.25	127.71	116.07
9	D	607	CHL	C1C-CHC-C4B	3.25	127.71	116.07
9	D	608	CHL	OBD-CAD-CBD	-3.25	121.05	125.82
9	C	609	CHL	C1C-CHC-C4B	3.25	127.70	116.07
9	F	601	CHL	C1C-CHC-C4B	3.25	127.70	116.07
9	B	606	CHL	C4D-CHA-CBD	-3.25	105.69	108.97
9	H	609	CHL	CAA-C2A-C3A	-3.25	104.22	113.00
9	H	601	CHL	C12-C11-C10	-3.25	98.73	113.28
9	D	605	CHL	C1C-CHC-C4B	3.25	127.69	116.07
9	J	605	CHL	C1C-CHC-C4B	3.25	127.68	116.07
9	J	606	CHL	C1C-CHC-C4B	3.25	127.68	116.07
9	I	606	CHL	OBD-CAD-CBD	-3.25	121.06	125.82
9	C	606	CHL	C1C-CHC-C4B	3.24	127.68	116.07
9	G	607	CHL	O2D-CGD-CBD	3.24	114.51	110.95
9	J	605	CHL	C1C-C2C-CMC	-3.24	120.95	126.80
9	G	601	CHL	C1C-C2C-CMC	-3.24	120.96	126.80
9	I	607	CHL	C1C-CHC-C4B	3.24	127.67	116.07
9	E	607	CHL	CBA-CAA-C2A	3.24	123.32	113.78
10	C	602	CLA	CED-O2D-CGD	3.24	123.27	115.92
10	E	603	CLA	C6-C5-C3	3.24	121.36	113.47
10	E	611	CLA	CAA-C2A-C1A	3.24	122.58	111.97
9	E	605	CHL	OBD-CAD-CBD	-3.24	121.07	125.82
9	D	607	CHL	OBD-CAD-CBD	-3.24	121.08	125.82
9	E	607	CHL	OBD-CAD-CBD	-3.24	121.08	125.82
9	F	609	CHL	CMB-C2B-C3B	3.23	131.14	124.68
9	B	607	CHL	CBA-CAA-C2A	3.23	123.30	113.78
10	B	604	CLA	C4-C3-C5	-3.23	109.62	115.23
9	D	609	CHL	CMB-C2B-C3B	3.23	131.14	124.68
9	J	607	CHL	C12-C11-C10	-3.23	98.80	113.28
9	D	606	CHL	C4D-CHA-CBD	-3.23	105.71	108.97
9	B	607	CHL	C1C-C2C-CMC	-3.23	120.98	126.80
7	C	2630	LHG	O10-C23-C24	-3.23	111.16	123.78
10	G	613	CLA	O2A-CGA-CBA	3.22	121.67	111.83
9	G	608	CHL	C1C-CHC-C4B	3.22	127.61	116.07
9	J	609	CHL	C1-C2-C3	3.22	131.48	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	605	CHL	C4D-CHA-CBD	-3.22	105.72	108.97
8	E	4632	DGD	O2G-C1B-C2B	3.22	118.45	111.48
10	A	612	CLA	C16-C15-C13	3.22	126.67	115.97
10	E	611	CLA	CAA-CBA-CGA	3.22	122.35	113.21
9	F	606	CHL	CBA-CAA-C2A	-3.22	104.30	113.78
9	H	605	CHL	C4D-CHA-CBD	-3.22	105.72	108.97
10	D	602	CLA	O2A-CGA-CBA	3.22	121.64	111.83
9	A	609	CHL	C1C-C2C-CMC	-3.22	121.00	126.80
5	E	2622	XAT	O24-C25-C24	3.22	116.50	113.49
9	I	606	CHL	C4D-CHA-CBD	-3.21	105.73	108.97
10	D	602	CLA	CMC-C2C-C1C	3.21	130.05	125.03
9	G	608	CHL	OBD-CAD-CBD	-3.21	121.11	125.82
10	H	604	CLA	CMB-C2B-C3B	3.21	134.10	126.55
10	H	611	CLA	CAA-C2A-C1A	3.21	122.48	111.97
10	C	614	CLA	CBA-CAA-C2A	3.21	123.33	113.79
10	A	611	CLA	CAA-CBA-CGA	3.21	122.31	113.21
9	G	606	CHL	C1C-CHC-C4B	3.20	127.54	116.07
7	I	8630	LHG	C27-C26-C25	3.20	130.55	114.37
9	I	605	CHL	C4D-CHA-CBD	-3.20	105.74	108.97
9	D	607	CHL	C6-C5-C3	3.20	121.26	113.47
9	D	609	CHL	C1C-CHC-C4B	3.20	127.52	116.07
9	H	609	CHL	C4C-CHD-C1D	3.20	127.52	116.07
9	I	608	CHL	O2D-CGD-CBD	3.20	114.46	110.95
9	I	608	CHL	C4D-CHA-CBD	-3.20	105.74	108.97
9	D	606	CHL	CED-O2D-CGD	3.20	123.17	115.92
9	A	607	CHL	C1C-CHC-C4B	3.20	127.51	116.07
9	B	609	CHL	C1C-CHC-C4B	3.20	127.51	116.07
10	I	602	CLA	C11-C10-C8	-3.20	105.33	115.97
9	A	607	CHL	C1C-C2C-CMC	-3.20	121.04	126.80
4	C	2620	LUT	C18-C5-C4	-3.20	108.54	114.42
9	I	608	CHL	C1C-CHC-C4B	3.20	127.51	116.07
10	F	614	CLA	CBA-CAA-C2A	3.20	123.31	113.79
9	G	607	CHL	OBD-CAD-CBD	-3.20	121.13	125.82
9	B	605	CHL	C1C-C2C-CMC	-3.20	121.04	126.80
9	A	601	CHL	C14-C13-C15	3.19	122.65	111.27
9	J	609	CHL	C1C-CHC-C4B	3.19	127.49	116.07
4	E	4621	LUT	C38-C25-C24	-3.19	115.81	123.36
9	G	606	CHL	CBA-CAA-C2A	3.19	123.18	113.78
9	J	608	CHL	C1C-CHC-C4B	3.19	127.48	116.07
9	A	605	CHL	C4D-CHA-CBD	-3.19	105.75	108.97
7	E	4630	LHG	C27-C26-C25	3.19	130.48	114.37
9	B	608	CHL	C1-C2-C3	3.19	131.42	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	606	CHL	CED-O2D-CGD	3.19	123.14	115.92
9	F	605	CHL	C4D-CHA-CBD	-3.18	105.76	108.97
9	E	605	CHL	C4D-CHA-CBD	-3.18	105.76	108.97
10	C	603	CLA	CAA-CBA-CGA	3.18	122.24	113.21
9	J	609	CHL	CMB-C2B-C3B	3.18	131.04	124.68
9	G	605	CHL	C1C-CHC-C4B	3.18	127.45	116.07
9	G	601	CHL	OBD-CAD-CBD	-3.18	121.16	125.82
9	E	608	CHL	C16-C15-C13	3.18	126.53	115.97
10	I	612	CLA	C16-C15-C13	3.18	126.53	115.97
2	J	9633	BNG	C1'-O1-C1	3.18	119.11	113.68
10	G	604	CLA	C6-C7-C8	3.18	126.52	115.97
9	E	601	CHL	C4-C3-C5	-3.18	109.71	115.23
4	H	7621	LUT	C3-C4-C5	3.18	120.08	112.18
9	C	606	CHL	OBD-CAD-CBD	-3.17	121.17	125.82
9	E	609	CHL	C14-C13-C15	3.17	122.58	111.27
9	B	601	CHL	OBD-CAD-CBD	-3.17	121.17	125.82
9	C	601	CHL	C1C-C2C-CMC	-3.17	121.09	126.80
9	C	601	CHL	C4D-CHA-CBD	-3.17	105.77	108.97
9	D	601	CHL	C16-C15-C13	3.17	126.49	115.97
10	H	614	CLA	CBA-CAA-C2A	3.16	123.20	113.79
9	C	608	CHL	C4D-CHA-CBD	-3.16	105.78	108.97
10	D	602	CLA	C11-C10-C8	-3.16	105.46	115.97
10	B	602	CLA	CMC-C2C-C1C	3.16	129.97	125.03
9	D	609	CHL	C1-C2-C3	3.16	131.37	126.20
9	A	606	CHL	C5-C3-C4	-3.16	107.32	114.59
9	B	607	CHL	CED-O2D-CGD	3.16	123.07	115.92
10	A	604	CLA	CBA-CAA-C2A	3.16	123.18	113.79
9	C	607	CHL	C1C-C2C-CMC	-3.15	121.12	126.80
10	C	612	CLA	C16-C15-C13	3.15	126.44	115.97
9	H	608	CHL	O2A-CGA-CBA	3.15	121.44	111.83
10	B	612	CLA	C16-C15-C13	3.15	126.43	115.97
9	B	608	CHL	C4-C3-C5	-3.15	109.76	115.23
4	F	5621	LUT	C18-C5-C4	-3.15	108.63	114.42
4	I	8620	LUT	C21-C26-C27	3.15	116.44	112.83
9	D	609	CHL	C4C-CHD-C1D	3.15	127.33	116.07
8	D	5632	DGD	C6D-O5D-C1E	3.15	120.54	113.80
9	F	601	CHL	C1C-C2C-CMC	-3.15	121.13	126.80
9	J	606	CHL	OBD-CAD-CBD	-3.15	121.21	125.82
4	D	3621	LUT	C1-C2-C3	3.15	120.49	113.59
10	F	604	CLA	O1D-CGD-CBD	-3.14	118.32	124.52
2	C	2633	BNG	C1'-O1-C1	3.14	119.05	113.68
9	B	601	CHL	C4D-CHA-CBD	-3.14	105.80	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	4630	LHG	O10-C23-C24	-3.14	111.49	123.78
9	H	609	CHL	C4D-CHA-CBD	-3.14	105.80	108.97
9	I	608	CHL	OBD-CAD-CBD	-3.14	121.21	125.82
9	J	607	CHL	C4D-CHA-CBD	-3.14	105.80	108.97
9	F	609	CHL	C1C-CHC-C4B	3.14	127.30	116.07
9	D	609	CHL	CED-O2D-CGD	3.14	123.04	115.92
9	J	609	CHL	C4C-CHD-C1D	3.14	127.30	116.07
9	E	609	CHL	CAA-CBA-CGA	3.14	122.11	113.21
9	F	609	CHL	OBD-CAD-CBD	-3.14	121.22	125.82
10	J	603	CLA	CAA-CBA-CGA	3.13	122.11	113.21
9	E	609	CHL	C4C-CHD-C1D	3.13	127.28	116.07
9	A	609	CHL	OBD-CAD-CBD	-3.13	121.23	125.82
9	G	608	CHL	CBA-CAA-C2A	3.13	123.00	113.78
9	G	605	CHL	C1C-C2C-CMC	-3.13	121.16	126.80
9	F	608	CHL	C1C-C2C-CMC	-3.13	121.16	126.80
9	F	608	CHL	O2A-CGA-CBA	3.13	121.38	111.83
10	I	602	CLA	C7-C6-C5	3.13	121.60	113.26
9	H	606	CHL	OBD-CAD-CBD	-3.13	121.23	125.82
9	E	607	CHL	C1C-CHC-C4B	3.13	127.25	116.07
9	I	607	CHL	CBA-CAA-C2A	3.12	122.98	113.78
9	F	608	CHL	C4D-CHA-CBD	-3.12	105.82	108.97
10	A	610	CLA	C14-C13-C15	3.12	122.41	111.27
9	E	609	CHL	C1C-CHC-C4B	3.12	127.24	116.07
10	H	602	CLA	CED-O2D-CGD	3.12	122.99	115.92
10	I	604	CLA	C1-C2-C3	3.12	131.31	126.20
10	A	613	CLA	C6-C5-C3	3.12	121.07	113.47
9	F	605	CHL	C1C-C2C-CMC	-3.12	121.18	126.80
9	F	609	CHL	C4C-CHD-C1D	3.12	127.23	116.07
9	J	607	CHL	C4-C3-C5	-3.12	109.82	115.23
9	F	608	CHL	C4C-CHD-C1D	3.12	127.22	116.07
9	D	608	CHL	C4D-CHA-CBD	-3.11	105.83	108.97
10	D	611	CLA	CED-O2D-CGD	3.11	122.98	115.92
9	I	601	CHL	CMB-C2B-C3B	3.11	130.91	124.68
9	E	608	CHL	C4D-CHA-CBD	-3.11	105.83	108.97
9	B	609	CHL	C4C-CHD-C1D	3.11	127.21	116.07
9	G	601	CHL	C4D-CHA-CBD	-3.11	105.83	108.97
10	A	603	CLA	CAA-C2A-C3A	-3.11	104.59	113.00
9	I	609	CHL	C4C-CHD-C1D	3.11	127.20	116.07
10	I	610	CLA	CED-O2D-CGD	3.11	122.97	115.92
9	G	608	CHL	C4D-CHA-CBD	-3.11	105.83	108.97
10	J	610	CLA	C14-C13-C15	3.11	122.36	111.27
9	J	608	CHL	C4D-CHA-CBD	-3.11	105.83	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	606	CHL	C4C-CHD-C1D	3.11	127.19	116.07
9	I	609	CHL	C4D-CHA-CBD	-3.11	105.83	108.97
10	C	602	CLA	C12-C11-C10	-3.11	99.35	113.28
9	E	605	CHL	CED-O2D-CGD	3.11	122.96	115.92
10	B	612	CLA	C14-C13-C15	3.11	122.34	111.27
9	A	608	CHL	C4D-CHA-CBD	-3.10	105.84	108.97
10	F	610	CLA	CED-O2D-CGD	3.10	122.96	115.92
10	D	602	CLA	C14-C13-C15	3.10	122.34	111.27
9	I	606	CHL	C1-C2-C3	3.10	131.78	126.76
10	E	613	CLA	O2A-CGA-CBA	3.10	121.29	111.83
10	F	602	CLA	C14-C13-C15	3.10	122.33	111.27
9	H	607	CHL	C1C-C2C-CMC	-3.10	121.21	126.80
9	D	609	CHL	C4D-CHA-CBD	-3.10	105.84	108.97
10	A	604	CLA	CED-O2D-CGD	3.10	122.94	115.92
9	A	601	CHL	C4D-CHA-CBD	-3.10	105.84	108.97
10	D	603	CLA	O1D-CGD-CBD	-3.10	118.41	124.52
9	D	609	CHL	OBD-CAD-CBD	-3.10	121.28	125.82
9	I	601	CHL	C11-C12-C13	3.10	126.26	115.97
10	B	603	CLA	O2A-CGA-CBA	3.10	121.27	111.83
9	B	605	CHL	C4D-CHA-CBD	-3.09	105.85	108.97
9	D	601	CHL	C4C-CHD-C1D	3.09	127.14	116.07
9	H	608	CHL	C4-C3-C5	-3.09	109.86	115.23
9	H	608	CHL	C1C-CHC-C4B	3.09	127.14	116.07
9	C	609	CHL	C4C-CHD-C1D	3.09	127.13	116.07
10	E	604	CLA	O1A-CGA-CBA	-3.09	111.70	123.78
9	F	607	CHL	C5-C3-C2	3.09	128.10	121.17
9	H	608	CHL	C4C-CHD-C1D	3.09	127.11	116.07
2	B	1633	BNG	C1'-O1-C1	3.09	118.95	113.68
10	B	613	CLA	C6-C5-C3	3.09	120.98	113.47
7	J	9630	LHG	O10-C23-C24	-3.08	111.72	123.78
9	F	606	CHL	OBD-CAD-CBD	-3.08	121.30	125.82
9	F	607	CHL	C7-C6-C5	-3.08	105.05	113.26
10	J	604	CLA	CAA-CBA-CGA	3.08	121.96	113.21
9	B	608	CHL	C4D-CHA-CBD	-3.08	105.86	108.97
9	G	606	CHL	C4C-CHD-C1D	3.08	127.09	116.07
9	C	608	CHL	O2A-CGA-CBA	3.08	121.22	111.83
9	E	607	CHL	C4C-CHD-C1D	3.08	127.09	116.07
9	C	605	CHL	C4D-CHA-CBD	-3.08	105.86	108.97
9	D	601	CHL	C4D-CHA-CBD	-3.08	105.86	108.97
9	E	601	CHL	OBD-CAD-CBD	-3.08	121.31	125.82
9	E	609	CHL	CMB-C2B-C3B	3.08	130.83	124.68
9	G	609	CHL	C4C-CHD-C1D	3.07	127.07	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	608	CHL	O2A-CGA-CBA	3.07	121.20	111.83
9	G	601	CHL	C4C-CHD-C1D	3.07	127.06	116.07
9	C	608	CHL	CBA-CAA-C2A	3.07	122.82	113.78
4	F	5621	LUT	C1-C2-C3	3.07	120.33	113.59
9	D	609	CHL	O2D-CGD-CBD	3.07	114.32	110.95
5	E	2622	XAT	C7-C8-C9	3.07	130.29	125.53
8	H	6632	DGD	C3D-C4D-C5D	3.07	115.80	110.23
9	B	607	CHL	C12-C11-C10	-3.07	99.53	113.28
9	A	606	CHL	OBD-CAD-CBD	-3.07	121.32	125.82
9	J	609	CHL	C1A-CHA-C4D	3.07	124.10	118.98
9	C	609	CHL	OBD-CAD-CBD	-3.07	121.33	125.82
9	F	601	CHL	C4D-CHA-CBD	-3.06	105.88	108.97
9	G	609	CHL	C4D-CHA-CBD	-3.06	105.88	108.97
9	F	609	CHL	C1-C2-C3	3.06	131.22	126.20
8	A	632	DGD	O2G-C1B-C2B	3.06	118.11	111.48
10	J	604	CLA	O1D-CGD-CBD	-3.06	118.48	124.52
9	B	605	CHL	CED-O2D-CGD	3.06	122.86	115.92
9	H	601	CHL	C4D-CHA-CBD	-3.06	105.88	108.97
9	C	601	CHL	C4C-CHD-C1D	3.06	127.00	116.07
9	A	605	CHL	C4C-CHD-C1D	3.06	127.00	116.07
9	D	605	CHL	C4D-CHA-CBD	-3.05	105.89	108.97
9	J	609	CHL	CBC-CAC-C3C	-3.05	108.50	112.87
8	E	4632	DGD	C3D-C4D-C5D	3.05	115.76	110.23
2	F	5633	BNG	C1'-O1-C1	3.05	118.89	113.68
9	A	601	CHL	C4C-CHD-C1D	3.05	126.98	116.07
10	E	613	CLA	C12-C11-C10	-3.05	99.62	113.28
9	F	607	CHL	C4C-CHD-C1D	3.05	126.97	116.07
9	E	605	CHL	C4C-CHD-C1D	3.05	126.97	116.07
10	I	610	CLA	C14-C13-C15	3.05	122.13	111.27
9	H	605	CHL	C4C-CHD-C1D	3.05	126.97	116.07
9	H	601	CHL	OBD-CAD-CBD	-3.04	121.36	125.82
4	A	621	LUT	C1-C2-C3	3.04	120.26	113.59
9	G	608	CHL	C16-C15-C13	3.04	126.07	115.97
2	H	7633	BNG	C1'-O1-C1	3.04	118.87	113.68
10	J	604	CLA	O1A-CGA-CBA	-3.04	111.90	123.78
9	B	605	CHL	C4C-CHD-C1D	3.04	126.94	116.07
9	G	605	CHL	C4D-CHA-CBD	-3.04	105.91	108.97
9	A	601	CHL	CMB-C2B-C3B	3.04	130.75	124.68
9	F	601	CHL	C4C-CHD-C1D	3.04	126.94	116.07
9	I	609	CHL	C1C-CHC-C4B	3.04	126.93	116.07
7	B	1630	LHG	C27-C26-C25	3.04	129.71	114.37
9	E	601	CHL	C4D-CHA-CBD	-3.04	105.91	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	606	CHL	O1D-CGD-CBD	-3.03	120.12	124.72
9	F	609	CHL	CED-O2D-CGD	3.03	122.80	115.92
9	A	608	CHL	C4C-CHD-C1D	3.03	126.92	116.07
10	D	611	CLA	CAA-C2A-C3A	-3.03	104.81	113.00
10	B	604	CLA	O2D-CGD-CBD	3.03	116.52	111.23
9	C	608	CHL	C4C-CHD-C1D	3.03	126.90	116.07
2	G	6633	BNG	C1'-O1-C1	3.03	118.85	113.68
10	J	613	CLA	C6-C5-C3	3.03	120.84	113.47
10	E	613	CLA	CBA-CAA-C2A	3.03	122.79	113.79
9	G	608	CHL	C4C-CHD-C1D	3.03	126.89	116.07
4	J	9621	LUT	C18-C5-C4	-3.02	108.86	114.42
9	F	605	CHL	CED-O2D-CGD	3.02	122.77	115.92
9	D	607	CHL	CBC-CAC-C3C	-3.02	108.54	112.87
9	I	608	CHL	C4C-CHD-C1D	3.02	126.88	116.07
9	H	609	CHL	C1A-CHA-C4D	3.02	124.02	118.98
2	A	633	BNG	C1'-O1-C1	3.02	118.84	113.68
9	I	607	CHL	O2D-CGD-CBD	3.02	114.27	110.95
4	F	5620	LUT	C18-C5-C4	-3.02	108.87	114.42
9	H	606	CHL	C4C-CHD-C1D	3.02	126.87	116.07
9	H	608	CHL	C4D-CHA-CBD	-3.02	105.92	108.97
9	A	609	CHL	C4C-CHD-C1D	3.02	126.86	116.07
9	B	607	CHL	C4C-CHD-C1D	3.02	126.86	116.07
9	C	607	CHL	C4C-CHD-C1D	3.02	126.86	116.07
4	G	6621	LUT	C1-C2-C3	3.01	120.21	113.59
10	F	603	CLA	O1D-CGD-CBD	-3.01	118.57	124.52
10	D	613	CLA	C4-C3-C5	-3.01	110.00	115.23
9	C	609	CHL	C4D-CHA-CBD	-3.01	105.93	108.97
10	A	604	CLA	O1D-CGD-CBD	-3.01	118.58	124.52
9	B	601	CHL	C4C-CHD-C1D	3.01	126.83	116.07
9	C	605	CHL	C4C-CHD-C1D	3.01	126.83	116.07
9	J	605	CHL	C4C-CHD-C1D	3.01	126.83	116.07
9	B	609	CHL	C4D-CHA-CBD	-3.01	105.94	108.97
9	J	601	CHL	C11-C12-C13	3.01	125.96	115.97
10	D	604	CLA	C1-C2-C3	3.00	131.12	126.20
7	J	9630	LHG	O7-C7-C8	3.00	117.98	111.48
9	E	607	CHL	C12-C11-C10	-3.00	99.82	113.28
9	A	601	CHL	C16-C15-C13	3.00	125.95	115.97
10	A	602	CLA	C3B-C4B-NB	-3.00	107.85	110.53
9	B	608	CHL	CMB-C2B-C3B	3.00	130.68	124.68
9	F	605	CHL	C4C-CHD-C1D	3.00	126.81	116.07
9	F	606	CHL	C4C-CHD-C1D	3.00	126.80	116.07
9	D	605	CHL	C4C-CHD-C1D	3.00	126.80	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2621	LUT	C38-C25-C24	-3.00	116.27	123.36
10	C	613	CLA	C1-C2-C3	3.00	131.10	126.20
4	I	8621	LUT	C1-C2-C3	3.00	120.16	113.59
9	I	601	CHL	C4C-CHD-C1D	2.99	126.78	116.07
9	G	605	CHL	C4C-CHD-C1D	2.99	126.78	116.07
9	H	609	CHL	CMB-C2B-C3B	2.99	130.66	124.68
10	E	603	CLA	CED-O2D-CGD	2.99	122.70	115.92
9	C	606	CHL	C4C-CHD-C1D	2.99	126.77	116.07
10	H	610	CLA	C14-C13-C15	2.99	121.93	111.27
9	E	608	CHL	C4C-CHD-C1D	2.99	126.76	116.07
9	J	609	CHL	CHA-C1A-C2A	-2.99	126.29	133.31
8	G	9632	DGD	C3D-C4D-C5D	2.99	115.65	110.23
10	C	603	CLA	CBA-CAA-C2A	2.99	122.68	113.79
7	H	7630	LHG	O7-C7-C8	2.99	117.94	111.48
9	H	608	CHL	CMB-C2B-C3B	2.99	130.65	124.68
9	D	608	CHL	C4C-CHD-C1D	2.99	126.75	116.07
9	E	601	CHL	C6-C5-C3	2.99	120.74	113.47
10	J	614	CLA	CBA-CAA-C2A	2.98	122.67	113.79
9	J	609	CHL	C4D-CHA-CBD	-2.98	105.96	108.97
10	F	603	CLA	C6-C5-C3	2.98	120.73	113.47
10	H	604	CLA	O1A-CGA-CBA	-2.98	112.12	123.78
9	C	601	CHL	OBD-CAD-CBD	-2.98	121.45	125.82
10	D	614	CLA	CBA-CAA-C2A	2.98	122.66	113.79
9	I	606	CHL	C4C-CHD-C1D	2.98	126.73	116.07
10	G	604	CLA	CED-O2D-CGD	2.98	122.67	115.92
9	J	601	CHL	C4C-CHD-C1D	2.98	126.73	116.07
9	D	606	CHL	C4C-CHD-C1D	2.98	126.72	116.07
4	E	4621	LUT	C1-C2-C3	2.97	120.12	113.59
9	F	608	CHL	C4-C3-C5	-2.97	110.07	115.23
9	J	608	CHL	C4C-CHD-C1D	2.97	126.70	116.07
9	H	605	CHL	O2D-CGD-CBD	2.97	114.21	110.95
10	J	603	CLA	C5-C3-C2	2.97	127.83	121.17
10	G	602	CLA	C12-C11-C10	-2.97	99.97	113.28
9	D	606	CHL	OMC-CMC-C2C	2.97	130.28	125.12
9	A	606	CHL	C4C-CHD-C1D	2.97	126.68	116.07
6	H	7623	NEX	C24-C23-C22	2.97	116.34	110.79
7	H	7630	LHG	O10-C23-C24	-2.96	112.19	123.78
4	I	8621	LUT	C18-C5-C4	-2.96	108.97	114.42
10	C	613	CLA	C6-C5-C3	2.96	120.69	113.47
10	F	610	CLA	C3B-C4B-NB	-2.96	107.89	110.53
10	F	602	CLA	C9-C8-C7	2.96	121.83	111.27
10	C	613	CLA	CBA-CAA-C2A	2.96	122.60	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	602	CLA	CED-O2D-CGD	2.96	122.63	115.92
9	E	601	CHL	C4C-CHD-C1D	2.96	126.66	116.07
10	H	604	CLA	CAA-CBA-CGA	2.96	121.61	113.21
10	I	602	CLA	CMC-C2C-C1C	2.96	129.66	125.03
7	C	2630	LHG	C27-C26-C25	2.96	129.32	114.37
9	C	609	CHL	C1A-CHA-C4D	2.96	123.92	118.98
9	A	607	CHL	C4C-CHD-C1D	2.96	126.65	116.07
9	H	601	CHL	CMB-C2B-C3B	2.96	130.59	124.68
9	D	609	CHL	C1A-CHA-C4D	2.95	123.91	118.98
10	H	602	CLA	O2A-CGA-CBA	2.95	120.84	111.83
9	B	608	CHL	C4C-CHD-C1D	2.95	126.64	116.07
10	B	604	CLA	CBA-CAA-C2A	2.95	122.58	113.79
8	H	6632	DGD	O2G-C1B-C2B	2.95	117.86	111.48
10	F	614	CLA	CAA-CBA-CGA	2.95	121.58	113.21
4	D	3620	LUT	C3-C4-C5	2.95	119.51	112.18
10	A	612	CLA	C14-C13-C15	2.94	121.76	111.27
9	I	605	CHL	C4C-CHD-C1D	2.94	126.58	116.07
9	E	609	CHL	CHA-C1A-C2A	-2.94	126.41	133.31
10	G	602	CLA	C11-C12-C13	-2.94	106.20	115.97
7	B	1630	LHG	O7-C7-C8	2.94	117.83	111.48
9	D	608	CHL	O2A-CGA-CBA	2.94	120.78	111.83
9	G	608	CHL	CMB-C2B-C3B	2.93	130.54	124.68
10	F	610	CLA	CMC-C2C-C1C	2.93	129.62	125.03
10	A	612	CLA	O2A-CGA-CBA	2.93	120.78	111.83
9	I	605	CHL	C1A-CHA-C4D	2.93	123.87	118.98
9	H	608	CHL	C1C-C2C-CMC	-2.93	121.52	126.80
9	H	608	CHL	C16-C15-C13	2.93	125.70	115.97
10	D	603	CLA	C1-C2-C3	2.93	131.00	126.20
9	A	609	CHL	C1A-CHA-C4D	2.93	123.87	118.98
9	B	609	CHL	C1A-CHA-C4D	2.93	123.86	118.98
9	C	606	CHL	CBC-CAC-C3C	-2.93	108.68	112.87
9	B	609	CHL	CHA-C1A-C2A	-2.93	126.44	133.31
9	H	601	CHL	C4C-CHD-C1D	2.93	126.54	116.07
10	I	614	CLA	CBA-CAA-C2A	2.93	122.50	113.79
10	G	614	CLA	O2A-CGA-CBA	2.93	120.75	111.83
10	I	602	CLA	C12-C11-C10	-2.92	100.17	113.28
10	F	602	CLA	C11-C12-C13	-2.92	106.24	115.97
2	I	8633	BNG	C1'-O1-C1	2.92	118.67	113.68
9	G	607	CHL	C4C-CHD-C1D	2.92	126.53	116.07
10	A	603	CLA	C4-C3-C5	-2.92	110.16	115.23
7	G	6630	LHG	C27-C26-C25	2.92	129.14	114.37
9	F	607	CHL	OBD-CAD-CBD	-2.92	121.54	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	606	CHL	O1A-CGA-CBA	-2.92	112.36	123.78
9	B	606	CHL	C4C-CHD-C1D	2.92	126.51	116.07
9	D	608	CHL	CBA-CAA-C2A	2.92	122.37	113.78
10	H	614	CLA	O2A-CGA-CBA	2.92	120.73	111.83
9	A	608	CHL	C14-C13-C15	2.91	121.67	111.27
9	D	607	CHL	C4C-CHD-C1D	2.91	126.49	116.07
9	A	609	CHL	CHA-C1A-C2A	-2.91	126.47	133.31
10	J	612	CLA	CED-O2D-CGD	2.91	122.52	115.92
10	E	610	CLA	C1-C2-C3	2.91	130.97	126.20
9	H	607	CHL	C4-C3-C5	-2.91	110.18	115.23
8	H	7632	DGD	C3D-C4D-C5D	2.91	115.51	110.23
10	F	603	CLA	CED-O2D-CGD	2.91	122.52	115.92
10	C	613	CLA	C4-C3-C5	-2.91	110.18	115.23
10	H	604	CLA	CBA-CAA-C2A	2.91	122.44	113.79
10	E	614	CLA	CAA-CBA-CGA	2.91	121.46	113.21
4	H	7620	LUT	C21-C26-C27	2.91	116.17	112.83
9	I	607	CHL	C4C-CHD-C1D	2.91	126.47	116.07
9	G	609	CHL	C1A-CHA-C4D	2.90	123.83	118.98
7	D	3630	LHG	C27-C26-C25	2.90	129.04	114.37
9	E	601	CHL	C11-C12-C13	2.90	125.61	115.97
9	F	609	CHL	C1A-CHA-C4D	2.90	123.82	118.98
10	J	612	CLA	O2A-CGA-CBA	2.89	120.66	111.83
10	F	604	CLA	O1A-CGA-CBA	-2.89	112.46	123.78
9	G	609	CHL	CHA-C1A-C2A	-2.89	126.51	133.31
10	I	603	CLA	CED-O2D-CGD	2.89	122.48	115.92
4	G	6620	LUT	C21-C26-C27	2.89	116.15	112.83
7	G	6630	LHG	O7-C7-C8	2.89	117.74	111.48
9	H	605	CHL	OBD-CAD-CBD	-2.89	121.58	125.82
10	F	611	CLA	CAA-C2A-C1A	2.89	121.45	111.97
9	A	608	CHL	O2A-CGA-CBA	2.89	120.65	111.83
10	I	602	CLA	O2A-CGA-CBA	2.89	120.65	111.83
9	J	607	CHL	C4C-CHD-C1D	2.89	126.41	116.07
10	G	604	CLA	C1-C2-C3	2.89	130.93	126.20
7	C	2630	LHG	O7-C7-C8	2.89	117.73	111.48
9	F	609	CHL	C4D-CHA-CBD	-2.89	106.06	108.97
9	J	609	CHL	OBD-CAD-CBD	-2.89	121.59	125.82
9	H	607	CHL	C4C-CHD-C1D	2.88	126.39	116.07
9	C	601	CHL	C11-C12-C13	2.88	125.55	115.97
9	C	607	CHL	C14-C13-C12	2.88	121.55	111.27
10	I	610	CLA	C3B-C4B-NB	-2.88	107.96	110.53
10	J	602	CLA	C3B-C4B-NB	-2.88	107.96	110.53
9	E	601	CHL	C12-C11-C10	-2.88	100.37	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	602	CLA	O2A-CGA-CBA	2.88	120.61	111.83
10	E	610	CLA	C3B-C4B-NB	-2.88	107.96	110.53
4	J	9621	LUT	C1-C2-C3	2.88	119.91	113.59
9	E	605	CHL	CAA-C2A-C3A	-2.88	105.22	113.00
9	I	609	CHL	CMB-C2B-C3B	2.88	130.43	124.68
9	I	609	CHL	C1A-CHA-C4D	2.88	123.78	118.98
10	E	613	CLA	CMB-C2B-C3B	2.88	133.31	126.55
9	D	608	CHL	C1A-CHA-C4D	2.87	123.77	118.98
9	F	609	CHL	CHA-C1A-C2A	-2.87	126.57	133.31
9	A	608	CHL	O1D-CGD-CBD	-2.87	120.38	124.72
7	F	5630	LHG	C27-C26-C25	2.86	128.85	114.37
9	C	609	CHL	CHA-C1A-C2A	-2.86	126.58	133.31
9	I	601	CHL	OBD-CAD-CBD	-2.86	121.62	125.82
9	C	607	CHL	O2D-CGD-CBD	2.86	114.09	110.95
9	A	609	CHL	CMB-C2B-C3B	2.86	130.40	124.68
5	C	7622	XAT	C38-C25-C24	-2.86	111.03	114.24
10	B	602	CLA	O2A-CGA-CBA	2.86	120.56	111.83
10	F	603	CLA	O2A-CGA-CBA	2.86	120.55	111.83
10	G	612	CLA	CED-O2D-CGD	2.86	122.40	115.92
10	G	602	CLA	C14-C13-C15	2.86	121.46	111.27
8	H	6632	DGD	C3G-O3G-C1D	2.86	119.92	113.80
9	F	601	CHL	C9-C8-C10	2.86	121.46	111.27
9	E	607	CHL	O2D-CGD-CBD	2.86	114.08	110.95
10	G	604	CLA	CBA-CAA-C2A	2.85	122.28	113.79
9	E	606	CHL	C4C-CHD-C1D	2.85	126.28	116.07
10	B	612	CLA	CED-O2D-CGD	2.85	122.38	115.92
9	A	601	CHL	OBD-CAD-CBD	-2.85	121.64	125.82
9	C	606	CHL	CED-O2D-CGD	2.85	122.38	115.92
9	J	609	CHL	CED-O2D-CGD	2.85	122.38	115.92
7	H	7630	LHG	C27-C26-C25	2.85	128.77	114.37
9	C	609	CHL	C14-C13-C15	2.85	121.42	111.27
9	A	609	CHL	C4D-CHA-CBD	-2.85	106.10	108.97
10	I	604	CLA	O1A-CGA-CBA	-2.85	112.65	123.78
9	B	605	CHL	OBD-CAD-CBD	-2.85	121.65	125.82
4	D	3621	LUT	C18-C5-C4	-2.84	109.19	114.42
10	C	614	CLA	O2A-CGA-CBA	2.84	120.51	111.83
9	I	608	CHL	C1A-CHA-C4D	2.84	123.73	118.98
9	H	607	CHL	C1A-CHA-C4D	2.84	123.72	118.98
10	F	603	CLA	CAA-C2A-C3A	-2.84	105.32	113.00
8	B	1632	DGD	C3D-C4D-C5D	2.84	115.38	110.23
9	G	607	CHL	C1A-CHA-C4D	2.84	123.72	118.98
9	J	607	CHL	OBD-CAD-CBD	-2.84	121.66	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1621	LUT	C1-C2-C3	2.84	119.82	113.59
10	E	610	CLA	CED-O2D-CGD	2.84	122.35	115.92
10	J	612	CLA	C14-C13-C15	2.84	121.39	111.27
10	E	602	CLA	C12-C11-C10	-2.83	100.59	113.28
10	C	610	CLA	C14-C13-C12	2.83	121.36	111.27
8	D	5632	DGD	C3G-C2G-C1G	-2.83	105.19	111.78
10	C	604	CLA	O1D-CGD-CBD	-2.83	118.94	124.52
8	E	4632	DGD	C4D-C3D-C2D	2.83	115.79	110.83
9	C	601	CHL	C1A-CHA-C4D	2.83	123.70	118.98
9	G	607	CHL	C4-C3-C5	-2.83	110.32	115.23
8	G	9632	DGD	C3G-O3G-C1D	2.83	119.85	113.80
9	F	601	CHL	CMB-C2B-C3B	2.83	130.33	124.68
10	C	610	CLA	C3B-C4B-NB	-2.83	108.01	110.53
9	E	606	CHL	C1A-CHA-C4D	2.82	123.69	118.98
9	B	607	CHL	OBD-CAD-CBD	-2.82	121.68	125.82
9	H	609	CHL	OBD-CAD-CBD	-2.82	121.68	125.82
9	I	609	CHL	C1C-C2C-CMC	-2.82	121.71	126.80
9	H	609	CHL	C16-C15-C13	2.82	125.35	115.97
9	B	601	CHL	C1A-CHA-C4D	2.82	123.69	118.98
9	C	606	CHL	C5-C3-C4	-2.82	108.09	114.59
9	H	609	CHL	CAA-CBA-CGA	2.82	121.21	113.21
9	D	609	CHL	CHA-C1A-C2A	-2.82	126.69	133.31
10	G	610	CLA	C1-C2-C3	2.82	130.81	126.20
9	F	608	CHL	CBA-CAA-C2A	2.82	122.07	113.78
9	J	601	CHL	OBD-CAD-CBD	-2.81	121.70	125.82
2	E	4633	BNG	C1'-O1-C1	2.81	118.48	113.68
10	E	602	CLA	C14-C13-C15	2.81	121.29	111.27
9	H	609	CHL	CHA-C1A-C2A	-2.81	126.71	133.31
9	H	601	CHL	C11-C12-C13	2.81	125.30	115.97
10	D	604	CLA	C4-C3-C5	-2.81	110.36	115.23
5	J	3622	XAT	C38-C25-C24	-2.81	111.09	114.24
9	I	609	CHL	CHA-C1A-C2A	-2.80	126.72	133.31
10	B	611	CLA	O2D-CGD-CBD	2.80	116.13	111.23
9	A	609	CHL	CAA-CBA-CGA	2.80	121.16	113.21
10	G	613	CLA	C5-C3-C2	2.80	127.46	121.17
10	B	603	CLA	C6-C5-C3	2.80	120.29	113.47
10	D	604	CLA	C9-C8-C10	2.80	121.25	111.27
10	D	602	CLA	C9-C8-C10	-2.80	101.30	111.27
10	A	614	CLA	O2A-CGA-CBA	2.80	120.36	111.83
10	H	602	CLA	C11-C10-C8	-2.79	106.67	115.97
9	F	607	CHL	CED-O2D-CGD	2.79	122.25	115.92
9	F	607	CHL	C6-C5-C3	2.79	120.27	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	603	CLA	CAA-CBA-CGA	2.79	121.13	113.21
9	B	608	CHL	C1A-CHA-C4D	2.79	123.64	118.98
9	F	605	CHL	C1A-CHA-C4D	2.79	123.64	118.98
9	B	606	CHL	C1A-CHA-C4D	2.79	123.64	118.98
10	J	610	CLA	C3B-C4B-NB	-2.79	108.04	110.53
9	H	606	CHL	C1A-CHA-C4D	2.79	123.64	118.98
9	F	607	CHL	O2A-CGA-O1A	-2.79	116.65	123.63
10	J	612	CLA	C7-C6-C5	-2.79	105.83	113.26
10	E	602	CLA	CMC-C2C-C1C	2.79	129.39	125.03
10	I	603	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
9	J	605	CHL	C1A-CHA-C4D	2.78	123.63	118.98
5	F	6622	XAT	C7-C8-C9	2.78	129.85	125.53
10	J	602	CLA	C6-C7-C8	-2.78	106.72	115.97
10	B	603	CLA	C9-C8-C10	-2.78	101.37	111.27
9	G	609	CHL	CBC-CAC-C3C	-2.78	108.90	112.87
9	G	607	CHL	C14-C13-C12	2.78	121.17	111.27
9	C	607	CHL	O2A-CGA-O1A	-2.78	116.68	123.63
10	B	602	CLA	C3B-C4B-NB	-2.78	108.05	110.53
9	F	601	CHL	C1A-CHA-C4D	2.77	123.61	118.98
9	D	601	CHL	C9-C8-C10	2.77	121.16	111.27
9	B	609	CHL	CMB-C2B-C3B	2.77	130.22	124.68
9	D	606	CHL	C1A-CHA-C4D	2.77	123.61	118.98
10	F	602	CLA	C6-C7-C8	-2.77	106.75	115.97
9	D	605	CHL	C1A-CHA-C4D	2.77	123.61	118.98
10	H	602	CLA	C7-C6-C5	2.77	120.65	113.26
10	F	610	CLA	C14-C13-C15	2.77	121.15	111.27
9	E	609	CHL	C1A-CHA-C4D	2.77	123.61	118.98
9	B	609	CHL	OBD-CAD-CBD	-2.77	121.76	125.82
8	H	7632	DGD	C3G-C2G-C1G	-2.77	105.33	111.78
10	J	613	CLA	O2A-CGA-CBA	2.77	120.28	111.83
10	I	611	CLA	C9-C8-C10	2.77	121.14	111.27
9	J	608	CHL	C1A-CHA-C4D	2.77	123.60	118.98
10	A	610	CLA	CMC-C2C-C1C	2.77	129.36	125.03
10	B	612	CLA	O1D-CGD-CBD	-2.77	119.06	124.52
8	D	3632	DGD	O2G-C1B-C2B	2.77	117.47	111.48
9	G	601	CHL	C1A-CHA-C4D	2.77	123.60	118.98
9	H	608	CHL	OBD-CAD-CBD	-2.77	121.77	125.82
7	A	630	LHG	C27-C26-C25	2.76	128.34	114.37
10	G	602	CLA	CED-O2D-CGD	2.76	122.19	115.92
10	A	612	CLA	CED-O2D-CGD	2.76	122.19	115.92
10	G	610	CLA	C3B-C4B-NB	-2.76	108.06	110.53
9	J	606	CHL	C1A-CHA-C4D	2.76	123.59	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	602	CLA	C3B-C4B-NB	-2.76	108.07	110.53
9	C	608	CHL	C1A-CHA-C4D	2.76	123.59	118.98
9	E	608	CHL	C1A-CHA-C4D	2.76	123.59	118.98
9	D	607	CHL	O2A-CGA-O1A	-2.76	116.73	123.63
9	A	607	CHL	C1A-CHA-C4D	2.76	123.58	118.98
10	A	610	CLA	C3B-C4B-NB	-2.76	108.07	110.53
5	B	1622	XAT	O24-C25-C24	2.75	116.07	113.49
9	D	601	CHL	CHA-C1A-C2A	-2.75	126.84	133.31
10	H	614	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
9	G	607	CHL	C7-C6-C5	-2.75	105.93	113.26
8	D	3632	DGD	C4D-C3D-C2D	2.75	115.66	110.83
10	H	604	CLA	CED-O2D-CGD	2.75	122.15	115.92
9	E	609	CHL	C4D-CHA-CBD	-2.75	106.20	108.97
4	A	621	LUT	C7-C8-C9	2.75	130.30	126.23
10	B	611	CLA	CMB-C2B-C1B	-2.75	121.24	125.42
6	C	2623	NEX	C26-C27-C28	2.75	131.80	125.99
9	I	605	CHL	CMB-C2B-C3B	2.75	130.17	124.68
8	B	2632	DGD	C3D-C4D-C5D	2.74	115.21	110.23
9	A	605	CHL	C1A-CHA-C4D	2.74	123.56	118.98
9	I	608	CHL	CHA-C1A-C2A	-2.74	126.87	133.31
10	J	611	CLA	CED-O2D-CGD	2.74	122.14	115.92
10	B	613	CLA	C1-C2-C3	2.74	130.69	126.20
9	E	607	CHL	O2A-CGA-O1A	-2.74	116.78	123.63
9	A	606	CHL	C1A-CHA-C4D	2.74	123.55	118.98
9	I	601	CHL	C1A-CHA-C4D	2.74	123.55	118.98
9	J	607	CHL	C1A-CHA-C4D	2.74	123.55	118.98
10	F	602	CLA	CED-O2D-CGD	2.74	122.12	115.92
8	G	9632	DGD	C6D-O5D-C1E	2.74	119.67	113.80
10	G	611	CLA	CAA-CBA-CGA	2.74	120.98	113.21
9	H	605	CHL	C1A-CHA-C4D	2.73	123.55	118.98
10	H	604	CLA	C6-C7-C8	2.73	125.05	115.97
9	F	606	CHL	C1A-CHA-C4D	2.73	123.54	118.98
10	H	614	CLA	CED-O2D-CGD	2.73	122.11	115.92
9	F	605	CHL	CMB-C2B-C3B	2.73	130.14	124.68
9	J	609	CHL	C16-C15-C13	2.73	125.04	115.97
10	C	602	CLA	C6-C7-C8	-2.73	106.89	115.97
8	E	4632	DGD	C6D-O5D-C1E	2.73	119.65	113.80
9	F	608	CHL	C1A-CHA-C4D	2.73	123.54	118.98
9	G	609	CHL	O2D-CGD-CBD	2.73	113.94	110.95
9	C	606	CHL	CHA-C1A-C2A	-2.73	126.90	133.31
10	A	614	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
9	I	606	CHL	C1A-CHA-C4D	2.73	123.53	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	609	CHL	C14-C13-C15	2.73	121.00	111.27
10	C	603	CLA	O2A-CGA-CBA	2.73	120.15	111.83
9	H	608	CHL	C1-C2-C3	2.73	130.66	126.20
9	D	608	CHL	C5-C3-C2	-2.72	115.05	121.17
9	J	608	CHL	CHA-C1A-C2A	-2.72	126.91	133.31
9	H	608	CHL	C1A-CHA-C4D	2.72	123.52	118.98
9	I	607	CHL	C1A-CHA-C4D	2.72	123.52	118.98
10	F	614	CLA	O2A-CGA-CBA	2.72	120.13	111.83
9	C	605	CHL	C1A-CHA-C4D	2.72	123.52	118.98
9	A	609	CHL	CAA-C2A-C3A	-2.72	105.66	113.00
9	E	607	CHL	C4-C3-C5	-2.72	110.51	115.23
8	I	8632	DGD	C3G-O3G-C1D	2.71	119.62	113.80
9	D	601	CHL	C1A-CHA-C4D	2.71	123.51	118.98
9	B	605	CHL	C1A-CHA-C4D	2.71	123.51	118.98
9	D	605	CHL	O2D-CGD-CBD	2.71	113.93	110.95
8	H	7632	DGD	C4D-C3D-C2D	2.71	115.59	110.83
9	D	607	CHL	C1A-CHA-C4D	2.71	123.51	118.98
9	E	605	CHL	C1A-CHA-C4D	2.71	123.51	118.98
5	A	622	XAT	C7-C8-C9	2.71	129.74	125.53
9	D	606	CHL	CHA-C1A-C2A	-2.71	126.94	133.31
8	E	4632	DGD	C3G-C2G-C1G	-2.71	105.47	111.78
10	E	612	CLA	C14-C13-C15	2.71	120.93	111.27
10	G	610	CLA	CMC-C2C-C1C	2.71	129.27	125.03
10	C	610	CLA	C1-C2-C3	2.71	130.63	126.20
9	A	606	CHL	CHA-C1A-C2A	-2.71	126.95	133.31
10	C	602	CLA	C3B-C4B-NB	-2.71	108.11	110.53
9	I	607	CHL	C5-C3-C2	2.71	127.24	121.17
10	E	612	CLA	O2A-CGA-CBA	2.71	120.08	111.83
9	G	601	CHL	C7-C6-C5	-2.70	106.05	113.26
9	C	601	CHL	CMB-C2B-C3B	2.70	130.09	124.68
10	H	602	CLA	C3B-C4B-NB	-2.70	108.12	110.53
9	G	609	CHL	OBD-CAD-CBD	-2.70	121.86	125.82
4	D	3620	LUT	C1-C2-C3	2.70	119.52	113.59
9	J	601	CHL	C14-C13-C12	2.70	120.91	111.27
9	G	601	CHL	C1-C2-C3	2.70	130.62	126.20
10	H	614	CLA	CAA-CBA-CGA	2.70	120.88	113.21
9	E	606	CHL	CHA-C1A-C2A	-2.70	126.97	133.31
10	J	603	CLA	O2A-CGA-CBA	2.70	120.07	111.83
4	F	5620	LUT	C3-C4-C5	2.70	118.90	112.18
7	J	9630	LHG	C27-C26-C25	2.70	128.01	114.37
8	A	632	DGD	C3G-C2G-C1G	-2.70	105.49	111.78
9	G	605	CHL	C1A-CHA-C4D	2.70	123.48	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	603	CLA	C7-C6-C5	-2.70	106.07	113.26
8	B	2632	DGD	C3G-C2G-C1G	-2.70	105.50	111.78
10	D	612	CLA	C14-C13-C15	2.70	120.88	111.27
10	D	612	CLA	CED-O2D-CGD	2.70	122.03	115.92
8	I	8632	DGD	C6D-O5D-C1E	2.69	119.57	113.80
9	D	607	CHL	CED-O2D-CGD	2.69	122.02	115.92
7	F	5630	LHG	O10-C23-C24	-2.69	113.25	123.78
5	J	3622	XAT	O24-C25-C24	2.69	116.01	113.49
9	F	601	CHL	CHA-C1A-C2A	-2.69	126.99	133.31
5	F	6622	XAT	C37-C21-C22	-2.69	104.24	108.97
9	G	606	CHL	CHA-C1A-C2A	-2.69	126.99	133.31
10	F	602	CLA	C3B-C4B-NB	-2.69	108.13	110.53
8	I	8632	DGD	C3G-C2G-C1G	-2.69	105.52	111.78
9	D	609	CHL	C6-C5-C3	2.69	120.01	113.47
10	D	610	CLA	C3B-C4B-NB	-2.68	108.13	110.53
9	G	608	CHL	C1A-CHA-C4D	2.68	123.46	118.98
10	D	612	CLA	C11-C10-C8	2.68	124.89	115.97
9	H	601	CHL	C6-C5-C3	2.68	120.00	113.47
9	G	601	CHL	CMB-C2B-C3B	2.68	130.04	124.68
10	D	612	CLA	C4-C3-C5	-2.68	110.58	115.23
10	G	603	CLA	C16-C15-C13	2.68	124.87	115.97
10	C	611	CLA	C4-C3-C5	-2.68	110.58	115.23
9	E	609	CHL	OBD-CAD-CBD	-2.68	121.89	125.82
10	E	603	CLA	O2A-CGA-CBA	2.68	120.00	111.83
9	D	607	CHL	CHA-C1A-C2A	-2.68	127.02	133.31
10	E	610	CLA	C14-C13-C15	2.68	120.82	111.27
9	G	609	CHL	C16-C15-C13	2.68	124.87	115.97
9	B	606	CHL	CHA-C1A-C2A	-2.68	127.02	133.31
8	B	1632	DGD	C3G-C2G-C1G	-2.68	105.55	111.78
6	J	9623	NEX	C24-C23-C22	2.68	115.80	110.79
4	A	620	LUT	C3-C4-C5	2.68	118.84	112.18
8	B	1632	DGD	C6D-O5D-C1E	2.67	119.53	113.80
9	I	609	CHL	OBD-CAD-CBD	-2.67	121.90	125.82
9	E	607	CHL	CED-O2D-CGD	2.67	121.97	115.92
9	D	608	CHL	CHA-C1A-C2A	-2.67	127.04	133.31
10	G	614	CLA	C3B-C4B-NB	-2.67	108.15	110.53
10	B	610	CLA	C3B-C4B-NB	-2.67	108.15	110.53
10	F	602	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
9	C	607	CHL	C1A-CHA-C4D	2.67	123.43	118.98
9	H	601	CHL	C1A-CHA-C4D	2.67	123.43	118.98
9	A	608	CHL	C1A-CHA-C4D	2.67	123.43	118.98
9	D	601	CHL	C14-C13-C15	-2.67	101.77	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	606	CHL	C1A-CHA-C4D	2.66	123.42	118.98
9	H	607	CHL	O2A-CGA-O1A	-2.66	116.97	123.63
8	A	632	DGD	C6D-O5D-C1E	2.66	119.50	113.80
8	D	3632	DGD	C6D-O5D-C1E	2.66	119.50	113.80
10	B	613	CLA	C4-C3-C5	-2.66	110.61	115.23
9	J	606	CHL	O1A-CGA-CBA	-2.66	113.38	123.78
10	C	603	CLA	C1-C2-C3	2.66	130.55	126.20
6	G	6623	NEX	C16-C1-C6	2.66	112.85	110.47
10	G	602	CLA	C6-C7-C8	-2.66	107.14	115.97
9	B	607	CHL	C5-C3-C2	2.65	127.13	121.17
4	C	2621	LUT	C18-C5-C4	-2.65	109.54	114.42
10	E	602	CLA	C3B-C4B-NB	-2.65	108.16	110.53
10	B	614	CLA	O2A-CGA-CBA	2.65	119.92	111.83
9	F	606	CHL	CHA-C1A-C2A	-2.65	127.09	133.31
8	E	4632	DGD	C3G-O3G-C1D	2.65	119.47	113.80
9	G	601	CHL	C9-C8-C10	2.65	120.71	111.27
10	I	614	CLA	CAA-CBA-CGA	2.65	120.73	113.21
9	A	607	CHL	C4-C3-C5	-2.65	110.63	115.23
9	E	607	CHL	C1A-CHA-C4D	2.65	123.40	118.98
8	B	2632	DGD	C4D-C3D-C2D	2.65	115.47	110.83
9	A	601	CHL	C1-C2-C3	2.65	130.53	126.20
9	A	601	CHL	C1A-CHA-C4D	2.65	123.40	118.98
10	I	611	CLA	CAA-C2A-C1A	2.65	120.64	111.97
9	I	608	CHL	C16-C15-C13	2.65	124.76	115.97
4	E	4621	LUT	C18-C5-C6	2.64	127.37	124.48
9	B	601	CHL	CHA-C1A-C2A	-2.64	127.10	133.31
6	G	6623	NEX	C24-C23-C22	2.64	115.73	110.79
10	A	610	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
9	C	601	CHL	CHA-C1A-C2A	-2.64	127.10	133.31
4	C	2620	LUT	C21-C26-C27	2.64	115.86	112.83
10	F	603	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
5	B	5622	XAT	O24-C25-C24	2.64	115.97	113.49
10	B	603	CLA	C20-C18-C19	-2.64	98.75	110.53
9	A	605	CHL	CHA-C1A-C2A	-2.64	127.11	133.31
8	A	632	DGD	C3G-O3G-C1D	2.64	119.45	113.80
10	H	613	CLA	C5-C3-C2	2.64	127.09	121.17
9	D	605	CHL	CMB-C2B-C3B	2.64	129.95	124.68
4	D	3621	LUT	C1-C6-C5	-2.64	119.03	122.64
9	A	607	CHL	CED-O2D-CGD	2.64	121.89	115.92
9	J	607	CHL	CED-O2D-CGD	2.64	121.89	115.92
9	G	601	CHL	CHA-C1A-C2A	-2.64	127.12	133.31
10	G	610	CLA	C16-C15-C13	2.63	124.72	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	5623	NEX	C16-C1-C6	2.63	112.83	110.47
9	A	607	CHL	O2A-CGA-O1A	-2.63	117.04	123.63
9	B	607	CHL	C1A-CHA-C4D	2.63	123.37	118.98
10	H	614	CLA	C3B-C4B-NB	-2.63	108.18	110.53
10	G	604	CLA	O1A-CGA-CBA	-2.63	113.50	123.78
9	D	607	CHL	C14-C13-C12	2.63	120.64	111.27
10	D	602	CLA	C3B-C4B-NB	-2.63	108.18	110.53
9	F	608	CHL	CHA-C1A-C2A	-2.63	127.14	133.31
10	F	613	CLA	C6-C5-C3	2.63	119.87	113.47
8	D	3632	DGD	C3G-O3G-C1D	2.63	119.43	113.80
8	H	6632	DGD	C6D-O5D-C1E	2.63	119.43	113.80
6	A	623	NEX	C16-C1-C6	2.63	112.82	110.47
10	D	602	CLA	C5-C3-C2	-2.63	115.27	121.17
9	F	607	CHL	C1A-CHA-C4D	2.62	123.36	118.98
10	J	613	CLA	C5-C3-C2	2.62	127.06	121.17
9	J	607	CHL	O2A-CGA-O1A	-2.62	117.06	123.63
10	J	603	CLA	C16-C15-C13	2.62	124.69	115.97
9	E	601	CHL	C1A-CHA-C4D	2.62	123.36	118.98
10	J	602	CLA	C14-C13-C15	2.62	120.62	111.27
9	D	608	CHL	CMB-C2B-C3B	2.62	129.92	124.68
8	B	2632	DGD	C3G-O3G-C1D	2.62	119.41	113.80
10	I	602	CLA	C3B-C4B-NB	-2.62	108.19	110.53
10	E	603	CLA	C1-C2-C3	2.62	130.49	126.20
10	G	611	CLA	C4-C3-C5	-2.62	110.68	115.23
9	A	601	CHL	CHA-C1A-C2A	-2.62	127.16	133.31
9	F	605	CHL	CHA-C1A-C2A	-2.62	127.16	133.31
9	G	608	CHL	CHA-C1A-C2A	-2.62	127.16	133.31
10	I	613	CLA	C6-C5-C3	2.62	119.84	113.47
10	B	612	CLA	C4-C3-C5	-2.61	110.69	115.23
9	B	605	CHL	CHA-C1A-C2A	-2.61	127.17	133.31
9	D	607	CHL	CBA-CAA-C2A	2.61	121.47	113.78
8	D	3632	DGD	C3D-C4D-C5D	2.61	114.97	110.23
9	H	606	CHL	CHA-C1A-C2A	-2.61	127.17	133.31
9	C	606	CHL	C1A-CHA-C4D	2.61	123.34	118.98
4	D	3621	LUT	C7-C8-C9	2.61	130.09	126.23
10	B	604	CLA	O1D-CGD-CBD	-2.61	119.38	124.52
9	B	608	CHL	C16-C15-C13	2.61	124.63	115.97
8	D	3632	DGD	C3G-C2G-C1G	-2.61	105.71	111.78
10	F	603	CLA	C4-C3-C5	-2.61	110.71	115.23
9	G	605	CHL	O2D-CGD-CBD	2.60	113.81	110.95
9	H	609	CHL	C14-C13-C15	2.60	120.56	111.27
10	C	614	CLA	CAA-CBA-CGA	2.60	120.60	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	605	CHL	CHA-C1A-C2A	-2.60	127.19	133.31
5	D	8622	XAT	O24-C25-C24	2.60	115.93	113.49
10	A	602	CLA	C12-C11-C10	-2.60	101.61	113.28
9	J	601	CHL	C1A-CHA-C4D	2.60	123.32	118.98
9	J	606	CHL	CHA-C1A-C2A	-2.60	127.20	133.31
9	I	601	CHL	CHA-C1A-C2A	-2.60	127.21	133.31
9	E	601	CHL	CHA-C1A-C2A	-2.60	127.21	133.31
10	F	603	CLA	C3B-C4B-NB	-2.60	108.21	110.53
9	F	609	CHL	C14-C13-C15	2.59	120.52	111.27
10	H	610	CLA	C3B-C4B-NB	-2.59	108.22	110.53
4	F	5620	LUT	C21-C26-C27	2.59	115.80	112.83
9	E	608	CHL	CMB-C2B-C3B	2.59	129.85	124.68
5	H	4622	XAT	C7-C8-C9	2.59	129.54	125.53
9	E	605	CHL	CMB-C2B-C3B	2.59	129.85	124.68
6	I	8623	NEX	C16-C1-C6	2.58	112.78	110.47
9	J	607	CHL	CHA-C1A-C2A	-2.58	127.24	133.31
9	G	609	CHL	C14-C13-C15	2.58	120.48	111.27
10	E	602	CLA	C4-C3-C5	2.58	119.71	115.23
10	G	612	CLA	C16-C15-C13	2.58	124.53	115.97
9	G	605	CHL	CMB-C2B-C3B	2.58	129.84	124.68
10	I	604	CLA	CBA-CAA-C2A	2.58	121.46	113.79
9	G	607	CHL	C6-C5-C3	2.58	119.74	113.47
10	F	613	CLA	O2A-CGA-CBA	2.58	119.69	111.83
9	C	608	CHL	CHA-C1A-C2A	-2.58	127.26	133.31
8	H	7632	DGD	O2G-C1B-C2B	2.57	117.05	111.48
9	F	605	CHL	O1D-CGD-CBD	-2.57	120.82	124.72
10	C	611	CLA	CED-O2D-CGD	2.57	121.75	115.92
9	G	607	CHL	O2A-CGA-O1A	-2.57	117.19	123.63
9	G	605	CHL	CHA-C1A-C2A	-2.57	127.27	133.31
9	H	601	CHL	CHA-C1A-C2A	-2.57	127.27	133.31
9	I	607	CHL	O2A-CGA-O1A	-2.57	117.20	123.63
9	H	608	CHL	CHA-C1A-C2A	-2.57	127.28	133.31
9	J	601	CHL	CHA-C1A-C2A	-2.57	127.28	133.31
9	B	607	CHL	O2A-CGA-O1A	-2.56	117.21	123.63
10	F	604	CLA	C6-C5-C3	2.56	119.71	113.47
9	I	606	CHL	CHA-C1A-C2A	-2.56	127.29	133.31
9	B	609	CHL	CBC-CAC-C3C	-2.56	109.20	112.87
9	E	601	CHL	CMB-C2B-C3B	2.56	129.80	124.68
10	H	604	CLA	C11-C10-C8	2.56	124.48	115.97
9	C	601	CHL	C7-C6-C5	-2.56	106.44	113.26
9	H	606	CHL	C5-C3-C4	-2.56	108.70	114.59
9	E	605	CHL	CHA-C1A-C2A	-2.56	127.30	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	H	603	CLA	O2A-CGA-CBA	2.56	119.64	111.83
9	D	605	CHL	CHA-C1A-C2A	-2.56	127.30	133.31
8	H	7632	DGD	C6D-O5D-C1E	2.55	119.27	113.80
10	A	602	CLA	C9-C8-C10	-2.55	102.18	111.27
8	G	9632	DGD	C3G-C2G-C1G	-2.55	105.84	111.78
9	I	605	CHL	CHA-C1A-C2A	-2.55	127.32	133.31
9	F	607	CHL	C12-C11-C10	-2.55	101.86	113.28
8	H	7632	DGD	O3G-C1D-C2D	2.55	112.14	108.27
9	D	606	CHL	O1D-CGD-CBD	-2.55	120.86	124.72
9	E	607	CHL	C14-C13-C12	2.55	120.35	111.27
8	B	1632	DGD	C3G-O3G-C1D	2.54	119.24	113.80
10	A	604	CLA	O1A-CGA-CBA	-2.54	113.84	123.78
9	G	607	CHL	O1D-CGD-CBD	-2.54	120.87	124.72
10	F	604	CLA	C6-C7-C8	2.54	124.40	115.97
10	I	610	CLA	C11-C10-C8	-2.54	107.53	115.97
9	A	601	CHL	C6-C5-C3	2.54	119.65	113.47
10	C	602	CLA	C11-C12-C13	-2.54	107.54	115.97
9	D	607	CHL	C12-C11-C10	-2.53	101.92	113.28
10	G	602	CLA	C9-C8-C10	-2.53	102.25	111.27
8	B	1632	DGD	C6D-C5D-C4D	2.53	117.38	112.07
6	I	8623	NEX	C24-C23-C22	2.53	115.52	110.79
9	D	606	CHL	C5-C3-C4	-2.53	108.78	114.59
10	D	610	CLA	CMC-C2C-C1C	2.52	128.98	125.03
8	B	2632	DGD	C6D-O5D-C1E	2.52	119.21	113.80
9	J	605	CHL	CMB-C2B-C3B	2.52	129.73	124.68
10	F	614	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
5	D	8622	XAT	C37-C21-C22	-2.52	104.54	108.97
4	G	6621	LUT	C18-C5-C4	-2.52	109.78	114.42
9	H	605	CHL	CHA-C1A-C2A	-2.52	127.39	133.31
5	I	9622	XAT	C7-C8-C9	2.52	129.44	125.53
8	H	7632	DGD	C3G-O3G-C1D	2.52	119.19	113.80
10	E	610	CLA	CMC-C2C-C1C	2.51	128.96	125.03
10	C	604	CLA	C6-C7-C8	2.51	124.31	115.97
9	F	608	CHL	C14-C13-C15	2.51	120.23	111.27
10	I	613	CLA	O2A-CGA-CBA	2.51	119.49	111.83
10	I	612	CLA	C11-C12-C13	2.51	124.31	115.97
10	G	614	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
10	B	614	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
10	A	602	CLA	C14-C13-C15	2.51	120.21	111.27
9	B	608	CHL	CHA-C1A-C2A	-2.51	127.42	133.31
10	C	604	CLA	CBA-CAA-C2A	2.51	121.25	113.79
10	A	613	CLA	O2A-CGA-CBA	2.50	119.47	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	612	CLA	C4-C3-C5	-2.50	110.88	115.23
10	H	613	CLA	O2A-CGA-CBA	2.50	119.47	111.83
6	F	5623	NEX	C24-C23-C22	2.50	115.47	110.79
9	E	608	CHL	CHA-C1A-C2A	-2.50	127.43	133.31
10	G	602	CLA	C11-C10-C8	-2.50	107.65	115.97
8	E	4632	DGD	C6D-C5D-C4D	2.50	117.32	112.07
6	H	7623	NEX	C16-C1-C6	2.50	112.71	110.47
10	J	610	CLA	CMC-C2C-C1C	2.50	128.94	125.03
9	A	609	CHL	CED-O2D-CGD	2.50	121.58	115.92
9	J	609	CHL	O1D-CGD-CBD	-2.50	120.94	124.72
10	B	603	CLA	C1-C2-C3	2.50	130.29	126.20
10	I	611	CLA	C3B-C4B-NB	-2.50	108.30	110.53
9	I	609	CHL	C14-C13-C15	2.50	120.17	111.27
6	B	1623	NEX	C16-C1-C6	2.49	112.70	110.47
5	H	4622	XAT	O24-C25-C24	2.49	115.83	113.49
10	I	602	CLA	C9-C8-C10	-2.49	102.39	111.27
9	E	608	CHL	C1-C2-C3	2.49	130.28	126.20
10	C	603	CLA	CAC-C3C-C4C	2.49	128.03	124.79
9	I	606	CHL	C5-C3-C4	-2.49	108.86	114.59
10	E	611	CLA	CED-O2D-CGD	2.49	121.56	115.92
10	B	611	CLA	C4-C3-C5	-2.49	110.91	115.23
10	G	613	CLA	C1-C2-C3	2.49	130.28	126.20
9	C	605	CHL	O1D-CGD-CBD	-2.49	120.95	124.72
10	A	603	CLA	C1-C2-C3	2.49	130.27	126.20
10	D	611	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
5	C	7622	XAT	C37-C21-C22	-2.48	104.60	108.97
9	B	607	CHL	CHA-C1A-C2A	-2.48	127.47	133.31
4	B	1620	LUT	C3-C4-C5	2.48	118.36	112.18
4	A	621	LUT	C1-C6-C5	-2.48	119.24	122.64
9	C	607	CHL	C12-C11-C10	-2.48	102.16	113.28
10	H	612	CLA	C14-C13-C15	2.48	120.11	111.27
8	D	5632	DGD	C3D-C4D-C5D	2.48	114.73	110.23
8	E	4632	DGD	O3G-C1D-C2D	2.48	112.04	108.27
10	F	610	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
9	A	609	CHL	O2D-CGD-CBD	2.48	113.67	110.95
9	I	605	CHL	CAA-C2A-C3A	-2.48	106.30	113.00
10	H	614	CLA	CMC-C2C-C1C	2.48	128.91	125.03
8	D	5632	DGD	C3G-O3G-C1D	2.48	119.11	113.80
10	E	602	CLA	C5-C3-C2	-2.48	115.61	121.17
9	J	609	CHL	C14-C13-C15	2.48	120.10	111.27
10	I	610	CLA	C2A-C1A-CHA	2.47	128.16	123.87
10	H	610	CLA	C11-C10-C8	-2.47	107.74	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	607	CHL	O1D-CGD-CBD	-2.47	120.97	124.72
10	G	602	CLA	C7-C6-C5	2.47	119.85	113.26
5	D	8622	XAT	C15-C35-C34	-2.47	118.46	123.52
10	J	614	CLA	O2A-CGA-CBA	2.47	119.37	111.83
9	A	608	CHL	CHA-C1A-C2A	-2.47	127.50	133.31
10	C	603	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
10	H	610	CLA	C1-C2-C3	2.47	130.24	126.20
10	C	602	CLA	C11-C10-C8	-2.47	107.76	115.97
9	H	607	CHL	CMD-C2D-C3D	2.47	129.61	124.68
10	H	602	CLA	C11-C12-C13	-2.46	107.77	115.97
6	A	623	NEX	C24-C23-C22	2.46	115.40	110.79
5	F	6622	XAT	C38-C25-C24	-2.46	111.47	114.24
9	C	605	CHL	CHA-C1A-C2A	-2.46	127.53	133.31
9	C	607	CHL	CMD-C2D-C3D	2.46	129.60	124.68
10	B	610	CLA	C1D-ND-C4D	-2.46	104.58	106.31
8	G	9632	DGD	C4D-C3D-C2D	2.46	115.15	110.83
9	F	608	CHL	C16-C15-C13	2.46	124.14	115.97
10	A	610	CLA	C2A-C1A-CHA	2.46	128.13	123.87
10	B	613	CLA	O2A-CGA-CBA	2.46	119.32	111.83
9	G	606	CHL	C5-C3-C4	-2.45	108.94	114.59
10	I	611	CLA	CED-O2D-CGD	2.45	121.48	115.92
6	J	9623	NEX	C16-C1-C6	2.45	112.67	110.47
5	I	9622	XAT	C27-C28-C29	-2.45	121.72	125.53
10	A	613	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
10	J	613	CLA	CMB-C2B-C3B	2.45	132.32	126.55
10	D	604	CLA	C6-C7-C8	2.45	124.11	115.97
10	J	614	CLA	C3B-C4B-NB	-2.45	108.34	110.53
7	E	4630	LHG	O7-C7-C8	2.45	116.78	111.48
10	A	614	CLA	CAA-CBA-CGA	2.45	120.16	113.21
9	G	607	CHL	CHA-C1A-C2A	-2.45	127.56	133.31
8	G	9632	DGD	O3G-C1D-C2D	2.45	111.99	108.27
10	H	602	CLA	C9-C8-C7	2.45	119.99	111.27
9	D	601	CHL	C6-C5-C3	2.45	119.42	113.47
10	I	604	CLA	CAA-C2A-C1A	2.44	119.99	111.97
4	G	6621	LUT	C1-C6-C5	-2.44	119.30	122.64
10	H	603	CLA	C1-C2-C3	2.44	130.19	126.20
10	F	604	CLA	CAA-C2A-C1A	2.44	119.97	111.97
9	H	605	CHL	CED-O2D-CGD	2.44	121.45	115.92
10	B	602	CLA	C12-C11-C10	-2.44	102.36	113.28
10	D	611	CLA	C6-C7-C8	2.44	124.06	115.97
6	E	4623	NEX	C16-C1-C6	2.44	112.65	110.47
9	H	607	CHL	CHA-C1A-C2A	-2.44	127.59	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	611	CLA	CMB-C2B-C1B	-2.44	121.71	125.42
9	I	606	CHL	CED-O2D-CGD	2.43	121.44	115.92
10	F	611	CLA	C3B-C4B-NB	-2.43	108.36	110.53
8	H	6632	DGD	C4D-C3D-C2D	2.43	115.10	110.83
10	B	614	CLA	CED-O2D-CGD	2.43	121.43	115.92
10	B	604	CLA	C9-C8-C10	2.43	119.93	111.27
8	H	6632	DGD	O3G-C1D-C2D	2.42	111.95	108.27
9	D	609	CHL	CAA-CBA-CGA	2.42	120.09	113.21
10	D	603	CLA	C3B-C4B-NB	-2.42	108.37	110.53
10	B	611	CLA	C9-C8-C10	2.42	119.91	111.27
10	E	611	CLA	C9-C8-C10	2.42	119.90	111.27
10	A	610	CLA	O2D-CGD-CBD	2.42	115.46	111.23
10	E	602	CLA	C11-C10-C8	-2.42	107.93	115.97
9	C	601	CHL	C16-C15-C13	2.42	124.00	115.97
9	A	607	CHL	CHA-C1A-C2A	-2.42	127.63	133.31
9	C	607	CHL	CHA-C1A-C2A	-2.41	127.64	133.31
9	F	609	CHL	CAA-C2A-C3A	-2.41	106.48	113.00
6	F	5623	NEX	C1-C2-C3	2.41	118.88	113.59
8	H	6632	DGD	C3G-C2G-C1G	-2.41	106.16	111.78
9	C	608	CHL	C6-C7-C8	-2.41	107.96	115.97
7	D	3630	LHG	O10-C23-C24	-2.41	114.36	123.78
10	D	614	CLA	C3B-C4B-NB	-2.41	108.38	110.53
10	G	612	CLA	C3B-C4B-NB	-2.41	108.38	110.53
9	G	605	CHL	CED-O2D-CGD	2.40	121.36	115.92
9	I	608	CHL	CMB-C2B-C3B	2.40	129.48	124.68
4	A	620	LUT	C1-C2-C3	2.40	118.86	113.59
4	F	5621	LUT	C1-C6-C5	-2.40	119.36	122.64
10	A	603	CLA	C16-C15-C13	2.40	123.94	115.97
9	J	605	CHL	CAA-C2A-C3A	-2.40	106.52	113.00
9	J	601	CHL	C7-C6-C5	-2.40	106.88	113.26
9	B	601	CHL	CMD-C2D-C3D	2.40	129.47	124.68
8	B	2632	DGD	O3G-C1D-C2D	2.39	111.91	108.27
10	C	614	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
9	F	609	CHL	C6-C5-C3	2.39	119.28	113.47
9	B	607	CHL	C16-C15-C13	-2.39	108.04	115.97
10	E	613	CLA	C3B-C4B-NB	-2.38	108.40	110.53
4	I	8620	LUT	C3-C4-C5	2.38	118.11	112.18
5	B	1622	XAT	C27-C28-C29	-2.38	121.83	125.53
9	A	605	CHL	O1D-CGD-CBD	-2.38	121.11	124.72
7	I	8630	LHG	O7-C7-C8	2.38	116.64	111.48
6	I	8623	NEX	C1-C2-C3	2.38	118.82	113.59
10	D	612	CLA	C3B-C4B-NB	-2.38	108.40	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	605	CHL	CMB-C2B-C3B	2.38	129.44	124.68
10	D	602	CLA	C11-C12-C13	-2.38	108.05	115.97
10	E	603	CLA	C12-C11-C10	-2.38	102.61	113.28
10	A	614	CLA	C3B-C4B-NB	-2.38	108.41	110.53
10	J	611	CLA	C12-C11-C10	-2.38	102.62	113.28
9	F	607	CHL	O1D-CGD-CBD	-2.38	121.12	124.72
9	C	608	CHL	CMB-C2B-C3B	2.38	129.43	124.68
10	J	610	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
9	B	609	CHL	CAA-CBA-CGA	2.38	119.96	113.21
10	F	610	CLA	C2A-C1A-CHA	2.38	127.99	123.87
10	C	603	CLA	C3B-C4B-NB	-2.38	108.41	110.53
10	J	614	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
9	D	606	CHL	OBD-CAD-C3D	2.37	131.60	127.89
10	D	603	CLA	O2A-CGA-CBA	2.37	119.07	111.83
10	B	604	CLA	C6-C7-C8	2.37	123.85	115.97
10	H	613	CLA	CAA-CBA-CGA	2.37	119.94	113.21
10	A	602	CLA	C4-C3-C5	2.37	119.34	115.23
9	G	607	CHL	CED-O2D-CGD	2.37	121.29	115.92
10	G	610	CLA	C2A-C1A-CHA	2.37	127.98	123.87
9	H	607	CHL	CED-O2D-CGD	2.37	121.29	115.92
6	H	7623	NEX	C1-C2-C3	2.37	118.78	113.59
10	H	612	CLA	CED-O2D-CGD	2.37	121.28	115.92
9	J	608	CHL	CMB-C2B-C3B	2.37	129.41	124.68
9	C	601	CHL	C14-C13-C12	2.37	119.71	111.27
9	G	609	CHL	CMB-C2B-C3B	2.37	129.41	124.68
9	F	608	CHL	CMB-C2B-C3B	2.36	129.41	124.68
9	I	607	CHL	CHA-C1A-C2A	-2.36	127.76	133.31
4	B	1620	LUT	C1-C2-C3	2.36	118.78	113.59
9	J	607	CHL	C5-C3-C2	2.36	126.47	121.17
9	B	606	CHL	CMD-C2D-C3D	2.36	129.40	124.68
9	C	608	CHL	C14-C13-C15	2.36	119.68	111.27
10	D	614	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
10	B	614	CLA	CBA-CAA-C2A	2.36	120.80	113.79
10	A	611	CLA	C11-C12-C13	2.35	123.79	115.97
4	F	5620	LUT	C1-C2-C3	2.35	118.75	113.59
9	E	606	CHL	C5-C3-C4	-2.35	109.18	114.59
10	H	613	CLA	C1-C2-C3	2.35	130.05	126.20
10	C	603	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
9	E	607	CHL	CHA-C1A-C2A	-2.35	127.79	133.31
9	A	606	CHL	O1D-CGD-CBD	-2.35	121.16	124.72
10	F	612	CLA	C3B-C4B-NB	-2.35	108.43	110.53
10	C	613	CLA	O2A-CGA-CBA	2.35	118.99	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	601	CHL	CMB-C2B-C3B	2.35	129.37	124.68
9	H	607	CHL	C14-C13-C12	2.35	119.64	111.27
10	F	612	CLA	CMB-C2B-C1B	-2.34	121.85	125.42
9	A	605	CHL	CAA-C2A-C3A	-2.34	106.67	113.00
10	H	613	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
4	D	3621	LUT	C18-C5-C6	2.34	127.04	124.48
9	E	605	CHL	O2D-CGD-CBD	2.34	113.52	110.95
9	I	601	CHL	C12-C11-C10	-2.34	102.79	113.28
10	C	611	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
10	D	610	CLA	C2A-C1A-CHA	2.34	127.92	123.87
8	D	5632	DGD	C6D-C5D-C4D	2.34	116.97	112.07
9	E	605	CHL	O2A-CGA-O1A	-2.34	117.78	123.63
9	G	605	CHL	O2A-CGA-O1A	-2.34	117.78	123.63
10	H	611	CLA	O2D-CGD-CBD	2.34	115.32	111.23
6	A	623	NEX	C1-C2-C3	2.34	118.72	113.59
10	H	610	CLA	C2A-C1A-CHA	2.34	127.92	123.87
10	G	610	CLA	C14-C13-C12	2.34	119.61	111.27
9	I	605	CHL	O2D-CGD-CBD	2.34	113.51	110.95
10	E	613	CLA	C5-C3-C2	2.34	126.41	121.17
4	E	4621	LUT	C18-C5-C4	-2.33	110.13	114.42
10	B	614	CLA	C3B-C4B-NB	-2.33	108.45	110.53
8	D	5632	DGD	O3G-C1D-C2D	2.33	111.82	108.27
10	I	602	CLA	C6-C7-C8	-2.33	108.21	115.97
10	J	610	CLA	C2A-C1A-CHA	2.33	127.91	123.87
10	F	604	CLA	CED-O2D-CGD	2.33	121.20	115.92
5	B	5622	XAT	C37-C21-C22	-2.33	104.87	108.97
10	I	602	CLA	C11-C12-C13	-2.33	108.22	115.97
9	J	605	CHL	O2A-CGA-O1A	-2.33	117.81	123.63
5	C	7622	XAT	C37-C21-C36	2.33	110.75	107.37
9	J	607	CHL	C6-C5-C3	2.33	119.14	113.47
10	B	610	CLA	C2A-C1A-CHA	2.33	127.90	123.87
10	B	611	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
9	B	607	CHL	C1-C2-C3	-2.32	122.39	126.20
10	D	602	CLA	C12-C11-C10	-2.32	102.87	113.28
10	F	614	CLA	C3B-C4B-NB	-2.32	108.46	110.53
10	C	612	CLA	C11-C12-C13	2.32	123.68	115.97
4	E	4620	LUT	C3-C4-C5	2.32	117.95	112.18
10	A	611	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
10	I	612	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
10	H	611	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
6	C	2623	NEX	C16-C1-C6	2.32	112.55	110.47
9	F	606	CHL	O1A-CGA-CBA	-2.32	114.72	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1622	XAT	C38-C25-C24	-2.32	111.64	114.24
10	E	614	CLA	C3B-C4B-NB	-2.32	108.46	110.53
9	D	606	CHL	O2A-CGA-O1A	-2.31	117.84	123.63
10	C	614	CLA	C3B-C4B-NB	-2.31	108.47	110.53
9	C	607	CHL	CED-O2D-CGD	2.31	121.16	115.92
9	A	607	CHL	C3C-C4C-NC	-2.31	109.00	114.65
10	F	612	CLA	CBA-CAA-C2A	2.31	120.67	113.79
9	F	607	CHL	C1-C2-C3	-2.31	122.41	126.20
4	G	6620	LUT	C1-C2-C3	2.31	118.66	113.59
9	D	607	CHL	C3C-C4C-NC	-2.31	109.01	114.65
10	E	604	CLA	O2D-CGD-CBD	2.31	115.27	111.23
9	I	607	CHL	C6-C5-C3	2.31	119.09	113.47
10	G	614	CLA	CAA-CBA-CGA	2.31	119.76	113.21
9	J	609	CHL	CAA-CBA-CGA	2.31	119.76	113.21
9	J	607	CHL	C14-C13-C12	2.31	119.49	111.27
6	G	6623	NEX	C38-C25-C24	-2.30	111.65	114.24
10	B	603	CLA	C3B-C4B-NB	-2.30	108.47	110.53
6	D	3623	NEX	C24-C23-C22	2.30	115.10	110.79
10	E	612	CLA	C3B-C4B-NB	-2.30	108.48	110.53
9	F	607	CHL	CHA-C1A-C2A	-2.30	127.90	133.31
10	J	602	CLA	C9-C8-C10	-2.30	103.07	111.27
9	C	607	CHL	OBD-CAD-C3D	2.30	131.48	127.89
10	H	602	CLA	C9-C8-C10	-2.30	103.09	111.27
10	E	611	CLA	C3B-C4B-NB	-2.30	108.48	110.53
9	B	606	CHL	OBD-CAD-C3D	2.30	131.47	127.89
10	E	610	CLA	C2A-C1A-CHA	2.29	127.85	123.87
8	I	8632	DGD	O3G-C1D-C2D	2.29	111.75	108.27
10	B	611	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
10	G	612	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
10	C	611	CLA	C12-C11-C10	-2.29	103.02	113.28
10	I	611	CLA	C4-C3-C5	-2.29	111.25	115.23
10	G	603	CLA	C7-C6-C5	-2.29	107.16	113.26
10	A	603	CLA	C3B-C4B-NB	-2.29	108.49	110.53
9	C	605	CHL	O2A-CGA-O1A	-2.29	117.90	123.63
9	I	607	CHL	C7-C6-C5	-2.29	107.16	113.26
9	H	605	CHL	CAA-C2A-C3A	-2.29	106.82	113.00
9	E	608	CHL	C14-C13-C15	2.29	119.42	111.27
10	I	611	CLA	C4D-CHA-C1A	2.29	123.97	121.24
9	F	609	CHL	C16-C15-C13	2.29	123.56	115.97
10	F	611	CLA	C4-C3-C5	-2.29	111.26	115.23
6	G	6623	NEX	C1-C2-C3	2.28	118.61	113.59
9	J	607	CHL	C7-C6-C5	-2.28	107.17	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	605	CHL	CMB-C2B-C3B	2.28	129.25	124.68
9	C	608	CHL	OBD-CAD-C3D	2.28	131.45	127.89
9	J	608	CHL	OBD-CAD-C3D	2.28	131.45	127.89
10	A	612	CLA	CBA-CAA-C2A	2.28	120.58	113.79
9	C	607	CHL	C3C-C4C-NC	-2.28	109.07	114.65
9	D	601	CHL	CBC-CAC-C3C	-2.28	109.61	112.87
4	B	1620	LUT	C21-C26-C27	2.28	115.45	112.83
10	I	612	CLA	C14-C13-C15	2.28	119.40	111.27
10	A	611	CLA	C9-C8-C10	2.28	119.40	111.27
5	H	4622	XAT	C37-C21-C22	-2.28	104.96	108.97
8	D	5632	DGD	C4D-C3D-C2D	2.28	114.83	110.83
10	J	611	CLA	CAA-CBA-CGA	2.28	119.68	113.21
10	D	610	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
4	D	3620	LUT	C21-C26-C27	2.28	115.44	112.83
10	F	604	CLA	C9-C8-C10	2.28	119.39	111.27
8	A	632	DGD	C6D-C5D-C4D	2.28	116.84	112.07
9	G	609	CHL	CAA-C2A-C3A	-2.27	106.85	113.00
10	I	611	CLA	C16-C15-C13	2.27	123.52	115.97
9	E	601	CHL	C14-C13-C15	2.27	119.38	111.27
10	I	611	CLA	C11-C12-C13	2.27	123.51	115.97
10	E	614	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
9	E	606	CHL	O1D-CGD-CBD	-2.27	121.28	124.72
9	B	608	CHL	C3C-C4C-NC	-2.27	109.11	114.65
10	E	603	CLA	CAA-C2A-C1A	2.27	119.41	111.97
9	G	607	CHL	C3C-C4C-NC	-2.27	109.11	114.65
9	I	605	CHL	C3C-C4C-NC	-2.27	109.11	114.65
10	F	602	CLA	O2A-CGA-CBA	2.27	118.75	111.83
9	H	608	CHL	C14-C13-C15	2.27	119.36	111.27
4	H	7620	LUT	C3-C4-C5	2.27	117.83	112.18
9	H	607	CHL	C3C-C4C-NC	-2.27	109.11	114.65
10	H	612	CLA	C3B-C4B-NB	-2.27	108.51	110.53
10	F	603	CLA	CAA-C2A-C1A	2.27	119.40	111.97
9	F	601	CHL	C6-C5-C3	2.27	118.99	113.47
9	E	608	CHL	OBD-CAD-C3D	2.26	131.43	127.89
10	A	612	CLA	C3B-C4B-NB	-2.26	108.51	110.53
9	G	608	CHL	C14-C13-C15	2.26	119.34	111.27
9	D	601	CHL	OBD-CAD-C3D	2.26	131.42	127.89
10	E	610	CLA	C1D-ND-C4D	-2.26	104.73	106.31
10	C	611	CLA	C3B-C4B-NB	-2.26	108.51	110.53
9	A	608	CHL	CMB-C2B-C3B	2.26	129.19	124.68
9	D	608	CHL	C3C-C4C-NC	-2.26	109.13	114.65
9	D	609	CHL	C3C-C4C-NC	-2.26	109.14	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	611	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
9	I	606	CHL	CMD-C2D-C3D	2.25	129.19	124.68
9	C	606	CHL	O2A-CGA-O1A	-2.25	117.99	123.63
10	F	611	CLA	C9-C8-C10	2.25	119.31	111.27
9	D	605	CHL	C3C-C4C-NC	-2.25	109.14	114.65
4	C	2620	LUT	C3-C4-C5	2.25	117.79	112.18
9	B	605	CHL	CAA-C2A-C3A	-2.25	106.92	113.00
9	J	608	CHL	C14-C13-C15	2.25	119.30	111.27
10	E	603	CLA	C11-C12-C13	2.25	123.45	115.97
10	G	604	CLA	C12-C11-C10	-2.25	103.19	113.28
9	G	609	CHL	C3C-C4C-NC	-2.25	109.16	114.65
10	D	603	CLA	C16-C17-C18	2.25	125.96	115.94
10	C	614	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
10	G	613	CLA	C6-C5-C3	2.25	118.94	113.47
9	J	601	CHL	CMB-C2B-C3B	2.24	129.17	124.68
10	F	603	CLA	C1-C2-C3	2.24	129.87	126.20
9	D	605	CHL	OBD-CAD-C3D	2.24	131.39	127.89
9	H	601	CHL	C4-C3-C5	-2.24	111.34	115.23
9	F	606	CHL	O2A-CGA-O1A	-2.24	118.03	123.63
9	I	607	CHL	C3C-C4C-NC	-2.24	109.18	114.65
10	A	613	CLA	C12-C11-C10	-2.24	103.25	113.28
9	D	606	CHL	O1A-CGA-CBA	-2.24	115.03	123.78
9	B	605	CHL	C3C-C4C-NC	-2.24	109.19	114.65
10	D	611	CLA	C3B-C4B-NB	-2.24	108.53	110.53
5	F	6622	XAT	C37-C21-C36	2.24	110.62	107.37
10	I	614	CLA	C3B-C4B-NB	-2.23	108.53	110.53
4	I	8620	LUT	C1-C2-C3	2.23	118.49	113.59
9	B	606	CHL	O1D-CGD-CBD	-2.23	121.34	124.72
10	J	612	CLA	C3B-C4B-NB	-2.23	108.54	110.53
9	D	601	CHL	C3C-C4C-NC	-2.23	109.19	114.65
9	I	608	CHL	C14-C13-C15	2.23	119.23	111.27
8	B	1632	DGD	O3G-C1D-C2D	2.23	111.66	108.27
10	A	614	CLA	CMD-C2D-C1D	2.23	128.65	124.73
10	E	613	CLA	C6-C5-C3	2.23	118.90	113.47
10	E	611	CLA	C4-C3-C5	-2.23	111.36	115.23
9	J	605	CHL	C3C-C4C-NC	-2.23	109.20	114.65
10	G	614	CLA	CMC-C2C-C1C	2.23	128.51	125.03
10	J	611	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
10	I	611	CLA	CBA-CAA-C2A	2.23	120.42	113.79
6	B	1623	NEX	C24-C23-C22	2.22	114.95	110.79
10	E	604	CLA	C1-C2-C3	2.22	129.84	126.20
10	F	611	CLA	O2A-CGA-O1A	-2.22	118.07	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	G	601	CHL	C3C-C4C-NC	-2.22	109.22	114.65
4	G	6621	LUT	C18-C5-C6	2.22	126.91	124.48
10	G	611	CLA	O2D-CGD-CBD	2.22	115.11	111.23
10	J	613	CLA	C4D-CHA-C1A	2.22	123.89	121.24
10	E	613	CLA	C11-C10-C8	2.22	123.33	115.97
10	H	603	CLA	C3B-C4B-NB	-2.22	108.55	110.53
9	B	601	CHL	C4-C3-C5	-2.22	111.38	115.23
10	B	603	CLA	C4-C3-C5	-2.22	111.38	115.23
9	B	609	CHL	O2A-CGA-CBA	2.22	118.59	111.83
9	C	605	CHL	C3C-C4C-NC	-2.21	109.24	114.65
9	D	605	CHL	O2A-CGA-O1A	-2.21	118.09	123.63
9	C	606	CHL	CMD-C2D-C3D	2.21	129.10	124.68
10	B	602	CLA	C11-C12-C13	-2.21	108.61	115.97
10	H	614	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
10	I	604	CLA	C11-C10-C8	2.21	123.31	115.97
10	C	610	CLA	C11-C10-C8	-2.21	108.62	115.97
4	C	2621	LUT	C1-C6-C5	-2.21	119.62	122.64
9	F	605	CHL	C3C-C4C-NC	-2.21	109.25	114.65
9	E	605	CHL	C3C-C4C-NC	-2.21	109.26	114.65
6	E	4623	NEX	C1-C2-C3	2.21	118.43	113.59
10	H	610	CLA	C1D-ND-C4D	-2.21	104.76	106.31
10	J	611	CLA	C3B-C4B-NB	-2.21	108.56	110.53
10	H	610	CLA	CAA-CBA-CGA	2.21	119.47	113.21
10	H	604	CLA	CBC-CAC-C3C	-2.20	106.44	112.42
9	G	608	CHL	C3C-C4C-NC	-2.20	109.26	114.65
10	A	602	CLA	C9-C8-C7	2.20	119.13	111.27
10	I	611	CLA	O2D-CGD-CBD	2.20	115.08	111.23
9	B	601	CHL	C3C-C4C-NC	-2.20	109.27	114.65
10	D	603	CLA	CAA-CBA-CGA	2.20	119.46	113.21
10	G	611	CLA	C4D-CHA-C1A	2.20	123.87	121.24
5	J	3622	XAT	C36-C21-C22	-2.20	105.10	108.97
6	J	9623	NEX	C1-C2-C3	2.20	118.42	113.59
5	E	2622	XAT	C27-C28-C29	-2.20	122.11	125.53
9	I	609	CHL	C6-C5-C3	2.20	118.83	113.47
10	C	610	CLA	C2A-C1A-CHA	2.20	127.69	123.87
10	F	604	CLA	C2B-C1B-NB	-2.20	108.04	110.33
9	F	609	CHL	O1D-CGD-CBD	-2.20	121.39	124.72
9	F	605	CHL	O2A-CGA-O1A	-2.20	118.12	123.63
10	A	613	CLA	CAA-CBA-CGA	2.20	119.45	113.21
9	H	605	CHL	CMB-C2B-C3B	2.20	129.08	124.68
10	I	602	CLA	C4D-CHA-C1A	2.20	123.86	121.24
9	E	607	CHL	C3C-C4C-NC	-2.20	109.28	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	609	CHL	C3C-C4C-NC	-2.20	109.28	114.65
10	H	602	CLA	C4D-CHA-C1A	2.20	123.86	121.24
9	I	605	CHL	OBD-CAD-C3D	2.19	131.31	127.89
10	D	611	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
9	B	601	CHL	C16-C15-C13	2.19	123.26	115.97
9	E	607	CHL	O1D-CGD-CBD	-2.19	121.40	124.72
9	I	605	CHL	O2A-CGA-O1A	-2.19	118.14	123.63
9	G	605	CHL	C3C-C4C-NC	-2.19	109.29	114.65
8	I	8632	DGD	C6D-C5D-C4D	2.19	116.67	112.07
9	A	607	CHL	O2D-CGD-CBD	2.19	113.35	110.95
9	J	606	CHL	O2D-CGD-CBD	2.19	113.35	110.95
10	B	611	CLA	C4D-CHA-C1A	2.19	123.86	121.24
10	E	613	CLA	C2B-C1B-NB	-2.19	108.06	110.33
4	G	6620	LUT	C1-C6-C5	-2.19	119.65	122.64
10	E	602	CLA	C9-C8-C10	-2.19	103.48	111.27
10	J	610	CLA	O1A-CGA-CBA	-2.19	115.23	123.78
9	C	608	CHL	C3C-C4C-NC	-2.19	109.30	114.65
10	E	613	CLA	CAA-C2A-C1A	2.19	119.14	111.97
10	E	611	CLA	C4D-CHA-C1A	2.19	123.85	121.24
9	B	609	CHL	C3C-C4C-NC	-2.19	109.31	114.65
10	I	603	CLA	O2A-CGA-CBA	2.19	118.50	111.83
9	F	608	CHL	OBD-CAD-C3D	2.18	131.30	127.89
9	B	608	CHL	C14-C13-C15	2.18	119.06	111.27
8	H	7632	DGD	C6D-C5D-C4D	2.18	116.65	112.07
9	A	608	CHL	C3C-C4C-NC	-2.18	109.32	114.65
9	J	607	CHL	C3C-C4C-NC	-2.18	109.32	114.65
9	F	607	CHL	C14-C13-C12	2.18	119.05	111.27
10	C	612	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
9	G	605	CHL	OBD-CAD-C3D	2.18	131.29	127.89
10	G	612	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
10	C	614	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
5	B	5622	XAT	C37-C21-C36	2.18	110.53	107.37
9	A	605	CHL	C3C-C4C-NC	-2.18	109.33	114.65
9	H	605	CHL	C3C-C4C-NC	-2.18	109.33	114.65
10	J	613	CLA	CAA-CBA-CGA	2.18	119.39	113.21
10	D	612	CLA	C11-C12-C13	2.18	123.19	115.97
9	B	605	CHL	O2A-CGA-O1A	-2.17	118.19	123.63
9	E	608	CHL	C3C-C4C-NC	-2.17	109.34	114.65
9	A	607	CHL	OBD-CAD-C3D	2.17	131.28	127.89
9	E	606	CHL	C3C-C4C-NC	-2.17	109.34	114.65
9	I	608	CHL	C3C-C4C-NC	-2.17	109.34	114.65
10	E	602	CLA	C4D-CHA-C1A	2.17	123.83	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	5622	XAT	C27-C28-C29	-2.17	122.16	125.53
10	E	610	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
9	A	605	CHL	OBD-CAD-C3D	2.17	131.28	127.89
9	E	606	CHL	OBD-CAD-C3D	2.17	131.28	127.89
10	A	603	CLA	C16-C17-C18	2.17	125.62	115.94
10	D	611	CLA	C4D-CHA-C1A	2.17	123.83	121.24
9	J	609	CHL	C3C-C4C-NC	-2.17	109.35	114.65
10	G	611	CLA	C3B-C4B-NB	-2.17	108.59	110.53
6	B	1623	NEX	C1-C2-C3	2.17	118.35	113.59
9	C	605	CHL	OBD-CAD-C3D	2.17	131.27	127.89
10	J	611	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
9	A	608	CHL	OBD-CAD-C3D	2.17	131.27	127.89
9	F	601	CHL	OBD-CAD-C3D	2.17	131.27	127.89
10	H	603	CLA	C9-C8-C10	-2.16	103.56	111.27
10	D	613	CLA	C1-C2-C3	2.16	129.74	126.20
9	H	609	CHL	C3C-C4C-NC	-2.16	109.36	114.65
5	D	8622	XAT	C37-C21-C36	2.16	110.51	107.37
10	E	612	CLA	CMC-C2C-C1C	2.16	128.41	125.03
10	D	610	CLA	C11-C10-C8	-2.16	108.78	115.97
9	F	601	CHL	C3C-C4C-NC	-2.16	109.37	114.65
4	A	620	LUT	C35-C15-C14	-2.16	119.10	123.52
9	F	609	CHL	OBD-CAD-C3D	2.16	131.26	127.89
10	I	614	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
10	G	614	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
10	J	612	CLA	CBA-CAA-C2A	2.16	120.21	113.79
10	G	611	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
9	B	606	CHL	C3C-C4C-NC	-2.16	109.38	114.65
10	A	603	CLA	CAA-CBA-CGA	2.16	119.33	113.21
10	B	612	CLA	C3B-C4B-NB	-2.16	108.61	110.53
9	H	601	CHL	C3C-C4C-NC	-2.16	109.38	114.65
10	J	604	CLA	CAA-C2A-C1A	2.15	119.03	111.97
10	A	611	CLA	C3B-C4B-NB	-2.15	108.61	110.53
10	H	604	CLA	CAA-C2A-C1A	2.15	119.03	111.97
9	B	601	CHL	OBD-CAD-C3D	2.15	131.25	127.89
10	B	604	CLA	CBC-CAC-C3C	-2.15	106.58	112.42
9	A	601	CHL	C3C-C4C-NC	-2.15	109.39	114.65
5	A	622	XAT	O24-C25-C24	2.15	115.51	113.49
9	J	608	CHL	C3C-C4C-NC	-2.15	109.39	114.65
9	A	609	CHL	C3C-C4C-NC	-2.15	109.40	114.65
9	C	609	CHL	C3C-C4C-NC	-2.15	109.40	114.65
10	J	612	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
10	C	612	CLA	C3B-C4B-NB	-2.15	108.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	611	CLA	C6-C7-C8	2.15	123.11	115.97
10	H	611	CLA	C4D-CHA-C1A	2.15	123.81	121.24
9	H	606	CHL	O2A-CGA-O1A	-2.15	118.26	123.63
10	H	611	CLA	C1D-ND-C4D	-2.15	104.81	106.31
10	F	611	CLA	CED-O2D-CGD	2.15	120.78	115.92
10	J	612	CLA	C4-C3-C5	-2.15	111.50	115.23
4	D	3621	LUT	C22-C23-C24	2.14	114.37	111.18
4	I	8621	LUT	C22-C23-C24	2.14	114.37	111.18
5	E	2622	XAT	C37-C21-C22	-2.14	105.20	108.97
9	I	607	CHL	OBD-CAD-C3D	2.14	131.24	127.89
10	I	613	CLA	C5-C3-C2	2.14	125.98	121.17
10	B	611	CLA	C3B-C4B-NB	-2.14	108.62	110.53
9	D	609	CHL	O1D-CGD-CBD	-2.14	121.47	124.72
10	J	610	CLA	C14-C13-C12	2.14	118.91	111.27
10	B	613	CLA	CAA-C2A-C1A	2.14	118.99	111.97
10	G	604	CLA	CAA-C2A-C1A	2.14	118.99	111.97
9	H	607	CHL	C12-C11-C10	-2.14	103.69	113.28
9	B	606	CHL	CED-O2D-CGD	2.14	120.77	115.92
9	I	608	CHL	O1D-CGD-CBD	-2.14	121.48	124.72
8	D	5632	DGD	O1B-C1B-C2B	-2.14	115.42	123.78
9	F	605	CHL	OBD-CAD-C3D	2.14	131.23	127.89
9	D	601	CHL	C7-C6-C5	-2.14	107.56	113.26
8	A	632	DGD	O3G-C1D-C2D	2.14	111.52	108.27
9	D	606	CHL	C3C-C4C-NC	-2.14	109.43	114.65
9	A	606	CHL	O2A-CGA-O1A	-2.14	118.28	123.63
9	H	609	CHL	CBA-CAA-C2A	2.14	120.07	113.78
9	C	601	CHL	C3C-C4C-NC	-2.14	109.43	114.65
10	F	611	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
10	A	612	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
9	G	601	CHL	OBD-CAD-C3D	2.13	131.22	127.89
10	D	613	CLA	CAA-C2A-C1A	2.13	118.97	111.97
9	A	606	CHL	CMD-C2D-C3D	2.13	128.95	124.68
10	D	603	CLA	C6-C5-C3	2.13	118.66	113.47
10	H	611	CLA	C3B-C4B-NB	-2.13	108.63	110.53
9	F	607	CHL	C3C-C4C-NC	-2.13	109.44	114.65
9	F	608	CHL	C3C-C4C-NC	-2.13	109.44	114.65
10	I	613	CLA	C4D-CHA-C1A	2.13	123.79	121.24
6	D	3623	NEX	C4-C3-C2	-2.13	106.80	110.79
9	I	601	CHL	C3C-C4C-NC	-2.13	109.44	114.65
8	D	3632	DGD	O3G-C1D-C2D	2.13	111.51	108.27
10	A	602	CLA	C11-C12-C13	-2.13	108.89	115.97
9	J	605	CHL	OBD-CAD-C3D	2.13	131.21	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	H	603	CLA	C16-C17-C18	2.13	125.44	115.94
9	G	609	CHL	CAA-CBA-CGA	2.13	119.25	113.21
4	C	2621	LUT	C18-C5-C6	2.13	126.81	124.48
10	H	604	CLA	C12-C11-C10	-2.13	103.75	113.28
10	H	612	CLA	C4-C3-C2	2.13	129.09	123.63
10	F	614	CLA	CED-O2D-CGD	2.13	120.74	115.92
10	A	604	CLA	C2A-C1A-CHA	2.13	127.56	123.87
9	G	605	CHL	CMA-C3A-C4A	-2.13	110.03	114.61
10	J	603	CLA	C3B-C4B-NB	-2.13	108.63	110.53
9	D	601	CHL	CMB-C2B-C3B	2.12	128.93	124.68
8	I	8632	DGD	C4D-C3D-C2D	2.12	114.56	110.83
10	E	613	CLA	C4D-CHA-C1A	2.12	123.78	121.24
10	F	604	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
9	C	608	CHL	C16-C17-C18	2.12	125.41	115.94
9	E	608	CHL	CAA-C2A-C3A	-2.12	107.26	113.00
10	G	612	CLA	C4-C3-C5	-2.12	111.54	115.23
9	B	608	CHL	C16-C17-C18	2.12	125.41	115.94
10	C	611	CLA	CAA-C2A-C1A	2.12	118.93	111.97
10	E	611	CLA	C6-C7-C8	2.12	123.02	115.97
9	E	607	CHL	OBD-CAD-C3D	2.12	131.20	127.89
10	B	613	CLA	C3A-C2A-C1A	2.12	104.52	101.34
9	A	607	CHL	CMD-C2D-C3D	2.12	128.92	124.68
10	F	611	CLA	O2D-CGD-CBD	2.12	114.94	111.23
10	F	613	CLA	C1-C2-C3	2.12	129.67	126.20
10	J	603	CLA	C1-C2-C3	2.12	129.67	126.20
9	B	601	CHL	CAA-CBA-CGA	2.12	119.23	113.21
10	H	613	CLA	C6-C5-C3	2.12	118.63	113.47
10	F	612	CLA	C11-C12-C13	2.12	123.01	115.97
10	I	612	CLA	C3B-C4B-NB	-2.12	108.64	110.53
10	H	610	CLA	O1A-CGA-CBA	-2.12	115.50	123.78
9	J	606	CHL	C3C-C4C-NC	-2.12	109.47	114.65
10	A	602	CLA	O2A-CGA-CBA	2.12	118.29	111.83
10	B	604	CLA	C2A-C1A-CHA	2.12	127.54	123.87
9	B	607	CHL	CMD-C2D-C3D	2.12	128.91	124.68
9	E	606	CHL	O2A-CGA-O1A	-2.12	118.33	123.63
10	D	613	CLA	C5-C3-C2	2.12	125.92	121.17
6	F	5623	NEX	C38-C25-C24	-2.12	111.86	114.24
9	H	607	CHL	CBC-CAC-C3C	2.11	115.90	112.87
9	H	601	CHL	CAA-CBA-CGA	2.11	119.21	113.21
10	H	611	CLA	CAA-CBA-CGA	2.11	119.21	113.21
6	E	4623	NEX	O24-C25-C24	2.11	115.47	113.49
9	J	601	CHL	C6-C5-C3	2.11	118.61	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	605	CHL	CED-O2D-CGD	2.11	120.70	115.92
9	F	609	CHL	C12-C11-C10	-2.11	103.82	113.28
10	A	611	CLA	C16-C15-C13	2.11	122.98	115.97
9	F	606	CHL	CBC-CAC-C3C	-2.11	109.85	112.87
9	H	605	CHL	O2A-CGA-O1A	-2.11	118.35	123.63
9	G	606	CHL	OBD-CAD-C3D	2.11	131.18	127.89
9	B	609	CHL	C7-C6-C5	-2.11	107.64	113.26
9	B	607	CHL	C6-C5-C3	2.11	118.60	113.47
10	D	612	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
10	G	603	CLA	C3B-C4B-NB	-2.11	108.65	110.53
6	D	3623	NEX	C16-C1-C6	2.11	112.36	110.47
10	D	613	CLA	C3A-C2A-C1A	2.11	104.49	101.34
9	F	606	CHL	C3C-C4C-NC	-2.10	109.51	114.65
10	B	611	CLA	CAA-CBA-CGA	2.10	119.18	113.21
9	C	606	CHL	C3C-C4C-NC	-2.10	109.51	114.65
10	J	603	CLA	CAA-C2A-C1A	2.10	118.86	111.97
9	J	605	CHL	CBC-CAC-C3C	2.10	115.88	112.87
10	F	612	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
9	B	607	CHL	C3C-C4C-NC	-2.10	109.52	114.65
6	H	7623	NEX	C27-C28-C29	2.10	128.79	125.53
10	A	612	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
10	I	614	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
9	I	606	CHL	OBD-CAD-C3D	2.10	131.17	127.89
10	G	602	CLA	C4D-CHA-C1A	2.10	123.75	121.24
10	A	603	CLA	O2A-CGA-CBA	2.10	118.23	111.83
9	B	608	CHL	O2A-CGA-O1A	-2.10	118.38	123.63
8	I	8632	DGD	C3D-C4D-C5D	2.10	114.03	110.23
9	F	608	CHL	CMD-C2D-C3D	2.10	128.87	124.68
9	A	606	CHL	C3C-C4C-NC	-2.10	109.53	114.65
10	J	612	CLA	CAA-C2A-C3A	-2.10	107.34	113.00
10	H	612	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
10	D	603	CLA	C9-C8-C10	-2.09	103.81	111.27
8	B	1632	DGD	C4D-C3D-C2D	2.09	114.50	110.83
10	H	613	CLA	CMA-C3A-C4A	2.09	117.40	111.77
10	B	603	CLA	C11-C12-C13	2.09	122.92	115.97
10	E	604	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
10	G	604	CLA	C9-C8-C10	2.09	118.73	111.27
9	E	605	CHL	OBD-CAD-C3D	2.09	131.15	127.89
10	E	612	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
9	C	607	CHL	C10-C8-C7	2.09	122.66	112.07
10	C	612	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
10	A	604	CLA	C2B-C1B-NB	-2.09	108.16	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	601	CHL	O2A-CGA-CBA	2.09	118.19	111.83
10	I	613	CLA	C3A-C2A-C1A	2.09	104.46	101.34
9	D	608	CHL	OBD-CAD-C3D	2.08	131.14	127.89
9	A	609	CHL	OBD-CAD-C3D	2.08	131.14	127.89
9	E	609	CHL	C3C-C4C-NC	-2.08	109.56	114.65
8	B	2632	DGD	C6D-C5D-C4D	2.08	116.44	112.07
10	I	611	CLA	C1D-ND-C4D	-2.08	104.85	106.31
10	J	602	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
10	A	602	CLA	C6-C7-C8	-2.08	109.05	115.97
9	D	608	CHL	C1-C2-C3	2.08	129.61	126.20
10	E	604	CLA	CBA-CAA-C2A	2.08	119.98	113.79
9	H	606	CHL	CMD-C2D-C3D	2.08	128.84	124.68
10	E	604	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
9	J	606	CHL	OBD-CAD-C3D	2.08	131.14	127.89
10	H	610	CLA	C9-C8-C7	2.08	118.69	111.27
10	J	612	CLA	C4D-CHA-C1A	2.08	123.72	121.24
9	F	606	CHL	O1D-CGD-CBD	-2.08	121.57	124.72
10	A	611	CLA	C4D-CHA-C1A	2.08	123.72	121.24
10	J	612	CLA	C4-C3-C2	2.08	128.96	123.63
9	E	608	CHL	O2A-CGA-O1A	-2.07	118.44	123.63
9	D	601	CHL	O2A-CGA-CBA	2.07	118.16	111.83
10	A	614	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
10	A	612	CLA	C4-C3-C5	-2.07	111.63	115.23
9	H	607	CHL	OBD-CAD-C3D	2.07	131.13	127.89
10	A	611	CLA	C11-C10-C8	2.07	122.86	115.97
10	C	611	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
9	E	601	CHL	C3C-C4C-NC	-2.07	109.58	114.65
10	J	604	CLA	C2B-C1B-NB	-2.07	108.18	110.33
10	J	610	CLA	C16-C15-C13	2.07	122.86	115.97
9	J	601	CHL	C3C-C4C-NC	-2.07	109.58	114.65
9	I	601	CHL	C16-C15-C13	2.07	122.85	115.97
9	A	607	CHL	C14-C13-C12	2.07	118.66	111.27
9	D	605	CHL	CMA-C3A-C4A	-2.07	110.15	114.61
10	I	604	CLA	C2B-C1B-NB	-2.07	108.18	110.33
9	C	608	CHL	C20-C18-C19	-2.07	101.30	110.53
10	A	603	CLA	CED-O2D-CGD	2.07	120.61	115.92
10	G	612	CLA	CMC-C2C-C1C	2.07	128.26	125.03
9	B	608	CHL	CMA-C3A-C4A	-2.07	110.16	114.61
10	J	613	CLA	C3A-C2A-C1A	2.07	104.44	101.34
9	G	607	CHL	OBD-CAD-C3D	2.07	131.12	127.89
10	F	612	CLA	C4D-CHA-C1A	2.06	123.71	121.24
10	B	612	CLA	O2A-CGA-O1A	-2.06	118.46	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	609	CHL	C3C-C4C-NC	-2.06	109.61	114.65
10	J	613	CLA	C3B-C4B-NB	-2.06	108.69	110.53
10	H	613	CLA	C4D-CHA-C1A	2.06	123.70	121.24
10	D	604	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
9	I	601	CHL	CBC-CAC-C3C	-2.06	109.92	112.87
5	C	7622	XAT	O24-C25-C24	2.06	115.42	113.49
4	A	620	LUT	C21-C26-C27	2.06	115.20	112.83
10	J	610	CLA	C11-C10-C8	-2.06	109.11	115.97
4	F	5621	LUT	C7-C8-C9	2.06	129.29	126.23
10	B	604	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
9	F	601	CHL	C11-C10-C8	2.06	122.82	115.97
9	I	607	CHL	C14-C13-C12	2.06	118.62	111.27
10	G	604	CLA	C6-C5-C3	2.06	118.49	113.47
9	A	601	CHL	O2A-CGA-CBA	2.06	118.12	111.83
9	H	608	CHL	C3C-C4C-NC	-2.06	109.62	114.65
5	E	2622	XAT	C37-C21-C36	2.06	110.36	107.37
8	G	9632	DGD	C6D-C5D-C4D	2.06	116.39	112.07
10	E	614	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
9	G	607	CHL	CMD-C2D-C3D	2.06	128.79	124.68
9	G	608	CHL	O1D-CGD-CBD	-2.06	121.60	124.72
10	C	614	CLA	CMD-C2D-C1D	2.06	128.35	124.73
10	B	610	CLA	C11-C10-C8	-2.06	109.13	115.97
9	D	607	CHL	OBD-CAD-C3D	2.06	131.10	127.89
10	B	602	CLA	C7-C6-C5	2.06	118.74	113.26
9	D	606	CHL	CMD-C2D-C3D	2.05	128.79	124.68
10	E	604	CLA	C2A-C1A-CHA	2.05	127.43	123.87
6	A	623	NEX	C38-C25-C24	-2.05	111.94	114.24
10	I	611	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
9	A	608	CHL	CAA-C2A-C3A	-2.05	107.46	113.00
9	E	601	CHL	C7-C6-C5	-2.05	107.80	113.26
9	C	609	CHL	C6-C5-C3	2.05	118.46	113.47
10	C	614	CLA	C2A-C1A-CHA	2.05	127.42	123.87
10	E	614	CLA	C2A-C1A-CHA	2.05	127.42	123.87
10	D	614	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
10	I	603	CLA	C16-C17-C18	2.05	125.07	115.94
10	I	610	CLA	C1D-ND-C4D	-2.05	104.88	106.31
5	D	8622	XAT	C31-C30-C29	-2.05	124.41	127.28
10	D	612	CLA	C3A-C2A-C1A	2.04	104.40	101.34
10	I	610	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
10	E	614	CLA	C4D-CHA-C1A	2.04	123.68	121.24
9	F	607	CHL	CMD-C2D-C3D	2.04	128.76	124.68
10	E	612	CLA	C11-C12-C13	2.04	122.74	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	H	611	CLA	C6-C7-C8	2.04	122.74	115.97
10	G	613	CLA	C4D-CHA-C1A	2.04	123.67	121.24
9	A	609	CHL	CBA-CAA-C2A	2.04	119.78	113.78
10	H	610	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
9	E	601	CHL	CAA-CBA-CGA	2.04	118.99	113.21
10	H	613	CLA	C3A-C2A-C1A	2.04	104.39	101.34
10	I	610	CLA	C1-C2-C3	2.04	129.53	126.20
10	G	613	CLA	C3A-C2A-C1A	2.03	104.39	101.34
10	H	603	CLA	C6-C5-C3	2.03	118.42	113.47
9	I	601	CHL	C1-C2-C3	2.03	129.53	126.20
10	F	604	CLA	CMA-C3A-C2A	-2.03	106.12	113.98
9	F	609	CHL	C20-C18-C19	-2.03	101.47	110.53
10	J	604	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
10	E	610	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
10	A	610	CLA	C1D-ND-C4D	-2.03	104.89	106.31
10	F	604	CLA	C11-C10-C8	2.03	122.72	115.97
9	C	608	CHL	C11-C12-C13	2.03	122.71	115.97
10	H	612	CLA	CBA-CAA-C2A	2.03	119.83	113.79
10	E	603	CLA	C3B-C4B-NB	-2.03	108.72	110.53
10	J	602	CLA	C4D-CHA-C1A	2.03	123.66	121.24
9	C	607	CHL	C4-C3-C5	-2.03	111.71	115.23
10	I	603	CLA	C16-C15-C13	2.02	122.69	115.97
10	A	613	CLA	CMB-C2B-C3B	2.02	131.31	126.55
10	J	604	CLA	C6-C7-C8	2.02	122.69	115.97
9	I	608	CHL	C9-C8-C7	-2.02	104.06	111.27
4	J	9621	LUT	C22-C23-C24	2.02	114.19	111.18
9	B	608	CHL	OBD-CAD-C3D	2.02	131.05	127.89
10	C	612	CLA	C11-C10-C8	2.02	122.69	115.97
9	B	609	CHL	CAA-C2A-C3A	-2.02	107.53	113.00
10	A	613	CLA	C3A-C2A-C1A	2.02	104.37	101.34
10	B	613	CLA	C4D-CHA-C1A	2.02	123.66	121.24
9	A	606	CHL	O1A-CGA-CBA	-2.02	115.87	123.78
9	E	607	CHL	C1-C2-C3	-2.02	122.89	126.20
10	G	604	CLA	C4D-CHA-C1A	2.02	123.66	121.24
10	J	614	CLA	C2A-C1A-CHA	2.02	127.37	123.87
10	J	614	CLA	C4D-CHA-C1A	2.02	123.65	121.24
10	B	610	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
10	B	611	CLA	O1A-CGA-CBA	-2.02	115.89	123.78
9	G	606	CHL	C3C-C4C-NC	-2.02	109.72	114.65
10	J	610	CLA	C1D-ND-C4D	-2.02	104.90	106.31
10	C	602	CLA	C4D-CHA-C1A	2.02	123.65	121.24
10	J	604	CLA	C2A-C1A-CHA	2.02	127.37	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	613	CLA	C3A-C2A-C1A	2.02	104.36	101.34
10	B	603	CLA	C4D-CHA-C1A	2.02	123.65	121.24
10	H	604	CLA	C4D-CHA-C1A	2.02	123.65	121.24
10	I	602	CLA	C9-C8-C7	2.02	118.46	111.27
10	H	612	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
10	J	611	CLA	C2A-C1A-CHA	2.02	127.36	123.87
9	I	606	CHL	C3C-C4C-NC	-2.02	109.72	114.65
9	F	609	CHL	O2A-CGA-CBA	2.02	117.98	111.83
9	C	609	CHL	OBD-CAD-C3D	2.01	131.03	127.89
9	D	609	CHL	O2A-CGA-CBA	2.01	117.98	111.83
10	D	614	CLA	C2A-C1A-CHA	2.01	127.36	123.87
10	D	613	CLA	C4D-CHA-C1A	2.01	123.65	121.24
10	H	612	CLA	C4D-CHA-C1A	2.01	123.65	121.24
9	H	606	CHL	OBD-CAD-C3D	2.01	131.03	127.89
5	H	4622	XAT	C31-C30-C29	-2.01	124.45	127.28
7	H	7630	LHG	C26-C25-C24	2.01	120.53	113.13
9	I	601	CHL	CMD-C2D-C3D	2.01	128.71	124.68
10	J	612	CLA	C3A-C2A-C1A	2.01	104.35	101.34
10	A	613	CLA	C4D-CHA-C1A	2.01	123.64	121.24
10	D	614	CLA	CAA-CBA-CGA	2.01	118.92	113.21
10	I	604	CLA	C2A-C1A-CHA	2.01	127.36	123.87
9	C	609	CHL	C7-C6-C5	-2.01	107.91	113.26
10	F	603	CLA	CAC-C3C-C4C	2.01	127.40	124.79
10	D	611	CLA	C4-C3-C5	-2.01	111.74	115.23
10	C	614	CLA	C4D-CHA-C1A	2.01	123.64	121.24
10	F	612	CLA	C2A-C1A-CHA	2.01	127.35	123.87
10	D	613	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
10	B	614	CLA	C4D-CHA-C1A	2.01	123.64	121.24
10	G	611	CLA	C16-C15-C13	2.01	122.64	115.97
10	B	604	CLA	C2B-C1B-NB	-2.01	108.25	110.33
10	I	603	CLA	C3A-C2A-C1A	2.01	104.34	101.34
10	C	604	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
4	B	1620	LUT	C35-C15-C14	-2.01	119.42	123.52
8	D	3632	DGD	C6D-C5D-C4D	2.01	116.28	112.07
9	B	601	CHL	O2A-CGA-CBA	2.01	117.95	111.83
10	D	610	CLA	C14-C13-C12	2.01	118.42	111.27
10	G	602	CLA	CMB-C2B-C1B	-2.01	122.37	125.42
10	F	604	CLA	C4D-CHA-C1A	2.00	123.64	121.24
10	D	603	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
10	G	610	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
10	C	613	CLA	C3A-C2A-C1A	2.00	104.34	101.34

All (343) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	632	DGD	C5D
8	A	632	DGD	C2D
8	B	1632	DGD	C5D
8	B	1632	DGD	C2D
8	B	2632	DGD	C5D
8	B	2632	DGD	C2D
8	D	3632	DGD	C5D
8	D	3632	DGD	C2D
8	D	5632	DGD	C5D
8	D	5632	DGD	C2D
8	E	4632	DGD	C5D
8	E	4632	DGD	C2D
8	G	9632	DGD	C5D
8	G	9632	DGD	C2D
8	H	6632	DGD	C5D
8	H	6632	DGD	C2D
8	H	7632	DGD	C5D
8	H	7632	DGD	C2D
8	I	8632	DGD	C5D
8	I	8632	DGD	C2D
9	A	601	CHL	C8
9	A	601	CHL	ND
9	A	601	CHL	C13
9	A	601	CHL	NC
9	A	601	CHL	NA
9	A	605	CHL	ND
9	A	605	CHL	NA
9	A	605	CHL	NC
9	A	606	CHL	ND
9	A	606	CHL	NA
9	A	606	CHL	NC
9	A	607	CHL	ND
9	A	607	CHL	NA
9	A	607	CHL	NC
9	A	608	CHL	C8
9	A	608	CHL	ND
9	A	608	CHL	NA
9	A	608	CHL	NC
9	A	609	CHL	C8
9	A	609	CHL	ND
9	A	609	CHL	C13
9	A	609	CHL	NC
9	A	609	CHL	NA

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Mol	Chain	Res	Type	Atom
9	B	601	CHL	C8
9	B	601	CHL	ND
9	B	601	CHL	NA
9	B	601	CHL	NC
9	B	605	CHL	ND
9	B	605	CHL	NA
9	B	605	CHL	NC
9	B	606	CHL	ND
9	B	606	CHL	NA
9	B	606	CHL	NC
9	B	607	CHL	ND
9	B	607	CHL	NA
9	B	607	CHL	NC
9	B	608	CHL	C8
9	B	608	CHL	ND
9	B	608	CHL	NA
9	B	608	CHL	NC
9	B	609	CHL	C8
9	B	609	CHL	ND
9	B	609	CHL	C13
9	B	609	CHL	NC
9	B	609	CHL	NA
9	C	601	CHL	C8
9	C	601	CHL	ND
9	C	601	CHL	NA
9	C	601	CHL	NC
9	C	605	CHL	ND
9	C	605	CHL	NA
9	C	605	CHL	NC
9	C	606	CHL	ND
9	C	606	CHL	NA
9	C	606	CHL	NC
9	C	607	CHL	ND
9	C	607	CHL	NA
9	C	607	CHL	NC
9	C	608	CHL	C8
9	C	608	CHL	ND
9	C	608	CHL	NA
9	C	608	CHL	NC
9	C	609	CHL	C8
9	C	609	CHL	ND
9	C	609	CHL	C13

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Mol	Chain	Res	Type	Atom
9	C	609	CHL	NC
9	C	609	CHL	NA
9	D	601	CHL	C8
9	D	601	CHL	ND
9	D	601	CHL	NA
9	D	601	CHL	NC
9	D	605	CHL	ND
9	D	605	CHL	NA
9	D	605	CHL	NC
9	D	606	CHL	ND
9	D	606	CHL	NA
9	D	606	CHL	NC
9	D	607	CHL	ND
9	D	607	CHL	NA
9	D	607	CHL	NC
9	D	608	CHL	C8
9	D	608	CHL	ND
9	D	608	CHL	NA
9	D	608	CHL	NC
9	D	609	CHL	C8
9	D	609	CHL	C13
9	D	609	CHL	NC
9	D	609	CHL	ND
9	D	609	CHL	NA
9	E	601	CHL	C8
9	E	601	CHL	ND
9	E	601	CHL	NA
9	E	601	CHL	NC
9	E	605	CHL	ND
9	E	605	CHL	NA
9	E	605	CHL	NC
9	E	606	CHL	ND
9	E	606	CHL	NA
9	E	606	CHL	NC
9	E	607	CHL	ND
9	E	607	CHL	NA
9	E	607	CHL	NC
9	E	608	CHL	C8
9	E	608	CHL	ND
9	E	608	CHL	NA
9	E	608	CHL	NC
9	E	609	CHL	C8

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Mol	Chain	Res	Type	Atom
9	E	609	CHL	ND
9	E	609	CHL	C13
9	E	609	CHL	NC
9	E	609	CHL	NA
9	F	601	CHL	C8
9	F	601	CHL	ND
9	F	601	CHL	NA
9	F	601	CHL	NC
9	F	605	CHL	ND
9	F	605	CHL	NA
9	F	605	CHL	NC
9	F	606	CHL	ND
9	F	606	CHL	NA
9	F	606	CHL	NC
9	F	607	CHL	ND
9	F	607	CHL	NA
9	F	607	CHL	NC
9	F	608	CHL	C8
9	F	608	CHL	ND
9	F	608	CHL	NA
9	F	608	CHL	NC
9	F	609	CHL	C8
9	F	609	CHL	ND
9	F	609	CHL	C13
9	F	609	CHL	NC
9	F	609	CHL	NA
9	G	601	CHL	C8
9	G	601	CHL	ND
9	G	601	CHL	NA
9	G	601	CHL	NC
9	G	605	CHL	ND
9	G	605	CHL	NA
9	G	605	CHL	NC
9	G	606	CHL	ND
9	G	606	CHL	NA
9	G	606	CHL	NC
9	G	607	CHL	ND
9	G	607	CHL	NA
9	G	607	CHL	NC
9	G	608	CHL	C8
9	G	608	CHL	ND
9	G	608	CHL	NA

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Mol	Chain	Res	Type	Atom
9	G	608	CHL	NC
9	G	609	CHL	C8
9	G	609	CHL	C13
9	G	609	CHL	NC
9	G	609	CHL	ND
9	G	609	CHL	NA
9	H	601	CHL	C8
9	H	601	CHL	ND
9	H	601	CHL	NA
9	H	601	CHL	NC
9	H	605	CHL	ND
9	H	605	CHL	NA
9	H	605	CHL	NC
9	H	606	CHL	ND
9	H	606	CHL	NA
9	H	606	CHL	NC
9	H	607	CHL	ND
9	H	607	CHL	NA
9	H	607	CHL	NC
9	H	608	CHL	C8
9	H	608	CHL	ND
9	H	608	CHL	NA
9	H	608	CHL	NC
9	H	609	CHL	C8
9	H	609	CHL	C13
9	H	609	CHL	NC
9	H	609	CHL	ND
9	H	609	CHL	NA
9	I	601	CHL	C8
9	I	601	CHL	ND
9	I	601	CHL	NA
9	I	601	CHL	NC
9	I	605	CHL	ND
9	I	605	CHL	NA
9	I	605	CHL	NC
9	I	606	CHL	ND
9	I	606	CHL	NA
9	I	606	CHL	NC
9	I	607	CHL	ND
9	I	607	CHL	NA
9	I	607	CHL	NC
9	I	608	CHL	C8

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Mol	Chain	Res	Type	Atom
9	I	608	CHL	ND
9	I	608	CHL	NA
9	I	608	CHL	NC
9	I	609	CHL	C8
9	I	609	CHL	ND
9	I	609	CHL	C13
9	I	609	CHL	NC
9	I	609	CHL	NA
9	J	601	CHL	C8
9	J	601	CHL	ND
9	J	601	CHL	NA
9	J	601	CHL	NC
9	J	605	CHL	ND
9	J	605	CHL	NA
9	J	605	CHL	NC
9	J	606	CHL	ND
9	J	606	CHL	NA
9	J	606	CHL	NC
9	J	607	CHL	ND
9	J	607	CHL	NA
9	J	607	CHL	NC
9	J	608	CHL	C8
9	J	608	CHL	ND
9	J	608	CHL	NA
9	J	608	CHL	NC
9	J	609	CHL	C8
9	J	609	CHL	C13
9	J	609	CHL	NC
9	J	609	CHL	ND
9	J	609	CHL	NA
10	A	602	CLA	C8
10	A	602	CLA	ND
10	A	603	CLA	C8
10	A	603	CLA	ND
10	A	604	CLA	ND
10	A	610	CLA	ND
10	A	611	CLA	ND
10	A	612	CLA	ND
10	A	613	CLA	ND
10	A	614	CLA	ND
10	B	602	CLA	C8
10	B	602	CLA	ND

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Mol	Chain	Res	Type	Atom
10	B	603	CLA	C8
10	B	603	CLA	ND
10	B	604	CLA	ND
10	B	610	CLA	ND
10	B	611	CLA	ND
10	B	612	CLA	ND
10	B	613	CLA	ND
10	B	614	CLA	ND
10	C	602	CLA	C8
10	C	602	CLA	ND
10	C	603	CLA	C8
10	C	603	CLA	ND
10	C	604	CLA	ND
10	C	610	CLA	ND
10	C	611	CLA	ND
10	C	612	CLA	ND
10	C	613	CLA	ND
10	C	614	CLA	ND
10	D	602	CLA	C8
10	D	602	CLA	ND
10	D	603	CLA	C8
10	D	603	CLA	ND
10	D	604	CLA	ND
10	D	610	CLA	ND
10	D	611	CLA	ND
10	D	612	CLA	ND
10	D	613	CLA	ND
10	D	614	CLA	ND
10	E	602	CLA	C8
10	E	602	CLA	ND
10	E	603	CLA	C8
10	E	603	CLA	ND
10	E	604	CLA	ND
10	E	610	CLA	ND
10	E	611	CLA	ND
10	E	612	CLA	ND
10	E	613	CLA	ND
10	E	614	CLA	ND
10	F	602	CLA	C8
10	F	602	CLA	ND
10	F	603	CLA	C8
10	F	603	CLA	ND

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Mol	Chain	Res	Type	Atom
10	F	604	CLA	ND
10	F	610	CLA	ND
10	F	611	CLA	ND
10	F	612	CLA	ND
10	F	613	CLA	ND
10	F	614	CLA	ND
10	G	602	CLA	C8
10	G	602	CLA	ND
10	G	603	CLA	C8
10	G	603	CLA	ND
10	G	604	CLA	ND
10	G	610	CLA	ND
10	G	611	CLA	ND
10	G	612	CLA	ND
10	G	613	CLA	ND
10	G	614	CLA	ND
10	H	602	CLA	C8
10	H	602	CLA	ND
10	H	603	CLA	C8
10	H	603	CLA	ND
10	H	604	CLA	ND
10	H	610	CLA	ND
10	H	610	CLA	C13
10	H	611	CLA	ND
10	H	612	CLA	ND
10	H	613	CLA	ND
10	H	614	CLA	ND
10	I	602	CLA	C8
10	I	602	CLA	ND
10	I	603	CLA	C8
10	I	603	CLA	ND
10	I	604	CLA	ND
10	I	610	CLA	ND
10	I	610	CLA	C13
10	I	611	CLA	ND
10	I	612	CLA	ND
10	I	613	CLA	ND
10	I	614	CLA	ND
10	J	602	CLA	C8
10	J	602	CLA	ND
10	J	603	CLA	C8
10	J	603	CLA	ND

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Mol	Chain	Res	Type	Atom
10	J	604	CLA	ND
10	J	610	CLA	ND
10	J	611	CLA	ND
10	J	612	CLA	ND
10	J	613	CLA	ND
10	J	614	CLA	ND

All (2426) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	9633	BNG	C2-C1-O1-C1'
2	J	9633	BNG	O5-C1-O1-C1'
5	D	8622	XAT	O24-C26-C27-C28
5	H	4622	XAT	O24-C26-C27-C28
7	A	630	LHG	O1-C1-C2-O2
7	A	630	LHG	O1-C1-C2-C3
7	A	630	LHG	C4-O6-P-O3
7	A	630	LHG	C4-O6-P-O5
7	B	1630	LHG	O1-C1-C2-C3
7	B	1630	LHG	C1-C2-C3-O3
7	C	2630	LHG	O1-C1-C2-C3
7	D	3630	LHG	O1-C1-C2-C3
7	D	3630	LHG	C4-O6-P-O3
7	E	4630	LHG	O1-C1-C2-C3
7	E	4630	LHG	C1-C2-C3-O3
7	E	4630	LHG	C4-O6-P-O3
7	E	4630	LHG	C4-O6-P-O4
7	E	4630	LHG	C4-O6-P-O5
7	F	5630	LHG	O1-C1-C2-C3
7	F	5630	LHG	C4-O6-P-O3
7	G	6630	LHG	O1-C1-C2-O2
7	G	6630	LHG	O1-C1-C2-C3
7	G	6630	LHG	C4-O6-P-O3
7	G	6630	LHG	C4-O6-P-O5
7	G	6630	LHG	O10-C23-O8-C6
7	H	7630	LHG	O1-C1-C2-C3
7	I	8630	LHG	C4-O6-P-O3
7	I	8630	LHG	C4-O6-P-O4
7	I	8630	LHG	C4-O6-P-O5
7	J	9630	LHG	O1-C1-C2-O2
7	J	9630	LHG	O1-C1-C2-C3
7	J	9630	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
9	A	605	CHL	C1A-C2A-CAA-CBA
9	A	606	CHL	C1A-C2A-CAA-CBA
9	A	609	CHL	C1A-C2A-CAA-CBA
9	B	605	CHL	C1A-C2A-CAA-CBA
9	C	605	CHL	C1A-C2A-CAA-CBA
9	C	605	CHL	C3A-C2A-CAA-CBA
9	C	606	CHL	C1A-C2A-CAA-CBA
9	D	605	CHL	C1A-C2A-CAA-CBA
9	D	606	CHL	C1A-C2A-CAA-CBA
9	D	606	CHL	CBA-CGA-O2A-C1
9	D	606	CHL	O1A-CGA-O2A-C1
9	E	605	CHL	C1A-C2A-CAA-CBA
9	E	606	CHL	C1A-C2A-CAA-CBA
9	E	606	CHL	C3A-C2A-CAA-CBA
9	F	605	CHL	C1A-C2A-CAA-CBA
9	F	605	CHL	C3A-C2A-CAA-CBA
9	F	606	CHL	C1A-C2A-CAA-CBA
9	F	609	CHL	C1A-C2A-CAA-CBA
9	G	605	CHL	C1A-C2A-CAA-CBA
9	G	605	CHL	C3A-C2A-CAA-CBA
9	H	605	CHL	C1A-C2A-CAA-CBA
9	H	609	CHL	C1A-C2A-CAA-CBA
9	I	605	CHL	C1A-C2A-CAA-CBA
9	I	606	CHL	C1A-C2A-CAA-CBA
9	I	606	CHL	O1A-CGA-O2A-C1
9	I	609	CHL	C1A-C2A-CAA-CBA
9	J	605	CHL	C1A-C2A-CAA-CBA
10	A	602	CLA	C4-C3-C5-C6
10	A	604	CLA	C1A-C2A-CAA-CBA
10	A	611	CLA	C1A-C2A-CAA-CBA
10	B	602	CLA	CHA-CBD-CGD-O2D
10	B	604	CLA	C6-C7-C8-C10
10	B	612	CLA	C14-C13-C15-C16
10	C	611	CLA	C6-C7-C8-C10
10	D	604	CLA	C1A-C2A-CAA-CBA
10	D	611	CLA	C1A-C2A-CAA-CBA
10	D	612	CLA	CBD-CGD-O2D-CED
10	E	611	CLA	C1A-C2A-CAA-CBA
10	F	603	CLA	C1A-C2A-CAA-CBA
10	F	603	CLA	CHA-CBD-CGD-O1D
10	F	603	CLA	CHA-CBD-CGD-O2D
10	G	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
10	G	610	CLA	C14-C13-C15-C16
10	G	612	CLA	CBD-CGD-O2D-CED
10	I	603	CLA	C1A-C2A-CAA-CBA
10	I	603	CLA	C3A-C2A-CAA-CBA
10	I	604	CLA	C1A-C2A-CAA-CBA
10	I	611	CLA	C1A-C2A-CAA-CBA
10	I	612	CLA	CBD-CGD-O2D-CED
10	J	612	CLA	CBD-CGD-O2D-CED
10	J	613	CLA	C2B-C3B-CAB-CBB
10	J	613	CLA	C4B-C3B-CAB-CBB
9	A	609	CHL	CBD-CGD-O2D-CED
9	G	608	CHL	CBD-CGD-O2D-CED
9	I	605	CHL	CBD-CGD-O2D-CED
10	A	602	CLA	CBD-CGD-O2D-CED
10	F	612	CLA	CBD-CGD-O2D-CED
10	H	612	CLA	CBD-CGD-O2D-CED
7	A	630	LHG	O10-C23-O8-C6
7	I	8630	LHG	O10-C23-O8-C6
9	A	606	CHL	O1A-CGA-O2A-C1
9	A	607	CHL	O1A-CGA-O2A-C1
9	C	606	CHL	O1A-CGA-O2A-C1
9	C	607	CHL	O1A-CGA-O2A-C1
9	E	606	CHL	O1A-CGA-O2A-C1
9	G	607	CHL	O1A-CGA-O2A-C1
10	I	612	CLA	O1D-CGD-O2D-CED
7	A	630	LHG	C24-C23-O8-C6
7	I	8630	LHG	C24-C23-O8-C6
7	J	9630	LHG	C24-C23-O8-C6
9	A	606	CHL	CBA-CGA-O2A-C1
9	C	606	CHL	CBA-CGA-O2A-C1
9	E	606	CHL	CBA-CGA-O2A-C1
9	G	607	CHL	CBA-CGA-O2A-C1
10	A	612	CLA	CBD-CGD-O2D-CED
10	H	602	CLA	CBD-CGD-O2D-CED
7	B	1630	LHG	O10-C23-O8-C6
7	C	2630	LHG	O10-C23-O8-C6
7	D	3630	LHG	O10-C23-O8-C6
7	E	4630	LHG	O10-C23-O8-C6
7	F	5630	LHG	O10-C23-O8-C6
7	H	7630	LHG	O10-C23-O8-C6
7	J	9630	LHG	O10-C23-O8-C6
8	A	632	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
8	B	2632	DGD	O1A-C1A-O1G-C1G
8	D	5632	DGD	O1A-C1A-O1G-C1G
9	B	607	CHL	O1A-CGA-O2A-C1
9	D	607	CHL	O1A-CGA-O2A-C1
9	E	607	CHL	O1A-CGA-O2A-C1
9	F	606	CHL	O1A-CGA-O2A-C1
9	F	607	CHL	O1A-CGA-O2A-C1
9	H	605	CHL	O1A-CGA-O2A-C1
9	H	606	CHL	O1A-CGA-O2A-C1
9	H	607	CHL	O1A-CGA-O2A-C1
9	I	605	CHL	O1A-CGA-O2A-C1
9	I	607	CHL	O1A-CGA-O2A-C1
9	J	607	CHL	O1A-CGA-O2A-C1
10	D	612	CLA	O1D-CGD-O2D-CED
10	J	612	CLA	O1D-CGD-O2D-CED
10	G	612	CLA	O1D-CGD-O2D-CED
10	H	612	CLA	O1D-CGD-O2D-CED
10	E	612	CLA	CBD-CGD-O2D-CED
9	E	601	CHL	C3-C5-C6-C7
9	F	607	CHL	C3-C5-C6-C7
9	G	601	CHL	C3-C5-C6-C7
9	G	607	CHL	C3-C5-C6-C7
9	H	607	CHL	C3-C5-C6-C7
9	H	609	CHL	C3-C5-C6-C7
9	I	601	CHL	C3-C5-C6-C7
9	I	607	CHL	C3-C5-C6-C7
9	I	609	CHL	C3-C5-C6-C7
9	J	607	CHL	C3-C5-C6-C7
9	J	609	CHL	C3-C5-C6-C7
10	A	603	CLA	C3-C5-C6-C7
10	B	611	CLA	C3-C5-C6-C7
10	C	611	CLA	C3-C5-C6-C7
10	D	603	CLA	C3-C5-C6-C7
10	D	611	CLA	C3-C5-C6-C7
10	E	603	CLA	C3-C5-C6-C7
10	F	603	CLA	C3-C5-C6-C7
10	G	603	CLA	C3-C5-C6-C7
10	G	611	CLA	C3-C5-C6-C7
10	H	603	CLA	C3-C5-C6-C7
10	H	611	CLA	C3-C5-C6-C7
10	H	612	CLA	C3-C5-C6-C7
10	I	611	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
10	J	611	CLA	C3-C5-C6-C7
7	B	1630	LHG	C24-C23-O8-C6
7	C	2630	LHG	C24-C23-O8-C6
7	D	3630	LHG	C24-C23-O8-C6
7	E	4630	LHG	C24-C23-O8-C6
7	F	5630	LHG	C24-C23-O8-C6
7	G	6630	LHG	C24-C23-O8-C6
7	H	7630	LHG	C24-C23-O8-C6
9	A	607	CHL	CBA-CGA-O2A-C1
9	C	607	CHL	CBA-CGA-O2A-C1
9	D	607	CHL	CBA-CGA-O2A-C1
9	F	606	CHL	CBA-CGA-O2A-C1
9	H	607	CHL	CBA-CGA-O2A-C1
9	I	606	CHL	CBA-CGA-O2A-C1
9	I	607	CHL	CBA-CGA-O2A-C1
10	C	614	CLA	CBA-CGA-O2A-C1
10	G	614	CLA	CBA-CGA-O2A-C1
9	B	606	CHL	CBD-CGD-O2D-CED
9	C	609	CHL	CBD-CGD-O2D-CED
9	E	609	CHL	CBD-CGD-O2D-CED
9	F	601	CHL	CBD-CGD-O2D-CED
9	F	605	CHL	CBD-CGD-O2D-CED
9	J	609	CHL	CBD-CGD-O2D-CED
10	D	602	CLA	CBD-CGD-O2D-CED
10	G	602	CLA	CBD-CGD-O2D-CED
10	G	613	CLA	CBD-CGD-O2D-CED
10	I	614	CLA	CBD-CGD-O2D-CED
10	J	602	CLA	CBD-CGD-O2D-CED
10	C	602	CLA	C4-C3-C5-C6
10	D	602	CLA	C4-C3-C5-C6
10	E	602	CLA	C4-C3-C5-C6
10	G	602	CLA	C4-C3-C5-C6
10	H	602	CLA	C4-C3-C5-C6
10	I	602	CLA	C4-C3-C5-C6
10	A	602	CLA	C2-C3-C5-C6
10	D	602	CLA	C2-C3-C5-C6
10	G	602	CLA	C2-C3-C5-C6
10	H	602	CLA	C2-C3-C5-C6
10	I	602	CLA	C2-C3-C5-C6
9	A	601	CHL	C2A-CAA-CBA-CGA
9	B	601	CHL	C2A-CAA-CBA-CGA
9	E	601	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	F	601	CHL	C2A-CAA-CBA-CGA
9	G	601	CHL	C2A-CAA-CBA-CGA
9	H	601	CHL	C2A-CAA-CBA-CGA
9	I	601	CHL	C2A-CAA-CBA-CGA
10	A	603	CLA	C2A-CAA-CBA-CGA
10	B	603	CLA	C2A-CAA-CBA-CGA
10	C	603	CLA	C2A-CAA-CBA-CGA
10	D	603	CLA	C2A-CAA-CBA-CGA
10	E	603	CLA	C2A-CAA-CBA-CGA
10	F	603	CLA	C2A-CAA-CBA-CGA
10	G	603	CLA	C2A-CAA-CBA-CGA
10	H	603	CLA	C2A-CAA-CBA-CGA
10	I	603	CLA	C2A-CAA-CBA-CGA
10	J	603	CLA	C2A-CAA-CBA-CGA
9	A	607	CHL	C3-C5-C6-C7
9	D	601	CHL	C3-C5-C6-C7
10	A	611	CLA	C3-C5-C6-C7
10	B	603	CLA	C3-C5-C6-C7
10	E	611	CLA	C3-C5-C6-C7
10	F	611	CLA	C3-C5-C6-C7
8	A	632	DGD	C2A-C1A-O1G-C1G
8	B	2632	DGD	C2A-C1A-O1G-C1G
8	D	5632	DGD	C2A-C1A-O1G-C1G
9	B	605	CHL	CBA-CGA-O2A-C1
9	B	607	CHL	CBA-CGA-O2A-C1
9	C	605	CHL	CBA-CGA-O2A-C1
9	E	605	CHL	CBA-CGA-O2A-C1
9	E	607	CHL	CBA-CGA-O2A-C1
9	F	605	CHL	CBA-CGA-O2A-C1
9	F	607	CHL	CBA-CGA-O2A-C1
9	G	605	CHL	CBA-CGA-O2A-C1
9	H	605	CHL	CBA-CGA-O2A-C1
9	H	606	CHL	CBA-CGA-O2A-C1
9	I	605	CHL	CBA-CGA-O2A-C1
9	J	607	CHL	CBA-CGA-O2A-C1
10	E	614	CLA	CBA-CGA-O2A-C1
10	G	612	CLA	CBA-CGA-O2A-C1
10	H	614	CLA	CBA-CGA-O2A-C1
10	J	612	CLA	CBA-CGA-O2A-C1
2	H	7633	BNG	O5-C5-C6-O6
8	E	4632	DGD	O1A-C1A-O1G-C1G
9	A	605	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	B	605	CHL	O1A-CGA-O2A-C1
9	C	605	CHL	O1A-CGA-O2A-C1
9	D	605	CHL	O1A-CGA-O2A-C1
9	E	605	CHL	O1A-CGA-O2A-C1
9	G	605	CHL	O1A-CGA-O2A-C1
9	J	605	CHL	O1A-CGA-O2A-C1
10	C	614	CLA	O1A-CGA-O2A-C1
10	G	614	CLA	O1A-CGA-O2A-C1
10	H	614	CLA	O1A-CGA-O2A-C1
10	F	612	CLA	O1D-CGD-O2D-CED
9	D	607	CHL	C3-C5-C6-C7
9	H	601	CHL	C3-C5-C6-C7
10	C	603	CLA	C3-C5-C6-C7
10	I	603	CLA	C3-C5-C6-C7
9	F	609	CHL	CBD-CGD-O2D-CED
7	A	630	LHG	O2-C2-C3-O3
9	A	609	CHL	O1D-CGD-O2D-CED
9	G	608	CHL	O1D-CGD-O2D-CED
10	A	612	CLA	O1D-CGD-O2D-CED
10	E	612	CLA	O1D-CGD-O2D-CED
8	E	4632	DGD	C2A-C1A-O1G-C1G
8	G	9632	DGD	C2A-C1A-O1G-C1G
8	H	6632	DGD	C2A-C1A-O1G-C1G
9	A	605	CHL	CBA-CGA-O2A-C1
9	J	605	CHL	CBA-CGA-O2A-C1
10	B	611	CLA	CBA-CGA-O2A-C1
10	E	611	CLA	CBA-CGA-O2A-C1
10	I	614	CLA	CBA-CGA-O2A-C1
9	F	605	CHL	O1A-CGA-O2A-C1
10	E	614	CLA	O1A-CGA-O2A-C1
10	J	612	CLA	O1A-CGA-O2A-C1
9	E	609	CHL	O1D-CGD-O2D-CED
2	H	7633	BNG	C4-C5-C6-O6
9	F	606	CHL	CBD-CGD-O2D-CED
9	E	607	CHL	C3-C5-C6-C7
10	I	604	CLA	C3-C5-C6-C7
9	D	605	CHL	CBA-CGA-O2A-C1
10	I	612	CLA	CBA-CGA-O2A-C1
10	B	602	CLA	C4-C3-C5-C6
10	C	602	CLA	C2-C3-C5-C6
10	E	602	CLA	C2-C3-C5-C6
8	G	9632	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
8	H	6632	DGD	O1A-C1A-O1G-C1G
10	E	611	CLA	O1A-CGA-O2A-C1
10	G	612	CLA	O1A-CGA-O2A-C1
2	A	633	BNG	O5-C5-C6-O6
10	C	604	CLA	CBD-CGD-O2D-CED
9	D	608	CHL	C2A-CAA-CBA-CGA
9	E	608	CHL	C2A-CAA-CBA-CGA
10	J	611	CLA	C2A-CAA-CBA-CGA
9	B	606	CHL	O1A-CGA-O2A-C1
10	B	611	CLA	O1A-CGA-O2A-C1
10	H	612	CLA	O1A-CGA-O2A-C1
10	I	614	CLA	O1A-CGA-O2A-C1
8	A	632	DGD	O6D-C1D-O3G-C3G
9	I	605	CHL	O1D-CGD-O2D-CED
9	B	606	CHL	CBA-CGA-O2A-C1
10	B	612	CLA	CBA-CGA-O2A-C1
10	H	612	CLA	CBA-CGA-O2A-C1
9	B	609	CHL	CBD-CGD-O2D-CED
9	C	601	CHL	CBD-CGD-O2D-CED
9	C	606	CHL	CBD-CGD-O2D-CED
10	E	614	CLA	CBD-CGD-O2D-CED
2	C	2633	BNG	O5-C5-C6-O6
10	B	612	CLA	O1A-CGA-O2A-C1
10	I	612	CLA	O1A-CGA-O2A-C1
2	J	9633	BNG	O5-C5-C6-O6
9	J	609	CHL	O1D-CGD-O2D-CED
10	A	602	CLA	O1D-CGD-O2D-CED
10	B	603	CLA	CBD-CGD-O2D-CED
10	E	602	CLA	CBD-CGD-O2D-CED
10	A	612	CLA	C3-C5-C6-C7
10	A	612	CLA	O1A-CGA-O2A-C1
10	A	614	CLA	O1A-CGA-O2A-C1
7	A	630	LHG	C1-C2-C3-O3
9	C	609	CHL	O1D-CGD-O2D-CED
8	B	1632	DGD	C2A-C1A-O1G-C1G
8	D	3632	DGD	C2A-C1A-O1G-C1G
8	H	7632	DGD	C2A-C1A-O1G-C1G
8	I	8632	DGD	C2A-C1A-O1G-C1G
10	A	611	CLA	CBA-CGA-O2A-C1
10	A	612	CLA	CBA-CGA-O2A-C1
10	A	614	CLA	CBA-CGA-O2A-C1
10	C	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	C	612	CLA	CBA-CGA-O2A-C1
10	D	611	CLA	CBA-CGA-O2A-C1
10	D	612	CLA	CBA-CGA-O2A-C1
10	D	614	CLA	CBA-CGA-O2A-C1
10	E	612	CLA	CBA-CGA-O2A-C1
10	F	611	CLA	CBA-CGA-O2A-C1
10	G	611	CLA	CBA-CGA-O2A-C1
10	H	611	CLA	CBA-CGA-O2A-C1
10	J	611	CLA	CBA-CGA-O2A-C1
2	J	9633	BNG	C4-C5-C6-O6
10	F	602	CLA	C4-C3-C5-C6
10	J	602	CLA	C4-C3-C5-C6
10	B	602	CLA	C2-C3-C5-C6
10	F	602	CLA	C2-C3-C5-C6
10	J	602	CLA	C2-C3-C5-C6
9	D	609	CHL	C3-C5-C6-C7
9	J	601	CHL	C3-C5-C6-C7
9	A	608	CHL	CBD-CGD-O2D-CED
10	H	613	CLA	CBD-CGD-O2D-CED
9	A	608	CHL	C14-C13-C15-C16
9	B	601	CHL	C11-C12-C13-C14
9	C	608	CHL	C14-C13-C15-C16
9	D	601	CHL	C11-C10-C8-C9
9	D	608	CHL	C14-C13-C15-C16
9	E	609	CHL	C14-C13-C15-C16
9	F	601	CHL	C11-C10-C8-C9
9	F	601	CHL	C11-C12-C13-C14
9	F	607	CHL	C11-C10-C8-C9
9	F	608	CHL	C14-C13-C15-C16
9	F	609	CHL	C14-C13-C15-C16
9	G	601	CHL	C11-C10-C8-C9
9	G	607	CHL	C11-C10-C8-C9
9	G	608	CHL	C14-C13-C15-C16
9	G	609	CHL	C14-C13-C15-C16
9	H	608	CHL	C14-C13-C15-C16
9	H	609	CHL	C14-C13-C15-C16
9	I	608	CHL	C14-C13-C15-C16
9	J	601	CHL	C11-C12-C13-C14
9	J	608	CHL	C14-C13-C15-C16
9	J	609	CHL	C14-C13-C15-C16
10	A	610	CLA	C14-C13-C15-C16
10	A	612	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
10	B	610	CLA	C14-C13-C15-C16
10	C	610	CLA	C14-C13-C15-C16
10	D	610	CLA	C14-C13-C15-C16
10	D	612	CLA	C14-C13-C15-C16
10	E	612	CLA	C14-C13-C15-C16
10	E	613	CLA	C11-C10-C8-C9
10	F	610	CLA	C14-C13-C15-C16
10	F	612	CLA	C14-C13-C15-C16
10	I	611	CLA	C11-C10-C8-C9
10	I	612	CLA	C14-C13-C15-C16
10	J	612	CLA	C14-C13-C15-C16
10	G	613	CLA	O1D-CGD-O2D-CED
10	J	602	CLA	O1D-CGD-O2D-CED
8	A	632	DGD	C2D-C1D-O3G-C3G
8	B	2632	DGD	C2D-C1D-O3G-C3G
8	D	3632	DGD	C2D-C1D-O3G-C3G
8	E	4632	DGD	C2D-C1D-O3G-C3G
8	G	9632	DGD	C2D-C1D-O3G-C3G
8	I	8632	DGD	C2D-C1D-O3G-C3G
7	B	1630	LHG	O2-C2-C3-O3
9	F	601	CHL	O1D-CGD-O2D-CED
9	F	605	CHL	O1D-CGD-O2D-CED
10	F	612	CLA	CBA-CGA-O2A-C1
10	D	612	CLA	O1A-CGA-O2A-C1
10	F	611	CLA	O1A-CGA-O2A-C1
10	H	611	CLA	O1A-CGA-O2A-C1
10	J	611	CLA	O1A-CGA-O2A-C1
9	D	609	CHL	CBD-CGD-O2D-CED
9	F	609	CHL	O1D-CGD-O2D-CED
9	I	608	CHL	C2A-CAA-CBA-CGA
8	G	9632	DGD	C1B-C2B-C3B-C4B
8	D	3632	DGD	O1A-C1A-O1G-C1G
8	I	8632	DGD	O1A-C1A-O1G-C1G
10	A	611	CLA	O1A-CGA-O2A-C1
2	C	2633	BNG	C4-C5-C6-O6
2	D	3633	BNG	O5-C5-C6-O6
10	B	614	CLA	CBA-CGA-O2A-C1
10	J	614	CLA	CBA-CGA-O2A-C1
9	A	607	CHL	C10-C11-C12-C13
9	D	607	CHL	C10-C11-C12-C13
9	I	607	CHL	C5-C6-C7-C8
10	E	611	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
10	F	603	CLA	C5-C6-C7-C8
10	I	614	CLA	O1D-CGD-O2D-CED
2	B	1633	BNG	O5-C5-C6-O6
9	B	607	CHL	C10-C11-C12-C13
9	B	608	CHL	C8-C10-C11-C12
9	E	608	CHL	C8-C10-C11-C12
9	J	608	CHL	C13-C15-C16-C17
10	C	612	CLA	C8-C10-C11-C12
10	D	613	CLA	C13-C15-C16-C17
10	E	603	CLA	C5-C6-C7-C8
10	G	611	CLA	C5-C6-C7-C8
10	G	612	CLA	C8-C10-C11-C12
10	H	612	CLA	C8-C10-C11-C12
10	I	611	CLA	C10-C11-C12-C13
7	F	5630	LHG	O1-C1-C2-O2
10	C	612	CLA	O1A-CGA-O2A-C1
10	E	612	CLA	O1A-CGA-O2A-C1
10	C	604	CLA	C6-C7-C8-C10
10	F	604	CLA	C6-C7-C8-C10
10	G	604	CLA	C6-C7-C8-C10
10	H	604	CLA	C6-C7-C8-C10
2	E	4633	BNG	O5-C5-C6-O6
2	F	5633	BNG	O5-C5-C6-O6
8	B	2632	DGD	C1B-C2B-C3B-C4B
8	E	4632	DGD	C1B-C2B-C3B-C4B
8	G	9632	DGD	C1A-C2A-C3A-C4A
8	I	8632	DGD	C1B-C2B-C3B-C4B
2	G	6633	BNG	O5-C5-C6-O6
10	G	612	CLA	C3-C5-C6-C7
10	J	604	CLA	C3-C5-C6-C7
10	D	604	CLA	C13-C15-C16-C17
10	F	604	CLA	C13-C15-C16-C17
9	H	608	CHL	C15-C16-C17-C18
9	I	607	CHL	C10-C11-C12-C13
10	A	611	CLA	C5-C6-C7-C8
10	D	611	CLA	C5-C6-C7-C8
10	I	613	CLA	C13-C15-C16-C17
10	J	612	CLA	C8-C10-C11-C12
8	A	632	DGD	C1A-C2A-C3A-C4A
8	A	632	DGD	C1B-C2B-C3B-C4B
8	B	1632	DGD	C1A-C2A-C3A-C4A
8	B	2632	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
8	E	4632	DGD	C1A-C2A-C3A-C4A
8	H	6632	DGD	C1A-C2A-C3A-C4A
8	H	7632	DGD	O1A-C1A-O1G-C1G
10	B	614	CLA	O1A-CGA-O2A-C1
10	C	611	CLA	O1A-CGA-O2A-C1
10	G	611	CLA	O1A-CGA-O2A-C1
9	B	606	CHL	O1D-CGD-O2D-CED
9	C	601	CHL	C10-C11-C12-C13
9	H	607	CHL	C15-C16-C17-C18
9	H	608	CHL	C13-C15-C16-C17
9	J	607	CHL	C5-C6-C7-C8
10	H	610	CLA	C13-C15-C16-C17
10	H	611	CLA	C5-C6-C7-C8
10	H	611	CLA	C13-C15-C16-C17
10	I	612	CLA	C8-C10-C11-C12
9	A	608	CHL	C2A-CAA-CBA-CGA
9	B	608	CHL	C2A-CAA-CBA-CGA
9	C	608	CHL	C2A-CAA-CBA-CGA
9	G	608	CHL	C2A-CAA-CBA-CGA
9	H	608	CHL	C2A-CAA-CBA-CGA
9	J	606	CHL	C2A-CAA-CBA-CGA
9	J	608	CHL	C2A-CAA-CBA-CGA
10	H	611	CLA	C2A-CAA-CBA-CGA
10	J	604	CLA	C2A-CAA-CBA-CGA
9	A	607	CHL	C5-C6-C7-C8
9	J	601	CHL	C10-C11-C12-C13
9	J	607	CHL	C10-C11-C12-C13
10	A	611	CLA	C10-C11-C12-C13
10	A	612	CLA	C8-C10-C11-C12
10	B	611	CLA	C5-C6-C7-C8
10	F	612	CLA	C8-C10-C11-C12
10	H	613	CLA	C13-C15-C16-C17
10	J	611	CLA	C13-C15-C16-C17
7	I	8630	LHG	C23-C24-C25-C26
8	D	3632	DGD	C1B-C2B-C3B-C4B
8	H	6632	DGD	C1B-C2B-C3B-C4B
8	H	7632	DGD	C1A-C2A-C3A-C4A
8	I	8632	DGD	C1A-C2A-C3A-C4A
8	B	1632	DGD	O1A-C1A-O1G-C1G
10	F	612	CLA	O1A-CGA-O2A-C1
9	B	607	CHL	C3-C5-C6-C7
9	F	608	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	H	608	CHL	C3-C5-C6-C7
9	D	601	CHL	CBD-CGD-O2D-CED
9	H	608	CHL	CBD-CGD-O2D-CED
10	J	613	CLA	CBD-CGD-O2D-CED
8	B	2632	DGD	O6D-C1D-O3G-C3G
8	D	3632	DGD	O6D-C1D-O3G-C3G
8	G	9632	DGD	O6D-C1D-O3G-C3G
8	B	2632	DGD	O6E-C5E-C6E-O5E
9	A	601	CHL	C10-C11-C12-C13
9	A	607	CHL	C15-C16-C17-C18
9	B	608	CHL	C15-C16-C17-C18
9	C	607	CHL	C5-C6-C7-C8
9	E	601	CHL	C13-C15-C16-C17
9	E	607	CHL	C5-C6-C7-C8
9	E	607	CHL	C10-C11-C12-C13
9	E	607	CHL	C15-C16-C17-C18
9	F	607	CHL	C15-C16-C17-C18
9	F	608	CHL	C5-C6-C7-C8
9	G	607	CHL	C15-C16-C17-C18
9	G	608	CHL	C13-C15-C16-C17
9	G	608	CHL	C15-C16-C17-C18
9	H	601	CHL	C13-C15-C16-C17
9	H	607	CHL	C10-C11-C12-C13
9	I	601	CHL	C13-C15-C16-C17
9	I	608	CHL	C13-C15-C16-C17
9	I	608	CHL	C15-C16-C17-C18
10	A	611	CLA	C13-C15-C16-C17
10	C	611	CLA	C5-C6-C7-C8
10	C	611	CLA	C13-C15-C16-C17
10	E	603	CLA	C15-C16-C17-C18
10	E	612	CLA	C8-C10-C11-C12
10	F	603	CLA	C15-C16-C17-C18
10	F	611	CLA	C5-C6-C7-C8
10	G	603	CLA	C8-C10-C11-C12
10	G	613	CLA	C13-C15-C16-C17
10	H	603	CLA	C5-C6-C7-C8
10	I	603	CLA	C10-C11-C12-C13
10	I	611	CLA	C13-C15-C16-C17
10	J	613	CLA	C13-C15-C16-C17
10	D	611	CLA	O1A-CGA-O2A-C1
10	D	614	CLA	O1A-CGA-O2A-C1
10	J	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	A	604	CLA	C13-C15-C16-C17
10	E	604	CLA	C13-C15-C16-C17
10	H	604	CLA	C13-C15-C16-C17
10	I	604	CLA	C13-C15-C16-C17
9	C	601	CHL	C13-C15-C16-C17
9	F	607	CHL	C5-C6-C7-C8
9	F	608	CHL	C13-C15-C16-C17
9	H	607	CHL	C5-C6-C7-C8
10	J	611	CLA	C10-C11-C12-C13
9	A	608	CHL	O1D-CGD-O2D-CED
9	F	609	CHL	C3-C5-C6-C7
9	A	608	CHL	C13-C15-C16-C17
9	G	601	CHL	C13-C15-C16-C17
9	I	607	CHL	C15-C16-C17-C18
10	A	613	CLA	C13-C15-C16-C17
10	C	603	CLA	C5-C6-C7-C8
10	E	611	CLA	C5-C6-C7-C8
10	G	603	CLA	C5-C6-C7-C8
10	I	611	CLA	C5-C6-C7-C8
8	D	5632	DGD	C1A-C2A-C3A-C4A
8	H	7632	DGD	C1B-C2B-C3B-C4B
9	B	609	CHL	O1D-CGD-O2D-CED
9	A	601	CHL	C15-C16-C17-C18
10	F	611	CLA	C10-C11-C12-C13
10	F	614	CLA	CBA-CGA-O2A-C1
10	I	611	CLA	CBA-CGA-O2A-C1
10	J	614	CLA	CBD-CGD-O2D-CED
9	C	608	CHL	C8-C10-C11-C12
9	C	607	CHL	C3-C5-C6-C7
10	C	613	CLA	C3-C5-C6-C7
9	G	607	CHL	C10-C11-C12-C13
7	A	630	LHG	C23-C24-C25-C26
7	E	4630	LHG	C23-C24-C25-C26
7	J	9630	LHG	C23-C24-C25-C26
9	H	606	CHL	C2A-CAA-CBA-CGA
10	E	611	CLA	C2A-CAA-CBA-CGA
9	A	608	CHL	C8-C10-C11-C12
9	C	607	CHL	C15-C16-C17-C18
9	C	608	CHL	C15-C16-C17-C18
9	D	608	CHL	C15-C16-C17-C18
9	E	608	CHL	C13-C15-C16-C17
9	E	608	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	F	608	CHL	C15-C16-C17-C18
9	G	608	CHL	C8-C10-C11-C12
9	I	608	CHL	C8-C10-C11-C12
10	A	603	CLA	C13-C15-C16-C17
10	B	611	CLA	C13-C15-C16-C17
10	B	612	CLA	C8-C10-C11-C12
10	E	603	CLA	C10-C11-C12-C13
10	E	611	CLA	C10-C11-C12-C13
10	I	610	CLA	C13-C15-C16-C17
10	A	603	CLA	O1D-CGD-O2D-CED
9	D	609	CHL	O1D-CGD-O2D-CED
8	D	5632	DGD	C1B-C2B-C3B-C4B
9	B	607	CHL	C5-C6-C7-C8
9	B	608	CHL	C13-C15-C16-C17
9	C	607	CHL	C10-C11-C12-C13
9	D	608	CHL	C13-C15-C16-C17
9	F	607	CHL	C10-C11-C12-C13
9	J	608	CHL	C15-C16-C17-C18
10	A	612	CLA	C10-C11-C12-C13
10	E	613	CLA	C13-C15-C16-C17
9	B	601	CHL	C10-C11-C12-C13
9	D	607	CHL	C15-C16-C17-C18
10	C	603	CLA	C10-C11-C12-C13
10	D	611	CLA	C13-C15-C16-C17
10	F	611	CLA	C13-C15-C16-C17
10	G	611	CLA	C13-C15-C16-C17
10	B	603	CLA	O1D-CGD-O2D-CED
10	B	604	CLA	C13-C15-C16-C17
10	J	604	CLA	C13-C15-C16-C17
9	F	608	CHL	C8-C10-C11-C12
10	D	603	CLA	C10-C11-C12-C13
9	E	609	CHL	C3-C5-C6-C7
10	B	612	CLA	CBD-CGD-O2D-CED
9	I	609	CHL	C14-C13-C15-C16
2	B	1633	BNG	C2-C1-O1-C1'
2	F	5633	BNG	C2-C1-O1-C1'
2	I	8633	BNG	C2-C1-O1-C1'
8	B	1632	DGD	C2D-C1D-O3G-C3G
8	D	5632	DGD	C2D-C1D-O3G-C3G
8	H	6632	DGD	C2D-C1D-O3G-C3G
8	H	7632	DGD	C2D-C1D-O3G-C3G
7	E	4630	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
9	H	608	CHL	O1D-CGD-O2D-CED
9	D	607	CHL	C16-C17-C18-C19
9	D	608	CHL	C16-C17-C18-C19
10	B	603	CLA	C16-C17-C18-C19
9	H	608	CHL	C8-C10-C11-C12
10	I	603	CLA	C8-C10-C11-C12
10	J	614	CLA	O1D-CGD-O2D-CED
9	F	608	CHL	C2A-CAA-CBA-CGA
10	G	611	CLA	C2A-CAA-CBA-CGA
10	F	603	CLA	C10-C11-C12-C13
9	C	607	CHL	C16-C17-C18-C19
9	H	607	CHL	C16-C17-C18-C19
10	B	603	CLA	C16-C17-C18-C20
10	H	603	CLA	C16-C17-C18-C20
10	C	604	CLA	O1D-CGD-O2D-CED
10	F	614	CLA	O1A-CGA-O2A-C1
10	I	611	CLA	O1A-CGA-O2A-C1
9	B	601	CHL	C3-C5-C6-C7
10	E	612	CLA	C3-C5-C6-C7
10	J	612	CLA	C3-C5-C6-C7
9	D	608	CHL	C8-C10-C11-C12
2	F	5633	BNG	O5-C1-O1-C1'
2	I	8633	BNG	O5-C1-O1-C1'
8	B	1632	DGD	O6D-C1D-O3G-C3G
8	D	5632	DGD	O6D-C1D-O3G-C3G
8	E	4632	DGD	O6D-C1D-O3G-C3G
8	I	8632	DGD	O6D-C1D-O3G-C3G
9	B	607	CHL	C15-C16-C17-C18
10	G	603	CLA	C15-C16-C17-C18
9	F	606	CHL	O1D-CGD-O2D-CED
10	H	602	CLA	O1D-CGD-O2D-CED
7	B	1630	LHG	C23-C24-C25-C26
9	F	607	CHL	C16-C17-C18-C19
10	J	602	CLA	C5-C6-C7-C8
2	C	2633	BNG	C3'-C4'-C5'-C6'
7	F	5630	LHG	C9-C10-C11-C12
7	J	9630	LHG	C15-C16-C17-C18
8	B	1632	DGD	C5A-C6A-C7A-C8A
8	D	5632	DGD	C7A-C8A-C9A-CAA
10	A	603	CLA	CBD-CGD-O2D-CED
2	D	3633	BNG	C1'-C2'-C3'-C4'
2	D	3633	BNG	C5'-C6'-C7'-C8'

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Mol	Chain	Res	Type	Atoms
7	A	630	LHG	C15-C16-C17-C18
7	I	8630	LHG	C15-C16-C17-C18
7	J	9630	LHG	C34-C35-C36-C37
8	D	5632	DGD	C6B-C7B-C8B-C9B
8	G	9632	DGD	CCB-CDB-CEB-CFB
8	H	6632	DGD	C5A-C6A-C7A-C8A
10	D	602	CLA	O1D-CGD-O2D-CED
8	B	2632	DGD	C7A-C8A-C9A-CAA
8	I	8632	DGD	CAA-CBA-CCA-CDA
8	I	8632	DGD	CEA-CFA-CGA-CHA
2	H	7633	BNG	C5'-C6'-C7'-C8'
2	I	8633	BNG	C3'-C4'-C5'-C6'
7	B	1630	LHG	C15-C16-C17-C18
7	E	4630	LHG	C29-C30-C31-C32
7	H	7630	LHG	C9-C10-C11-C12
8	B	2632	DGD	CEA-CFA-CGA-CHA
8	D	3632	DGD	CDB-CEB-CFB-CGB
8	G	9632	DGD	CDB-CEB-CFB-CGB
8	H	7632	DGD	CDB-CEB-CFB-CGB
8	I	8632	DGD	CDB-CEB-CFB-CGB
7	B	1630	LHG	O1-C1-C2-O2
7	C	2630	LHG	O1-C1-C2-O2
7	D	3630	LHG	O1-C1-C2-O2
7	E	4630	LHG	O1-C1-C2-O2
7	H	7630	LHG	O1-C1-C2-O2
2	C	2633	BNG	C5'-C6'-C7'-C8'
2	J	9633	BNG	C3'-C4'-C5'-C6'
7	F	5630	LHG	C14-C15-C16-C17
8	A	632	DGD	C2A-C3A-C4A-C5A
8	E	4632	DGD	C7A-C8A-C9A-CAA
8	G	9632	DGD	C7A-C8A-C9A-CAA
10	A	613	CLA	C4B-C3B-CAB-CBB
10	E	613	CLA	C4B-C3B-CAB-CBB
7	D	3630	LHG	C23-C24-C25-C26
7	G	6630	LHG	C23-C24-C25-C26
7	H	7630	LHG	C23-C24-C25-C26
2	B	1633	BNG	C3'-C4'-C5'-C6'
7	I	8630	LHG	C9-C10-C11-C12
8	I	8632	DGD	CCB-CDB-CEB-CFB
9	B	608	CHL	C16-C17-C18-C19
9	C	607	CHL	C16-C17-C18-C20
9	D	607	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
9	E	608	CHL	C16-C17-C18-C19
9	H	607	CHL	C16-C17-C18-C20
9	H	608	CHL	C16-C17-C18-C19
9	I	607	CHL	C16-C17-C18-C20
10	B	613	CLA	C16-C17-C18-C19
10	B	611	CLA	C2A-CAA-CBA-CGA
7	B	1630	LHG	C14-C15-C16-C17
7	H	7630	LHG	C30-C31-C32-C33
7	I	8630	LHG	C34-C35-C36-C37
8	D	5632	DGD	C5A-C6A-C7A-C8A
8	E	4632	DGD	C6B-C7B-C8B-C9B
8	H	6632	DGD	CAA-CBA-CCA-CDA
8	H	7632	DGD	C5A-C6A-C7A-C8A
9	D	607	CHL	C5-C6-C7-C8
10	C	611	CLA	C15-C16-C17-C18
10	C	613	CLA	C13-C15-C16-C17
9	I	608	CHL	C12-C13-C15-C16
10	B	612	CLA	C11-C12-C13-C15
10	C	603	CLA	C11-C10-C8-C7
10	D	611	CLA	C6-C7-C8-C10
10	E	602	CLA	C11-C12-C13-C15
10	F	611	CLA	C6-C7-C8-C10
10	H	604	CLA	C11-C10-C8-C7
10	H	611	CLA	C6-C7-C8-C10
10	J	611	CLA	C6-C7-C8-C10
2	A	633	BNG	C3'-C4'-C5'-C6'
2	E	4633	BNG	C3'-C4'-C5'-C6'
8	A	632	DGD	CCB-CDB-CEB-CFB
8	D	3632	DGD	C6B-C7B-C8B-C9B
7	C	2630	LHG	C23-C24-C25-C26
7	F	5630	LHG	C23-C24-C25-C26
9	H	609	CHL	CBA-CGA-O2A-C1
10	B	603	CLA	C5-C6-C7-C8
2	F	5633	BNG	C3'-C4'-C5'-C6'
7	J	9630	LHG	C25-C26-C27-C28
8	H	6632	DGD	C7A-C8A-C9A-CAA
9	A	605	CHL	C3A-C2A-CAA-CBA
9	A	606	CHL	C3A-C2A-CAA-CBA
9	B	605	CHL	C3A-C2A-CAA-CBA
9	C	606	CHL	C3A-C2A-CAA-CBA
9	D	605	CHL	C3A-C2A-CAA-CBA
9	D	606	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	E	605	CHL	C3A-C2A-CAA-CBA
9	F	606	CHL	C3A-C2A-CAA-CBA
9	G	606	CHL	C3A-C2A-CAA-CBA
9	H	605	CHL	C3A-C2A-CAA-CBA
9	I	605	CHL	C3A-C2A-CAA-CBA
9	I	606	CHL	C3A-C2A-CAA-CBA
9	J	605	CHL	C3A-C2A-CAA-CBA
10	A	611	CLA	C3A-C2A-CAA-CBA
10	B	611	CLA	C3A-C2A-CAA-CBA
10	D	611	CLA	C3A-C2A-CAA-CBA
10	E	611	CLA	C3A-C2A-CAA-CBA
10	F	603	CLA	C3A-C2A-CAA-CBA
10	F	611	CLA	C3A-C2A-CAA-CBA
10	G	611	CLA	C3A-C2A-CAA-CBA
10	I	604	CLA	C3A-C2A-CAA-CBA
10	I	611	CLA	C3A-C2A-CAA-CBA
2	I	8633	BNG	C5'-C6'-C7'-C8'
2	J	9633	BNG	C5'-C6'-C7'-C8'
7	G	6630	LHG	C15-C16-C17-C18
7	I	8630	LHG	C32-C33-C34-C35
8	B	1632	DGD	C7A-C8A-C9A-CAA
8	G	9632	DGD	CEA-CFA-CGA-CHA
8	H	7632	DGD	C7A-C8A-C9A-CAA
2	I	8633	BNG	O5-C5-C6-O6
2	A	633	BNG	C5'-C6'-C7'-C8'
7	D	3630	LHG	C15-C16-C17-C18
9	B	609	CHL	C13-C15-C16-C17
9	D	607	CHL	C13-C15-C16-C17
9	J	608	CHL	C8-C10-C11-C12
9	J	609	CHL	C13-C15-C16-C17
10	B	611	CLA	C10-C11-C12-C13
10	D	603	CLA	C5-C6-C7-C8
10	G	611	CLA	C10-C11-C12-C13
10	I	603	CLA	C5-C6-C7-C8
9	C	601	CHL	O1D-CGD-O2D-CED
10	E	614	CLA	O1D-CGD-O2D-CED
10	G	602	CLA	O1D-CGD-O2D-CED
9	I	607	CHL	C16-C17-C18-C19
10	B	613	CLA	C16-C17-C18-C20
10	H	603	CLA	C16-C17-C18-C19
7	J	9630	LHG	C28-C29-C30-C31
8	A	632	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
10	H	610	CLA	C10-C11-C12-C13
10	G	614	CLA	CBD-CGD-O2D-CED
2	E	4633	BNG	C5'-C6'-C7'-C8'
7	E	4630	LHG	C15-C16-C17-C18
7	G	6630	LHG	C28-C29-C30-C31
9	A	609	CHL	CBA-CGA-O2A-C1
7	E	4630	LHG	C4-C5-C6-O8
2	G	6633	BNG	C3'-C4'-C5'-C6'
2	H	7633	BNG	C3'-C4'-C5'-C6'
7	E	4630	LHG	C14-C15-C16-C17
7	J	9630	LHG	C32-C33-C34-C35
8	D	3632	DGD	C2A-C3A-C4A-C5A
8	H	6632	DGD	CDB-CEB-CFB-CGB
8	I	8632	DGD	C5A-C6A-C7A-C8A
8	I	8632	DGD	C7A-C8A-C9A-CAA
10	A	604	CLA	C3-C5-C6-C7
10	J	603	CLA	C3-C5-C6-C7
8	B	1632	DGD	C1B-C2B-C3B-C4B
2	B	1633	BNG	C5'-C6'-C7'-C8'
2	G	6633	BNG	C5'-C6'-C7'-C8'
7	C	2630	LHG	C14-C15-C16-C17
7	C	2630	LHG	C30-C31-C32-C33
7	D	3630	LHG	C14-C15-C16-C17
7	D	3630	LHG	C28-C29-C30-C31
7	D	3630	LHG	C30-C31-C32-C33
7	G	6630	LHG	C9-C10-C11-C12
7	H	7630	LHG	C14-C15-C16-C17
7	H	7630	LHG	C15-C16-C17-C18
7	J	9630	LHG	C26-C27-C28-C29
8	A	632	DGD	C7A-C8A-C9A-CAA
8	E	4632	DGD	CAB-CBB-CCB-CDB
8	H	6632	DGD	CCB-CDB-CEB-CFB
8	H	7632	DGD	CAA-CBA-CCA-CDA
8	I	8632	DGD	C6B-C7B-C8B-C9B
9	H	609	CHL	O1A-CGA-O2A-C1
8	B	1632	DGD	CCB-CDB-CEB-CFB
8	D	5632	DGD	CAB-CBB-CCB-CDB
8	G	9632	DGD	CAA-CBA-CCA-CDA
8	H	7632	DGD	CAB-CBB-CCB-CDB
7	B	1630	LHG	C32-C33-C34-C35
7	J	9630	LHG	C14-C15-C16-C17
8	D	3632	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
8	D	5632	DGD	C2A-C3A-C4A-C5A
2	A	633	BNG	C1'-C2'-C3'-C4'
7	C	2630	LHG	C28-C29-C30-C31
7	G	6630	LHG	C14-C15-C16-C17
8	B	2632	DGD	CDB-CEB-CFB-CGB
10	E	613	CLA	C2B-C3B-CAB-CBB
7	G	6630	LHG	C32-C33-C34-C35
8	B	2632	DGD	CCB-CDB-CEB-CFB
8	G	9632	DGD	C5A-C6A-C7A-C8A
9	C	605	CHL	CBD-CGD-O2D-CED
7	G	6630	LHG	C8-C7-O7-C5
10	C	612	CLA	C10-C11-C12-C13
10	E	613	CLA	C8-C10-C11-C12
10	I	612	CLA	C3-C5-C6-C7
2	D	3633	BNG	C3'-C4'-C5'-C6'
7	F	5630	LHG	C33-C34-C35-C36
8	G	9632	DGD	C2A-C3A-C4A-C5A
8	H	6632	DGD	C6B-C7B-C8B-C9B
7	A	630	LHG	C14-C15-C16-C17
8	E	4632	DGD	CAA-CBA-CCA-CDA
2	A	633	BNG	C4-C5-C6-O6
8	D	3632	DGD	C1A-C2A-C3A-C4A
9	A	609	CHL	O1A-CGA-O2A-C1
9	G	609	CHL	O1A-CGA-O2A-C1
8	B	1632	DGD	C2A-C3A-C4A-C5A
10	B	613	CLA	C15-C16-C17-C18
9	B	608	CHL	C16-C17-C18-C20
7	E	4630	LHG	C28-C29-C30-C31
7	F	5630	LHG	C15-C16-C17-C18
8	B	2632	DGD	CAA-CBA-CCA-CDA
8	D	3632	DGD	C7A-C8A-C9A-CAA
8	E	4632	DGD	C5A-C6A-C7A-C8A
9	G	609	CHL	CBA-CGA-O2A-C1
9	B	608	CHL	C14-C13-C15-C16
10	D	602	CLA	C14-C13-C15-C16
10	J	610	CLA	C14-C13-C15-C16
7	H	7630	LHG	C28-C29-C30-C31
7	I	8630	LHG	C29-C30-C31-C32
8	B	1632	DGD	C6B-C7B-C8B-C9B
8	D	5632	DGD	CAA-CBA-CCA-CDA
10	J	603	CLA	C5-C6-C7-C8
7	B	1630	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	B	1632	DGD	CAA-CBA-CCA-CDA
8	E	4632	DGD	CDB-CEB-CFB-CGB
8	H	6632	DGD	O6D-C1D-O3G-C3G
8	H	6632	DGD	C2A-C3A-C4A-C5A
2	A	633	BNG	C2-C1-O1-C1'
2	C	2633	BNG	C2-C1-O1-C1'
2	D	3633	BNG	C2-C1-O1-C1'
2	E	4633	BNG	C2-C1-O1-C1'
2	G	6633	BNG	C2-C1-O1-C1'
2	H	7633	BNG	C2-C1-O1-C1'
9	J	607	CHL	C15-C16-C17-C18
2	E	4633	BNG	C1'-C2'-C3'-C4'
2	F	5633	BNG	C5'-C6'-C7'-C8'
7	J	9630	LHG	C18-C19-C20-C21
7	C	2630	LHG	C34-C35-C36-C37
9	A	609	CHL	C3-C5-C6-C7
9	G	607	CHL	C16-C17-C18-C19
10	E	613	CLA	C16-C17-C18-C19
10	F	611	CLA	C16-C17-C18-C19
10	G	611	CLA	C16-C17-C18-C19
10	G	613	CLA	C16-C17-C18-C19
10	J	613	CLA	C16-C17-C18-C19
7	A	630	LHG	C8-C7-O7-C5
8	H	7632	DGD	CCB-CDB-CEB-CFB
10	E	603	CLA	C13-C15-C16-C17
10	H	604	CLA	C5-C6-C7-C8
10	J	611	CLA	C5-C6-C7-C8
7	D	3630	LHG	C9-C10-C11-C12
9	B	609	CHL	C15-C16-C17-C18
8	D	3632	DGD	CAB-CBB-CCB-CDB
7	J	9630	LHG	C9-C10-C11-C12
8	D	3632	DGD	CCB-CDB-CEB-CFB
9	F	601	CHL	C3-C5-C6-C7
2	H	7633	BNG	C1'-C2'-C3'-C4'
7	A	630	LHG	C32-C33-C34-C35
7	H	7630	LHG	C34-C35-C36-C37
8	B	1632	DGD	CAB-CBB-CCB-CDB
9	B	609	CHL	C16-C17-C18-C20
9	D	609	CHL	C16-C17-C18-C20
9	F	607	CHL	C16-C17-C18-C20
10	B	611	CLA	C16-C17-C18-C20
10	D	610	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
10	F	611	CLA	C16-C17-C18-C20
10	G	611	CLA	C16-C17-C18-C20
10	G	613	CLA	C16-C17-C18-C20
10	J	613	CLA	C16-C17-C18-C20
7	G	6630	LHG	C34-C35-C36-C37
9	C	608	CHL	C13-C15-C16-C17
10	C	602	CLA	C5-C6-C7-C8
8	E	4632	DGD	CEA-CFA-CGA-CHA
2	B	1633	BNG	C1'-C2'-C3'-C4'
9	C	606	CHL	O1D-CGD-O2D-CED
7	E	4630	LHG	C34-C35-C36-C37
8	A	632	DGD	CAA-CBA-CCA-CDA
8	H	6632	DGD	CEA-CFA-CGA-CHA
10	A	612	CLA	C15-C16-C17-C18
10	D	604	CLA	C5-C6-C7-C8
10	H	611	CLA	C10-C11-C12-C13
8	B	2632	DGD	C5A-C6A-C7A-C8A
8	E	4632	DGD	C2A-C3A-C4A-C5A
9	J	606	CHL	CBA-CGA-O2A-C1
7	H	7630	LHG	C11-C10-C9-C8
8	D	5632	DGD	CDB-CEB-CFB-CGB
9	F	601	CHL	C13-C15-C16-C17
9	G	607	CHL	C5-C6-C7-C8
10	A	611	CLA	C8-C10-C11-C12
10	B	611	CLA	C8-C10-C11-C12
10	C	603	CLA	C13-C15-C16-C17
7	I	8630	LHG	C33-C34-C35-C36
8	G	9632	DGD	C2B-C3B-C4B-C5B
10	B	604	CLA	C5-C6-C7-C8
10	B	611	CLA	C15-C16-C17-C18
10	F	612	CLA	C10-C11-C12-C13
10	I	602	CLA	C5-C6-C7-C8
9	B	608	CHL	O1D-CGD-O2D-CED
7	G	6630	LHG	C11-C10-C9-C8
7	I	8630	LHG	C14-C15-C16-C17
8	H	6632	DGD	CAB-CBB-CCB-CDB
9	D	606	CHL	CBD-CGD-O2D-CED
8	B	1632	DGD	O1G-C1G-C2G-O2G
8	H	7632	DGD	O1G-C1G-C2G-O2G
8	I	8632	DGD	O1G-C1G-C2G-O2G
7	F	5630	LHG	C29-C30-C31-C32
8	B	2632	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
8	B	2632	DGD	C6B-C7B-C8B-C9B
9	I	609	CHL	CBA-CGA-O2A-C1
9	J	606	CHL	O1A-CGA-O2A-C1
7	A	630	LHG	C9-C10-C11-C12
7	B	1630	LHG	C13-C14-C15-C16
7	C	2630	LHG	C15-C16-C17-C18
10	D	603	CLA	C15-C16-C17-C18
10	H	602	CLA	C5-C6-C7-C8
10	J	613	CLA	C15-C16-C17-C18
7	A	630	LHG	C29-C30-C31-C32
7	D	3630	LHG	C16-C17-C18-C19
7	A	630	LHG	C28-C29-C30-C31
7	A	630	LHG	C11-C10-C9-C8
7	A	630	LHG	C34-C35-C36-C37
9	A	601	CHL	C3-C5-C6-C7
10	F	613	CLA	C13-C15-C16-C17
8	B	1632	DGD	CEA-CFA-CGA-CHA
8	E	4632	DGD	CCB-CDB-CEB-CFB
7	G	6630	LHG	C18-C19-C20-C21
8	B	2632	DGD	C2B-C3B-C4B-C5B
9	G	607	CHL	C16-C17-C18-C20
10	D	610	CLA	C16-C17-C18-C19
10	H	610	CLA	C16-C17-C18-C19
10	D	610	CLA	C13-C15-C16-C17
9	B	609	CHL	C3-C5-C6-C7
8	B	1632	DGD	CDB-CEB-CFB-CGB
10	B	611	CLA	C1A-C2A-CAA-CBA
10	F	611	CLA	C1A-C2A-CAA-CBA
10	G	611	CLA	C1A-C2A-CAA-CBA
10	H	604	CLA	C1A-C2A-CAA-CBA
10	H	611	CLA	C1A-C2A-CAA-CBA
7	F	5630	LHG	C13-C14-C15-C16
10	B	612	CLA	O1D-CGD-O2D-CED
7	C	2630	LHG	C25-C26-C27-C28
8	A	632	DGD	C5A-C6A-C7A-C8A
10	B	612	CLA	C10-C11-C12-C13
7	F	5630	LHG	O6-C4-C5-C6
7	I	8630	LHG	O6-C4-C5-C6
7	H	7630	LHG	C7-C8-C9-C10
10	B	612	CLA	C3-C5-C6-C7
10	D	602	CLA	C3-C5-C6-C7
10	I	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	A	601	CHL	C11-C10-C8-C7
9	A	609	CHL	C11-C12-C13-C15
9	B	601	CHL	C11-C12-C13-C15
9	B	608	CHL	C12-C13-C15-C16
9	C	601	CHL	C11-C12-C13-C15
9	C	608	CHL	C6-C7-C8-C10
9	C	608	CHL	C12-C13-C15-C16
9	D	608	CHL	C6-C7-C8-C10
9	D	608	CHL	C11-C12-C13-C15
9	D	609	CHL	C11-C12-C13-C15
9	D	609	CHL	C12-C13-C15-C16
9	E	608	CHL	C6-C7-C8-C10
9	E	608	CHL	C12-C13-C15-C16
9	F	608	CHL	C12-C13-C15-C16
9	G	601	CHL	C11-C10-C8-C7
9	G	601	CHL	C12-C13-C15-C16
9	G	608	CHL	C6-C7-C8-C10
9	G	608	CHL	C12-C13-C15-C16
9	H	608	CHL	C12-C13-C15-C16
9	I	608	CHL	C11-C12-C13-C15
9	I	609	CHL	C12-C13-C15-C16
9	J	601	CHL	C12-C13-C15-C16
9	J	607	CHL	C12-C13-C15-C16
9	J	608	CHL	C6-C7-C8-C10
9	J	608	CHL	C11-C12-C13-C15
9	J	608	CHL	C12-C13-C15-C16
9	J	609	CHL	C11-C12-C13-C15
10	A	612	CLA	C11-C12-C13-C15
10	B	602	CLA	C11-C12-C13-C15
10	B	611	CLA	C6-C7-C8-C10
10	C	602	CLA	C11-C10-C8-C7
10	C	602	CLA	C11-C12-C13-C15
10	C	610	CLA	C11-C12-C13-C15
10	C	613	CLA	C11-C12-C13-C15
10	D	602	CLA	C11-C12-C13-C15
10	D	612	CLA	C11-C12-C13-C15
10	E	612	CLA	C11-C12-C13-C15
10	F	602	CLA	C11-C10-C8-C7
10	F	613	CLA	C12-C13-C15-C16
10	G	610	CLA	C11-C12-C13-C15
10	G	611	CLA	C6-C7-C8-C10
10	H	610	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
10	H	612	CLA	C11-C12-C13-C15
10	H	613	CLA	C12-C13-C15-C16
10	I	602	CLA	C11-C10-C8-C7
10	I	602	CLA	C11-C12-C13-C15
10	I	603	CLA	C12-C13-C15-C16
10	J	604	CLA	C6-C7-C8-C10
10	J	612	CLA	C11-C12-C13-C15
7	F	5630	LHG	C25-C26-C27-C28
7	I	8630	LHG	C11-C10-C9-C8
8	A	632	DGD	CEA-CFA-CGA-CHA
8	H	6632	DGD	CEB-CFB-CGB-CHB
8	H	7632	DGD	CEA-CFA-CGA-CHA
9	C	608	CHL	C16-C17-C18-C19
10	B	611	CLA	C16-C17-C18-C19
9	B	609	CHL	O1A-CGA-O2A-C1
7	E	4630	LHG	C32-C33-C34-C35
9	G	606	CHL	CBA-CGA-O2A-C1
8	A	632	DGD	C6B-C7B-C8B-C9B
10	G	604	CLA	C13-C15-C16-C17
9	G	609	CHL	C8-C10-C11-C12
9	B	608	CHL	C4-C3-C5-C6
9	I	609	CHL	O1A-CGA-O2A-C1
10	F	612	CLA	C5-C6-C7-C8
9	A	601	CHL	C11-C10-C8-C9
9	A	607	CHL	C14-C13-C15-C16
9	B	607	CHL	C14-C13-C15-C16
9	C	608	CHL	C6-C7-C8-C9
9	D	608	CHL	C11-C12-C13-C14
9	D	609	CHL	C14-C13-C15-C16
9	F	607	CHL	C14-C13-C15-C16
9	F	609	CHL	C11-C12-C13-C14
9	G	601	CHL	C14-C13-C15-C16
9	G	607	CHL	C14-C13-C15-C16
9	G	609	CHL	C11-C12-C13-C14
9	H	601	CHL	C14-C13-C15-C16
9	I	601	CHL	C14-C13-C15-C16
9	I	608	CHL	C6-C7-C8-C9
10	B	602	CLA	C11-C10-C8-C9
10	B	611	CLA	C6-C7-C8-C9
10	B	612	CLA	C11-C12-C13-C14
10	C	602	CLA	C11-C10-C8-C9
10	D	602	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
10	D	603	CLA	C14-C13-C15-C16
10	D	604	CLA	C6-C7-C8-C9
10	D	612	CLA	C11-C12-C13-C14
10	E	602	CLA	C11-C10-C8-C9
10	F	602	CLA	C11-C10-C8-C9
10	F	611	CLA	C6-C7-C8-C9
10	G	603	CLA	C11-C12-C13-C14
10	H	602	CLA	C14-C13-C15-C16
10	H	604	CLA	C11-C10-C8-C9
10	H	611	CLA	C6-C7-C8-C9
10	H	612	CLA	C14-C13-C15-C16
10	I	602	CLA	C11-C10-C8-C9
10	I	611	CLA	C6-C7-C8-C9
10	J	603	CLA	C11-C12-C13-C14
7	D	3630	LHG	C11-C10-C9-C8
7	J	9630	LHG	C11-C10-C9-C8
8	I	8632	DGD	C2B-C3B-C4B-C5B
8	B	2632	DGD	CAB-CBB-CCB-CDB
9	B	609	CHL	CBA-CGA-O2A-C1
9	J	609	CHL	CBA-CGA-O2A-C1
7	F	5630	LHG	C32-C33-C34-C35
7	C	2630	LHG	C11-C10-C9-C8
7	C	2630	LHG	C4-C5-C6-O8
7	D	3630	LHG	C4-C5-C6-O8
9	I	608	CHL	O1D-CGD-O2D-CED
7	E	4630	LHG	C16-C17-C18-C19
9	H	608	CHL	C5-C6-C7-C8
7	B	1630	LHG	C28-C29-C30-C31
9	D	609	CHL	C16-C17-C18-C19
10	E	613	CLA	C16-C17-C18-C20
10	H	611	CLA	C16-C17-C18-C20
10	D	610	CLA	O1D-CGD-O2D-CED
9	A	608	CHL	CHA-CBD-CGD-O1D
9	D	605	CHL	CHA-CBD-CGD-O1D
9	D	608	CHL	CHA-CBD-CGD-O1D
9	D	608	CHL	CHA-CBD-CGD-O2D
9	E	605	CHL	CHA-CBD-CGD-O1D
9	E	609	CHL	CHA-CBD-CGD-O2D
9	F	607	CHL	CHA-CBD-CGD-O1D
9	G	607	CHL	CHA-CBD-CGD-O1D
9	H	608	CHL	CHA-CBD-CGD-O1D
9	J	608	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
9	J	608	CHL	CHA-CBD-CGD-O2D
10	B	613	CLA	C13-C15-C16-C17
9	G	606	CHL	O1A-CGA-O2A-C1
9	J	609	CHL	O1A-CGA-O2A-C1
7	G	6630	LHG	C30-C31-C32-C33
9	B	608	CHL	C2-C3-C5-C6
10	J	603	CLA	C2-C3-C5-C6
9	B	601	CHL	C13-C15-C16-C17
9	G	609	CHL	C13-C15-C16-C17
2	A	633	BNG	C4'-C5'-C6'-C7'
7	C	2630	LHG	C13-C14-C15-C16
10	C	611	CLA	C16-C17-C18-C19
10	C	604	CLA	C13-C15-C16-C17
7	B	1630	LHG	C29-C30-C31-C32
7	E	4630	LHG	C25-C26-C27-C28
7	H	7630	LHG	C16-C17-C18-C19
8	H	7632	DGD	CEB-CFB-CGB-CHB
9	B	607	CHL	C13-C15-C16-C17
9	D	605	CHL	C2A-CAA-CBA-CGA
10	C	611	CLA	C2A-CAA-CBA-CGA
8	A	632	DGD	CAB-CBB-CCB-CDB
7	D	3630	LHG	C25-C26-C27-C28
7	F	5630	LHG	C11-C10-C9-C8
2	J	9633	BNG	C1'-C2'-C3'-C4'
9	F	609	CHL	CBA-CGA-O2A-C1
9	F	608	CHL	O2A-C1-C2-C3
7	E	4630	LHG	C11-C10-C9-C8
7	F	5630	LHG	C34-C35-C36-C37
8	G	9632	DGD	C3B-C4B-C5B-C6B
10	H	612	CLA	C10-C11-C12-C13
10	J	603	CLA	C10-C11-C12-C13
10	C	611	CLA	C16-C17-C18-C20
10	J	603	CLA	C16-C17-C18-C20
7	B	1630	LHG	C7-C8-C9-C10
6	E	4623	NEX	C11-C10-C9-C8
8	A	632	DGD	C8B-C9B-CAB-CBB
9	B	607	CHL	O1D-CGD-O2D-CED
9	C	609	CHL	CBA-CGA-O2A-C1
2	C	2633	BNG	C6'-C7'-C8'-C9'
2	F	5633	BNG	C6'-C7'-C8'-C9'
8	I	8632	DGD	C2A-C3A-C4A-C5A
8	H	7632	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
10	J	613	CLA	C3-C5-C6-C7
10	I	611	CLA	C16-C17-C18-C19
2	H	7633	BNG	C4'-C5'-C6'-C7'
8	I	8632	DGD	C8B-C9B-CAB-CBB
2	E	4633	BNG	C6'-C7'-C8'-C9'
2	B	1633	BNG	C4'-C5'-C6'-C7'
7	A	630	LHG	C13-C14-C15-C16
7	E	4630	LHG	C10-C11-C12-C13
8	B	2632	DGD	C8A-C9A-CAA-CBA
8	E	4632	DGD	C7B-C8B-C9B-CAB
7	A	630	LHG	C30-C31-C32-C33
8	H	7632	DGD	C7B-C8B-C9B-CAB
10	I	603	CLA	O1D-CGD-O2D-CED
10	D	604	CLA	C2A-CAA-CBA-CGA
10	F	604	CLA	C2A-CAA-CBA-CGA
9	G	609	CHL	C3-C5-C6-C7
10	E	613	CLA	C3-C5-C6-C7
2	F	5633	BNG	C1'-C2'-C3'-C4'
2	G	6633	BNG	C1'-C2'-C3'-C4'
7	D	3630	LHG	C35-C36-C37-C38
10	E	602	CLA	C5-C6-C7-C8
9	A	607	CHL	C16-C17-C18-C19
9	A	609	CHL	C16-C17-C18-C20
9	E	608	CHL	C16-C17-C18-C20
9	I	608	CHL	C16-C17-C18-C19
9	I	608	CHL	CBD-CGD-O2D-CED
7	C	2630	LHG	C9-C10-C11-C12
8	B	1632	DGD	C8B-C9B-CAB-CBB
9	C	601	CHL	CBA-CGA-O2A-C1
2	G	6633	BNG	C6'-C7'-C8'-C9'
8	D	5632	DGD	CEA-CFA-CGA-CHA
8	D	5632	DGD	CCB-CDB-CEB-CFB
10	G	611	CLA	C15-C16-C17-C18
9	C	601	CHL	C3-C5-C6-C7
7	I	8630	LHG	C18-C19-C20-C21
7	H	7630	LHG	C19-C20-C21-C22
10	J	611	CLA	C16-C17-C18-C19
2	I	8633	BNG	C6'-C7'-C8'-C9'
2	D	3633	BNG	C4'-C5'-C6'-C7'
8	D	5632	DGD	C8B-C9B-CAB-CBB
7	A	630	LHG	O9-C7-O7-C5
7	G	6630	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
9	A	608	CHL	C6-C7-C8-C9
9	C	601	CHL	C11-C10-C8-C9
9	C	601	CHL	C14-C13-C15-C16
9	C	609	CHL	C11-C12-C13-C14
9	E	607	CHL	C14-C13-C15-C16
9	E	608	CHL	C6-C7-C8-C9
9	E	608	CHL	C14-C13-C15-C16
9	G	608	CHL	C6-C7-C8-C9
9	H	607	CHL	C14-C13-C15-C16
9	I	608	CHL	C11-C12-C13-C14
9	J	607	CHL	C14-C13-C15-C16
9	J	608	CHL	C6-C7-C8-C9
10	A	602	CLA	C11-C10-C8-C9
10	A	611	CLA	C11-C10-C8-C9
10	B	602	CLA	C11-C12-C13-C14
10	B	602	CLA	C14-C13-C15-C16
10	B	603	CLA	C11-C12-C13-C14
10	B	613	CLA	C14-C13-C15-C16
10	C	603	CLA	C11-C10-C8-C9
10	C	611	CLA	C6-C7-C8-C9
10	D	602	CLA	C11-C10-C8-C9
10	E	602	CLA	C11-C12-C13-C14
10	E	613	CLA	C11-C12-C13-C14
10	F	612	CLA	C11-C12-C13-C14
10	G	602	CLA	C11-C10-C8-C9
10	G	602	CLA	C11-C12-C13-C14
10	G	611	CLA	C6-C7-C8-C9
10	H	602	CLA	C11-C10-C8-C9
10	H	610	CLA	C11-C10-C8-C9
10	H	612	CLA	C11-C12-C13-C14
10	H	613	CLA	C14-C13-C15-C16
10	I	603	CLA	C14-C13-C15-C16
10	J	612	CLA	C11-C12-C13-C14
7	F	5630	LHG	C27-C28-C29-C30
9	E	601	CHL	C15-C16-C17-C18
10	F	611	CLA	C8-C10-C11-C12
10	G	612	CLA	C13-C15-C16-C17
10	H	613	CLA	C15-C16-C17-C18
10	J	612	CLA	C10-C11-C12-C13
2	D	3633	BNG	C6'-C7'-C8'-C9'
9	F	609	CHL	O1A-CGA-O2A-C1
7	G	6630	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
9	J	608	CHL	O1D-CGD-O2D-CED
7	B	1630	LHG	C25-C26-C27-C28
10	A	613	CLA	C15-C16-C17-C18
2	C	2633	BNG	C1'-C2'-C3'-C4'
8	H	6632	DGD	C8B-C9B-CAB-CBB
10	C	611	CLA	C10-C11-C12-C13
7	A	630	LHG	C18-C19-C20-C21
7	D	3630	LHG	O6-C4-C5-C6
7	H	7630	LHG	O6-C4-C5-C6
7	J	9630	LHG	O6-C4-C5-C6
7	H	7630	LHG	C25-C26-C27-C28
7	F	5630	LHG	C19-C20-C21-C22
9	A	601	CHL	C12-C13-C15-C16
9	A	608	CHL	C11-C12-C13-C15
9	A	608	CHL	C12-C13-C15-C16
9	A	609	CHL	C12-C13-C15-C16
9	B	608	CHL	C11-C12-C13-C15
9	B	609	CHL	C11-C12-C13-C15
9	B	609	CHL	C12-C13-C15-C16
9	D	601	CHL	C11-C10-C8-C7
9	D	608	CHL	C12-C13-C15-C16
9	E	601	CHL	C12-C13-C15-C16
9	E	608	CHL	C11-C12-C13-C15
9	E	609	CHL	C11-C12-C13-C15
9	F	609	CHL	C12-C13-C15-C16
9	G	608	CHL	C11-C12-C13-C15
9	G	609	CHL	C12-C13-C15-C16
9	H	609	CHL	C6-C7-C8-C10
9	H	609	CHL	C11-C12-C13-C15
9	H	609	CHL	C12-C13-C15-C16
9	I	609	CHL	C6-C7-C8-C10
9	J	601	CHL	C11-C12-C13-C15
9	J	609	CHL	C12-C13-C15-C16
10	A	602	CLA	C6-C7-C8-C10
10	A	602	CLA	C11-C12-C13-C15
10	A	603	CLA	C6-C7-C8-C10
10	A	603	CLA	C12-C13-C15-C16
10	A	612	CLA	C12-C13-C15-C16
10	B	602	CLA	C6-C7-C8-C10
10	B	612	CLA	C12-C13-C15-C16
10	D	603	CLA	C12-C13-C15-C16
10	D	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
10	D	610	CLA	C11-C10-C8-C7
10	E	612	CLA	C12-C13-C15-C16
10	E	613	CLA	C11-C12-C13-C15
10	F	602	CLA	C6-C7-C8-C10
10	F	602	CLA	C11-C12-C13-C15
10	F	603	CLA	C6-C7-C8-C10
10	F	610	CLA	C11-C10-C8-C7
10	F	612	CLA	C11-C12-C13-C15
10	G	602	CLA	C11-C12-C13-C15
10	G	603	CLA	C11-C12-C13-C15
10	G	612	CLA	C11-C12-C13-C15
10	H	602	CLA	C11-C12-C13-C15
10	I	603	CLA	C11-C12-C13-C15
10	I	610	CLA	C11-C10-C8-C7
10	I	612	CLA	C11-C12-C13-C15
10	J	602	CLA	C6-C7-C8-C10
10	J	602	CLA	C11-C12-C13-C15
10	J	603	CLA	C11-C12-C13-C15
10	J	612	CLA	C12-C13-C15-C16
10	I	611	CLA	C15-C16-C17-C18
10	J	611	CLA	C16-C17-C18-C20
7	C	2630	LHG	C27-C28-C29-C30
7	F	5630	LHG	C30-C31-C32-C33
7	I	8630	LHG	C27-C28-C29-C30
9	C	609	CHL	O1A-CGA-O2A-C1
8	H	7632	DGD	CFA-CGA-CHA-CIA
9	H	608	CHL	C4-C3-C5-C6
9	J	601	CHL	C3A-C2A-CAA-CBA
9	J	606	CHL	C3A-C2A-CAA-CBA
10	H	604	CLA	C3A-C2A-CAA-CBA
10	H	611	CLA	C3A-C2A-CAA-CBA
10	J	603	CLA	C4-C3-C5-C6
10	D	611	CLA	C15-C16-C17-C18
10	G	611	CLA	C8-C10-C11-C12
8	I	8632	DGD	CAB-CBB-CCB-CDB
9	H	608	CHL	C2-C3-C5-C6
7	E	4630	LHG	C9-C10-C11-C12
2	I	8633	BNG	C1'-C2'-C3'-C4'
8	B	2632	DGD	CEB-CFB-CGB-CHB
9	C	609	CHL	C8-C10-C11-C12
10	I	610	CLA	C8-C10-C11-C12
8	E	4632	DGD	CFA-CGA-CHA-CIA

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Mol	Chain	Res	Type	Atoms
9	C	601	CHL	O1A-CGA-O2A-C1
7	I	8630	LHG	C28-C29-C30-C31
8	H	7632	DGD	C6B-C7B-C8B-C9B
8	H	6632	DGD	O6E-C5E-C6E-O5E
10	I	602	CLA	CBD-CGD-O2D-CED
2	D	3633	BNG	C4-C5-C6-O6
7	H	7630	LHG	C4-C5-C6-O8
8	B	1632	DGD	O1G-C1G-C2G-C3G
8	H	7632	DGD	O1G-C1G-C2G-C3G
8	I	8632	DGD	O1G-C1G-C2G-C3G
8	D	3632	DGD	C5A-C6A-C7A-C8A
9	B	609	CHL	C16-C17-C18-C19
10	A	602	CLA	C16-C17-C18-C20
10	H	610	CLA	C16-C17-C18-C20
10	I	611	CLA	C16-C17-C18-C20
9	A	607	CHL	C13-C15-C16-C17
10	E	603	CLA	C8-C10-C11-C12
10	F	602	CLA	C5-C6-C7-C8
10	G	602	CLA	C5-C6-C7-C8
10	G	612	CLA	C10-C11-C12-C13
7	J	9630	LHG	C27-C28-C29-C30
7	C	2630	LHG	C11-C12-C13-C14
7	D	3630	LHG	C13-C14-C15-C16
10	H	613	CLA	O1D-CGD-O2D-CED
9	G	606	CHL	C1A-C2A-CAA-CBA
9	G	609	CHL	C1A-C2A-CAA-CBA
2	B	1633	BNG	C4-C5-C6-O6
7	J	9630	LHG	C30-C31-C32-C33
10	E	611	CLA	C4-C3-C5-C6
7	C	2630	LHG	C12-C13-C14-C15
8	H	6632	DGD	CBB-CCB-CDB-CEB
8	G	9632	DGD	C6B-C7B-C8B-C9B
8	H	6632	DGD	CFB-CGB-CHB-CIB
9	H	608	CHL	C16-C17-C18-C20
7	G	6630	LHG	C7-C8-C9-C10
8	D	3632	DGD	CEA-CFA-CGA-CHA
9	C	609	CHL	C3-C5-C6-C7
7	B	1630	LHG	C34-C35-C36-C37
7	I	8630	LHG	C25-C26-C27-C28
8	I	8632	DGD	C4A-C5A-C6A-C7A
9	E	609	CHL	C15-C16-C17-C18
10	D	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
7	B	1630	LHG	C19-C20-C21-C22
7	G	6630	LHG	C19-C20-C21-C22
10	G	614	CLA	O1D-CGD-O2D-CED
2	J	9633	BNG	C4'-C5'-C6'-C7'
9	C	608	CHL	C16-C17-C18-C20
10	B	612	CLA	C15-C16-C17-C18
7	A	630	LHG	O7-C5-C6-O8
7	B	1630	LHG	O7-C5-C6-O8
7	D	3630	LHG	O7-C5-C6-O8
7	F	5630	LHG	O7-C5-C6-O8
7	H	7630	LHG	O7-C5-C6-O8
8	D	3632	DGD	O1G-C1G-C2G-O2G
8	G	9632	DGD	O1G-C1G-C2G-O2G
8	H	6632	DGD	O1G-C1G-C2G-O2G
2	A	633	BNG	C6'-C7'-C8'-C9'
10	F	610	CLA	O1D-CGD-O2D-CED
7	C	2630	LHG	C29-C30-C31-C32
10	G	612	CLA	C4-C3-C5-C6
9	E	607	CHL	O1D-CGD-O2D-CED
7	H	7630	LHG	C13-C14-C15-C16
8	H	6632	DGD	C7B-C8B-C9B-CAB
8	H	7632	DGD	C4A-C5A-C6A-C7A
10	H	613	CLA	C8-C10-C11-C12
9	A	607	CHL	C16-C17-C18-C20
10	H	611	CLA	C16-C17-C18-C19
10	I	610	CLA	C16-C17-C18-C19
7	I	8630	LHG	C13-C14-C15-C16
8	B	2632	DGD	C4A-C5A-C6A-C7A
7	C	2630	LHG	C7-C8-C9-C10
7	I	8630	LHG	C7-C8-C9-C10
9	D	607	CHL	C14-C13-C15-C16
9	D	608	CHL	C6-C7-C8-C9
9	I	609	CHL	C11-C12-C13-C14
9	J	601	CHL	C11-C10-C8-C9
9	J	609	CHL	C11-C12-C13-C14
10	A	612	CLA	C11-C12-C13-C14
10	E	612	CLA	C11-C12-C13-C14
10	F	602	CLA	C11-C12-C13-C14
10	F	604	CLA	C6-C7-C8-C9
10	G	603	CLA	C11-C10-C8-C9
10	H	603	CLA	C14-C13-C15-C16
10	I	602	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
10	I	603	CLA	C11-C10-C8-C9
10	I	603	CLA	C11-C12-C13-C14
10	I	612	CLA	C11-C12-C13-C14
10	J	602	CLA	C11-C10-C8-C9
10	J	611	CLA	C6-C7-C8-C9
8	B	1632	DGD	CFA-CGA-CHA-CIA
7	F	5630	LHG	C16-C17-C18-C19
10	A	614	CLA	O1D-CGD-O2D-CED
8	H	6632	DGD	C6A-C7A-C8A-C9A
9	B	607	CHL	C16-C17-C18-C19
10	F	602	CLA	C3-C5-C6-C7
8	H	6632	DGD	CFA-CGA-CHA-CIA
8	I	8632	DGD	CFB-CGB-CHB-CIB
10	C	614	CLA	O2A-C1-C2-C3
10	I	614	CLA	O2A-C1-C2-C3
8	H	6632	DGD	C3B-C4B-C5B-C6B
2	B	1633	BNG	O1-C1'-C2'-C3'
7	D	3630	LHG	C19-C20-C21-C22
9	C	601	CHL	C2A-CAA-CBA-CGA
9	E	605	CHL	C2A-CAA-CBA-CGA
7	F	5630	LHG	C28-C29-C30-C31
9	D	601	CHL	C13-C15-C16-C17
10	E	613	CLA	C15-C16-C17-C18
10	F	613	CLA	C3-C5-C6-C7
10	B	604	CLA	C4-C3-C5-C6
10	G	611	CLA	C4-C3-C5-C6
7	J	9630	LHG	C19-C20-C21-C22
9	B	607	CHL	C16-C17-C18-C20
9	D	608	CHL	C16-C17-C18-C20
9	E	609	CHL	C16-C17-C18-C20
8	G	9632	DGD	C3A-C4A-C5A-C6A
8	D	5632	DGD	CFA-CGA-CHA-CIA
7	H	7630	LHG	C29-C30-C31-C32
8	B	2632	DGD	CBB-CCB-CDB-CEB
10	G	603	CLA	C10-C11-C12-C13
7	G	6630	LHG	C1-C2-C3-O3
7	C	2630	LHG	C16-C17-C18-C19
9	D	609	CHL	CBA-CGA-O2A-C1
2	I	8633	BNG	C4'-C5'-C6'-C7'
7	C	2630	LHG	O6-C4-C5-C6
9	D	601	CHL	C16-C17-C18-C20
10	F	603	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
10	I	611	CLA	C8-C10-C11-C12
9	A	601	CHL	C11-C12-C13-C15
9	C	601	CHL	C11-C10-C8-C7
9	C	608	CHL	C11-C12-C13-C15
9	E	609	CHL	C12-C13-C15-C16
9	F	601	CHL	C12-C13-C15-C16
9	F	608	CHL	C11-C12-C13-C15
9	H	608	CHL	C11-C12-C13-C15
9	I	609	CHL	C11-C12-C13-C15
9	J	601	CHL	C11-C10-C8-C7
10	A	604	CLA	C11-C12-C13-C15
10	B	610	CLA	C11-C10-C8-C7
10	C	602	CLA	C6-C7-C8-C10
10	C	604	CLA	C11-C12-C13-C15
10	C	610	CLA	C11-C10-C8-C7
10	C	612	CLA	C11-C12-C13-C15
10	E	603	CLA	C6-C7-C8-C10
10	E	610	CLA	C11-C10-C8-C7
10	F	604	CLA	C11-C12-C13-C15
10	G	603	CLA	C11-C10-C8-C7
10	G	604	CLA	C11-C12-C13-C15
10	G	610	CLA	C11-C10-C8-C7
10	I	603	CLA	C11-C10-C8-C7
10	J	610	CLA	C11-C10-C8-C7
8	I	8632	DGD	CFA-CGA-CHA-CIA
7	E	4630	LHG	C27-C28-C29-C30
10	D	612	CLA	C10-C11-C12-C13
10	J	613	CLA	C5-C6-C7-C8
10	I	611	CLA	C2A-CAA-CBA-CGA
8	H	7632	DGD	C2A-C3A-C4A-C5A
10	H	612	CLA	C4-C3-C5-C6
10	G	612	CLA	C2-C3-C5-C6
7	A	630	LHG	C35-C36-C37-C38
10	F	610	CLA	CBD-CGD-O2D-CED
7	B	1630	LHG	C26-C27-C28-C29
10	A	602	CLA	C10-C11-C12-C13
10	E	602	CLA	C15-C16-C17-C18
9	B	608	CHL	O2A-C1-C2-C3
9	H	608	CHL	O2A-C1-C2-C3
10	C	602	CLA	C10-C11-C12-C13
8	D	3632	DGD	CEB-CFB-CGB-CHB
7	B	1630	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
7	I	8630	LHG	C16-C17-C18-C19
9	D	609	CHL	O1A-CGA-O2A-C1
10	G	610	CLA	O1A-CGA-O2A-C1
9	A	608	CHL	C15-C16-C17-C18
10	B	602	CLA	C5-C6-C7-C8
10	E	611	CLA	C8-C10-C11-C12
7	G	6630	LHG	C13-C14-C15-C16
6	A	623	NEX	C11-C10-C9-C8
10	A	610	CLA	C15-C16-C17-C18
10	D	604	CLA	CAA-CBA-CGA-O2A
7	A	630	LHG	O6-C4-C5-O7
7	H	7630	LHG	O6-C4-C5-O7
8	D	3632	DGD	CFA-CGA-CHA-CIA
9	C	605	CHL	O1D-CGD-O2D-CED
7	B	1630	LHG	C4-C5-C6-O8
7	F	5630	LHG	C4-C5-C6-O8
7	I	8630	LHG	C4-C5-C6-O8
9	F	609	CHL	C8-C10-C11-C12
7	J	9630	LHG	C33-C34-C35-C36
10	H	612	CLA	C2-C3-C5-C6
7	D	3630	LHG	C29-C30-C31-C32
8	E	4632	DGD	CEB-CFB-CGB-CHB
10	D	612	CLA	C3-C5-C6-C7
10	G	613	CLA	C3-C5-C6-C7
7	E	4630	LHG	O7-C5-C6-O8
7	I	8630	LHG	O7-C5-C6-O8
10	J	610	CLA	C13-C15-C16-C17
9	A	601	CHL	C14-C13-C15-C16
9	I	601	CHL	C11-C12-C13-C14
10	A	603	CLA	C14-C13-C15-C16
10	A	611	CLA	C6-C7-C8-C9
10	C	613	CLA	C11-C12-C13-C14
10	D	611	CLA	C6-C7-C8-C9
10	F	613	CLA	C14-C13-C15-C16
9	A	601	CHL	C16-C17-C18-C20
8	H	6632	DGD	C4A-C5A-C6A-C7A
8	D	5632	DGD	C7B-C8B-C9B-CAB
9	A	608	CHL	O1A-CGA-O2A-C1
2	E	4633	BNG	C4'-C5'-C6'-C7'
7	A	630	LHG	C25-C26-C27-C28
9	J	601	CHL	C15-C16-C17-C18
10	A	602	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	F	603	CLA	C8-C10-C11-C12
7	B	1630	LHG	C30-C31-C32-C33
8	E	4632	DGD	C8B-C9B-CAB-CBB
10	C	613	CLA	C8-C10-C11-C12
10	I	613	CLA	C15-C16-C17-C18
9	C	608	CHL	C3-C5-C6-C7
10	E	604	CLA	C3-C5-C6-C7
10	E	602	CLA	O1D-CGD-O2D-CED
9	E	609	CHL	C16-C17-C18-C19
10	E	611	CLA	C16-C17-C18-C19
10	C	613	CLA	C15-C16-C17-C18
10	D	603	CLA	C8-C10-C11-C12
7	D	3630	LHG	C33-C34-C35-C36
2	E	4633	BNG	C4-C5-C6-O6
7	C	2630	LHG	C17-C18-C19-C20
9	C	607	CHL	C4-C3-C5-C6
10	F	604	CLA	C4-C3-C5-C6
10	G	611	CLA	C2-C3-C5-C6
8	A	632	DGD	C4A-C5A-C6A-C7A
10	E	612	CLA	C15-C16-C17-C18
8	I	8632	DGD	C9B-CAB-CBB-CCB
2	B	1633	BNG	C6'-C7'-C8'-C9'
10	J	603	CLA	C16-C17-C18-C19
7	C	2630	LHG	C26-C27-C28-C29
8	A	632	DGD	C6A-C7A-C8A-C9A
10	H	604	CLA	C3-C5-C6-C7
9	A	609	CHL	C4C-C3C-CAC-CBC
2	J	9633	BNG	C6'-C7'-C8'-C9'
7	E	4630	LHG	C33-C34-C35-C36
7	E	4630	LHG	C19-C20-C21-C22
9	A	609	CHL	C16-C17-C18-C19
9	B	601	CHL	C16-C17-C18-C20
9	E	607	CHL	C16-C17-C18-C19
2	H	7633	BNG	C6'-C7'-C8'-C9'
10	B	602	CLA	C4B-C3B-CAB-CBB
10	D	602	CLA	C4B-C3B-CAB-CBB
10	D	603	CLA	C1A-C2A-CAA-CBA
10	D	613	CLA	C1A-C2A-CAA-CBA
10	F	604	CLA	C1A-C2A-CAA-CBA
10	H	603	CLA	C1A-C2A-CAA-CBA
10	G	610	CLA	O1D-CGD-O2D-CED
10	H	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	F	608	CHL	C4-C3-C5-C6
10	G	604	CLA	C4-C3-C5-C6
10	J	611	CLA	C4-C3-C5-C6
10	D	602	CLA	C5-C6-C7-C8
9	F	608	CHL	C2-C3-C5-C6
10	B	604	CLA	C2-C3-C5-C6
8	A	632	DGD	C2B-C3B-C4B-C5B
9	G	606	CHL	C2A-CAA-CBA-CGA
10	F	611	CLA	C2A-CAA-CBA-CGA
8	H	7632	DGD	CBB-CCB-CDB-CEB
7	A	630	LHG	O6-C4-C5-C6
8	D	3632	DGD	CBB-CCB-CDB-CEB
10	C	612	CLA	C3-C5-C6-C7
9	B	608	CHL	C6-C7-C8-C10
9	C	609	CHL	C11-C10-C8-C7
9	F	601	CHL	C11-C10-C8-C7
9	F	608	CHL	C11-C10-C8-C7
9	F	609	CHL	C11-C10-C8-C7
9	J	609	CHL	C6-C7-C8-C10
10	D	602	CLA	C11-C10-C8-C7
10	D	603	CLA	C11-C10-C8-C7
10	E	602	CLA	C6-C7-C8-C10
10	E	602	CLA	C11-C10-C8-C7
10	F	604	CLA	C12-C13-C15-C16
10	G	602	CLA	C6-C7-C8-C10
10	H	602	CLA	C6-C7-C8-C10
10	H	604	CLA	C11-C12-C13-C15
10	H	610	CLA	C11-C12-C13-C15
10	I	602	CLA	C6-C7-C8-C10
10	I	610	CLA	C11-C12-C13-C15
10	I	613	CLA	C12-C13-C15-C16
10	J	610	CLA	C11-C12-C13-C15
8	B	1632	DGD	CFB-CGB-CHB-CIB
10	A	614	CLA	CBD-CGD-O2D-CED
7	G	6630	LHG	O2-C2-C3-O3
9	A	608	CHL	CBA-CGA-O2A-C1
7	B	1630	LHG	C11-C10-C9-C8
2	F	5633	BNG	C4-C5-C6-O6
8	B	2632	DGD	CFB-CGB-CHB-CIB
7	D	3630	LHG	C26-C27-C28-C29
7	B	1630	LHG	C35-C36-C37-C38
7	H	7630	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
9	E	609	CHL	O1A-CGA-O2A-C1
9	F	607	CHL	C4-C3-C5-C6
9	H	606	CHL	C3A-C2A-CAA-CBA
10	A	611	CLA	C4-C3-C5-C6
10	A	612	CLA	C4-C3-C5-C6
10	C	611	CLA	C4-C3-C5-C6
10	D	611	CLA	C4-C3-C5-C6
10	H	604	CLA	C4-C3-C5-C6
10	J	611	CLA	C3A-C2A-CAA-CBA
9	D	601	CHL	C16-C17-C18-C19
9	I	606	CHL	O1D-CGD-O2D-CED
7	A	630	LHG	C27-C28-C29-C30
9	E	609	CHL	C13-C15-C16-C17
8	H	6632	DGD	C2B-C3B-C4B-C5B
7	C	2630	LHG	O6-C4-C5-O7
7	D	3630	LHG	O6-C4-C5-O7
7	E	4630	LHG	O6-C4-C5-O7
7	F	5630	LHG	O6-C4-C5-O7
7	I	8630	LHG	O6-C4-C5-O7
7	J	9630	LHG	O6-C4-C5-O7
7	I	8630	LHG	C8-C7-O7-C5
9	A	608	CHL	C11-C12-C13-C14
9	F	608	CHL	C11-C10-C8-C9
9	J	608	CHL	C11-C12-C13-C14
10	A	603	CLA	C6-C7-C8-C9
10	B	602	CLA	C6-C7-C8-C9
10	C	602	CLA	C6-C7-C8-C9
10	C	612	CLA	C11-C12-C13-C14
10	E	611	CLA	C6-C7-C8-C9
10	F	604	CLA	C11-C12-C13-C14
10	G	604	CLA	C11-C12-C13-C14
10	G	610	CLA	C11-C10-C8-C9
10	H	602	CLA	C11-C12-C13-C14
10	H	613	CLA	C11-C12-C13-C14
10	I	610	CLA	C11-C10-C8-C9
10	J	602	CLA	C6-C7-C8-C9
10	J	602	CLA	C11-C12-C13-C14
8	G	9632	DGD	CAB-CBB-CCB-CDB
8	H	7632	DGD	C6A-C7A-C8A-C9A
8	D	3632	DGD	C8A-C9A-CAA-CBA
10	D	613	CLA	C15-C16-C17-C18
10	A	614	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
10	B	614	CLA	C1-C2-C3-C4
10	C	614	CLA	C1-C2-C3-C4
10	D	614	CLA	C1-C2-C3-C4
10	E	614	CLA	C1-C2-C3-C4
10	F	614	CLA	C1-C2-C3-C4
10	G	614	CLA	C1-C2-C3-C4
10	H	614	CLA	C1-C2-C3-C4
10	I	614	CLA	C1-C2-C3-C4
10	J	614	CLA	C1-C2-C3-C4
7	D	3630	LHG	C32-C33-C34-C35
10	C	603	CLA	O1D-CGD-O2D-CED
10	H	602	CLA	O1A-CGA-O2A-C1
7	C	2630	LHG	O7-C5-C6-O8
7	G	6630	LHG	O7-C5-C6-O8
7	H	7630	LHG	C27-C28-C29-C30
7	G	6630	LHG	C35-C36-C37-C38
9	J	609	CHL	C16-C17-C18-C20
10	D	603	CLA	C16-C17-C18-C20
7	D	3630	LHG	C27-C28-C29-C30
7	I	8630	LHG	C30-C31-C32-C33
8	B	2632	DGD	C8B-C9B-CAB-CBB
7	A	630	LHG	C4-C5-C6-O8
7	J	9630	LHG	C4-C5-C6-O8
8	G	9632	DGD	O1G-C1G-C2G-C3G
10	B	611	CLA	C4-C3-C5-C6
10	E	611	CLA	C2-C3-C5-C6
7	B	1630	LHG	C33-C34-C35-C36
10	C	604	CLA	CAD-CBD-CGD-O2D
10	H	602	CLA	C15-C16-C17-C18
7	C	2630	LHG	C33-C34-C35-C36
8	H	6632	DGD	C3A-C4A-C5A-C6A
9	I	608	CHL	C16-C17-C18-C20
10	A	602	CLA	C16-C17-C18-C19
7	A	630	LHG	C33-C34-C35-C36
9	D	601	CHL	C2A-CAA-CBA-CGA
9	I	605	CHL	C2A-CAA-CBA-CGA
10	A	611	CLA	C2A-CAA-CBA-CGA
9	E	608	CHL	O1A-CGA-O2A-C1
7	H	7630	LHG	C33-C34-C35-C36
8	D	3632	DGD	C8B-C9B-CAB-CBB
7	A	630	LHG	C4-O6-P-O4
7	B	1630	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
7	D	3630	LHG	C3-O3-P-O4
7	E	4630	LHG	C3-O3-P-O5
7	G	6630	LHG	C4-O6-P-O4
9	A	605	CHL	CHA-CBD-CGD-O1D
9	A	605	CHL	CHA-CBD-CGD-O2D
9	A	608	CHL	CHA-CBD-CGD-O2D
9	A	609	CHL	CHA-CBD-CGD-O2D
9	B	605	CHL	CHA-CBD-CGD-O2D
9	D	605	CHL	CHA-CBD-CGD-O2D
9	D	609	CHL	CHA-CBD-CGD-O2D
9	E	605	CHL	CHA-CBD-CGD-O2D
9	F	608	CHL	CHA-CBD-CGD-O2D
9	G	605	CHL	CHA-CBD-CGD-O2D
9	H	605	CHL	CHA-CBD-CGD-O2D
9	H	608	CHL	CHA-CBD-CGD-O2D
9	I	605	CHL	CHA-CBD-CGD-O2D
9	I	608	CHL	CHA-CBD-CGD-O1D
9	I	608	CHL	CHA-CBD-CGD-O2D
9	J	605	CHL	CHA-CBD-CGD-O1D
9	J	605	CHL	CHA-CBD-CGD-O2D
10	A	603	CLA	CHA-CBD-CGD-O1D
10	B	602	CLA	CHA-CBD-CGD-O1D
10	C	602	CLA	CHA-CBD-CGD-O2D
10	C	603	CLA	CHA-CBD-CGD-O1D
10	C	604	CLA	CAD-CBD-CGD-O1D
10	D	603	CLA	CHA-CBD-CGD-O1D
10	E	602	CLA	CHA-CBD-CGD-O2D
10	E	603	CLA	CHA-CBD-CGD-O1D
10	F	602	CLA	CHA-CBD-CGD-O1D
10	F	602	CLA	CHA-CBD-CGD-O2D
10	G	602	CLA	CHA-CBD-CGD-O1D
10	G	603	CLA	CHA-CBD-CGD-O1D
10	H	602	CLA	CHA-CBD-CGD-O2D
10	H	603	CLA	CHA-CBD-CGD-O1D
10	I	602	CLA	CHA-CBD-CGD-O2D
10	I	603	CLA	CHA-CBD-CGD-O1D
10	I	614	CLA	CAD-CBD-CGD-O1D
10	J	602	CLA	CHA-CBD-CGD-O1D
10	J	602	CLA	CHA-CBD-CGD-O2D
10	J	603	CLA	CHA-CBD-CGD-O1D
10	J	604	CLA	CAD-CBD-CGD-O1D
9	G	608	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
10	J	602	CLA	C3-C5-C6-C7
8	H	6632	DGD	C9A-CAA-CBA-CCA
8	H	6632	DGD	C5B-C6B-C7B-C8B
10	I	612	CLA	C4-C3-C5-C6
10	A	613	CLA	C2B-C3B-CAB-CBB
8	A	632	DGD	CFA-CGA-CHA-CIA
10	G	603	CLA	O1D-CGD-O2D-CED
10	E	611	CLA	C16-C17-C18-C20
9	D	601	CHL	O1D-CGD-O2D-CED
8	G	9632	DGD	CFA-CGA-CHA-CIA
8	B	2632	DGD	C4E-C5E-C6E-O5E
10	G	604	CLA	C2A-CAA-CBA-CGA
7	B	1630	LHG	C27-C28-C29-C30
8	G	9632	DGD	C5B-C6B-C7B-C8B
8	B	1632	DGD	CEB-CFB-CGB-CHB
9	B	608	CHL	C5-C6-C7-C8
10	A	614	CLA	O2A-C1-C2-C3
10	D	614	CLA	O2A-C1-C2-C3
8	B	1632	DGD	C4A-C5A-C6A-C7A
10	C	604	CLA	C4-C3-C5-C6
10	H	611	CLA	C4-C3-C5-C6
10	F	602	CLA	C10-C11-C12-C13
9	C	607	CHL	C2-C3-C5-C6
10	I	610	CLA	C16-C17-C18-C20
9	F	607	CHL	C8-C10-C11-C12
7	E	4630	LHG	O6-C4-C5-C6
10	E	612	CLA	C10-C11-C12-C13
9	B	609	CHL	C14-C13-C15-C16
9	J	609	CHL	C6-C7-C8-C9
10	A	611	CLA	C11-C12-C13-C14
10	B	604	CLA	C6-C7-C8-C9
10	C	602	CLA	C14-C13-C15-C16
10	D	613	CLA	C14-C13-C15-C16
10	E	602	CLA	C6-C7-C8-C9
10	E	602	CLA	C14-C13-C15-C16
10	F	602	CLA	C14-C13-C15-C16
10	F	603	CLA	C6-C7-C8-C9
10	F	613	CLA	C11-C12-C13-C14
10	G	612	CLA	C11-C12-C13-C14
9	A	607	CHL	C12-C13-C15-C16
9	A	608	CHL	C6-C7-C8-C10
9	G	609	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
9	G	609	CHL	C11-C12-C13-C15
9	I	608	CHL	C6-C7-C8-C10
10	B	603	CLA	C11-C12-C13-C15
10	C	613	CLA	C12-C13-C15-C16
10	D	610	CLA	C11-C12-C13-C15
10	D	613	CLA	C12-C13-C15-C16
10	F	613	CLA	C11-C12-C13-C15
10	G	602	CLA	C11-C10-C8-C7
10	H	613	CLA	C11-C12-C13-C15
10	I	611	CLA	C6-C7-C8-C10
6	B	1623	NEX	C11-C10-C9-C8
9	D	606	CHL	O1D-CGD-O2D-CED
7	G	6630	LHG	C25-C26-C27-C28
2	B	1633	BNG	O5-C1-O1-C1'
8	H	7632	DGD	O6D-C1D-O3G-C3G
2	G	6633	BNG	C4-C5-C6-O6
10	H	614	CLA	CBD-CGD-O2D-CED
10	F	612	CLA	C4-C3-C5-C6
8	H	6632	DGD	C8A-C9A-CAA-CBA
9	E	607	CHL	C16-C17-C18-C20
7	J	9630	LHG	O7-C5-C6-O8
10	C	612	CLA	C5-C6-C7-C8
10	F	611	CLA	C15-C16-C17-C18
8	G	9632	DGD	CFB-CGB-CHB-CIB
9	C	608	CHL	O1D-CGD-O2D-CED
10	C	604	CLA	C2A-CAA-CBA-CGA
7	I	8630	LHG	C26-C27-C28-C29
9	B	607	CHL	C4-C3-C5-C6
9	E	609	CHL	C4-C3-C5-C6
10	A	603	CLA	C4-C3-C5-C6
10	D	613	CLA	C16-C17-C18-C19
10	C	604	CLA	CAA-CBA-CGA-O2A
10	B	603	CLA	C15-C16-C17-C18
7	G	6630	LHG	C4-C5-C6-O8
8	D	3632	DGD	O1G-C1G-C2G-C3G
8	H	6632	DGD	O1G-C1G-C2G-C3G
10	J	613	CLA	O1D-CGD-O2D-CED
9	J	608	CHL	CBD-CGD-O2D-CED
10	F	602	CLA	C13-C15-C16-C17
9	J	609	CHL	C16-C17-C18-C19
10	H	613	CLA	C16-C17-C18-C19
7	H	7630	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
8	B	1632	DGD	C3A-C4A-C5A-C6A
7	F	5630	LHG	C7-C8-C9-C10
9	D	608	CHL	C3-C5-C6-C7
10	F	612	CLA	C3-C5-C6-C7
10	A	603	CLA	C5-C6-C7-C8
10	A	611	CLA	C2-C3-C5-C6
10	A	612	CLA	C2-C3-C5-C6
10	I	612	CLA	C2-C3-C5-C6
9	E	609	CHL	CBA-CGA-O2A-C1
7	J	9630	LHG	C13-C14-C15-C16
8	D	5632	DGD	CEB-CFB-CGB-CHB
10	B	602	CLA	C16-C17-C18-C20
9	B	608	CHL	C6-C7-C8-C9
9	C	607	CHL	C14-C13-C15-C16
9	C	609	CHL	C11-C10-C8-C9
9	F	609	CHL	C11-C10-C8-C9
9	H	609	CHL	C6-C7-C8-C9
9	I	607	CHL	C14-C13-C15-C16
10	A	602	CLA	C6-C7-C8-C9
10	A	602	CLA	C11-C12-C13-C14
10	A	613	CLA	C14-C13-C15-C16
10	C	604	CLA	C11-C12-C13-C14
10	D	603	CLA	C6-C7-C8-C9
10	E	603	CLA	C6-C7-C8-C9
10	G	613	CLA	C14-C13-C15-C16
10	H	602	CLA	C6-C7-C8-C9
10	I	613	CLA	C14-C13-C15-C16
10	J	610	CLA	C11-C10-C8-C9
8	D	5632	DGD	C2B-C3B-C4B-C5B
7	J	9630	LHG	C31-C32-C33-C34
10	E	610	CLA	O1D-CGD-O2D-CED
8	G	9632	DGD	O6E-C5E-C6E-O5E
8	E	4632	DGD	C8A-C9A-CAA-CBA
7	F	5630	LHG	C26-C27-C28-C29
8	G	9632	DGD	C8A-C9A-CAA-CBA
10	I	604	CLA	CBA-CGA-O2A-C1
9	I	601	CHL	O1A-CGA-O2A-C1
9	A	607	CHL	C4-C3-C5-C6
9	I	607	CHL	C4-C3-C5-C6
10	D	612	CLA	C4-C3-C5-C6
10	E	612	CLA	C4-C3-C5-C6
10	I	611	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	A	607	CHL	C2-C3-C5-C6
10	B	611	CLA	C2-C3-C5-C6
10	C	604	CLA	C2-C3-C5-C6
10	C	611	CLA	C2-C3-C5-C6
10	D	611	CLA	C2-C3-C5-C6
10	G	604	CLA	C2-C3-C5-C6
10	J	611	CLA	C2-C3-C5-C6
8	B	1632	DGD	O6E-C5E-C6E-O5E
10	A	604	CLA	CAA-CBA-CGA-O2A
9	H	601	CHL	C12-C13-C15-C16
9	H	608	CHL	C11-C10-C8-C7
10	A	602	CLA	C11-C10-C8-C7
10	A	611	CLA	C6-C7-C8-C10
10	B	602	CLA	C11-C10-C8-C7
10	G	604	CLA	C12-C13-C15-C16
9	J	601	CHL	C13-C15-C16-C17
10	G	613	CLA	C15-C16-C17-C18
9	B	608	CHL	CBD-CGD-O2D-CED
9	I	609	CHL	C8-C10-C11-C12
9	B	608	CHL	O1A-CGA-O2A-C1
8	D	3632	DGD	C7B-C8B-C9B-CAB
9	E	608	CHL	CBA-CGA-O2A-C1
7	I	8630	LHG	O9-C7-O7-C5
9	G	608	CHL	C16-C17-C18-C19
9	J	608	CHL	C16-C17-C18-C20
10	A	603	CLA	C16-C17-C18-C20
10	B	602	CLA	C16-C17-C18-C19
10	D	611	CLA	C16-C17-C18-C20
2	C	2633	BNG	C4'-C5'-C6'-C7'
8	A	632	DGD	O1G-C1G-C2G-O2G
8	E	4632	DGD	O1G-C1G-C2G-O2G
9	D	601	CHL	C3A-C2A-CAA-CBA
9	F	608	CHL	C3A-C2A-CAA-CBA
10	A	604	CLA	C4-C3-C5-C6
10	B	603	CLA	C4-C3-C5-C6
10	E	604	CLA	C4-C3-C5-C6
10	F	604	CLA	C3A-C2A-CAA-CBA
10	G	604	CLA	C3A-C2A-CAA-CBA
10	I	604	CLA	C4-C3-C5-C6
10	D	612	CLA	C2-C3-C5-C6
10	F	612	CLA	C2-C3-C5-C6
10	H	604	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	H	611	CLA	C2-C3-C5-C6
7	E	4630	LHG	C26-C27-C28-C29
10	H	613	CLA	C16-C17-C18-C20
2	C	2633	BNG	O5-C1-O1-C1'
2	D	3633	BNG	O5-C1-O1-C1'
2	E	4633	BNG	O5-C1-O1-C1'
2	H	7633	BNG	O5-C1-O1-C1'
6	A	623	NEX	C39-C29-C30-C31
6	B	1623	NEX	C39-C29-C30-C31
6	C	2623	NEX	C39-C29-C30-C31
6	D	3623	NEX	C39-C29-C30-C31
6	E	4623	NEX	C39-C29-C30-C31
6	F	5623	NEX	C39-C29-C30-C31
6	G	6623	NEX	C39-C29-C30-C31
6	H	7623	NEX	C39-C29-C30-C31
6	I	8623	NEX	C39-C29-C30-C31
6	J	9623	NEX	C39-C29-C30-C31
7	C	2630	LHG	C32-C33-C34-C35
8	B	1632	DGD	C8A-C9A-CAA-CBA
7	H	7630	LHG	C32-C33-C34-C35
9	A	609	CHL	C2-C1-O2A-CGA
9	H	606	CHL	C2-C1-O2A-CGA
9	B	608	CHL	C3-C5-C6-C7
10	I	613	CLA	C16-C17-C18-C20
10	C	602	CLA	C13-C15-C16-C17
10	H	612	CLA	C5-C6-C7-C8
7	I	8630	LHG	C12-C13-C14-C15
9	B	609	CHL	C4-C3-C5-C6
9	C	609	CHL	C4-C3-C5-C6
9	D	607	CHL	C4-C3-C5-C6
9	D	609	CHL	C4-C3-C5-C6
9	H	609	CHL	C4-C3-C5-C6
9	J	607	CHL	C4-C3-C5-C6
10	H	603	CLA	C4-C3-C5-C6
10	J	612	CLA	C4-C3-C5-C6
9	F	607	CHL	C2-C3-C5-C6
10	F	604	CLA	C2-C3-C5-C6
10	I	613	CLA	C16-C17-C18-C19
8	I	8632	DGD	C3A-C4A-C5A-C6A
8	H	7632	DGD	O6E-C5E-C6E-O5E
9	A	608	CHL	C3-C5-C6-C7
10	G	604	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	D	5632	DGD	C9A-CAA-CBA-CCA
9	B	601	CHL	C14-C13-C15-C16
9	C	601	CHL	C11-C12-C13-C14
9	C	607	CHL	C11-C10-C8-C9
9	I	609	CHL	C6-C7-C8-C9
9	J	601	CHL	C14-C13-C15-C16
10	A	604	CLA	C11-C12-C13-C14
10	B	611	CLA	C11-C10-C8-C9
10	C	613	CLA	C14-C13-C15-C16
10	D	603	CLA	C11-C10-C8-C9
10	H	610	CLA	C14-C13-C15-C16
10	I	602	CLA	C6-C7-C8-C9
10	I	602	CLA	C14-C13-C15-C16
10	I	610	CLA	C14-C13-C15-C16
10	I	613	CLA	C11-C12-C13-C14
7	I	8630	LHG	O1-C1-C2-C3
8	D	5632	DGD	CFB-CGB-CHB-CIB
7	B	1630	LHG	C17-C18-C19-C20
7	J	9630	LHG	C35-C36-C37-C38
9	B	606	CHL	C1A-C2A-CAA-CBA
9	B	609	CHL	C1A-C2A-CAA-CBA
9	C	609	CHL	C1A-C2A-CAA-CBA
9	D	609	CHL	C1A-C2A-CAA-CBA
9	E	609	CHL	C1A-C2A-CAA-CBA
9	J	609	CHL	C1A-C2A-CAA-CBA
10	A	611	CLA	C15-C16-C17-C18
10	J	604	CLA	C4-C3-C5-C6
9	B	607	CHL	C2-C3-C5-C6
9	D	607	CHL	C2-C3-C5-C6
9	E	609	CHL	C2-C3-C5-C6
9	I	607	CHL	C2-C3-C5-C6
10	A	604	CLA	C2-C3-C5-C6
7	I	8630	LHG	O1-C1-C2-O2
9	D	607	CHL	C2A-CAA-CBA-CGA
9	E	607	CHL	C2A-CAA-CBA-CGA
9	I	607	CHL	C2A-CAA-CBA-CGA
6	A	623	NEX	C28-C29-C30-C31
6	B	1623	NEX	C28-C29-C30-C31
6	C	2623	NEX	C28-C29-C30-C31
6	D	3623	NEX	C28-C29-C30-C31
6	E	4623	NEX	C28-C29-C30-C31
6	F	5623	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
6	G	6623	NEX	C28-C29-C30-C31
6	H	7623	NEX	C28-C29-C30-C31
6	I	8623	NEX	C28-C29-C30-C31
6	J	9623	NEX	C28-C29-C30-C31
10	A	603	CLA	C1A-C2A-CAA-CBA
10	C	603	CLA	C1A-C2A-CAA-CBA
10	C	604	CLA	C1A-C2A-CAA-CBA
10	J	611	CLA	C1A-C2A-CAA-CBA
7	A	630	LHG	C19-C20-C21-C22
7	A	630	LHG	C26-C27-C28-C29
10	C	602	CLA	C3-C5-C6-C7
2	A	633	BNG	O5-C1-O1-C1'
4	C	2621	LUT	C1-C6-C7-C8
4	D	3621	LUT	C1-C6-C7-C8
10	D	613	CLA	C16-C17-C18-C20
10	H	613	CLA	C3-C5-C6-C7
9	A	609	CHL	C4-C3-C5-C6
9	D	601	CHL	C4-C3-C5-C6
9	F	609	CHL	C4-C3-C5-C6
9	G	607	CHL	C4-C3-C5-C6
9	H	601	CHL	C4-C3-C5-C6
9	J	601	CHL	C4-C3-C5-C6
10	E	603	CLA	C4-C3-C5-C6
10	F	603	CLA	C4-C3-C5-C6
10	F	611	CLA	C4-C3-C5-C6
7	B	1630	LHG	O6-C4-C5-C6
7	G	6630	LHG	O6-C4-C5-C6
9	J	607	CHL	C2-C3-C5-C6
10	B	603	CLA	C2-C3-C5-C6
10	C	612	CLA	C2-C3-C5-C6
10	E	604	CLA	C2-C3-C5-C6
10	E	612	CLA	C2-C3-C5-C6
10	I	604	CLA	C2-C3-C5-C6
10	I	611	CLA	C2-C3-C5-C6
8	G	9632	DGD	CBB-CCB-CDB-CEB
8	D	5632	DGD	O6E-C5E-C6E-O5E
9	C	608	CHL	C11-C10-C8-C7
9	F	609	CHL	C11-C12-C13-C15
9	G	607	CHL	C12-C13-C15-C16
9	I	601	CHL	C11-C12-C13-C15
10	A	603	CLA	C11-C12-C13-C15
10	A	613	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
10	B	613	CLA	C12-C13-C15-C16
10	D	604	CLA	C11-C10-C8-C7
10	D	604	CLA	C11-C12-C13-C15
10	E	613	CLA	C12-C13-C15-C16
10	G	613	CLA	C12-C13-C15-C16
10	H	602	CLA	C11-C10-C8-C7
10	I	604	CLA	C12-C13-C15-C16
10	J	602	CLA	C11-C10-C8-C7
10	J	613	CLA	C12-C13-C15-C16
2	A	633	BNG	O1-C1'-C2'-C3'
7	G	6630	LHG	C27-C28-C29-C30
9	G	608	CHL	C16-C17-C18-C20
10	A	611	CLA	C16-C17-C18-C19
9	B	606	CHL	C2A-CAA-CBA-CGA
8	A	632	DGD	O6E-C5E-C6E-O5E
8	B	1632	DGD	C7B-C8B-C9B-CAB
2	H	7633	BNG	C2'-C3'-C4'-C5'
8	G	9632	DGD	C8B-C9B-CAB-CBB
7	I	8630	LHG	C19-C20-C21-C22
8	E	4632	DGD	CFB-CGB-CHB-CIB
10	I	613	CLA	C5-C6-C7-C8
9	H	607	CHL	C4-C3-C5-C6
9	J	609	CHL	C4-C3-C5-C6
10	D	604	CLA	C4-C3-C5-C6
10	D	602	CLA	C15-C16-C17-C18
9	B	609	CHL	C2-C3-C5-C6
9	C	609	CHL	C2-C3-C5-C6
9	D	609	CHL	C2-C3-C5-C6
9	H	609	CHL	C2-C3-C5-C6
10	A	603	CLA	C2-C3-C5-C6
10	F	611	CLA	C2-C3-C5-C6
10	G	602	CLA	C16-C17-C18-C20
9	G	601	CHL	C6-C7-C8-C9
10	J	613	CLA	C14-C13-C15-C16
10	D	611	CLA	C10-C11-C12-C13
10	H	611	CLA	C15-C16-C17-C18
8	H	6632	DGD	CCA-CDA-CEA-CFA
9	E	605	CHL	O1D-CGD-O2D-CED
8	D	3632	DGD	CFB-CGB-CHB-CIB
8	A	632	DGD	CBB-CCB-CDB-CEB
2	G	6633	BNG	O5-C1-O1-C1'
9	G	609	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	I	601	CHL	C4-C3-C5-C6
9	I	609	CHL	C4-C3-C5-C6
10	B	612	CLA	C4-C3-C5-C6
10	C	612	CLA	C4-C3-C5-C6
10	G	603	CLA	C4-C3-C5-C6
9	I	609	CHL	C2-C3-C5-C6
10	B	612	CLA	C2-C3-C5-C6
10	H	603	CLA	C2-C3-C5-C6
10	J	612	CLA	C2-C3-C5-C6
8	B	2632	DGD	C3B-C4B-C5B-C6B
10	C	603	CLA	C8-C10-C11-C12
10	A	610	CLA	O1D-CGD-O2D-CED
9	A	609	CHL	C15-C16-C17-C18
10	I	604	CLA	O1A-CGA-O2A-C1
7	A	630	LHG	C16-C17-C18-C19
7	G	6630	LHG	C26-C27-C28-C29
8	B	2632	DGD	C7B-C8B-C9B-CAB
8	B	1632	DGD	C1G-C2G-C3G-O3G
9	C	607	CHL	C2A-CAA-CBA-CGA
9	F	607	CHL	C2A-CAA-CBA-CGA
10	D	602	CLA	C10-C11-C12-C13
10	H	604	CLA	O1A-CGA-O2A-C1
9	F	601	CHL	C15-C16-C17-C18
10	E	611	CLA	C15-C16-C17-C18
9	J	608	CHL	C3-C5-C6-C7
7	G	6630	LHG	O6-C4-C5-O7
9	E	601	CHL	C4-C3-C5-C6
10	D	611	CLA	C16-C17-C18-C19
8	H	7632	DGD	C8A-C9A-CAA-CBA
2	J	9633	BNG	C2'-C3'-C4'-C5'
9	J	608	CHL	C16-C17-C18-C19
9	J	605	CHL	O1D-CGD-O2D-CED
9	C	608	CHL	CHA-CBD-CGD-O1D
9	E	608	CHL	CHA-CBD-CGD-O1D
9	F	601	CHL	CHA-CBD-CGD-O2D
9	D	609	CHL	C13-C15-C16-C17
10	H	602	CLA	C13-C15-C16-C17
7	B	1630	LHG	C12-C13-C14-C15
8	D	5632	DGD	C3A-C4A-C5A-C6A
8	H	7632	DGD	CFB-CGB-CHB-CIB
10	F	603	CLA	C16-C17-C18-C19
10	D	604	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	J	604	CLA	C2-C3-C5-C6
9	E	608	CHL	C3-C5-C6-C7
10	H	604	CLA	CBA-CGA-O2A-C1
9	B	607	CHL	C12-C13-C15-C16
9	I	609	CHL	C11-C10-C8-C7
10	D	612	CLA	C12-C13-C15-C16
8	D	3632	DGD	CDA-CEA-CFA-CGA
9	J	609	CHL	C15-C16-C17-C18
2	A	633	BNG	C2'-C3'-C4'-C5'
9	D	601	CHL	C6-C7-C8-C9
9	F	601	CHL	C14-C13-C15-C16
10	D	611	CLA	C14-C13-C15-C16
10	D	613	CLA	C11-C12-C13-C14
10	G	604	CLA	C6-C7-C8-C9
10	G	613	CLA	C11-C12-C13-C14
10	H	603	CLA	C11-C10-C8-C9
10	J	613	CLA	C11-C12-C13-C14
8	B	1632	DGD	C2G-C3G-O3G-C1D
8	I	8632	DGD	C2G-C3G-O3G-C1D
9	J	605	CHL	C2A-CAA-CBA-CGA
10	A	604	CLA	C2A-CAA-CBA-CGA
9	B	609	CHL	C2-C1-O2A-CGA
9	F	601	CHL	C2-C1-O2A-CGA
9	G	609	CHL	C2-C1-O2A-CGA
9	I	606	CHL	C2-C1-O2A-CGA
9	J	601	CHL	C2-C1-O2A-CGA
9	G	609	CHL	C16-C17-C18-C20
10	A	611	CLA	C16-C17-C18-C20
9	G	601	CHL	C4-C3-C5-C6
9	I	609	CHL	C3A-C2A-CAA-CBA
10	A	603	CLA	C3A-C2A-CAA-CBA
10	D	603	CLA	C3A-C2A-CAA-CBA
10	H	603	CLA	C3A-C2A-CAA-CBA
10	G	610	CLA	CBA-CGA-O2A-C1
9	I	608	CHL	O2A-C1-C2-C3
9	H	609	CHL	C13-C15-C16-C17
10	D	612	CLA	C8-C10-C11-C12
10	C	603	CLA	C16-C17-C18-C20
5	B	1622	XAT	O24-C26-C27-C28
5	B	5622	XAT	O24-C26-C27-C28
5	E	2622	XAT	O24-C26-C27-C28
5	F	6622	XAT	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
7	B	1630	LHG	O6-C4-C5-O7
10	B	614	CLA	O2A-C1-C2-C3
8	A	632	DGD	C8A-C9A-CAA-CBA
9	B	608	CHL	CBA-CGA-O2A-C1
10	I	603	CLA	C4-C3-C5-C6
10	F	614	CLA	C2A-CAA-CBA-CGA
10	H	604	CLA	C2A-CAA-CBA-CGA
9	C	607	CHL	C13-C15-C16-C17
2	G	6633	BNG	C4'-C5'-C6'-C7'
7	J	9630	LHG	C16-C17-C18-C19
8	B	1632	DGD	CBB-CCB-CDB-CEB
9	C	608	CHL	C11-C12-C13-C14
9	G	608	CHL	C11-C12-C13-C14
9	H	608	CHL	C11-C10-C8-C9
10	B	610	CLA	C11-C10-C8-C9
10	C	602	CLA	C11-C12-C13-C14
10	D	611	CLA	C11-C12-C13-C14
10	E	610	CLA	C14-C13-C15-C16
10	E	613	CLA	C14-C13-C15-C16
10	F	604	CLA	C14-C13-C15-C16
10	F	611	CLA	C11-C10-C8-C9
10	G	602	CLA	C6-C7-C8-C9
10	H	604	CLA	C11-C12-C13-C14
9	H	609	CHL	C16-C17-C18-C20
10	H	602	CLA	C16-C17-C18-C20
7	B	1630	LHG	O8-C23-C24-C25
7	H	7630	LHG	O8-C23-C24-C25
10	D	614	CLA	C2A-CAA-CBA-CGA
9	C	609	CHL	C12-C13-C15-C16
9	E	607	CHL	C12-C13-C15-C16
9	H	607	CHL	C12-C13-C15-C16
9	J	609	CHL	C11-C10-C8-C7
10	A	604	CLA	C6-C7-C8-C10
10	B	604	CLA	C12-C13-C15-C16
10	E	604	CLA	C12-C13-C15-C16
10	G	613	CLA	C11-C12-C13-C15
10	I	612	CLA	C12-C13-C15-C16
10	I	613	CLA	C11-C12-C13-C15
10	J	613	CLA	C11-C12-C13-C15
4	A	621	LUT	C1-C6-C7-C8
4	B	1621	LUT	C1-C6-C7-C8
4	B	1621	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	E	4621	LUT	C1-C6-C7-C8
4	F	5621	LUT	C1-C6-C7-C8
4	H	7621	LUT	C1-C6-C7-C8
4	I	8621	LUT	C1-C6-C7-C8
4	J	9620	LUT	C1-C6-C7-C8
4	J	9621	LUT	C1-C6-C7-C8
10	C	604	CLA	C2B-C3B-CAB-CBB
10	H	613	CLA	C2B-C3B-CAB-CBB
9	C	605	CHL	CAA-CBA-CGA-O2A
9	D	601	CHL	C2-C1-O2A-CGA
9	E	601	CHL	C2-C1-O2A-CGA
9	E	606	CHL	C2-C1-O2A-CGA
9	F	606	CHL	C2-C1-O2A-CGA
9	F	609	CHL	C2-C1-O2A-CGA
9	G	601	CHL	C2-C1-O2A-CGA
9	H	609	CHL	C2-C1-O2A-CGA
10	J	603	CLA	C13-C15-C16-C17
8	D	5632	DGD	CBB-CCB-CDB-CEB
7	D	3630	LHG	O8-C23-C24-C25
7	E	4630	LHG	O8-C23-C24-C25
9	I	605	CHL	CAA-CBA-CGA-O2A
9	G	609	CHL	C2-C3-C5-C6
10	C	613	CLA	C2-C3-C5-C6
8	G	9632	DGD	C9B-CAB-CBB-CCB
9	C	606	CHL	C1C-C2C-CMC-OMC
9	G	607	CHL	C2A-CAA-CBA-CGA
9	H	607	CHL	C2A-CAA-CBA-CGA
10	D	602	CLA	C13-C15-C16-C17
2	E	4633	BNG	O1-C1'-C2'-C3'
8	H	7632	DGD	O1G-C1A-C2A-C3A
9	H	605	CHL	CAA-CBA-CGA-O2A
8	I	8632	DGD	CBB-CCB-CDB-CEB
10	A	602	CLA	C15-C16-C17-C18
9	A	601	CHL	C13-C15-C16-C17
7	A	630	LHG	O8-C23-C24-C25
7	F	5630	LHG	O7-C7-C8-C9
8	D	3632	DGD	O1G-C1A-C2A-C3A
9	B	605	CHL	CAA-CBA-CGA-O2A
9	J	605	CHL	CAA-CBA-CGA-O2A
9	E	607	CHL	C4-C3-C5-C6
7	G	6630	LHG	O7-C7-C8-C9
7	G	6630	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
9	A	605	CHL	CAA-CBA-CGA-O2A
10	A	613	CLA	C16-C17-C18-C19
2	I	8633	BNG	C2'-C3'-C4'-C5'
8	D	5632	DGD	C3B-C4B-C5B-C6B
7	C	2630	LHG	O7-C7-C8-C9
10	H	614	CLA	O1D-CGD-O2D-CED
9	A	609	CHL	C6-C7-C8-C9
9	E	601	CHL	C14-C13-C15-C16
9	E	608	CHL	C11-C12-C13-C14
9	G	609	CHL	C6-C7-C8-C9
9	I	601	CHL	C6-C7-C8-C9
10	D	602	CLA	C6-C7-C8-C9
10	F	611	CLA	C11-C12-C13-C14
10	J	611	CLA	C11-C12-C13-C14
2	B	1633	BNG	C2'-C3'-C4'-C5'
7	H	7630	LHG	O7-C7-C8-C9
7	I	8630	LHG	O7-C7-C8-C9
10	C	602	CLA	CBD-CGD-O2D-CED
8	A	632	DGD	O1G-C1G-C2G-C3G
8	E	4632	DGD	O1G-C1G-C2G-C3G
10	H	613	CLA	C1A-C2A-CAA-CBA
9	E	601	CHL	CAA-CBA-CGA-O2A
10	D	613	CLA	CAA-CBA-CGA-O2A
10	F	612	CLA	CAA-CBA-CGA-O2A
10	J	603	CLA	CAA-CBA-CGA-O2A
8	D	5632	DGD	O1G-C1G-C2G-O2G
10	H	610	CLA	C8-C10-C11-C12
10	B	602	CLA	CBD-CGD-O2D-CED
9	I	601	CHL	CBA-CGA-O2A-C1
7	I	8630	LHG	O8-C23-C24-C25
10	D	611	CLA	C2A-CAA-CBA-CGA
7	A	630	LHG	O7-C7-C8-C9
7	F	5630	LHG	O8-C23-C24-C25
9	J	606	CHL	CAA-CBA-CGA-O2A
10	B	602	CLA	O1D-CGD-O2D-CED
2	F	5633	BNG	C4'-C5'-C6'-C7'
7	H	7630	LHG	C11-C12-C13-C14
9	A	606	CHL	C2-C1-O2A-CGA
9	D	606	CHL	C2-C1-O2A-CGA
9	J	609	CHL	C2-C1-O2A-CGA
7	D	3630	LHG	O7-C7-C8-C9
9	A	608	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
9	A	609	CHL	C6-C7-C8-C10
9	D	607	CHL	C11-C12-C13-C15
9	E	608	CHL	C11-C10-C8-C7
9	F	607	CHL	C12-C13-C15-C16
9	G	608	CHL	C11-C10-C8-C7
9	H	608	CHL	C6-C7-C8-C10
9	I	601	CHL	C6-C7-C8-C10
9	J	608	CHL	C11-C10-C8-C7
10	A	610	CLA	C11-C10-C8-C7
10	B	604	CLA	C11-C10-C8-C7
10	D	603	CLA	C6-C7-C8-C10
10	D	604	CLA	C12-C13-C15-C16
10	F	604	CLA	C11-C10-C8-C7
10	F	610	CLA	C6-C7-C8-C10
10	H	604	CLA	C12-C13-C15-C16
9	F	609	CHL	C2-C3-C5-C6
10	G	603	CLA	C2-C3-C5-C6
8	B	2632	DGD	C1G-C2G-O2G-C1B
8	B	2632	DGD	C3G-C2G-O2G-C1B
10	I	612	CLA	C10-C11-C12-C13
7	C	2630	LHG	O8-C23-C24-C25
10	J	612	CLA	C15-C16-C17-C18
9	H	605	CHL	C2A-CAA-CBA-CGA
9	J	609	CHL	C8-C10-C11-C12
10	E	614	CLA	O2A-C1-C2-C3
10	J	611	CLA	C15-C16-C17-C18
9	A	609	CHL	C3A-C2A-CAA-CBA
9	B	606	CHL	C3A-C2A-CAA-CBA
9	F	609	CHL	C3A-C2A-CAA-CBA
10	C	603	CLA	C3A-C2A-CAA-CBA
10	C	604	CLA	C3A-C2A-CAA-CBA
10	C	611	CLA	C3A-C2A-CAA-CBA
10	J	604	CLA	C3A-C2A-CAA-CBA
9	B	601	CHL	C16-C17-C18-C19
10	G	602	CLA	C16-C17-C18-C19
10	C	611	CLA	CAA-CBA-CGA-O2A
6	H	7623	NEX	C11-C10-C9-C8
7	A	630	LHG	O10-C23-C24-C25
7	D	3630	LHG	O10-C23-C24-C25
8	H	7632	DGD	O1A-C1A-C2A-C3A
9	B	605	CHL	CAA-CBA-CGA-O1A
9	H	605	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
10	D	604	CLA	CAA-CBA-CGA-O1A
9	D	605	CHL	CAA-CBA-CGA-O2A
9	G	605	CHL	CAA-CBA-CGA-O2A
7	E	4630	LHG	O10-C23-C24-C25
9	J	605	CHL	CAA-CBA-CGA-O1A
7	A	630	LHG	C7-C8-C9-C10
10	B	604	CLA	C2A-CAA-CBA-CGA
9	A	609	CHL	C11-C12-C13-C14
9	B	608	CHL	C11-C10-C8-C9
9	D	609	CHL	C11-C12-C13-C14
9	G	608	CHL	C11-C10-C8-C9
10	A	603	CLA	C11-C12-C13-C14
10	B	611	CLA	C11-C12-C13-C14
10	C	610	CLA	C11-C10-C8-C9
10	D	610	CLA	C11-C10-C8-C9
10	F	602	CLA	C6-C7-C8-C9
10	F	610	CLA	C11-C10-C8-C9
10	I	611	CLA	C11-C12-C13-C14
7	C	2630	LHG	O9-C7-C8-C9
7	G	6630	LHG	O10-C23-C24-C25
10	F	604	CLA	C5-C6-C7-C8
7	H	7630	LHG	O9-C7-C8-C9
7	I	8630	LHG	O9-C7-C8-C9
9	A	605	CHL	CAA-CBA-CGA-O1A
9	G	609	CHL	O1D-CGD-O2D-CED
8	D	3632	DGD	O1A-C1A-C2A-C3A
7	B	1630	LHG	O10-C23-C24-C25
7	H	7630	LHG	O10-C23-C24-C25
9	C	605	CHL	CAA-CBA-CGA-O1A
8	A	632	DGD	C2G-C3G-O3G-C1D
8	D	3632	DGD	C2G-C3G-O3G-C1D
7	D	3630	LHG	O9-C7-C8-C9
7	J	9630	LHG	O8-C23-C24-C25
10	A	602	CLA	CAA-CBA-CGA-O2A
10	C	614	CLA	O1D-CGD-O2D-CED
9	J	607	CHL	C16-C17-C18-C20
10	B	602	CLA	C13-C15-C16-C17
7	G	6630	LHG	O9-C7-C8-C9
10	I	612	CLA	C13-C15-C16-C17
10	E	603	CLA	CAA-CBA-CGA-O2A
8	B	2632	DGD	CFA-CGA-CHA-CIA
7	G	6630	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
7	A	630	LHG	O9-C7-C8-C9
9	D	605	CHL	CAA-CBA-CGA-O1A
9	I	605	CHL	CAA-CBA-CGA-O1A
10	F	612	CLA	CAA-CBA-CGA-O1A
10	C	603	CLA	CAD-CBD-CGD-O2D
10	D	603	CLA	CAD-CBD-CGD-O2D
10	E	603	CLA	CAD-CBD-CGD-O2D
10	F	612	CLA	CAD-CBD-CGD-O2D
10	H	603	CLA	CAD-CBD-CGD-O2D
10	I	604	CLA	CAD-CBD-CGD-O2D
10	I	614	CLA	CAD-CBD-CGD-O2D
10	J	603	CLA	CAD-CBD-CGD-O2D
9	E	605	CHL	CAA-CBA-CGA-O2A
10	B	613	CLA	CAA-CBA-CGA-O2A
10	F	613	CLA	CAA-CBA-CGA-O2A
7	C	2630	LHG	O10-C23-C24-C25
7	F	5630	LHG	O9-C7-C8-C9
9	J	606	CHL	CAA-CBA-CGA-O1A
7	C	2630	LHG	C19-C20-C21-C22
8	E	4632	DGD	O6D-C5D-C6D-O5D
8	A	632	DGD	C9B-CAB-CBB-CCB
10	F	602	CLA	CBA-CGA-O2A-C1
10	C	603	CLA	C15-C16-C17-C18
9	A	601	CHL	C2-C1-O2A-CGA
9	C	606	CHL	C2-C1-O2A-CGA
9	E	609	CHL	C2-C1-O2A-CGA
9	I	601	CHL	C2-C1-O2A-CGA
9	I	609	CHL	C2-C1-O2A-CGA
8	B	1632	DGD	O1G-C1A-C2A-C3A
2	D	3633	BNG	C2'-C3'-C4'-C5'
8	H	7632	DGD	C9A-CAA-CBA-CCA
7	I	8630	LHG	O10-C23-C24-C25
10	J	612	CLA	C5-C6-C7-C8
7	E	4630	LHG	O7-C7-C8-C9
10	B	603	CLA	CAA-CBA-CGA-O2A
8	I	8632	DGD	O6E-C5E-C6E-O5E
9	C	601	CHL	CAA-CBA-CGA-O2A
9	F	608	CHL	CAA-CBA-CGA-O2A
10	A	613	CLA	CAA-CBA-CGA-O2A
10	I	602	CLA	CAA-CBA-CGA-O2A
7	F	5630	LHG	O10-C23-C24-C25
9	E	605	CHL	CAA-CBA-CGA-O1A

There are no ring outliers.

122 monomers are involved in 159 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	611	CLA	3	0
9	F	608	CHL	1	0
10	E	610	CLA	1	0
9	G	609	CHL	1	0
10	D	604	CLA	1	0
10	C	602	CLA	1	0
10	I	603	CLA	3	0
10	A	602	CLA	1	0
10	B	610	CLA	2	0
10	F	613	CLA	1	0
10	C	612	CLA	2	0
9	C	608	CHL	2	0
10	D	612	CLA	2	0
10	E	602	CLA	1	0
10	J	610	CLA	1	0
10	E	612	CLA	2	0
10	H	612	CLA	2	0
10	H	603	CLA	3	0
9	I	606	CHL	1	0
6	G	6623	NEX	1	0
10	C	603	CLA	3	0
9	F	609	CHL	1	0
4	A	620	LUT	2	0
10	F	611	CLA	1	0
10	G	604	CLA	1	0
10	J	613	CLA	1	0
7	F	5630	LHG	3	0
10	B	612	CLA	2	0
9	I	601	CHL	2	0
10	H	610	CLA	2	0
10	I	602	CLA	1	0
9	E	601	CHL	1	0
10	H	602	CLA	2	0
10	J	603	CLA	2	0
9	J	605	CHL	1	0
5	F	6622	XAT	1	0
8	A	632	DGD	1	0
10	D	611	CLA	2	0
8	H	6632	DGD	1	0
4	J	9621	LUT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	3630	LHG	1	0
9	B	601	CHL	3	0
9	C	607	CHL	1	0
9	G	607	CHL	1	0
10	A	603	CLA	2	0
10	D	613	CLA	1	0
10	C	614	CLA	1	0
9	G	606	CHL	1	0
10	E	603	CLA	3	0
10	H	613	CLA	1	0
9	G	601	CHL	4	0
9	A	605	CHL	1	0
10	B	611	CLA	3	0
2	D	3633	BNG	1	0
9	A	601	CHL	2	0
9	B	606	CHL	1	0
9	H	609	CHL	1	0
10	A	611	CLA	3	0
10	J	611	CLA	3	0
8	D	5632	DGD	1	0
7	C	2630	LHG	1	0
10	F	602	CLA	1	0
7	H	7630	LHG	2	0
10	I	611	CLA	2	0
10	J	612	CLA	2	0
9	A	608	CHL	1	0
7	I	8630	LHG	3	0
10	C	604	CLA	1	0
4	C	2621	LUT	2	0
5	H	4622	XAT	1	0
5	B	1622	XAT	1	0
9	E	605	CHL	1	0
9	C	609	CHL	1	0
8	I	8632	DGD	1	0
4	D	3620	LUT	1	0
4	E	4621	LUT	1	0
10	B	603	CLA	4	0
10	I	612	CLA	1	0
9	H	601	CHL	1	0
9	J	609	CHL	1	0
10	G	603	CLA	2	0
10	C	610	CLA	1	0

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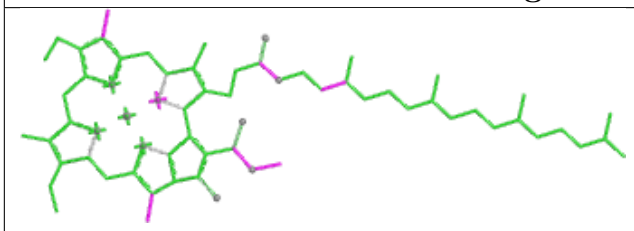
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	610	CLA	2	0
10	D	602	CLA	1	0
9	D	601	CHL	2	0
9	B	609	CHL	1	0
10	G	612	CLA	2	0
5	E	2622	XAT	2	0
9	B	605	CHL	1	0
10	F	603	CLA	2	0
10	G	602	CLA	1	0
5	J	3622	XAT	1	0
10	J	614	CLA	1	0
4	A	621	LUT	2	0
4	E	4620	LUT	2	0
10	C	611	CLA	3	0
4	F	5620	LUT	1	0
4	I	8621	LUT	2	0
10	E	611	CLA	1	0
10	B	602	CLA	2	0
10	C	613	CLA	1	0
10	G	611	CLA	3	0
4	B	1621	LUT	2	0
10	J	602	CLA	1	0
5	I	9622	XAT	1	0
10	A	612	CLA	2	0
4	H	7621	LUT	2	0
9	I	605	CHL	1	0
4	F	5621	LUT	2	0
7	A	630	LHG	2	0
4	I	8620	LUT	2	0
9	F	601	CHL	3	0
7	B	1630	LHG	3	0
7	G	6630	LHG	2	0
4	D	3621	LUT	1	0
9	G	608	CHL	1	0
10	A	610	CLA	2	0
9	H	605	CHL	1	0
4	G	6621	LUT	1	0
7	E	4630	LHG	1	0
9	C	601	CHL	1	0
4	B	1620	LUT	2	0

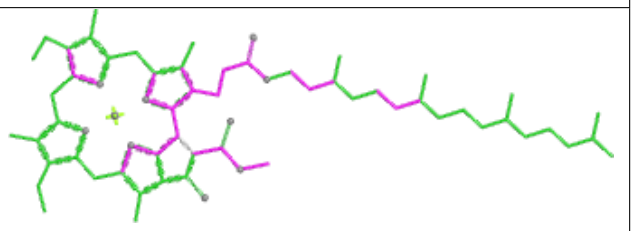
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

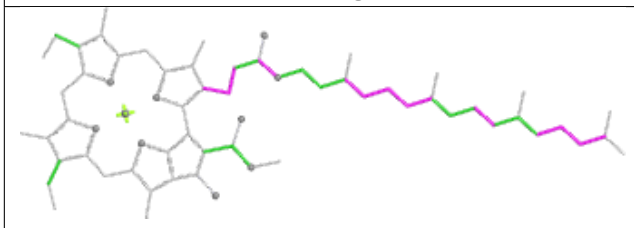
Ligand CLA H 611



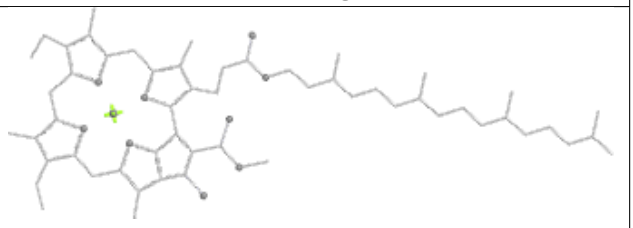
Bond lengths



Bond angles

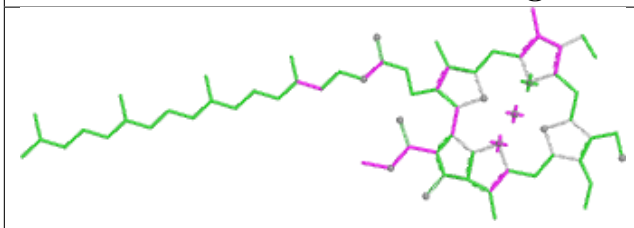


Torsions

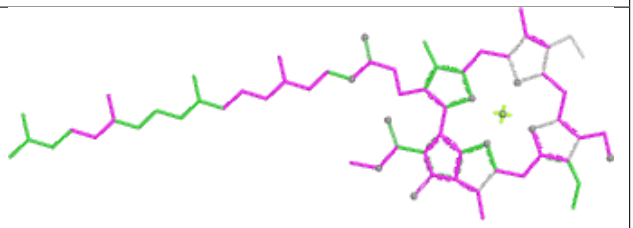


Rings

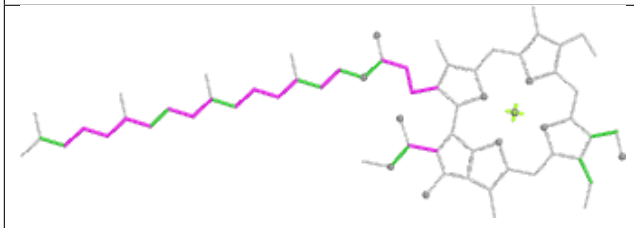
Ligand CHL F 608



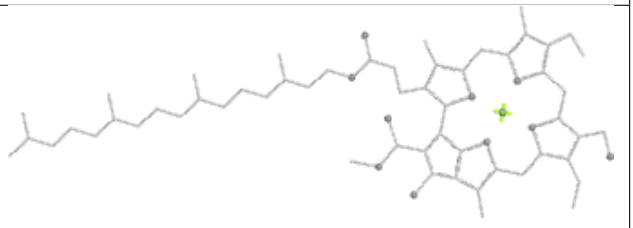
Bond lengths



Bond angles

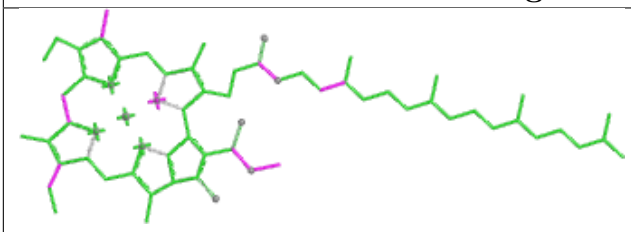


Torsions

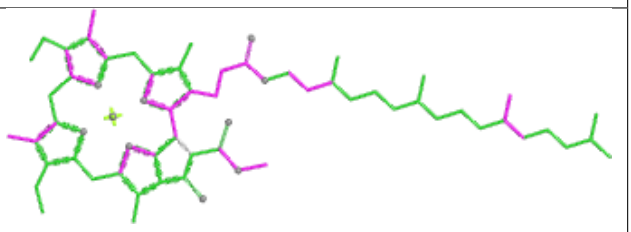


Rings

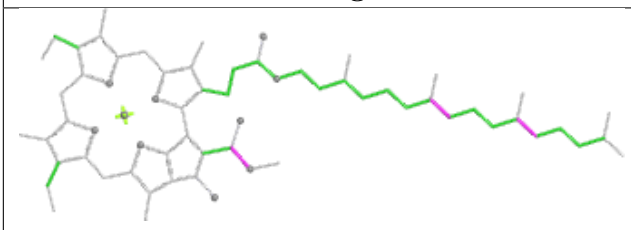
Ligand CLA E 610



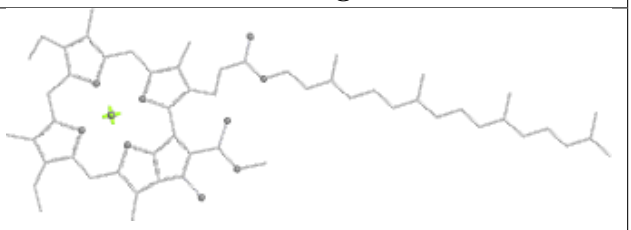
Bond lengths



Bond angles

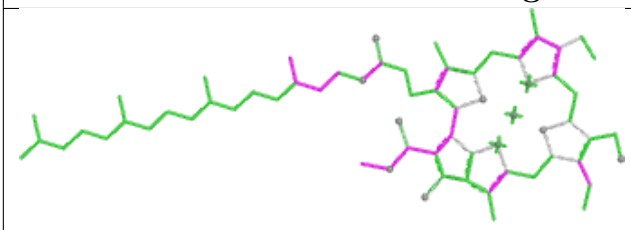


Torsions

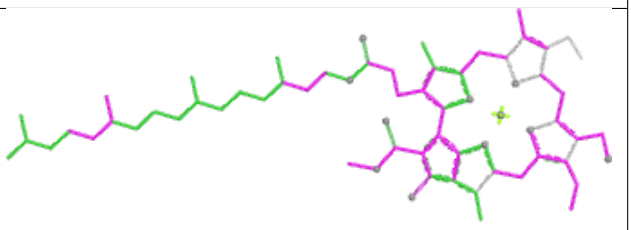


Rings

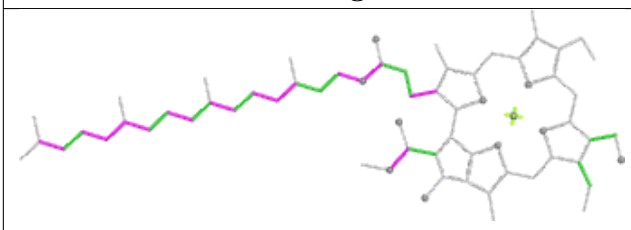
Ligand CHL G 609



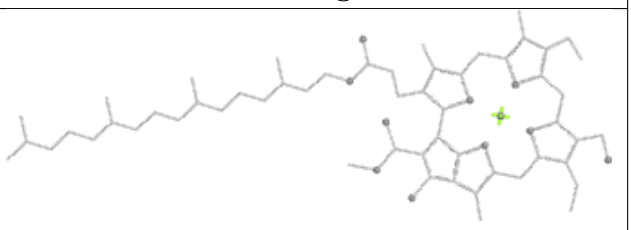
Bond lengths



Bond angles

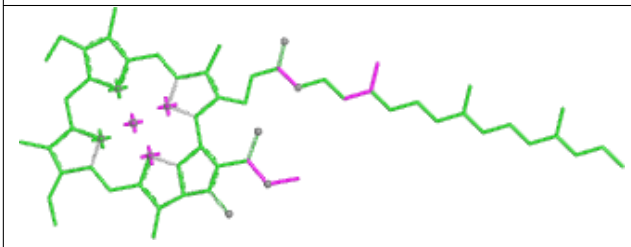


Torsions

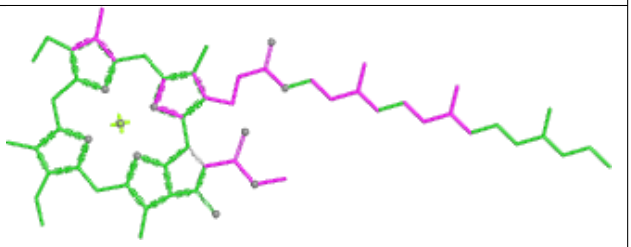


Rings

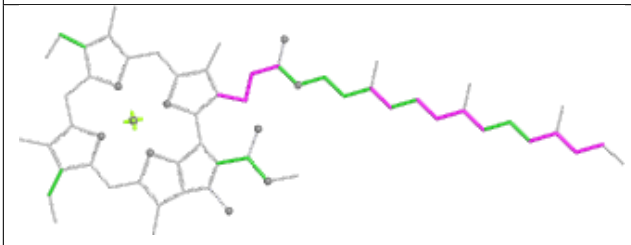
Ligand CLA D 604



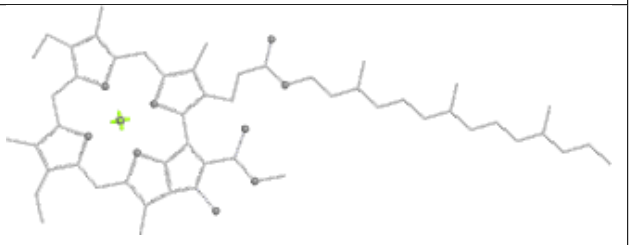
Bond lengths



Bond angles

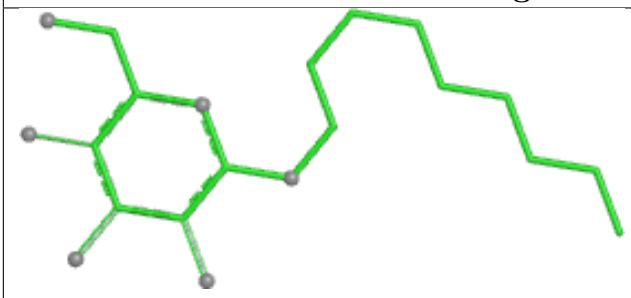


Torsions



Rings

Ligand BNG E 4633



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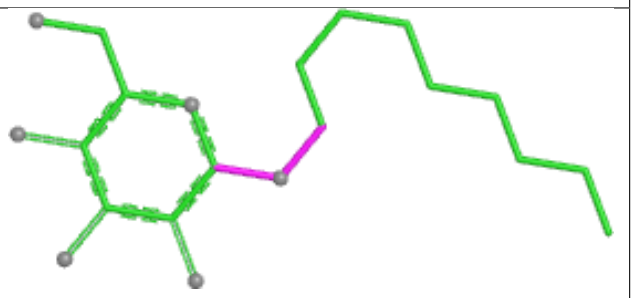
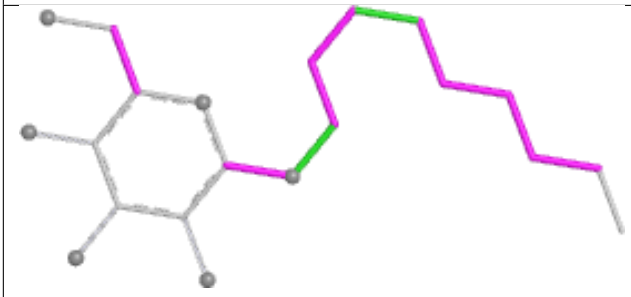


Bond angles



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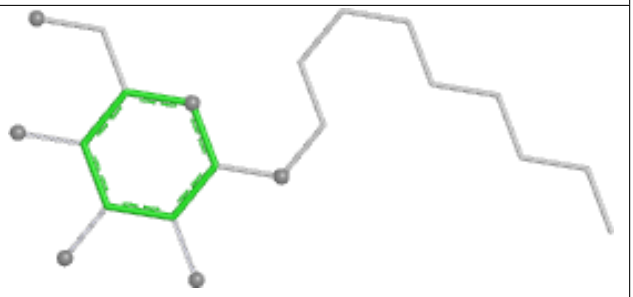
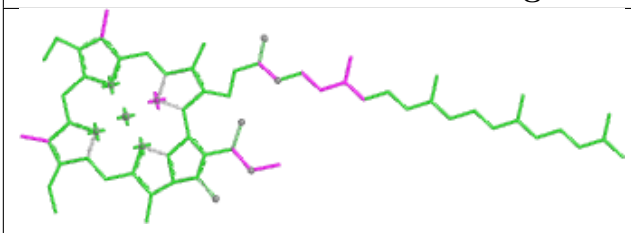


Rings

Ligand CLA A 613



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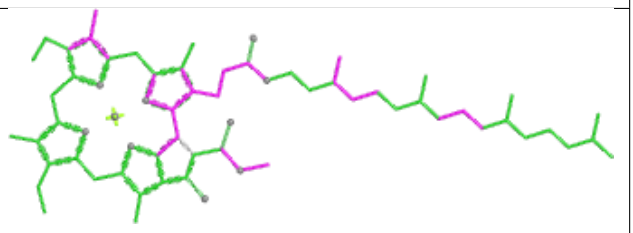
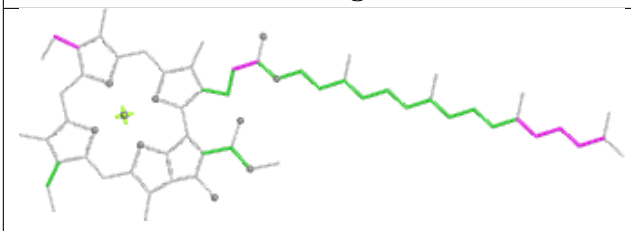
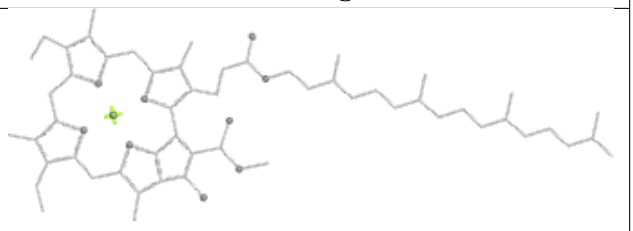


Bond angles

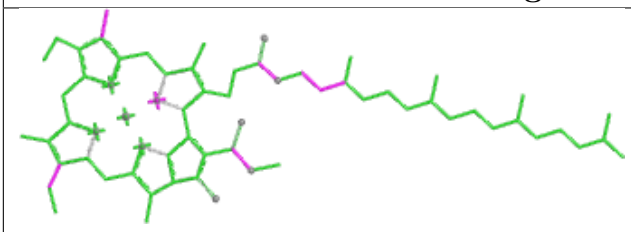


Torsions

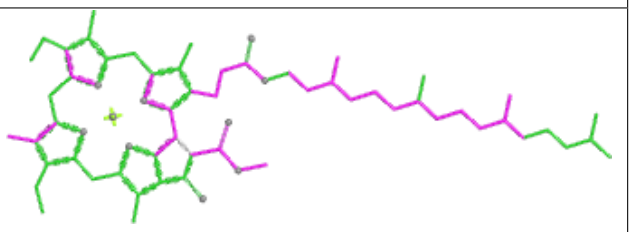


Rings

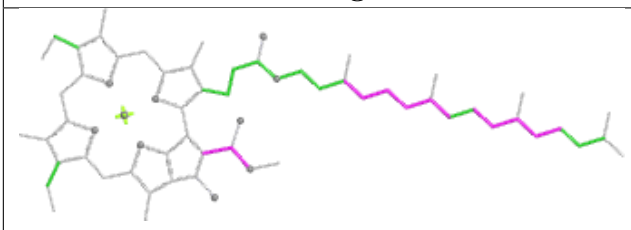
Ligand CLA C 602



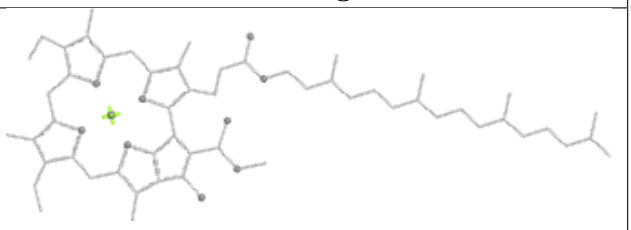
Bond lengths



Bond angles



Torsions

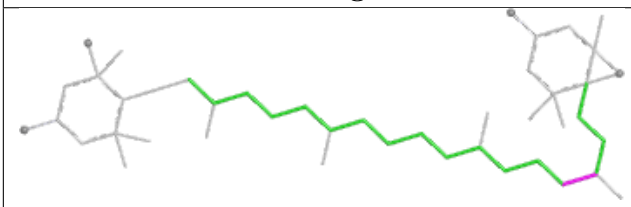


Rings

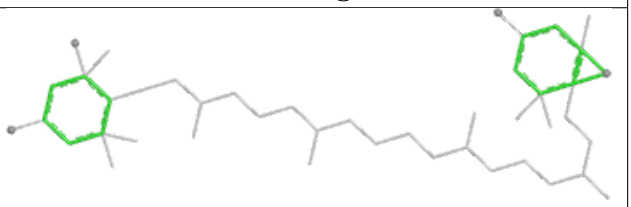
Ligand NEX F 5623

Bond lengths

Bond angles

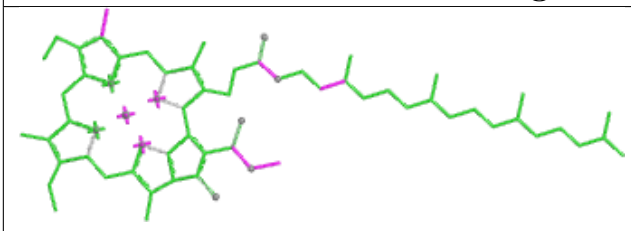


Torsions

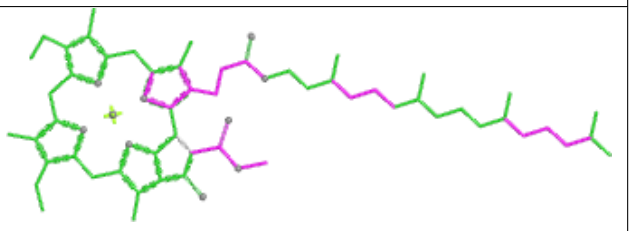


Rings

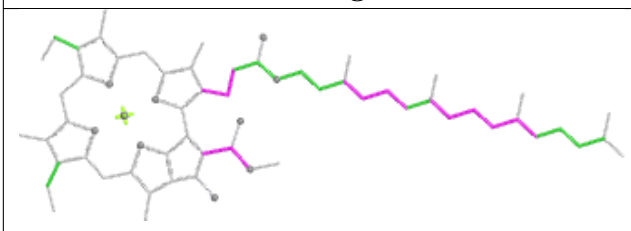
Ligand CLA I 603



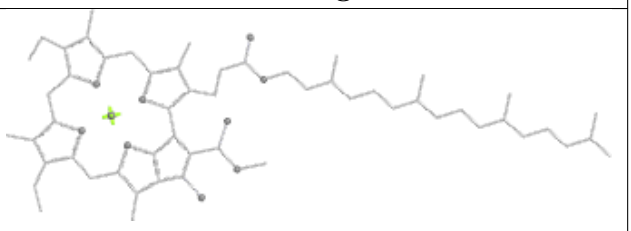
Bond lengths



Bond angles

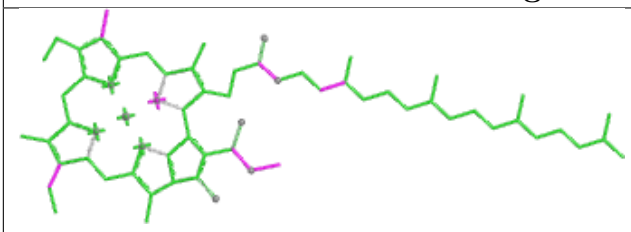


Torsions

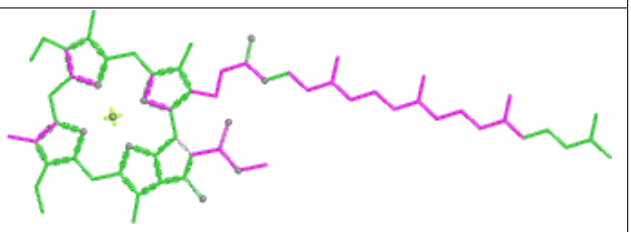


Rings

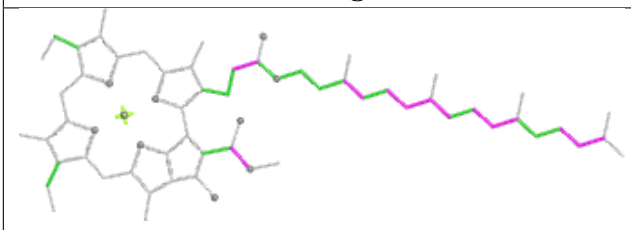
Ligand CLA A 602



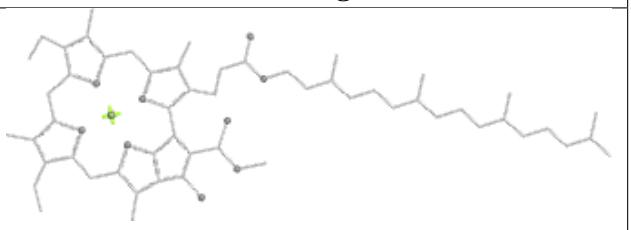
Bond lengths



Bond angles



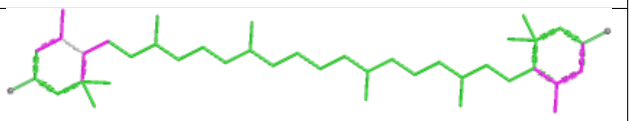
Torsions



Rings

Ligand LUT C 2620

Bond lengths



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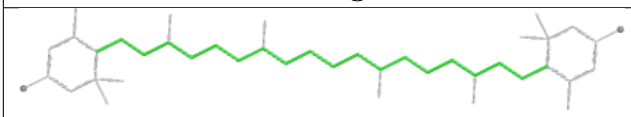

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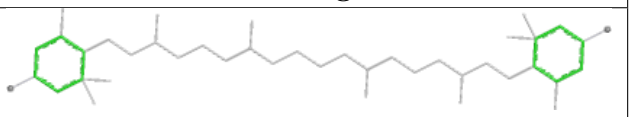
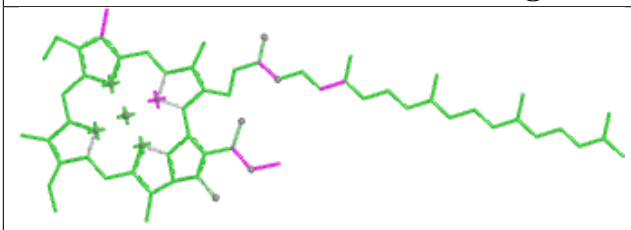


Rings

Ligand CLA B 610



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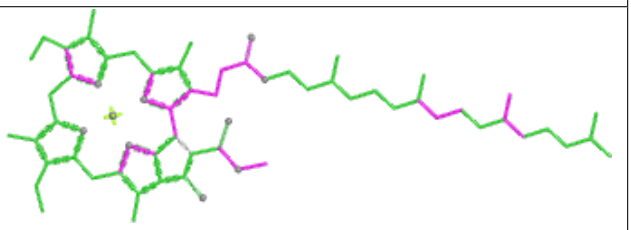

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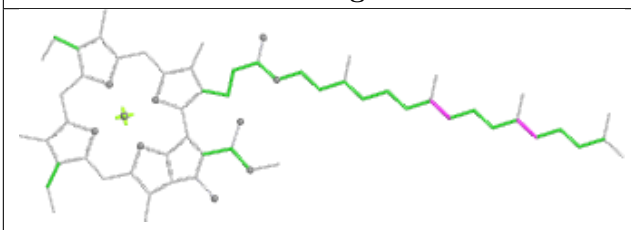

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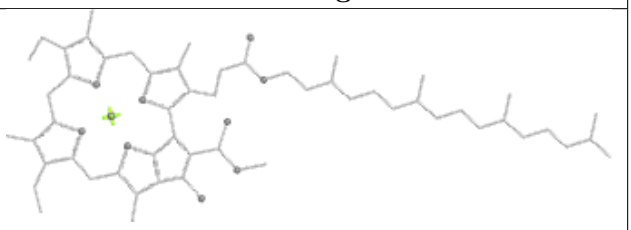
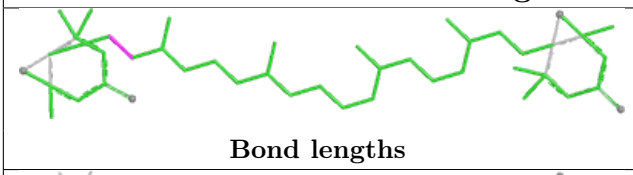


Rings

Ligand XAT D 8622



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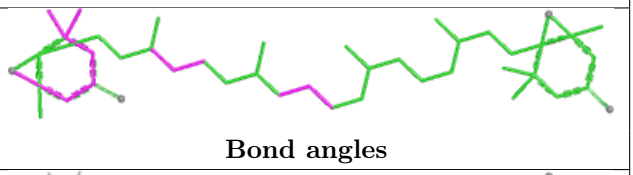

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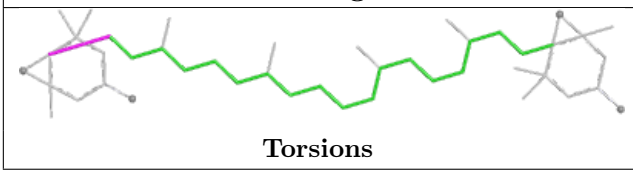

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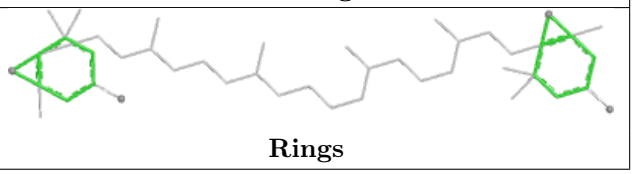
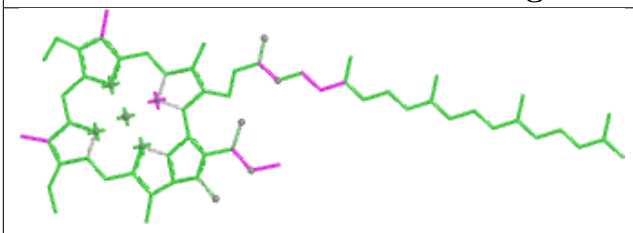


Rings

Ligand CLA F 613



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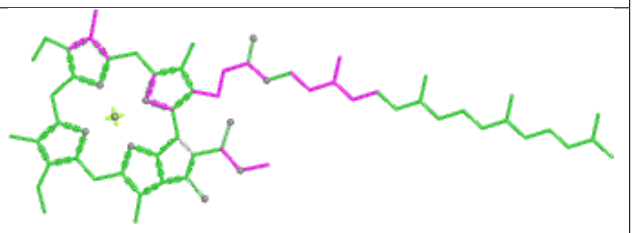
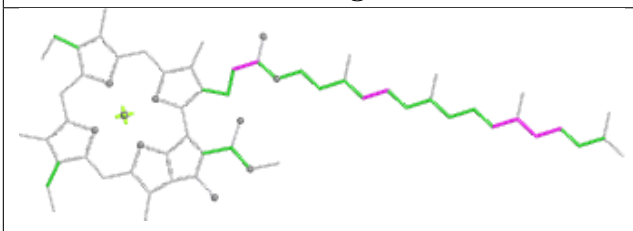


Bond angles



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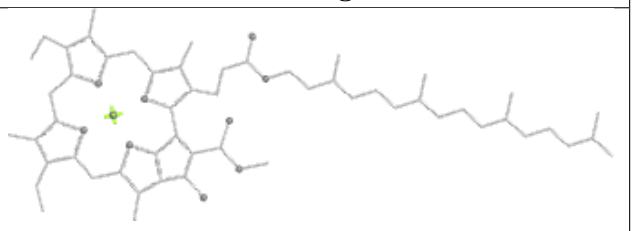
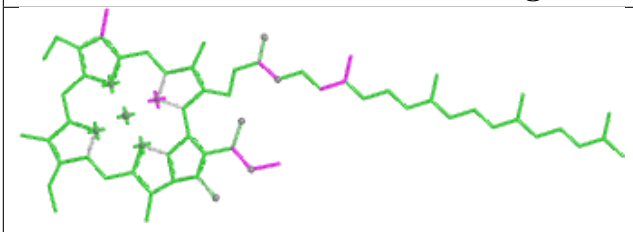


Rings

Ligand CLA C 612



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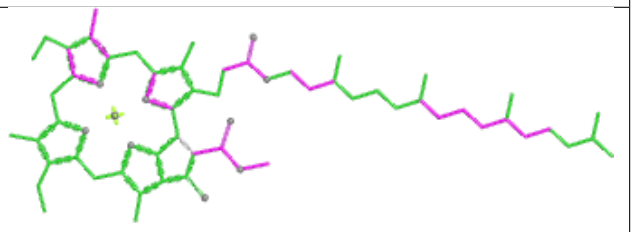

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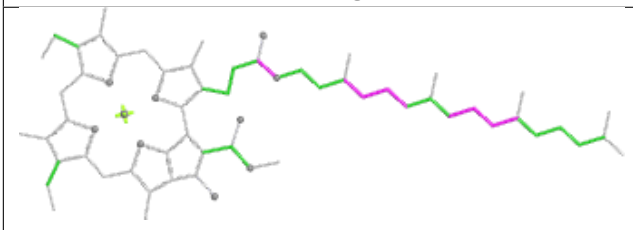

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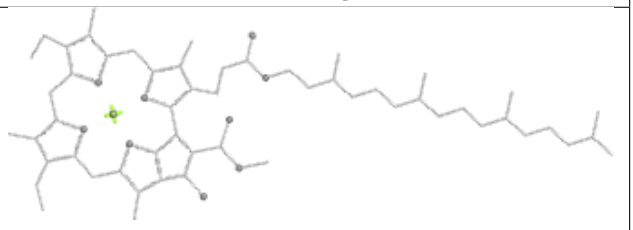
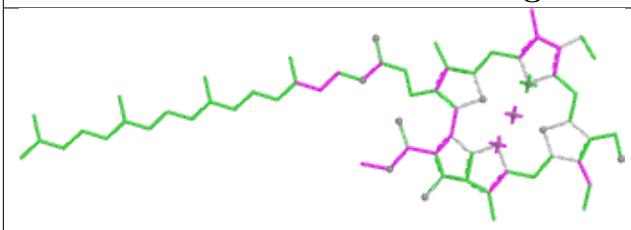


Rings

Ligand CHL C 608



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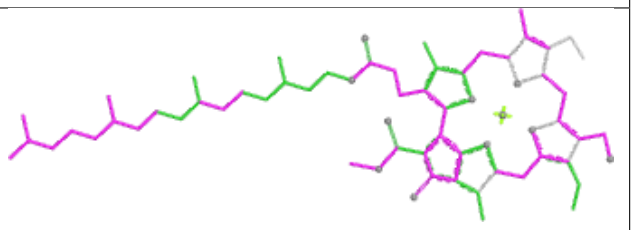
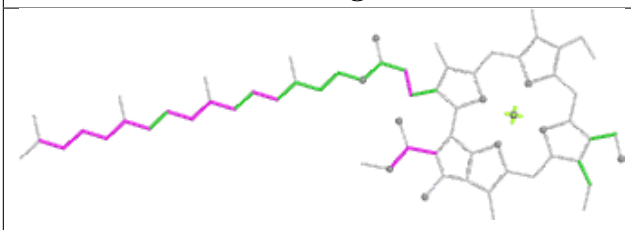


Bond angles



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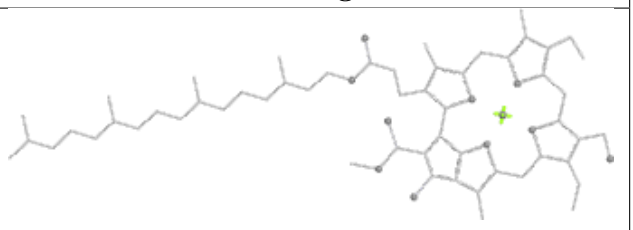
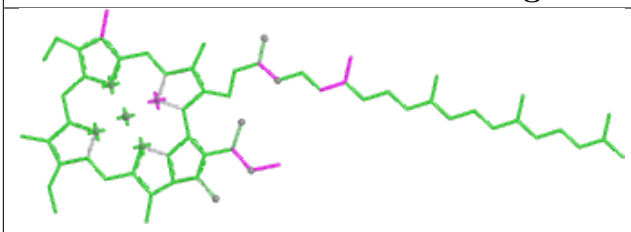


Rings

Ligand CLA D 612



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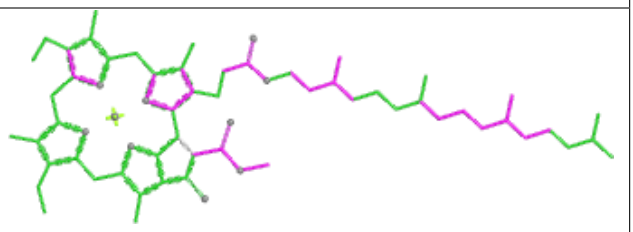

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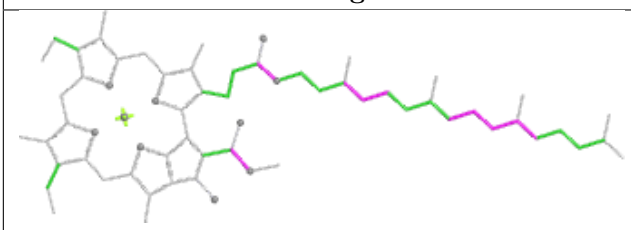

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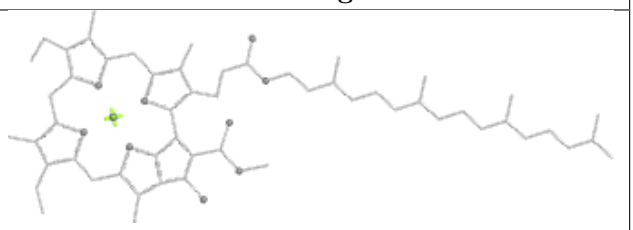
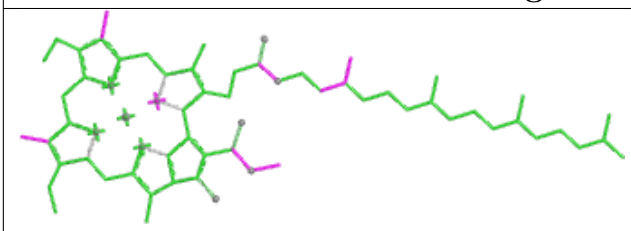


Rings

Ligand CLA E 602



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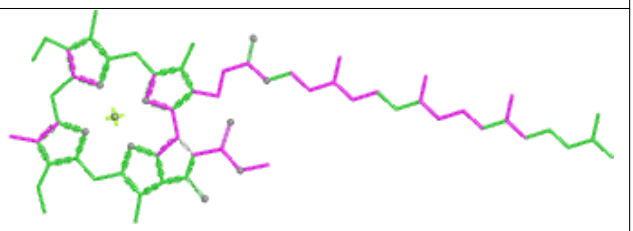

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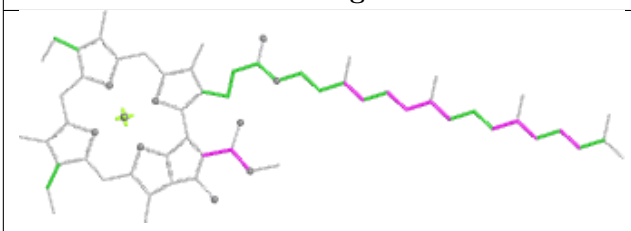

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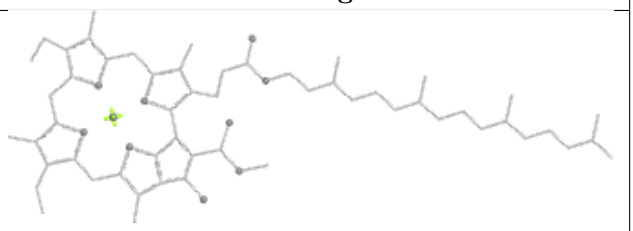
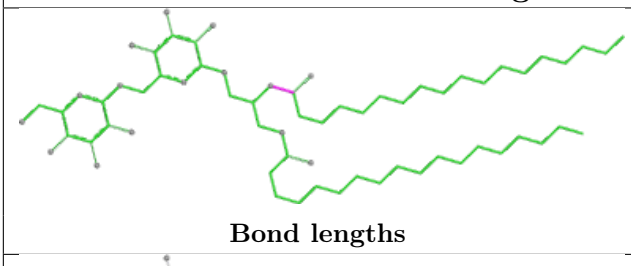


Rings

Ligand DGD E 4632



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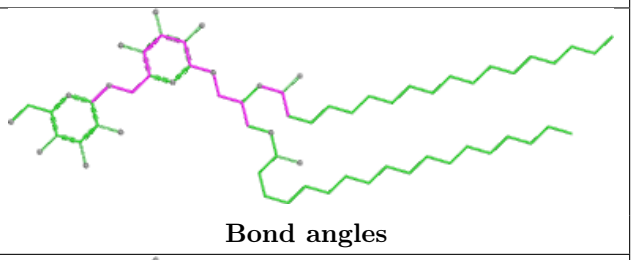

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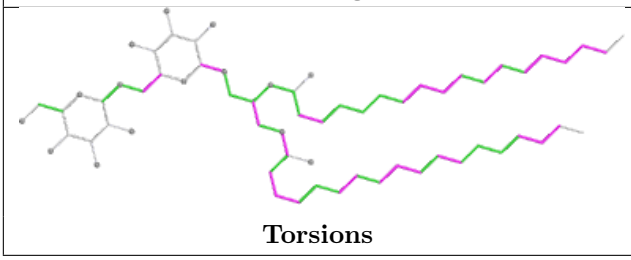

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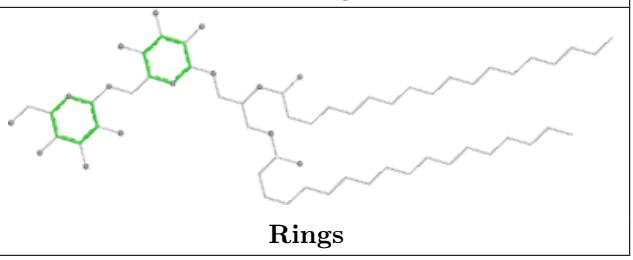
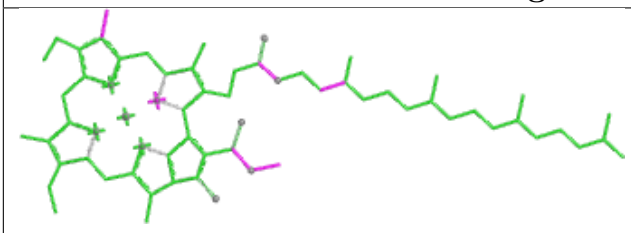


Rings

Ligand CLA J 610



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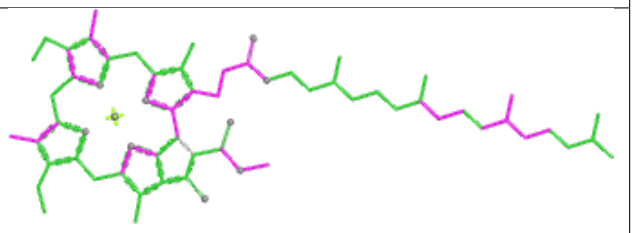

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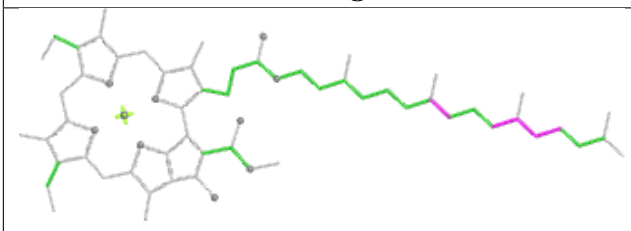

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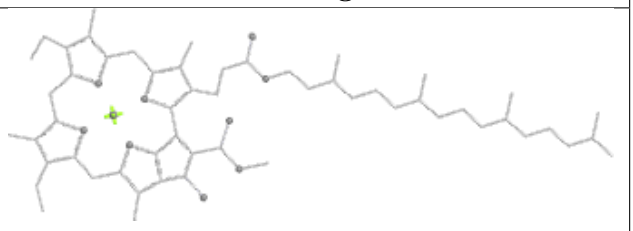
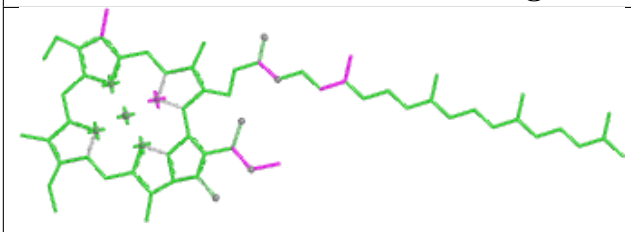


Rings

Ligand CLA E 612



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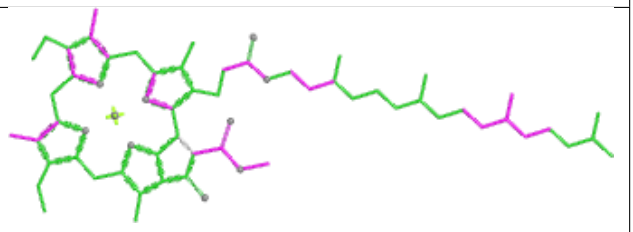
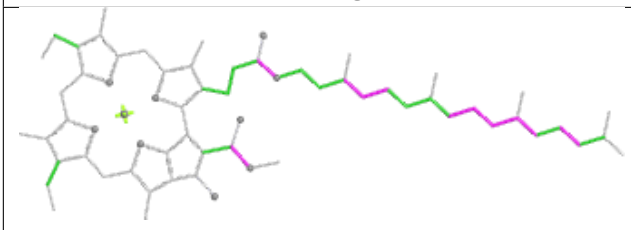


Bond angles



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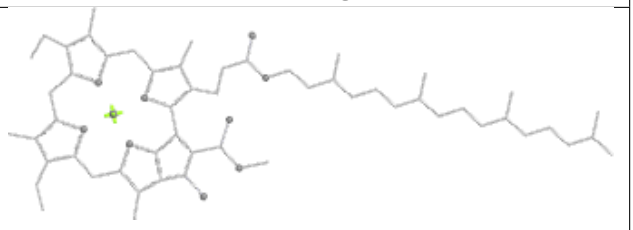
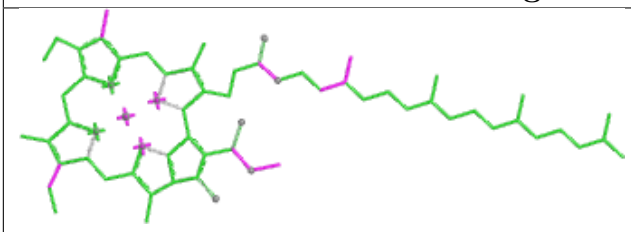


Rings

Ligand CLA H 612



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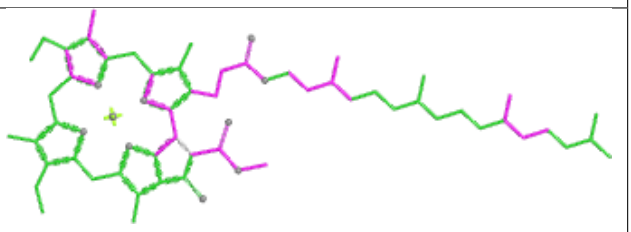
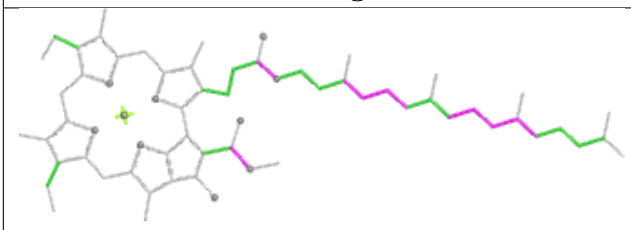
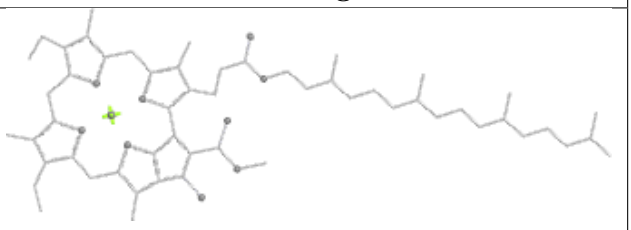


Bond angles

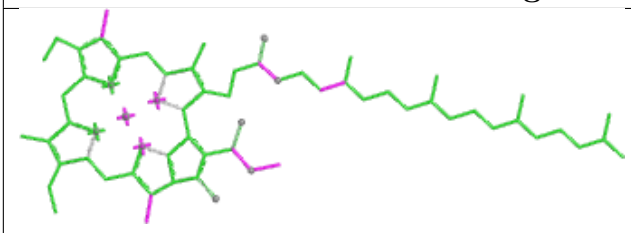


Torsions



Rings

Ligand CLA H 603



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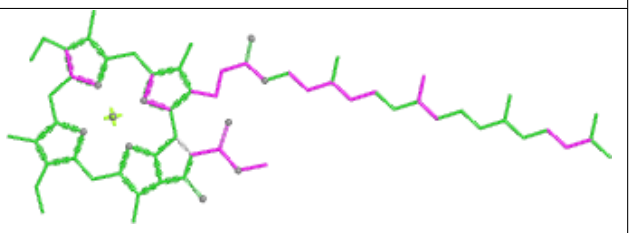
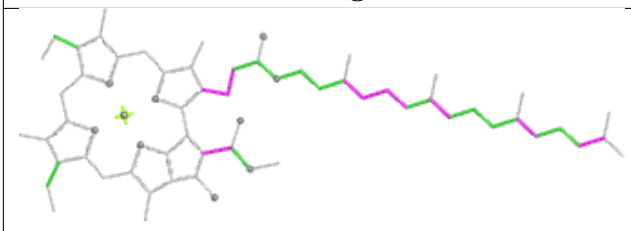


Bond angles



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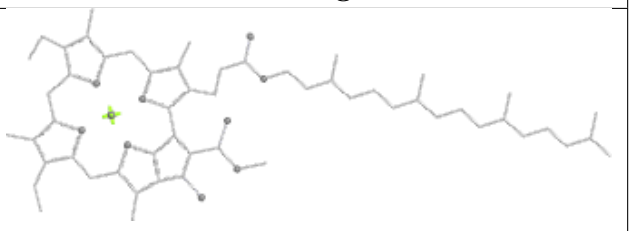
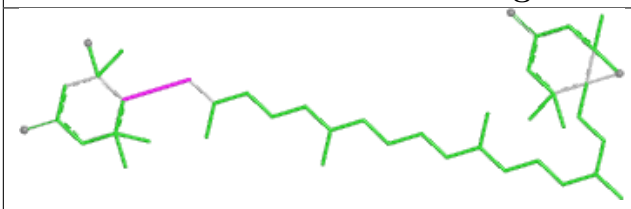
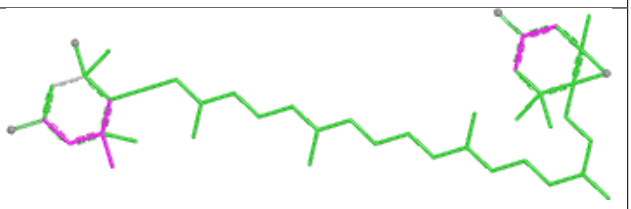


Rings

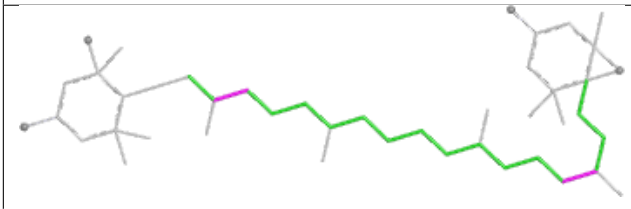
Ligand NEX B 1623



Bond lengths



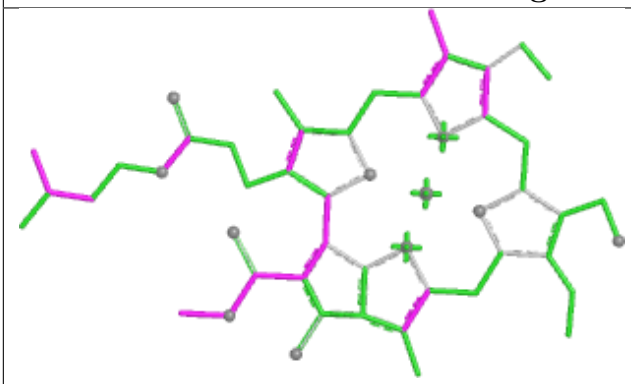
Bond angles



Torsions

Rings

Ligand CHL I 606



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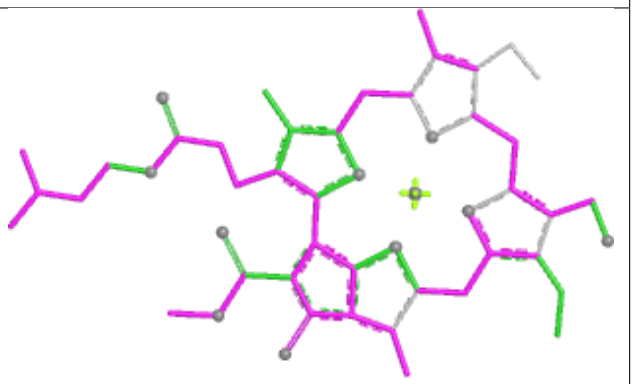
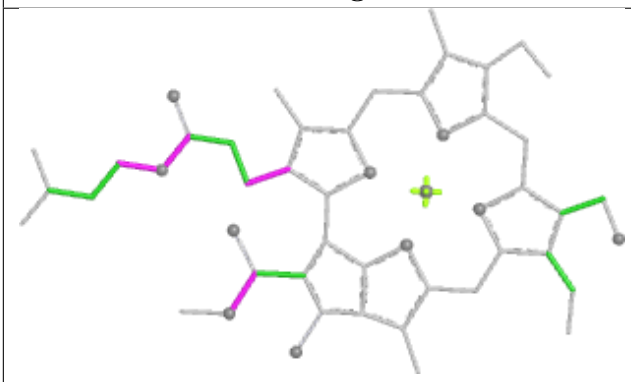
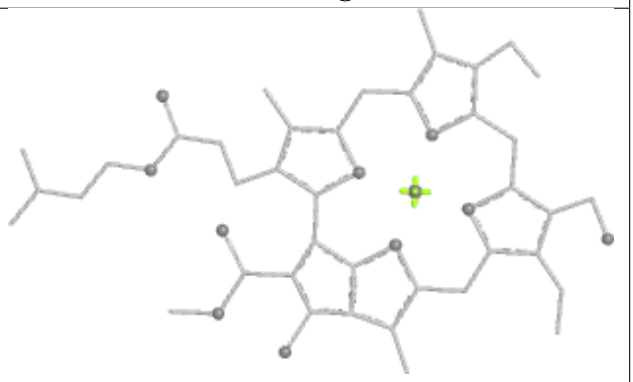


Bond angles

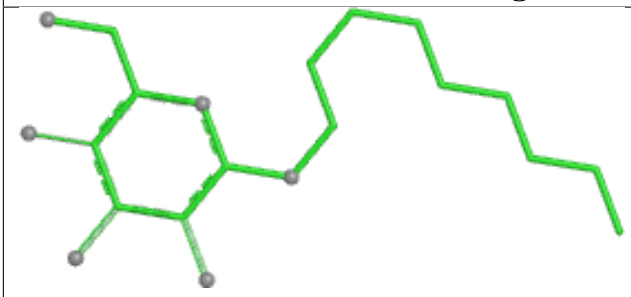


Torsions



Rings

Ligand BNG H 7633



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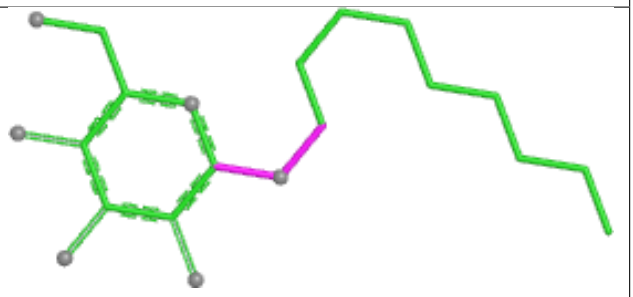
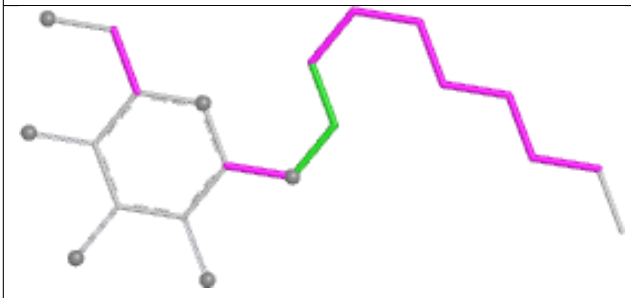
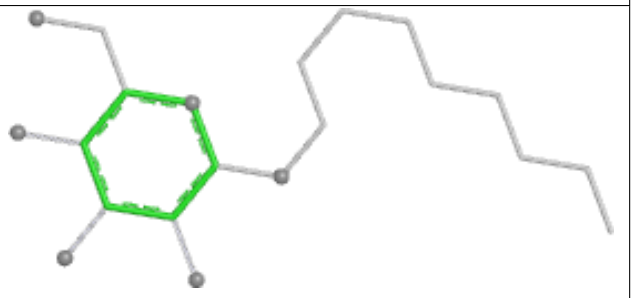


Bond angles

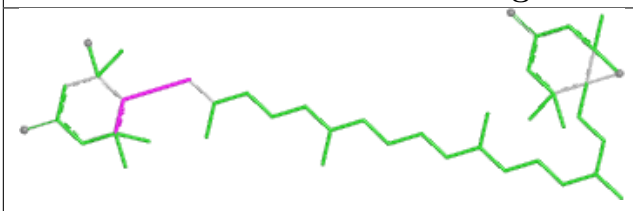


Torsions



Rings

Ligand NEX G 6623



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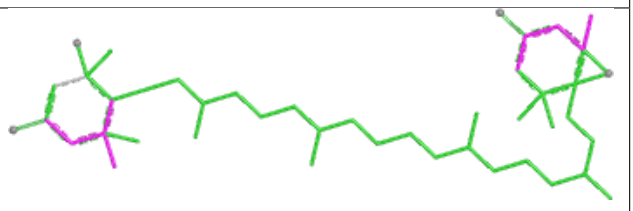
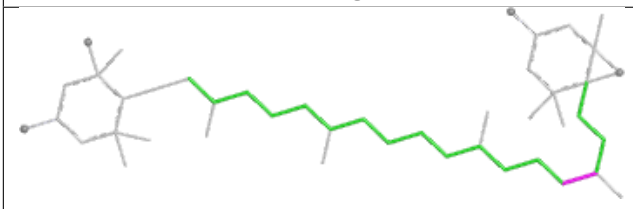


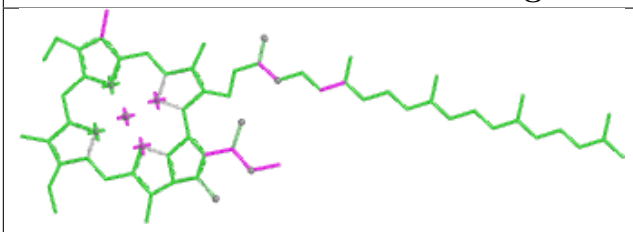
Bond angles



Torsions

Rings

Ligand CLA C 603



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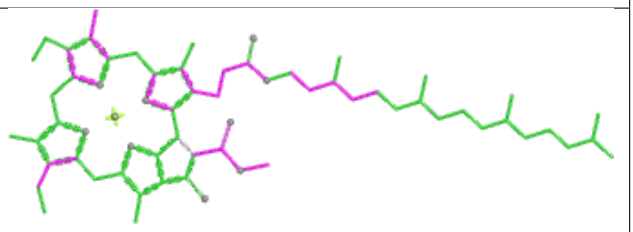
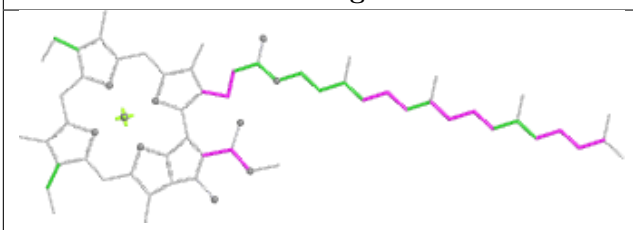


Bond angles



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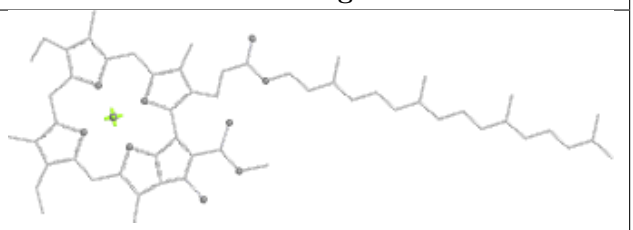
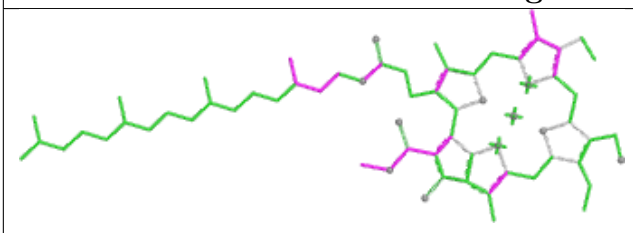


Rings

Ligand CHL F 609



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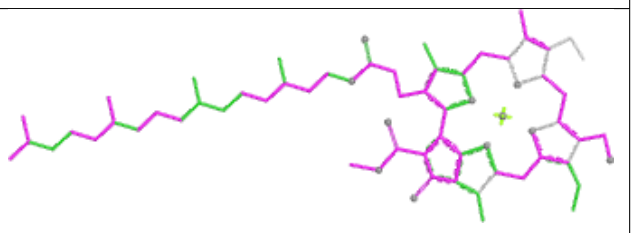
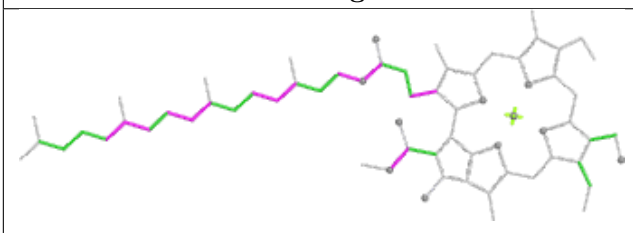


Bond angles



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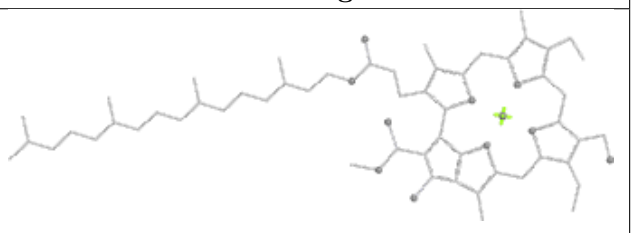
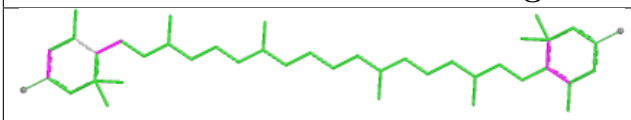


Rings

Ligand LUT A 620



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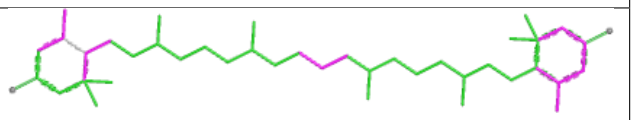

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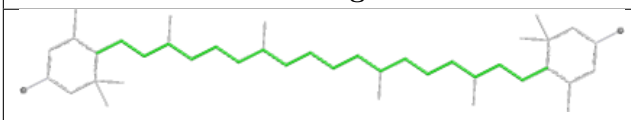

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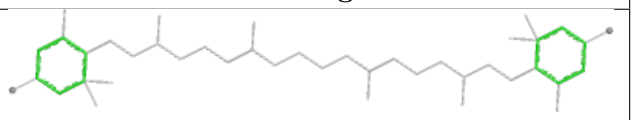
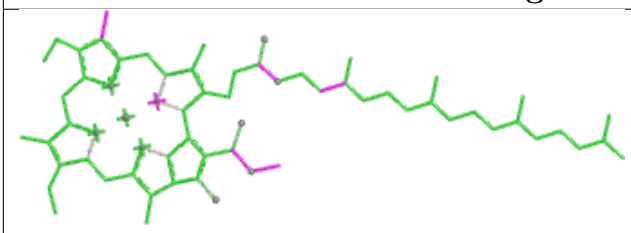


Rings

Ligand CLA F 611



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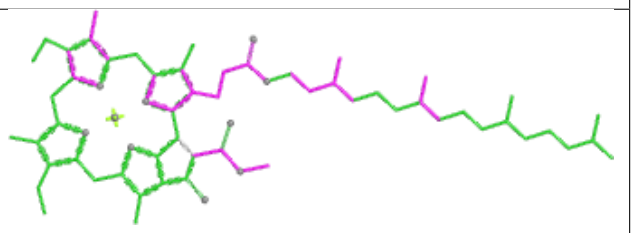
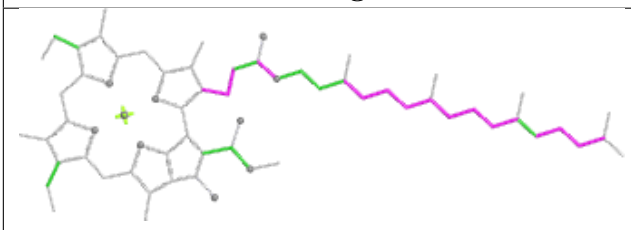


Bond angles



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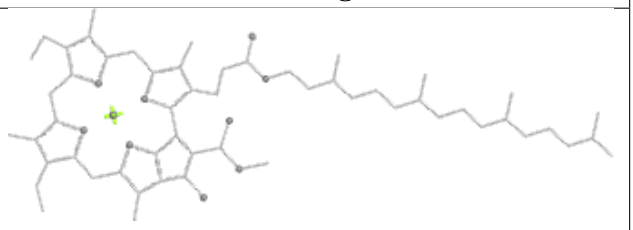
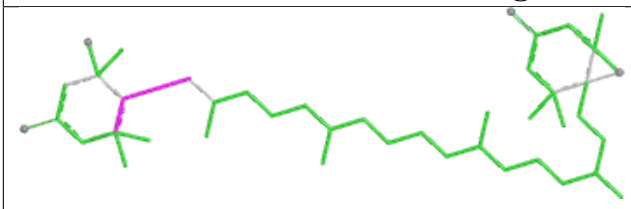


Rings

Ligand NEX H 7623



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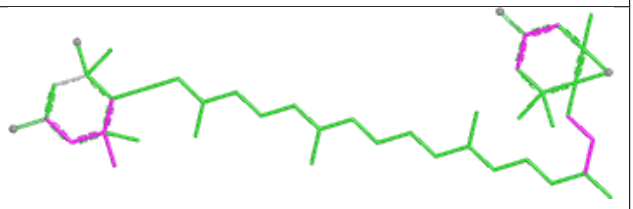
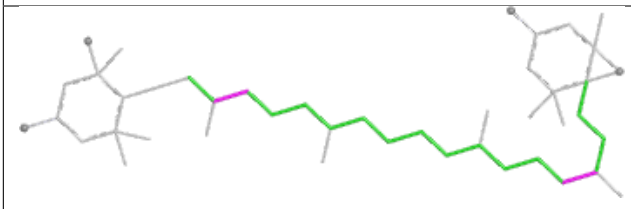


Bond angles



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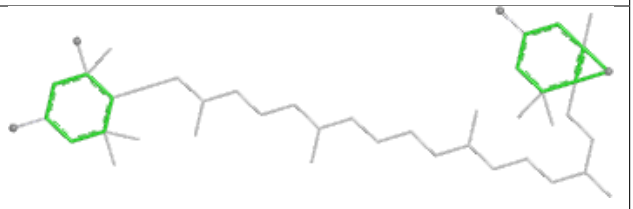
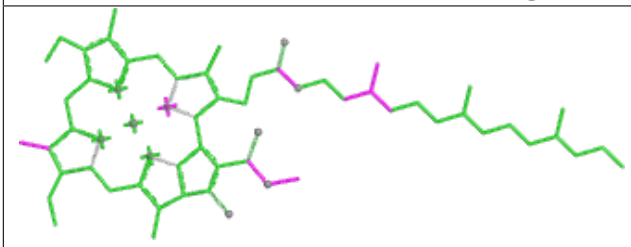


Rings

Ligand CLA G 604



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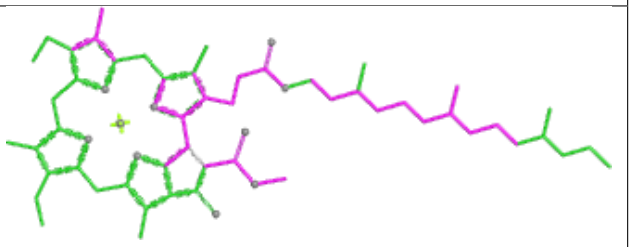

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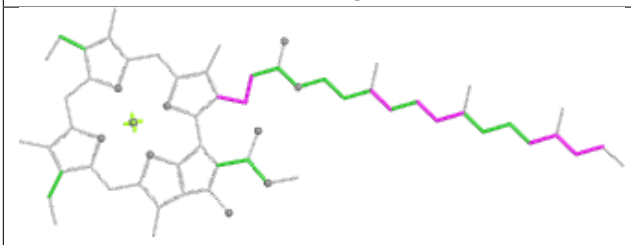

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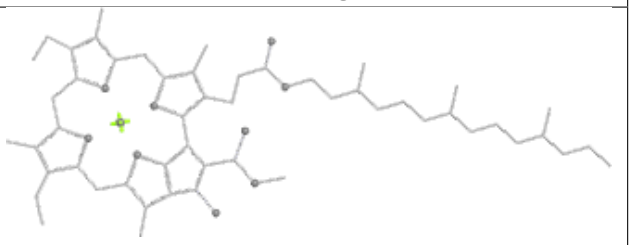
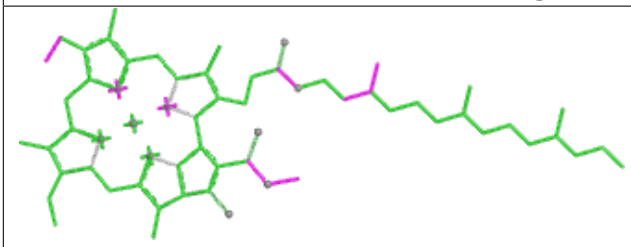


Rings

Ligand CLA I 604



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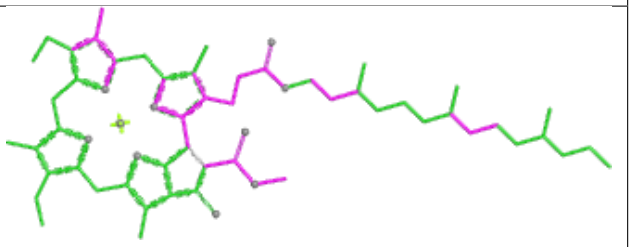
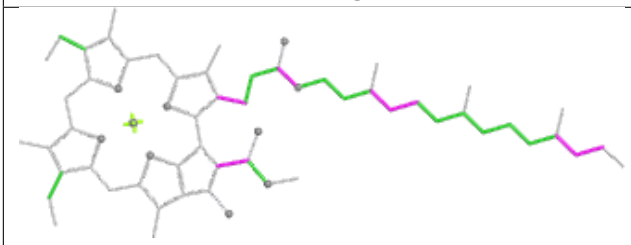


Bond angles



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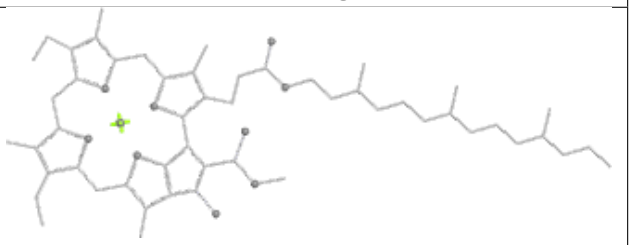
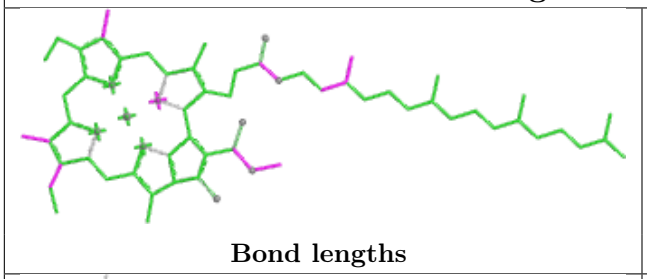


Rings

Ligand CLA J 613



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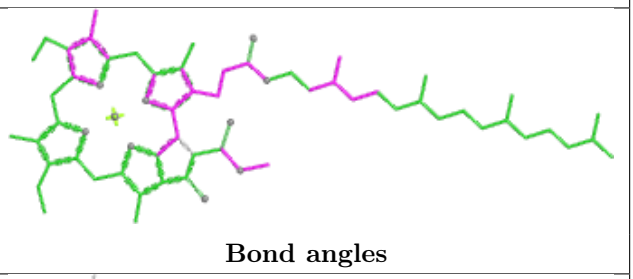
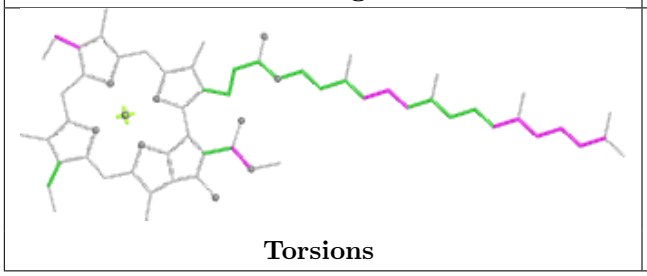


Bond angles



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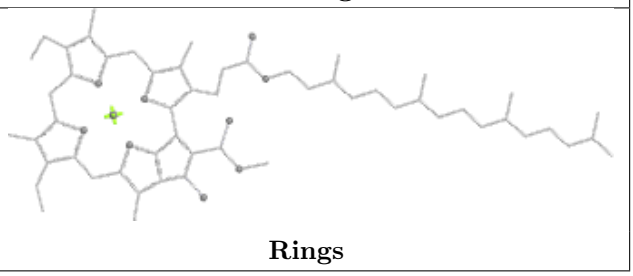
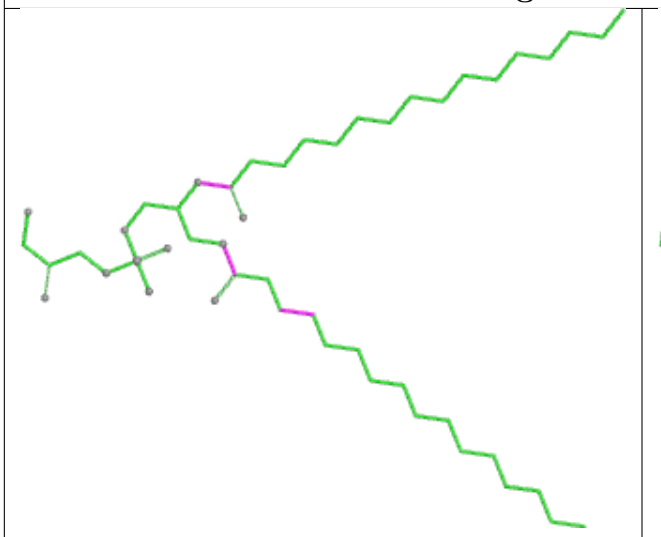


Rings

Ligand LHG F 5630



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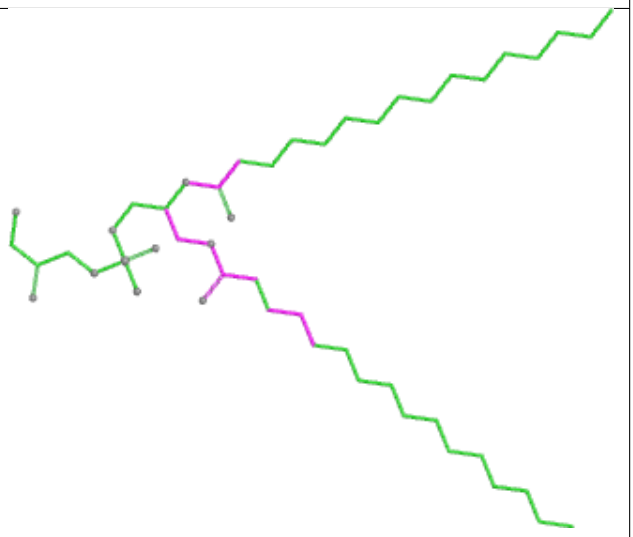
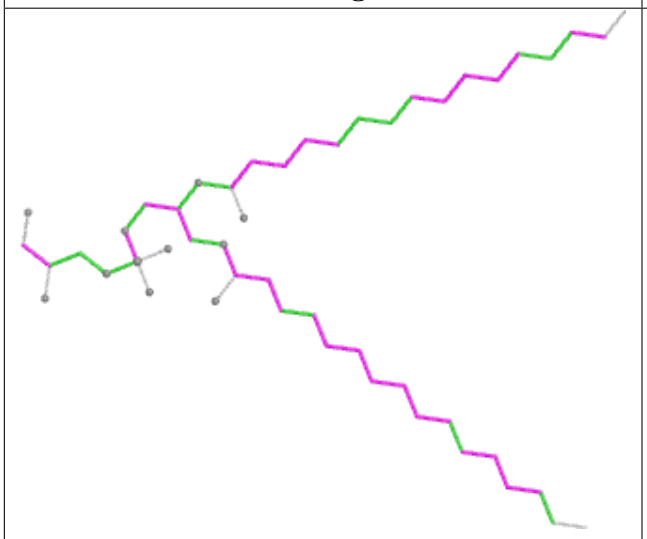


Bond angles



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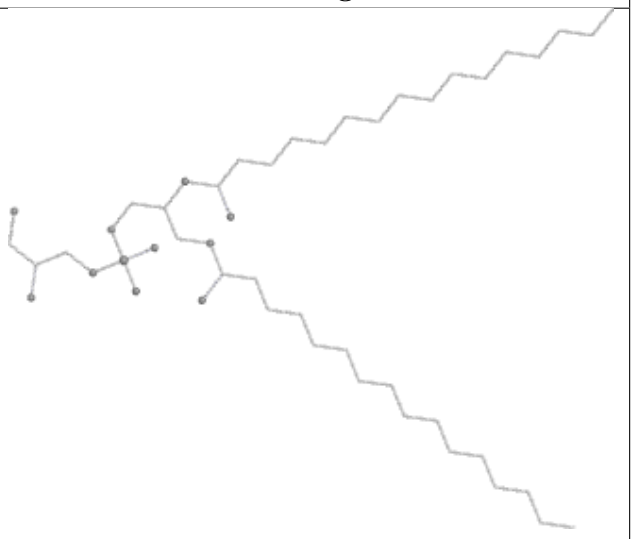
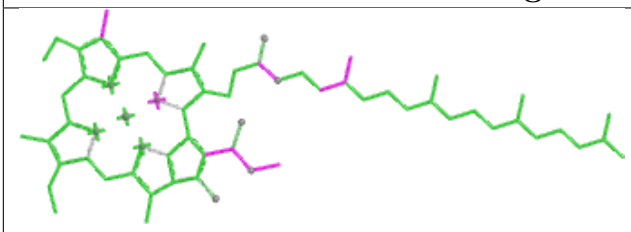


Rings

Ligand CLA B 612



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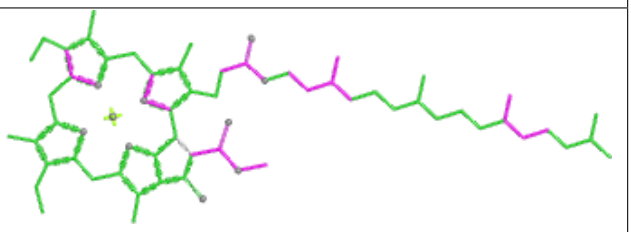
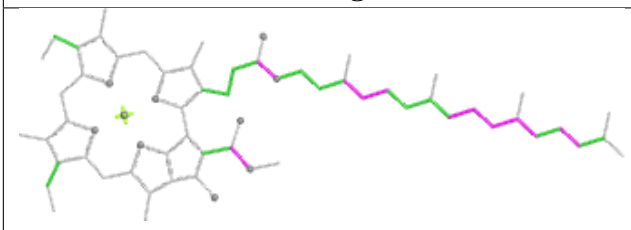


Bond angles



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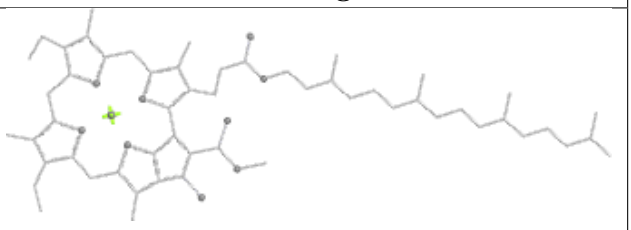
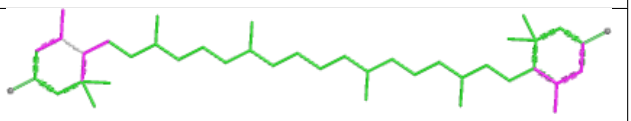


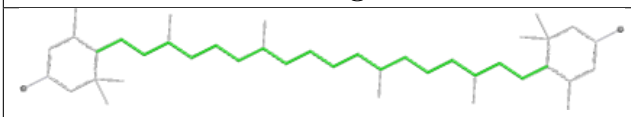
Rings

Ligand LUT H 7620

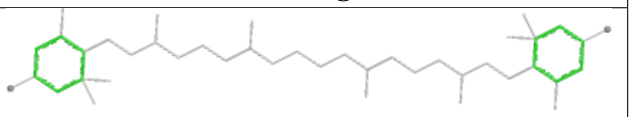
Bond lengths



Bond angles

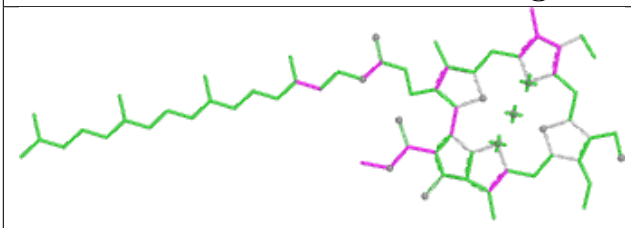


Torsions

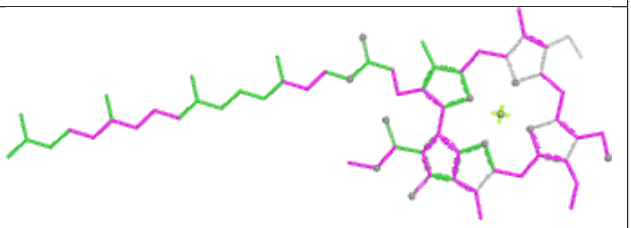


Rings

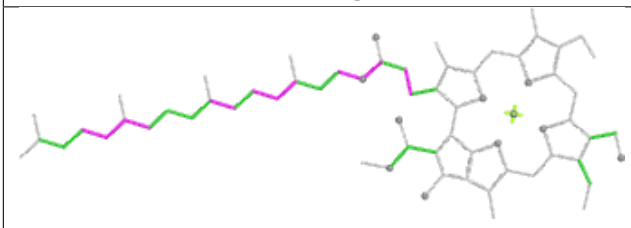
Ligand CHL I 601



Bond lengths



Bond angles



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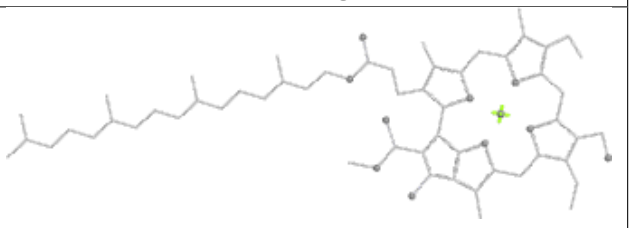
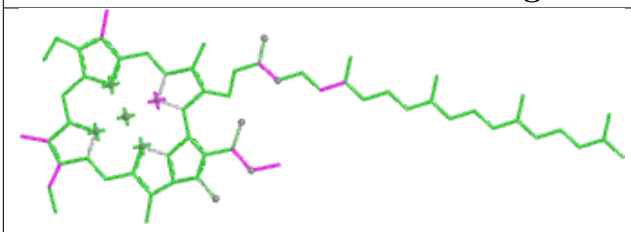


Rings

Ligand CLA H 610



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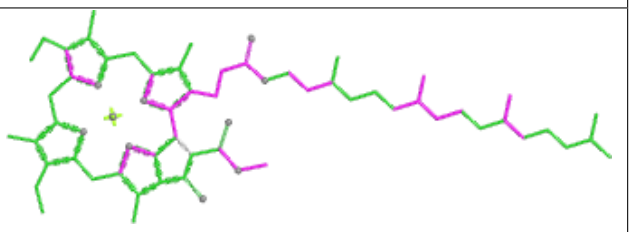

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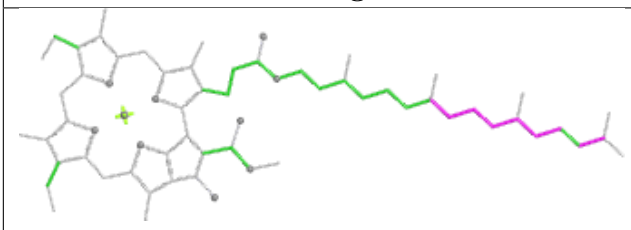

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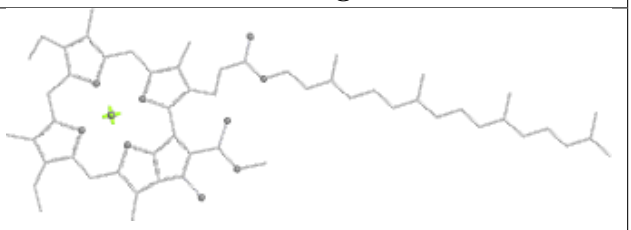
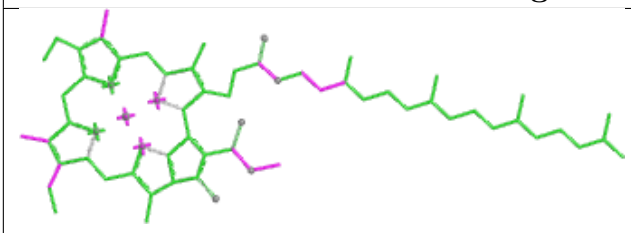


Rings

Ligand CLA I 602



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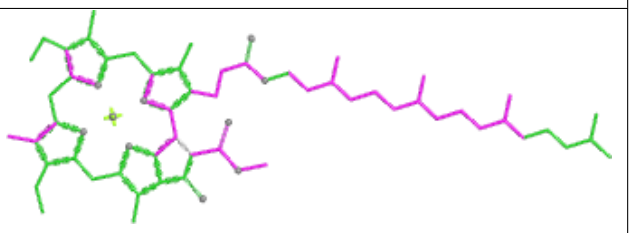

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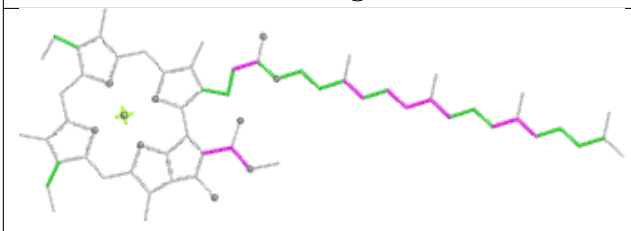

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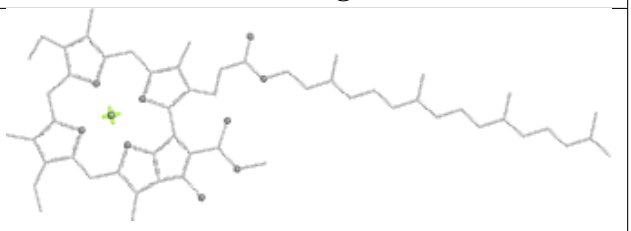
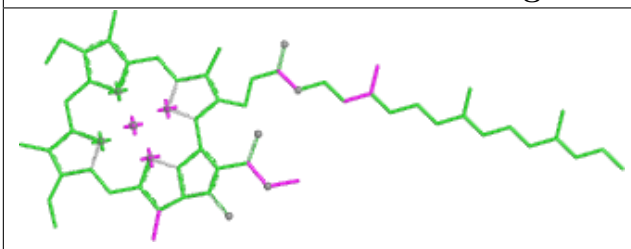


Rings

Ligand CLA H 604



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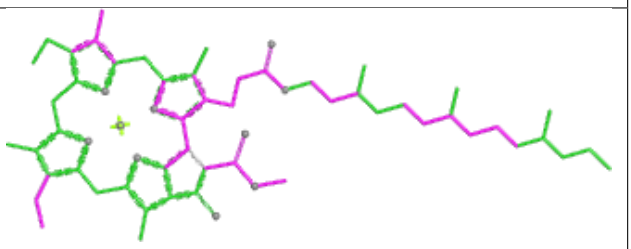
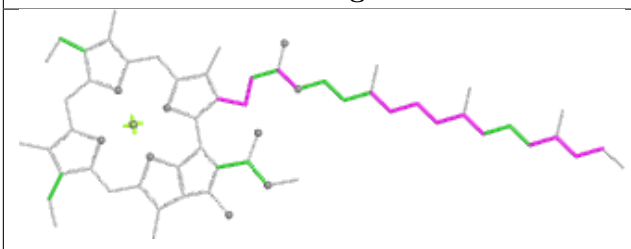


Bond angles



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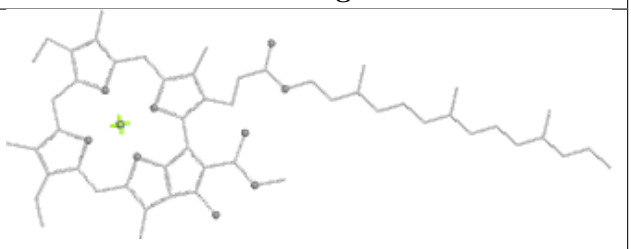
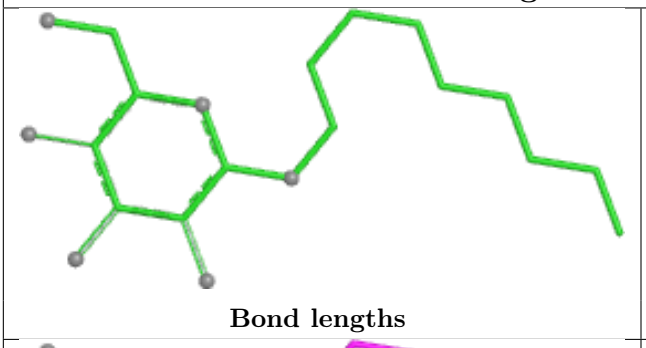


Rings

Ligand BNG A 633



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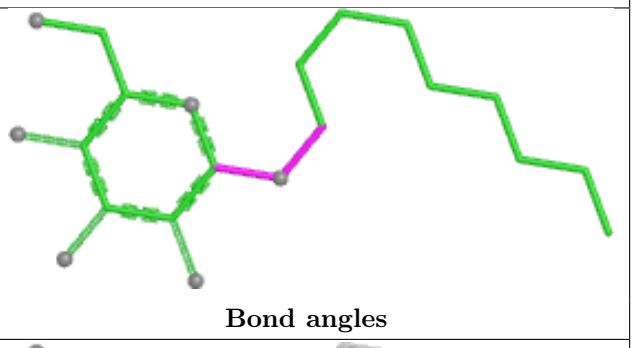
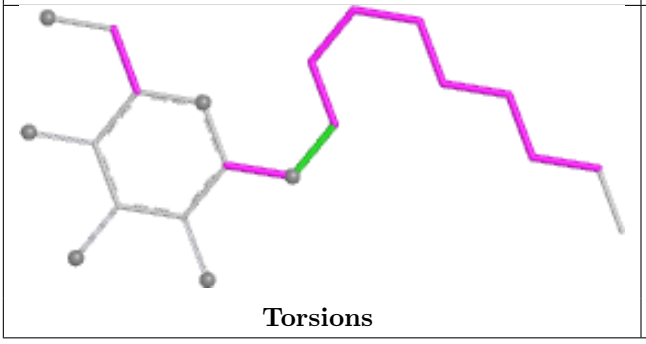


Bond angles



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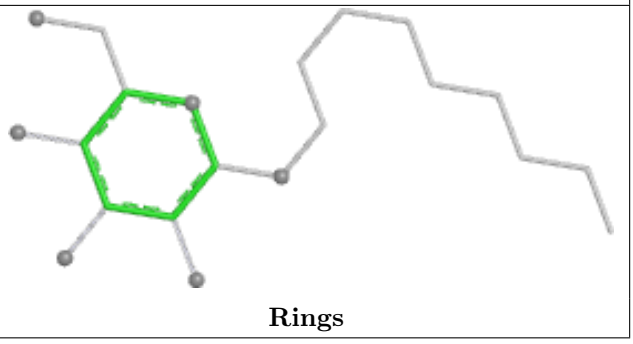
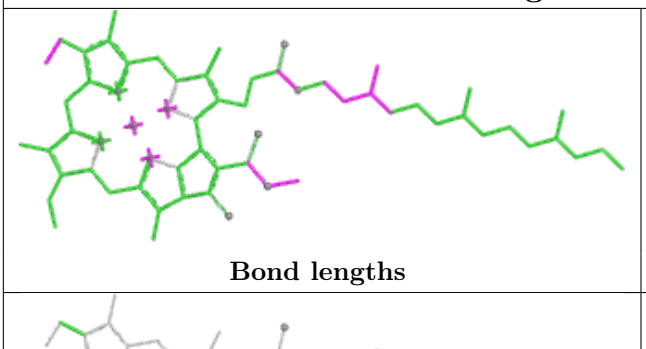


Rings

Ligand CLA E 604



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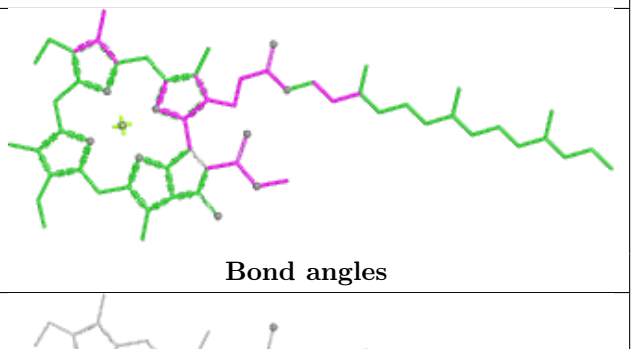

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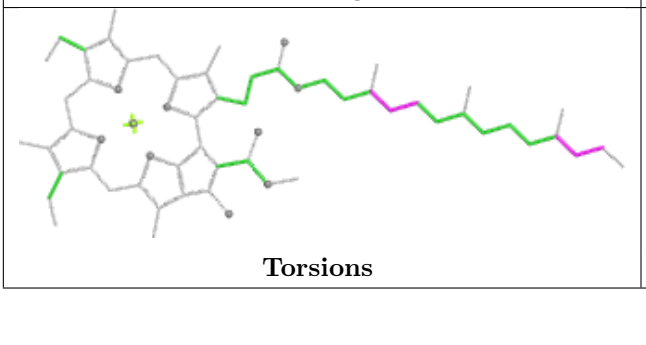

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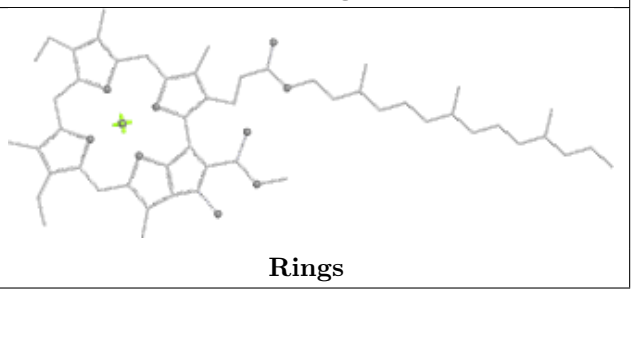
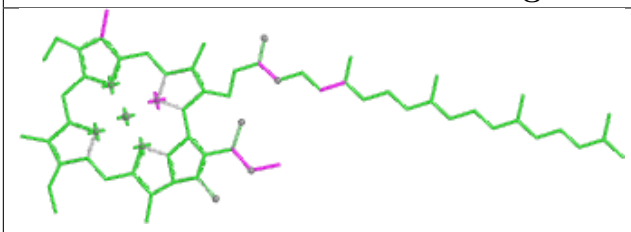


Rings

Ligand CLA D 610



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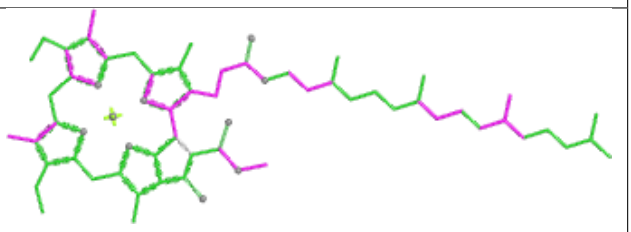

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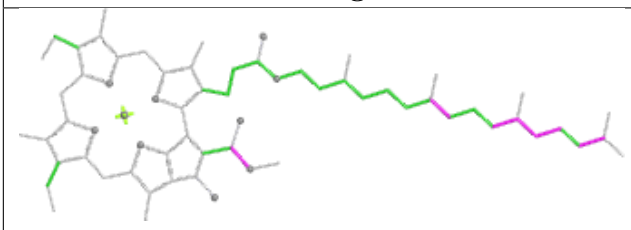

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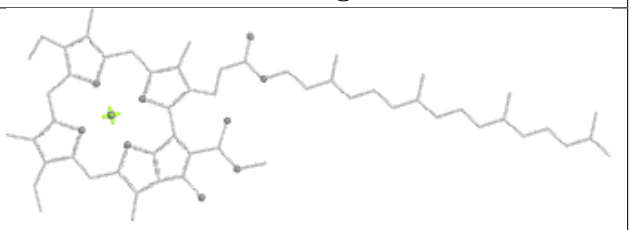
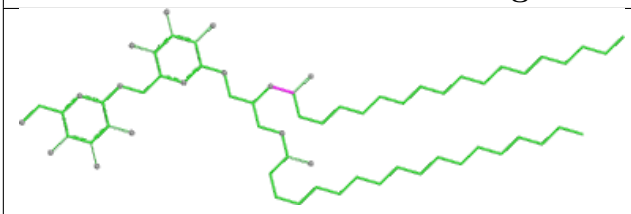


Rings

Ligand DGD B 2632



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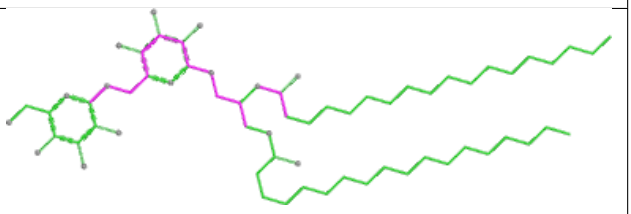

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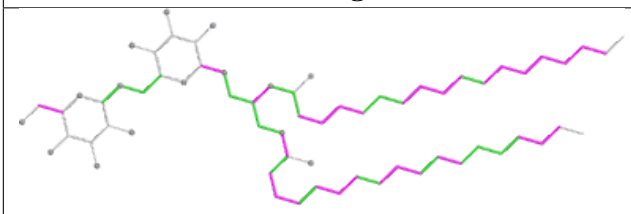

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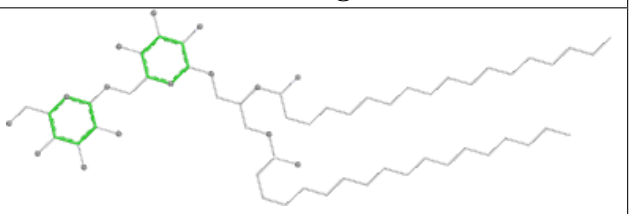
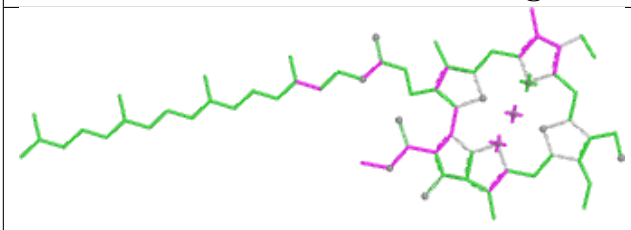


Rings

Ligand CHL E 601



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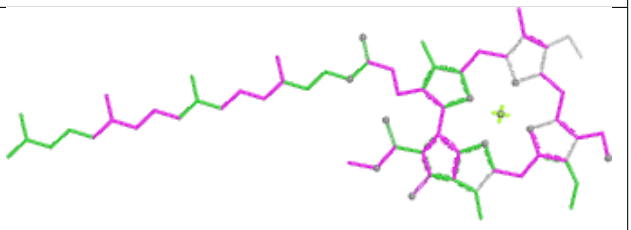

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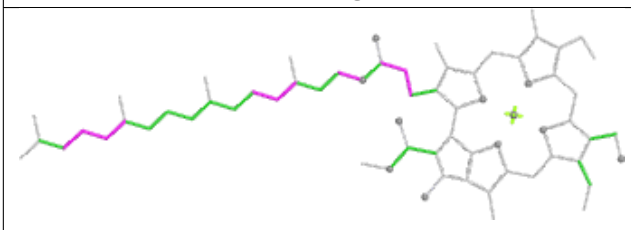

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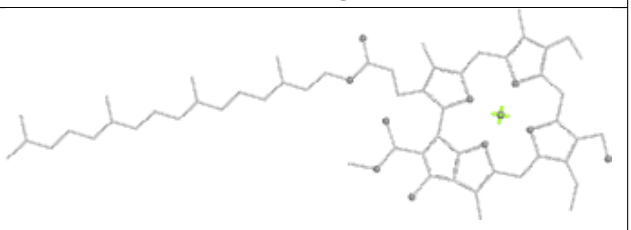
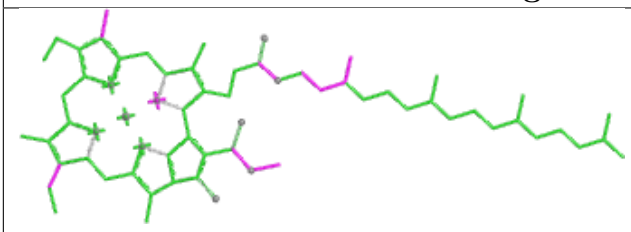


Rings

Ligand CLA H 602



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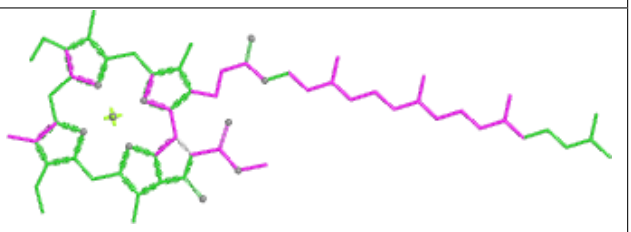

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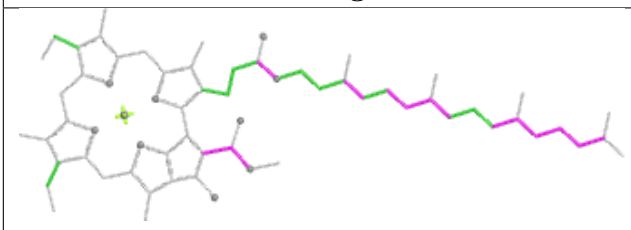

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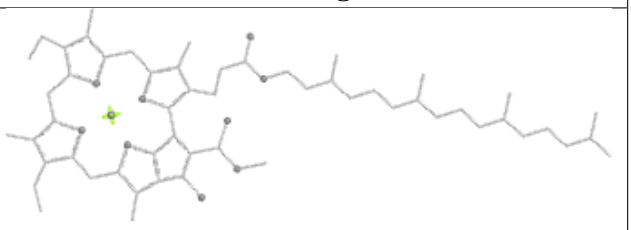
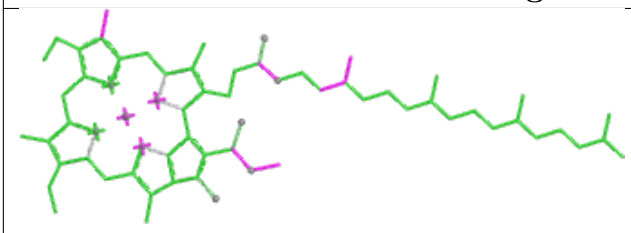


Rings

Ligand CLA F 612



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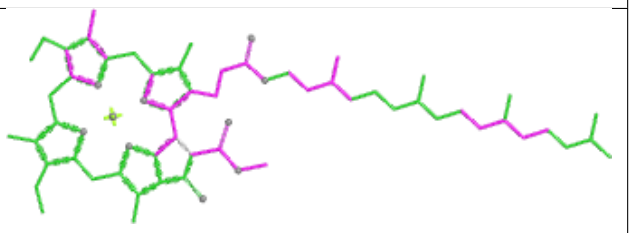

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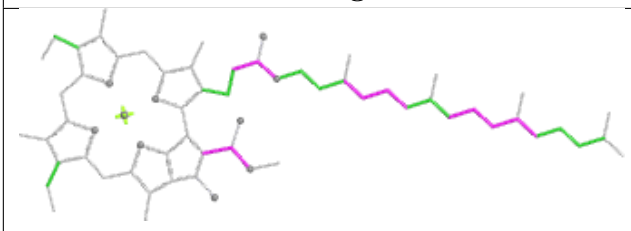

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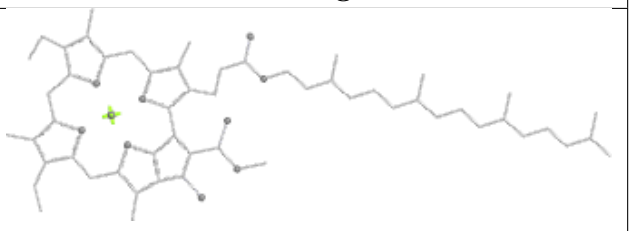
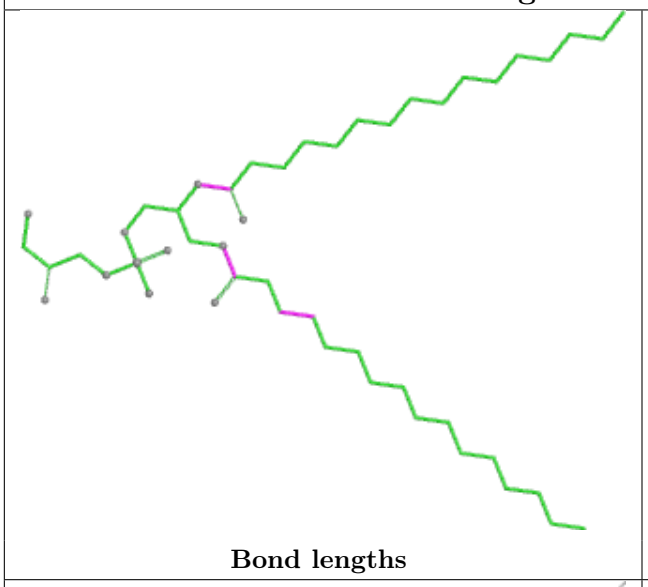


Rings

Ligand LHG J 9630



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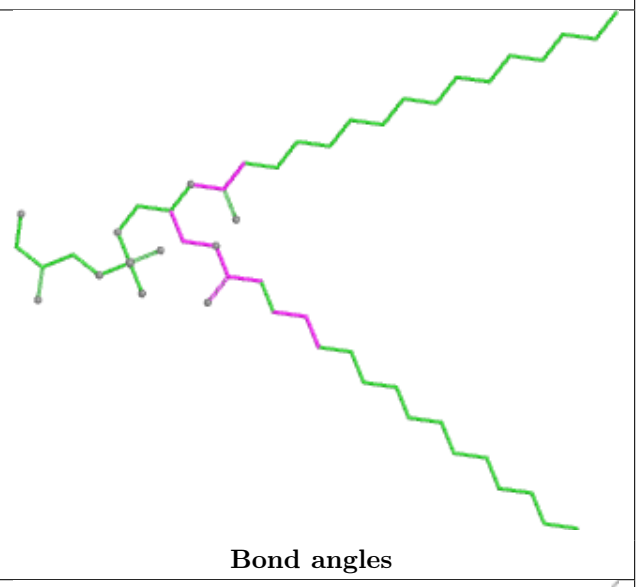
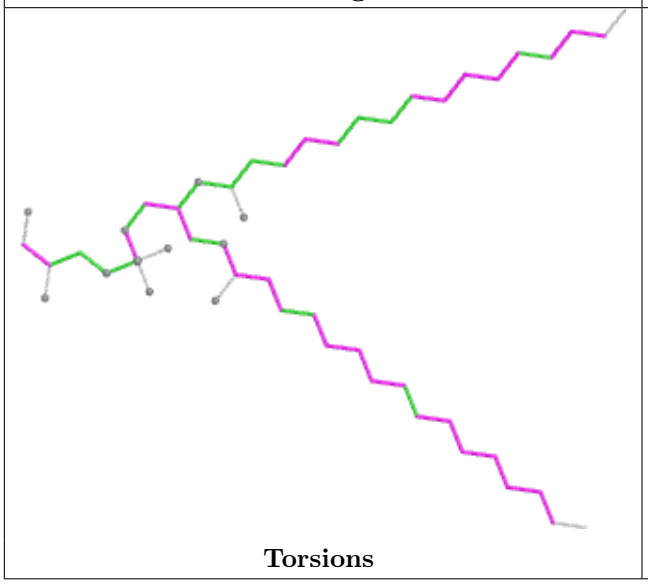


Bond angles



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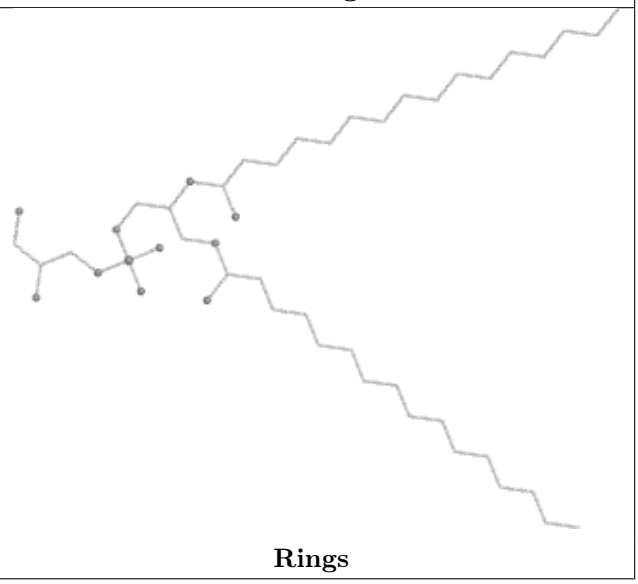
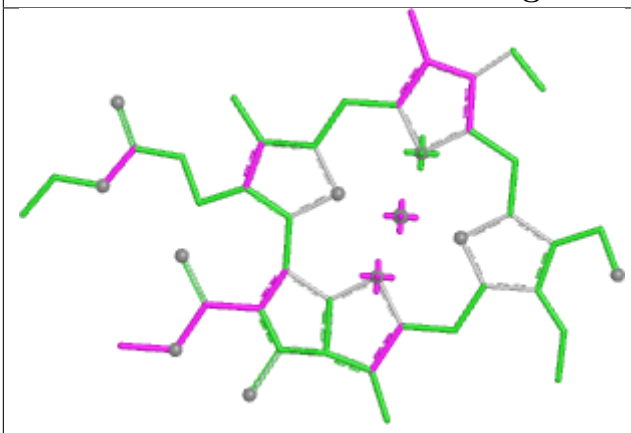


Rings

Ligand CHL G 605



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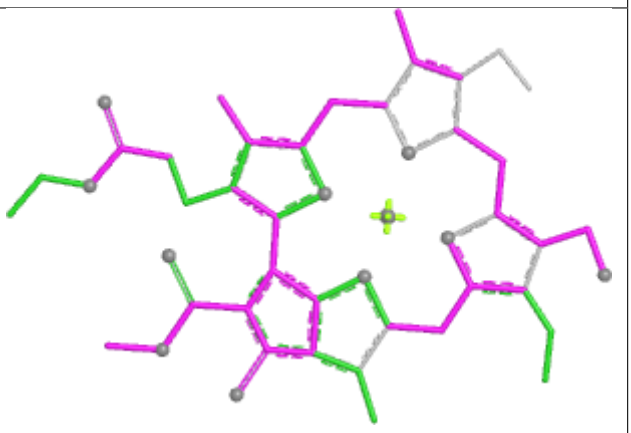
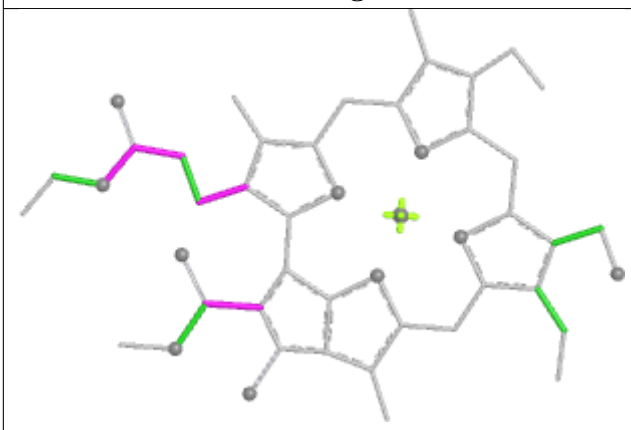


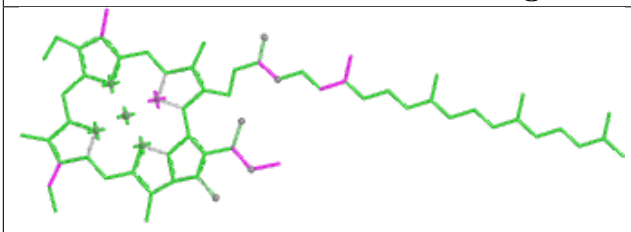
Bond angles



Torsions

Rings

Ligand CLA G 610



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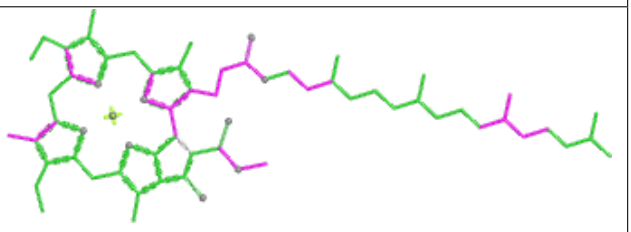

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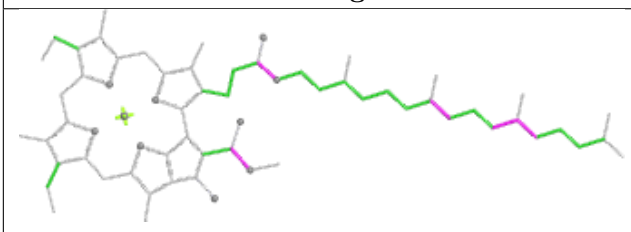
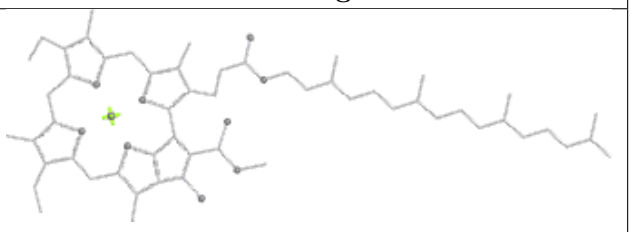
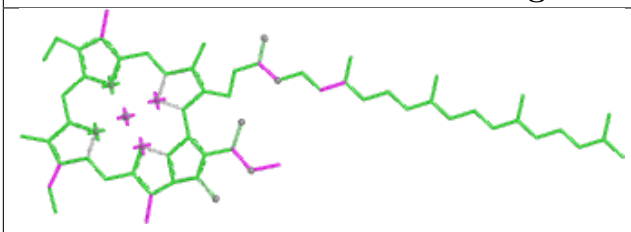


Torsions



Rings

Ligand CLA J 603



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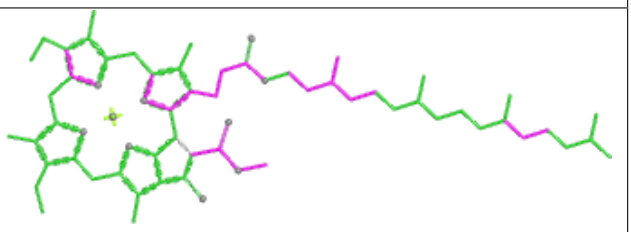
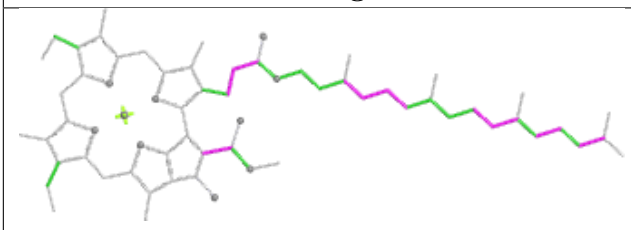
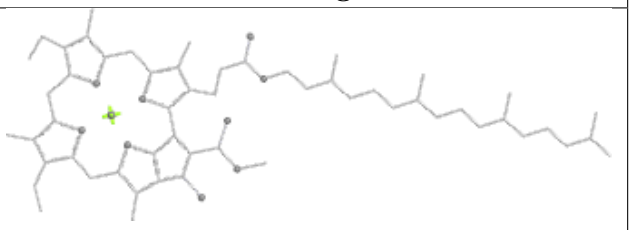


Bond angles

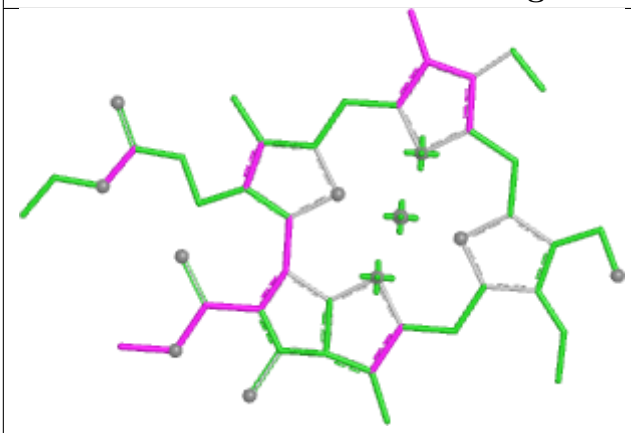


Torsions



Rings

Ligand CHL J 605



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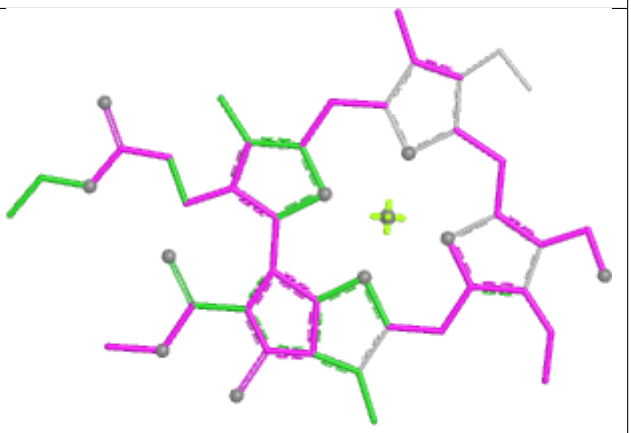
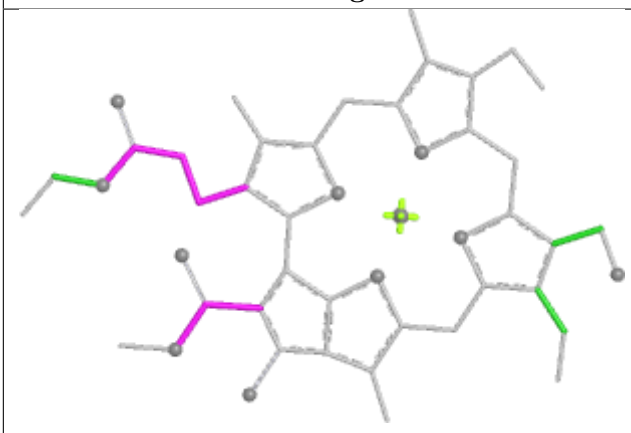
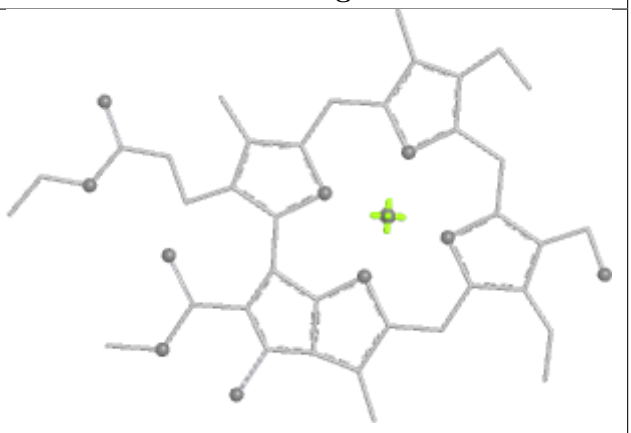


Bond angles

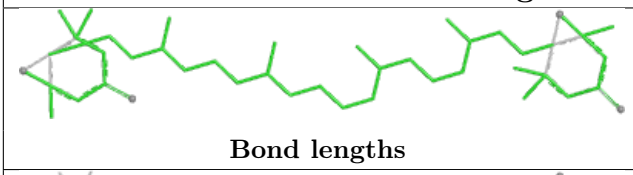


Torsions



Rings

Ligand XAT F 6622



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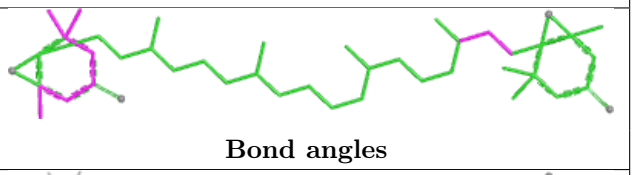
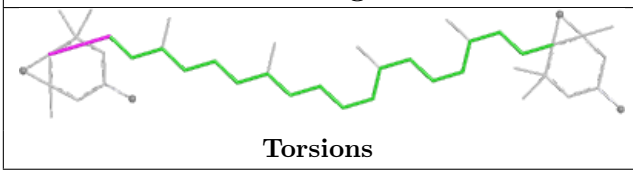
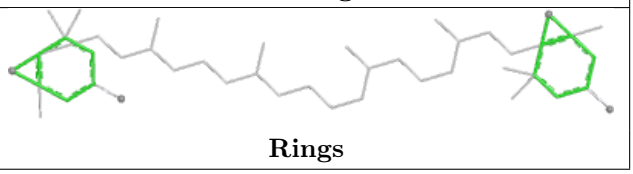


Bond angles

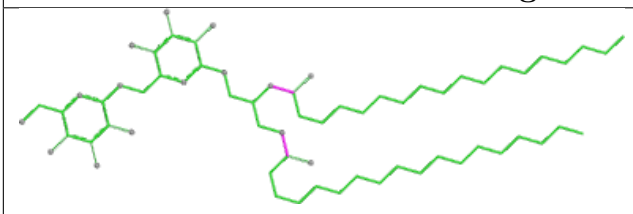


Torsions



Rings

Ligand DGD A 632



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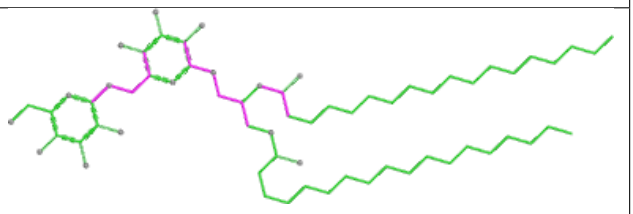
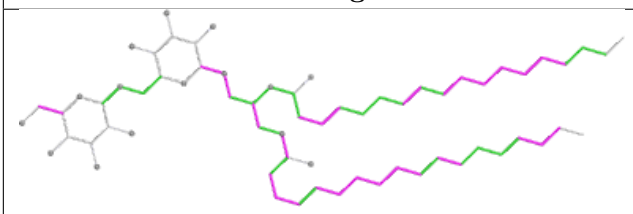
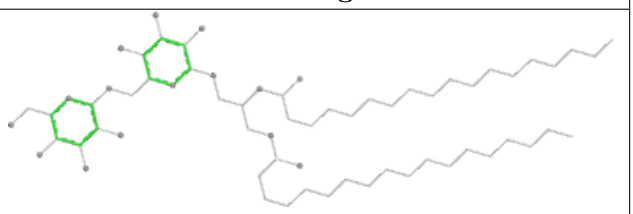


Bond angles

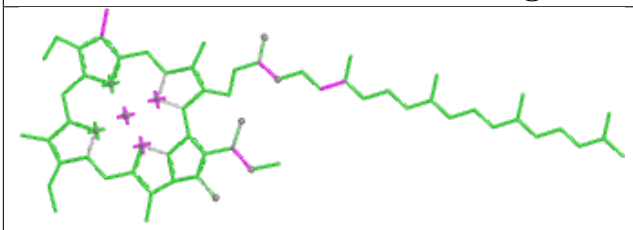


Torsions



Rings

Ligand CLA D 611



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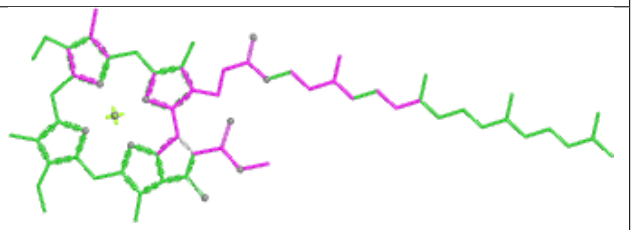
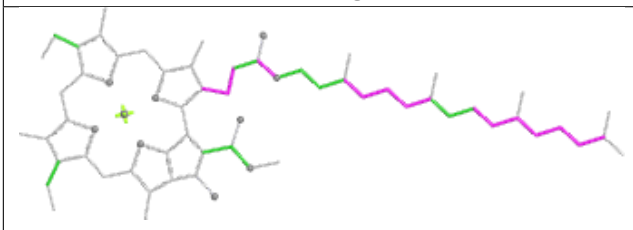
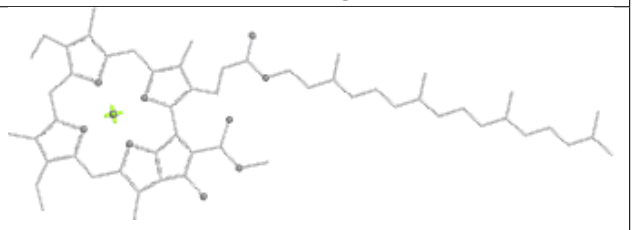


Bond angles

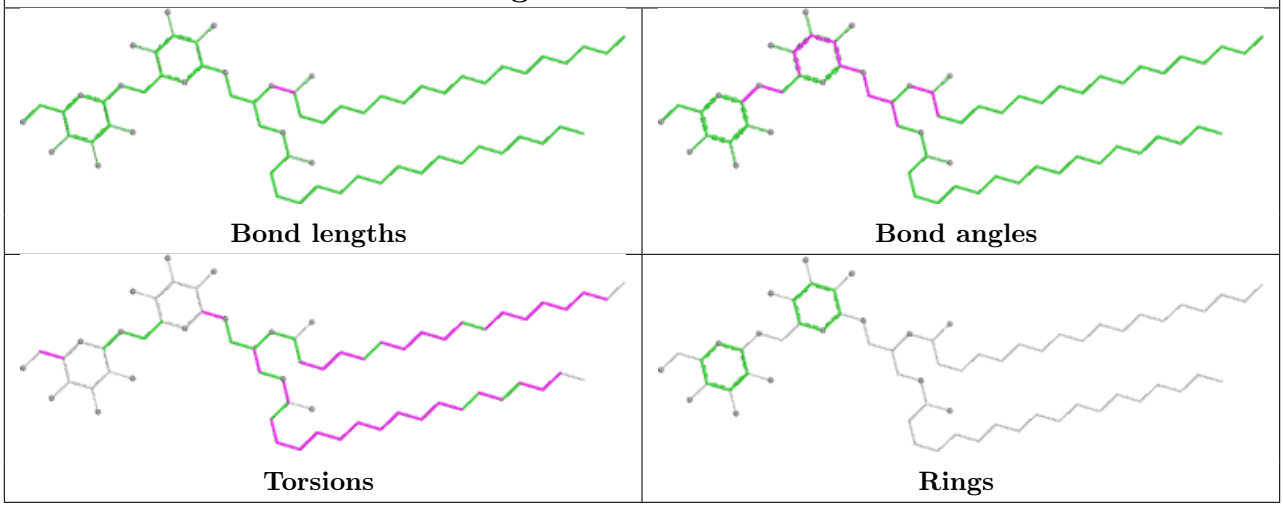


Torsions

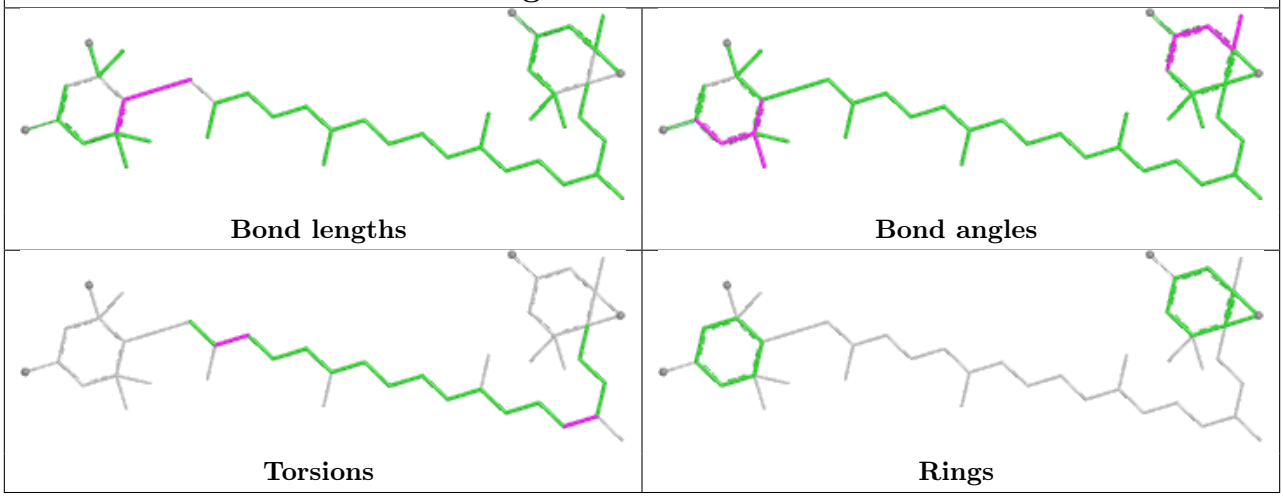


Rings

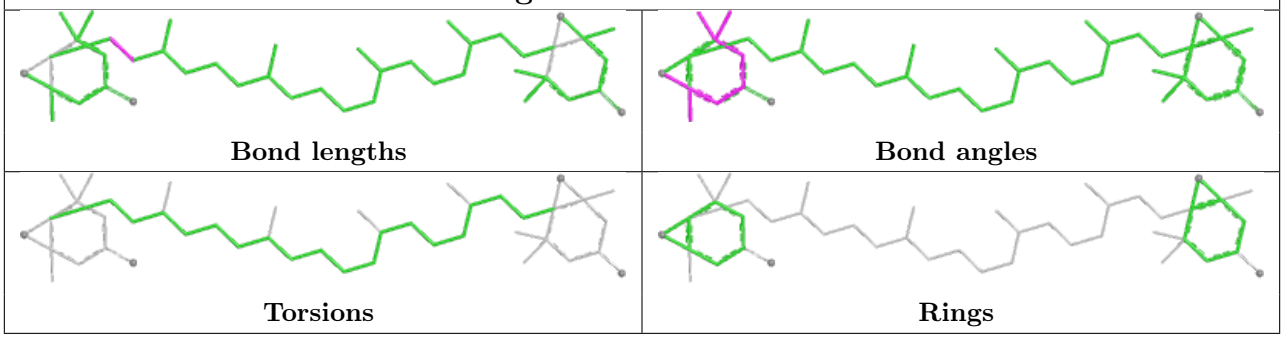
Ligand DGD H 6632



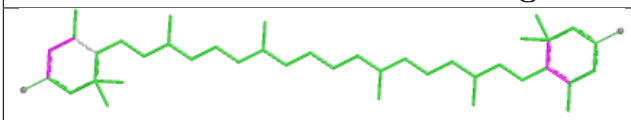
Ligand NEX A 623



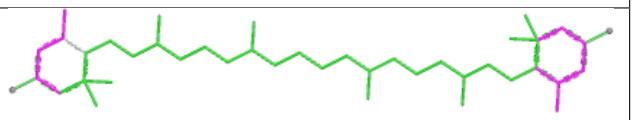
Ligand XAT C 7622



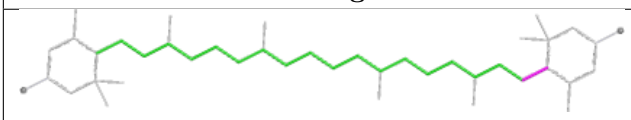
Ligand LUT J 9621



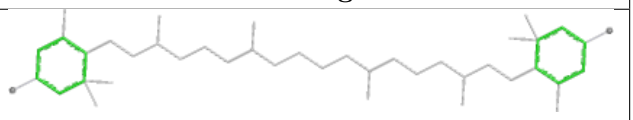
Bond lengths



Bond angles

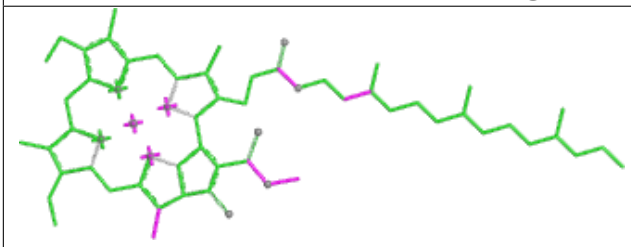


Torsions



Rings

Ligand CLA B 604



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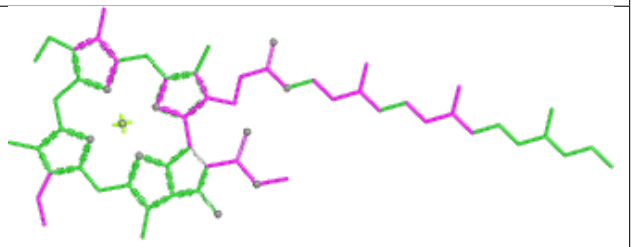
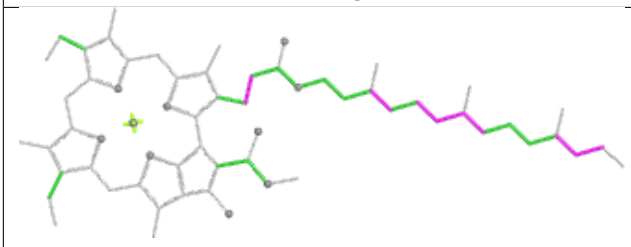
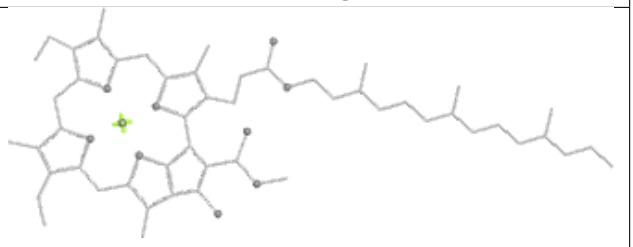


Bond angles

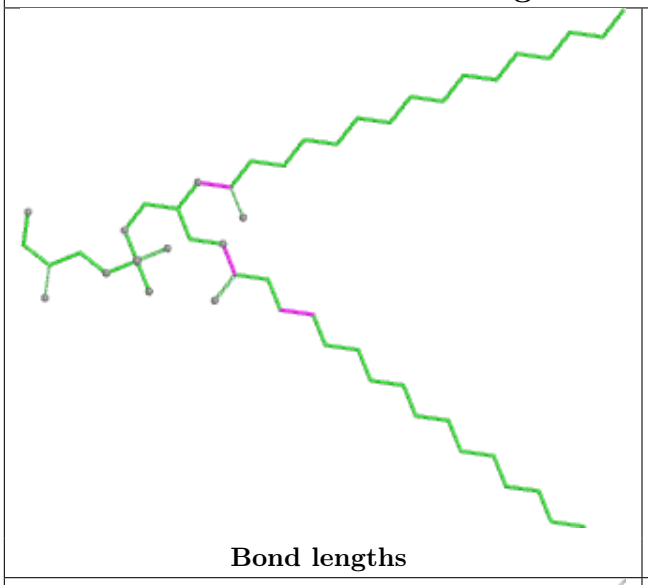


Torsions



Rings

Ligand LHG D 3630



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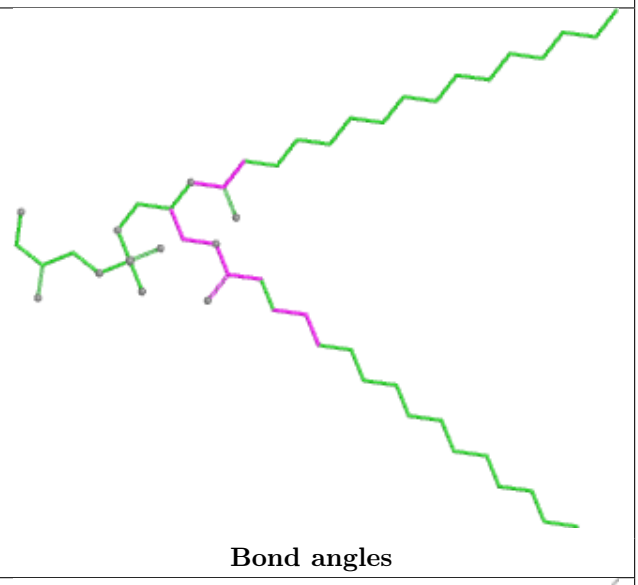
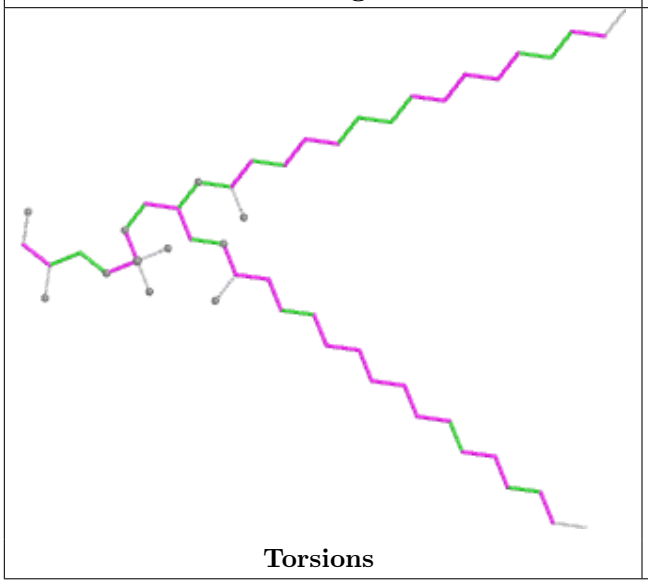


Bond angles



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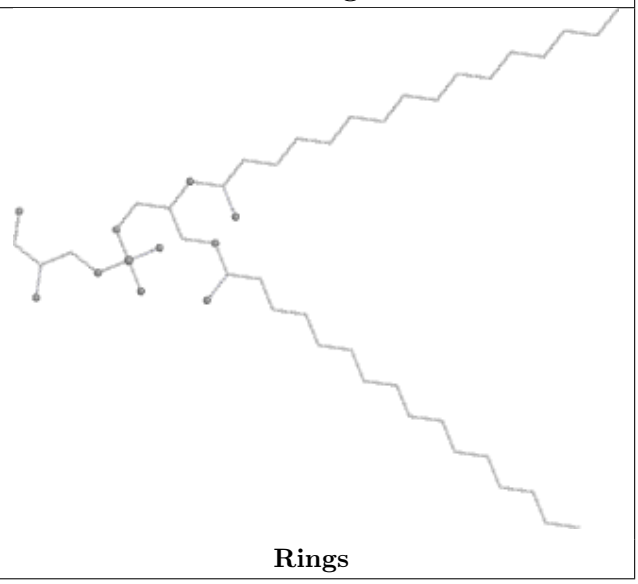
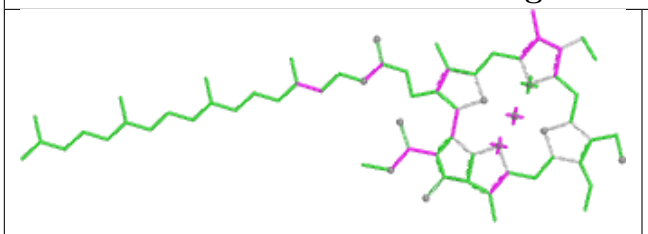


Rings

Ligand CHL B 601



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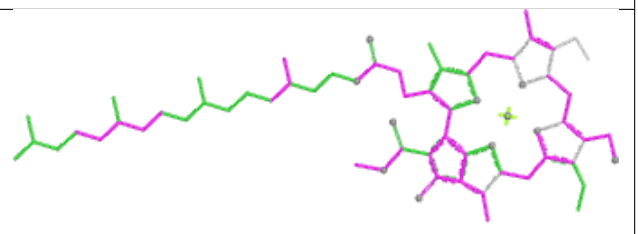
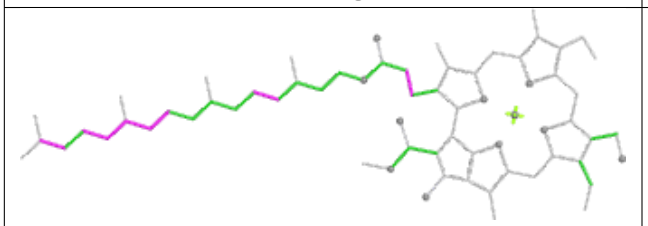
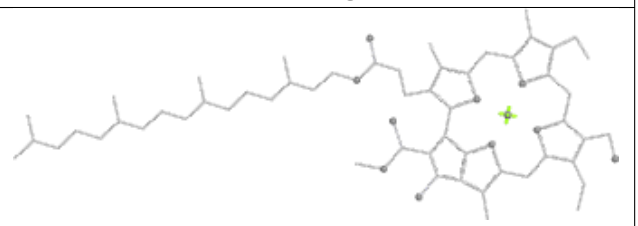


Bond angles

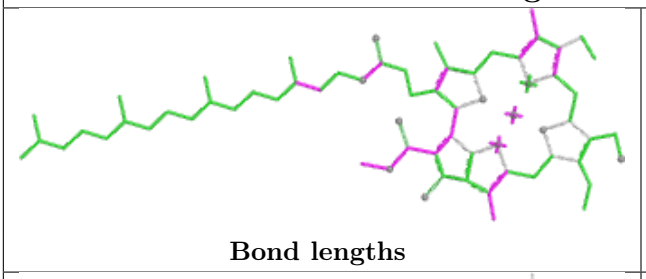


Torsions



Rings

Ligand CHL C 607



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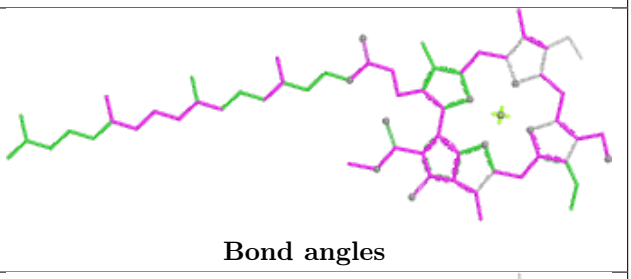
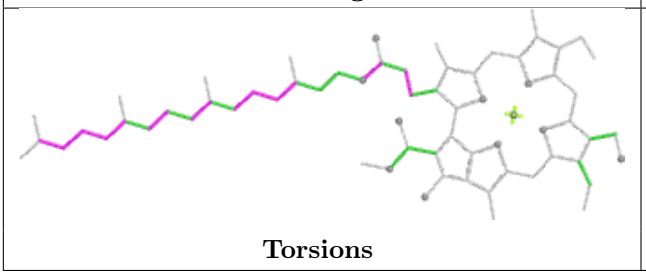
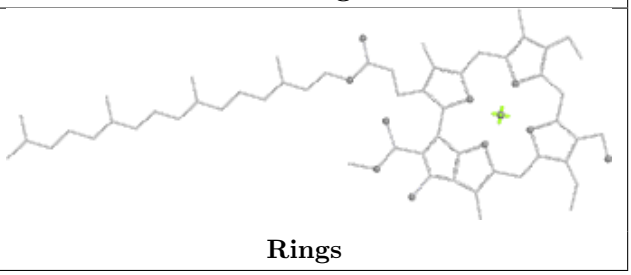


Bond angles

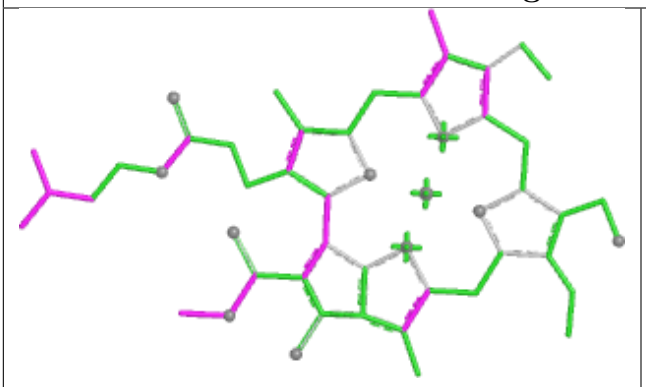


Torsions

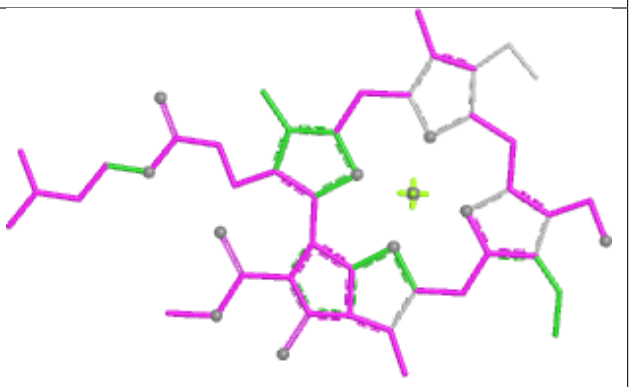


Rings

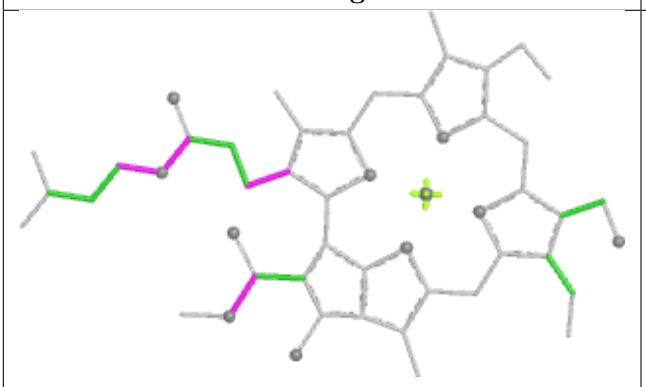
Ligand CHL D 606



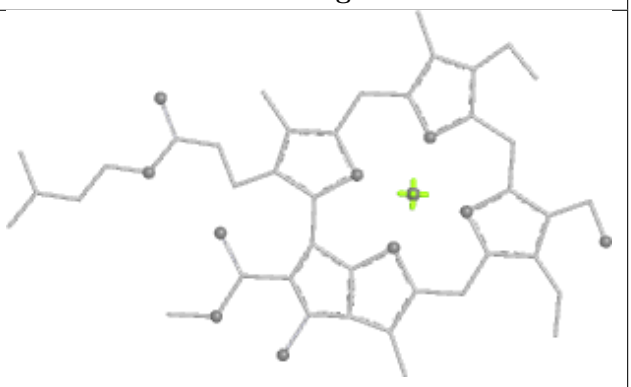
Bond lengths



Bond angles

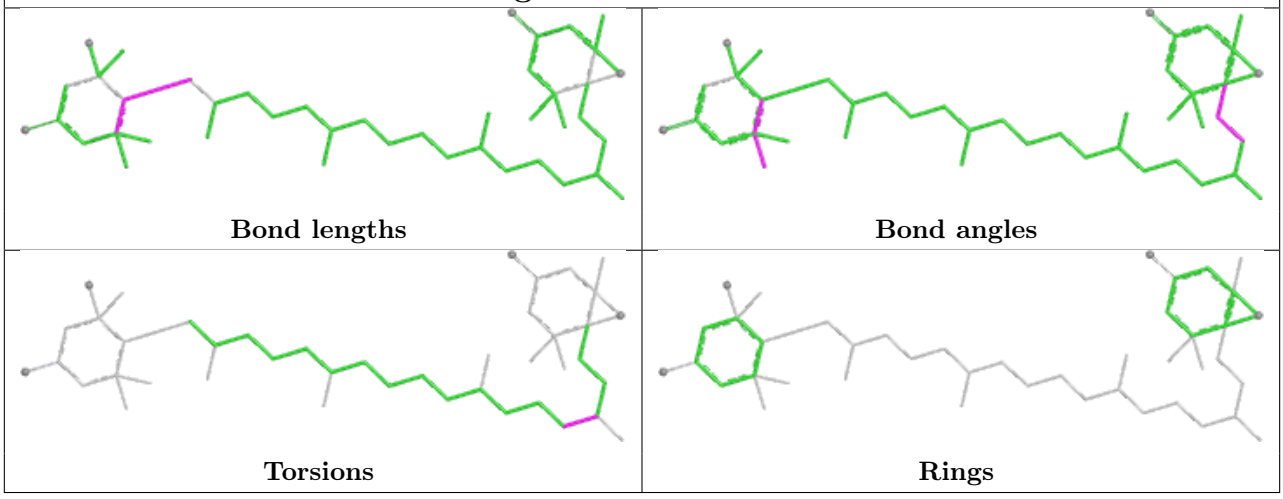


Torsions

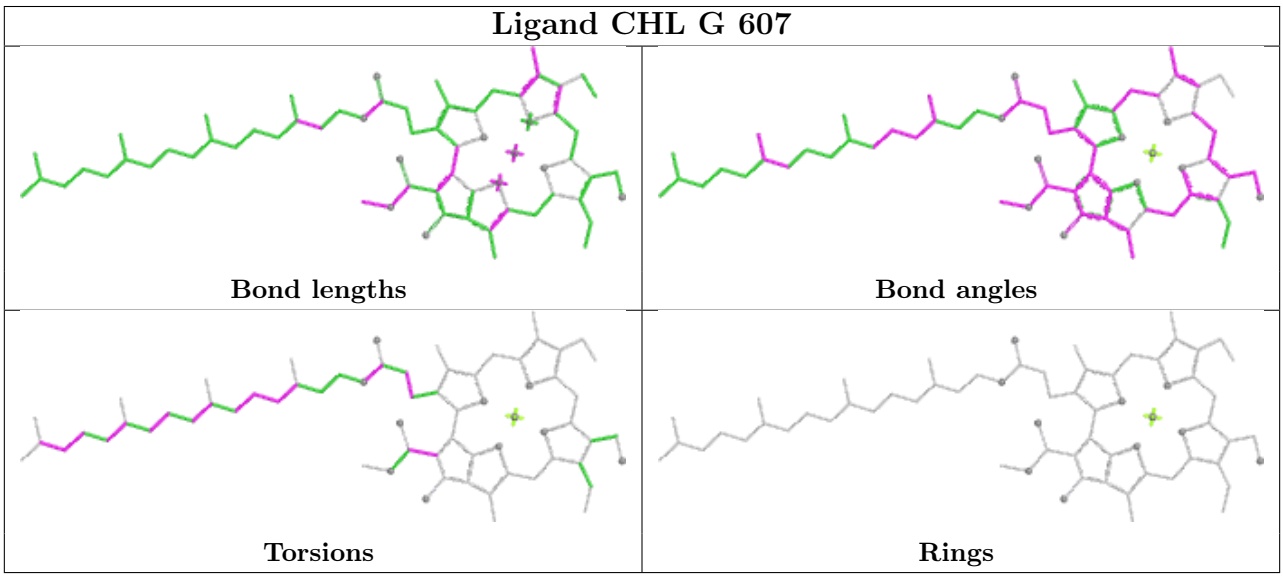


Rings

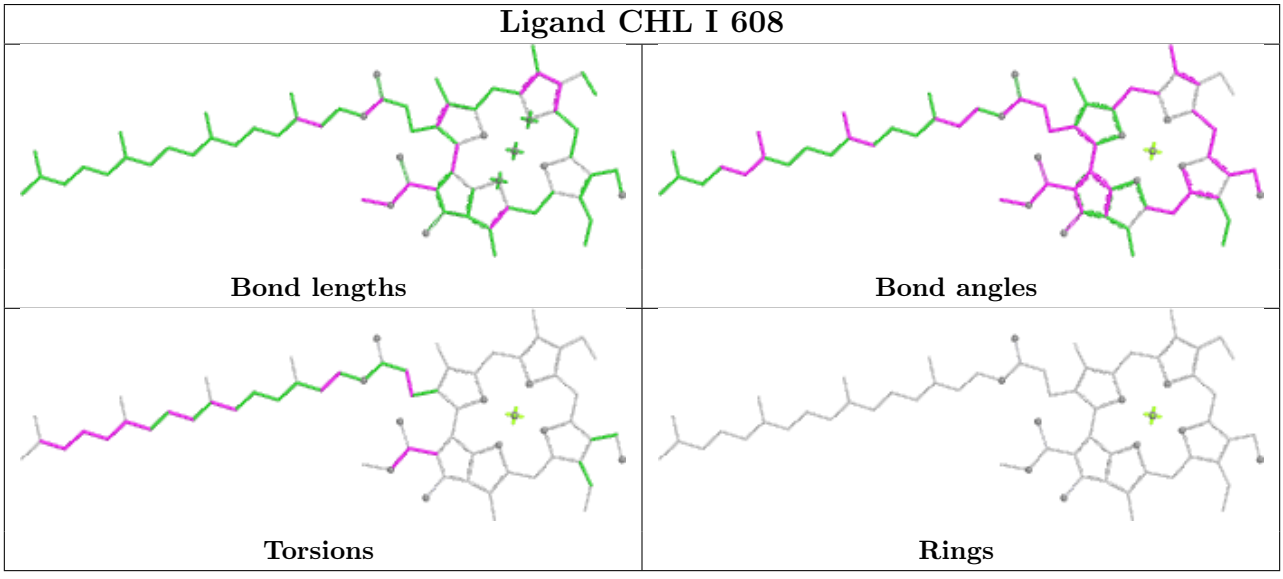
Ligand NEX C 2623



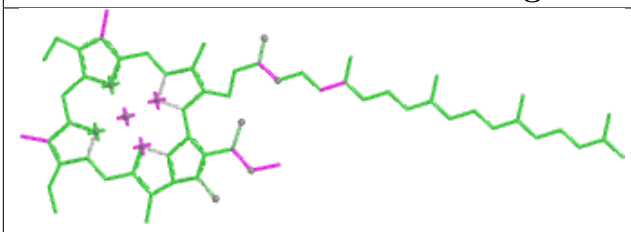
Ligand CHL G 607



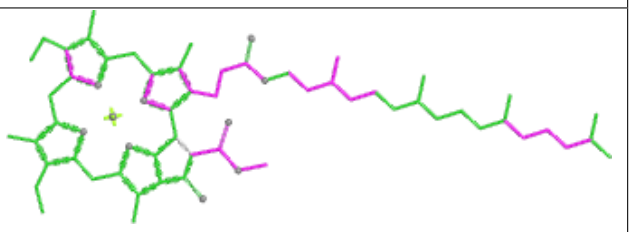
Ligand CHL I 608



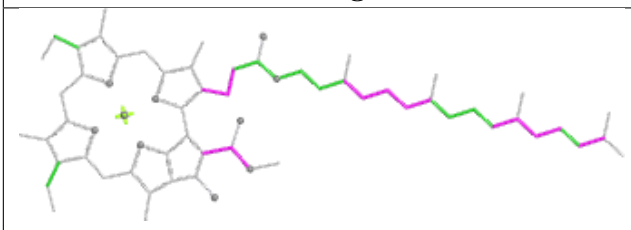
Ligand CLA A 603



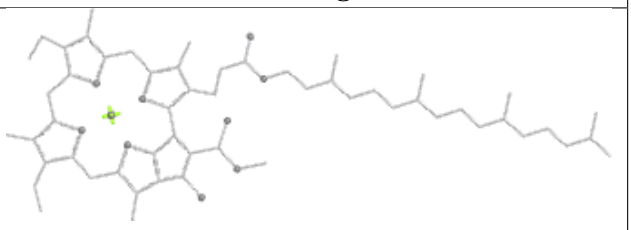
Bond lengths



Bond angles

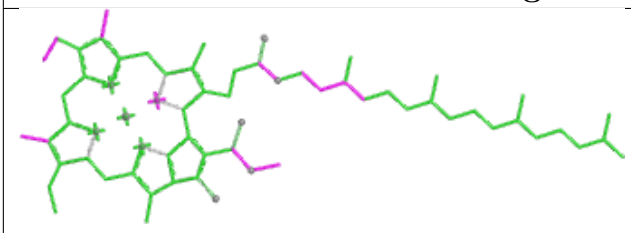


Torsions

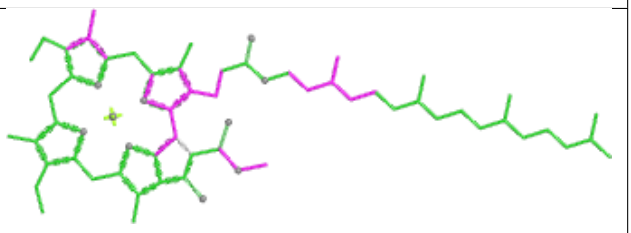


Rings

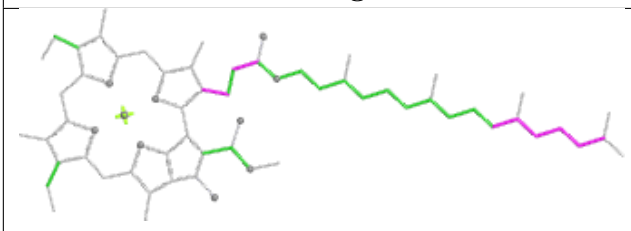
Ligand CLA D 613



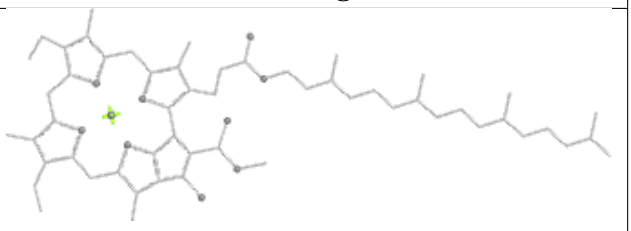
Bond lengths



Bond angles

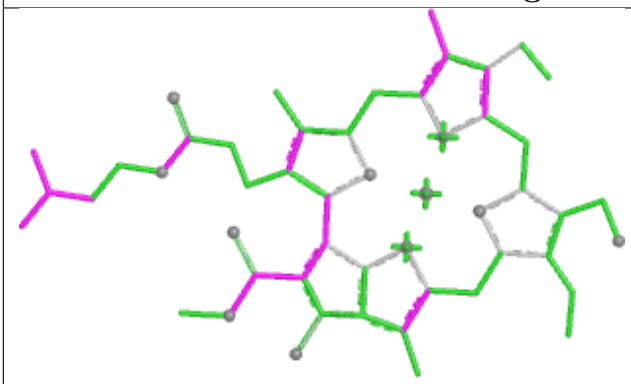


Torsions



Rings

Ligand CHL C 606



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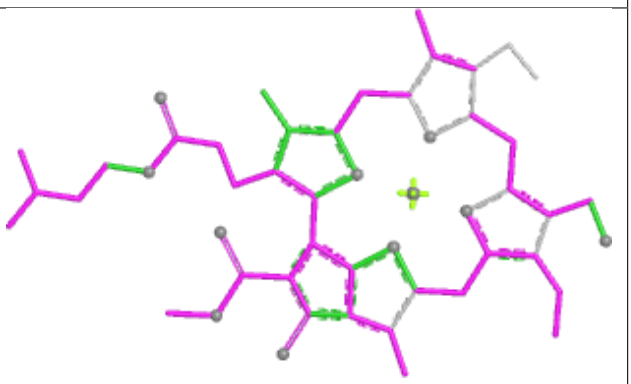
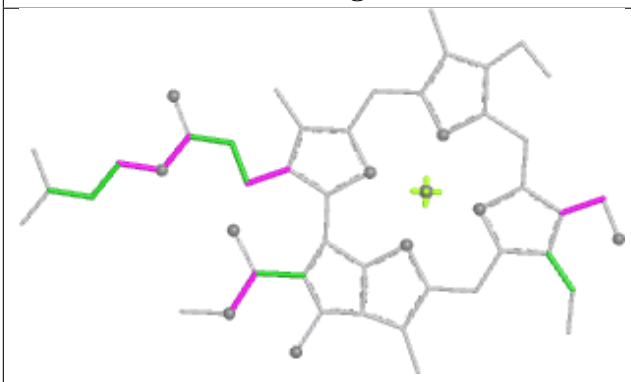


Bond angles



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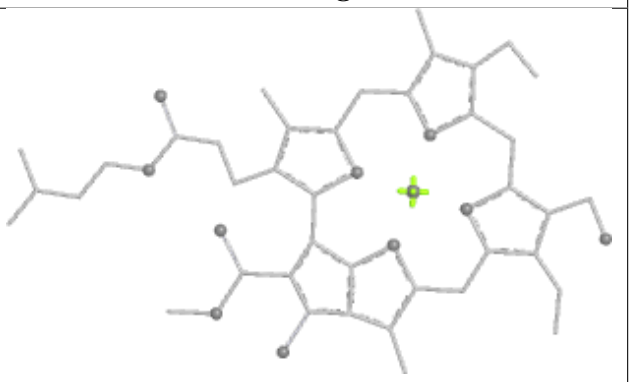
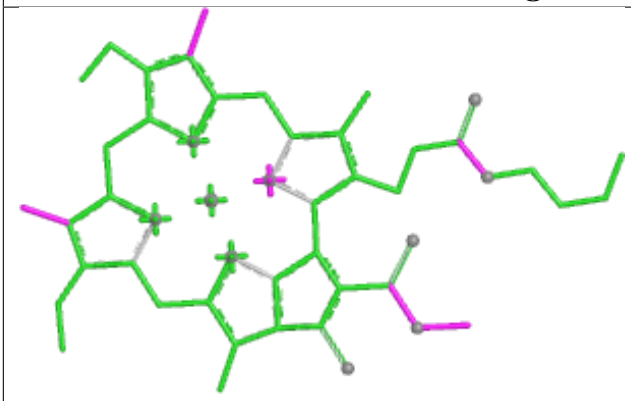


Rings

Ligand CLA C 614



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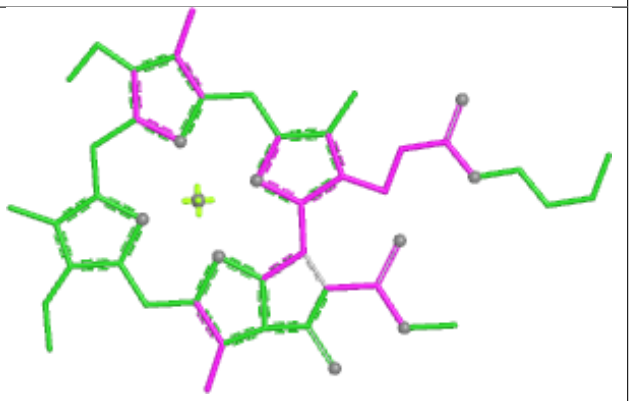
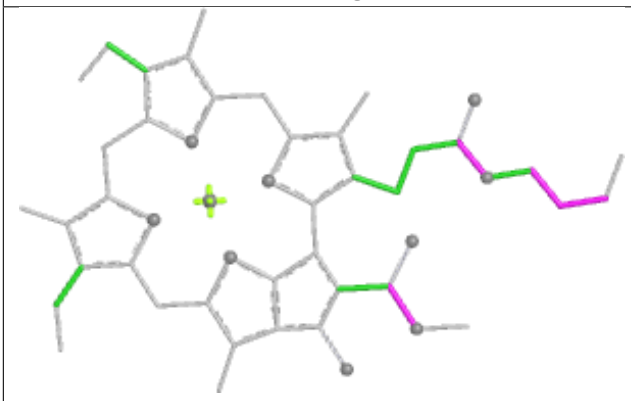


Bond angles



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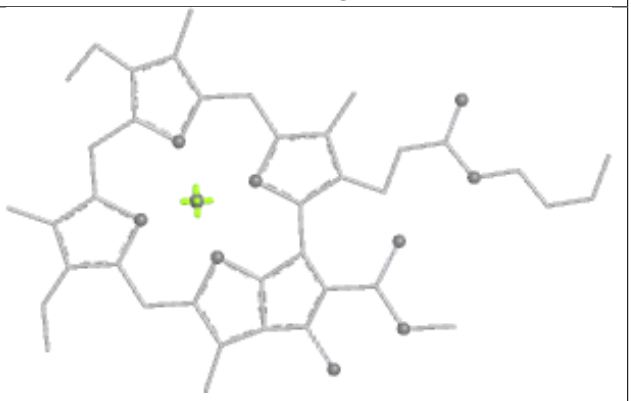
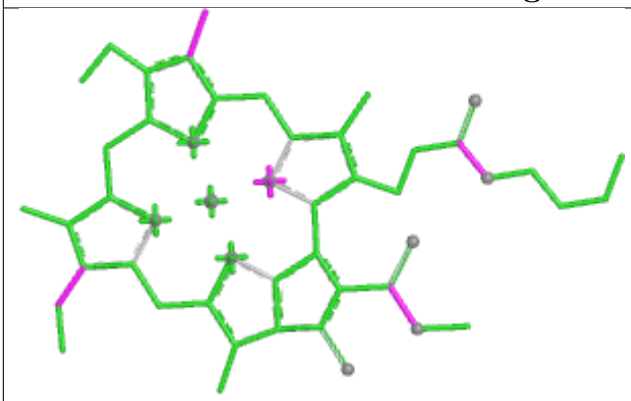


Rings

Ligand CLA D 614



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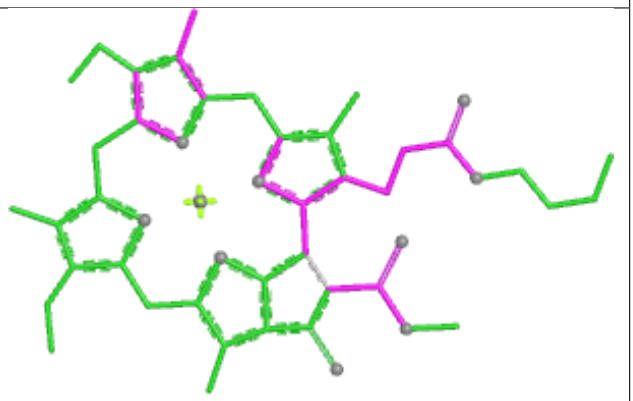
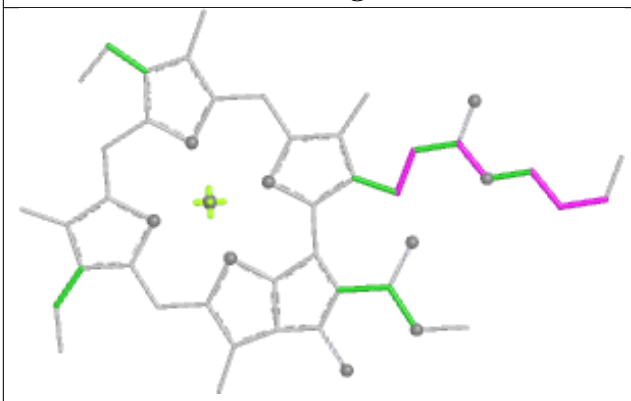


Bond angles



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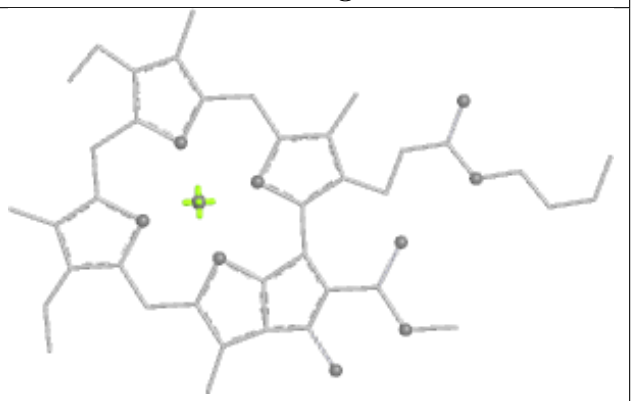
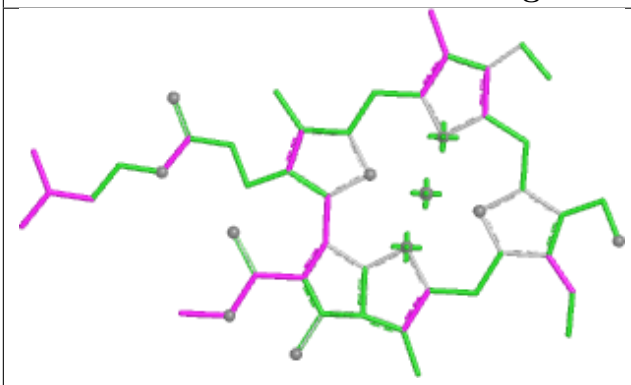


Rings

Ligand CHL G 606



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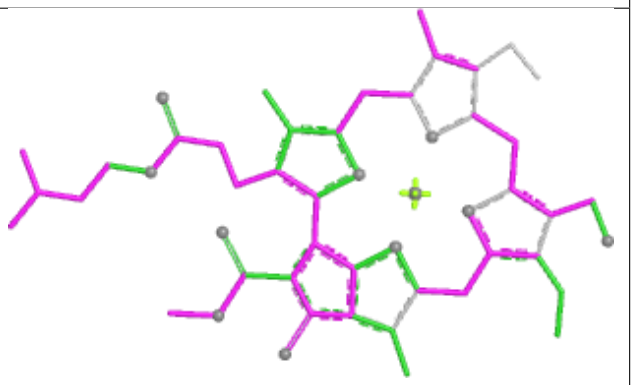

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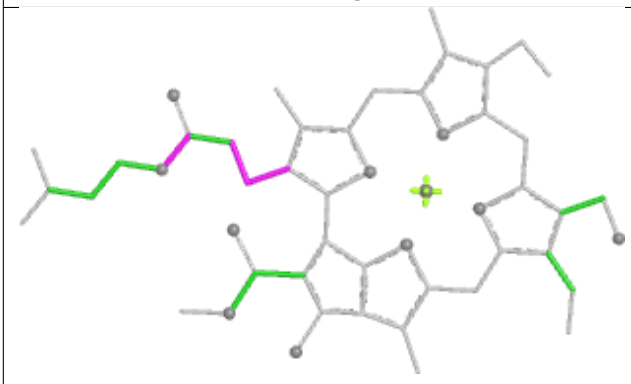

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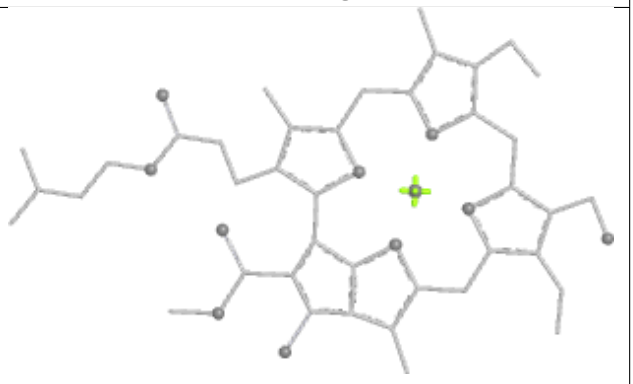
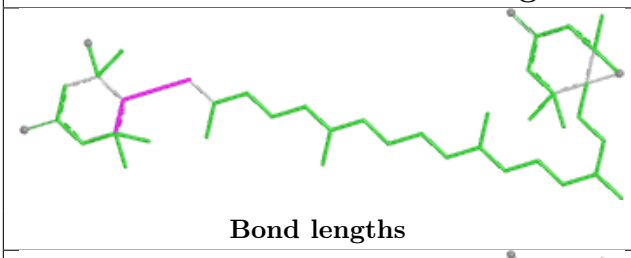


Rings

Ligand NEX I 8623



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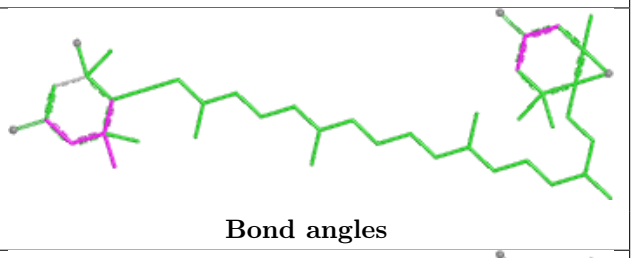
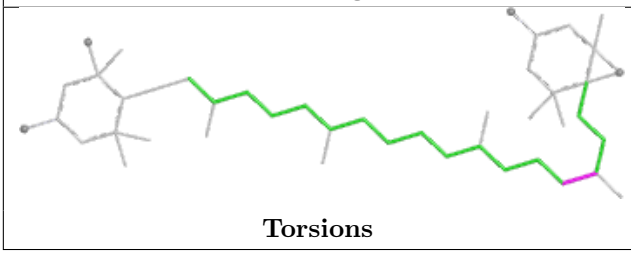


Bond angles



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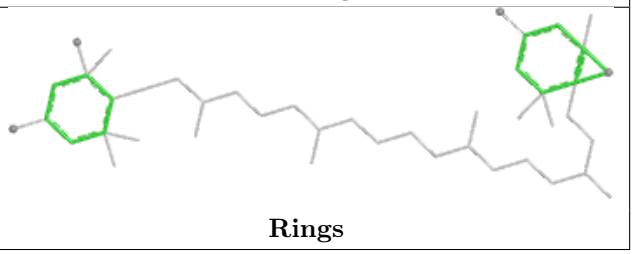
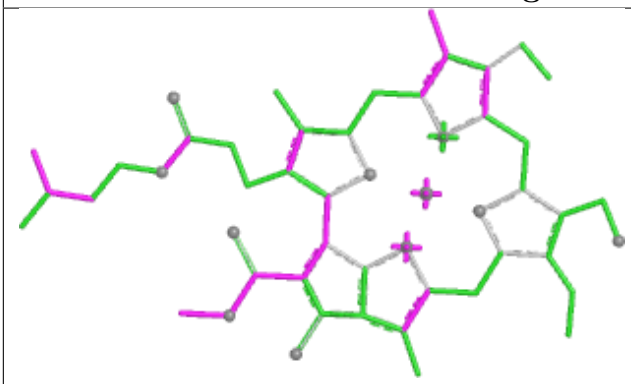


Rings

Ligand CHL H 606



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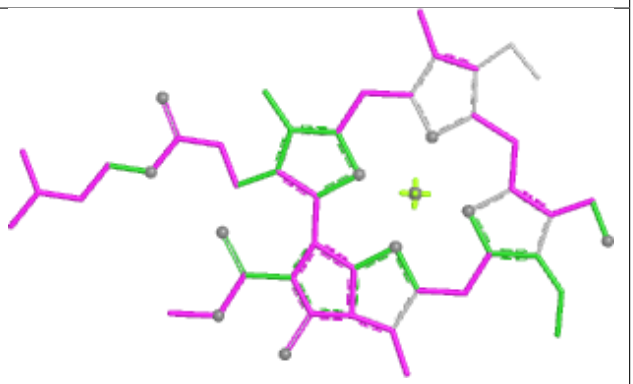
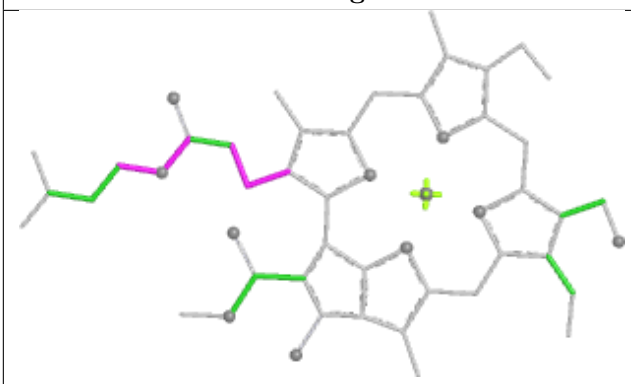


Bond angles



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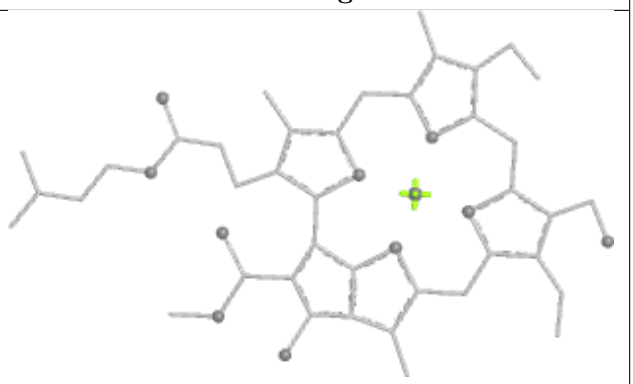
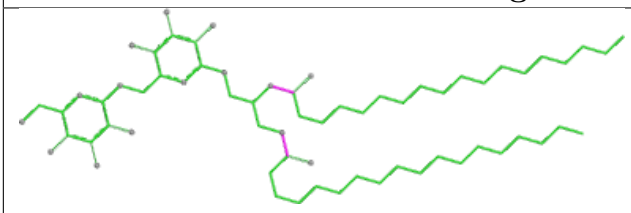


Rings

Ligand DGD G 9632



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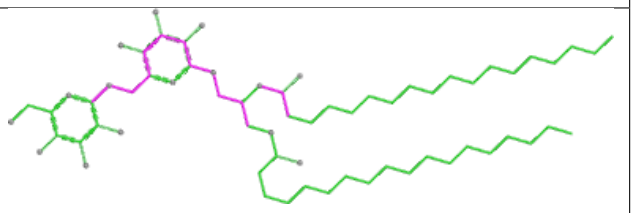

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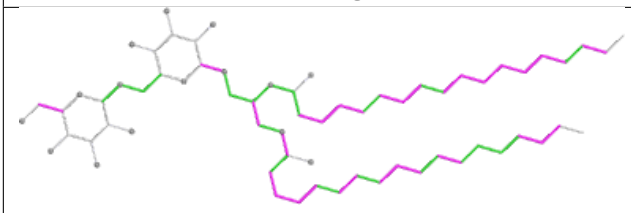

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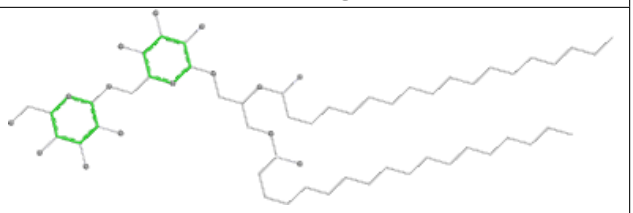
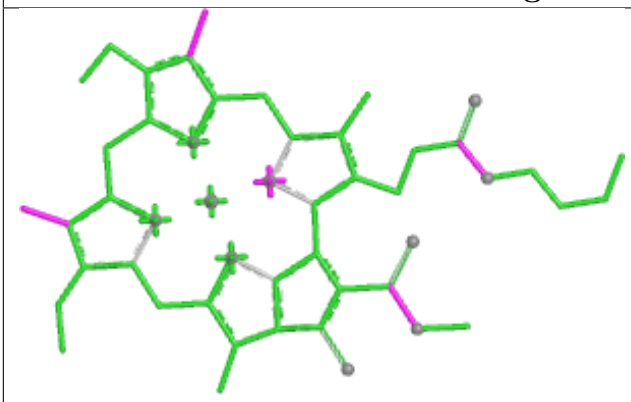


Rings

Ligand CLA A 614



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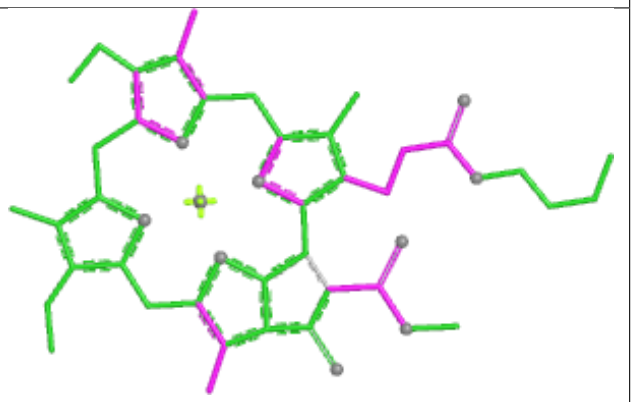
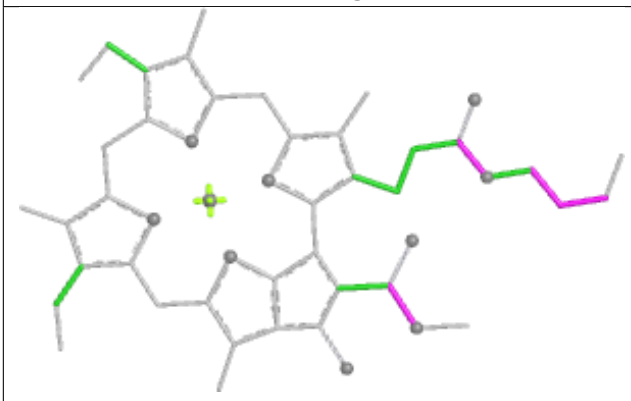


Bond angles



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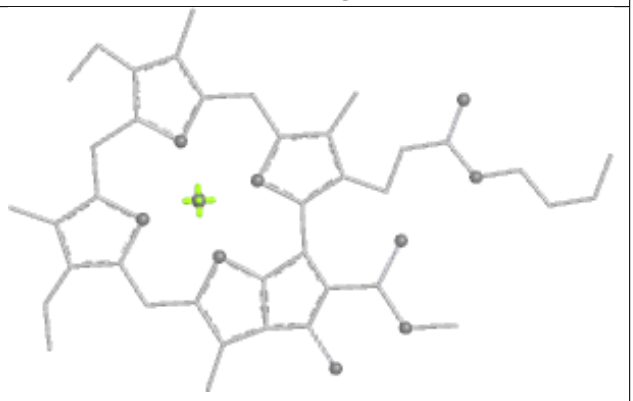
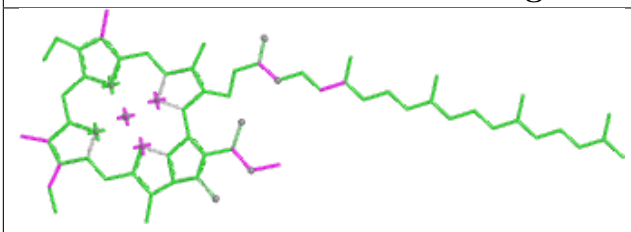


Rings

Ligand CLA E 603



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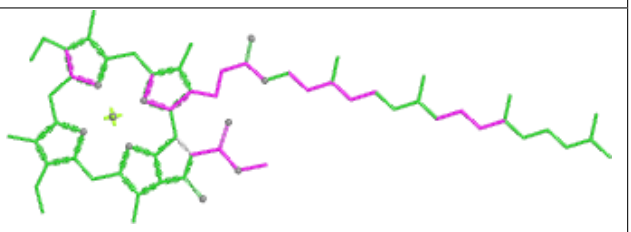

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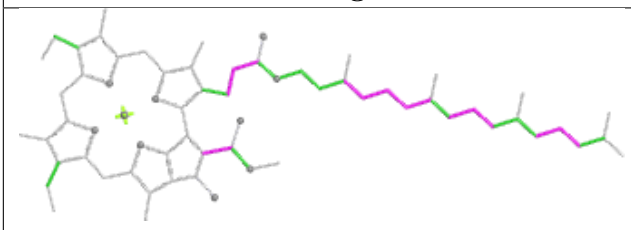

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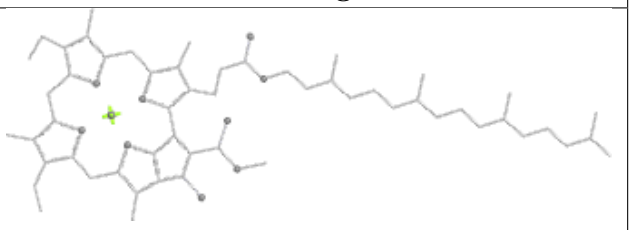
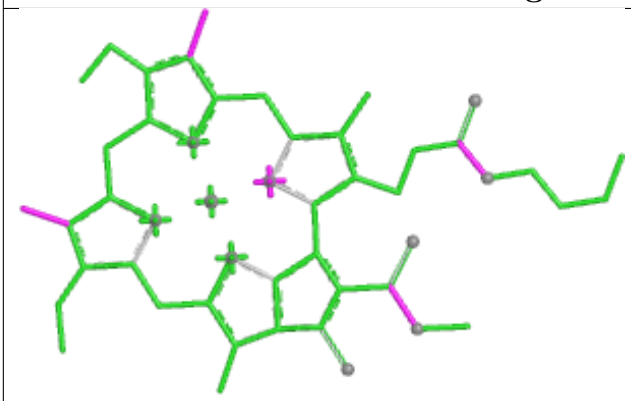


Rings

Ligand CLA E 614



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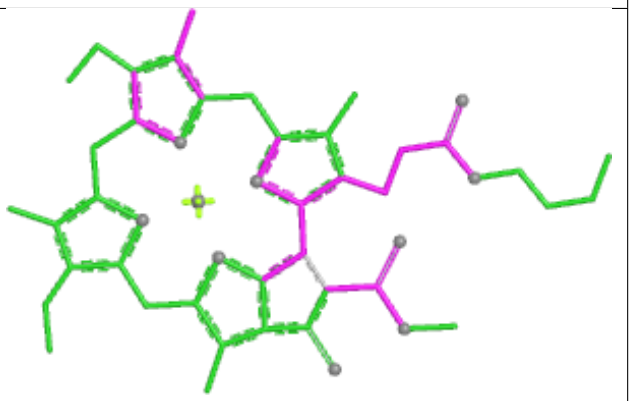

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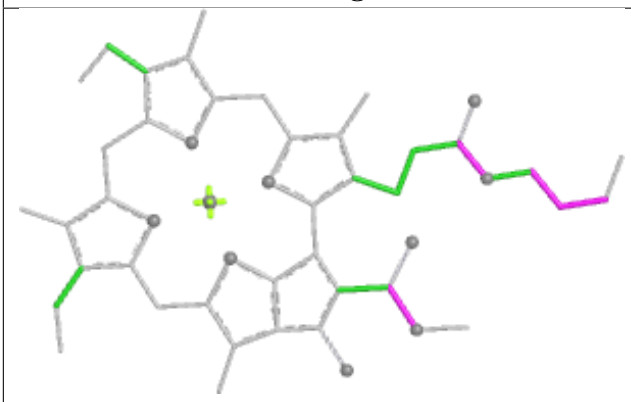

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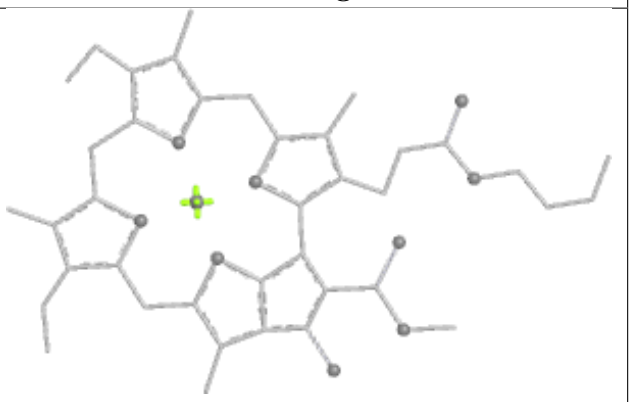
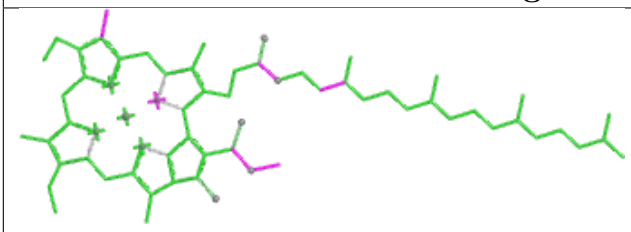


Rings

Ligand CLA H 613



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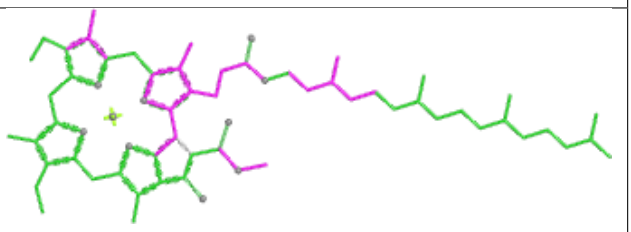
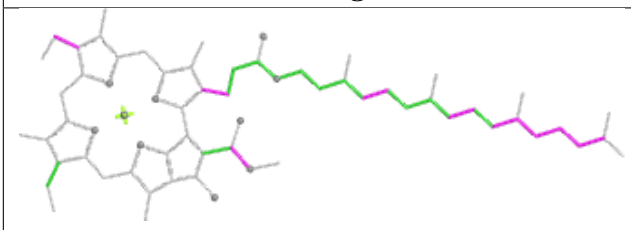
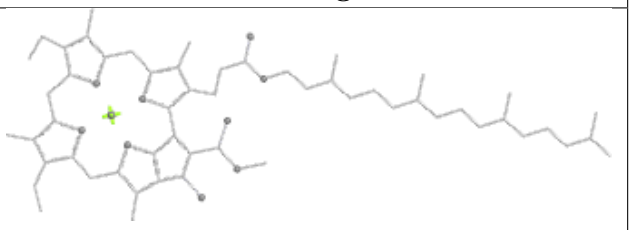


Bond angles

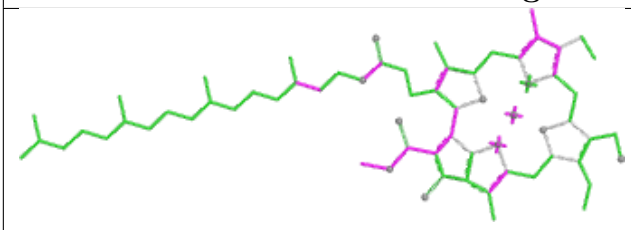


Torsions



Rings

Ligand CHL G 601



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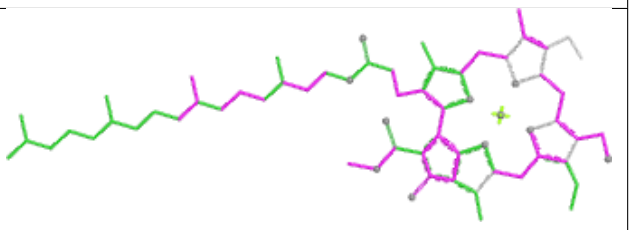
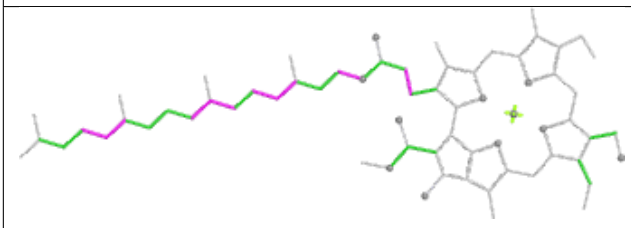


Bond angles



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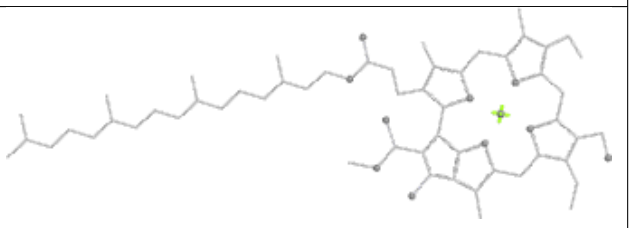
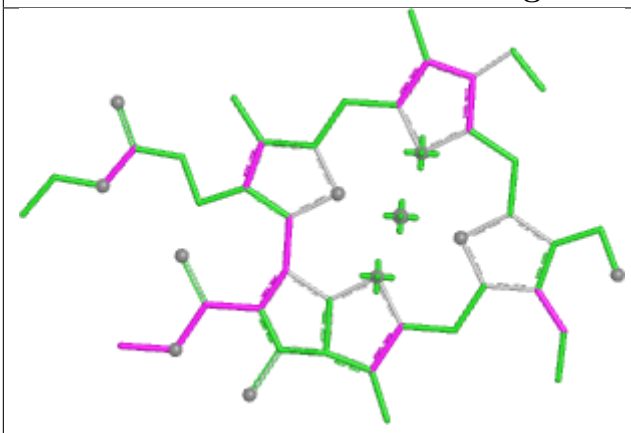


Rings

Ligand CHL A 605



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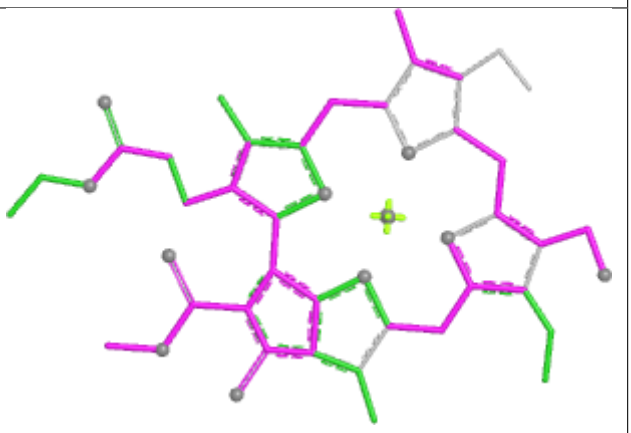
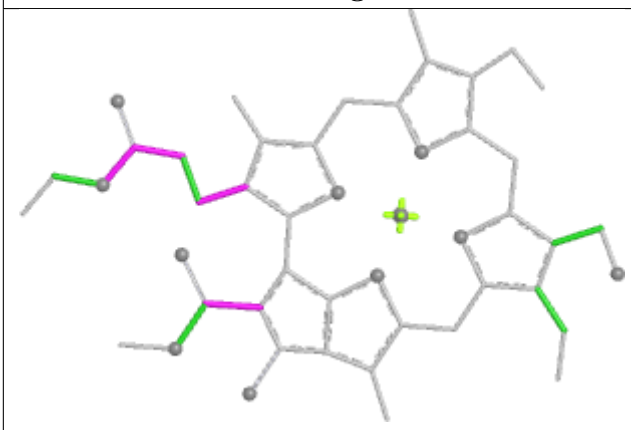


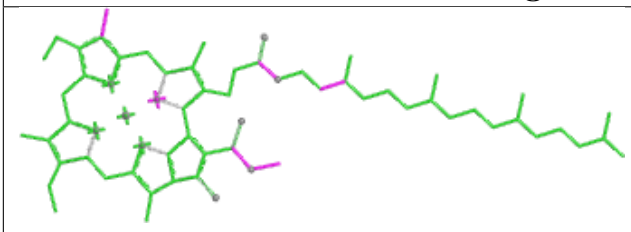
Bond angles



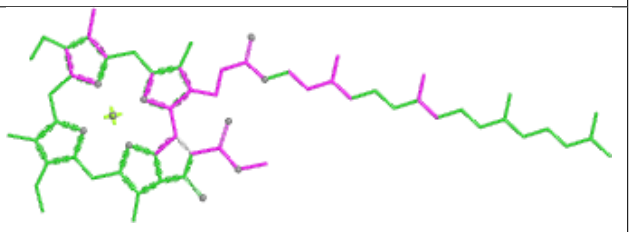
Torsions

Rings

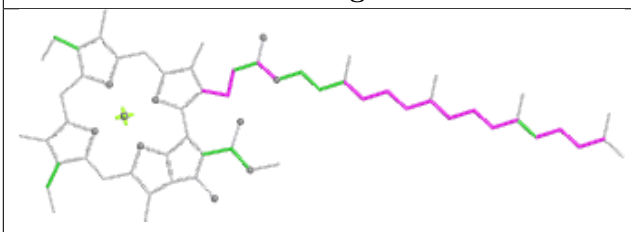
Ligand CLA B 611



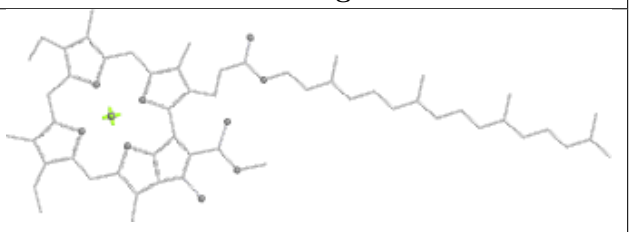
Bond lengths



Bond angles

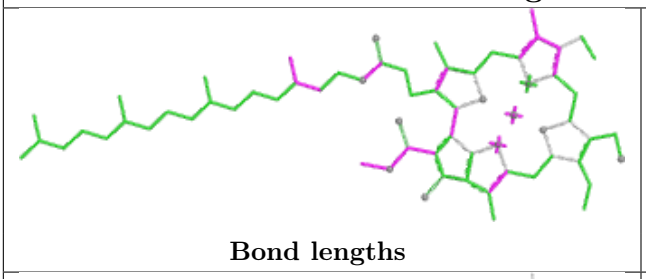


Torsions



Rings

Ligand CHL E 608



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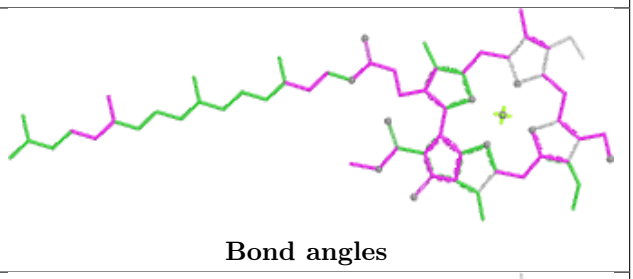
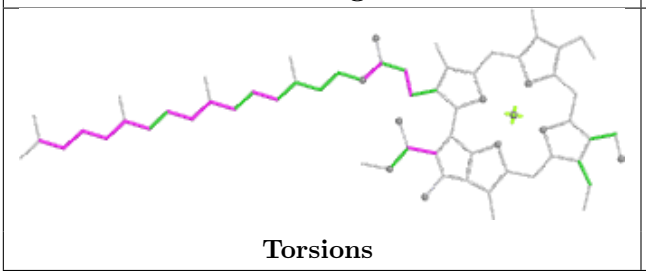


Bond angles



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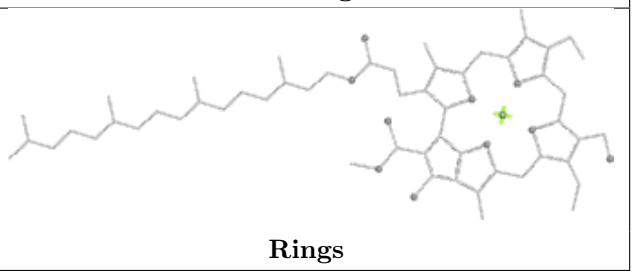
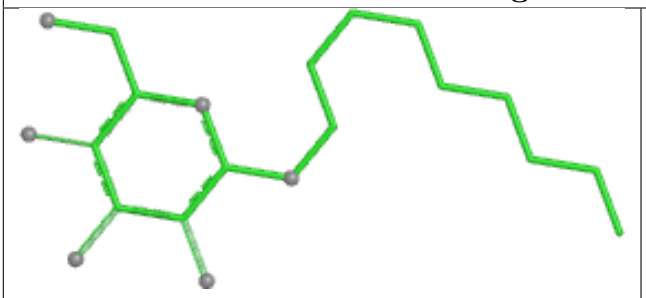


Rings

Ligand BNG D 3633



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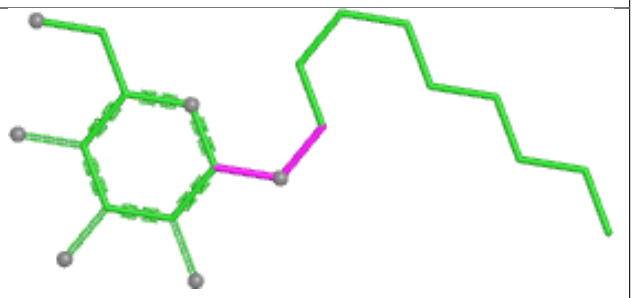
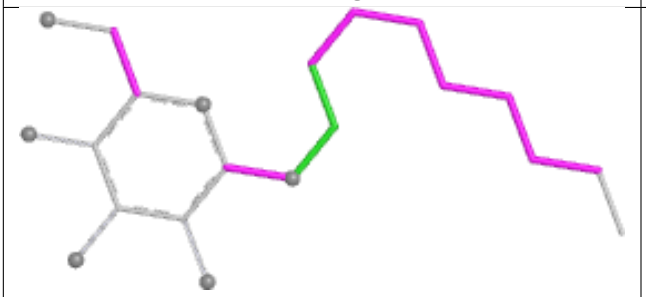


Bond angles



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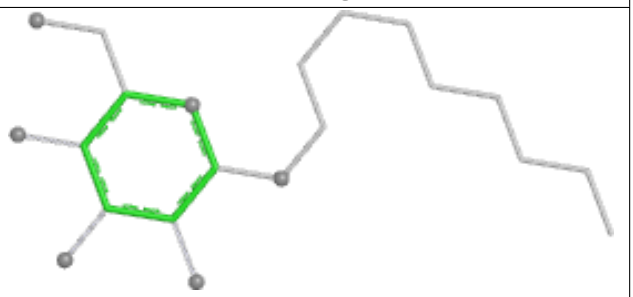
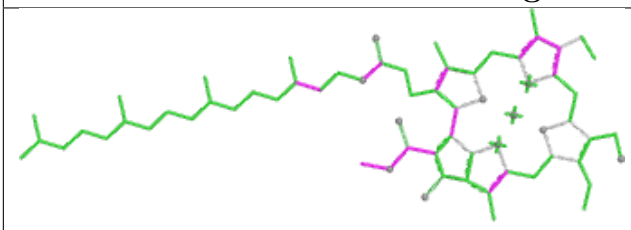


Rings

Ligand CHL A 601



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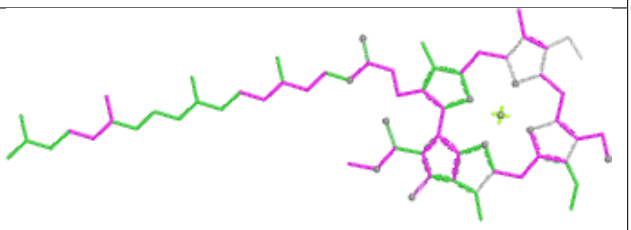
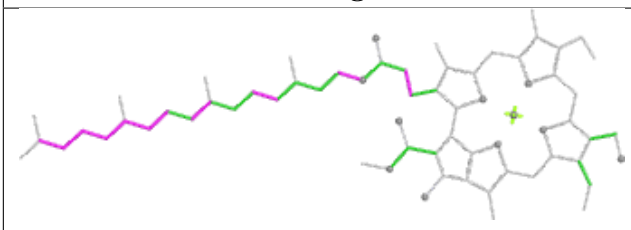


Bond angles



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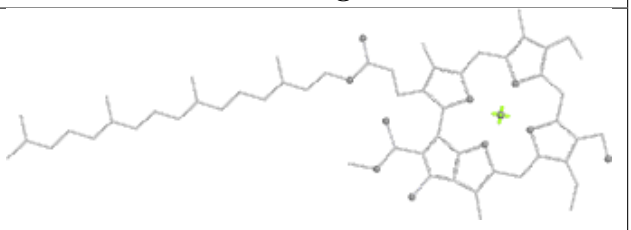
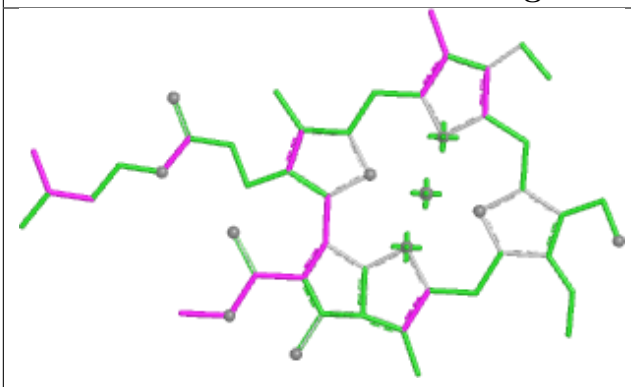
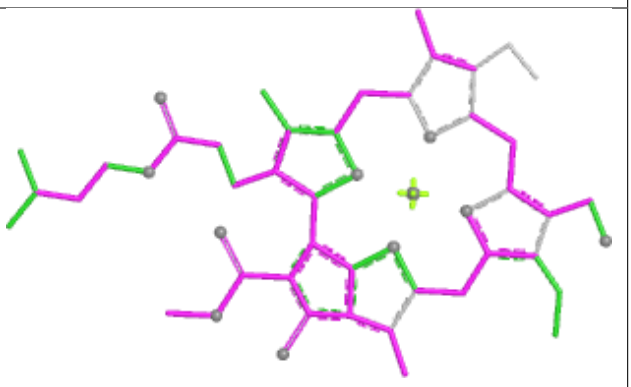


Rings

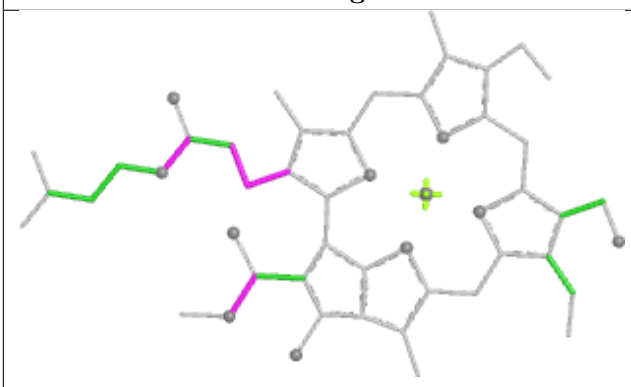
Ligand CHL B 606



Bond lengths



Bond angles



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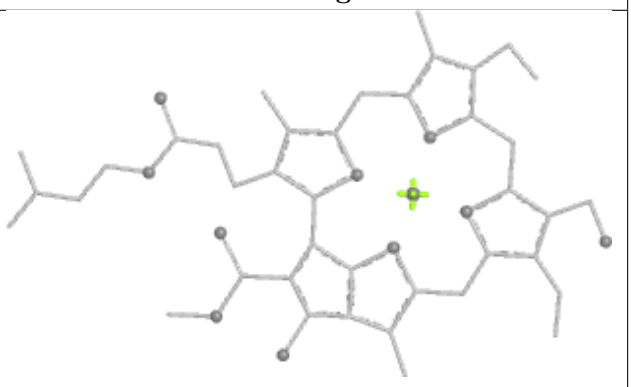
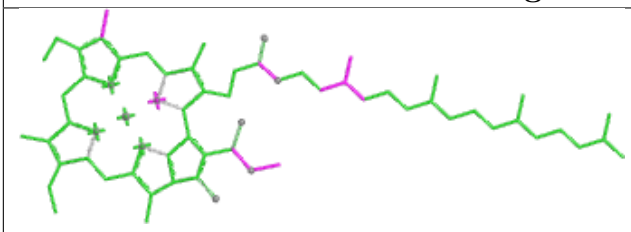


Rings

Ligand CLA B 613



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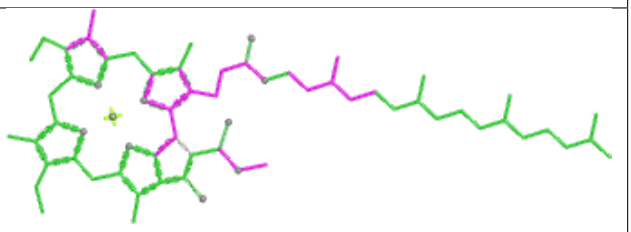
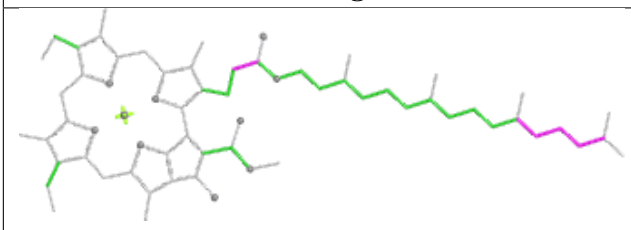


Bond angles



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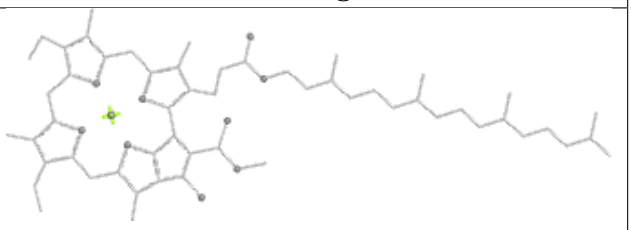
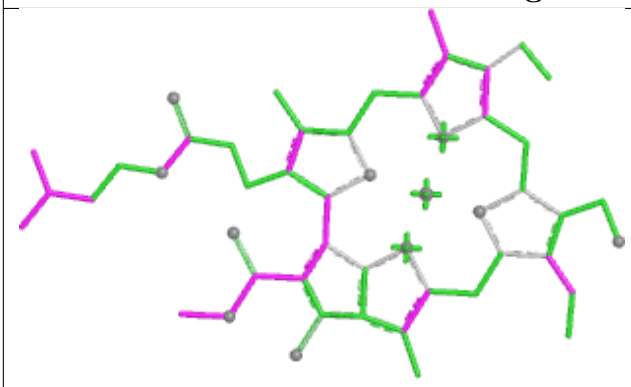


Rings

Ligand CHL E 606



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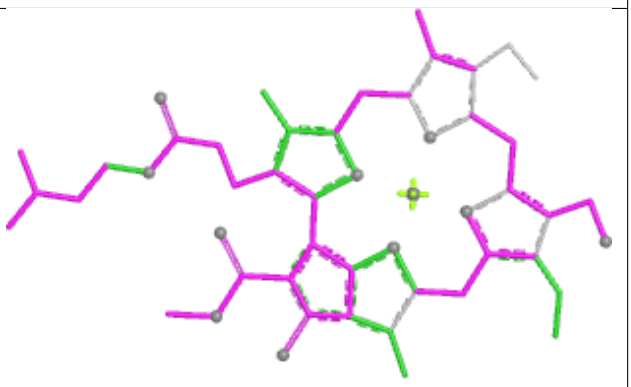
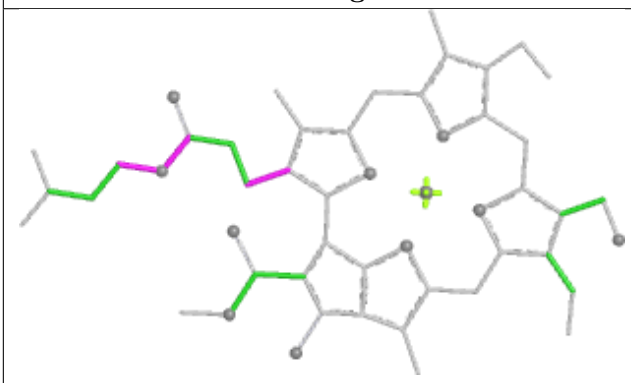


Bond angles



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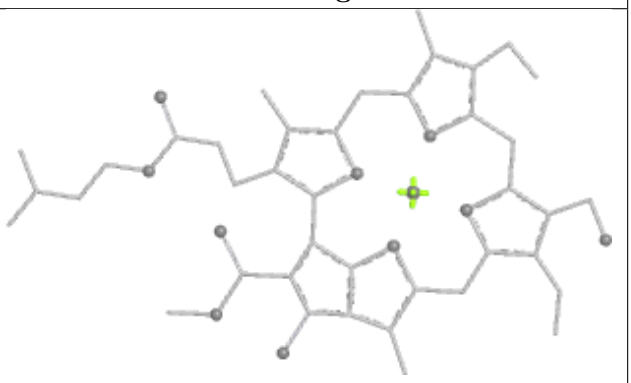
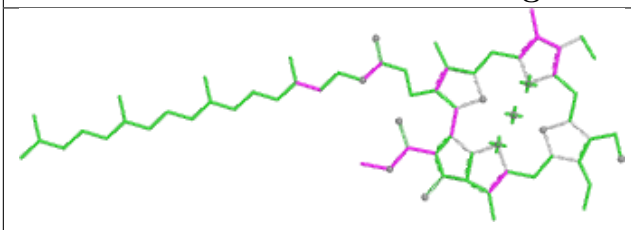


Rings

Ligand CHL H 609



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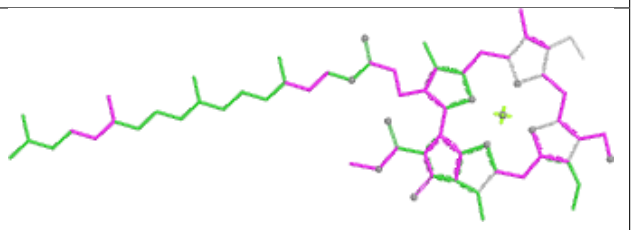
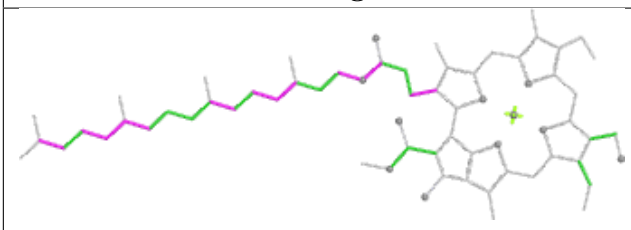


Bond angles



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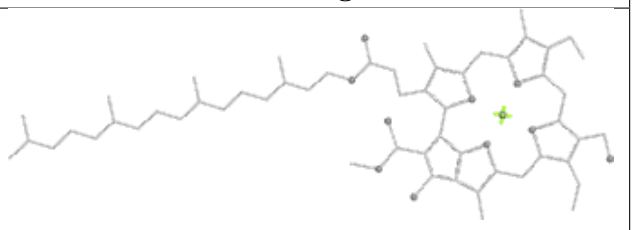
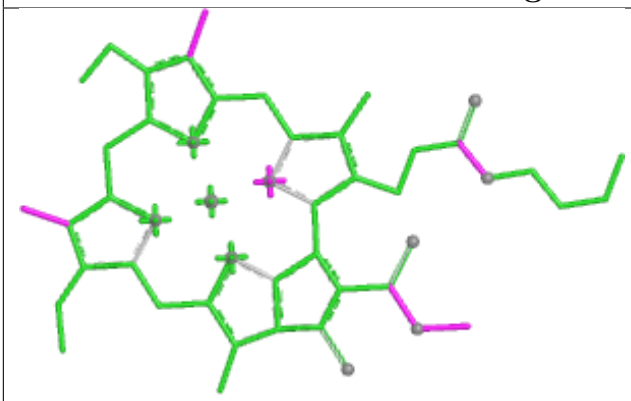
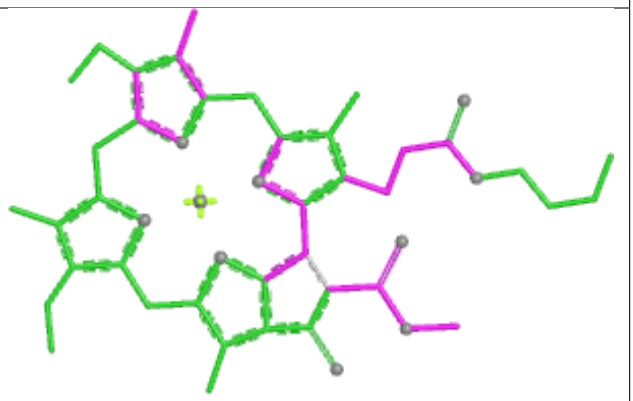


Rings

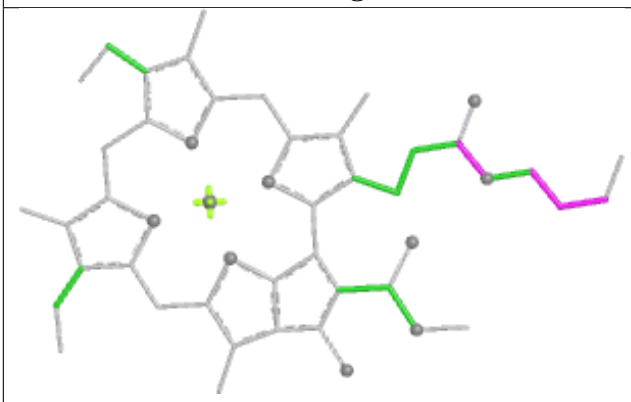
Ligand CLA B 614



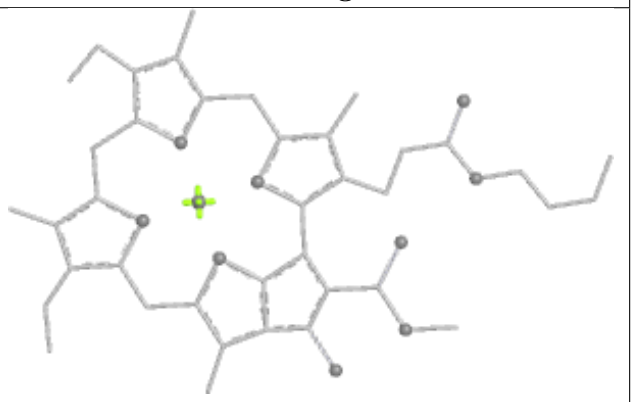
Bond lengths



Bond angles

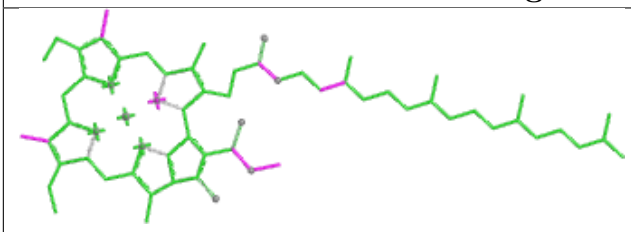


Torsions



Rings

Ligand CLA E 613



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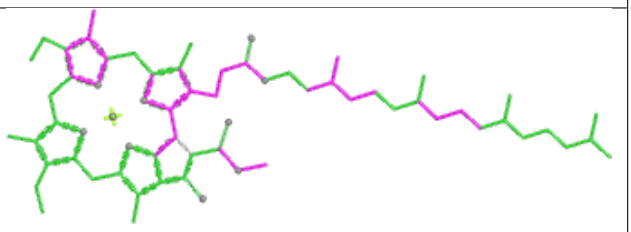
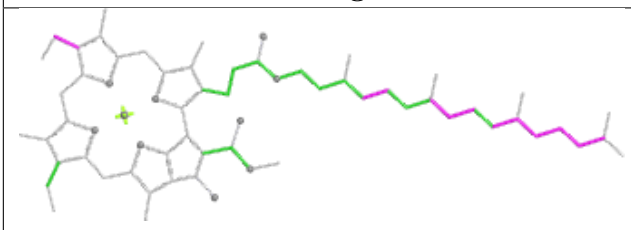


Bond angles



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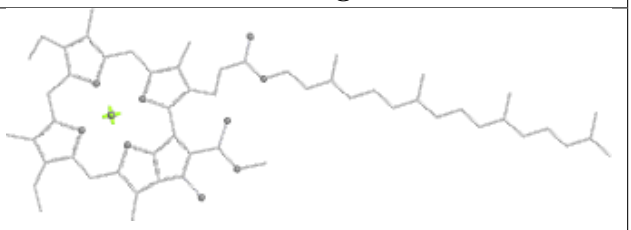
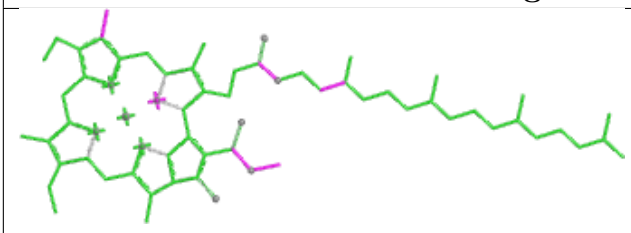


Rings

Ligand CLA A 611



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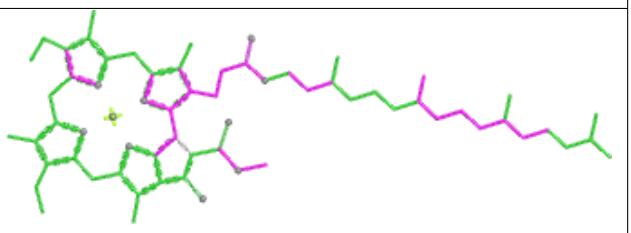
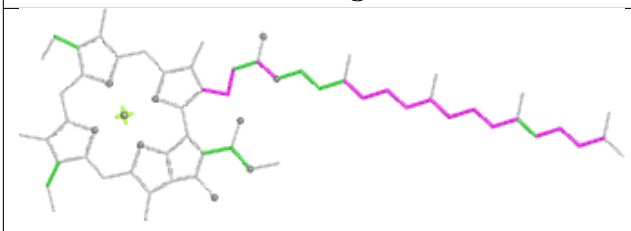
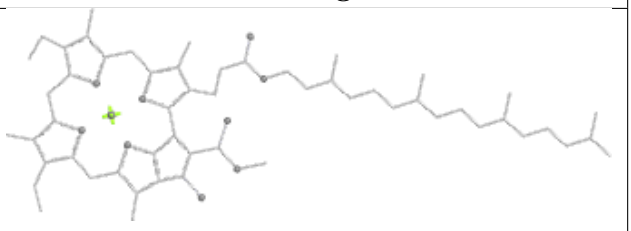


Bond angles

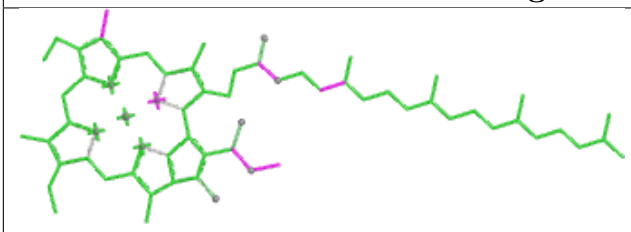


Torsions



Rings

Ligand CLA J 611



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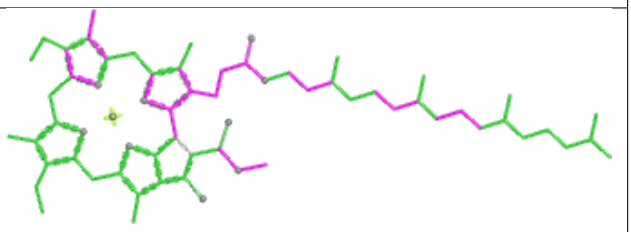
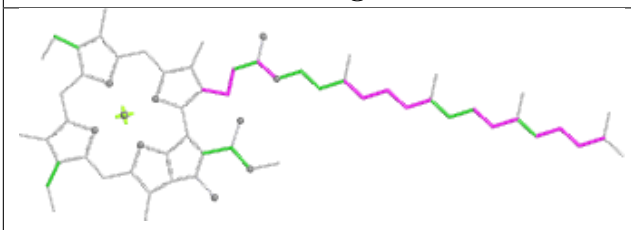
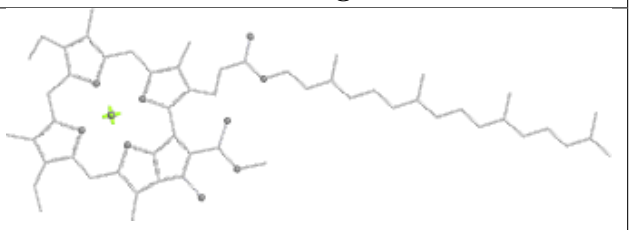


Bond angles

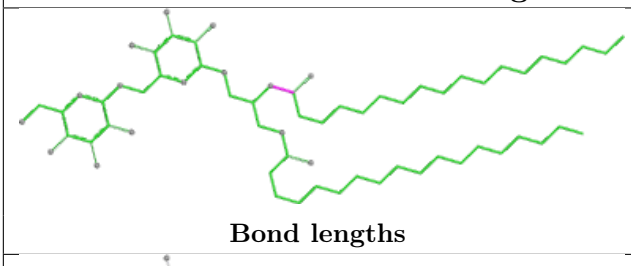


Torsions

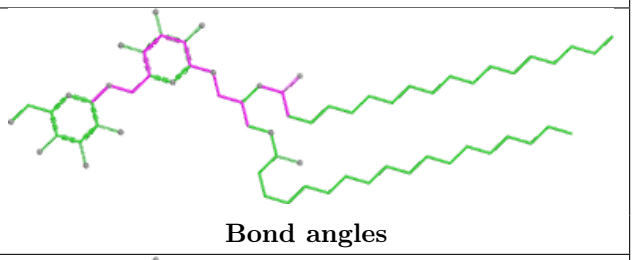


Rings

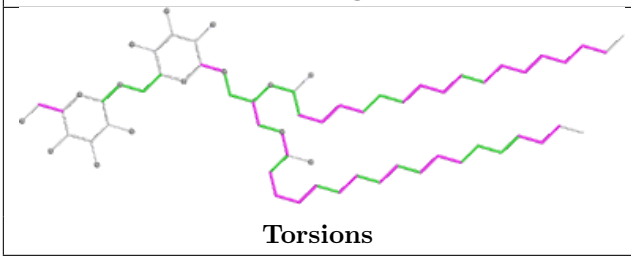
Ligand DGD D 5632



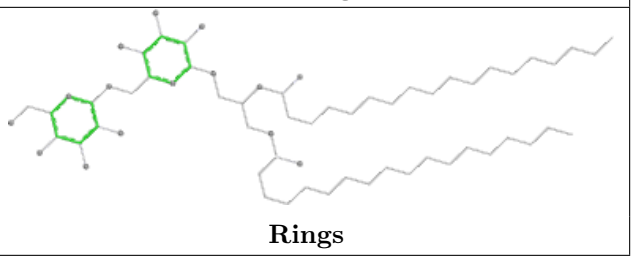
Bond lengths



Bond angles

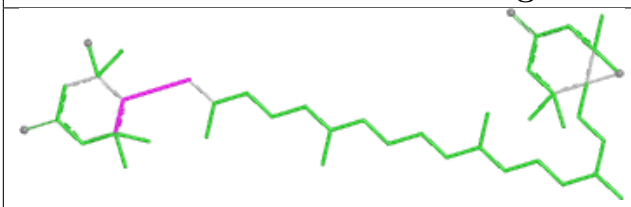


Torsions

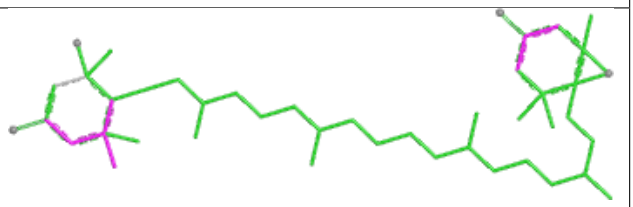


Rings

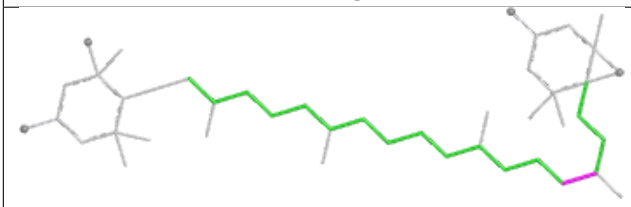
Ligand NEX J 9623



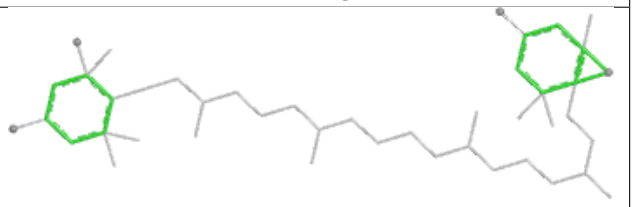
Bond lengths



Bond angles

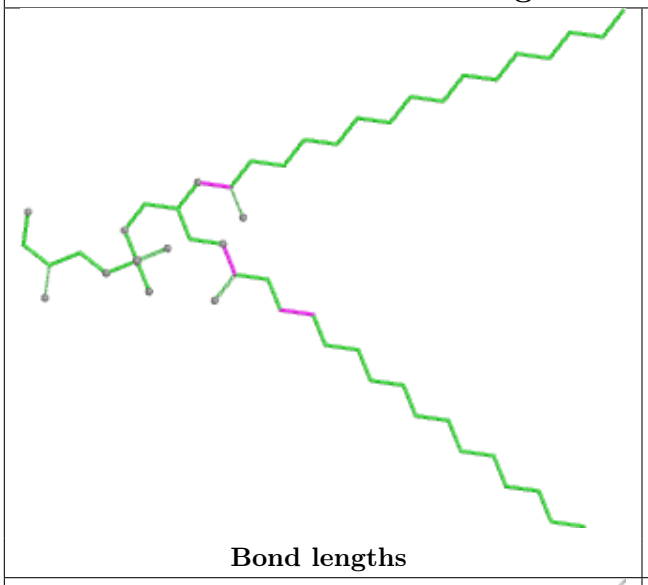


Torsions

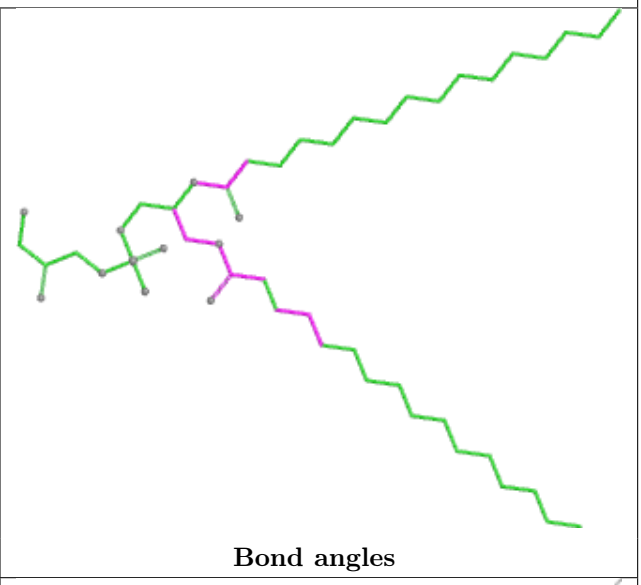


Rings

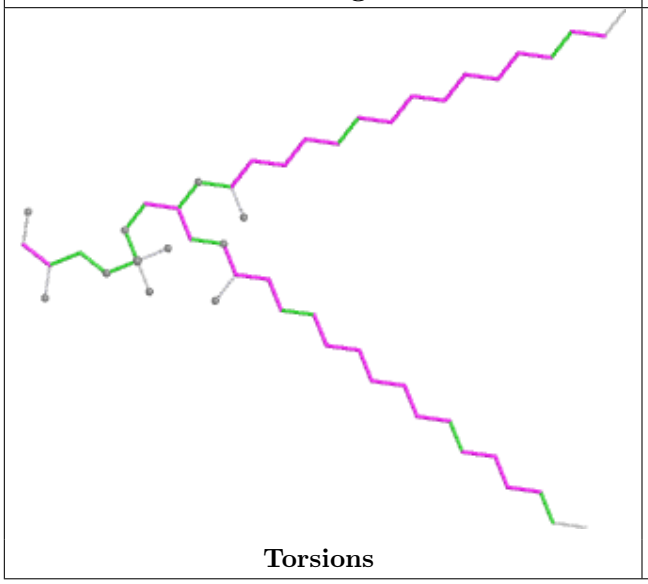
Ligand LHG C 2630



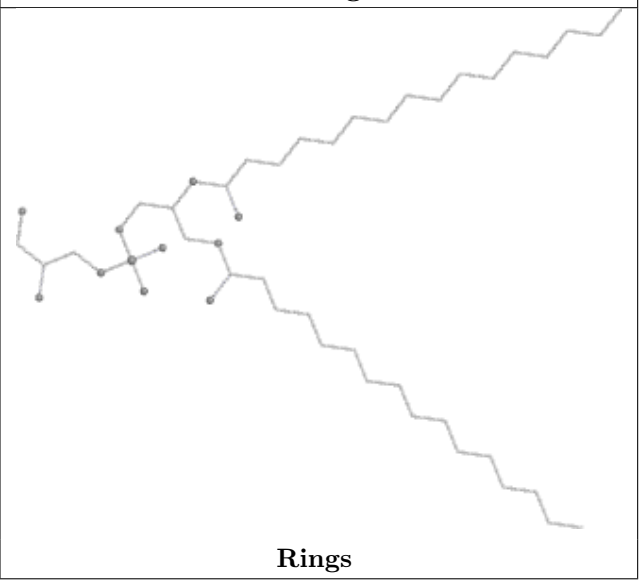
Bond lengths



Bond angles

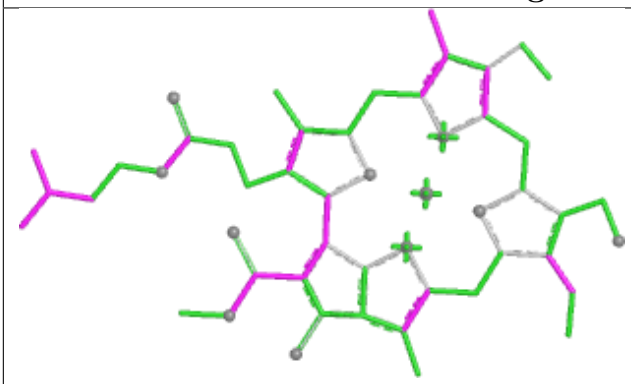


Torsions



Rings

Ligand CHL J 606



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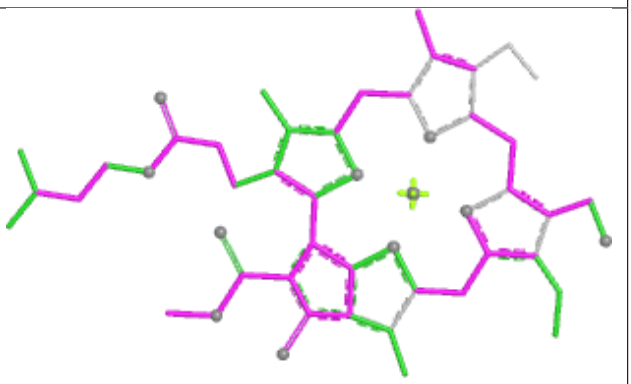
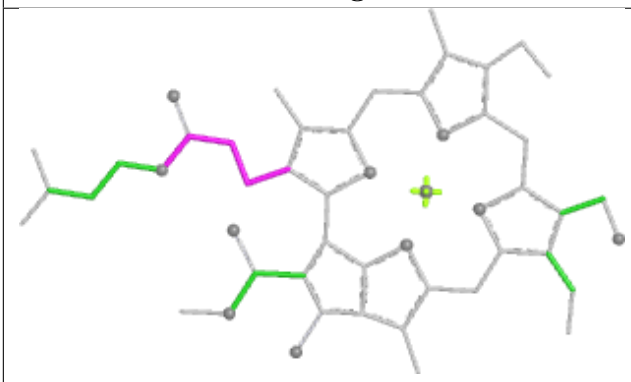


Bond angles



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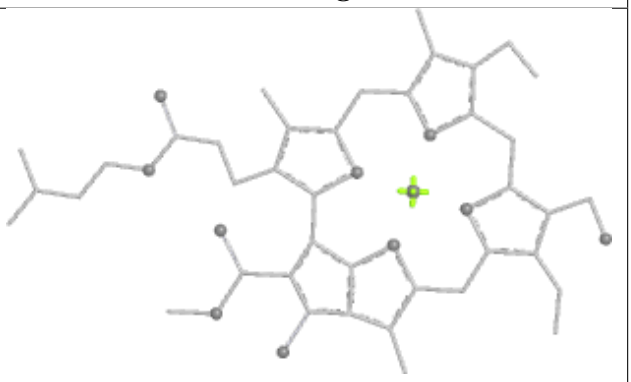
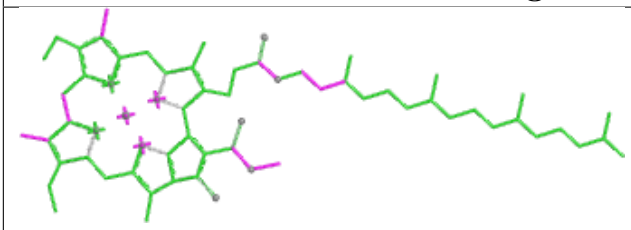


Rings

Ligand CLA F 602



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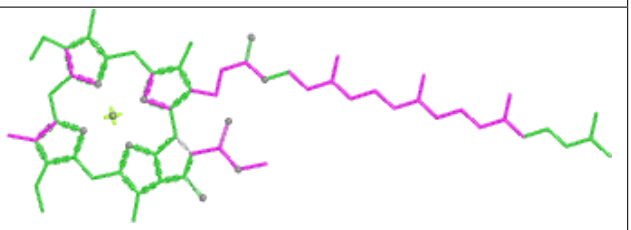
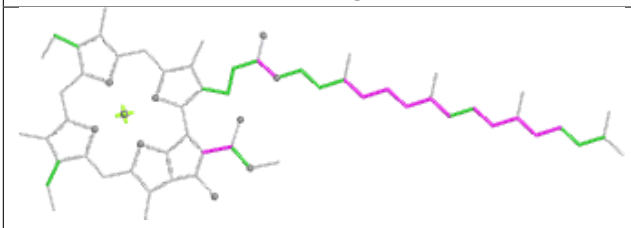


Bond angles



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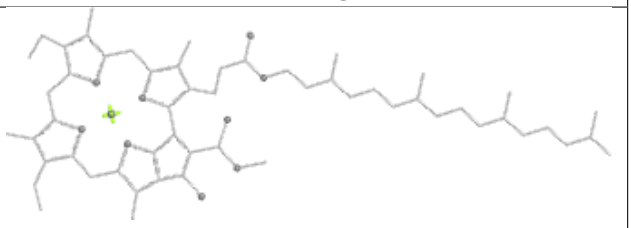
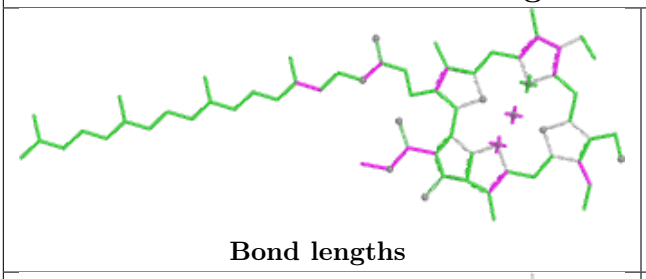


Rings

Ligand CHL B 608



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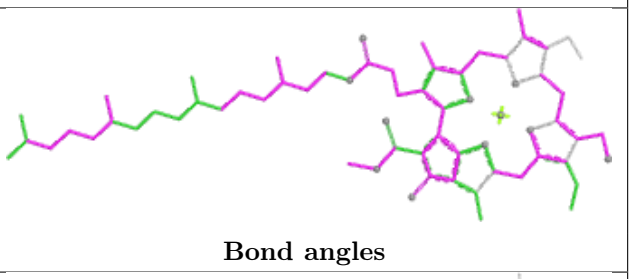
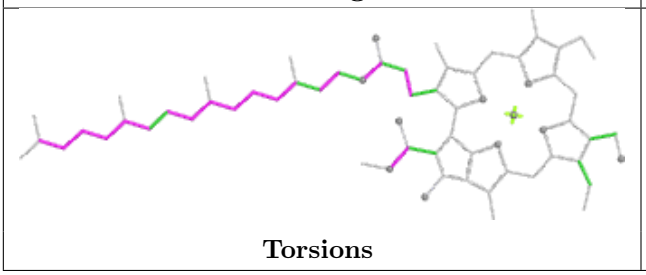


Bond angles



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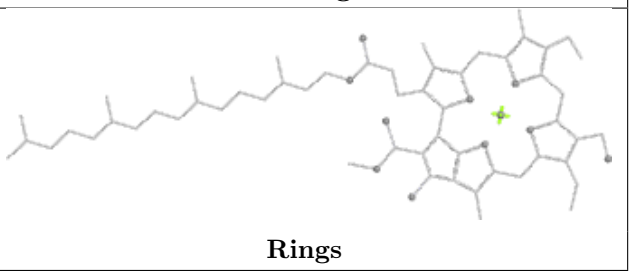
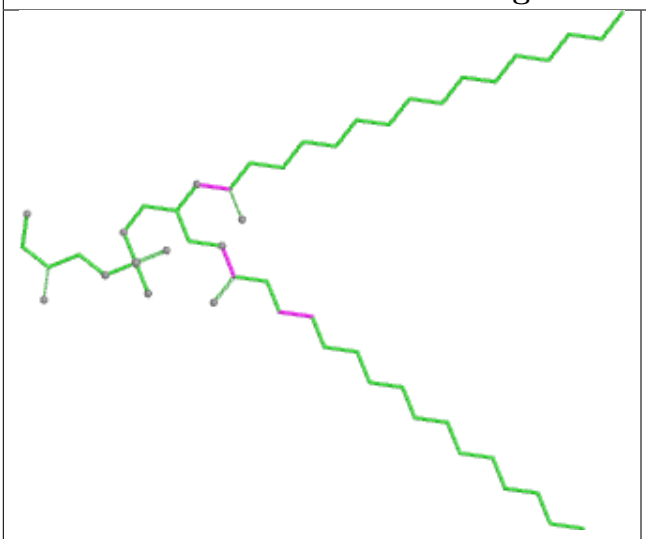


Rings

Ligand LHG H 7630



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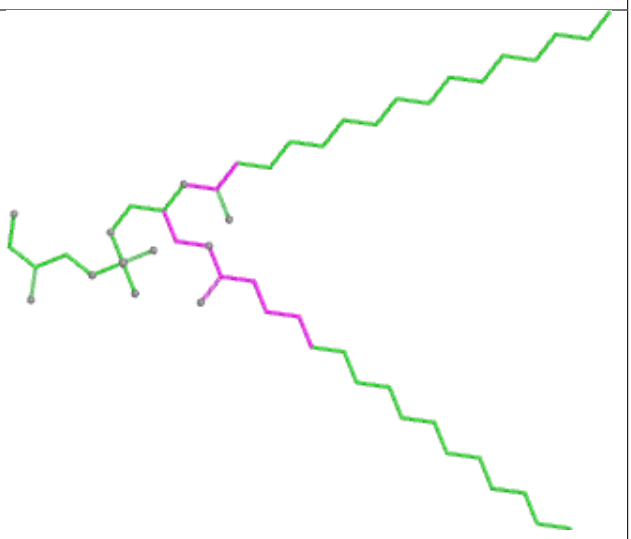

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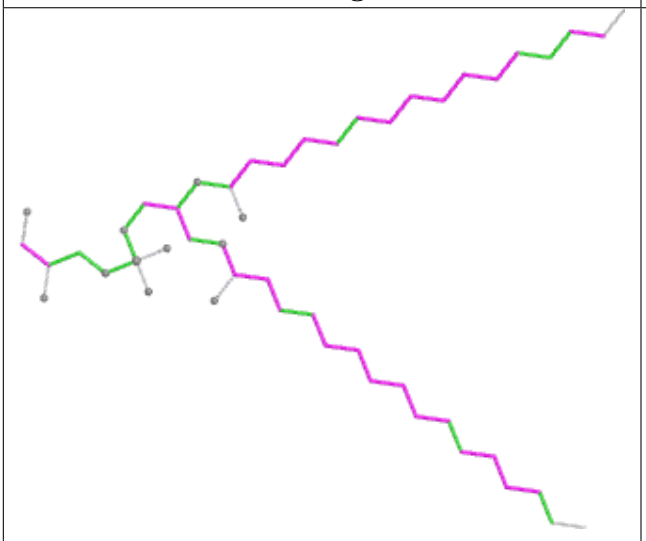

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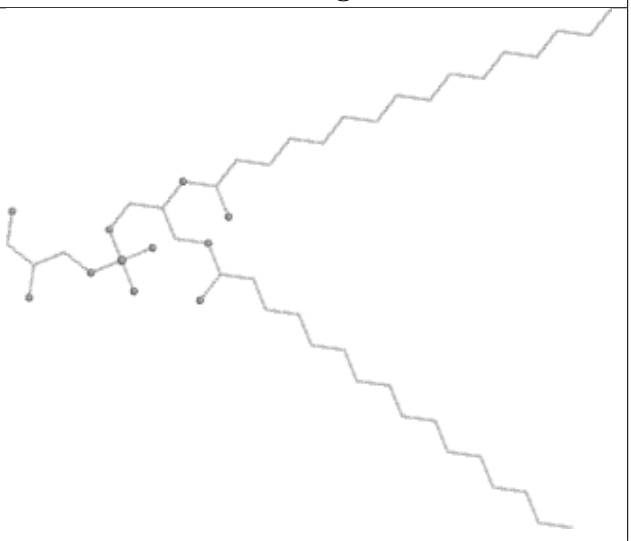
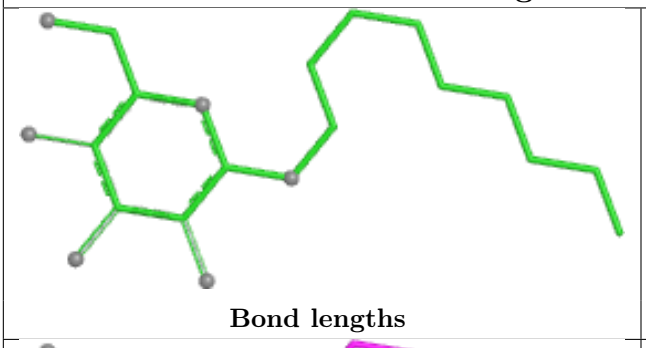


Rings

Ligand BNG J 9633



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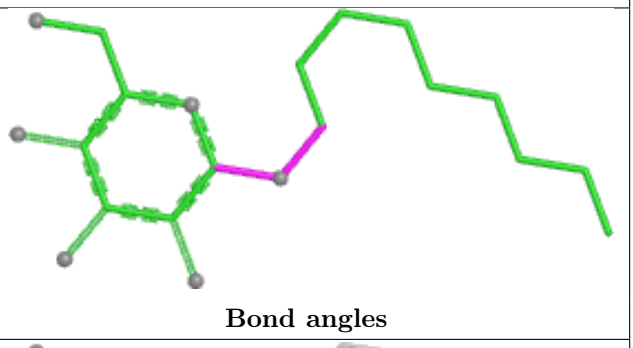
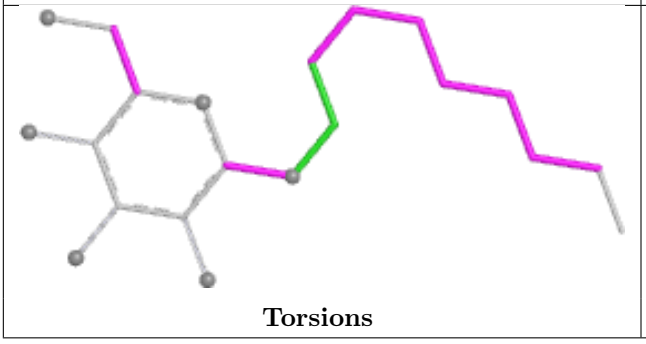


Bond angles



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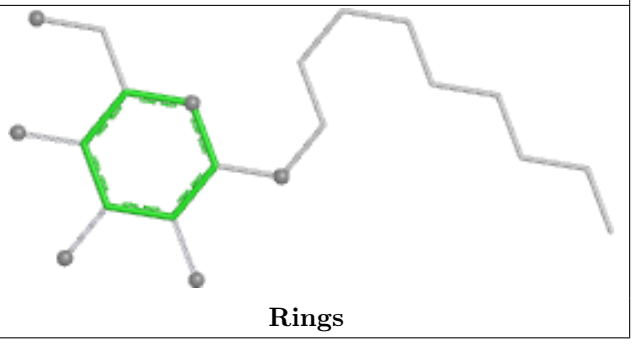
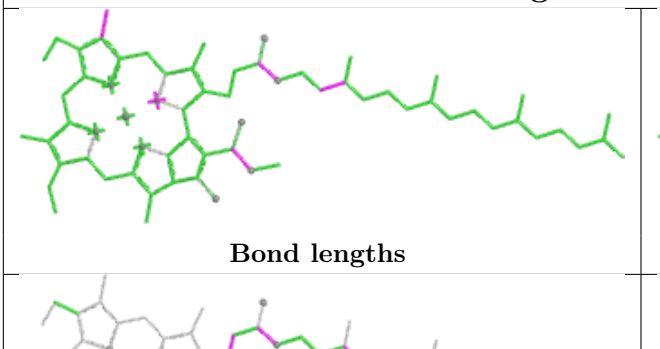


Rings

Ligand CLA I 611



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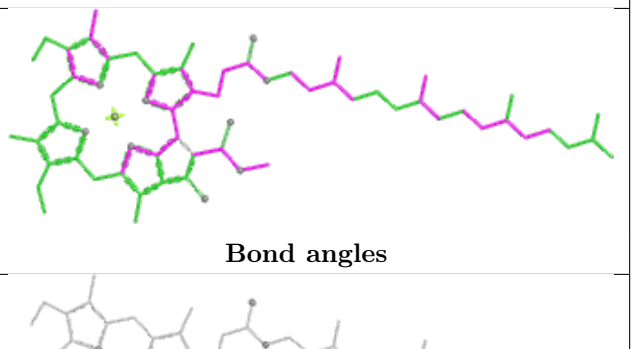

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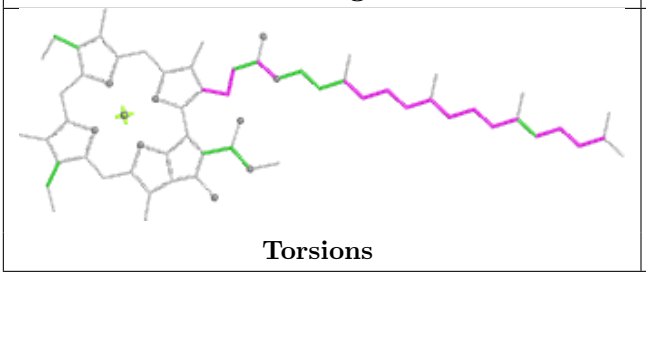

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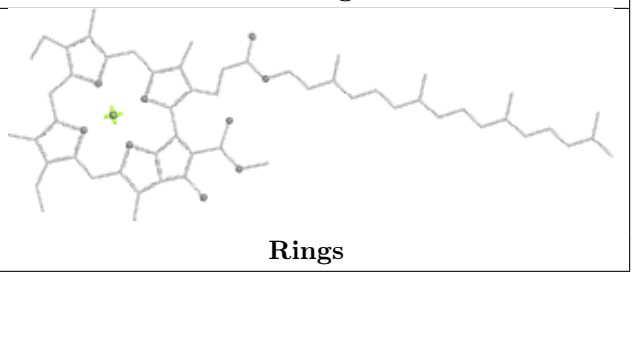
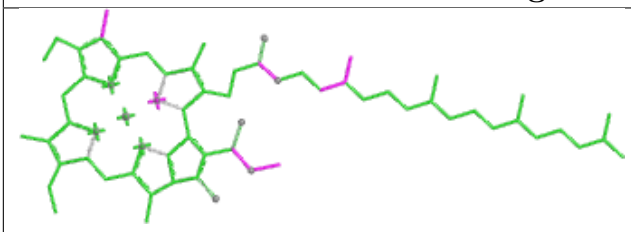


Rings

Ligand CLA J 612



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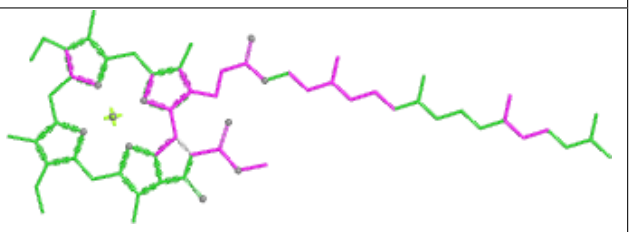

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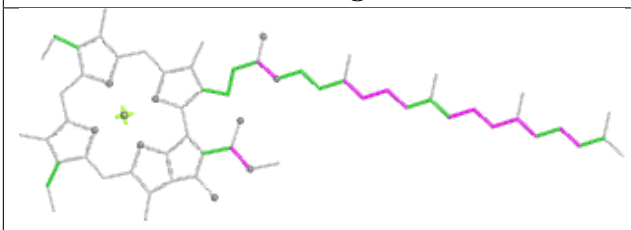

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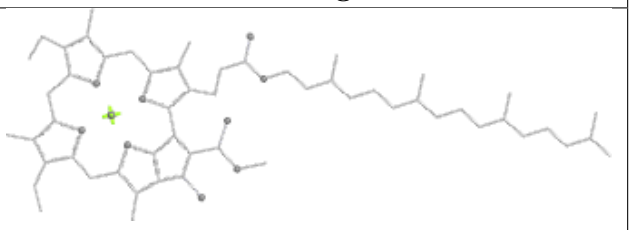
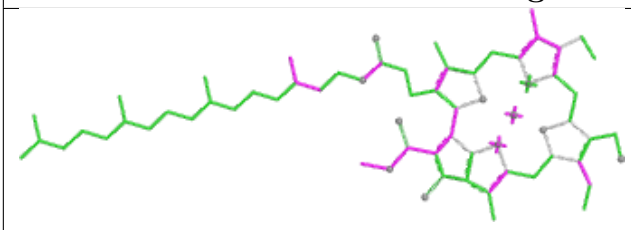


Rings

Ligand CHL J 608



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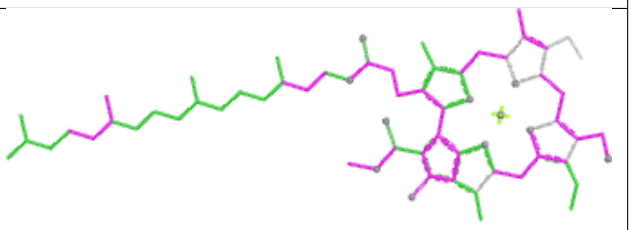
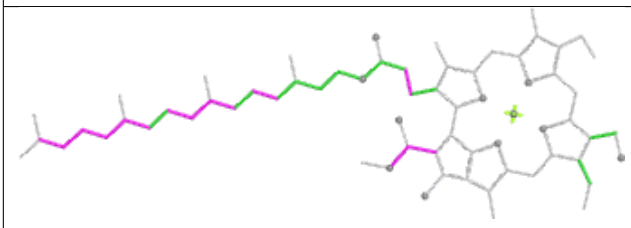


Bond angles



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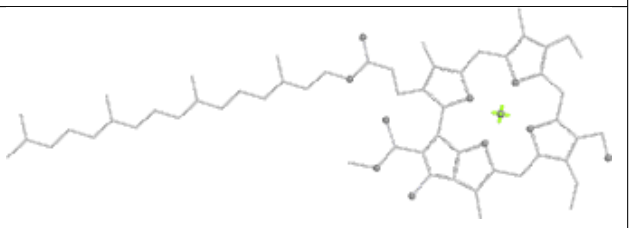
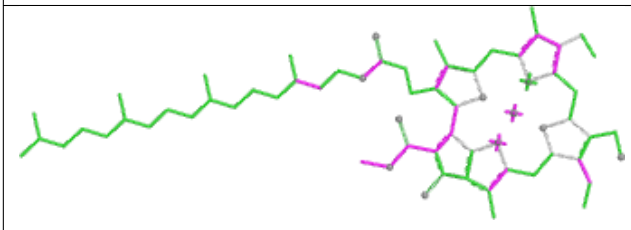


Rings

Ligand CHL A 608



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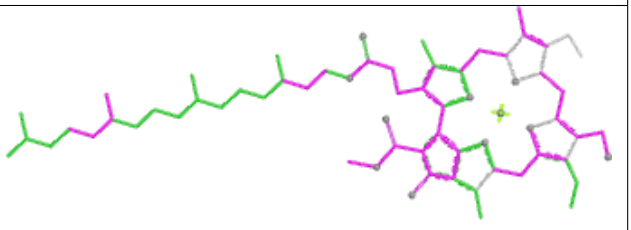

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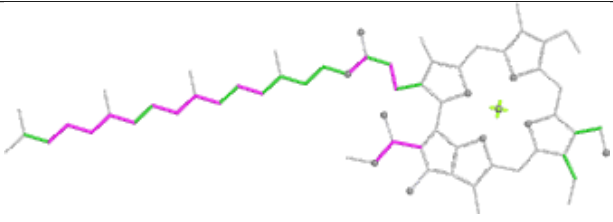

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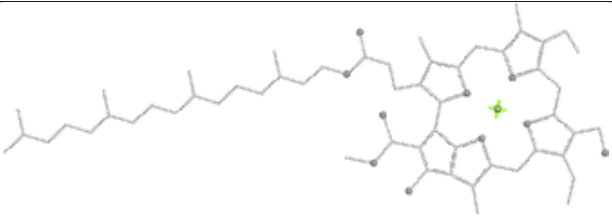
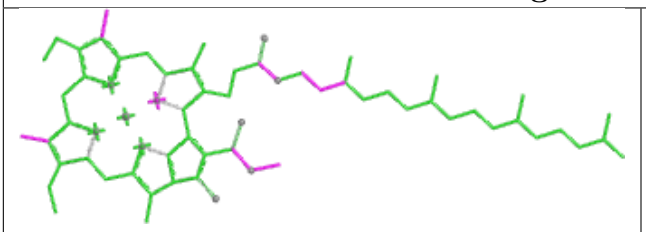


Rings

Ligand CLA I 613



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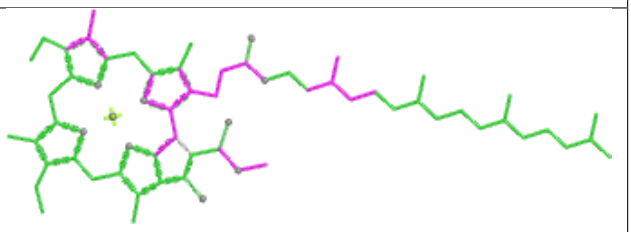

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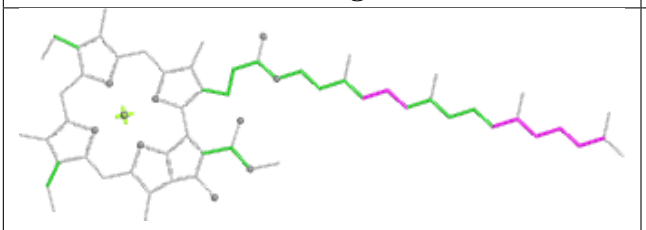

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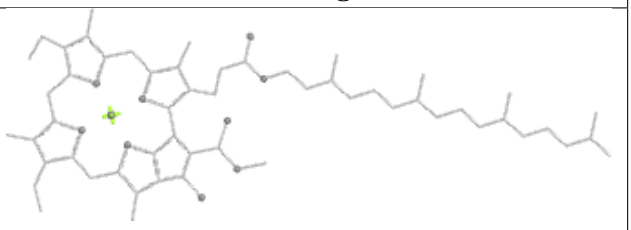
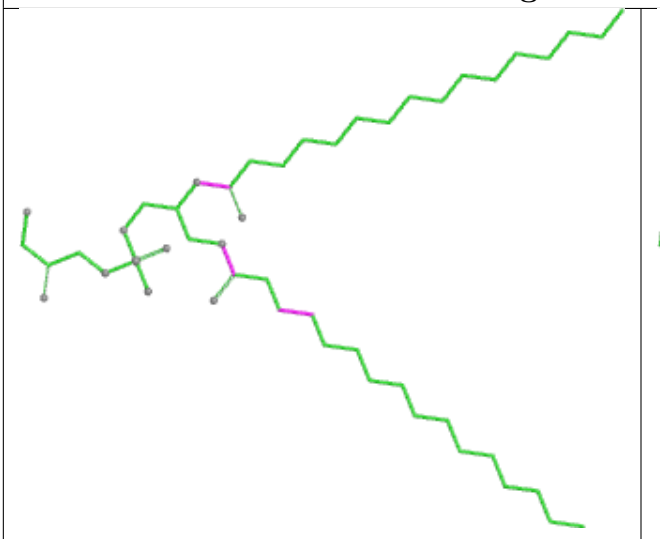


Rings

Ligand LHG I 8630



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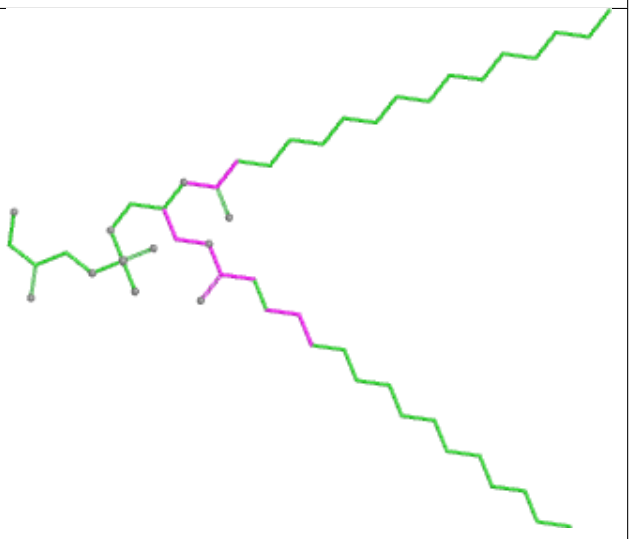
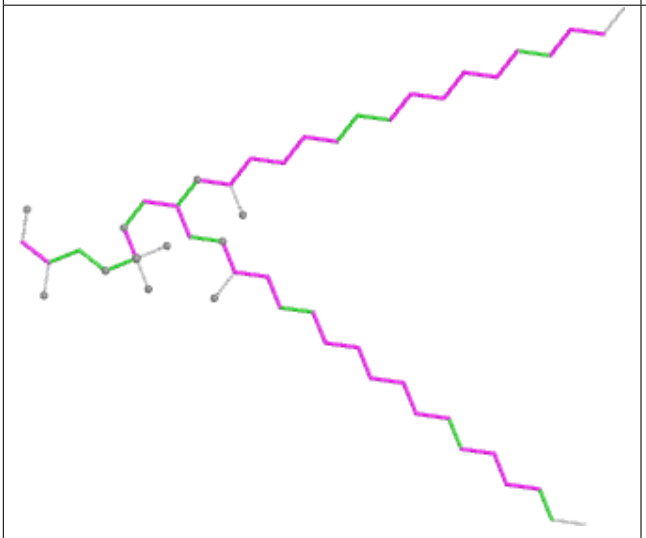
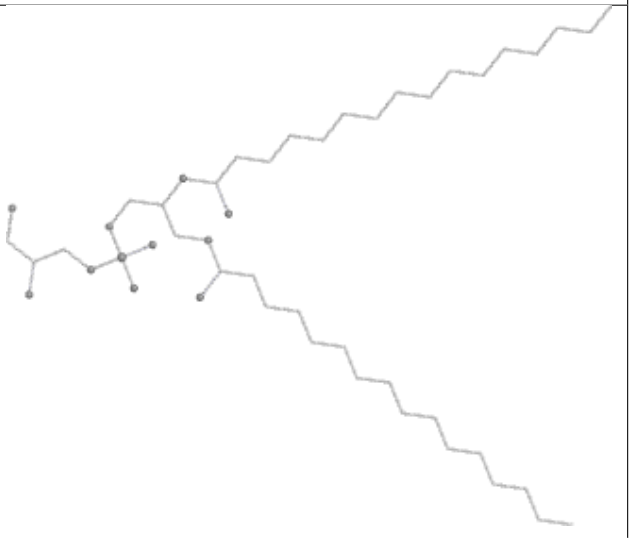


Bond angles

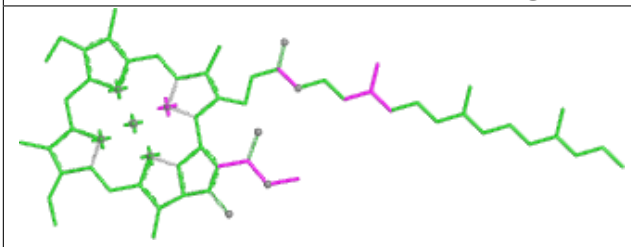


Torsions



Rings

Ligand CLA C 604



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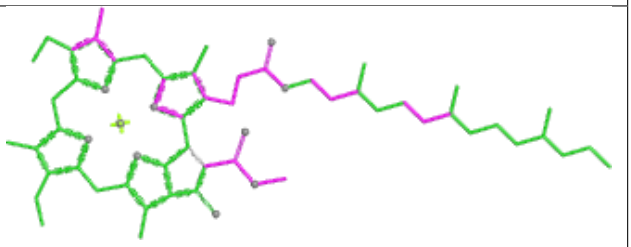
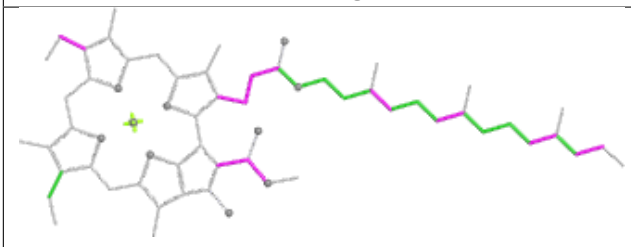
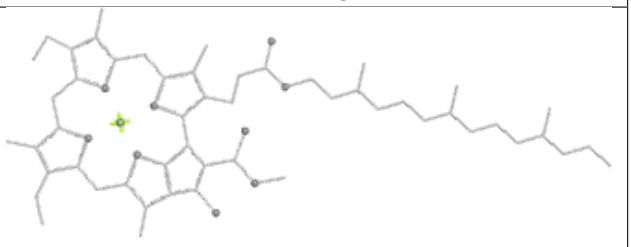


Bond angles

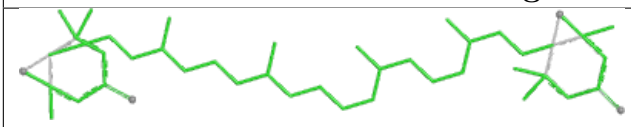


Torsions

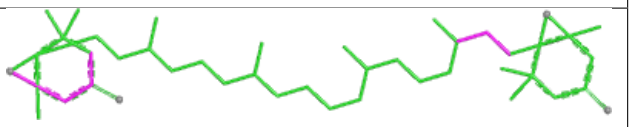


Rings

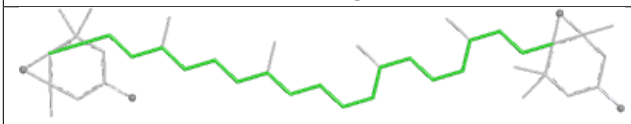
Ligand XAT A 622



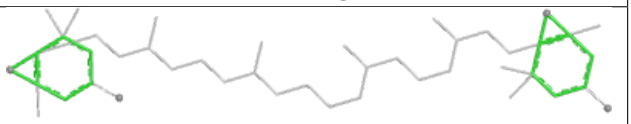
Bond lengths



Bond angles

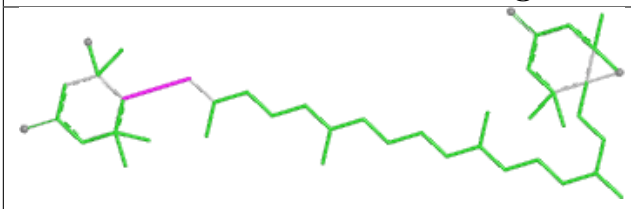


Torsions

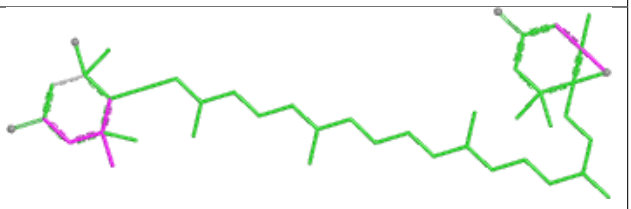


Rings

Ligand NEX E 4623

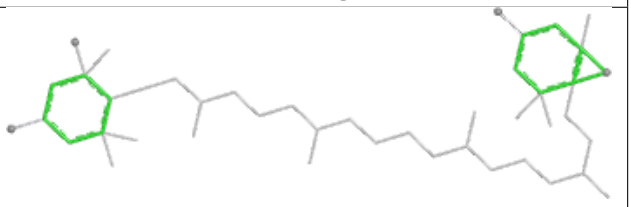


Bond lengths



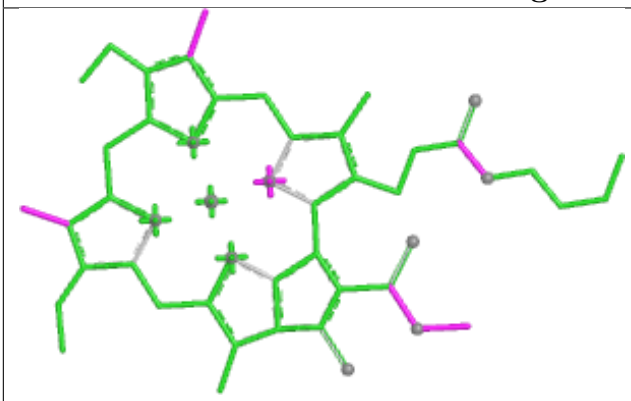
Bond angles

Torsions



Rings

Ligand CLA I 614



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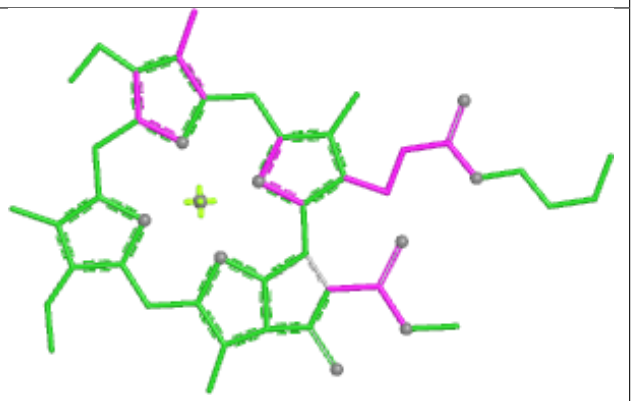
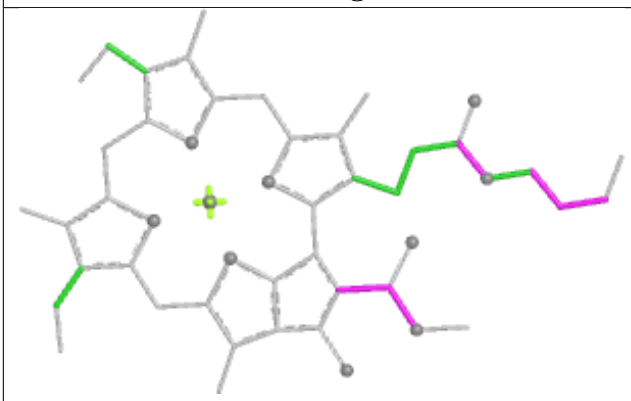


Bond angles



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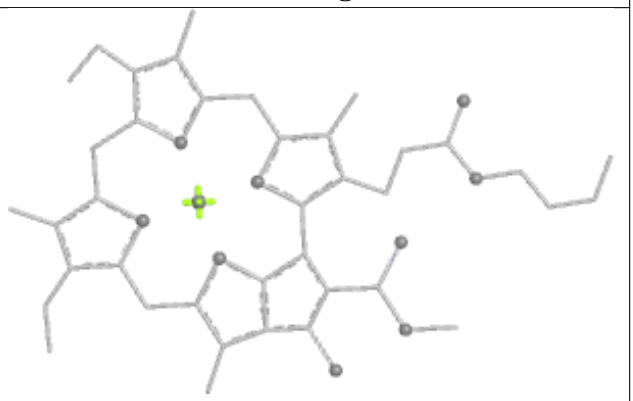
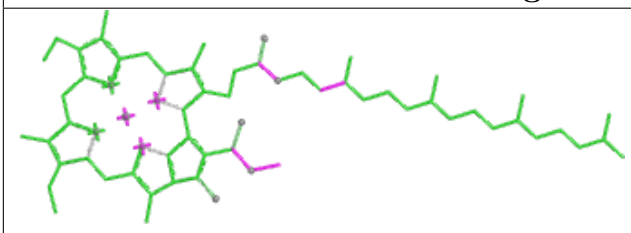


Rings

Ligand CLA D 603



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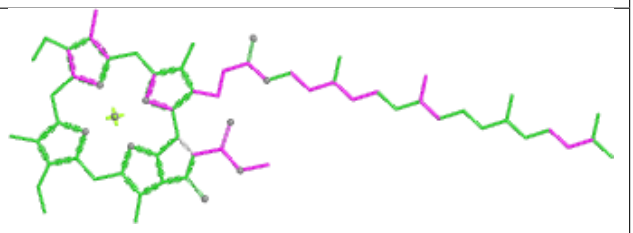
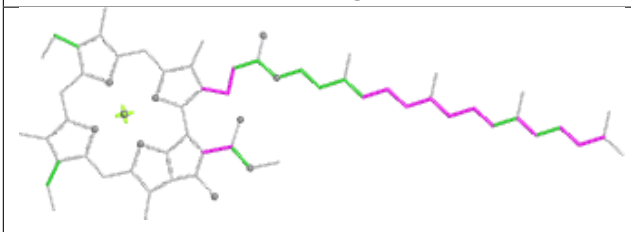


Bond angles



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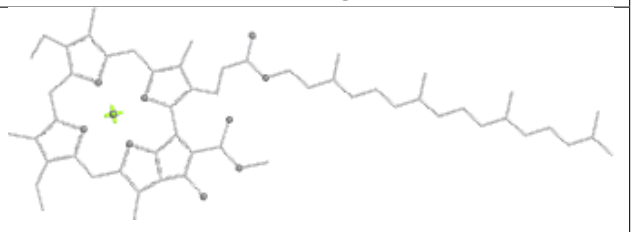
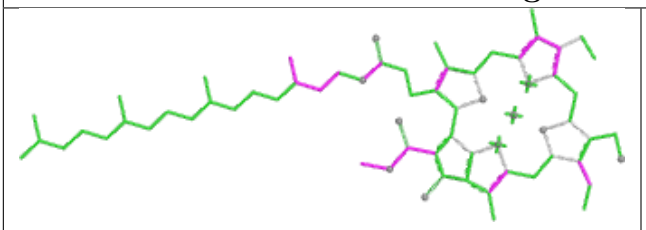


Rings

Ligand CHL A 609



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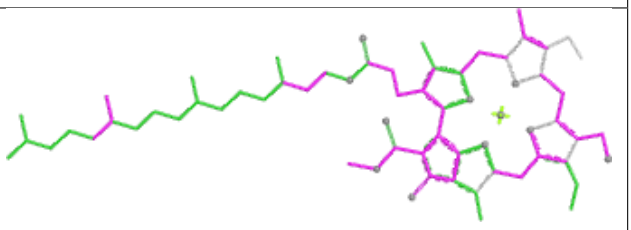
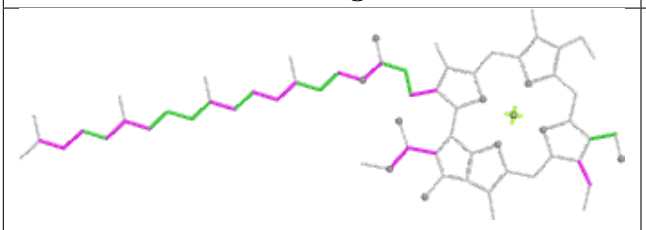


Bond angles



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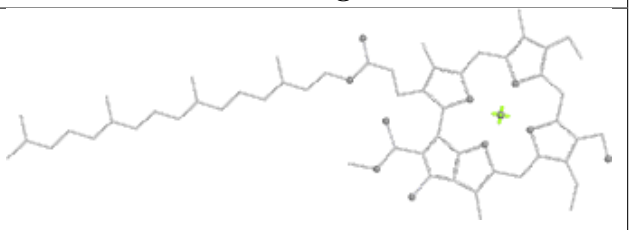
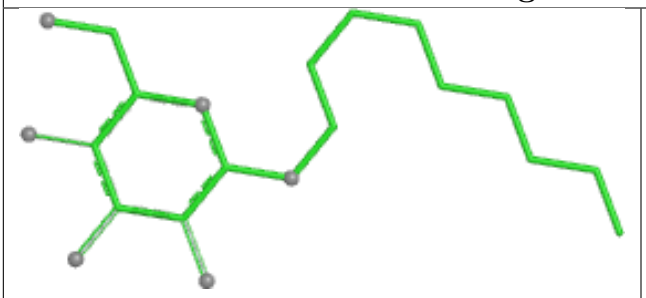


Rings

Ligand BNG I 8633



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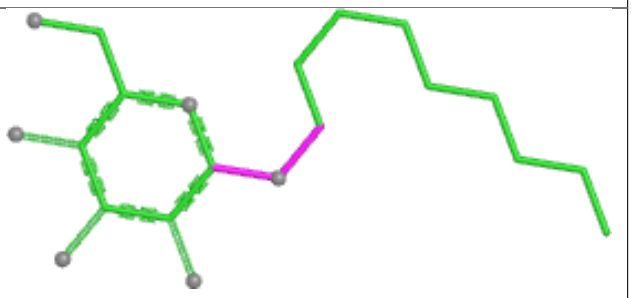
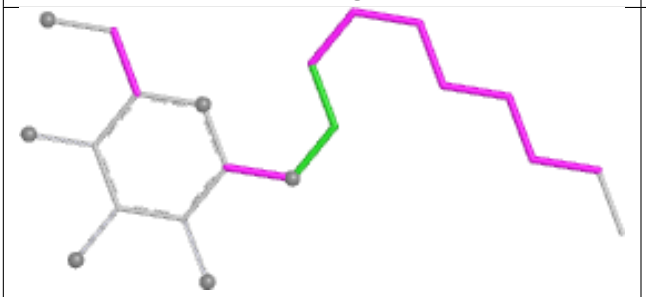


Bond angles



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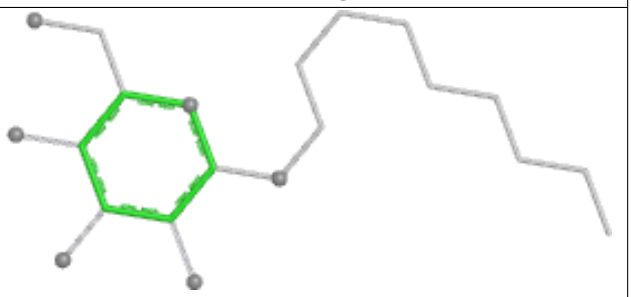
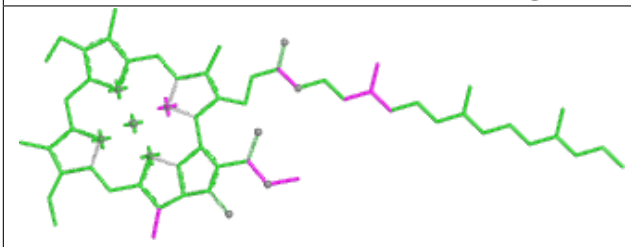


Rings

Ligand CLA F 604



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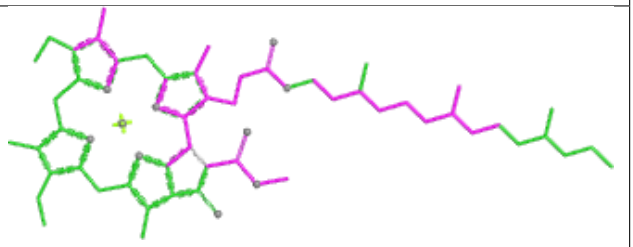
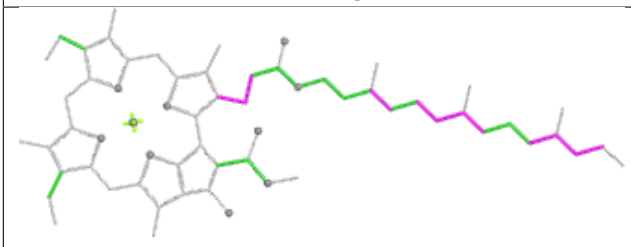


Bond angles



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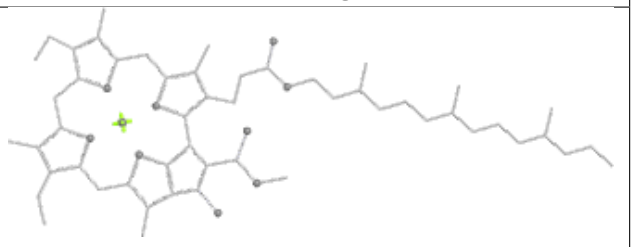
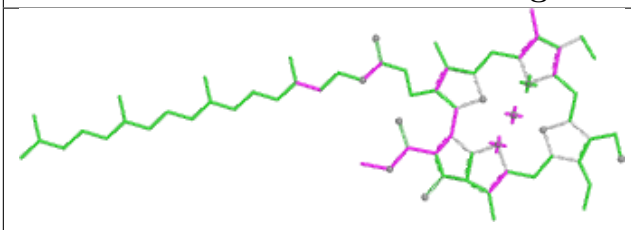


Rings

Ligand CHL I 607



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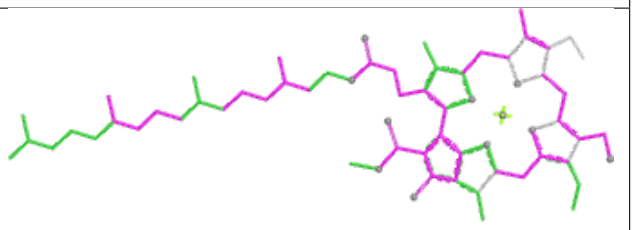
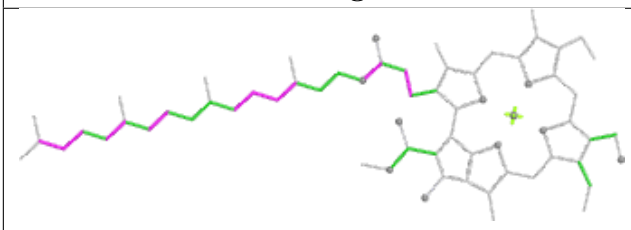


Bond angles



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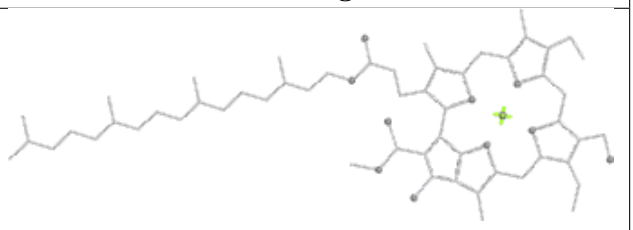
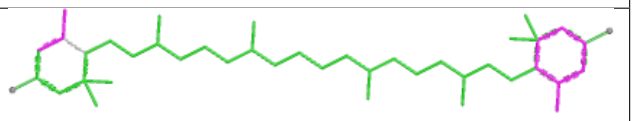


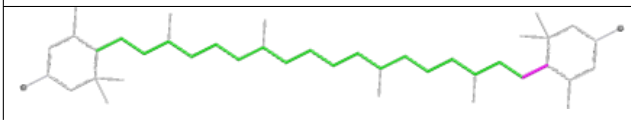
Rings

Ligand LUT C 2621

Bond lengths



Bond angles



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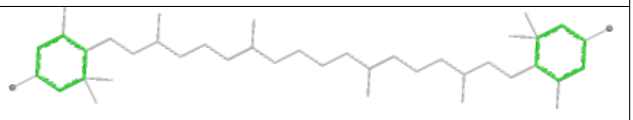
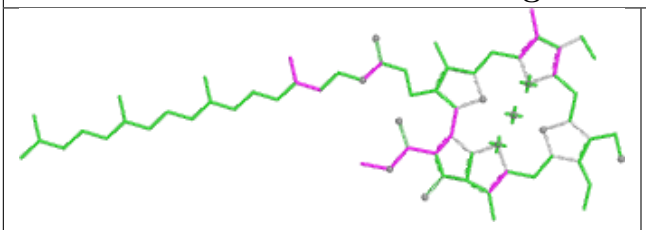


Rings

Ligand CHL D 607



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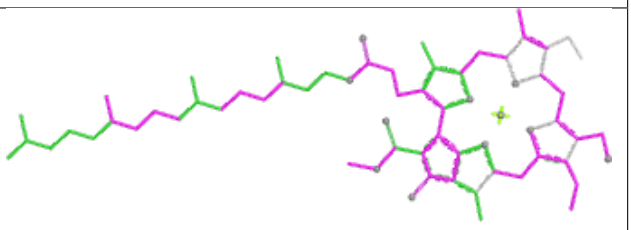
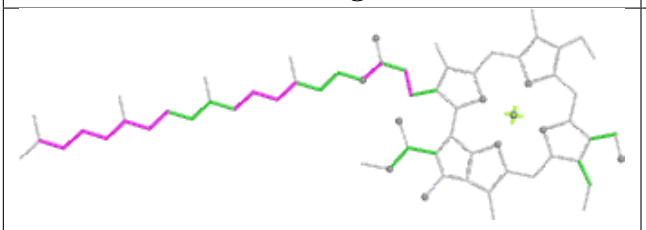


Bond angles



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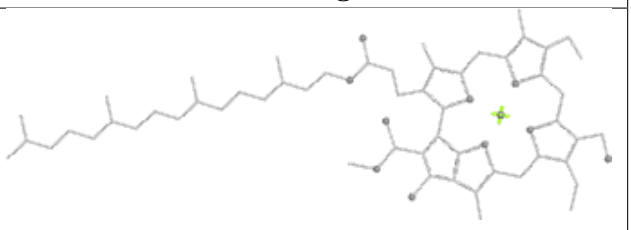
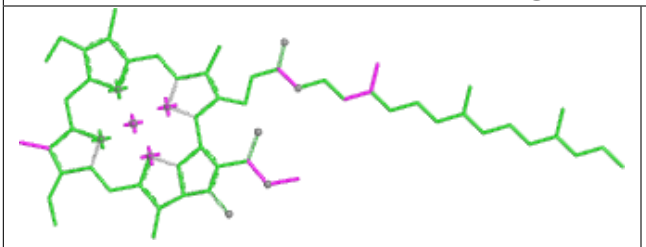


Rings

Ligand CLA J 604



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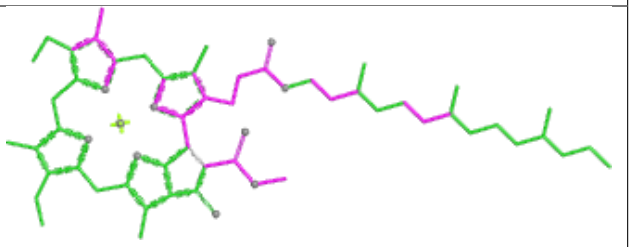

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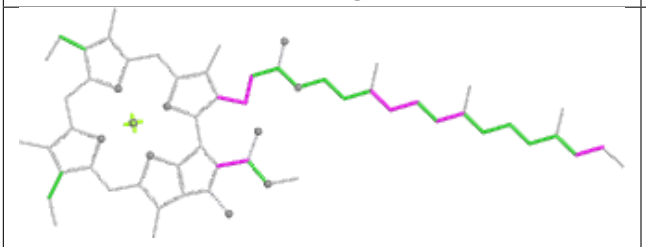

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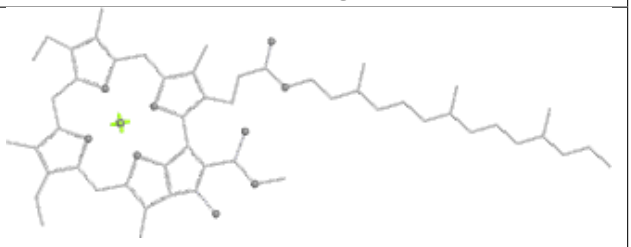
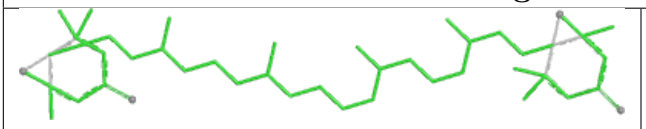


Rings

Ligand XAT H 4622



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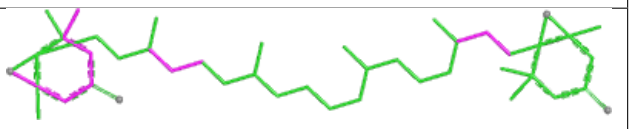
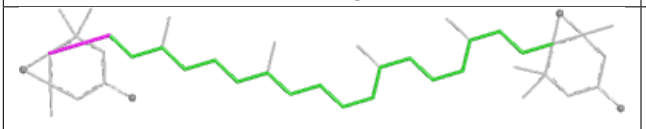


Bond angles



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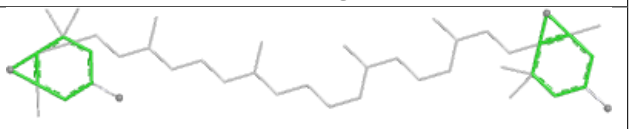
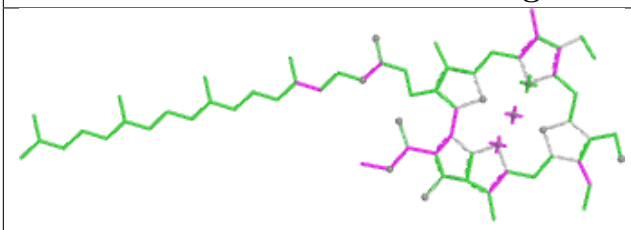


Rings

Ligand CHL H 607



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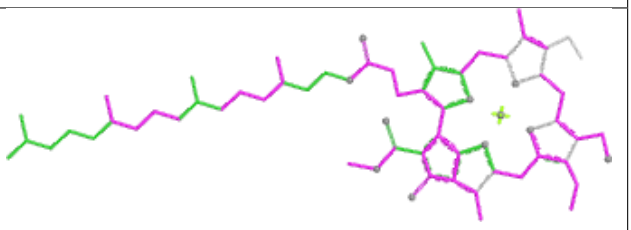
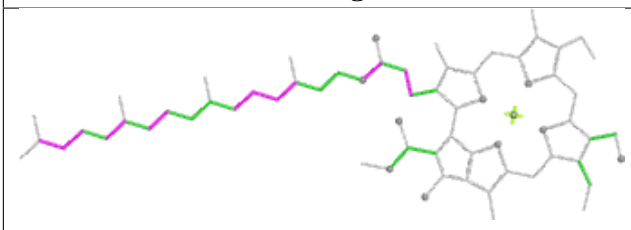


Bond angles



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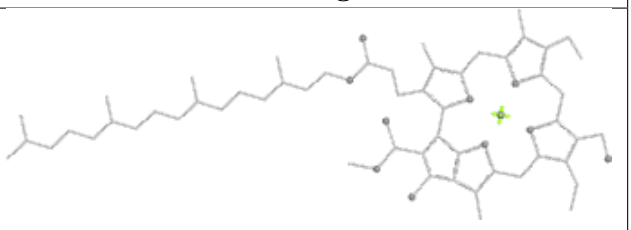
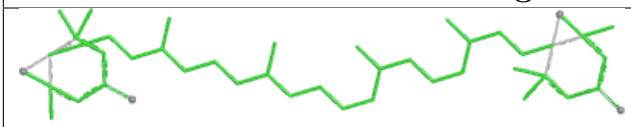


Rings

Ligand XAT B 1622



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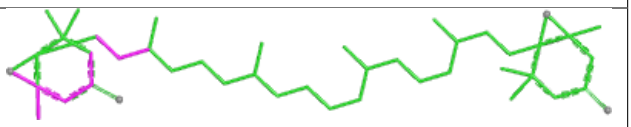
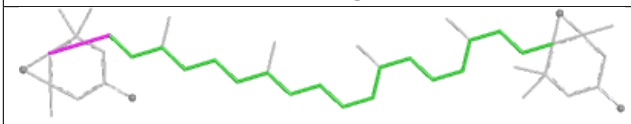
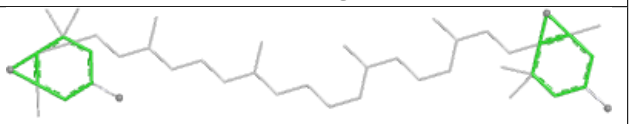


Bond angles

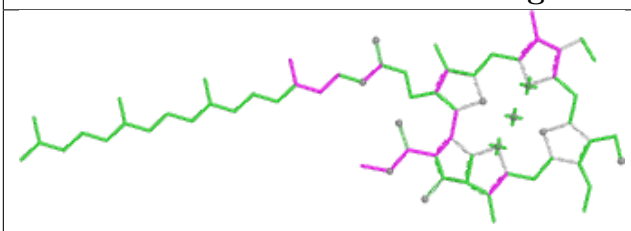


Torsions

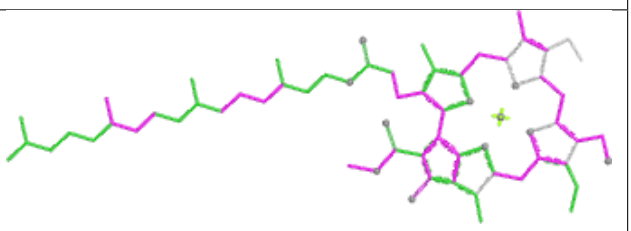


Rings

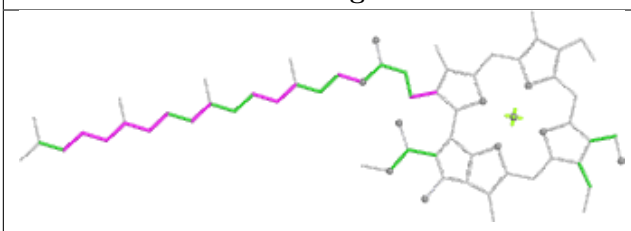
Ligand CHL J 601



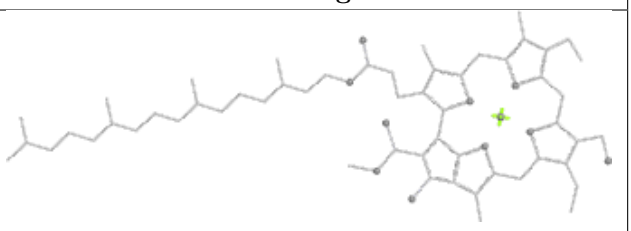
Bond lengths



Bond angles

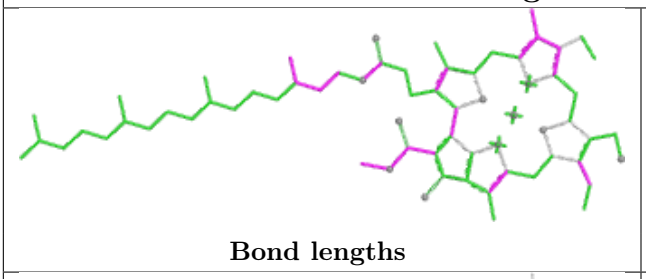


Torsions



Rings

Ligand CHL D 608



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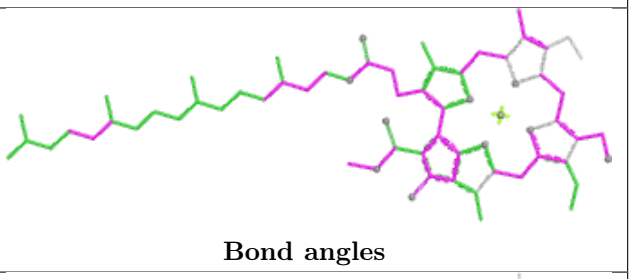
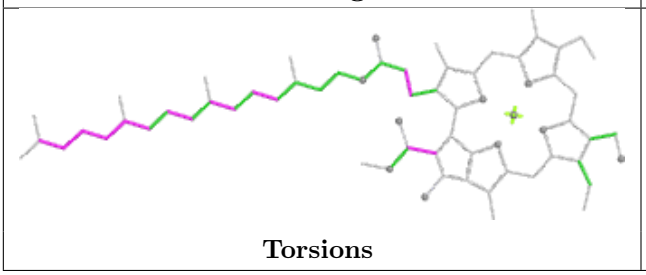
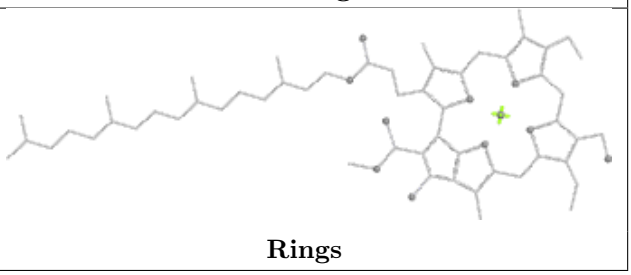


Bond angles

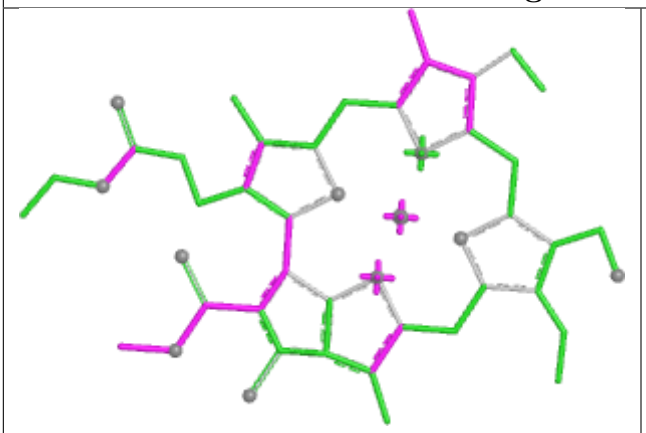


Torsions



Rings

Ligand CHL E 605



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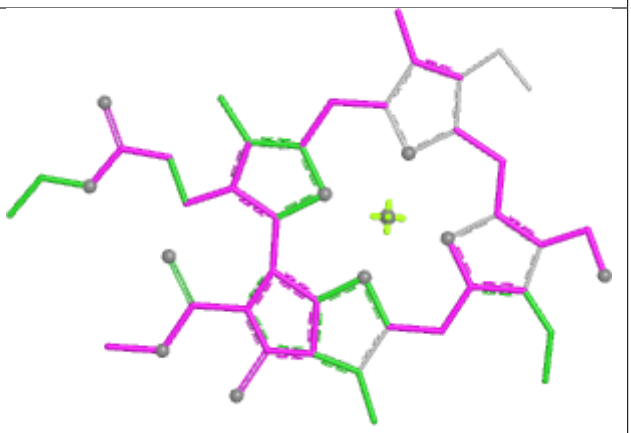

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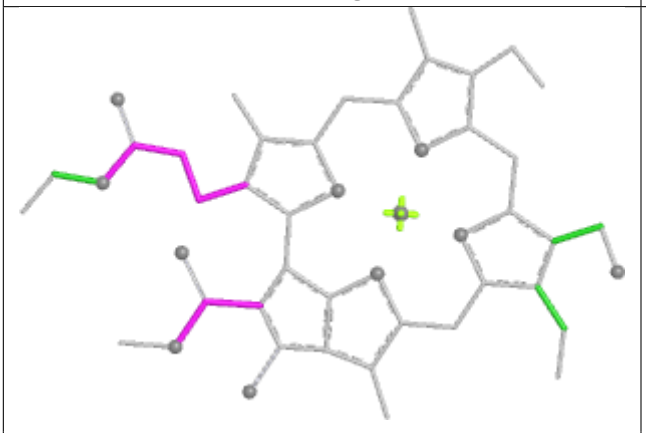

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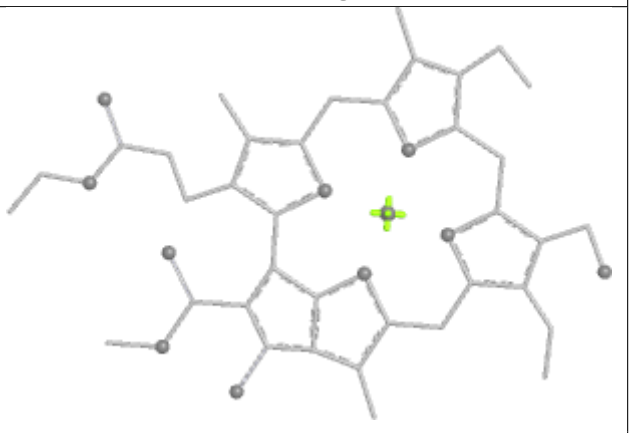
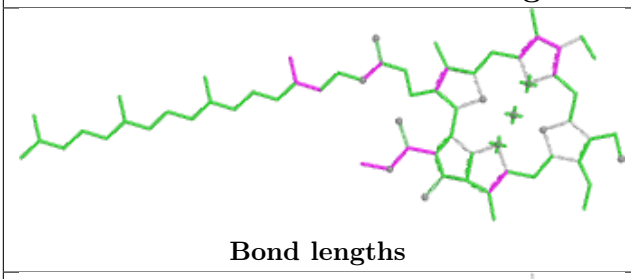


Rings

Ligand CHL D 609



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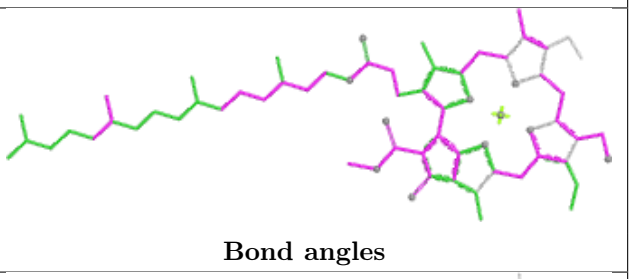

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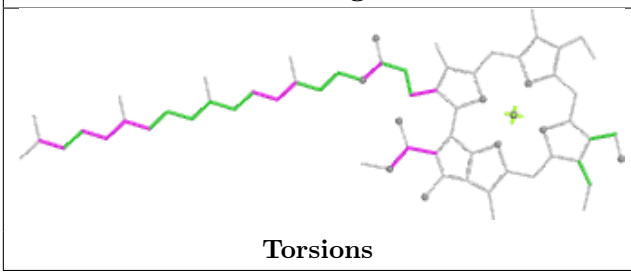

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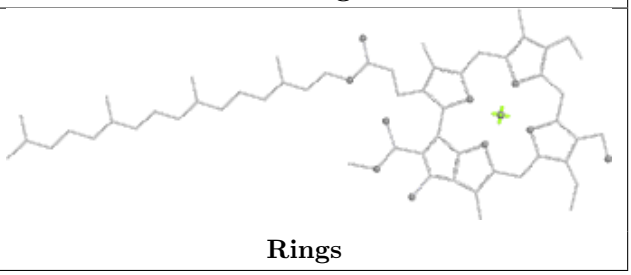
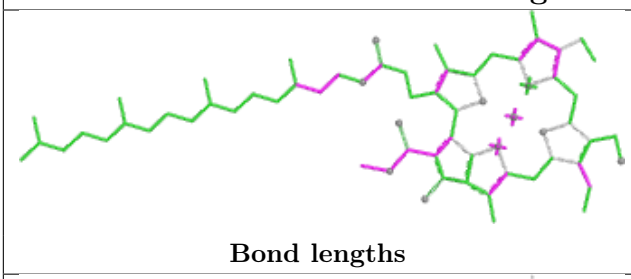


Rings

Ligand CHL I 609



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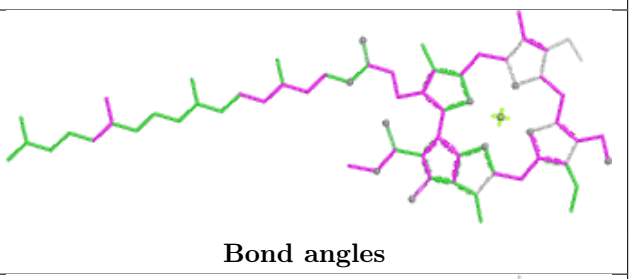
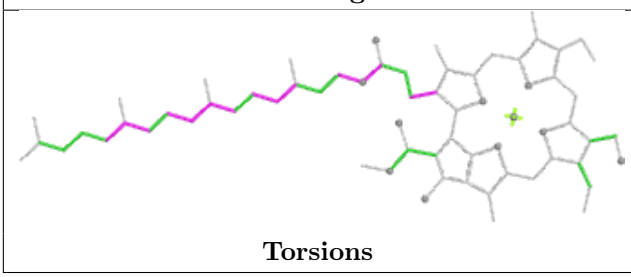


Bond angles



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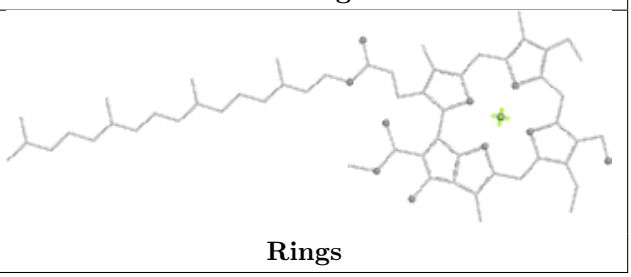
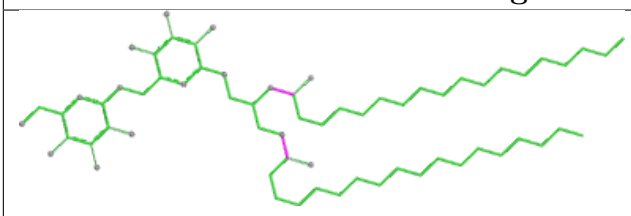


Rings

Ligand DGD D 3632



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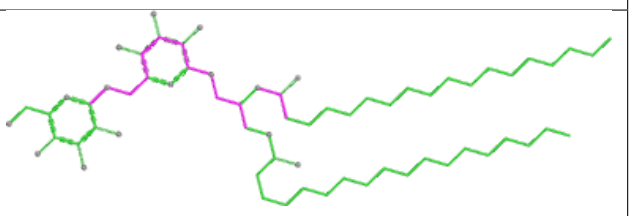

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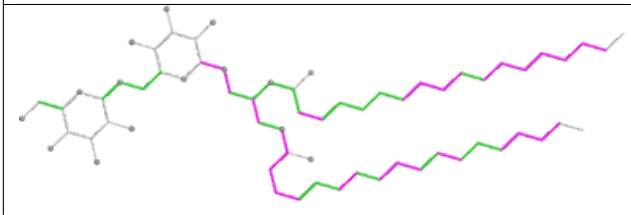

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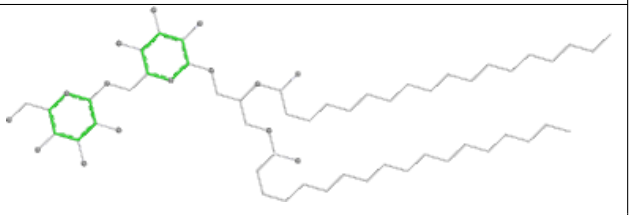
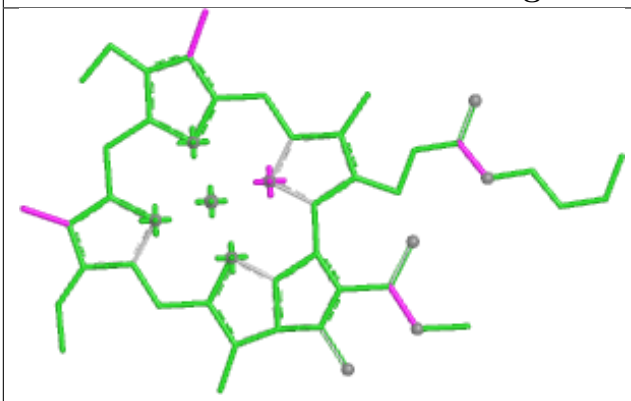


Rings

Ligand CLA H 614



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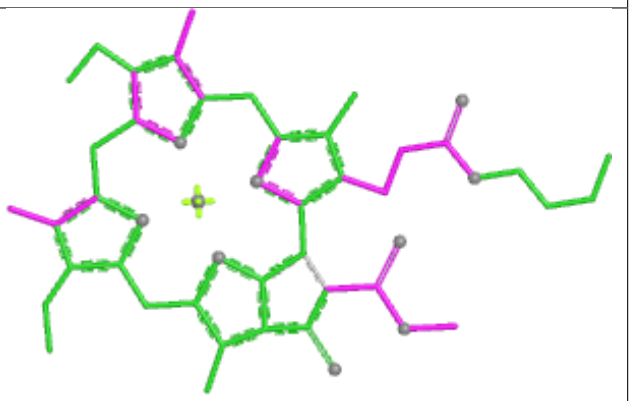
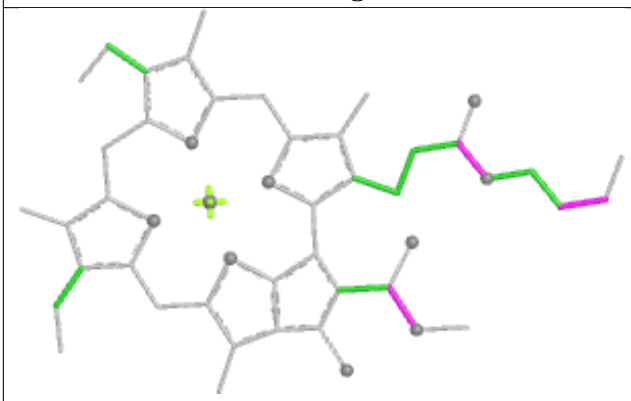


Bond angles



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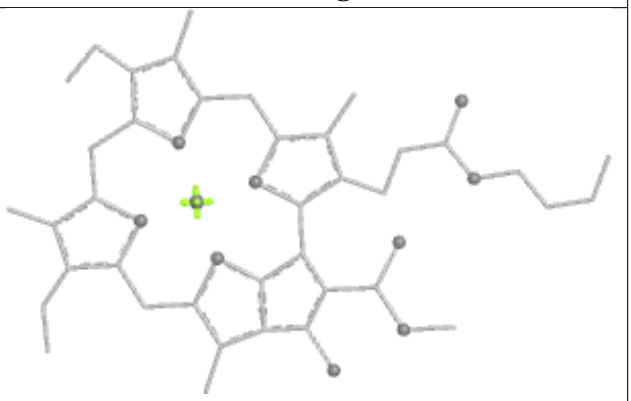
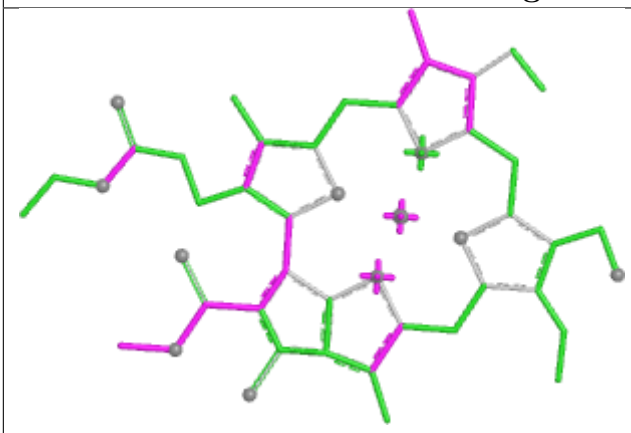


Rings

Ligand CHL D 605



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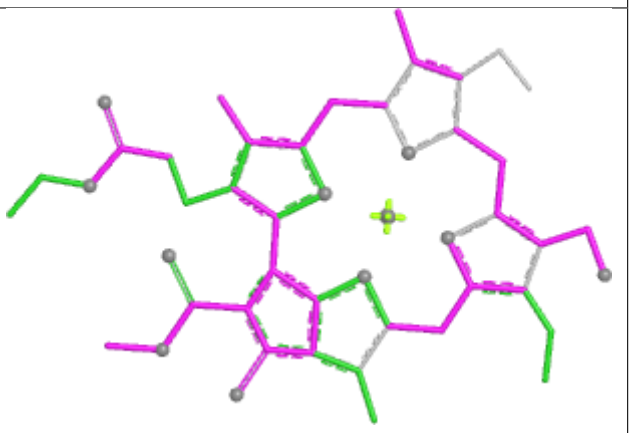

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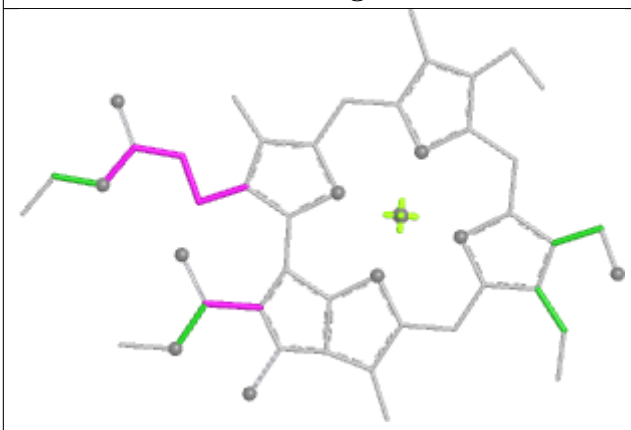
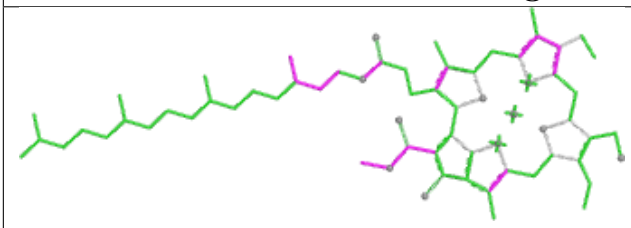


Torsions

Rings

Ligand CHL C 609



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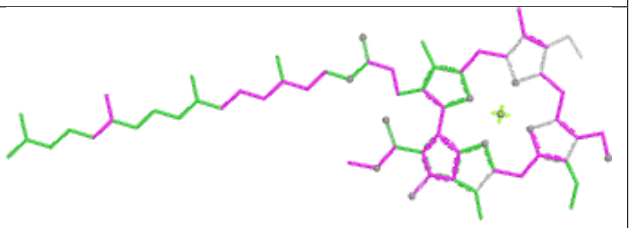

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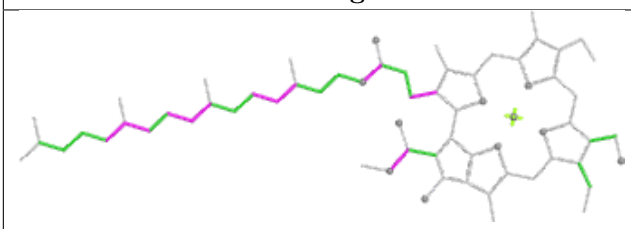

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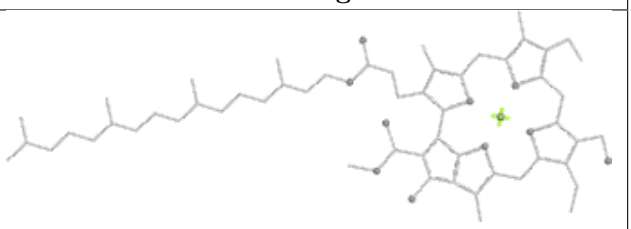
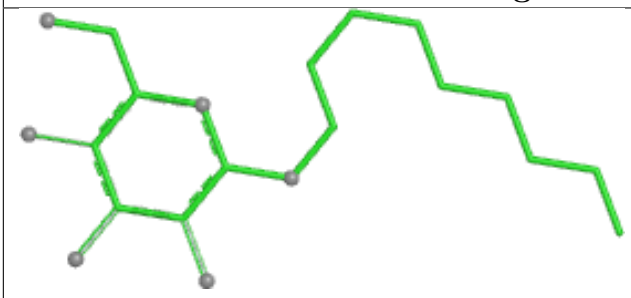


Rings

Ligand BNG F 5633



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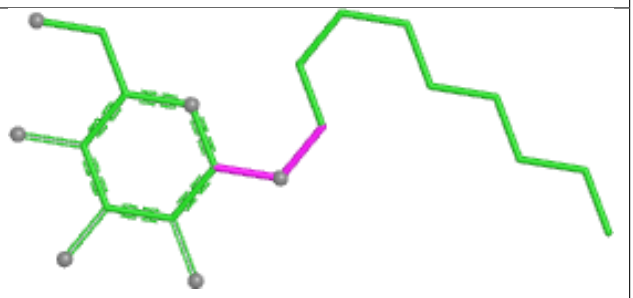

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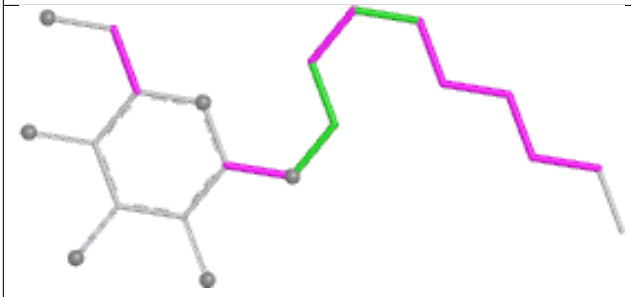

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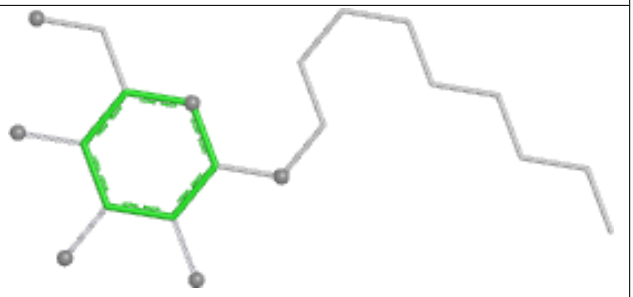
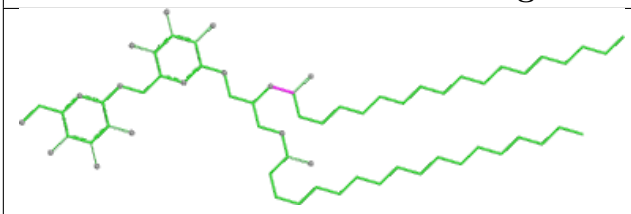


Rings

Ligand DGD I 8632



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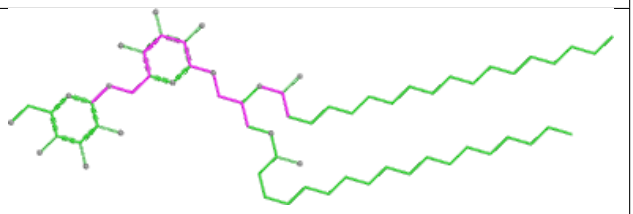

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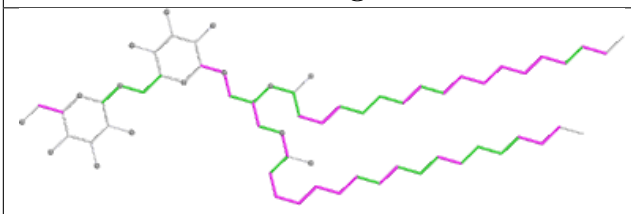

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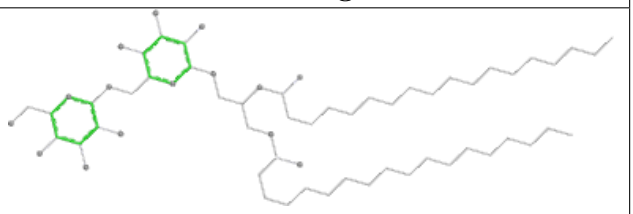
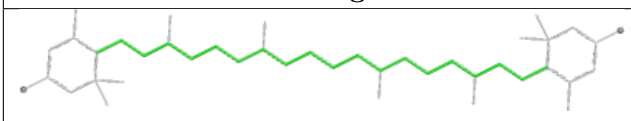


Rings

Ligand LUT D 3620

Bond lengths

Bond angles



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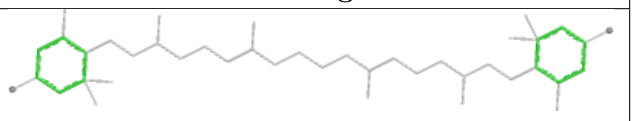
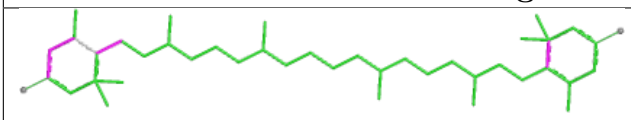


Rings

Ligand LUT E 4621



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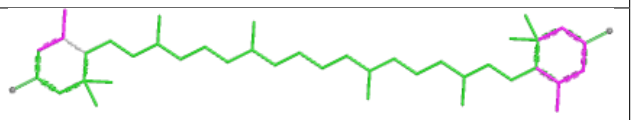
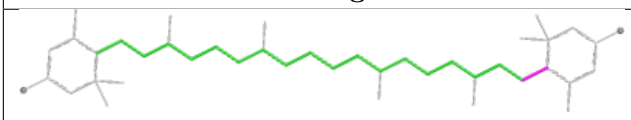


Bond angles



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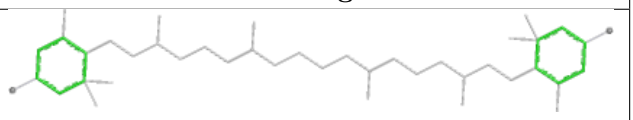
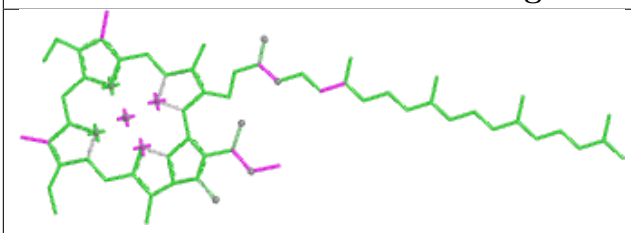


Rings

Ligand CLA B 603



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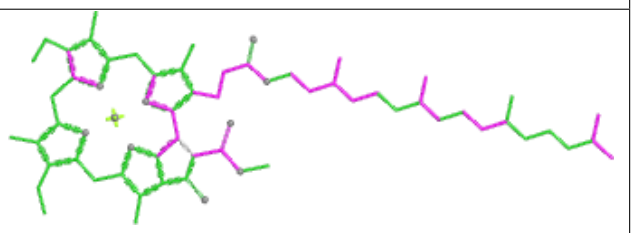
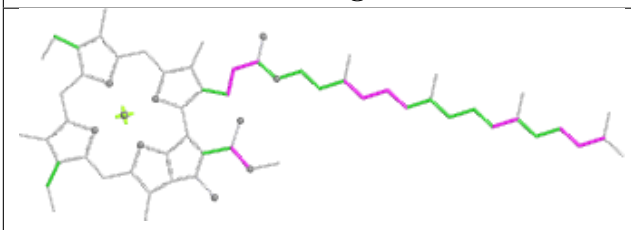


Bond angles



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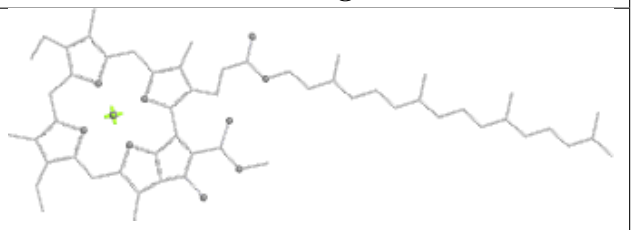
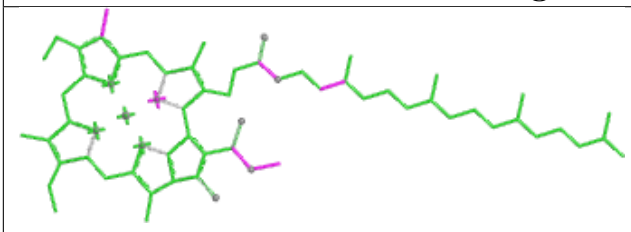
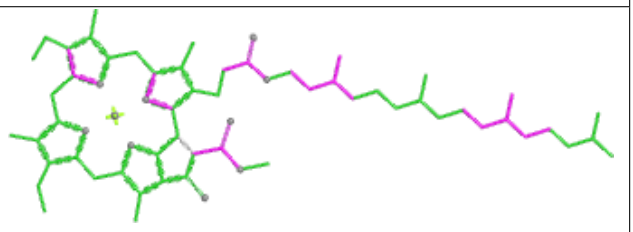


Rings

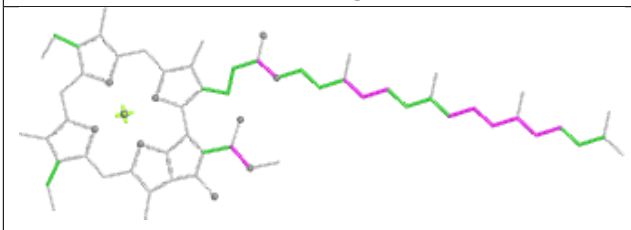
Ligand CLA I 612



Bond lengths



Bond angles



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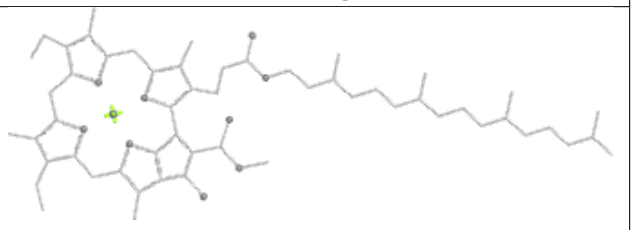
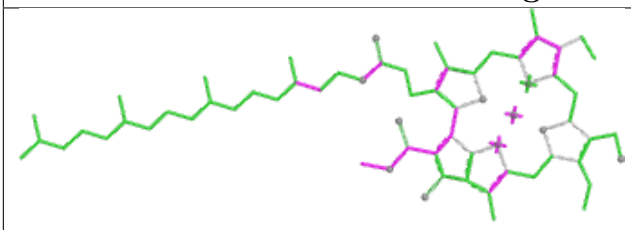


Rings

Ligand CHL H 601



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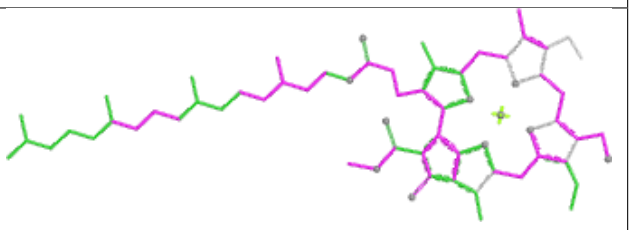
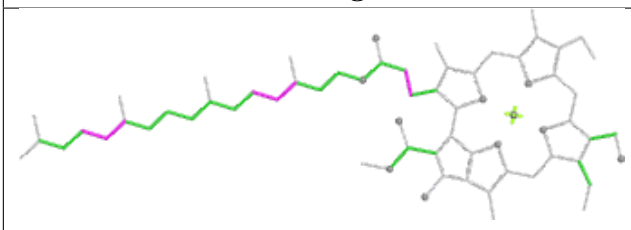


Bond angles



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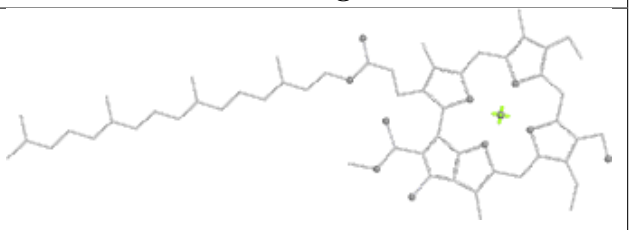
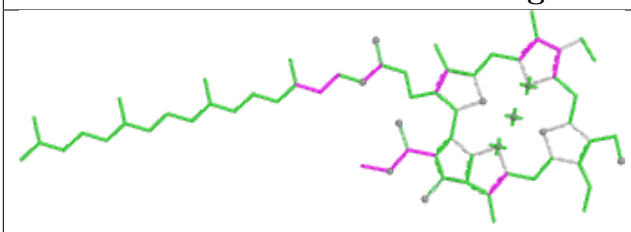
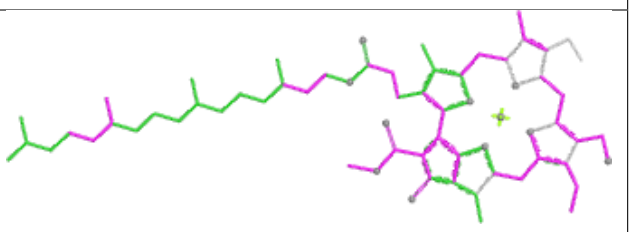


Rings

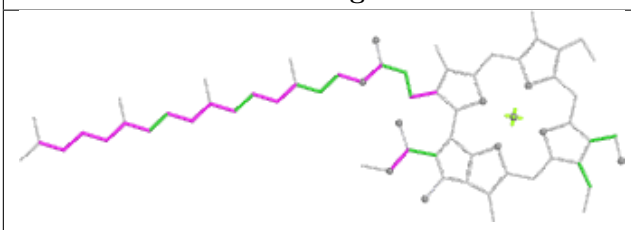
Ligand CHL J 609



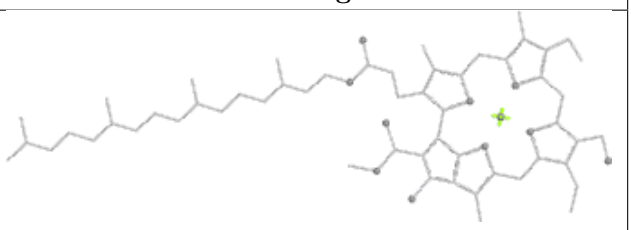
Bond lengths



Bond angles

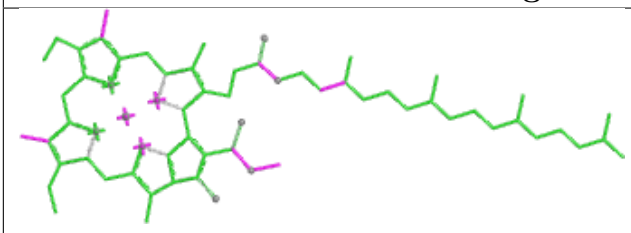


Torsions



Rings

Ligand CLA G 603



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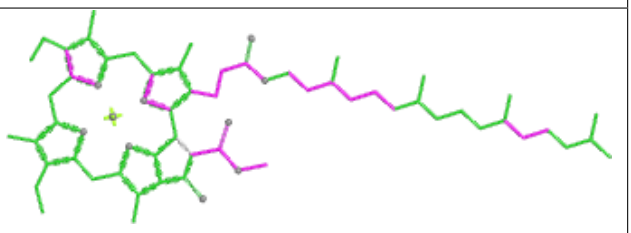
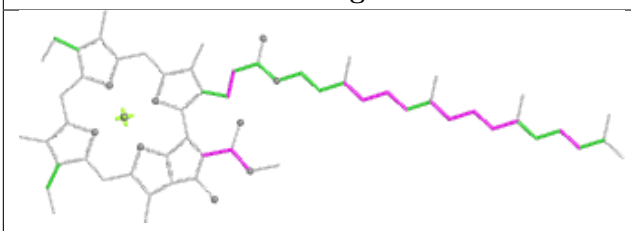


Bond angles



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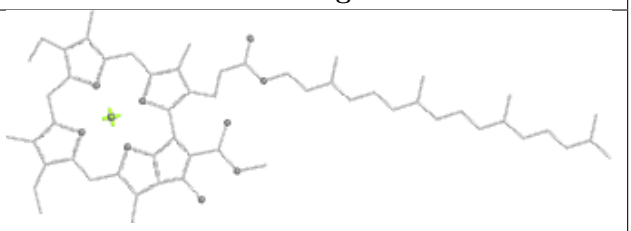
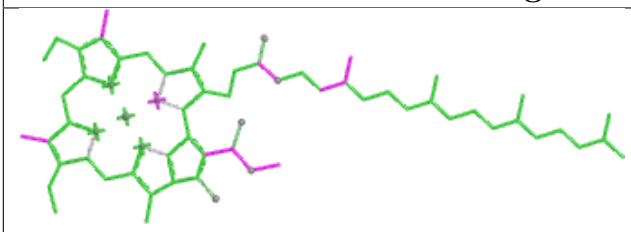


Rings

Ligand CLA C 610



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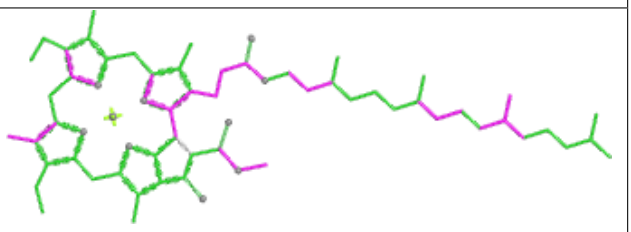
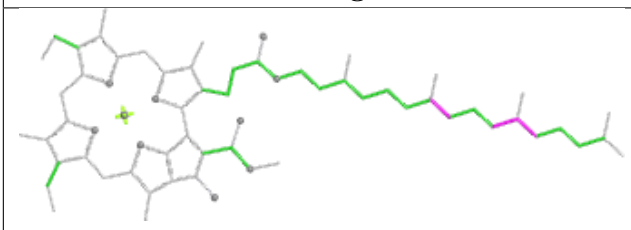


Bond angles



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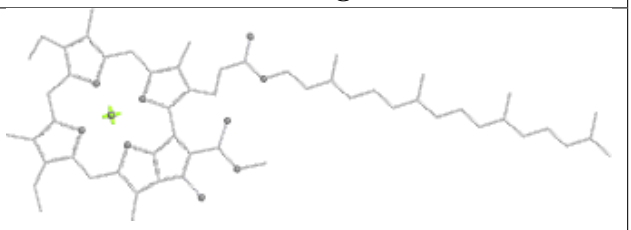
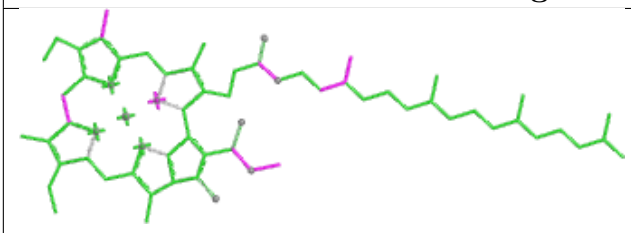


Rings

Ligand CLA I 610



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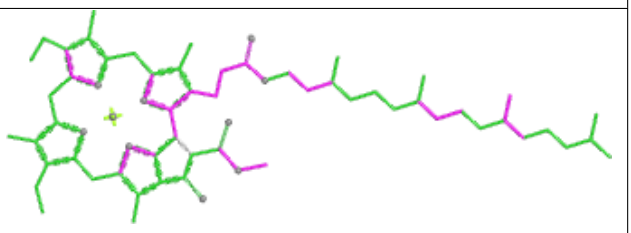
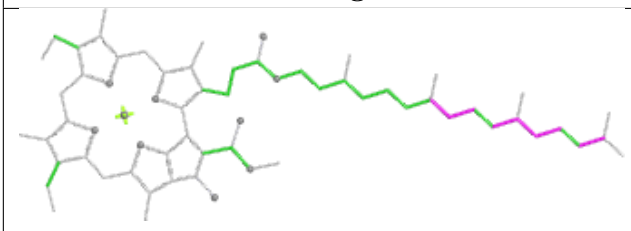


Bond angles



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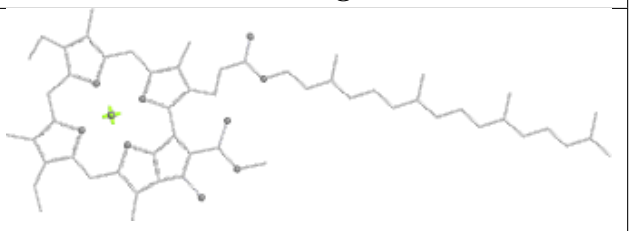
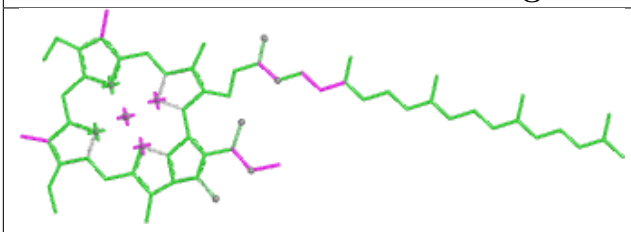


Rings

Ligand CLA D 602



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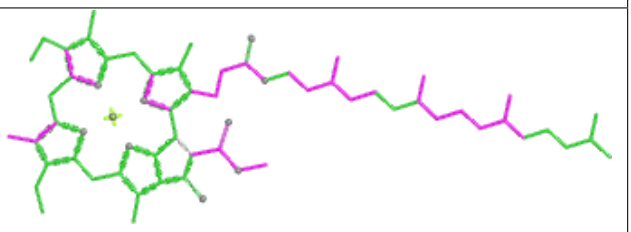
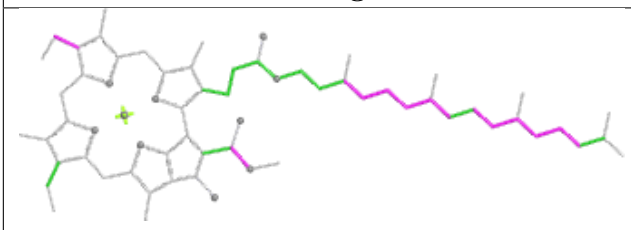


Bond angles



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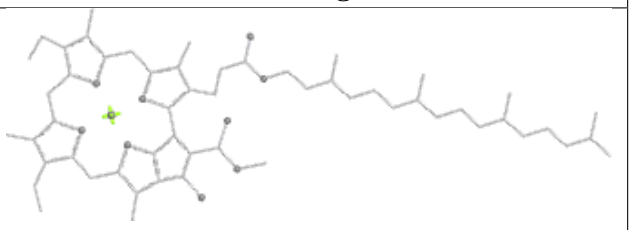
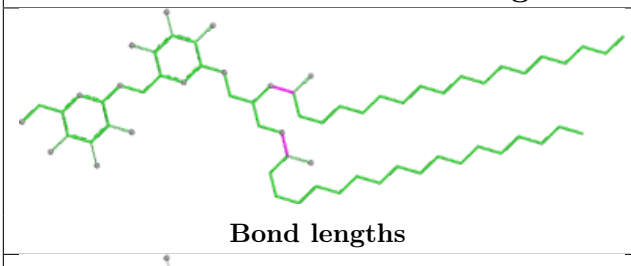


Rings

Ligand DGD B 1632



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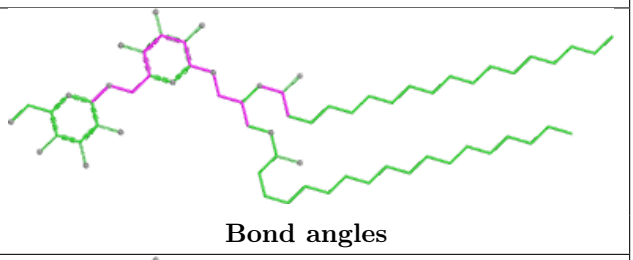
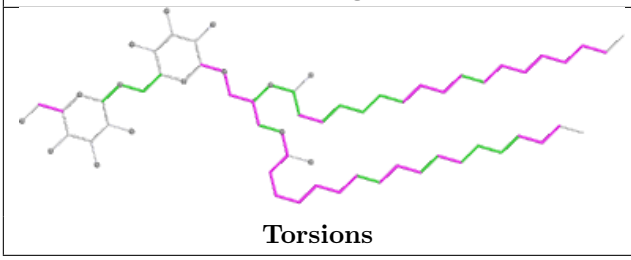


Bond angles



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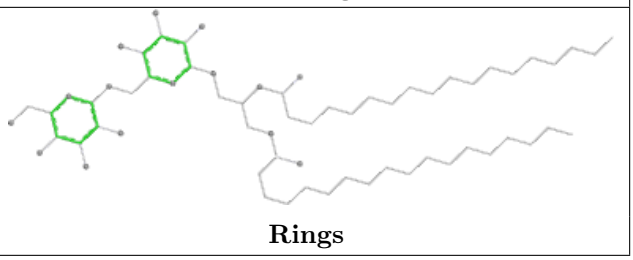
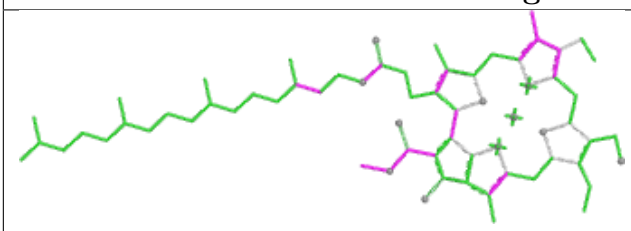


Rings

Ligand CHL D 601



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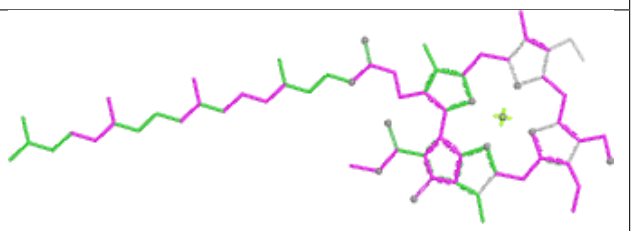

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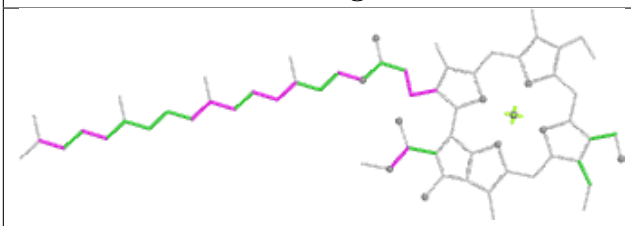

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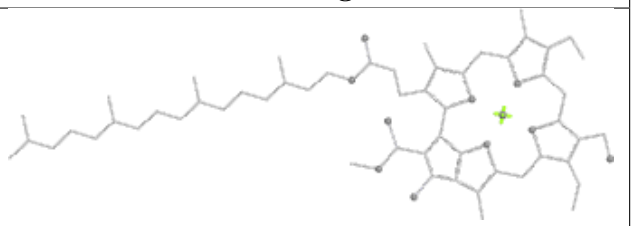
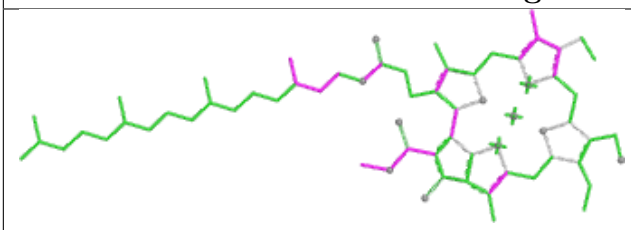


Rings

Ligand CHL B 609



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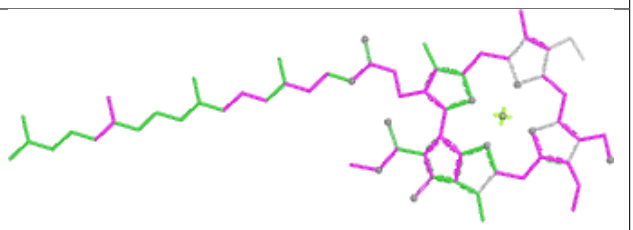
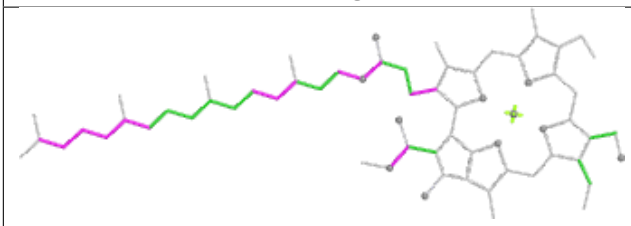


Bond angles



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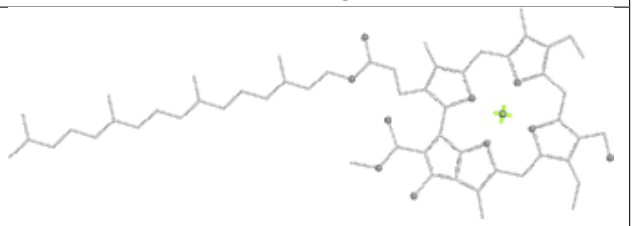
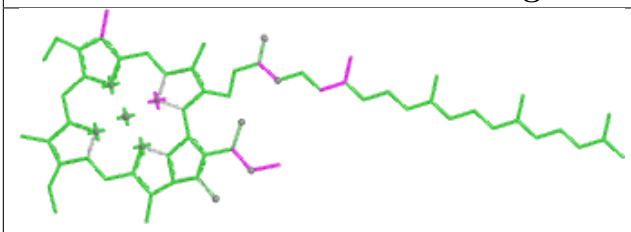


Rings

Ligand CLA G 612



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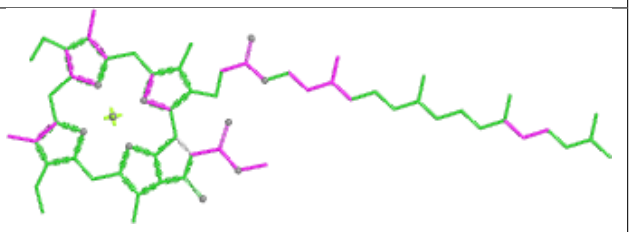

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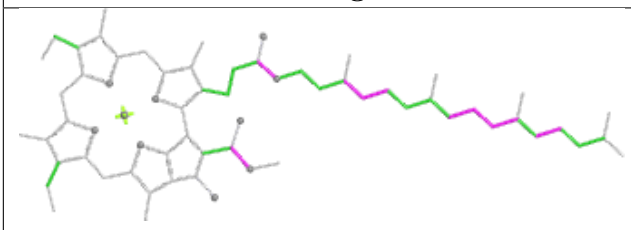

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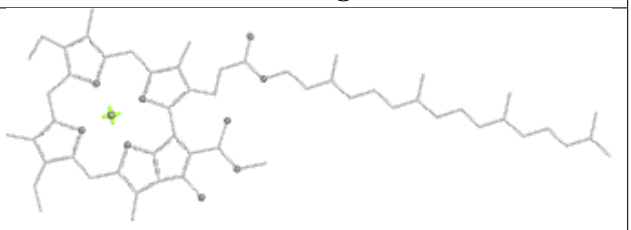

Rings

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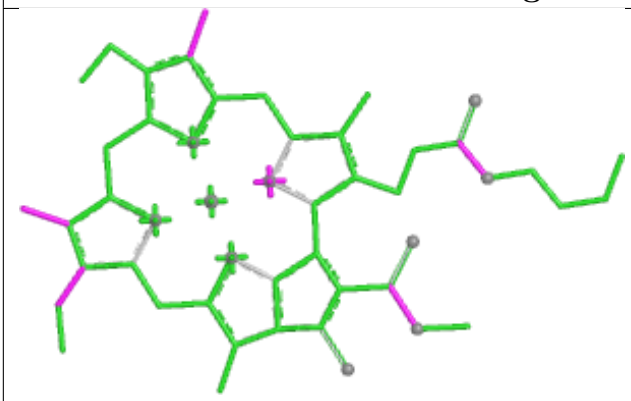

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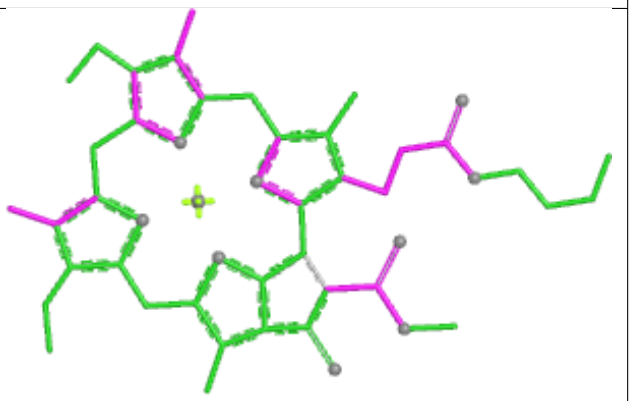

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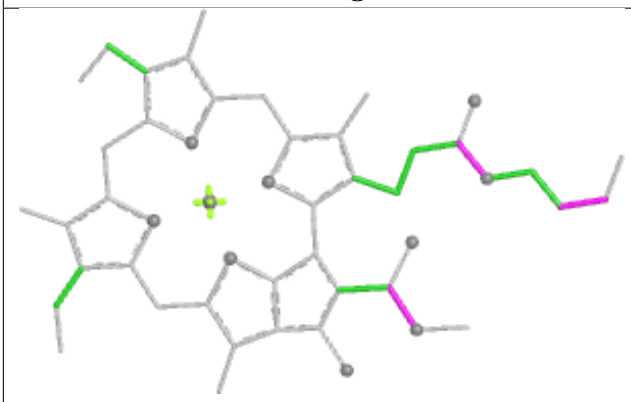

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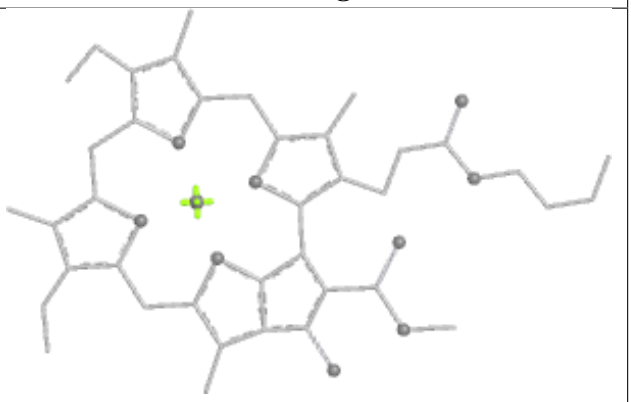
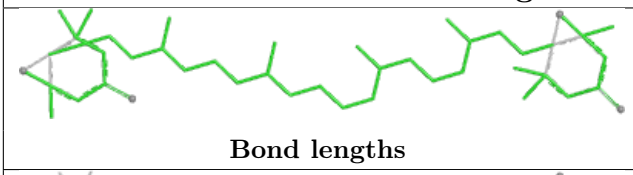


Rings

Ligand XAT E 2622



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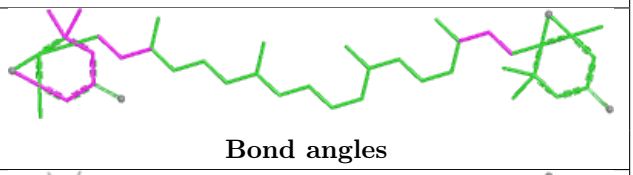

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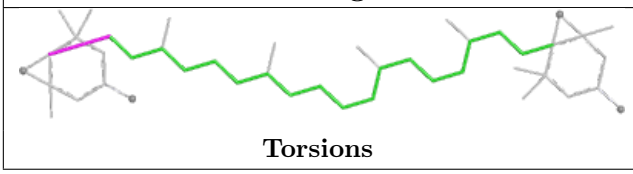

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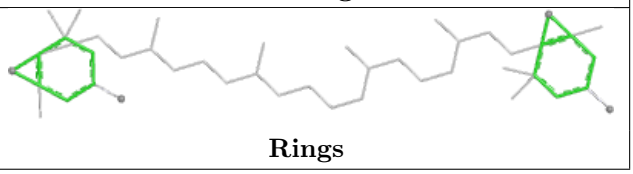
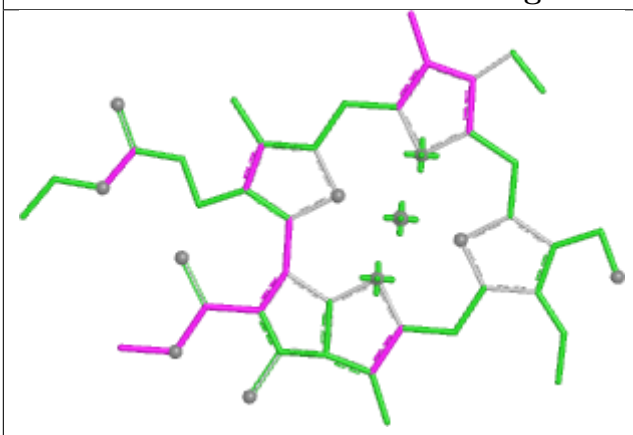


Rings

Ligand CHL B 605



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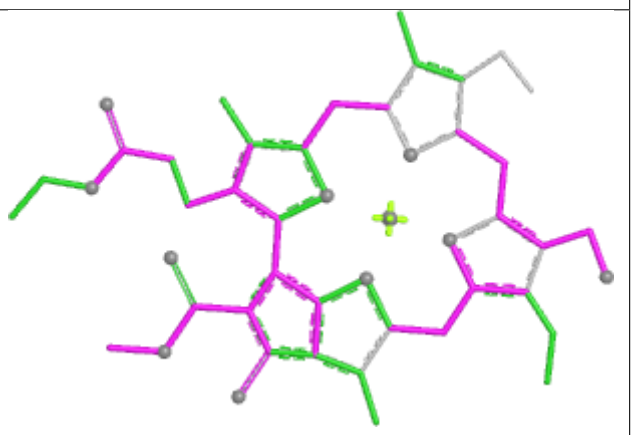
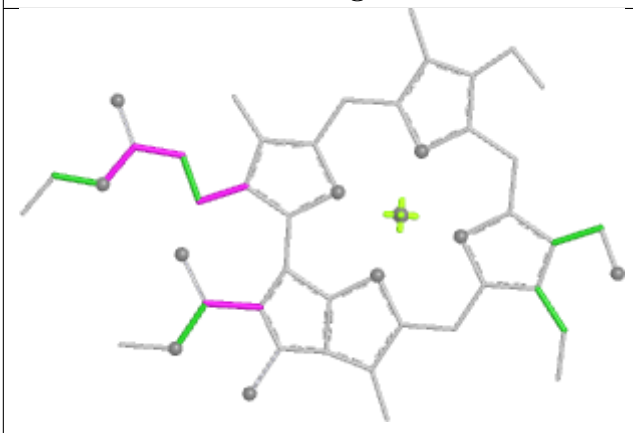
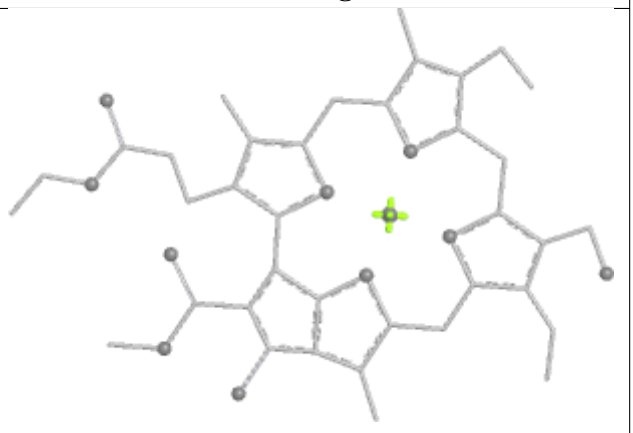


Bond angles

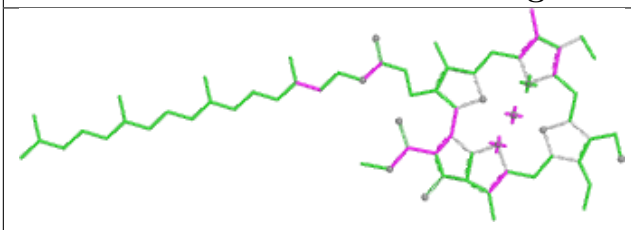


Torsions



Rings

Ligand CHL J 607



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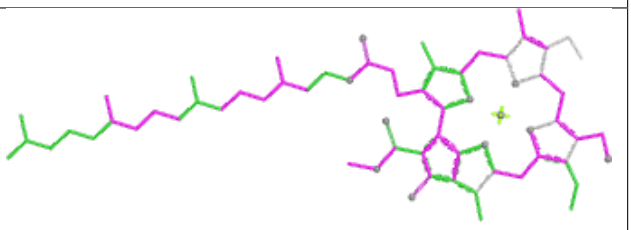
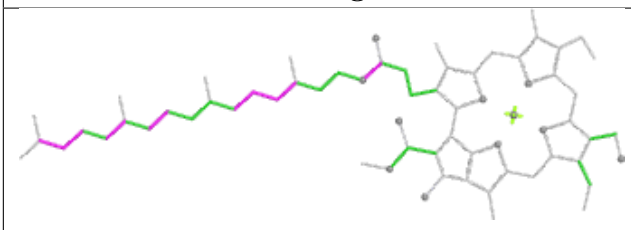


Bond angles



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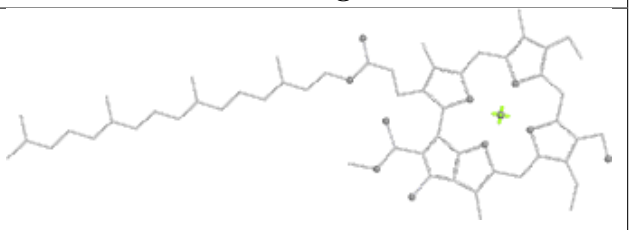
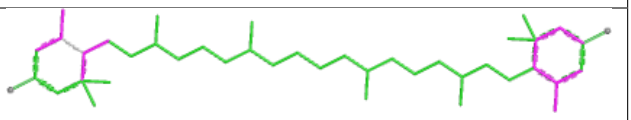


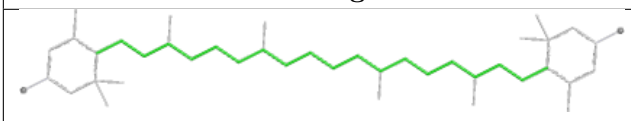
Rings

Ligand LUT G 6620

Bond lengths



Bond angles



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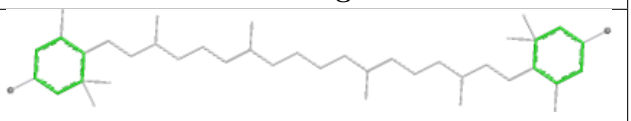
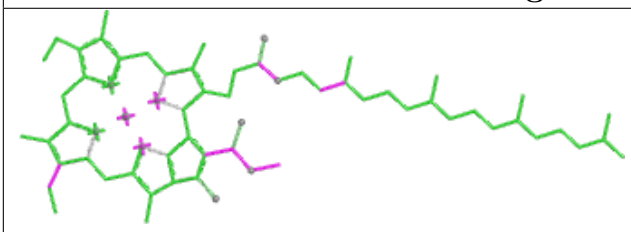
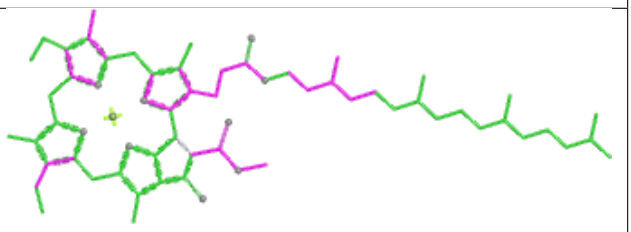


Rings

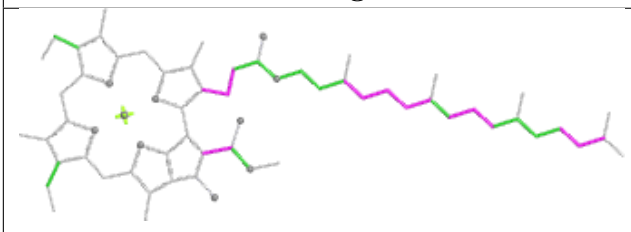
Ligand CLA F 603



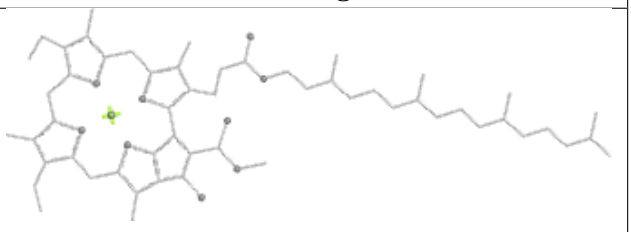
Bond lengths



Bond angles

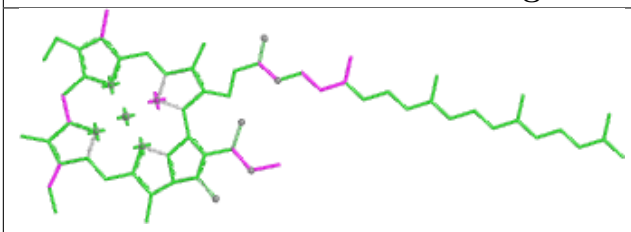


Torsions

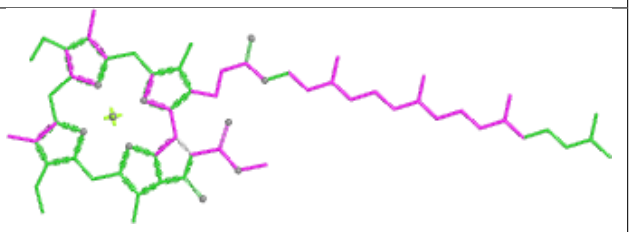


Rings

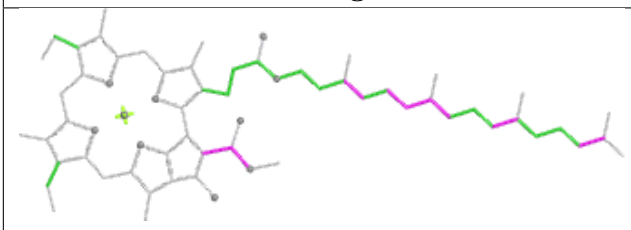
Ligand CLA G 602



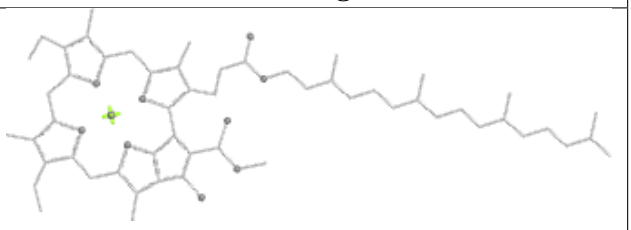
Bond lengths



Bond angles



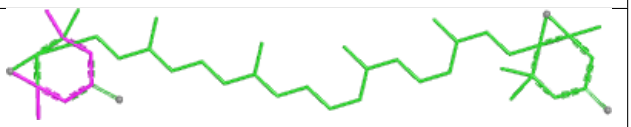
Torsions



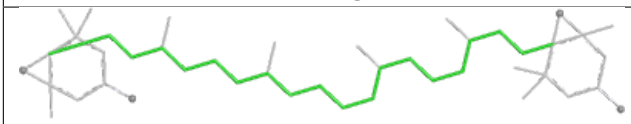
Rings

Ligand XAT J 3622

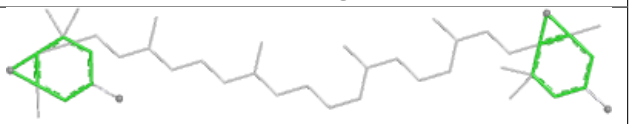
Bond lengths



Bond angles

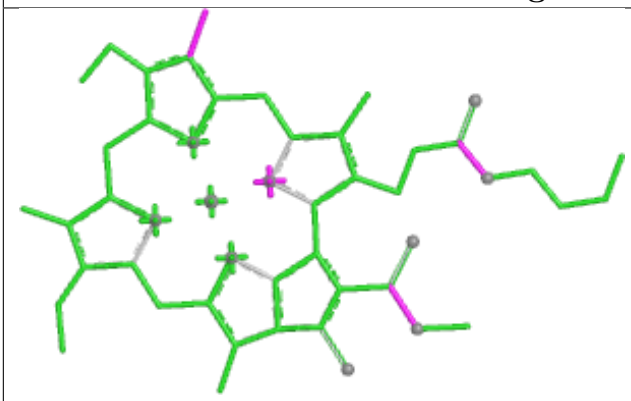


Torsions



Rings

Ligand CLA J 614



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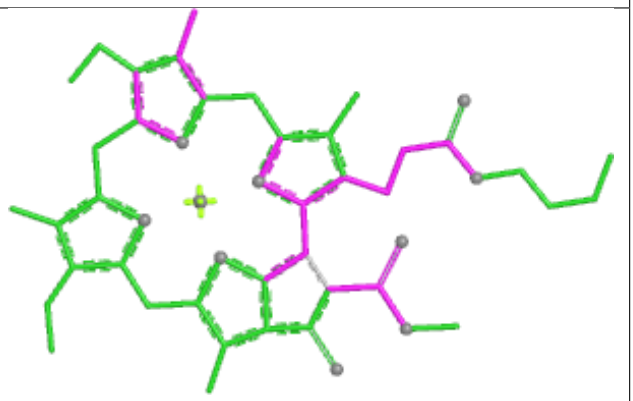
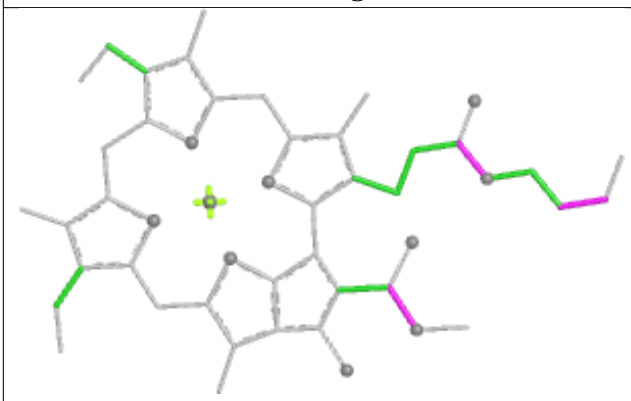
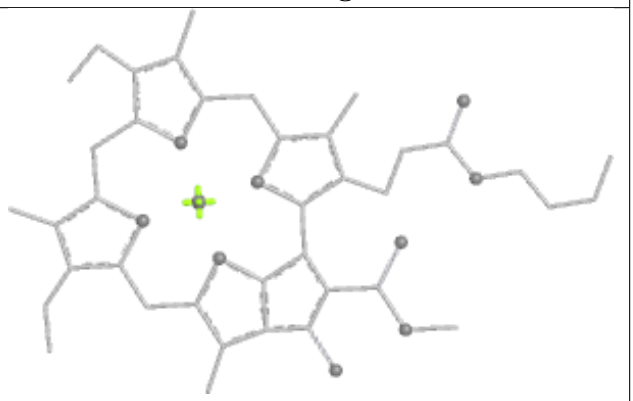


Bond angles



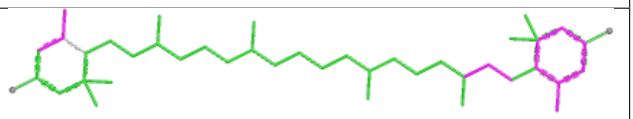
Torsions



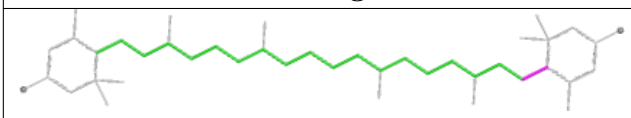
Rings

Ligand LUT A 621

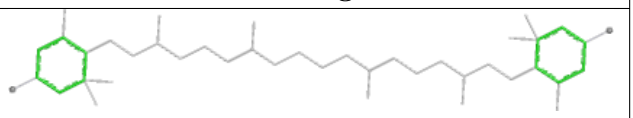
Bond lengths



Bond angles



Torsions

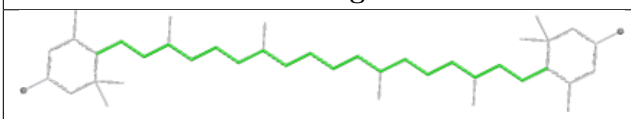


Rings

Ligand LUT E 4620

Bond lengths

Bond angles



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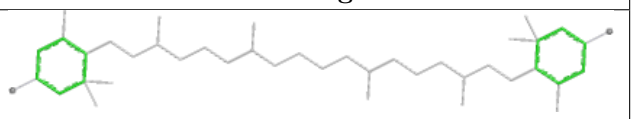
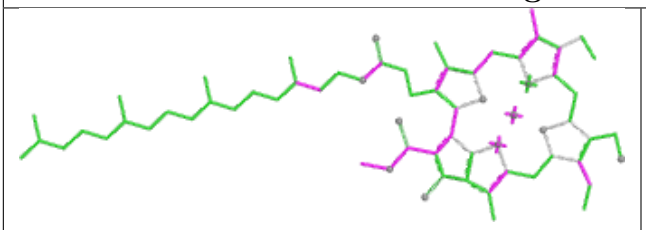
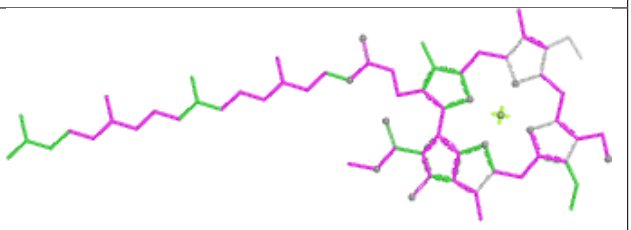


Rings

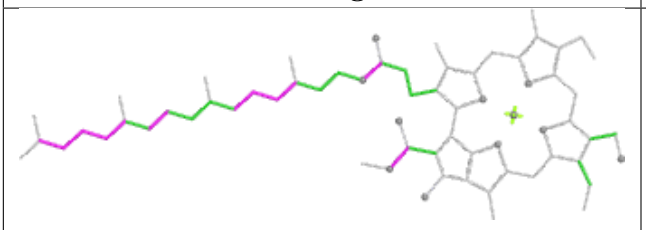
Ligand CHL B 607



Bond lengths



Bond angles



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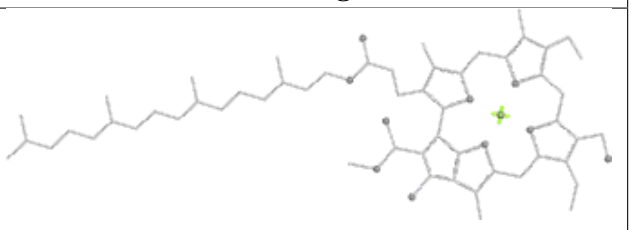
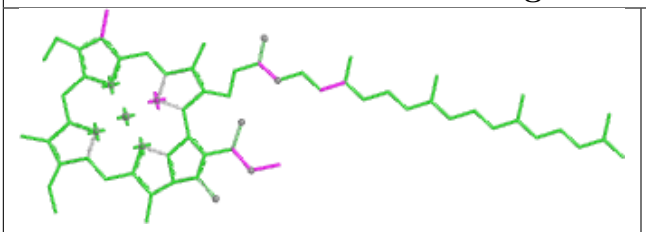
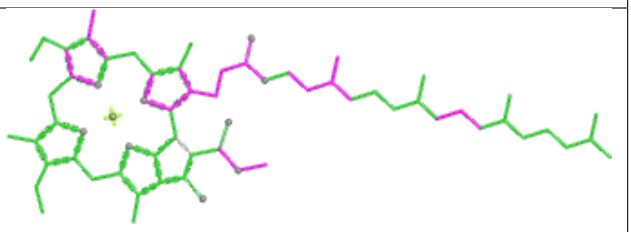


Rings

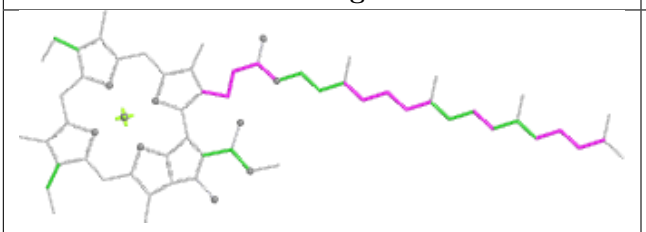
Ligand CLA C 611



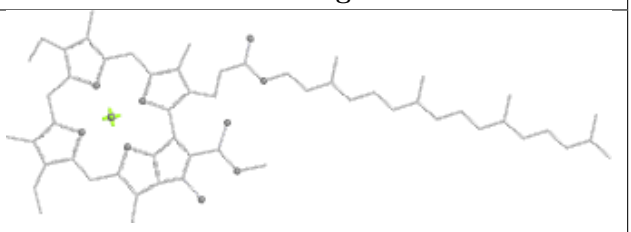
Bond lengths



Bond angles

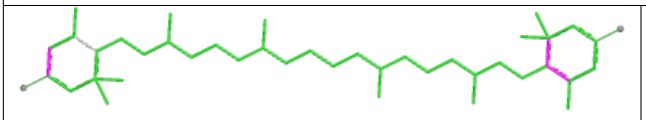


Torsions

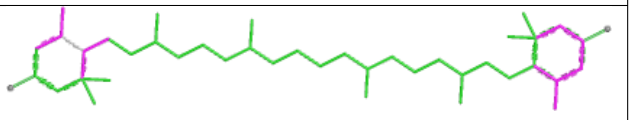


Rings

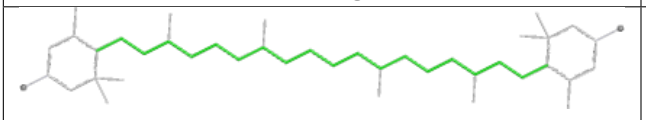
Ligand LUT F 5620



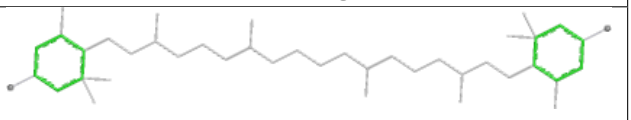
Bond lengths



Bond angles

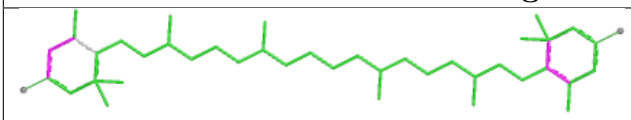


Torsions

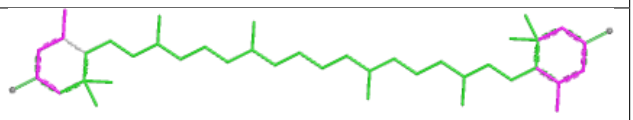


Rings

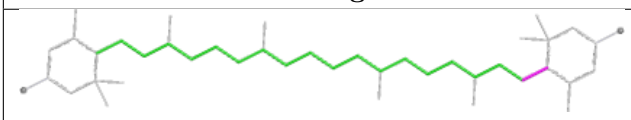
Ligand LUT I 8621



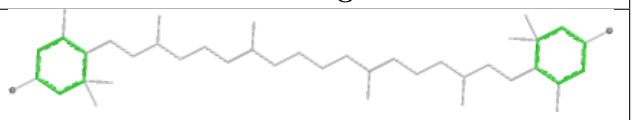
Bond lengths



Bond angles

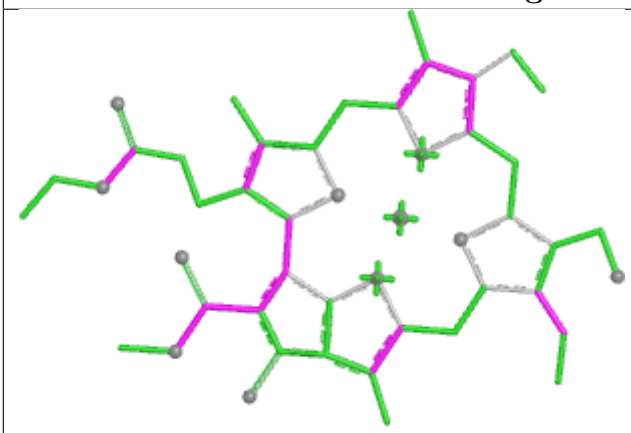


Torsions



Rings

Ligand CHL F 605



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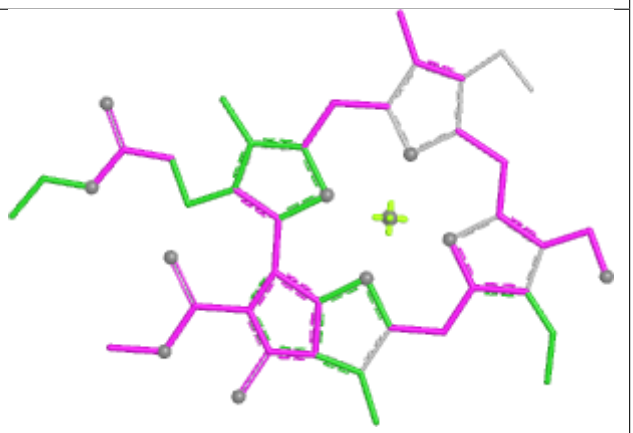
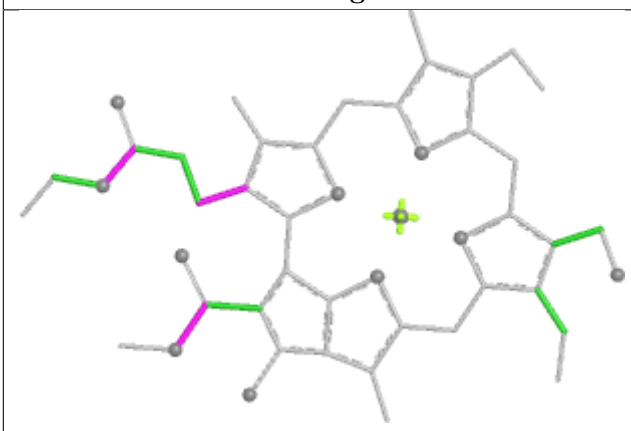


Bond angles



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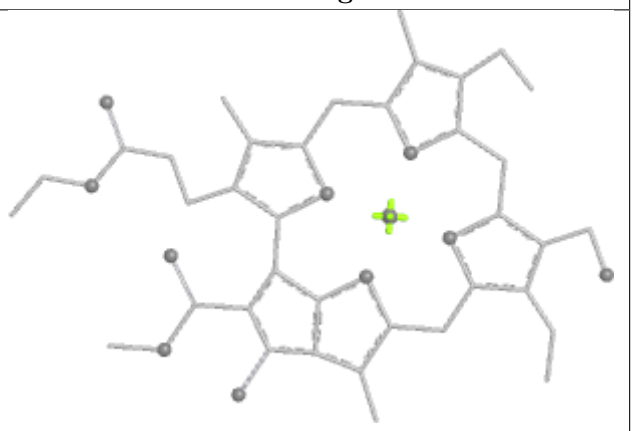
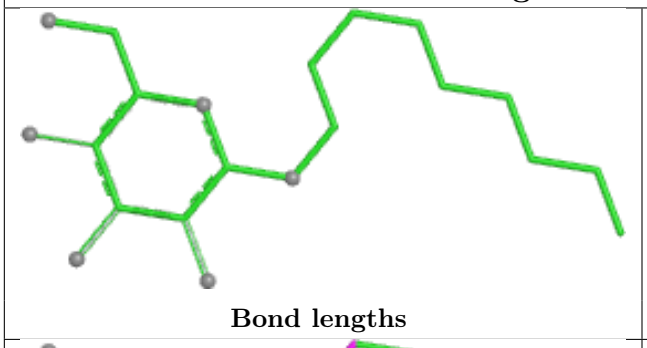


Rings

Ligand BNG C 2633



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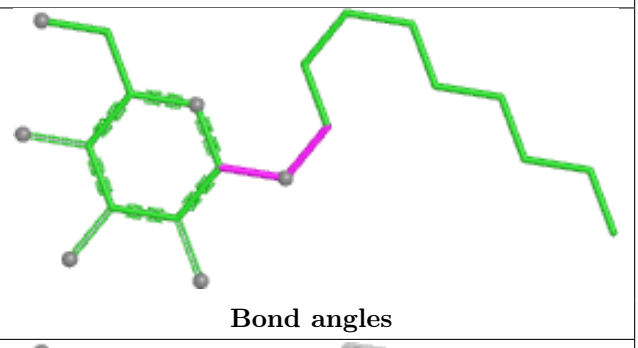
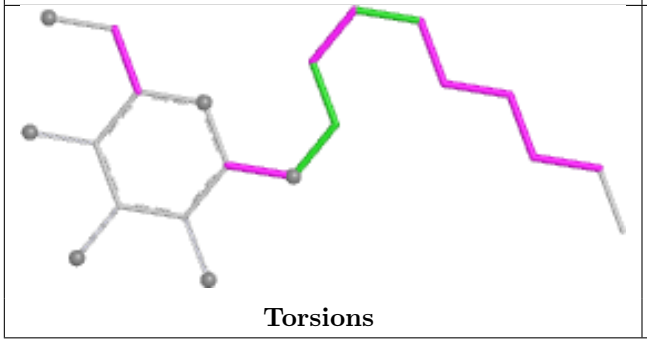


Bond angles



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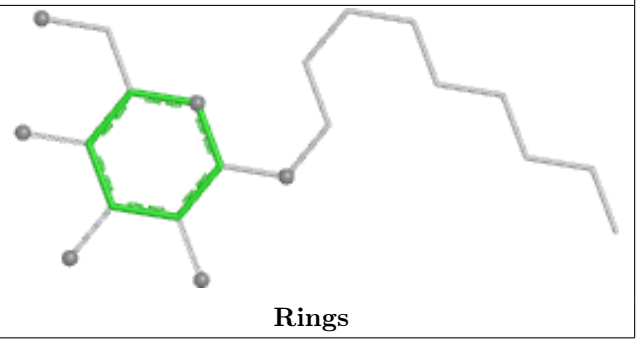
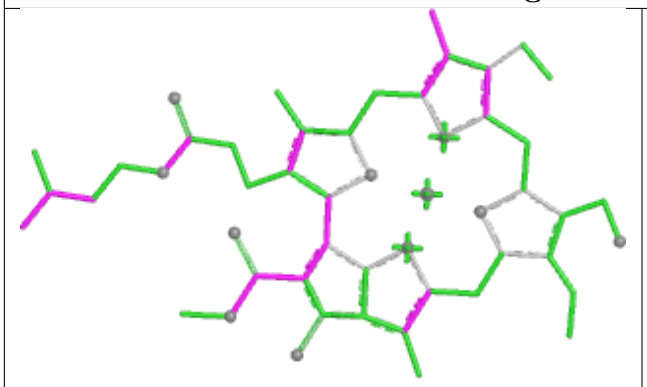
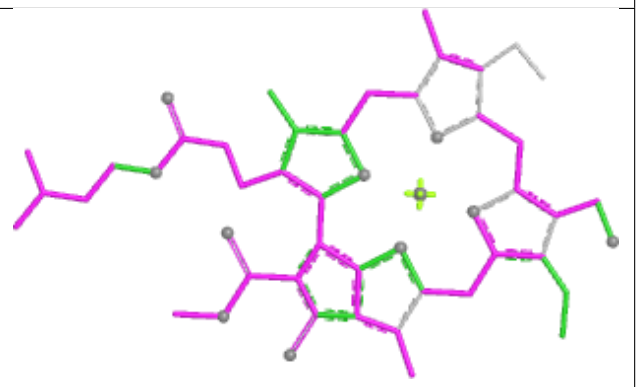


Rings

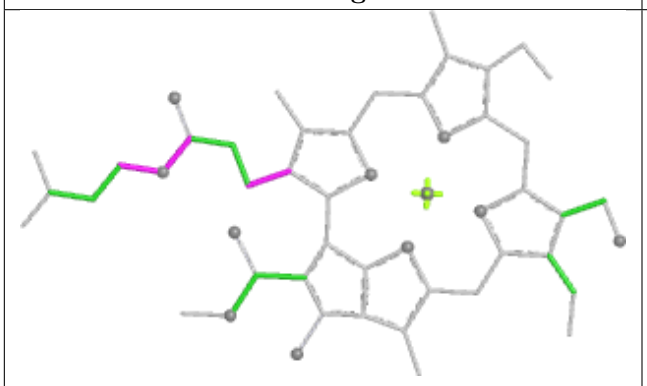
Ligand CHL A 606



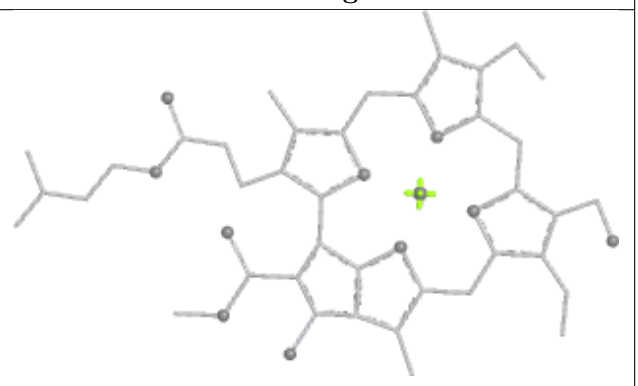
Bond lengths



Bond angles

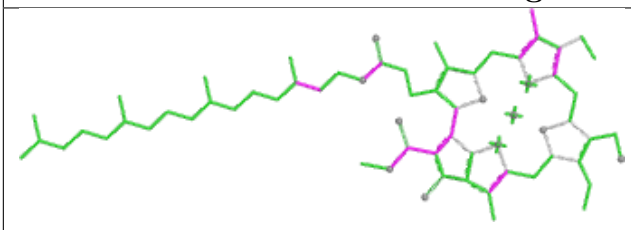


Torsions

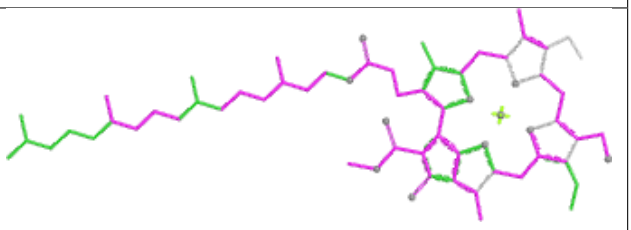


Rings

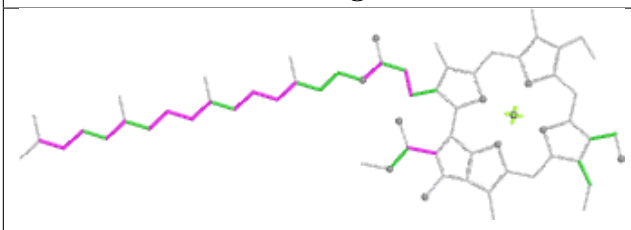
Ligand CHL F 607



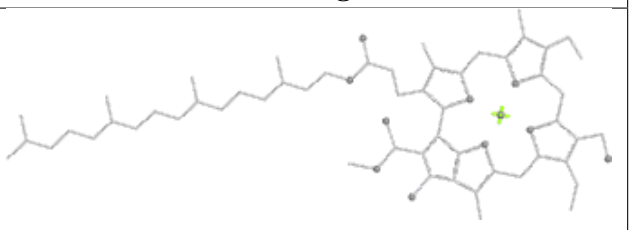
Bond lengths



Bond angles

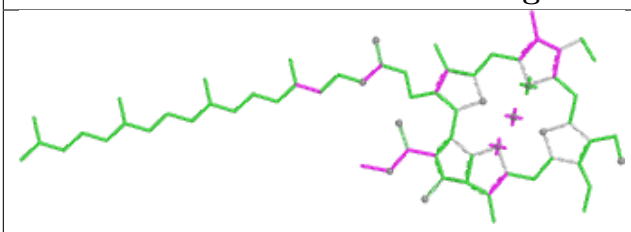


Torsions

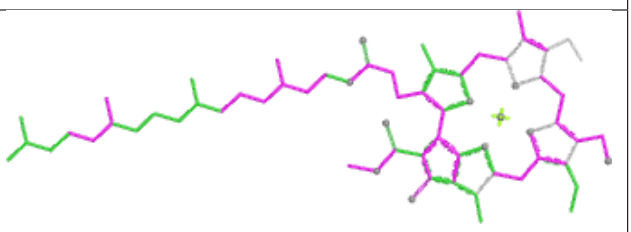


Rings

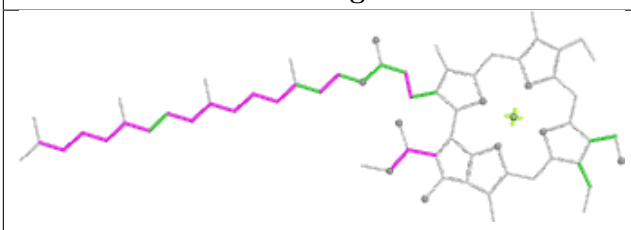
Ligand CHL H 608



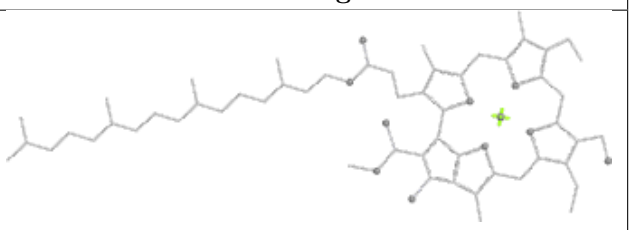
Bond lengths



Bond angles

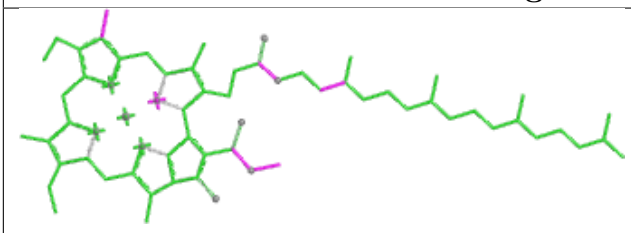


Torsions

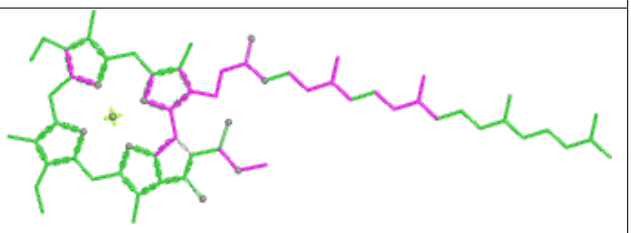


Rings

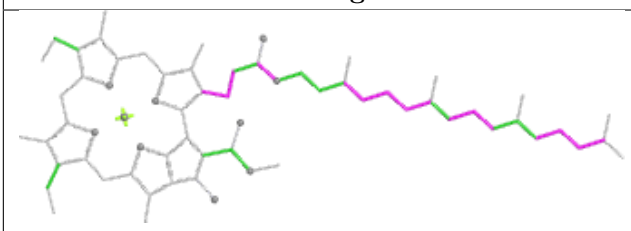
Ligand CLA E 611



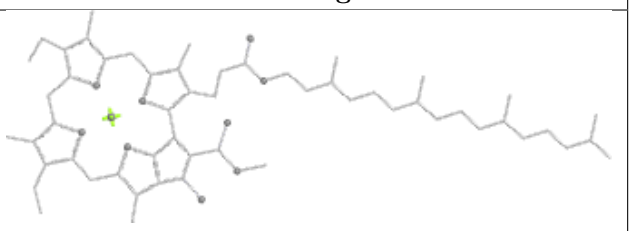
Bond lengths



Bond angles

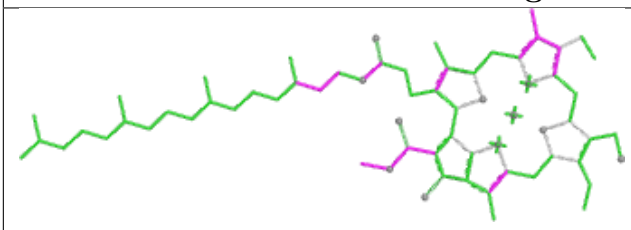


Torsions

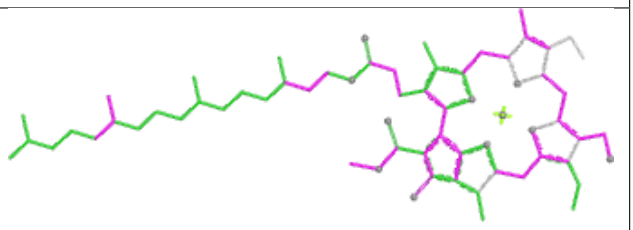


Rings

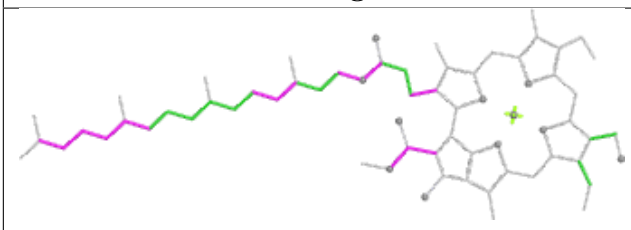
Ligand CHL E 609



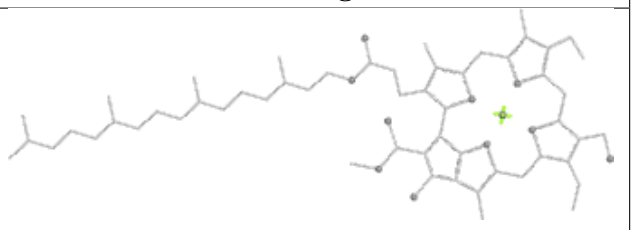
Bond lengths



Bond angles

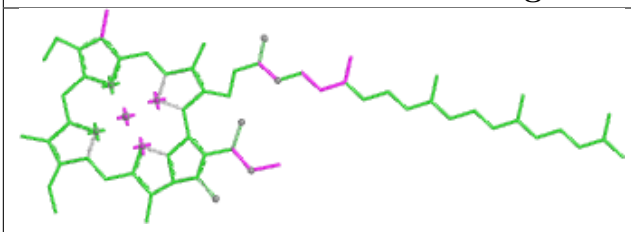


Torsions



Rings

Ligand CLA B 602



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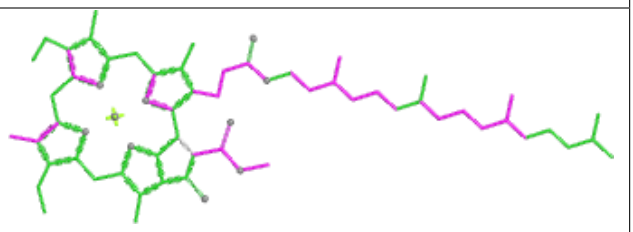
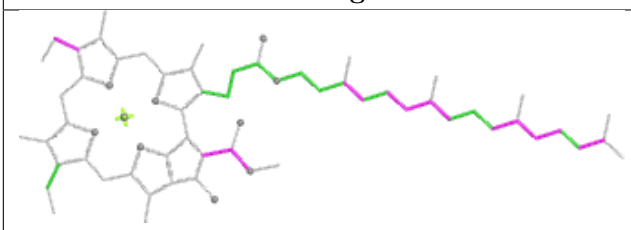
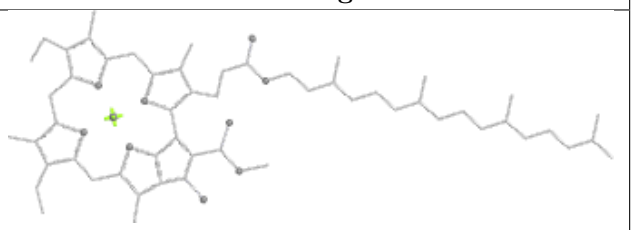


Bond angles

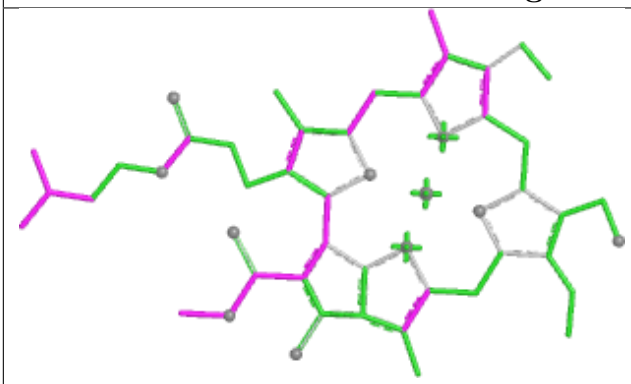


Torsions



Rings

Ligand CHL F 606



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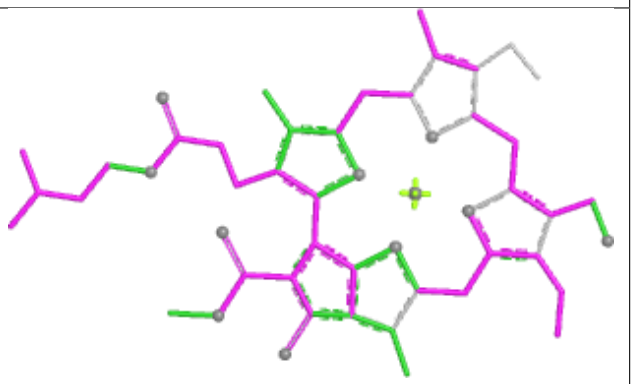
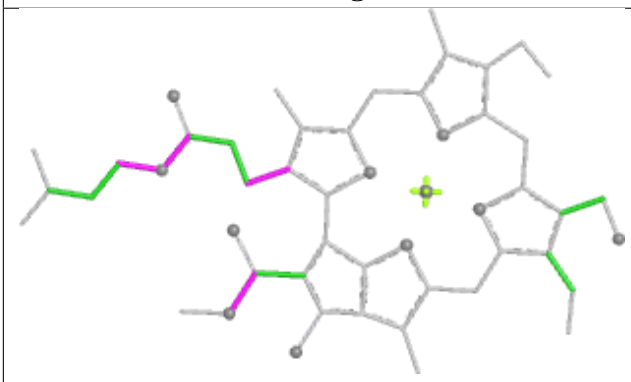
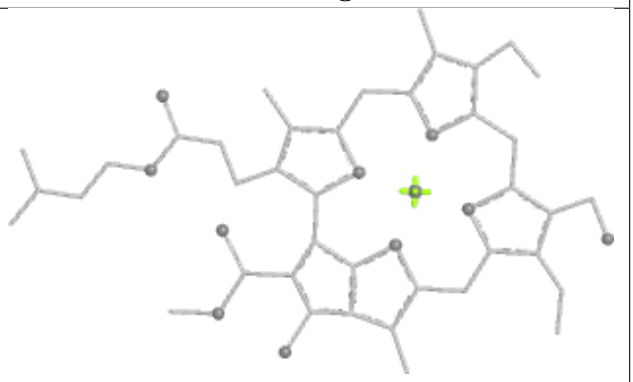


Bond angles

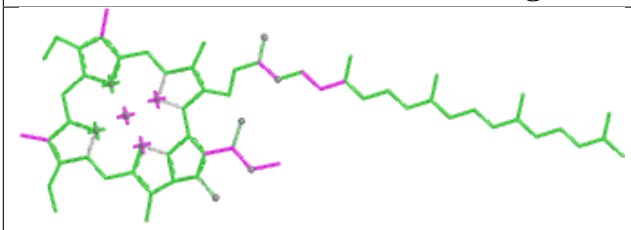


Torsions



Rings

Ligand CLA C 613



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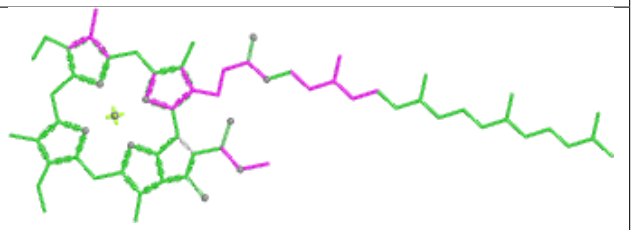
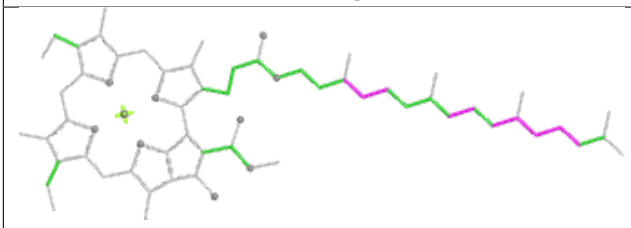


Bond angles



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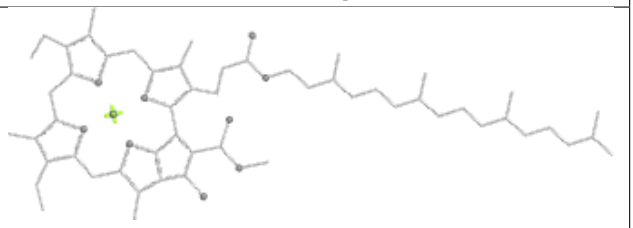
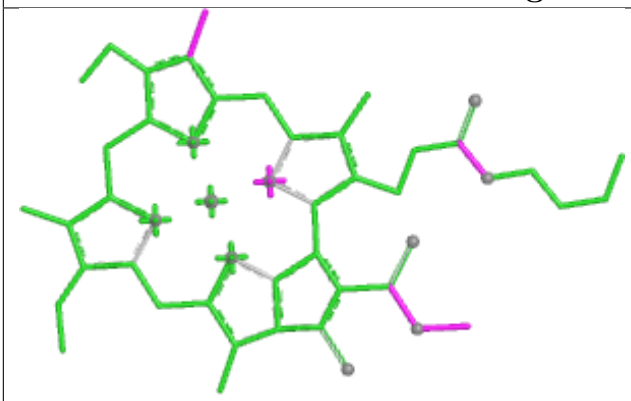


Rings

Ligand CLA F 614



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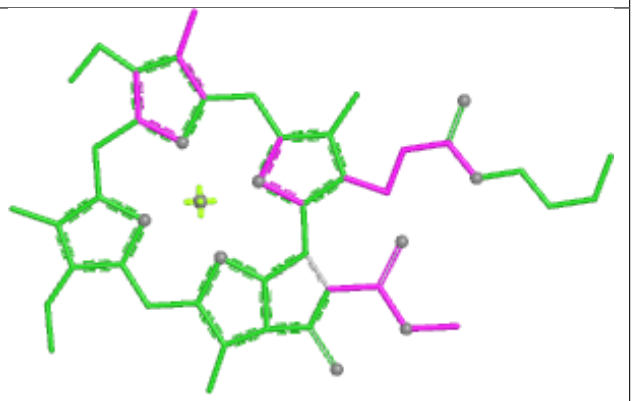
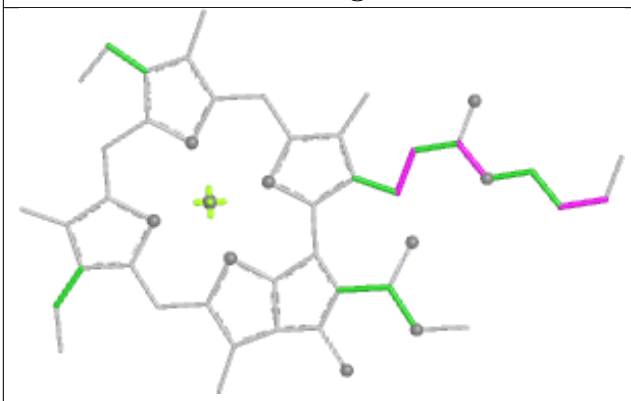


Bond angles



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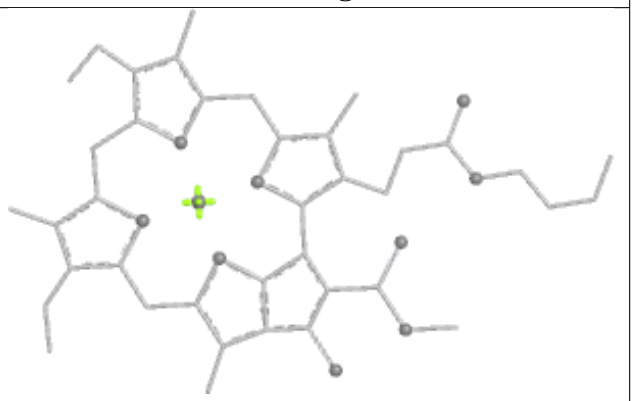
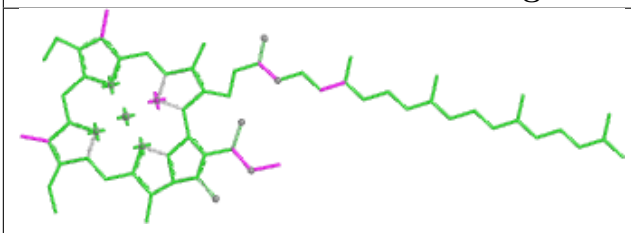
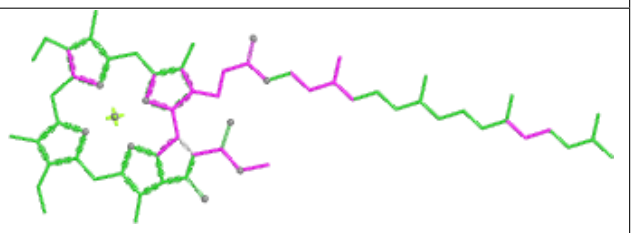


Rings

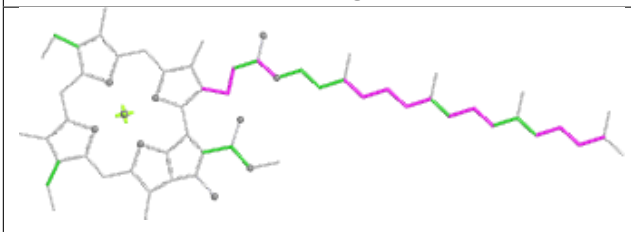
Ligand CLA G 611



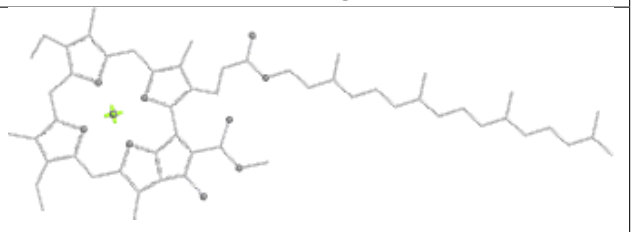
Bond lengths



Bond angles

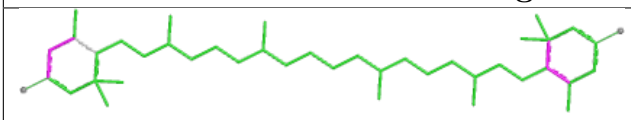


Torsions



Rings

Ligand LUT B 1621



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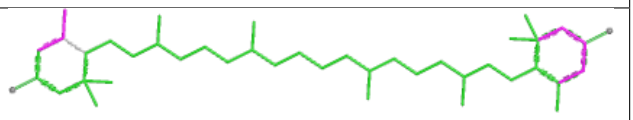
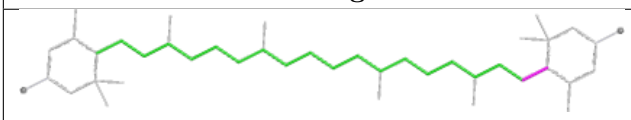


Bond angles



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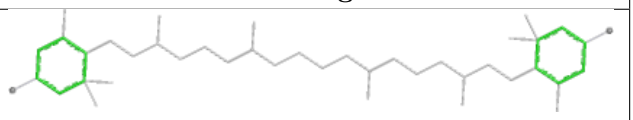
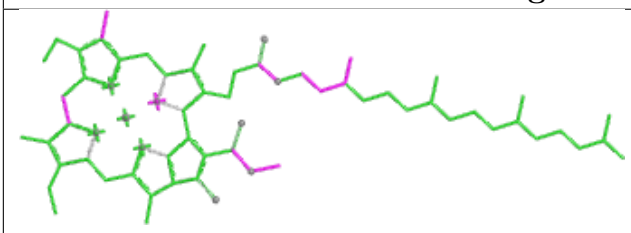


Rings

Ligand CLA J 602



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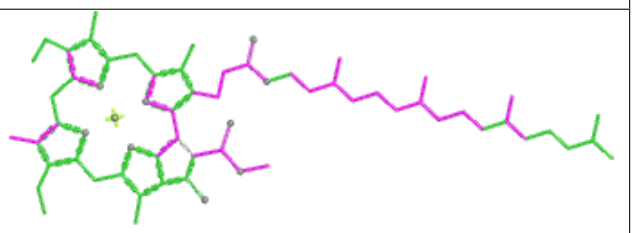
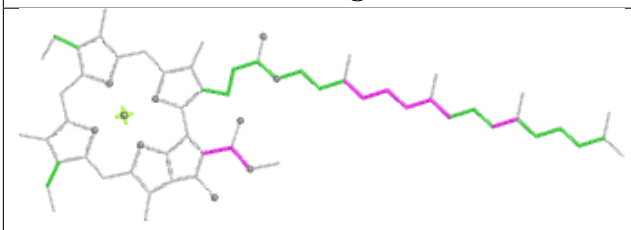


Bond angles



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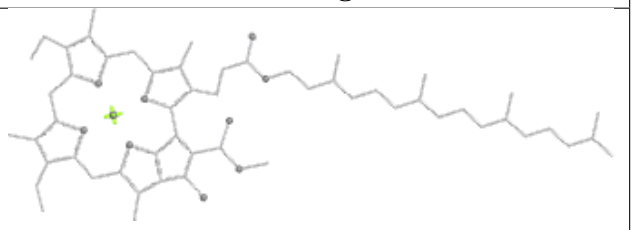
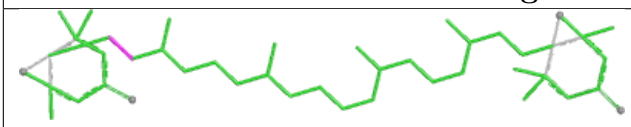


Rings

Ligand XAT I 9622



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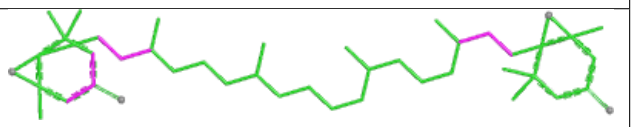
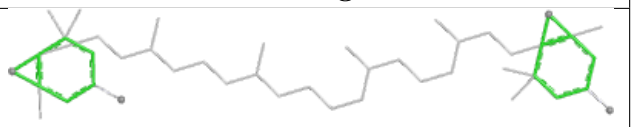


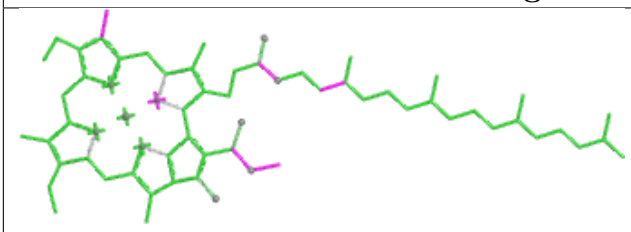
Bond angles

Torsions



Rings

Ligand CLA A 612



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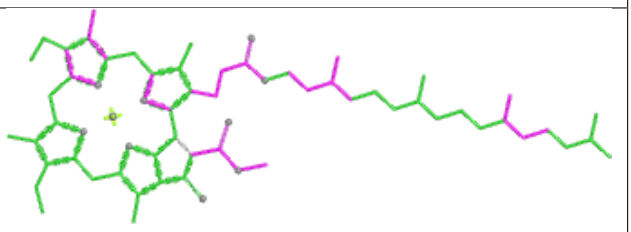
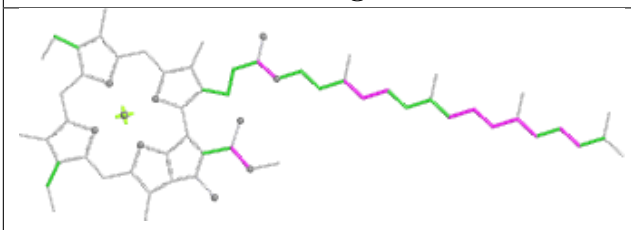


Bond angles



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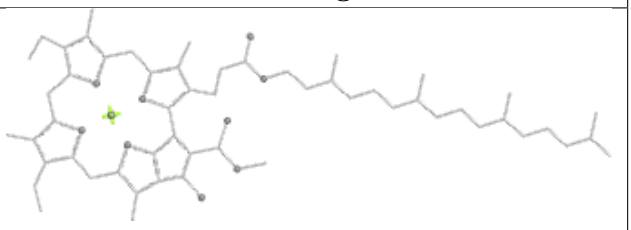
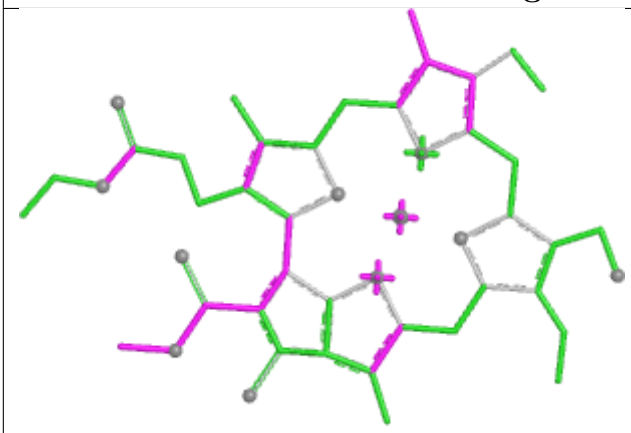


Rings

Ligand CHL C 605



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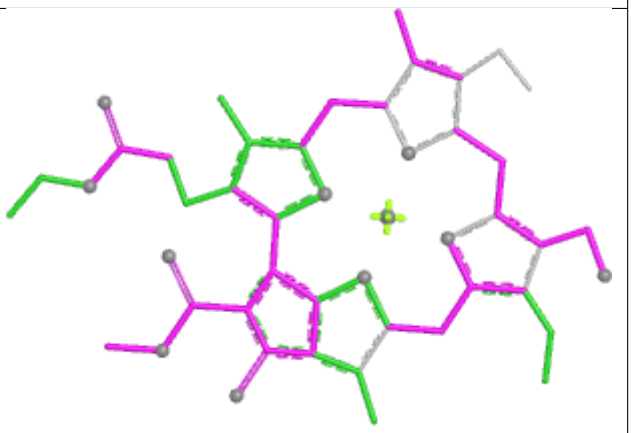
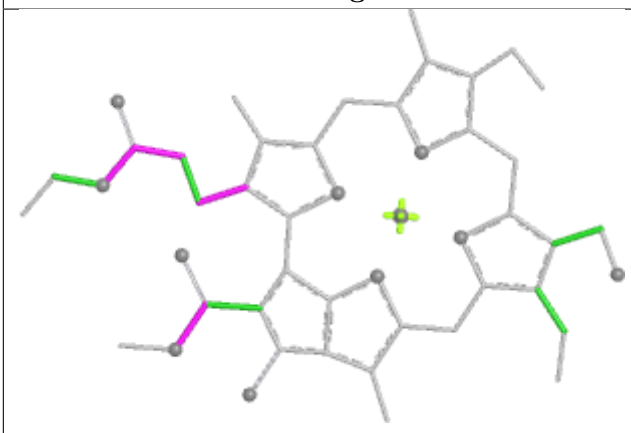
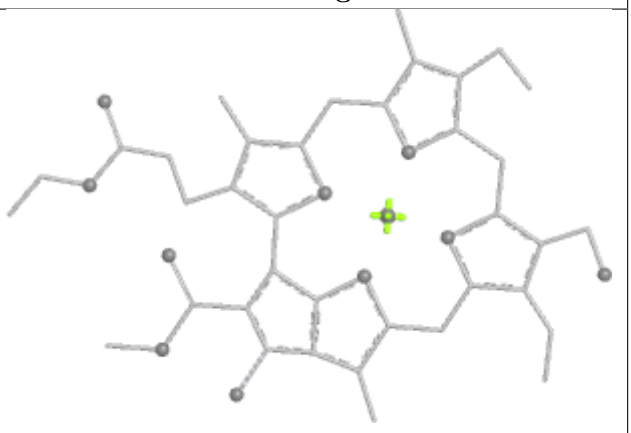


Bond angles

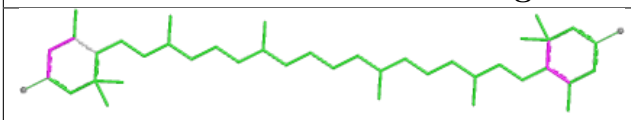


Torsions



Rings

Ligand LUT H 7621



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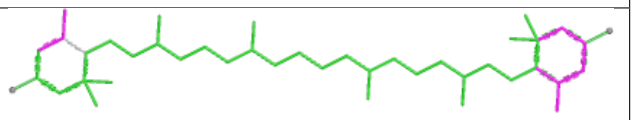
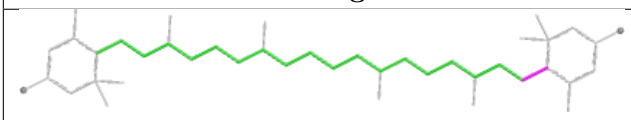


Bond angles



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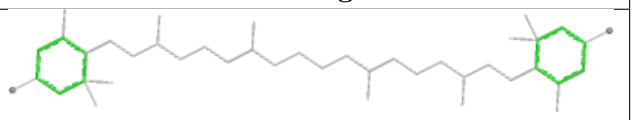
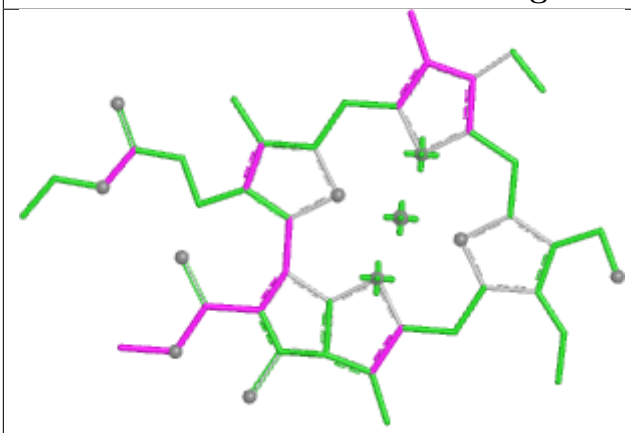


Rings

Ligand CHL I 605



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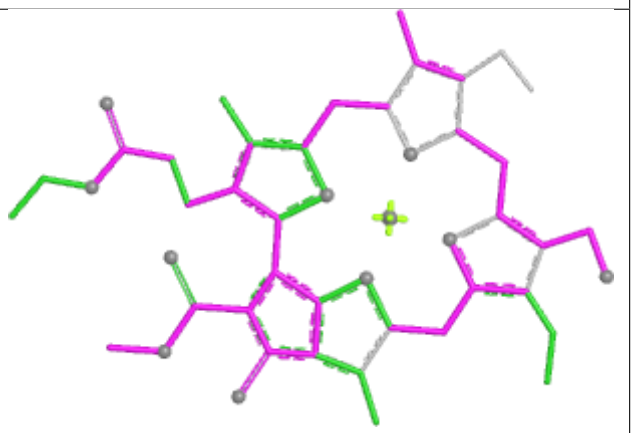
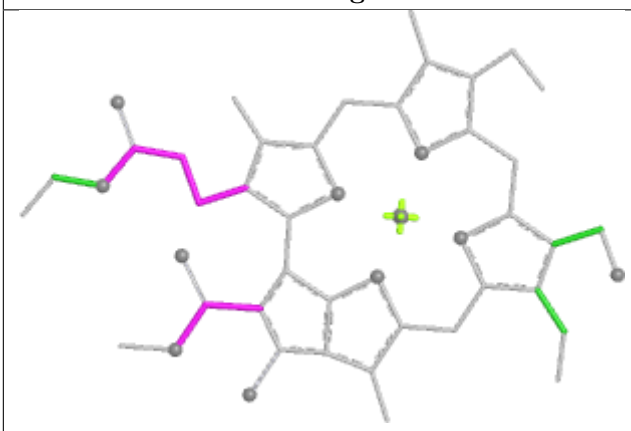
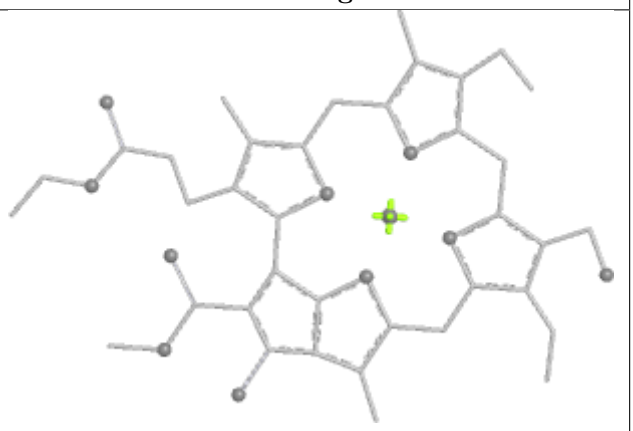


Bond angles



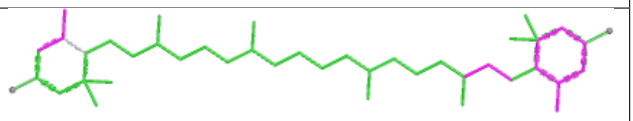
Torsions



Rings

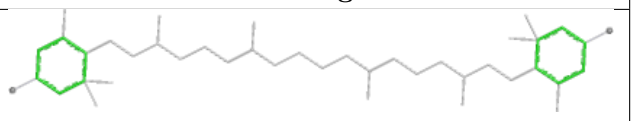
Ligand LUT F 5621

Bond lengths



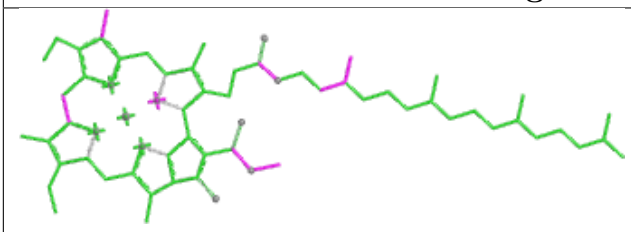
Bond angles

Torsions

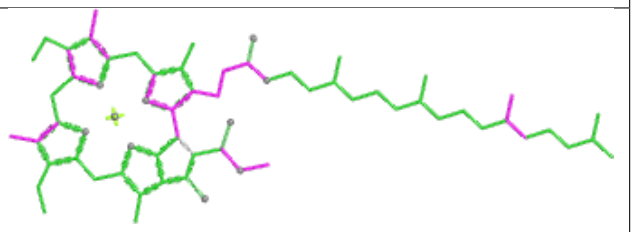


Rings

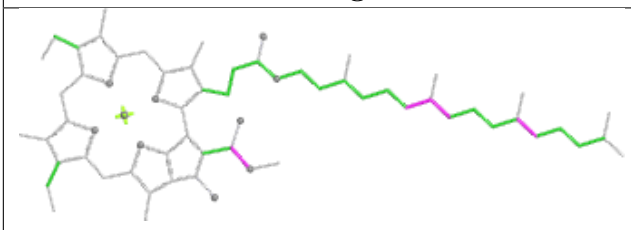
Ligand CLA F 610



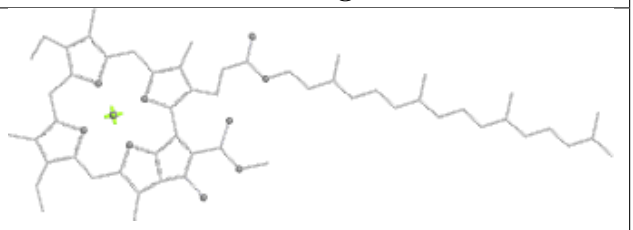
Bond lengths



Bond angles

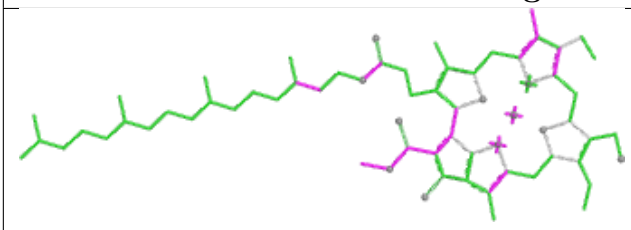


Torsions



Rings

Ligand CHL A 607



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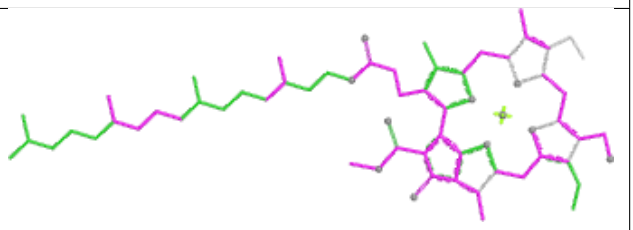
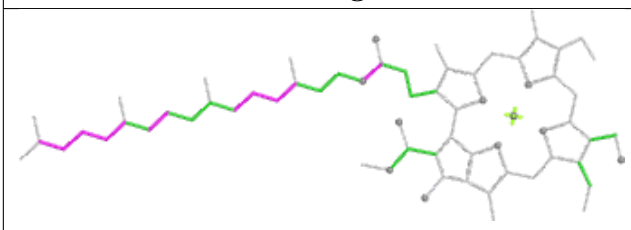
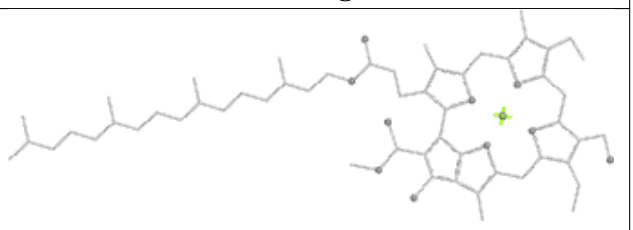


Bond angles

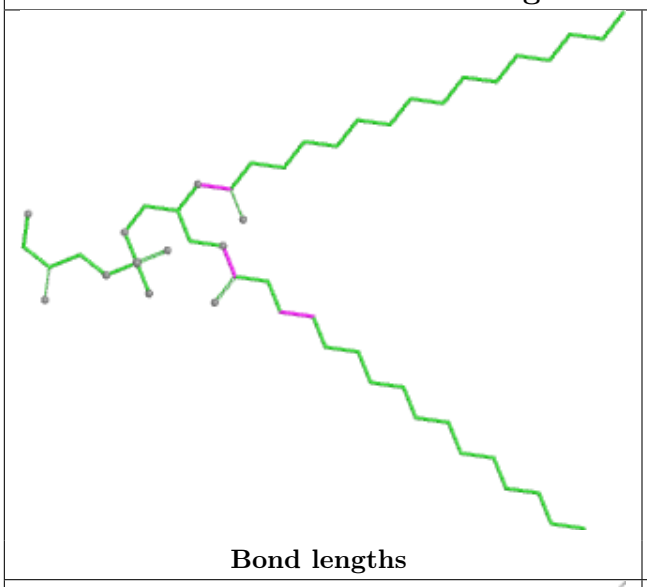


Torsions



Rings

Ligand LHG A 630



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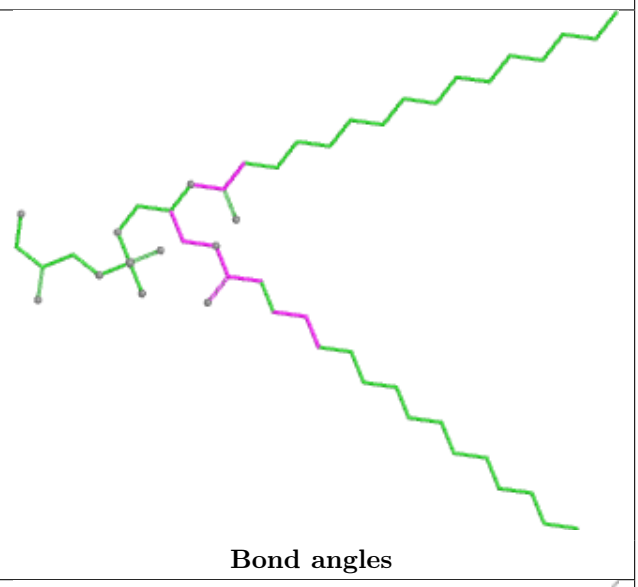
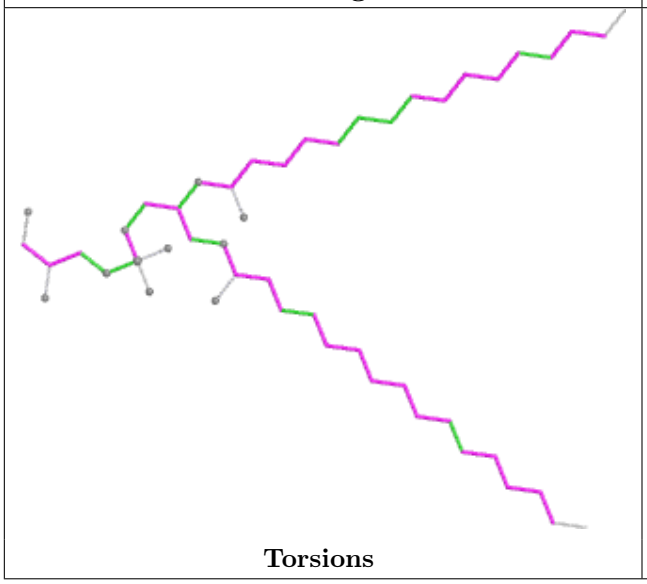
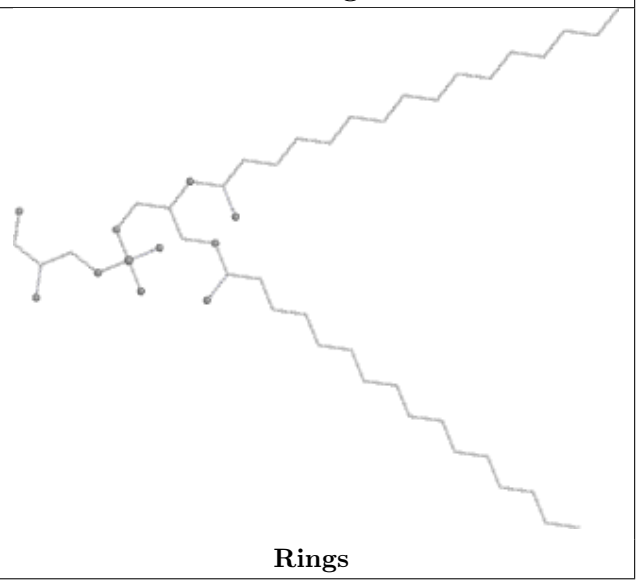


Bond angles

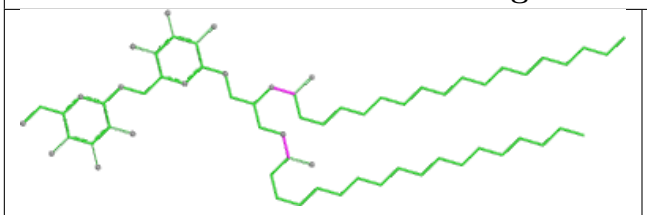


Torsions



Rings

Ligand DGD H 7632



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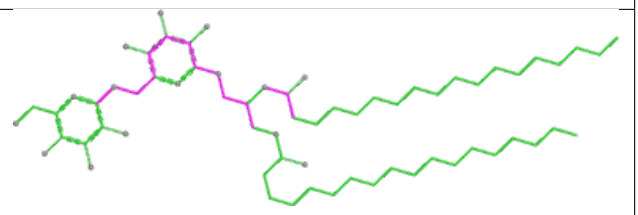
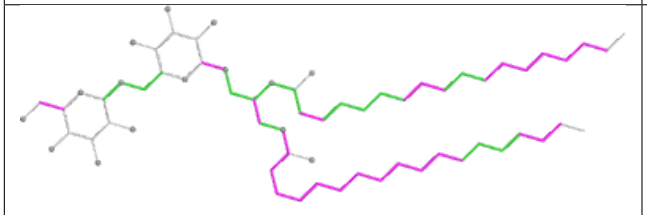


Bond angles



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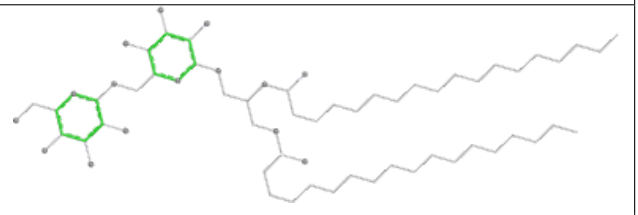
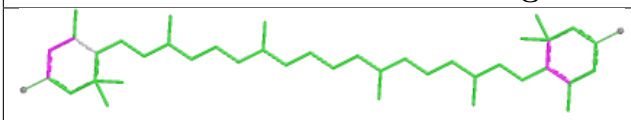


Rings

Ligand LUT I 8620



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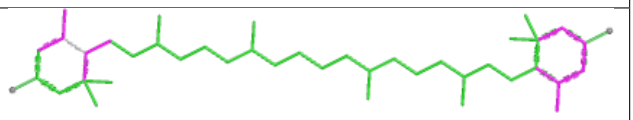
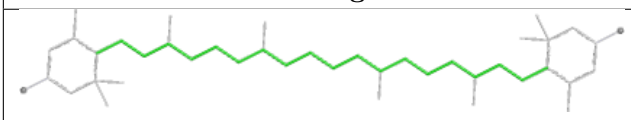


Bond angles



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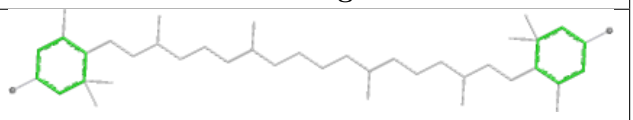
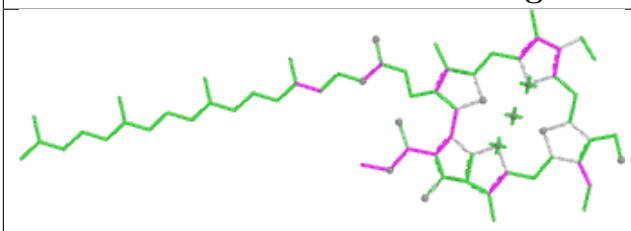


Rings

Ligand CHL F 601



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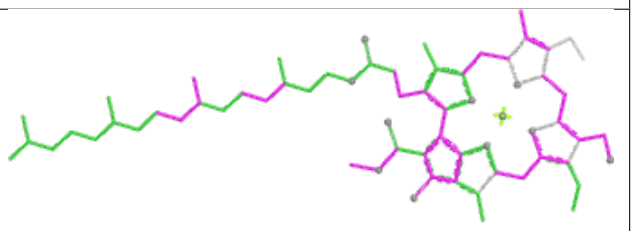
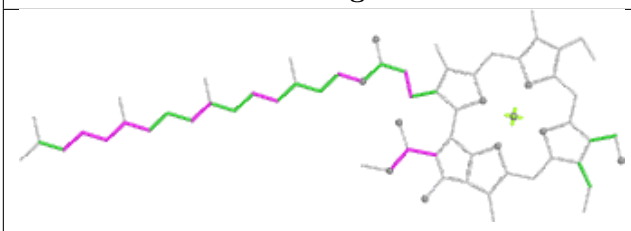


Bond angles



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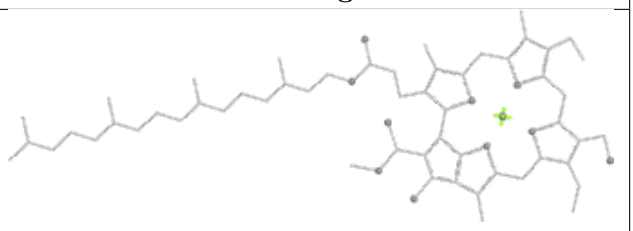
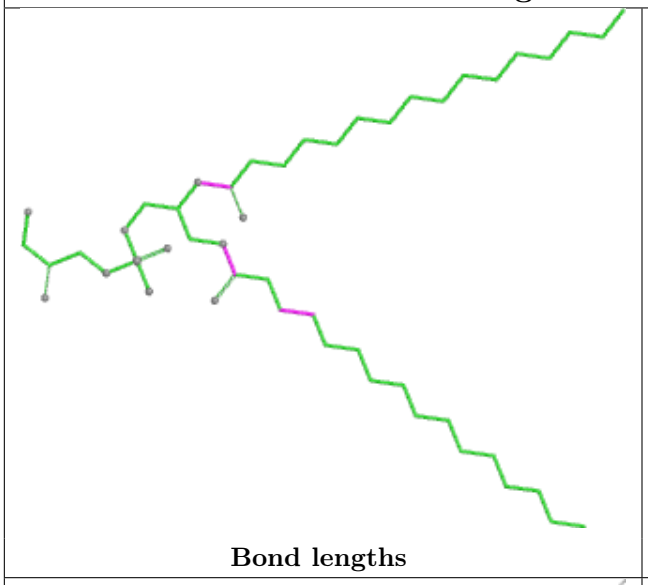


Rings

Ligand LHG B 1630



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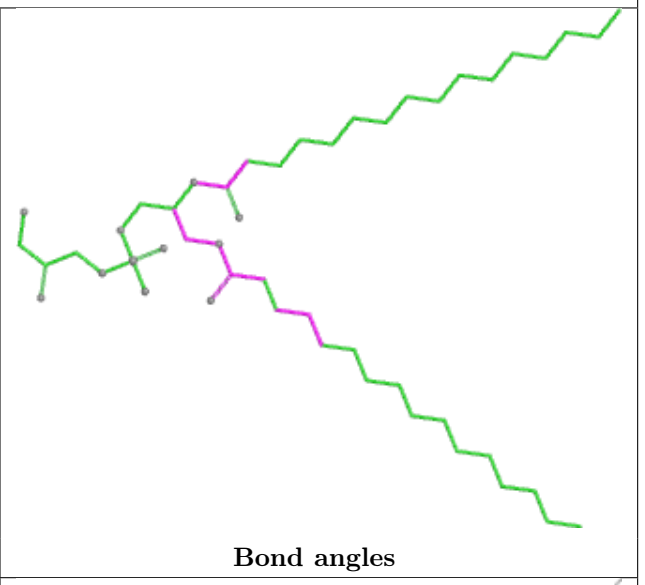
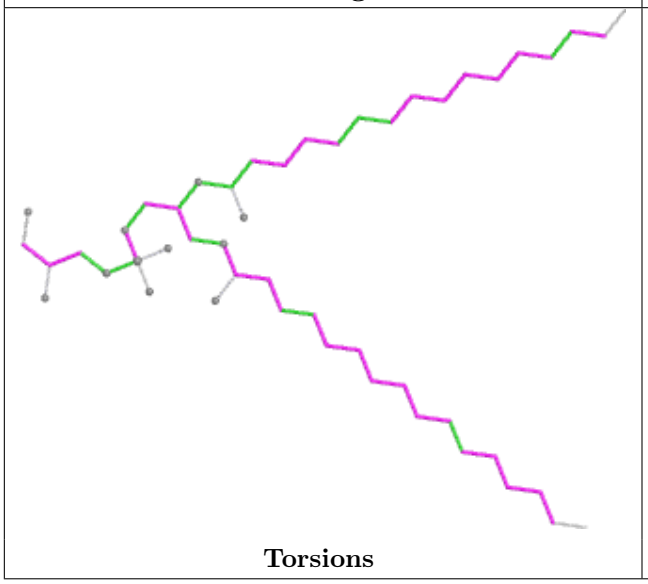


Bond angles



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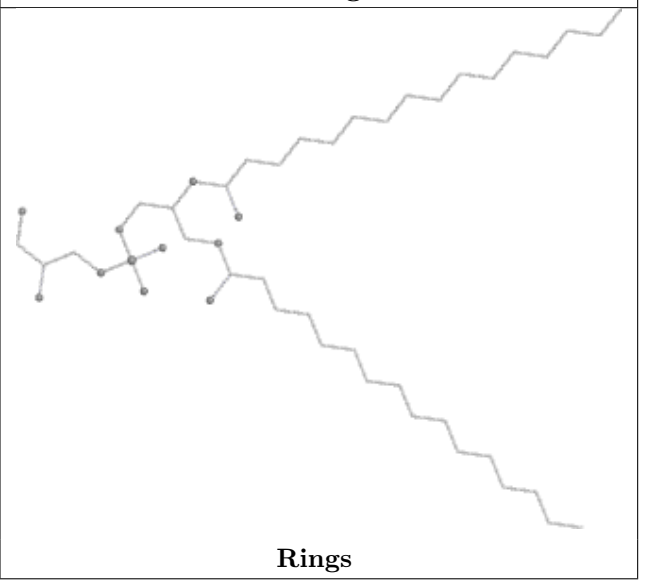
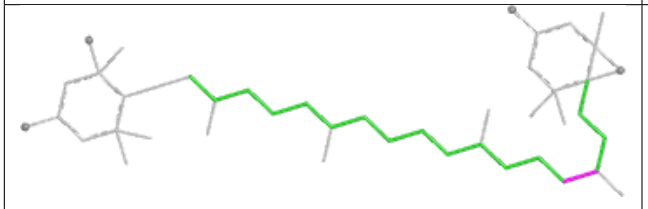


Rings

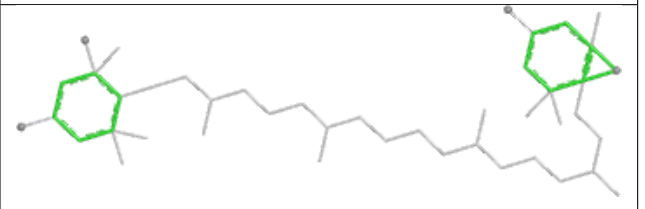
Ligand NEX D 3623

Bond lengths

Bond angles

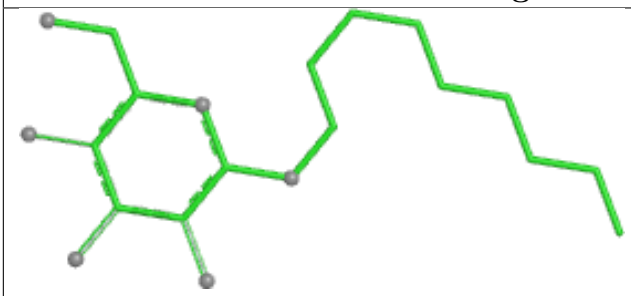


Torsions

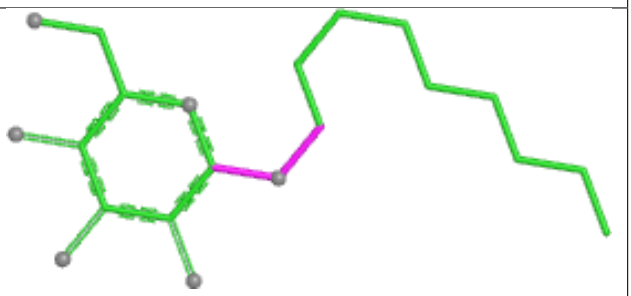


Rings

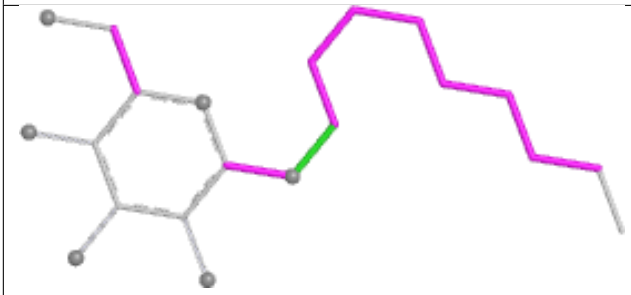
Ligand BNG B 1633



Bond lengths



Bond angles



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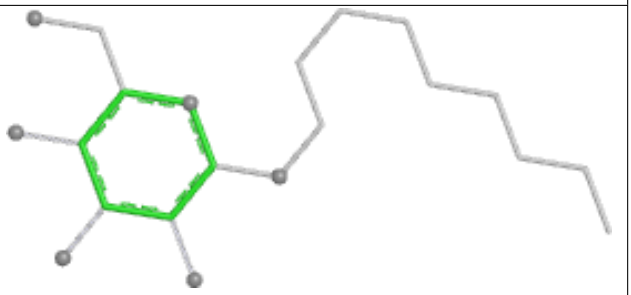
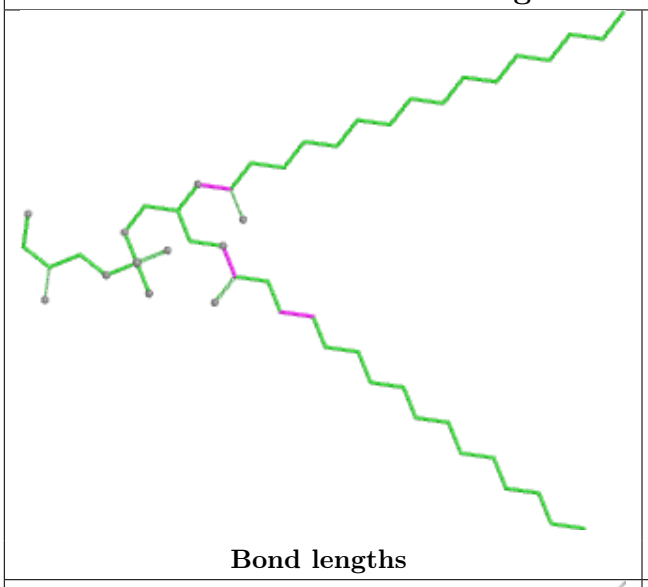


Rings

Ligand LHG G 6630



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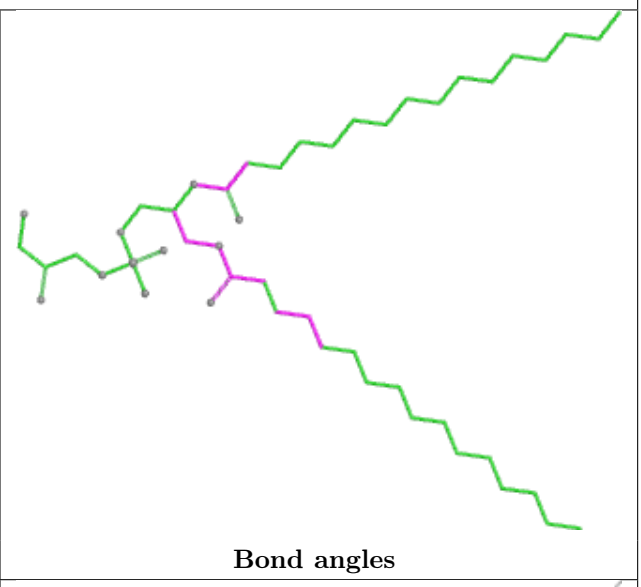
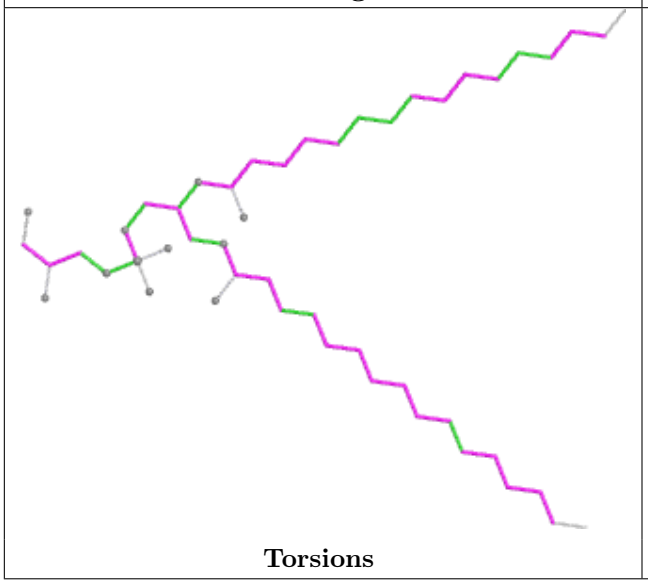


Bond angles



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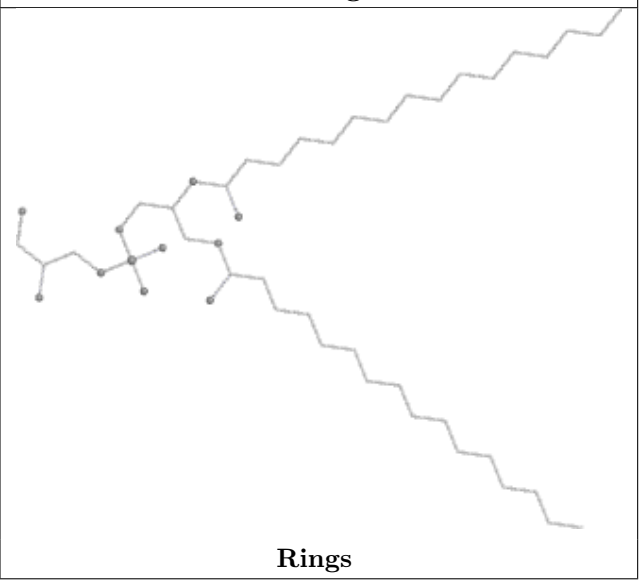
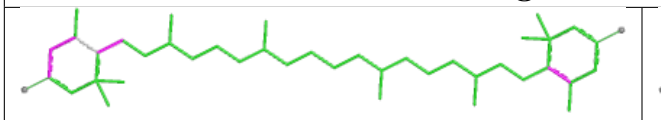


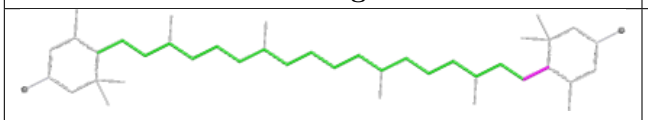
Rings

Ligand LUT D 3621



Bond lengths

Bond angles



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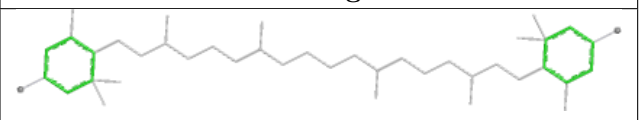
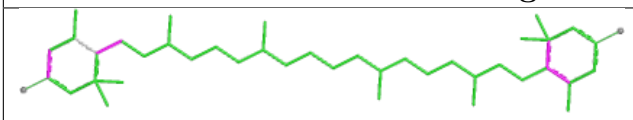


Rings

Ligand LUT J 9620



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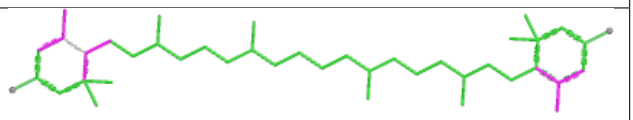
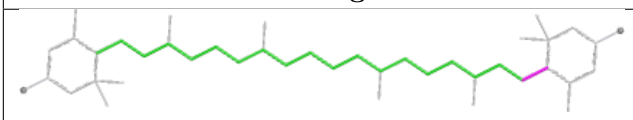


Bond angles



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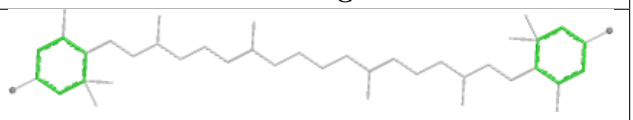
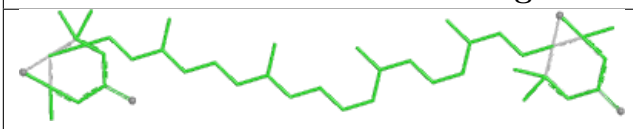
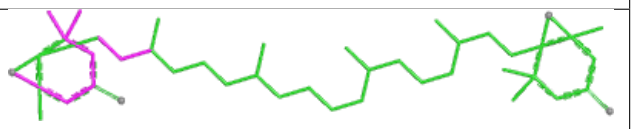


Rings

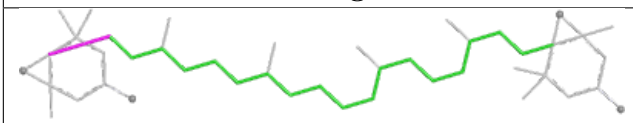
Ligand XAT B 5622



Bond lengths



Bond angles



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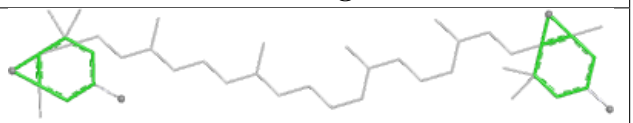
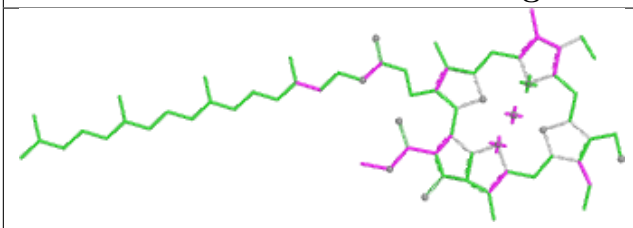
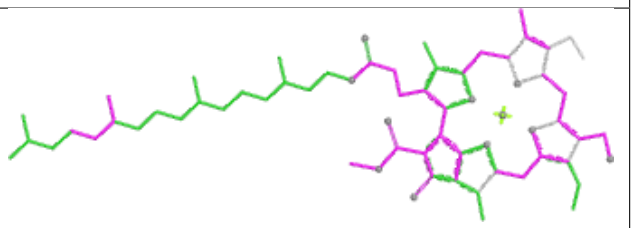


Rings

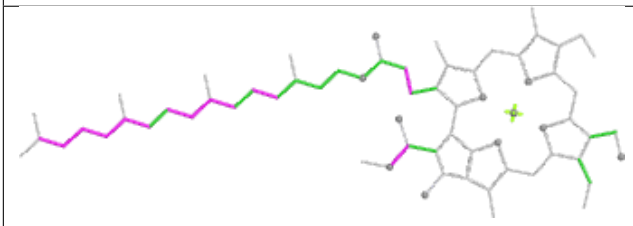
Ligand CHL G 608



Bond lengths



Bond angles



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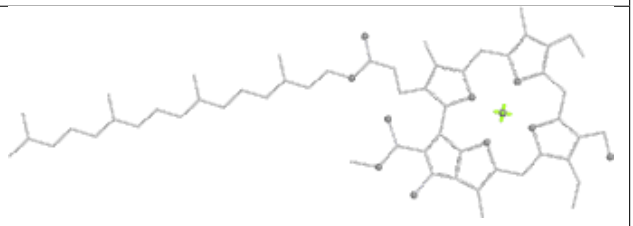
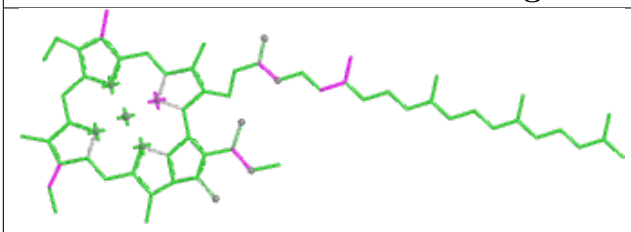
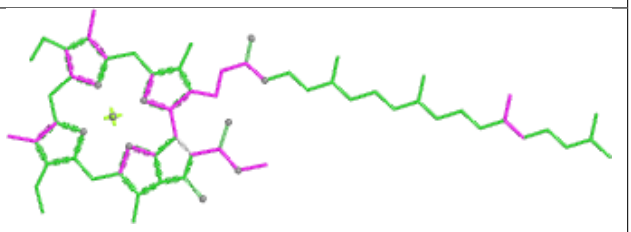


Rings

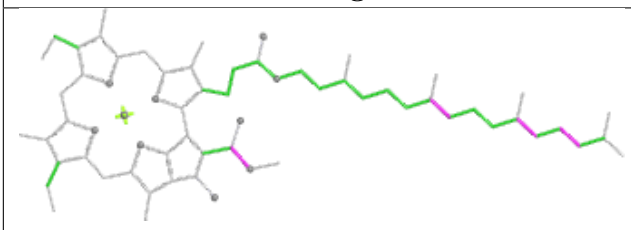
Ligand CLA A 610



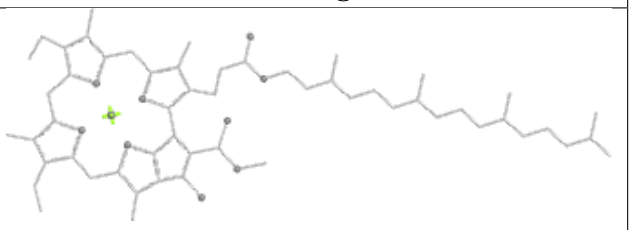
Bond lengths



Bond angles

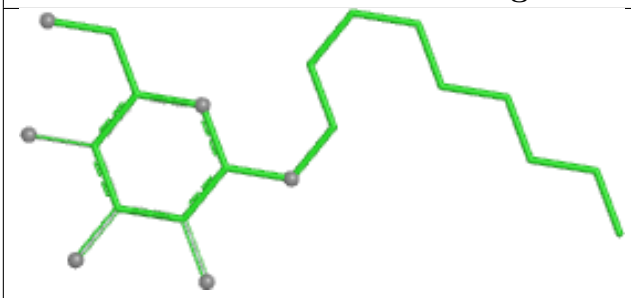


Torsions

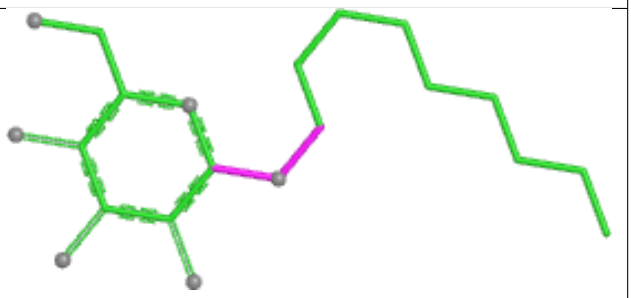


Rings

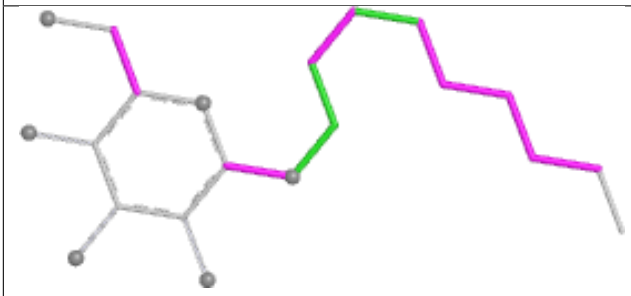
Ligand BNG G 6633



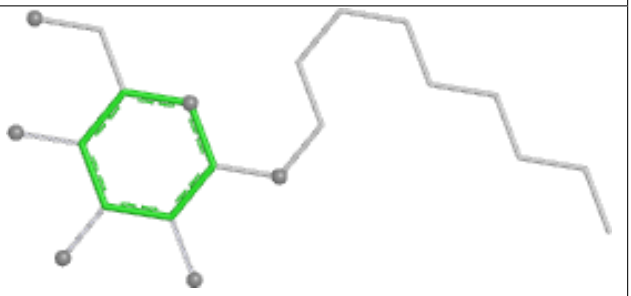
Bond lengths



Bond angles

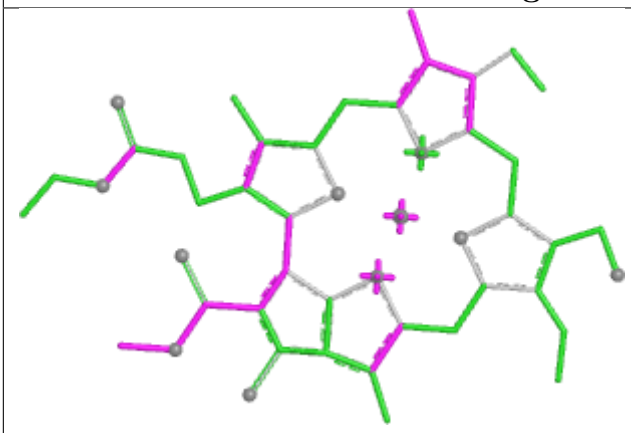


Torsions

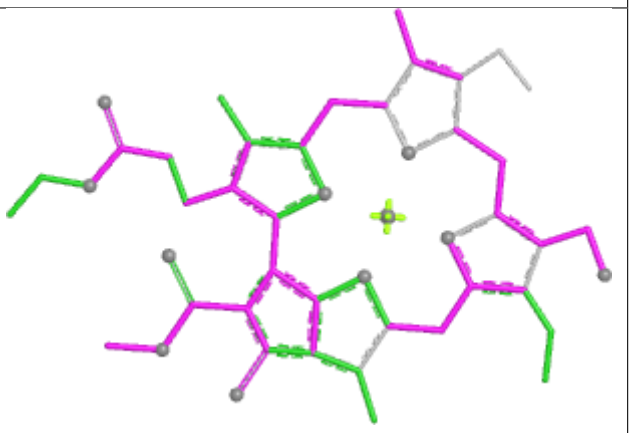


Rings

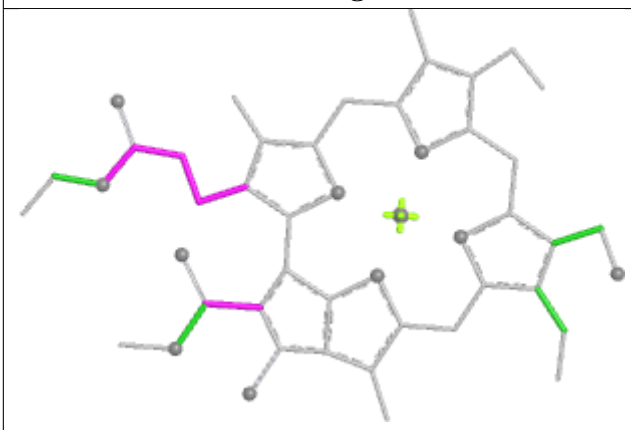
Ligand CHL H 605



Bond lengths



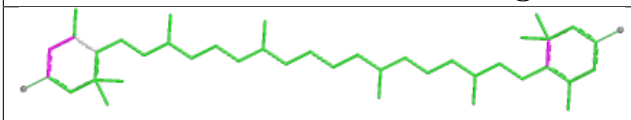
Bond angles



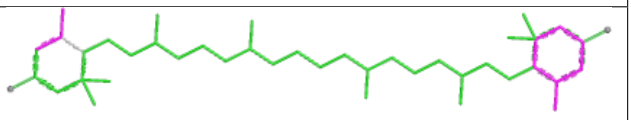
Torsions

Rings

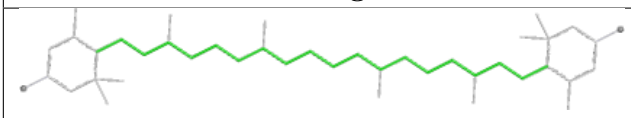
Ligand LUT G 6621



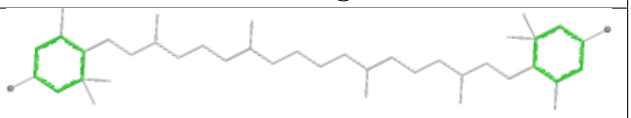
Bond lengths



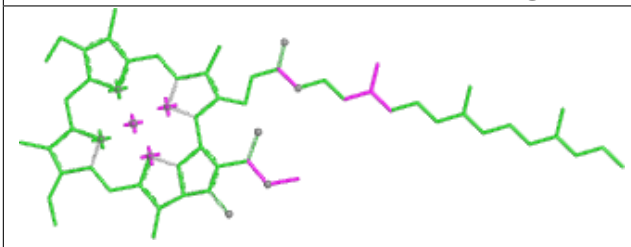
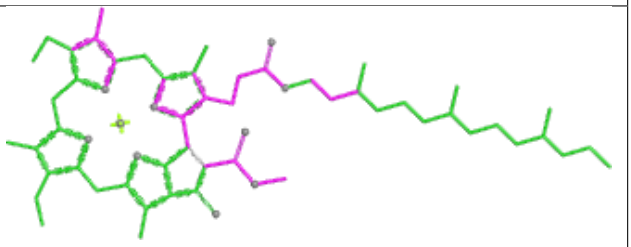
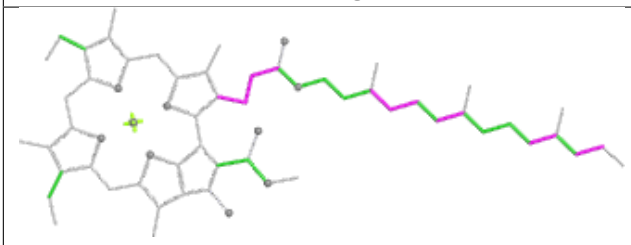
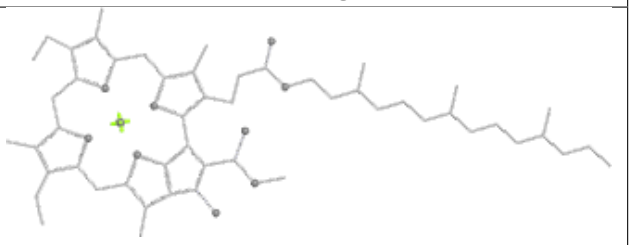
Bond angles

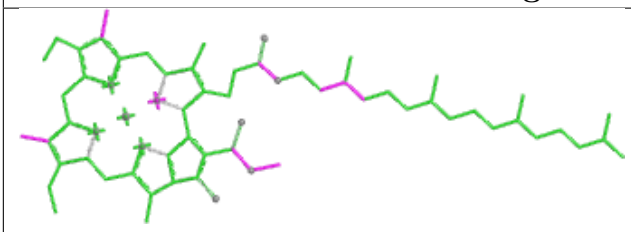
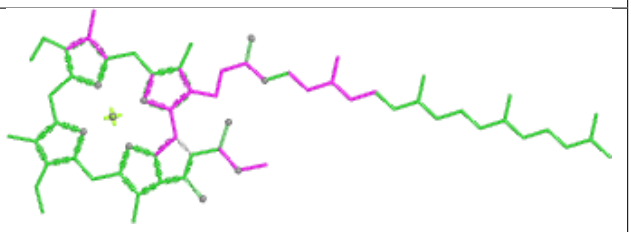
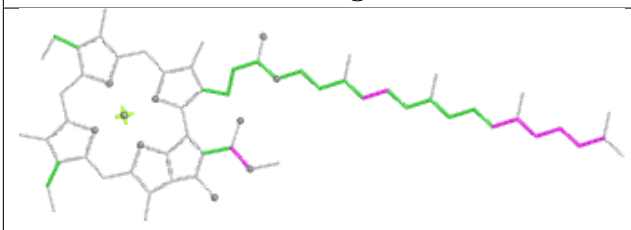
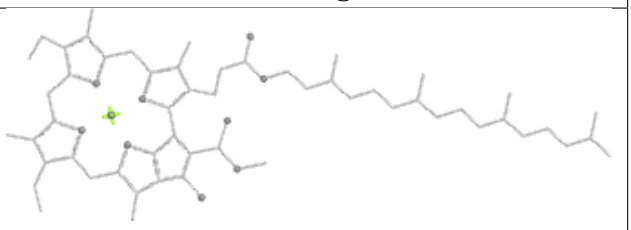


Torsions

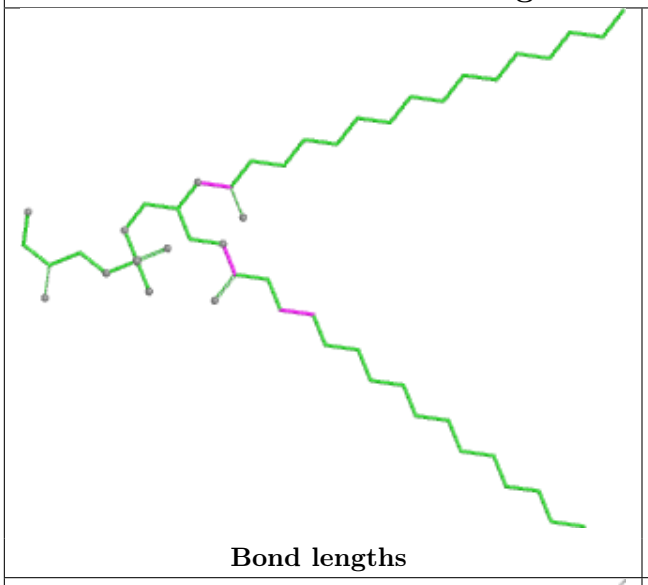


Rings

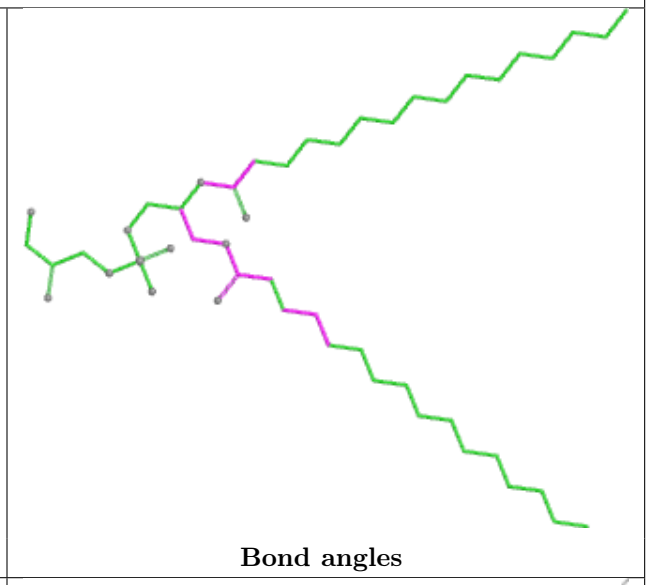
Ligand CLA A 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

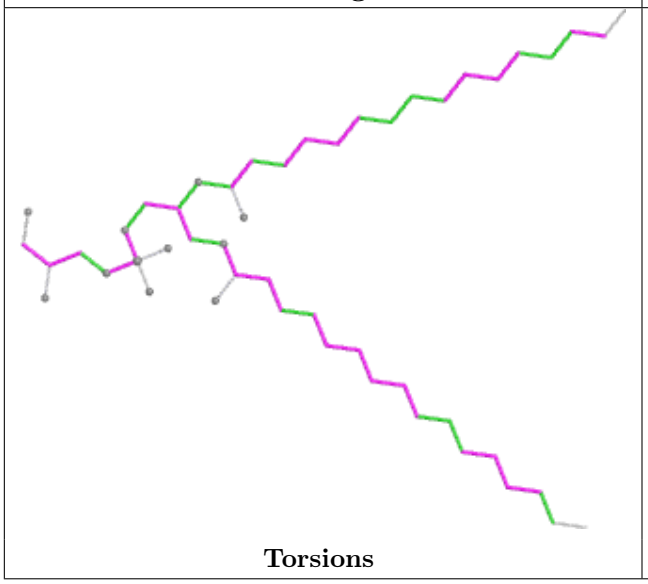
Ligand LHG E 4630



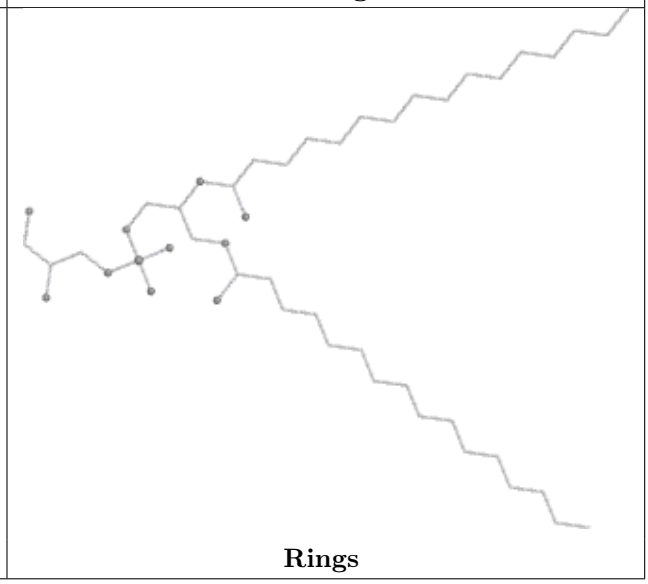
Bond lengths



Bond angles

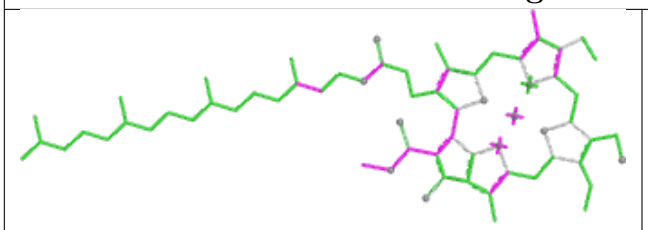


Torsions

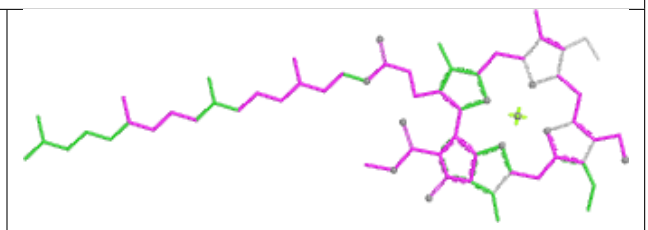


Rings

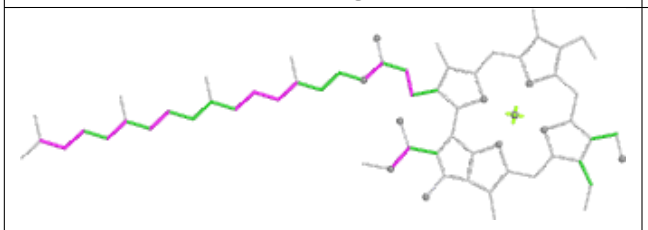
Ligand CHL E 607



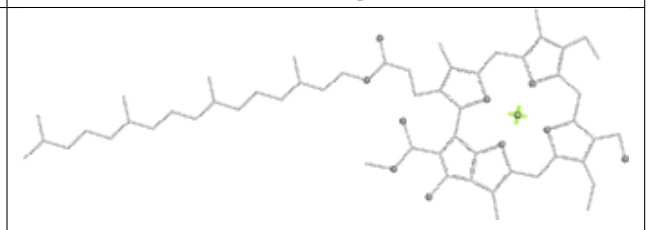
Bond lengths



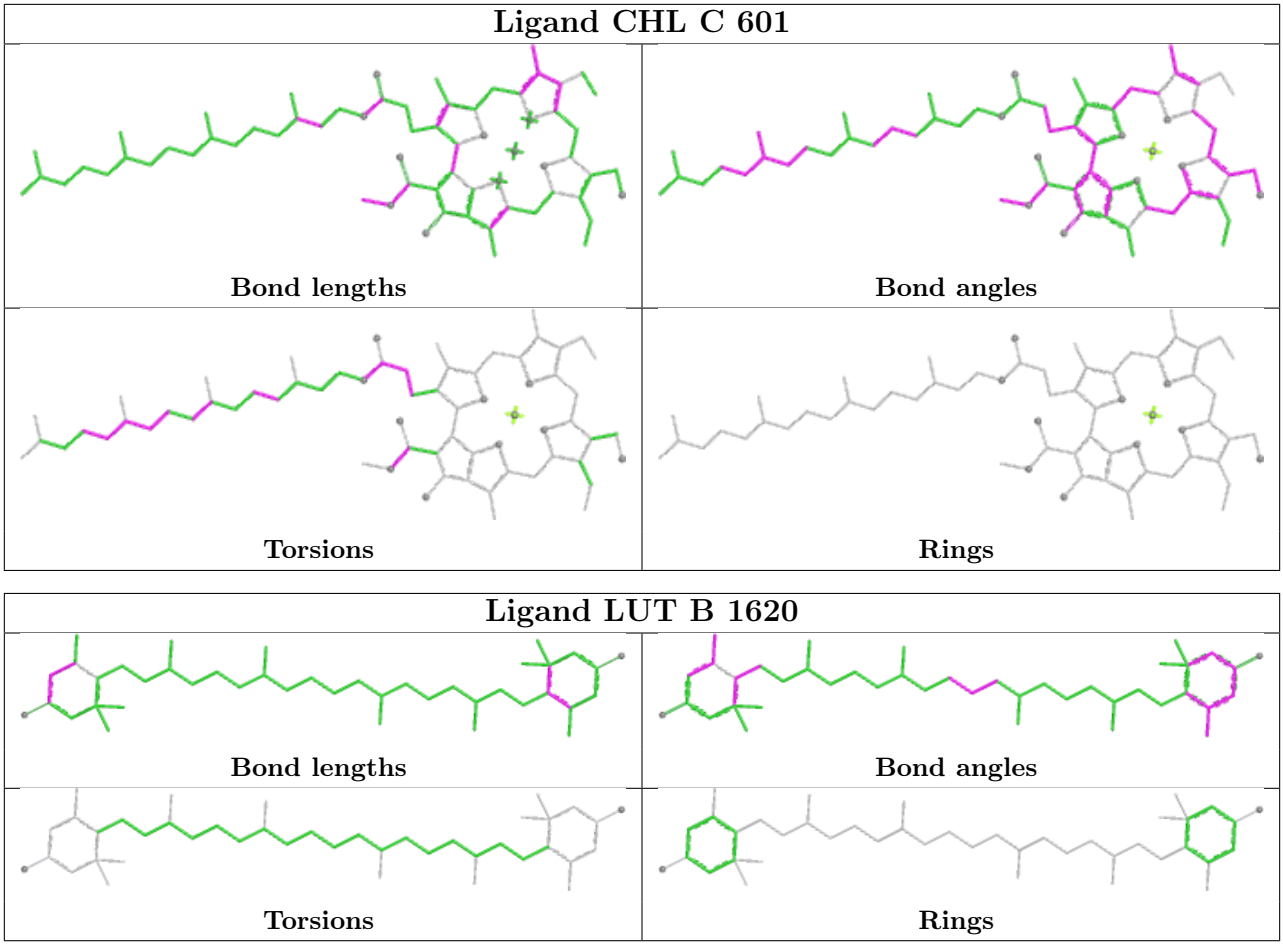
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	218/232 (93%)	-0.43	2 (0%)	81	80	18, 31, 53, 67	0
1	B	218/232 (93%)	-0.65	1 (0%)	87	86	15, 23, 42, 50	0
1	C	218/232 (93%)	-0.66	2 (0%)	81	80	14, 23, 40, 53	0
1	D	218/232 (93%)	-0.60	2 (0%)	81	80	16, 26, 44, 60	0
1	E	218/232 (93%)	-0.62	1 (0%)	87	86	14, 25, 41, 54	0
1	F	219/232 (94%)	-0.63	2 (0%)	81	80	14, 24, 42, 69	0
1	G	218/232 (93%)	-0.56	1 (0%)	87	86	16, 27, 47, 59	0
1	H	218/232 (93%)	-0.47	3 (1%)	73	71	18, 27, 49, 58	0
1	I	218/232 (93%)	-0.59	2 (0%)	81	80	17, 26, 45, 61	0
1	J	218/232 (93%)	-0.65	1 (0%)	87	86	15, 24, 42, 52	0
All	All	2181/2320 (94%)	-0.59	17 (0%)	82	81	14, 26, 46, 69	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	231	GLY	6.1
1	F	14	SER	4.3
1	A	231	GLY	4.1
1	G	231	GLY	4.1
1	D	231	GLY	3.9
1	F	232	LYS	3.5
1	J	231	GLY	3.2
1	H	107	GLU	2.9
1	C	107	GLU	2.6
1	A	153	ASP	2.5
1	I	231	GLY	2.5
1	H	149	GLY	2.5
1	B	107	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	14	SER	2.3
1	I	223	ASN	2.2
1	H	169	ASP	2.2
1	D	223	ASN	2.1

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BNG	D	3633	21/21	0.63	0.23	61,86,92,92	0
2	BNG	B	1633	21/21	0.64	0.23	63,86,92,93	0
2	BNG	C	2633	21/21	0.66	0.23	59,85,92,93	0
2	BNG	G	6633	21/21	0.69	0.22	75,96,102,104	0
2	BNG	A	633	21/21	0.70	0.19	72,92,95,96	0
2	BNG	H	7633	21/21	0.71	0.20	71,90,97,99	0
2	BNG	I	8633	21/21	0.72	0.19	67,86,93,93	0
2	BNG	J	9633	21/21	0.72	0.21	63,83,92,93	0
3	NA	A	634	1/1	0.72	0.43	1,1,1,1	1
2	BNG	E	4633	21/21	0.73	0.21	65,89,96,97	0
2	BNG	F	5633	21/21	0.78	0.18	55,83,91,91	0
8	DGD	A	632	66/66	0.86	0.14	26,46,79,80	0
8	DGD	H	7632	66/66	0.87	0.14	30,50,82,83	0
8	DGD	B	2632	66/66	0.88	0.13	21,44,77,79	0
8	DGD	D	3632	66/66	0.88	0.13	20,47,77,79	0
8	DGD	E	4632	66/66	0.88	0.14	27,41,87,89	0
8	DGD	G	9632	66/66	0.88	0.15	23,48,83,86	0
8	DGD	H	6632	66/66	0.88	0.14	24,49,83,84	0
8	DGD	B	1632	66/66	0.88	0.14	20,45,80,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	CLA	A	611	65/65	0.88	0.12	40,48,78,78	0
8	DGD	I	8632	66/66	0.89	0.13	24,49,85,86	0
9	CHL	I	605	48/66	0.89	0.10	29,32,60,73	0
8	DGD	D	5632	66/66	0.89	0.14	23,43,89,91	0
9	CHL	F	605	48/66	0.90	0.09	26,29,59,72	0
10	CLA	B	611	65/65	0.90	0.11	24,31,69,69	0
10	CLA	D	611	65/65	0.90	0.12	25,34,65,66	0
10	CLA	C	611	65/65	0.91	0.11	28,33,76,77	0
5	XAT	B	5622	44/44	0.91	0.08	12,22,27,31	0
10	CLA	G	611	65/65	0.91	0.11	33,39,75,77	0
10	CLA	H	611	65/65	0.91	0.11	33,39,71,72	0
7	LHG	A	630	49/49	0.92	0.10	39,47,61,63	0
9	CHL	G	608	66/66	0.92	0.10	27,31,67,68	0
9	CHL	H	608	66/66	0.92	0.09	28,31,69,72	0
7	LHG	B	1630	49/49	0.92	0.10	32,40,55,60	0
7	LHG	D	3630	49/49	0.92	0.10	30,36,55,60	0
7	LHG	E	4630	49/49	0.92	0.09	28,37,52,55	0
7	LHG	G	6630	49/49	0.92	0.09	31,38,57,61	0
7	LHG	H	7630	49/49	0.92	0.10	30,37,57,62	0
10	CLA	D	612	65/65	0.92	0.09	22,30,83,85	0
10	CLA	E	611	65/65	0.92	0.10	26,32,70,72	0
5	XAT	A	622	44/44	0.92	0.08	16,26,34,38	0
10	CLA	H	610	65/65	0.92	0.09	24,32,69,74	0
5	XAT	D	8622	44/44	0.92	0.08	18,23,30,33	0
10	CLA	I	611	65/65	0.92	0.10	27,33,71,72	0
9	CHL	G	605	48/66	0.93	0.08	24,27,59,75	0
9	CHL	G	606	51/66	0.93	0.07	15,23,59,60	0
6	NEX	H	7623	44/44	0.93	0.11	28,46,82,84	0
5	XAT	B	1622	44/44	0.93	0.08	17,23,28,30	0
5	XAT	E	2622	44/44	0.93	0.08	16,22,27,30	0
9	CHL	J	605	48/66	0.93	0.08	20,26,59,71	0
9	CHL	J	606	51/66	0.93	0.07	16,22,60,62	0
10	CLA	A	610	65/65	0.93	0.09	27,36,73,78	0
5	XAT	F	6622	44/44	0.93	0.08	15,22,29,32	0
10	CLA	A	612	65/65	0.93	0.09	33,38,86,88	0
10	CLA	A	614	49/65	0.93	0.08	20,27,59,66	0
5	XAT	H	4622	44/44	0.93	0.08	20,24,30,34	0
7	LHG	F	5630	49/49	0.93	0.08	25,33,48,52	0
10	CLA	C	612	65/65	0.93	0.09	20,31,82,85	0
5	XAT	I	9622	44/44	0.93	0.07	15,22,29,32	0
6	NEX	A	623	44/44	0.93	0.11	27,53,90,91	0
7	LHG	J	9630	49/49	0.93	0.09	26,35,54,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	CLA	F	612	65/65	0.93	0.09	22,28,79,81	0
9	CHL	A	608	66/66	0.93	0.09	30,35,67,68	0
9	CHL	C	606	51/66	0.93	0.08	16,22,63,64	0
6	NEX	G	6623	44/44	0.93	0.10	30,42,80,82	0
10	CLA	H	612	65/65	0.93	0.09	24,34,86,87	0
9	CHL	F	608	66/66	0.93	0.08	22,28,63,65	0
9	CHL	H	605	48/66	0.94	0.08	24,30,60,73	0
9	CHL	H	606	51/66	0.94	0.08	17,22,67,69	0
6	NEX	I	8623	44/44	0.94	0.09	27,36,77,80	0
7	LHG	I	8630	49/49	0.94	0.08	29,34,55,57	0
9	CHL	I	606	51/66	0.94	0.07	15,19,62,64	0
9	CHL	I	608	66/66	0.94	0.08	21,26,66,67	0
6	NEX	J	9623	44/44	0.94	0.10	22,40,85,86	0
9	CHL	A	605	48/66	0.94	0.08	19,25,57,71	0
9	CHL	J	608	66/66	0.94	0.08	19,26,67,68	0
10	CLA	A	603	65/65	0.94	0.07	20,26,77,78	0
9	CHL	A	606	51/66	0.94	0.07	19,24,66,67	0
6	NEX	B	1623	44/44	0.94	0.09	19,36,75,78	0
9	CHL	C	605	48/66	0.94	0.08	25,29,58,72	0
6	NEX	C	2623	44/44	0.94	0.10	17,35,85,87	0
10	CLA	B	610	65/65	0.94	0.08	19,25,62,68	0
9	CHL	C	608	66/66	0.94	0.08	23,28,60,61	0
10	CLA	B	612	65/65	0.94	0.08	18,27,88,89	0
10	CLA	C	610	65/65	0.94	0.08	15,21,65,70	0
9	CHL	D	605	48/66	0.94	0.08	23,29,57,71	0
9	CHL	D	608	66/66	0.94	0.08	24,29,65,67	0
9	CHL	E	605	48/66	0.94	0.08	20,25,58,71	0
9	CHL	E	606	51/66	0.94	0.07	18,21,60,62	0
10	CLA	E	610	65/65	0.94	0.08	17,25,59,66	0
9	CHL	E	607	66/66	0.94	0.08	16,20,51,51	0
10	CLA	E	612	65/65	0.94	0.08	19,25,80,82	0
10	CLA	E	614	49/65	0.94	0.07	15,23,57,68	0
10	CLA	F	604	62/65	0.94	0.08	17,21,76,81	0
10	CLA	F	611	65/65	0.94	0.09	20,26,73,75	0
7	LHG	C	2630	49/49	0.94	0.09	24,30,48,50	0
10	CLA	G	603	65/65	0.94	0.08	17,22,69,71	0
10	CLA	G	610	65/65	0.94	0.08	24,31,73,79	0
9	CHL	F	606	51/66	0.94	0.07	13,21,61,62	0
10	CLA	G	612	65/65	0.94	0.09	22,33,89,91	0
10	CLA	H	604	62/65	0.94	0.08	18,25,69,74	0
6	NEX	D	3623	44/44	0.94	0.09	22,34,76,79	0
6	NEX	E	4623	44/44	0.94	0.09	16,30,74,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	XAT	J	3622	44/44	0.94	0.07	17,24,29,31	0
10	CLA	H	614	49/65	0.94	0.07	16,26,60,68	0
10	CLA	I	610	65/65	0.94	0.08	21,26,62,68	0
5	XAT	C	7622	44/44	0.94	0.07	17,23,31,34	0
10	CLA	I	612	65/65	0.94	0.09	23,30,87,90	0
10	CLA	J	603	65/65	0.94	0.07	13,20,71,72	0
10	CLA	J	604	62/65	0.94	0.08	15,22,72,76	0
10	CLA	J	611	65/65	0.94	0.09	20,26,68,69	0
10	CLA	J	614	49/65	0.94	0.08	14,22,57,67	0
10	CLA	C	604	62/65	0.95	0.08	15,21,70,75	0
9	CHL	A	607	66/66	0.95	0.07	17,20,48,49	0
9	CHL	H	601	66/66	0.95	0.07	28,31,32,36	0
9	CHL	D	606	51/66	0.95	0.07	16,22,60,61	0
10	CLA	C	614	49/65	0.95	0.07	14,18,54,65	0
10	CLA	D	603	65/65	0.95	0.07	14,21,74,75	0
10	CLA	D	610	65/65	0.95	0.07	21,26,64,69	0
9	CHL	D	607	66/66	0.95	0.07	11,14,52,57	0
9	CHL	H	607	66/66	0.95	0.07	12,18,49,50	0
10	CLA	D	614	49/65	0.95	0.07	10,21,54,64	0
10	CLA	E	604	62/65	0.95	0.08	18,23,75,79	0
6	NEX	F	5623	44/44	0.95	0.09	21,33,78,81	0
9	CHL	H	609	66/66	0.95	0.07	21,26,45,51	0
9	CHL	I	601	66/66	0.95	0.07	22,26,34,35	0
9	CHL	D	609	66/66	0.95	0.07	18,23,42,46	0
10	CLA	F	603	65/65	0.95	0.07	14,22,74,77	0
9	CHL	E	601	66/66	0.95	0.06	23,28,31,33	0
10	CLA	F	610	65/65	0.95	0.07	15,20,63,68	0
9	CHL	I	607	66/66	0.95	0.07	11,17,53,56	0
9	CHL	A	609	66/66	0.95	0.07	23,27,50,54	0
10	CLA	G	602	65/65	0.95	0.07	17,21,44,46	0
9	CHL	B	601	66/66	0.95	0.07	22,26,37,38	0
10	CLA	G	604	62/65	0.95	0.08	17,24,75,79	0
9	CHL	B	606	51/66	0.95	0.07	11,20,60,62	0
9	CHL	J	607	66/66	0.95	0.07	12,17,45,47	0
9	CHL	E	608	66/66	0.95	0.07	14,19,67,69	0
10	CLA	G	614	49/65	0.95	0.07	12,22,58,67	0
10	CLA	H	602	65/65	0.95	0.07	20,23,47,48	0
10	CLA	H	603	65/65	0.95	0.07	15,19,78,79	0
10	CLA	A	602	65/65	0.95	0.07	20,30,52,54	0
9	CHL	C	601	66/66	0.95	0.07	17,22,32,33	0
10	CLA	A	604	62/65	0.95	0.07	18,25,74,79	0
9	CHL	A	601	66/66	0.95	0.07	31,36,39,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	CHL	F	607	66/66	0.95	0.07	13,19,41,43	0
10	CLA	I	602	65/65	0.95	0.07	17,21,52,57	0
10	CLA	I	604	62/65	0.95	0.08	20,25,77,81	0
4	LUT	G	6621	42/42	0.95	0.07	16,21,23,25	0
9	CHL	G	601	66/66	0.95	0.06	27,32,36,40	0
10	CLA	B	604	62/65	0.95	0.08	19,22,75,78	0
10	CLA	I	614	49/65	0.95	0.07	20,23,58,67	0
9	CHL	C	607	66/66	0.95	0.07	15,18,46,49	0
4	LUT	G	6620	42/42	0.95	0.07	16,25,36,37	0
10	CLA	J	610	65/65	0.95	0.07	18,24,64,67	0
9	CHL	G	607	66/66	0.95	0.07	15,17,49,51	0
10	CLA	J	612	65/65	0.95	0.08	18,25,79,82	0
10	CLA	B	614	49/65	0.95	0.07	10,22,59,69	0
9	CHL	J	609	66/66	0.96	0.06	13,19,39,43	0
9	CHL	F	609	66/66	0.96	0.07	14,22,43,47	0
10	CLA	E	613	65/65	0.96	0.07	15,18,54,57	0
4	LUT	E	4620	42/42	0.96	0.06	16,21,29,30	0
10	CLA	F	602	65/65	0.96	0.06	9,17,42,48	0
4	LUT	F	5620	42/42	0.96	0.06	15,22,26,26	0
9	CHL	C	609	66/66	0.96	0.06	15,22,41,42	0
9	CHL	D	601	66/66	0.96	0.06	22,27,30,32	0
4	LUT	F	5621	42/42	0.96	0.06	11,19,22,24	0
10	CLA	A	613	65/65	0.96	0.07	15,19,46,49	0
10	CLA	F	613	65/65	0.96	0.06	14,17,45,48	0
10	CLA	F	614	49/65	0.96	0.06	12,20,57,68	0
9	CHL	G	609	66/66	0.96	0.06	18,25,42,46	0
10	CLA	B	602	65/65	0.96	0.07	16,21,51,54	0
10	CLA	B	603	65/65	0.96	0.07	10,19,74,76	0
4	LUT	A	620	42/42	0.96	0.06	19,26,38,39	0
4	LUT	A	621	42/42	0.96	0.06	17,20,25,26	0
4	LUT	H	7620	42/42	0.96	0.06	16,22,35,36	0
4	LUT	I	8620	42/42	0.96	0.06	15,23,35,36	0
4	LUT	J	9620	42/42	0.96	0.06	11,18,34,35	0
10	CLA	C	602	65/65	0.96	0.06	10,19,38,39	0
10	CLA	C	603	65/65	0.96	0.07	12,18,76,78	0
9	CHL	B	605	48/66	0.96	0.07	23,26,58,74	0
4	LUT	J	9621	42/42	0.96	0.06	14,19,21,24	0
9	CHL	B	607	66/66	0.96	0.06	13,16,44,45	0
9	CHL	B	608	66/66	0.96	0.07	16,22,63,63	0
9	CHL	E	609	66/66	0.96	0.06	16,19,40,43	0
10	CLA	I	603	65/65	0.96	0.07	16,20,64,65	0
10	CLA	D	602	65/65	0.96	0.06	13,20,45,46	0

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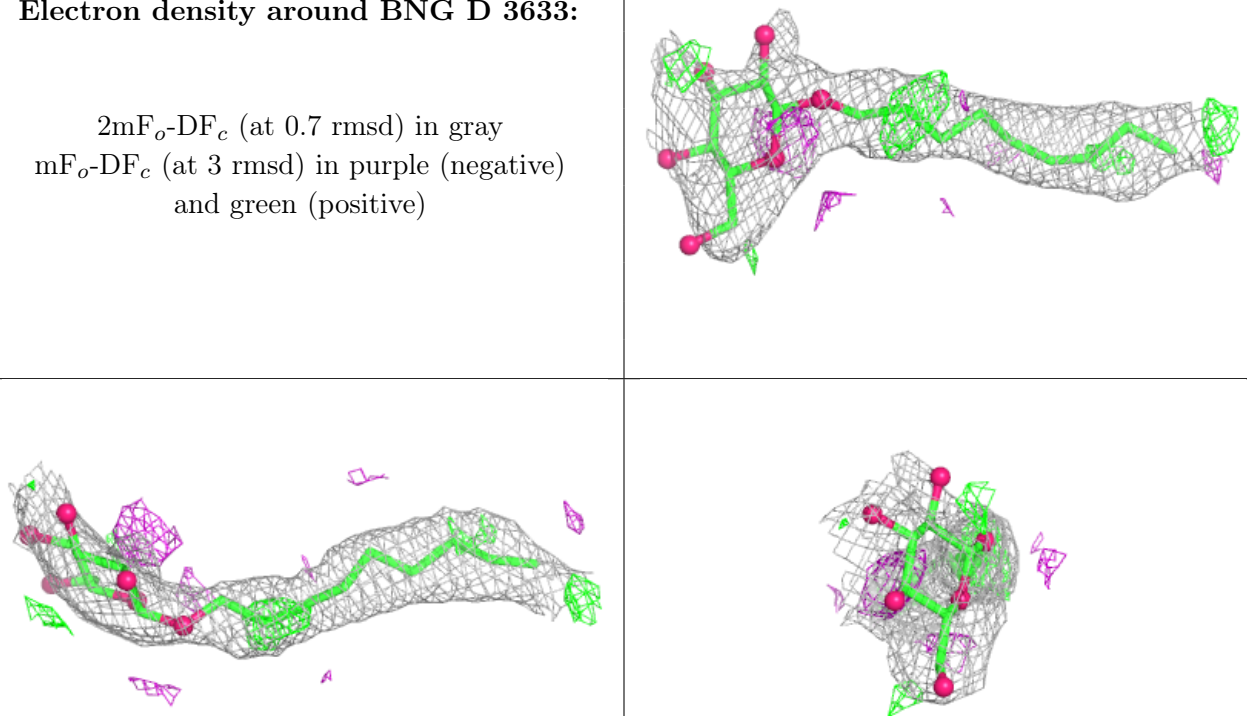
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	CHL	F	601	66/66	0.96	0.06	22,24,32,33	0
10	CLA	D	604	62/65	0.96	0.07	20,25,66,70	0
9	CHL	I	609	66/66	0.96	0.07	17,20,45,50	0
10	CLA	I	613	65/65	0.96	0.07	15,19,49,51	0
9	CHL	J	601	66/66	0.96	0.06	19,23,29,33	0
10	CLA	J	602	65/65	0.96	0.06	12,17,47,48	0
9	CHL	B	609	66/66	0.96	0.07	14,20,43,47	0
4	LUT	C	2620	42/42	0.96	0.06	18,23,28,29	0
10	CLA	E	602	65/65	0.96	0.06	13,20,48,49	0
10	CLA	E	603	65/65	0.96	0.07	11,20,73,74	0
4	LUT	D	3620	42/42	0.96	0.06	18,24,35,36	0
4	LUT	D	3621	42/42	0.96	0.06	11,19,23,23	0
10	CLA	B	613	65/65	0.97	0.06	13,17,52,56	0
10	CLA	D	613	65/65	0.97	0.06	15,18,50,52	0
10	CLA	C	613	65/65	0.97	0.06	13,15,43,47	0
4	LUT	B	1621	42/42	0.97	0.05	8,14,23,25	0
4	LUT	H	7621	42/42	0.97	0.06	13,20,24,25	0
10	CLA	H	613	65/65	0.97	0.06	10,17,55,57	0
4	LUT	B	1620	42/42	0.97	0.05	13,19,30,30	0
4	LUT	I	8621	42/42	0.97	0.05	12,20,22,24	0
10	CLA	G	613	65/65	0.97	0.06	14,17,55,56	0
4	LUT	C	2621	42/42	0.97	0.06	13,18,21,22	0
10	CLA	J	613	65/65	0.97	0.06	11,17,56,59	0
4	LUT	E	4621	42/42	0.97	0.06	11,16,22,24	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.

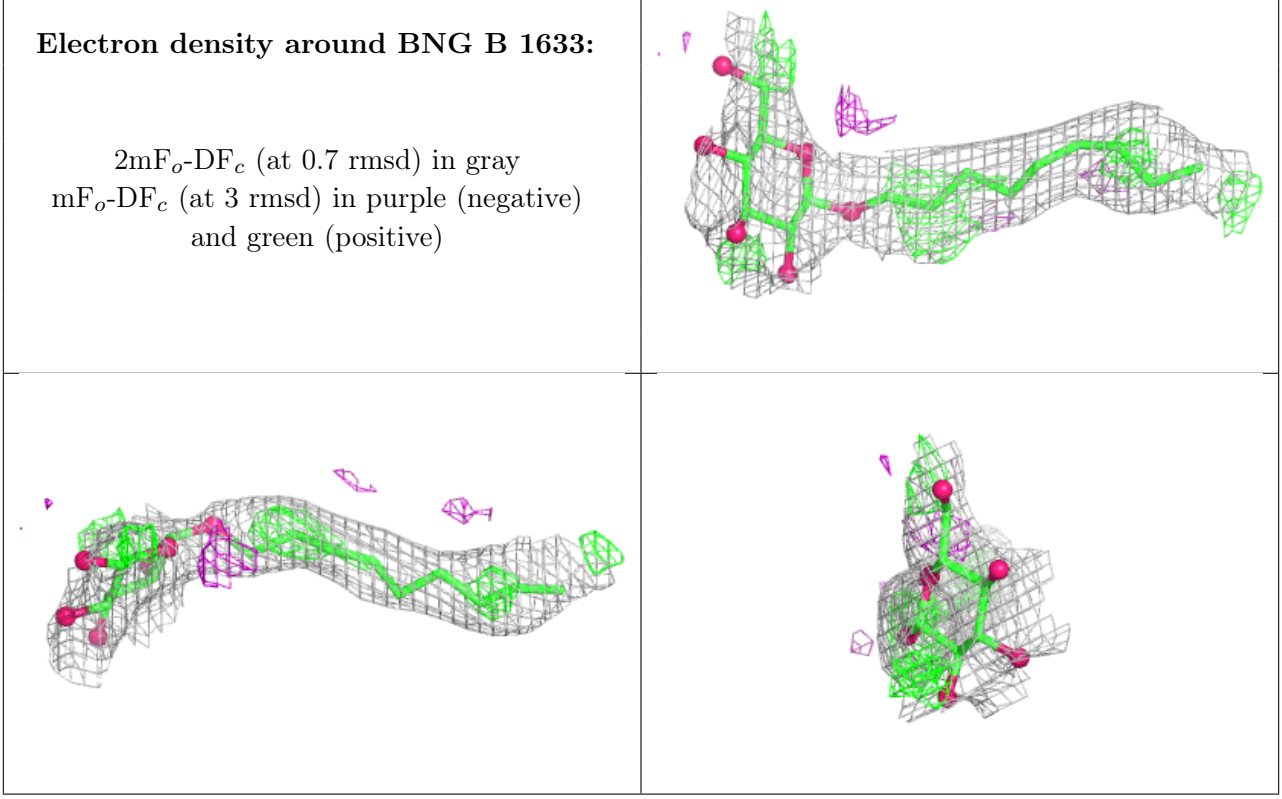
Electron density around BNG D 3633:

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



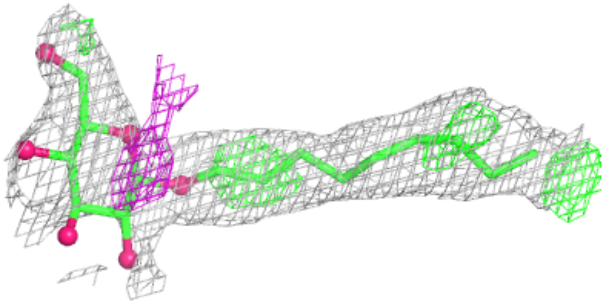
Electron density around BNG B 1633:

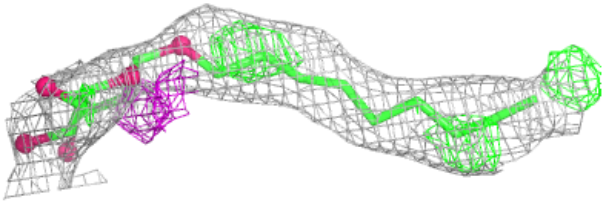
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

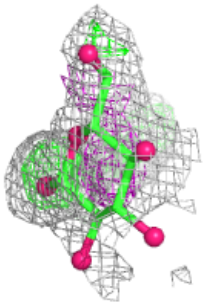


Electron density around BNG C 2633:

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

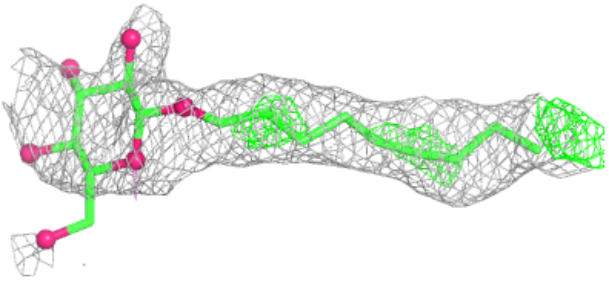


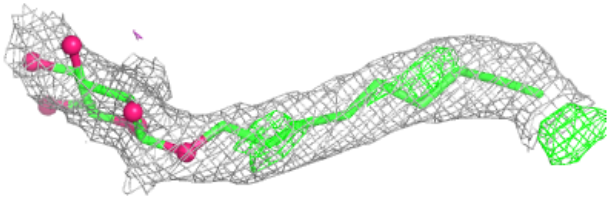


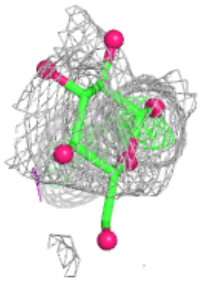


Electron density around BNG G 6633:

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

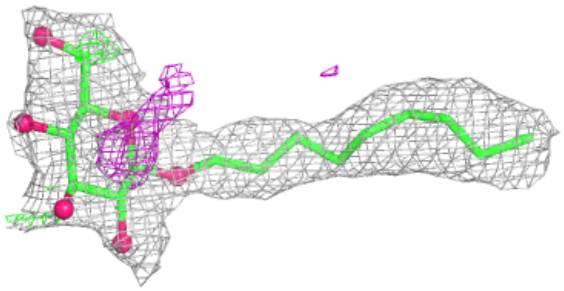


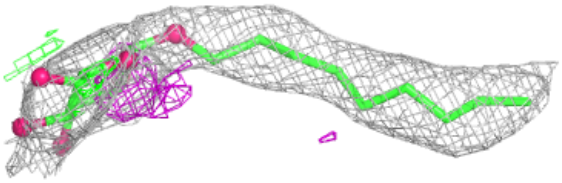


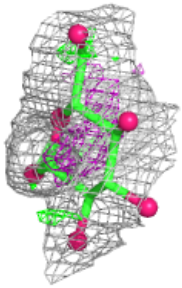


Electron density around BNG A 633:

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

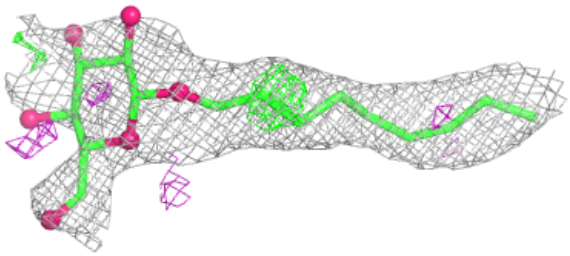


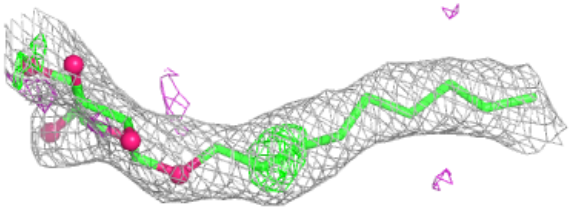


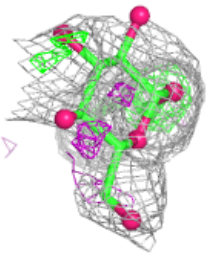


Electron density around BNG H 7633:

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

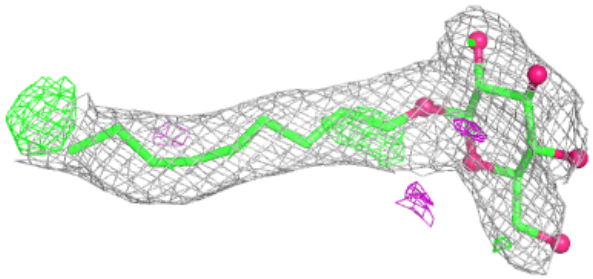


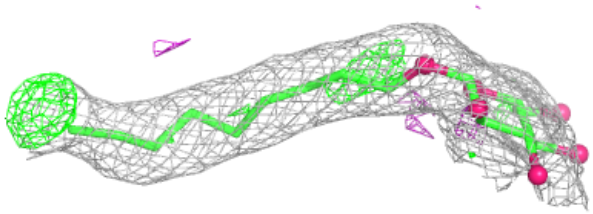


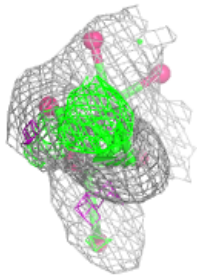


Electron density around BNG I 8633:

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

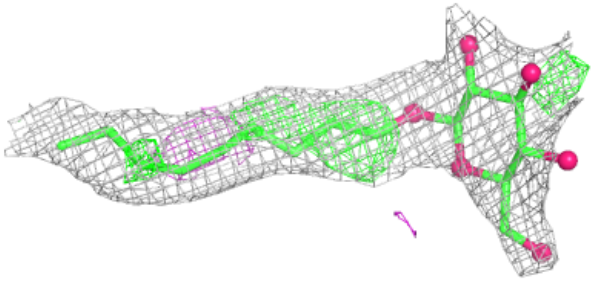


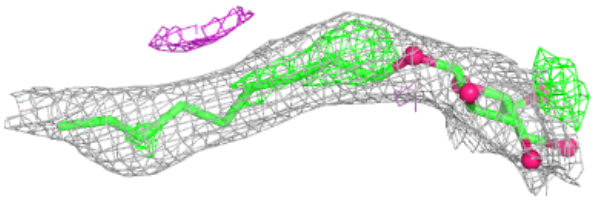


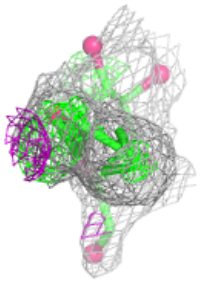


Electron density around BNG J 9633:

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

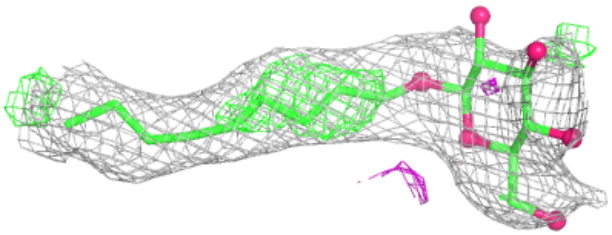


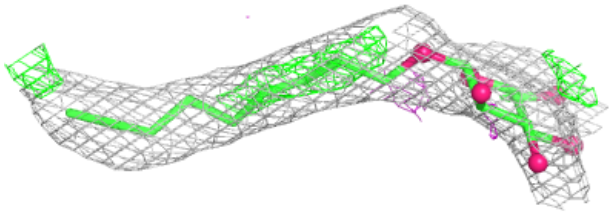


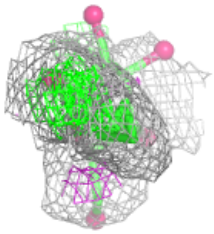


Electron density around BNG E 4633:

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

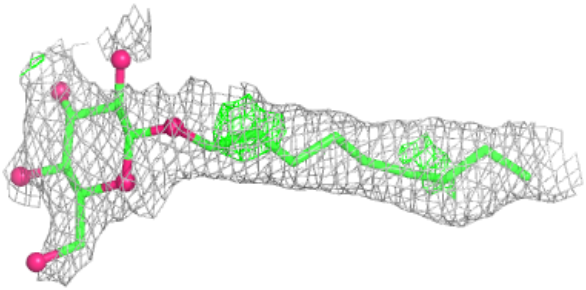


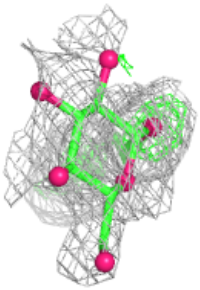




Electron density around BNG F 5633:

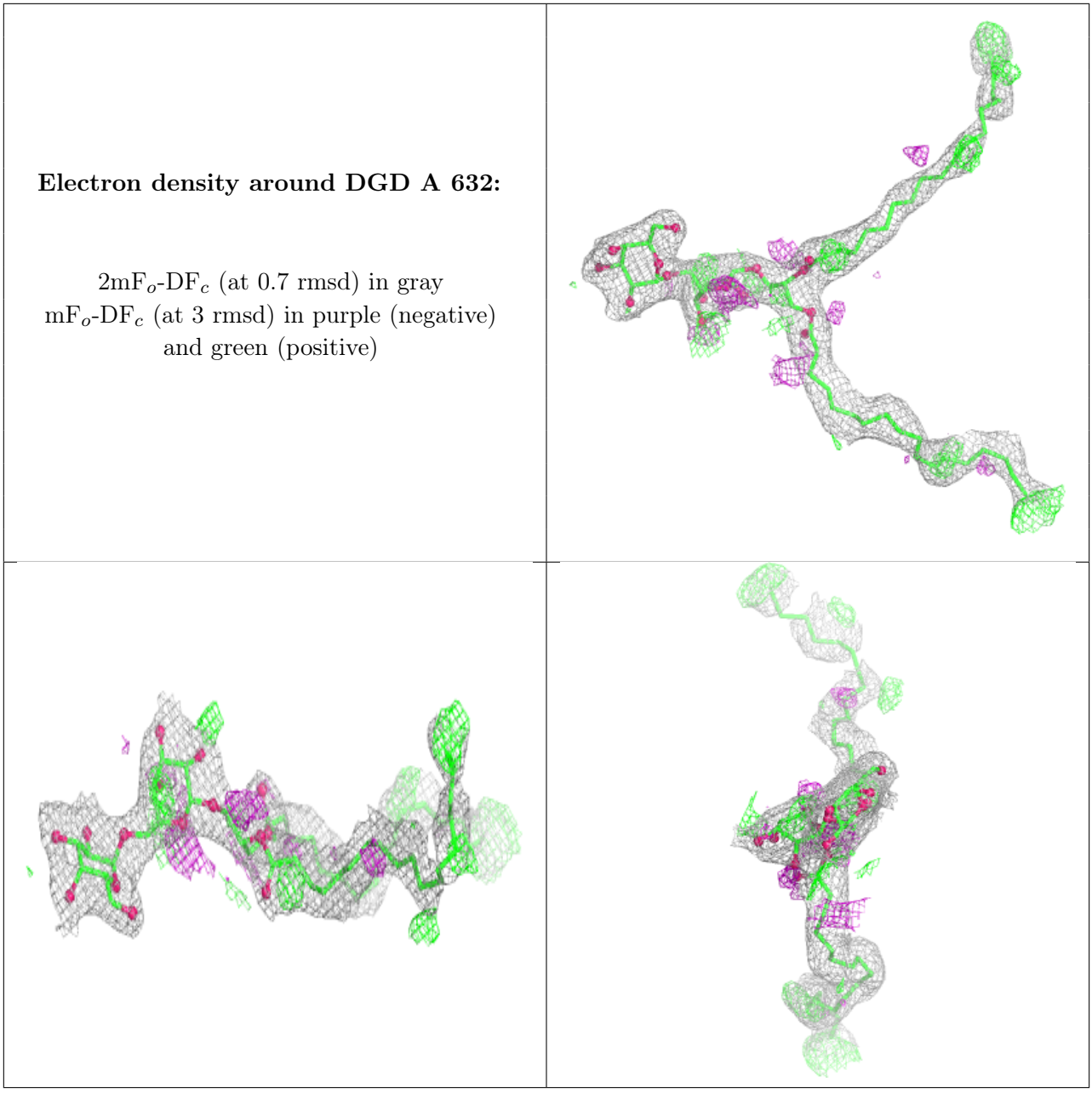
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





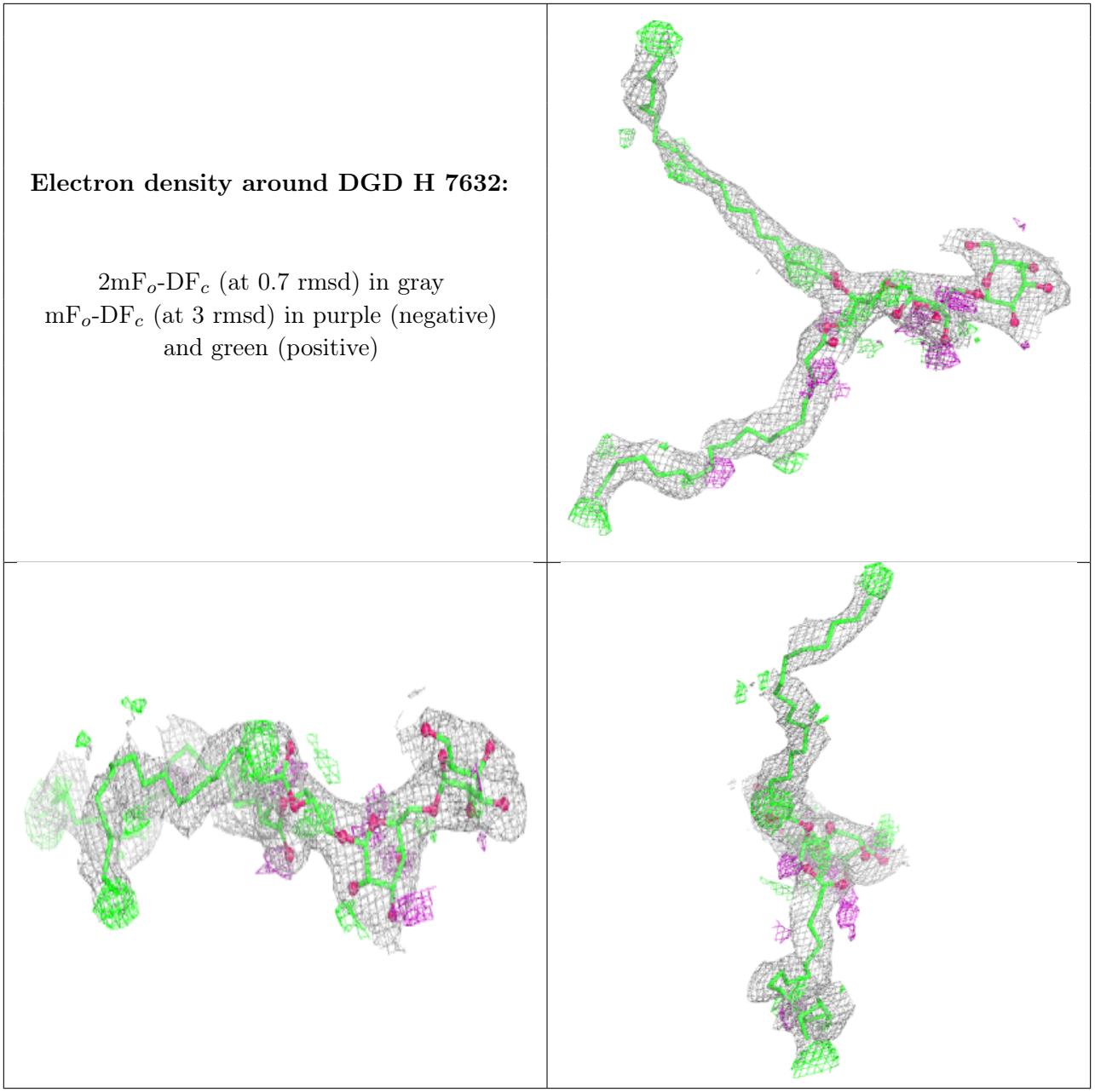
Electron density around DGD A 632:

$2mF_o$-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 H 7632:

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

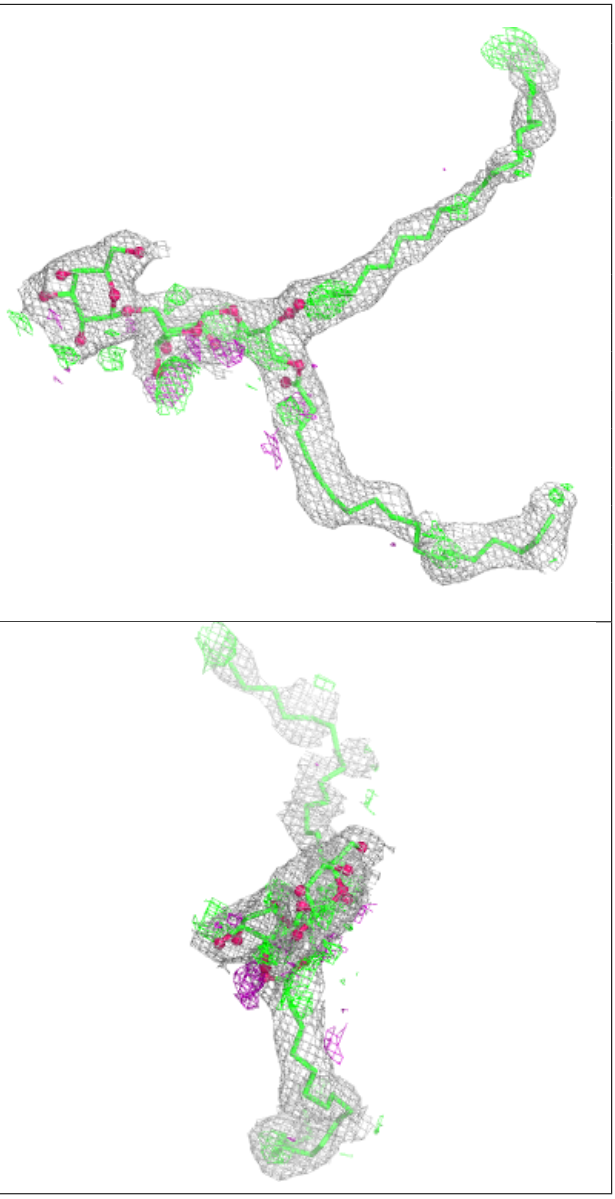


Electron density around DGD B 2632:

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

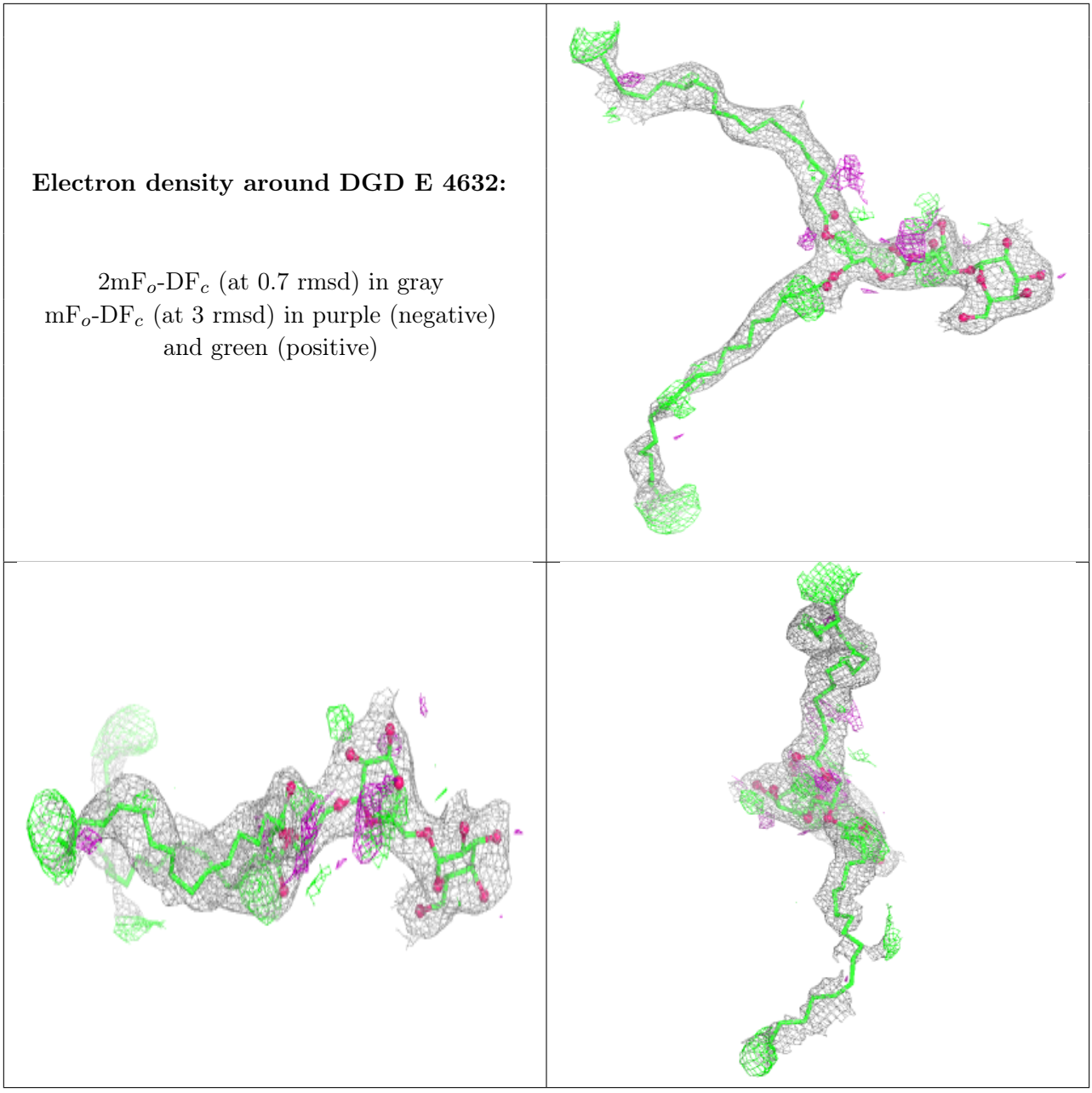
Electron density around DGD D 3632:

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



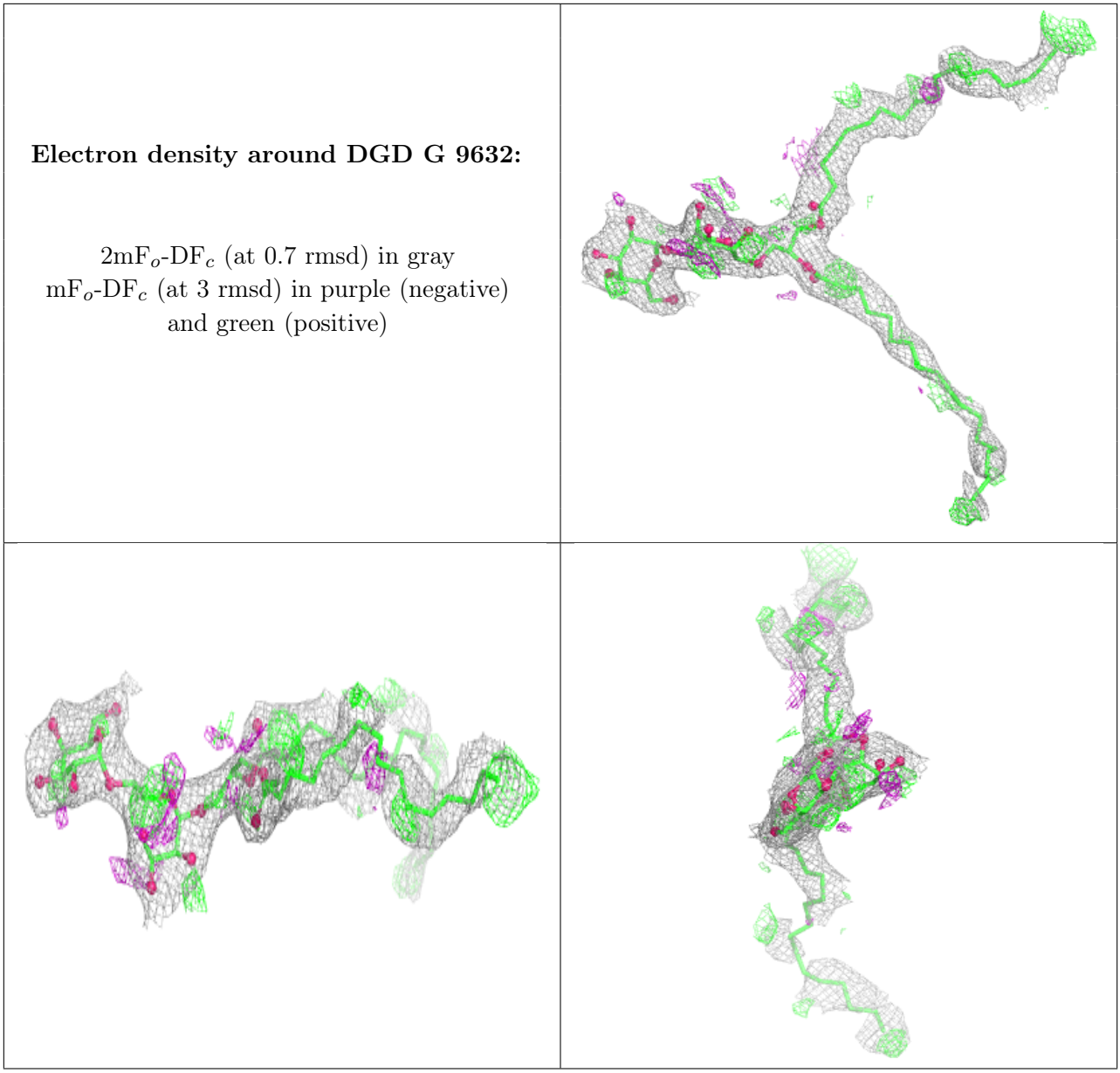
Electron density around DGD E 4632:

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



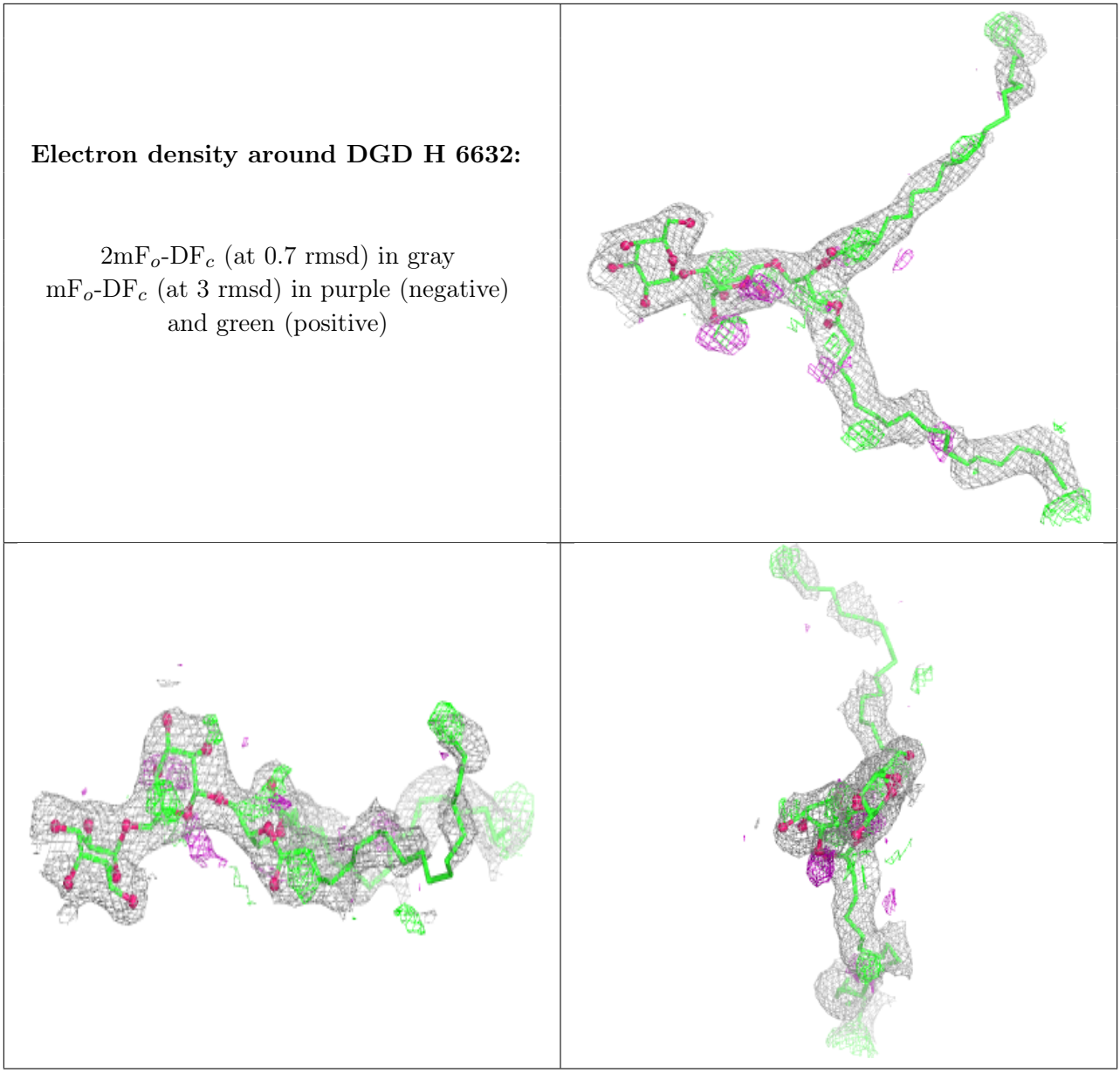
Electron density around DGD G 9632:

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



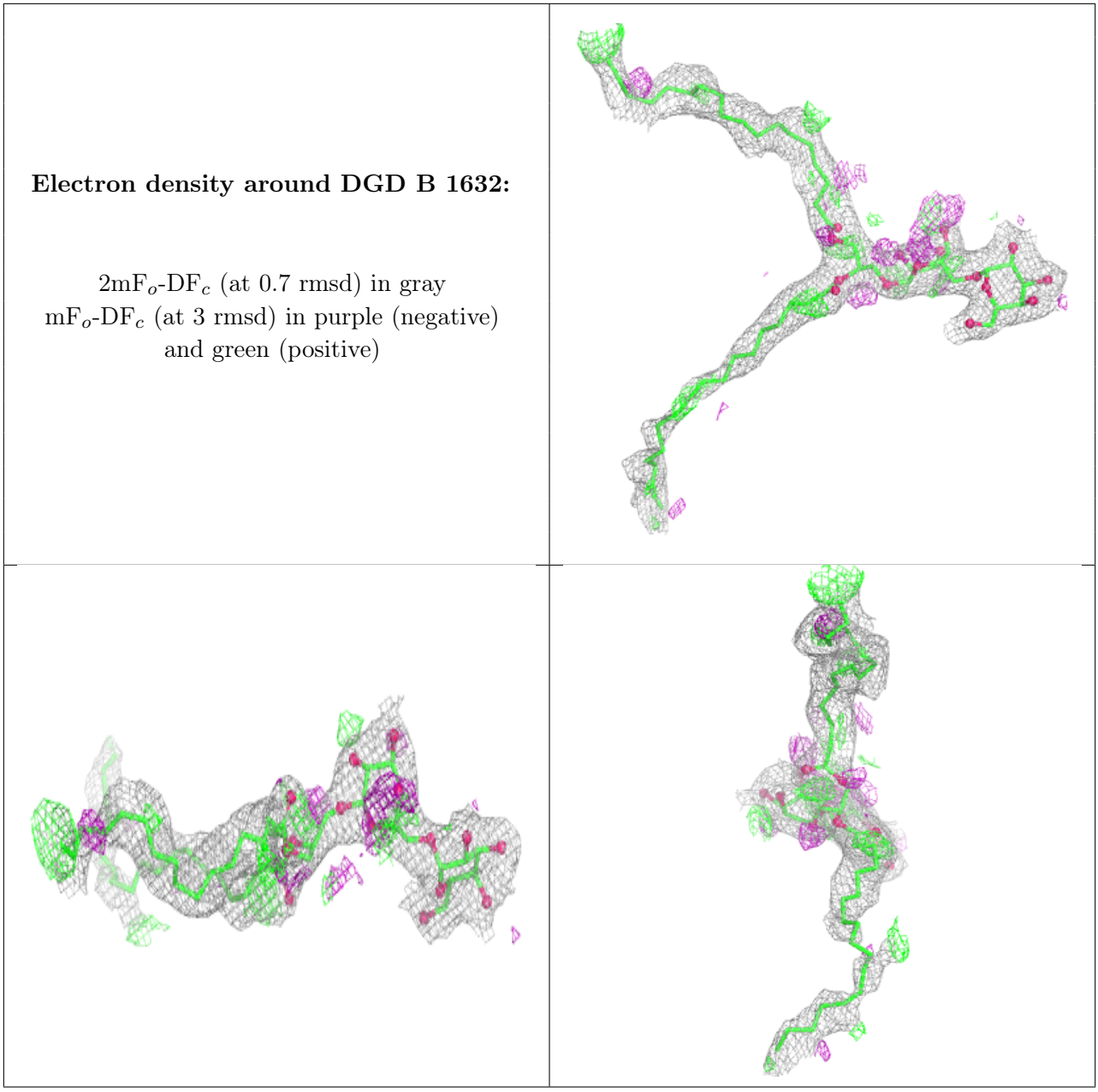
Electron density around DGD H 6632:

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



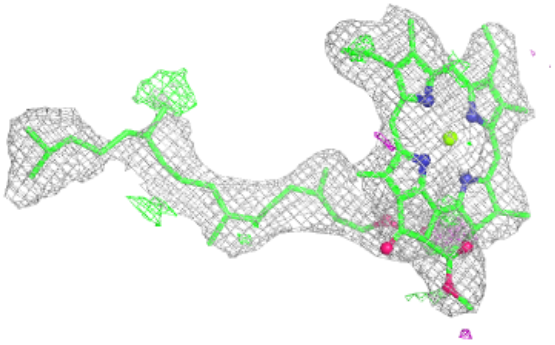
Electron density around DGD B 1632:

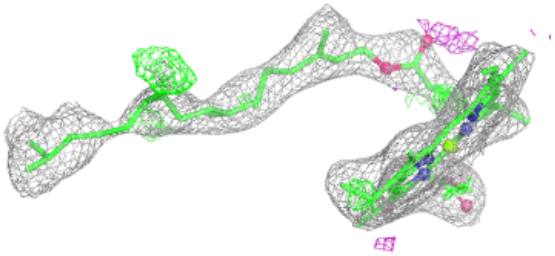
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

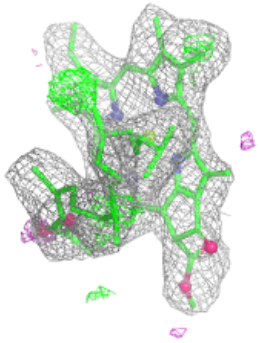


Electron density around CLA A 611:

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

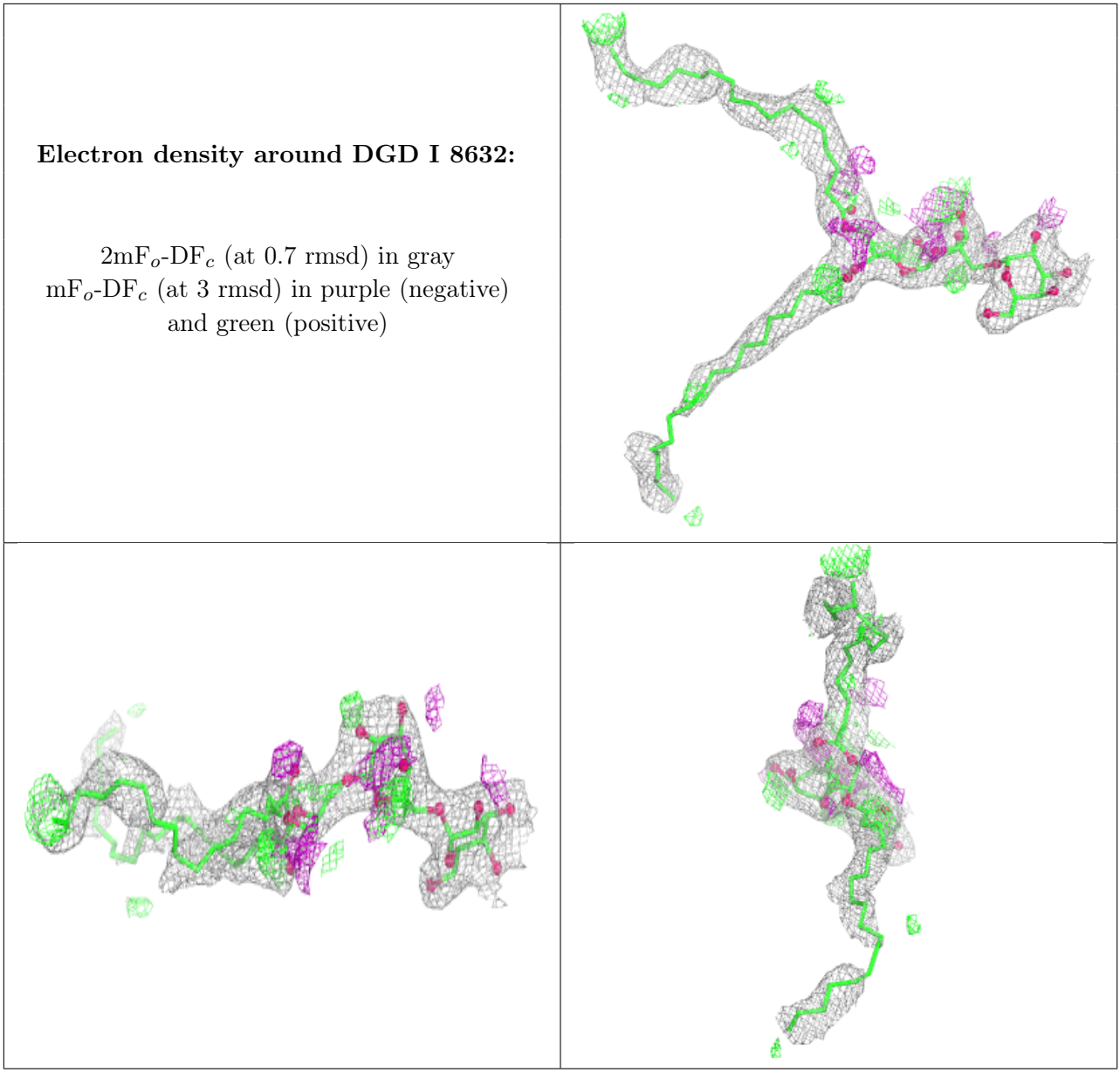






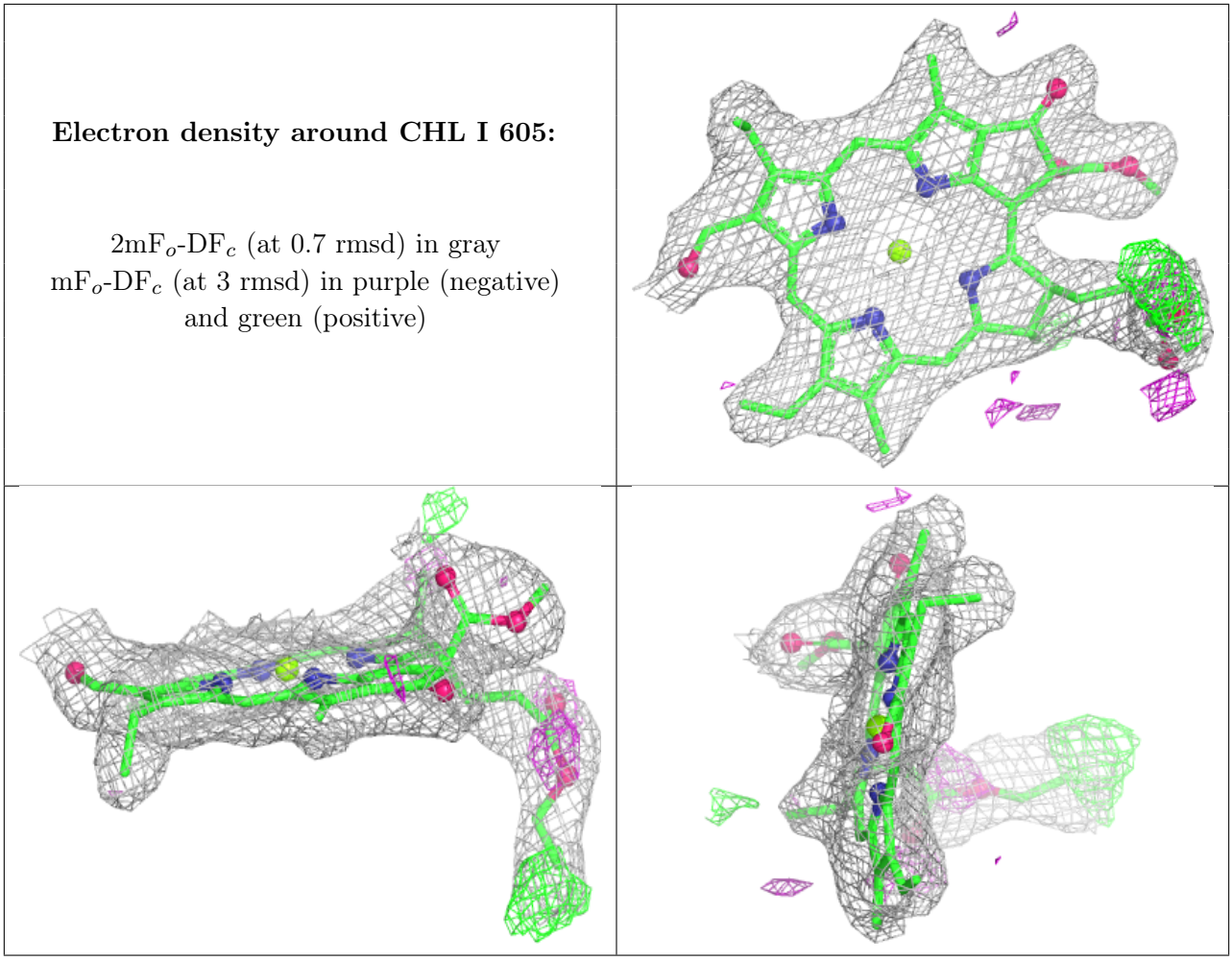
Electron density around DGD I 8632:

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



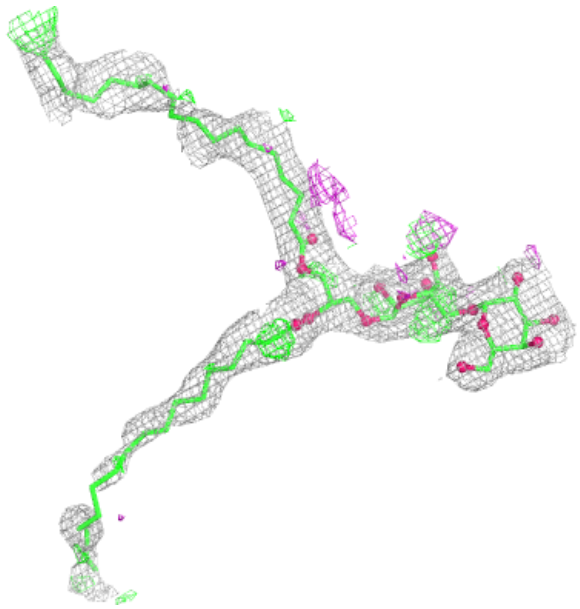
Electron density around CHL I 605:

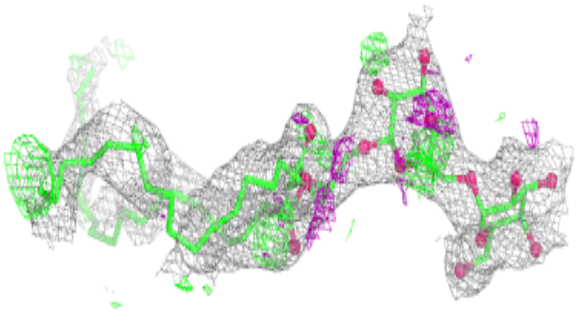
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

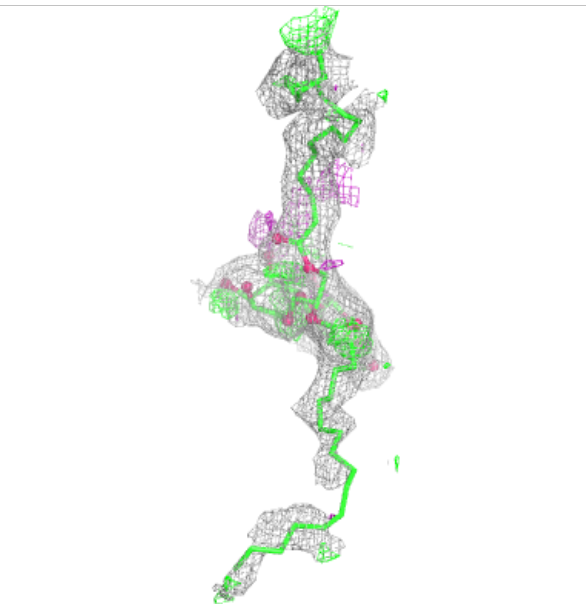


Electron density around DGD D 5632:

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

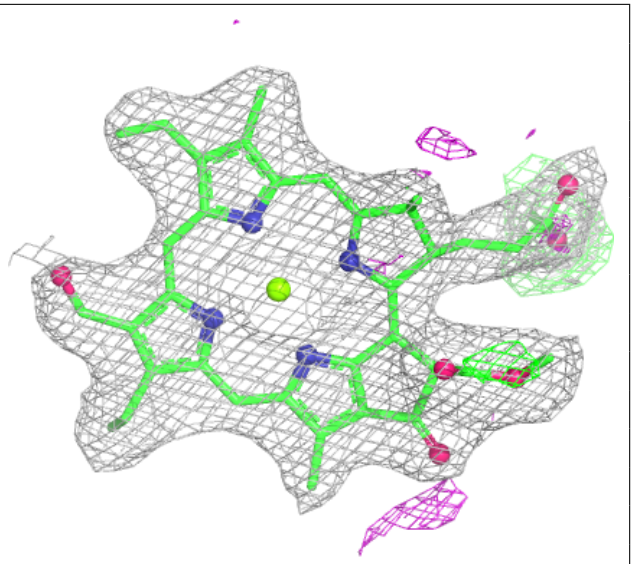


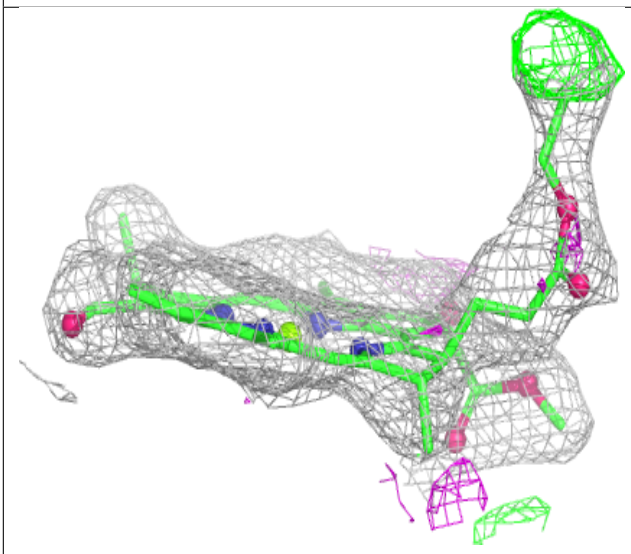


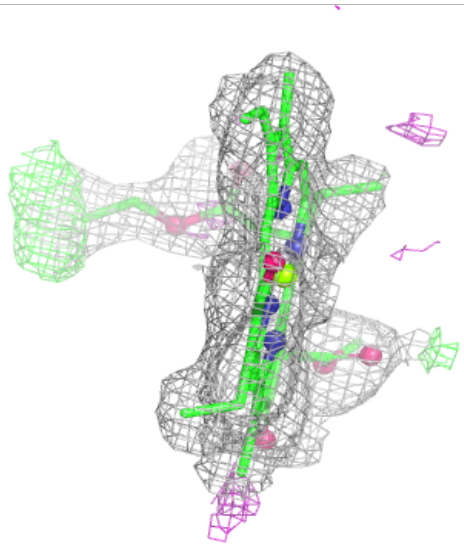


Electron density around CHL F 605:

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

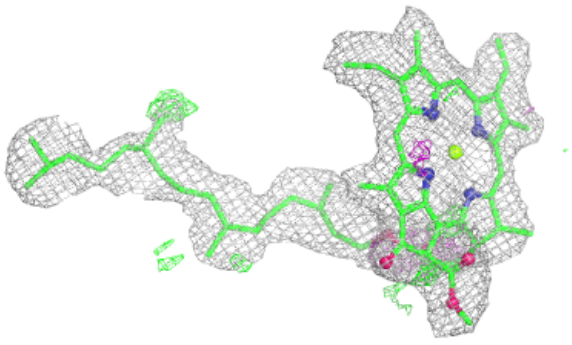


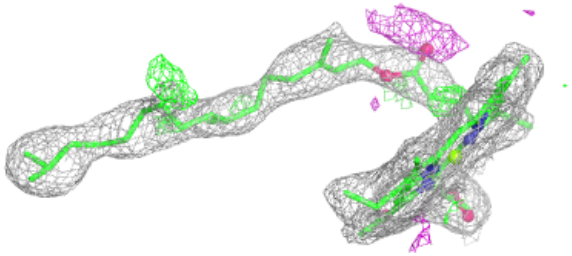


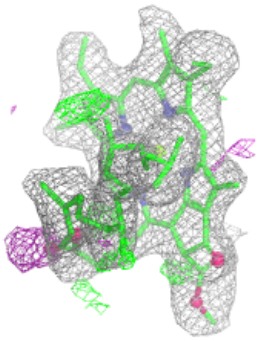


Electron density around CLA B 611:

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

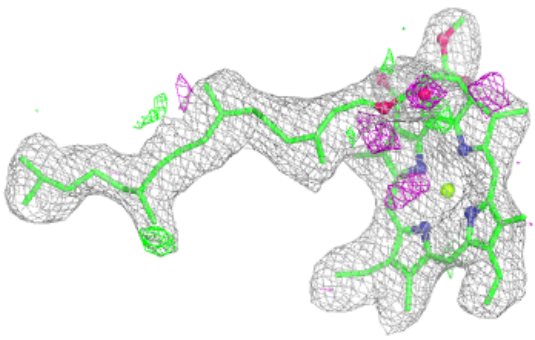


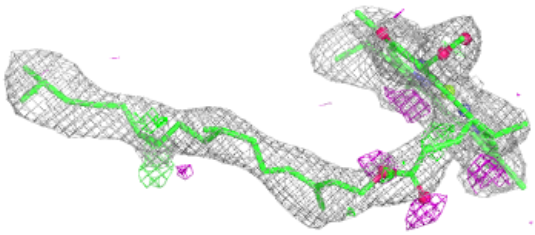


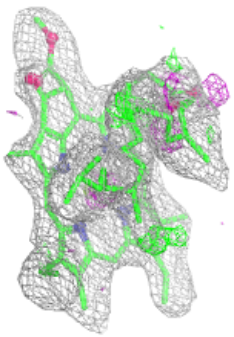


Electron density around CLA D 611:

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

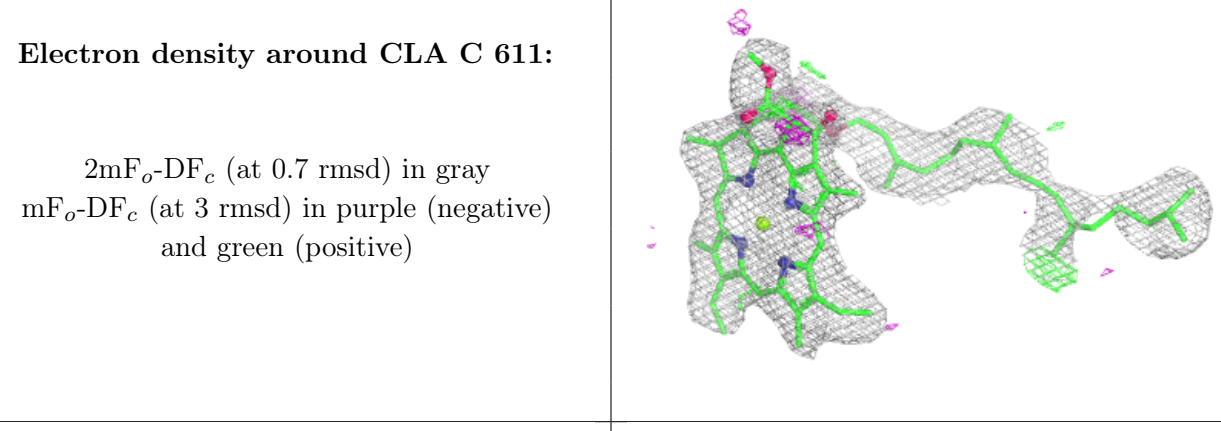






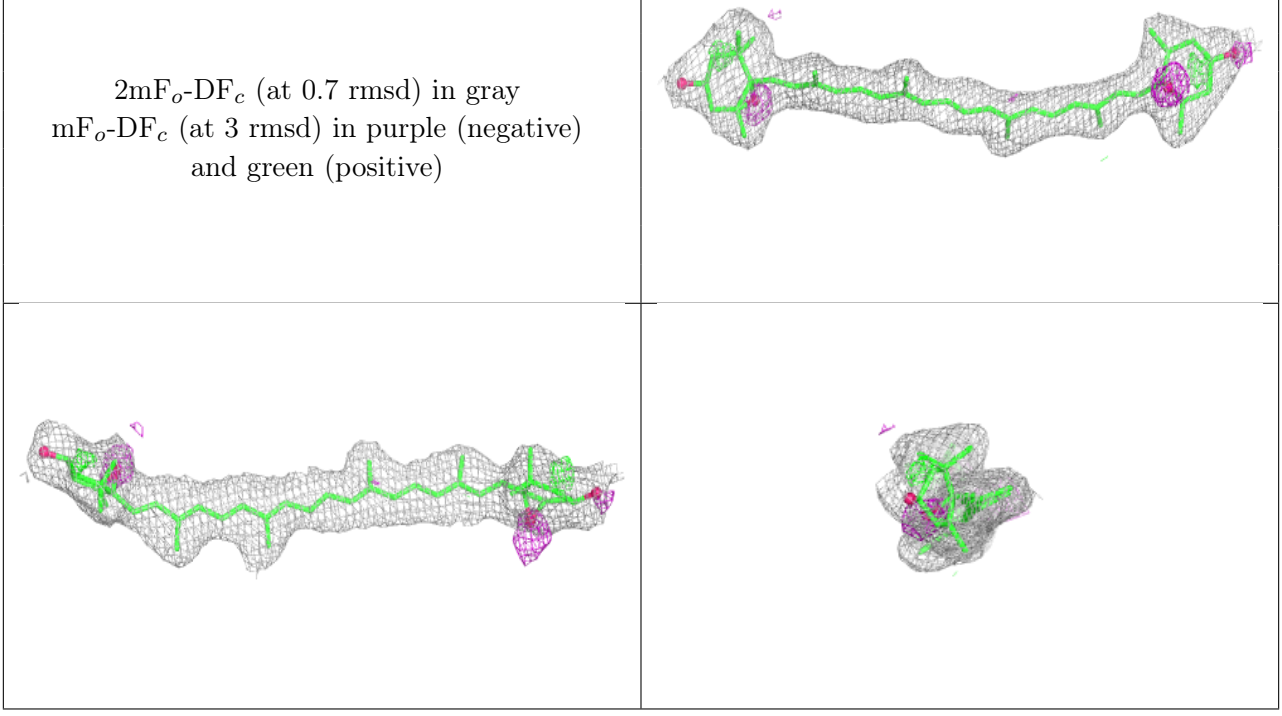
Electron density around CLA C 611:

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



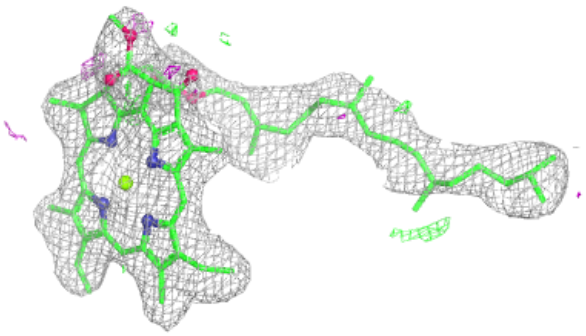
Electron density around XAT B 5622:

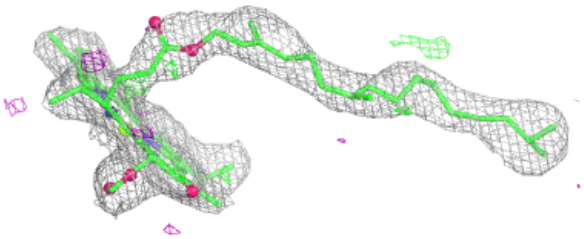
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

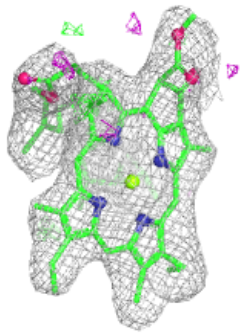


Electron density around CLA G 611:

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

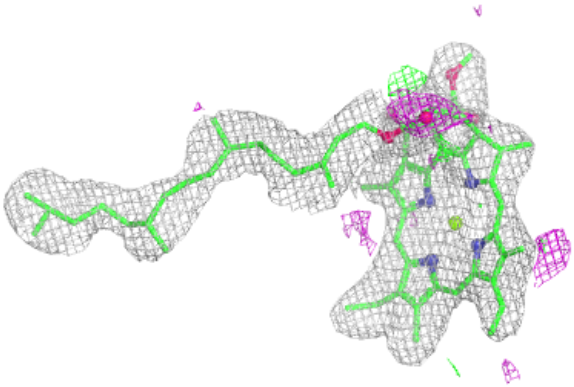


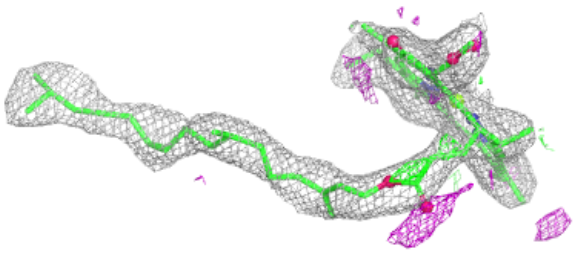


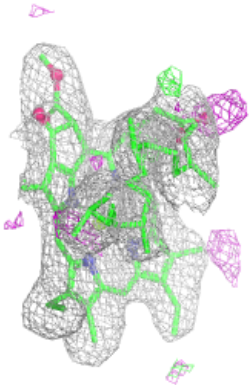


Electron density around CLA H 611:

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

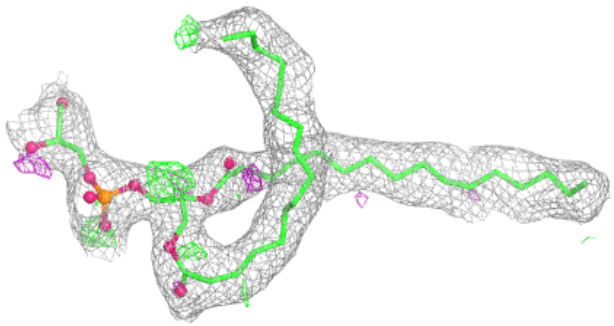


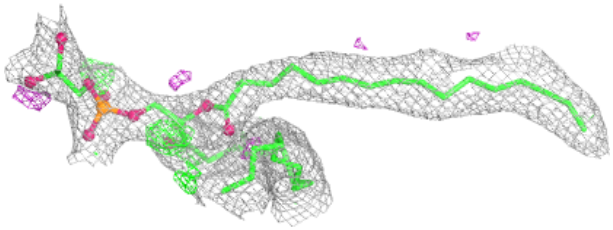




Electron density around LHG A 630:

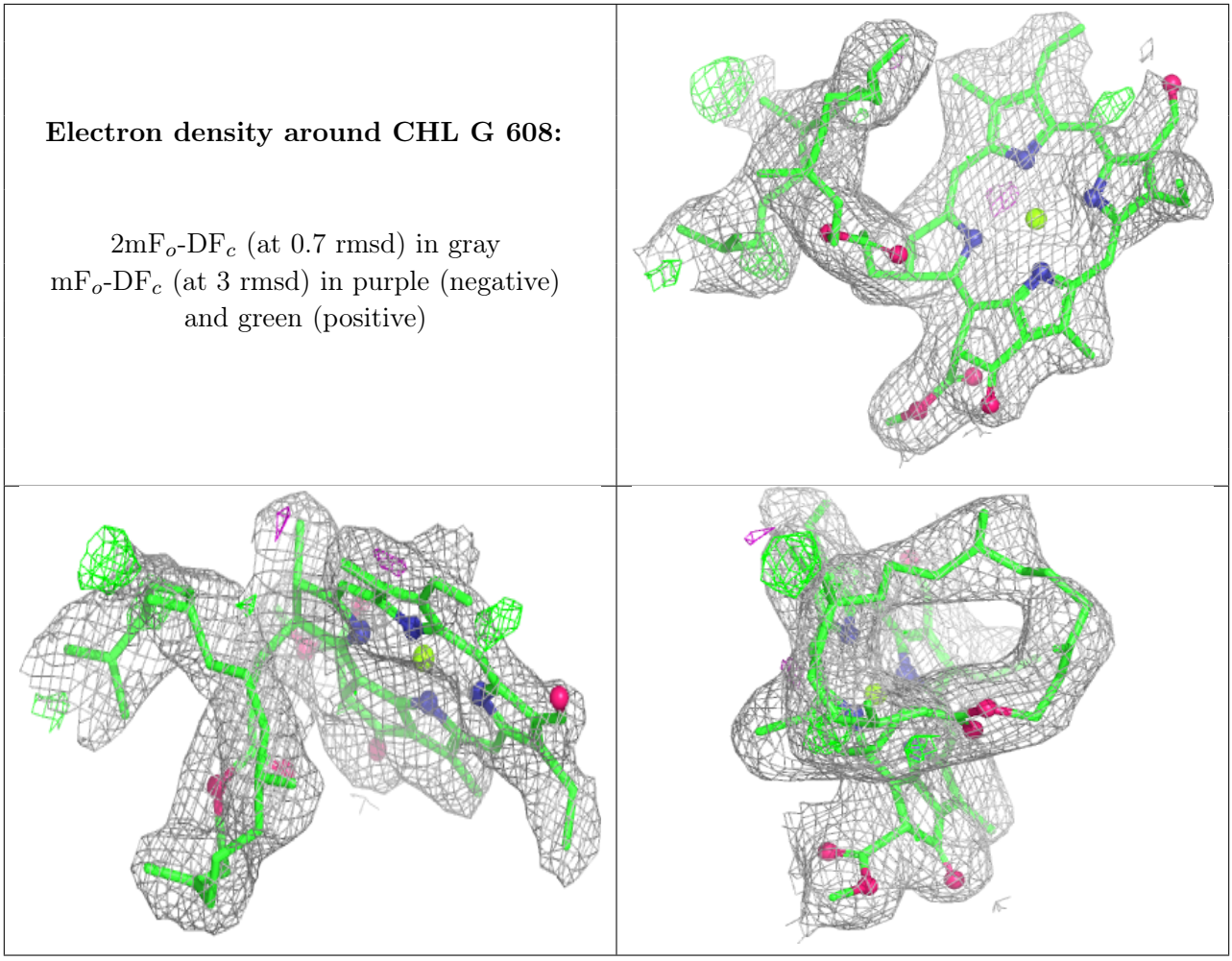
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





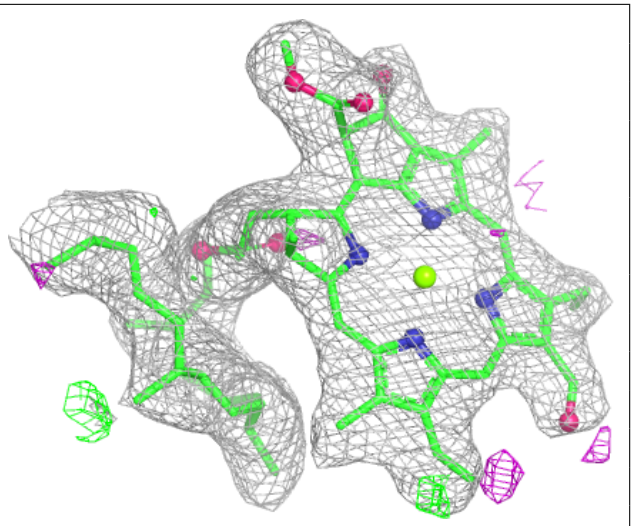
Electron density around CHL G 608:

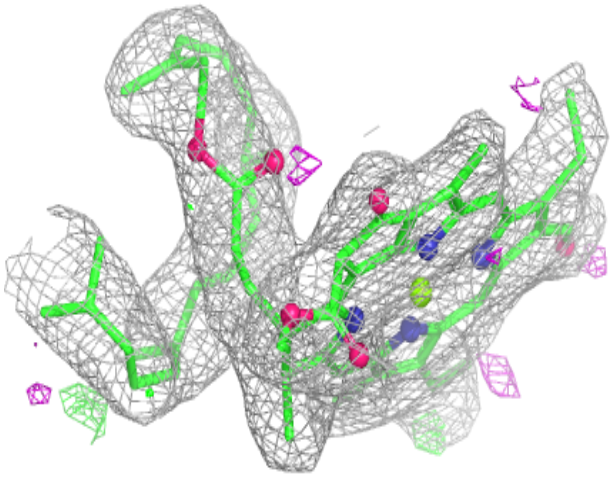
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

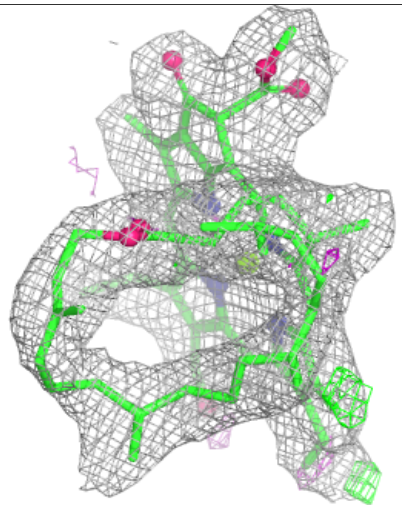


Electron density around CHL H 608:

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

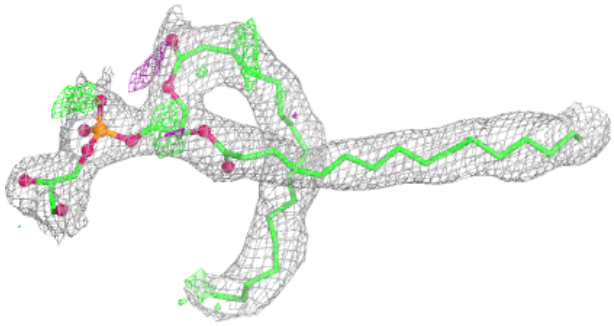


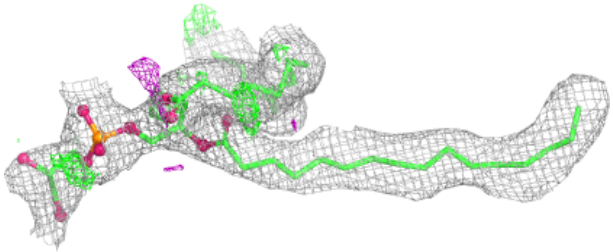


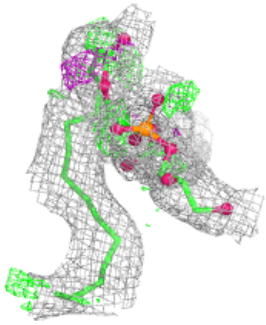


Electron density around LHG B 1630:

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

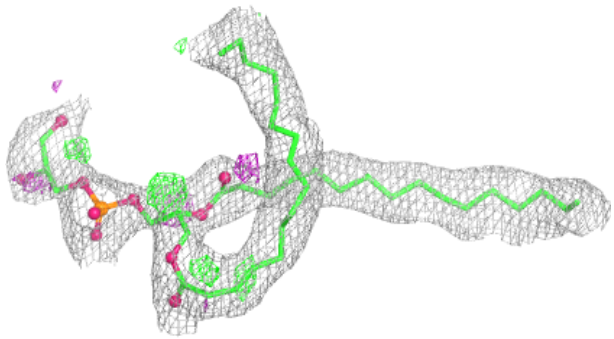


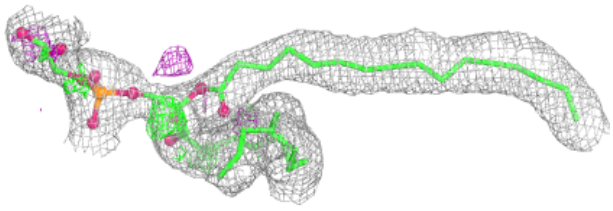


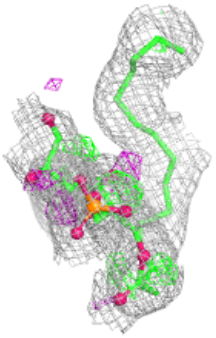


Electron density around LHG D 3630:

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

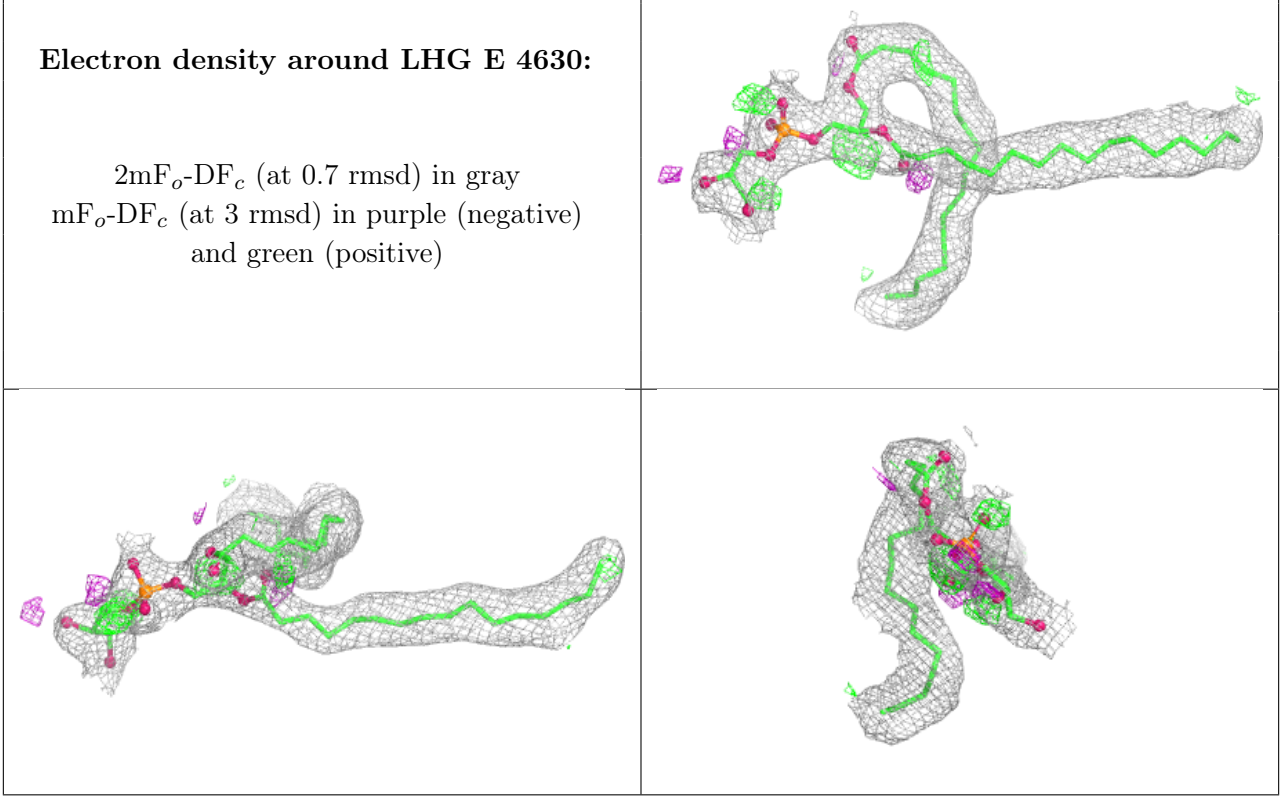






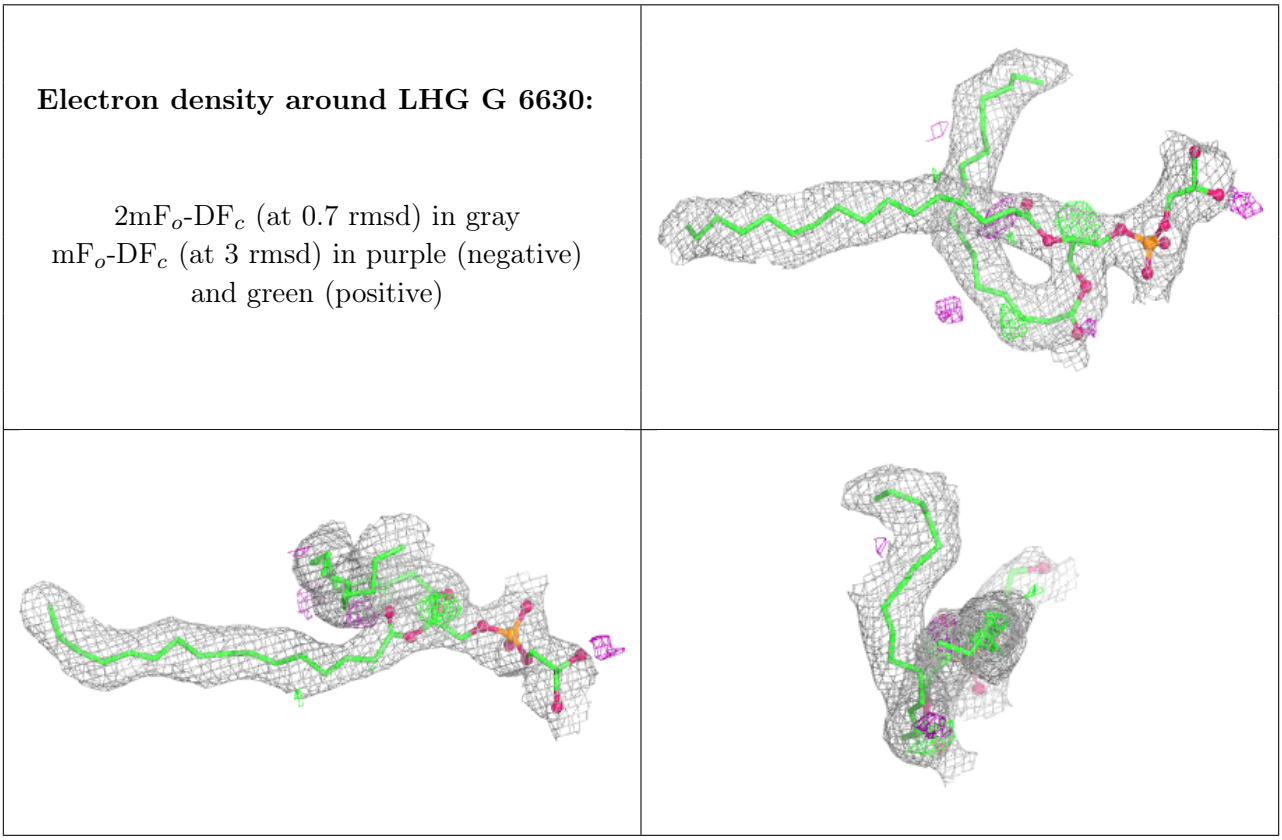
Electron density around LHG E 4630:

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



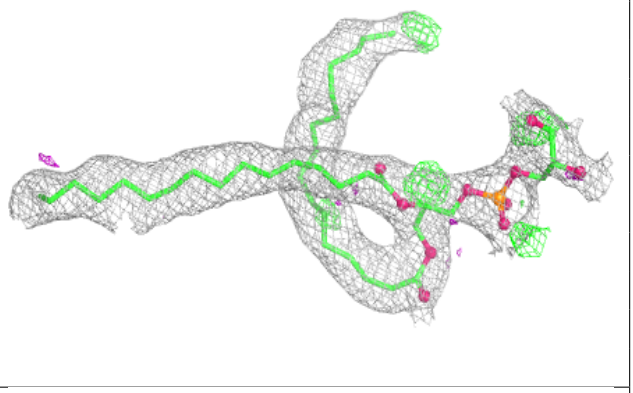
Electron density around LHG G 6630:

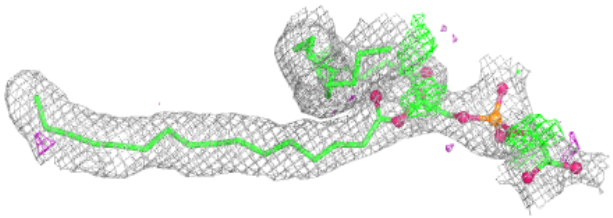
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG H 7630:

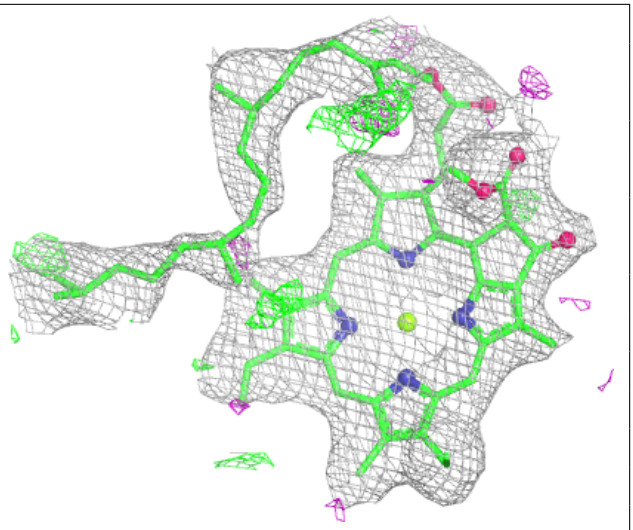
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

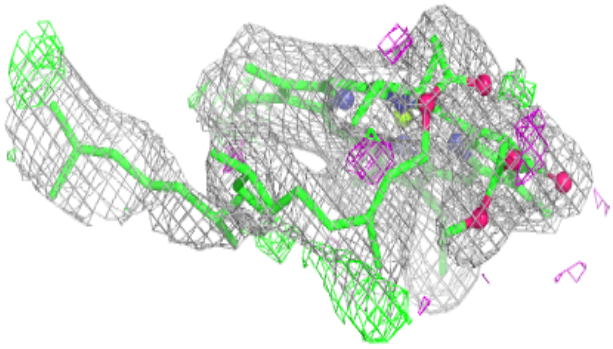


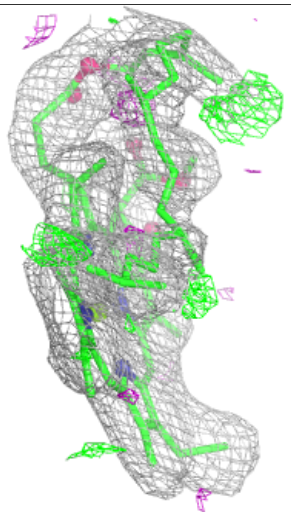


Electron density around CLA D 612:

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

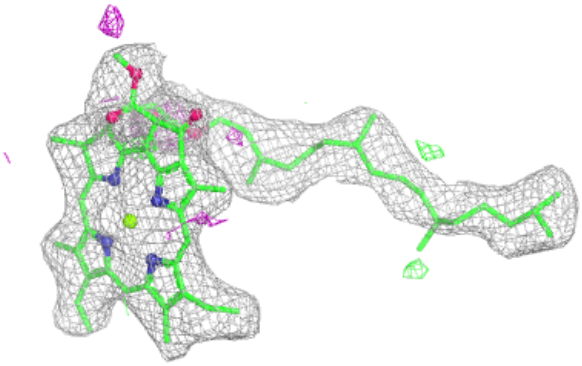


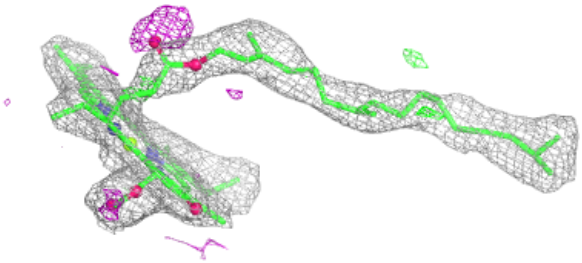


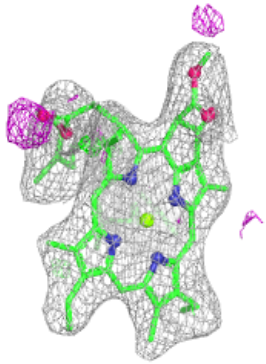


Electron density around CLA E 611:

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

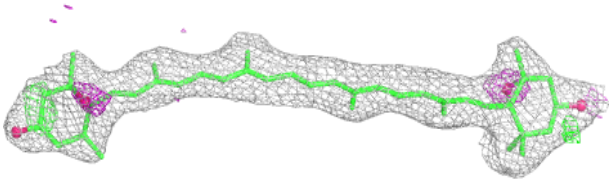


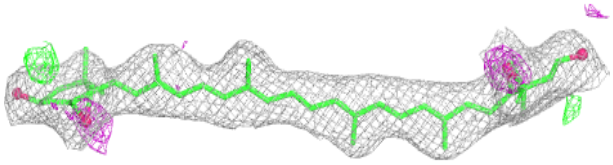


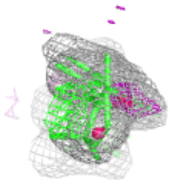


Electron density around XAT A 622:

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

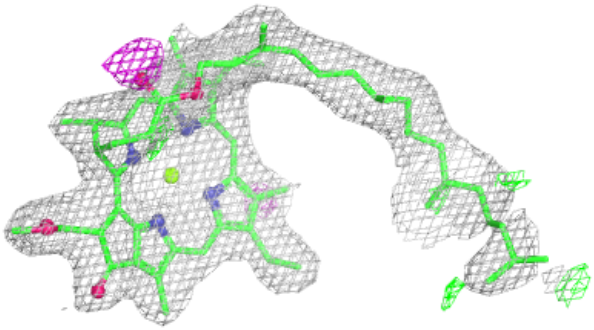


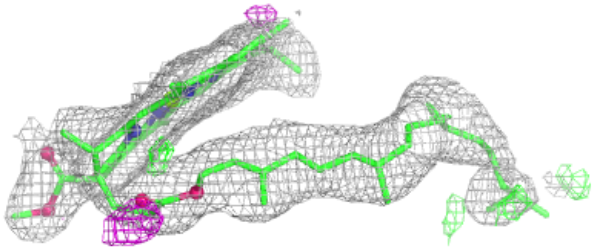


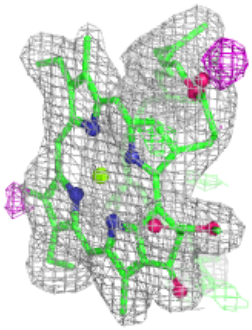


Electron density around CLA H 610:

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

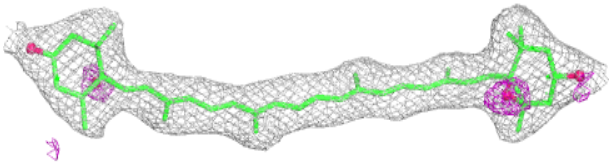


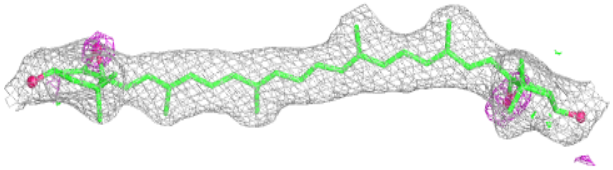


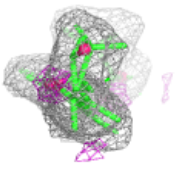


Electron density around XAT D 8622:

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

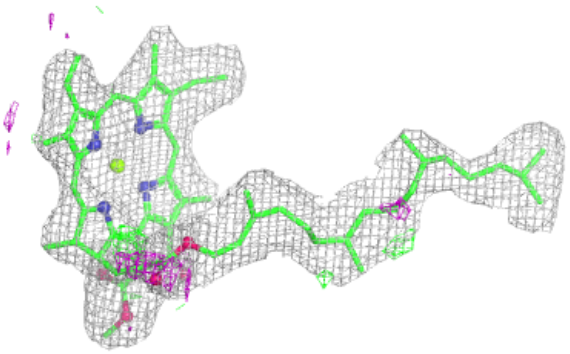


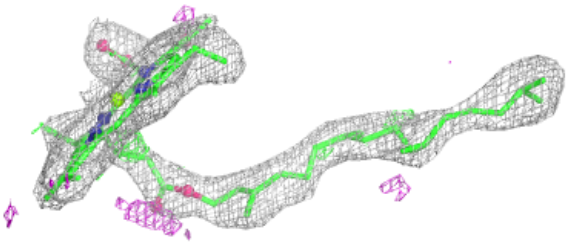


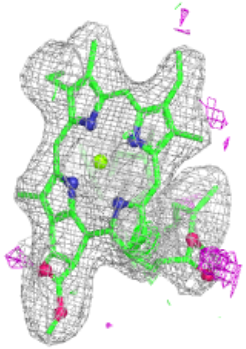


Electron density around CLA I 611:

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

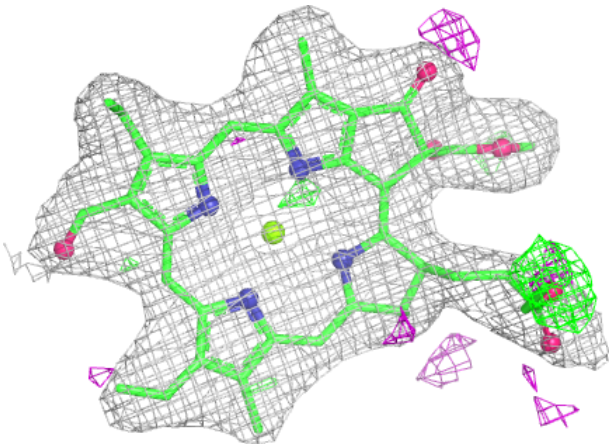


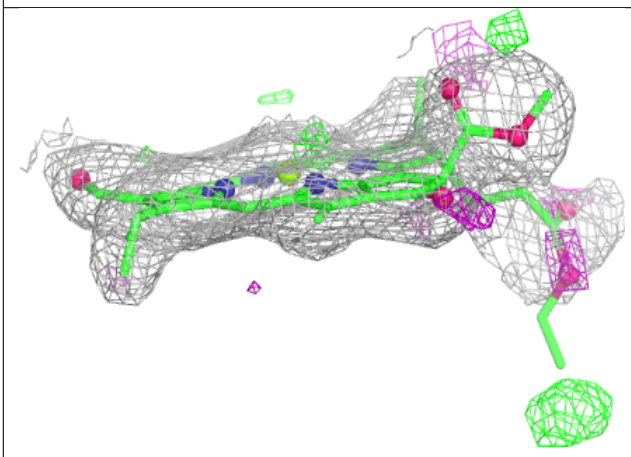


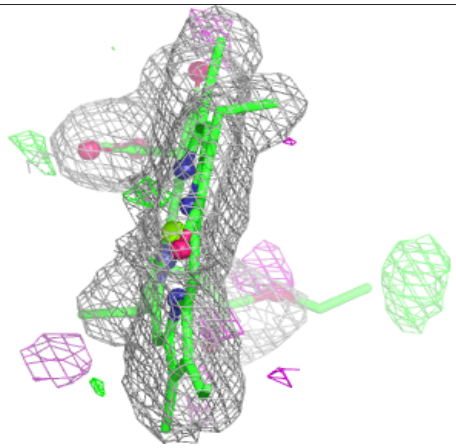


Electron density around CHL G 605:

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

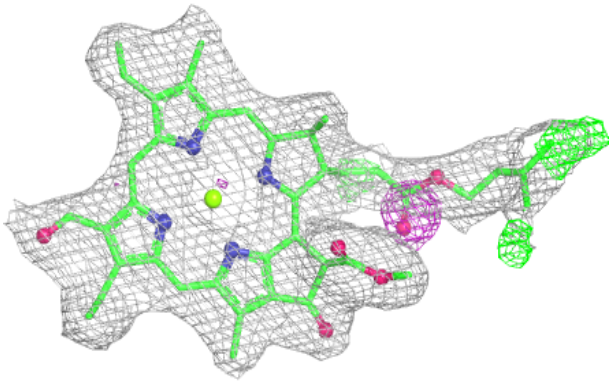


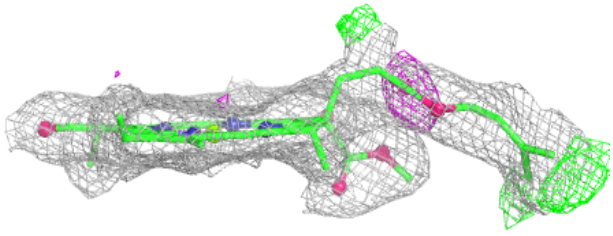




Electron density around CHL G 606:

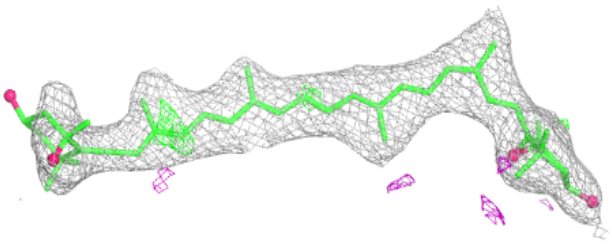
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

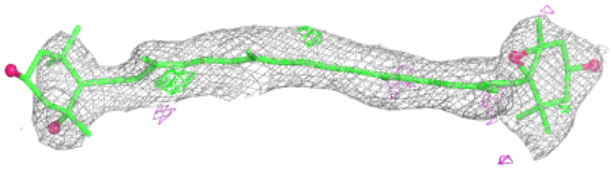


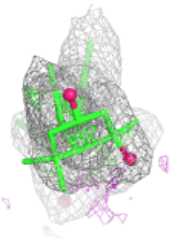


Electron density around NEX H 7623:

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

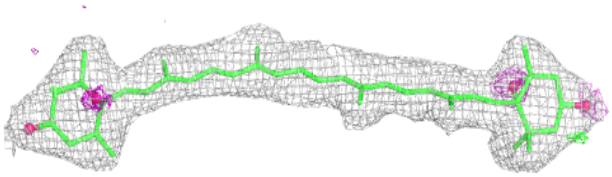


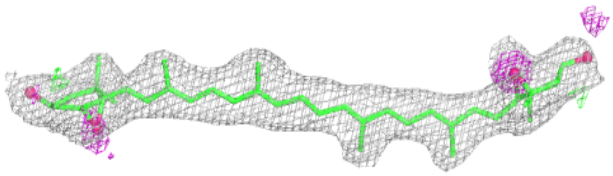


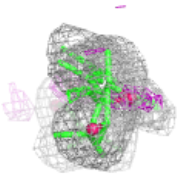


Electron density around XAT B 1622:

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

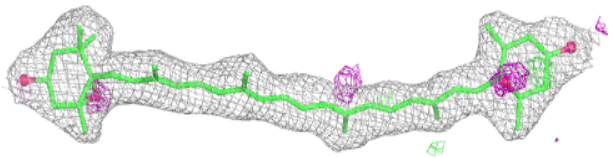


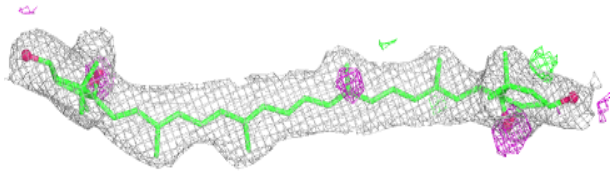


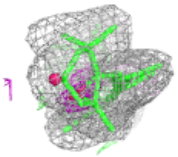


Electron density around XAT E 2622:

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

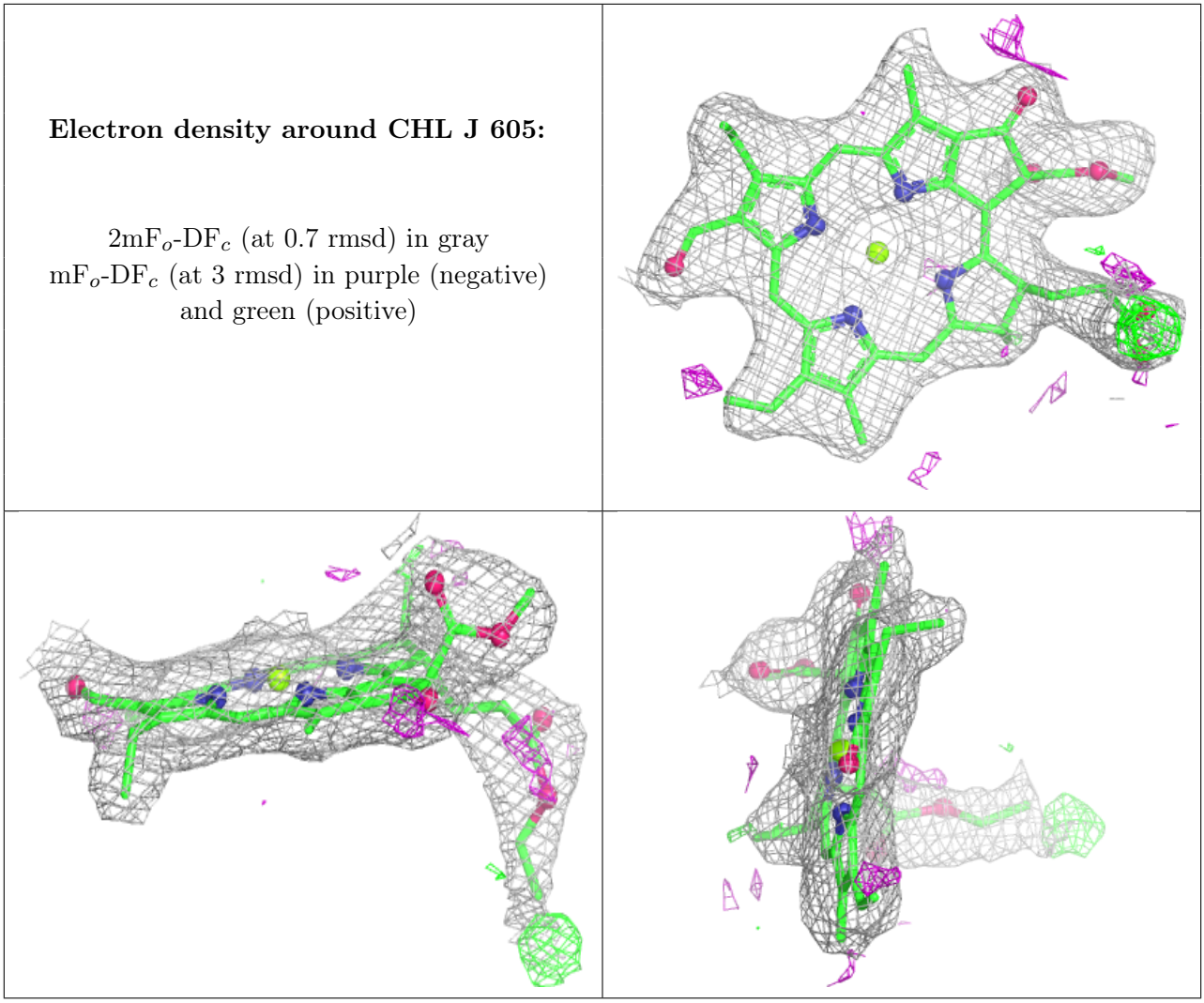






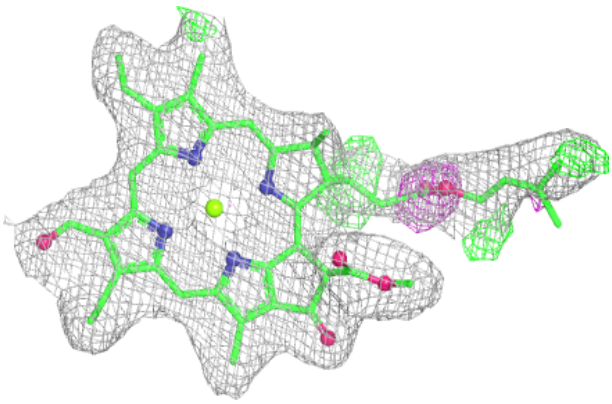
Electron density around CHL J 605:

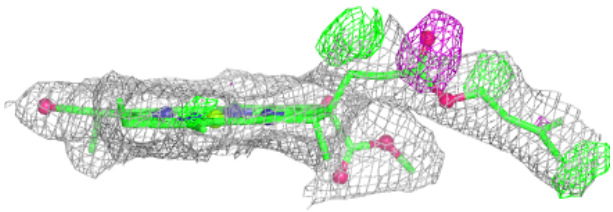
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

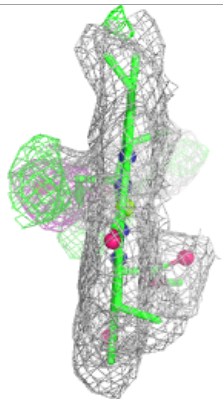


Electron density around CHL J 606:

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

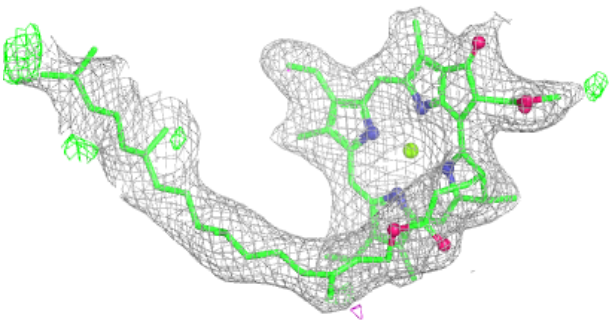


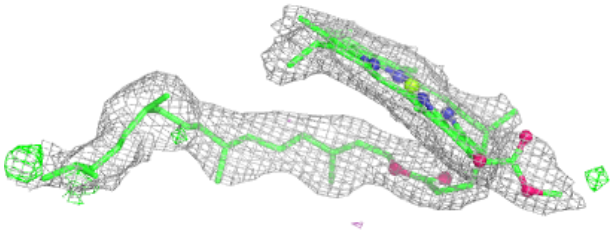




Electron density around CLA A 610:

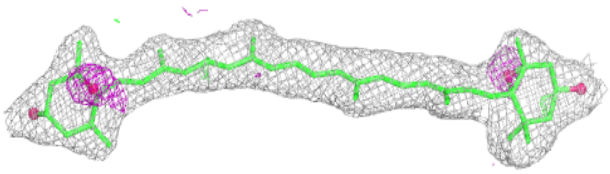
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

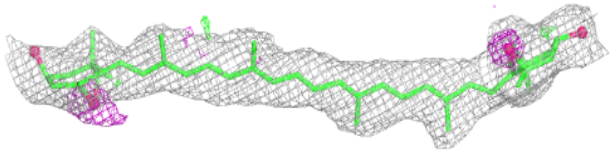


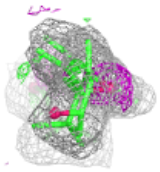


Electron density around XAT F 6622:

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

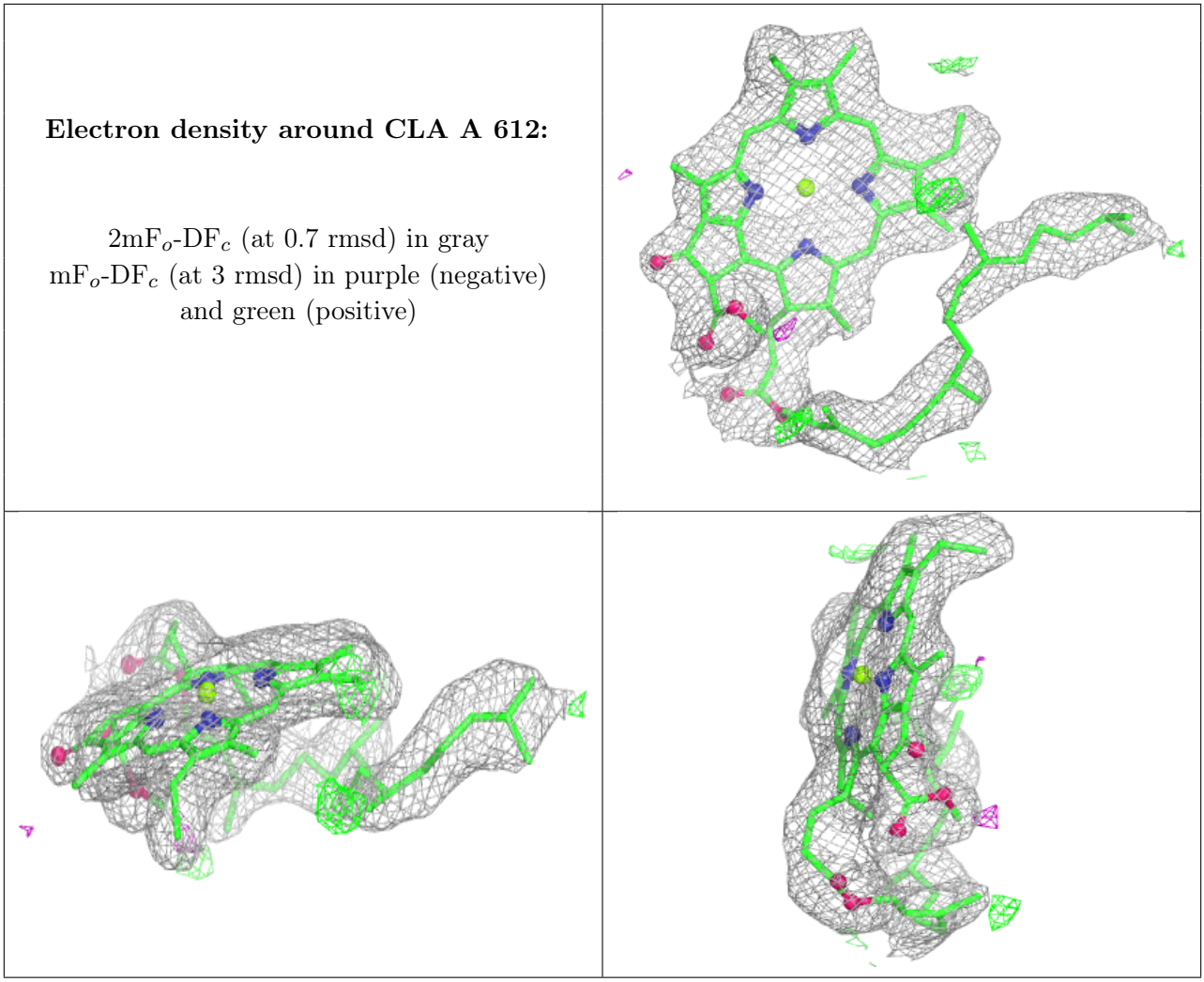






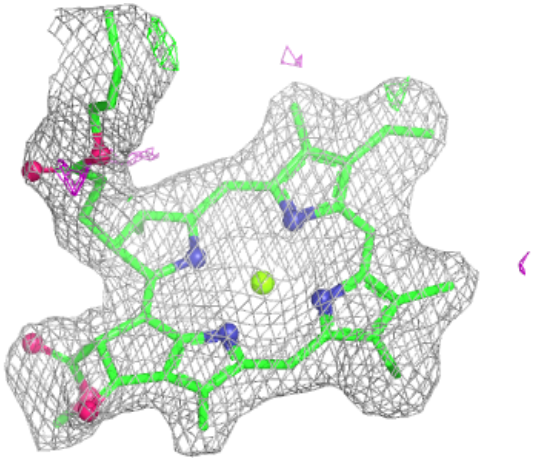
Electron density around CLA A 612:

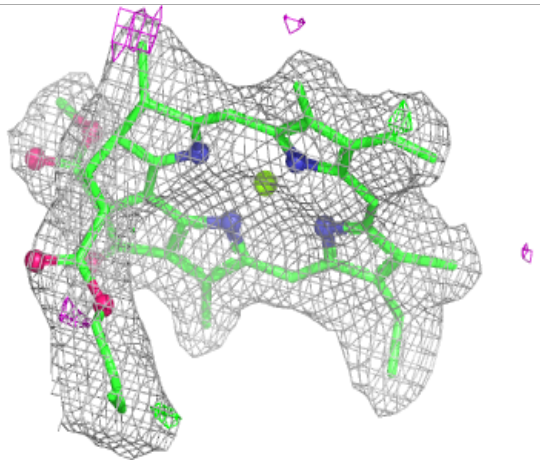
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

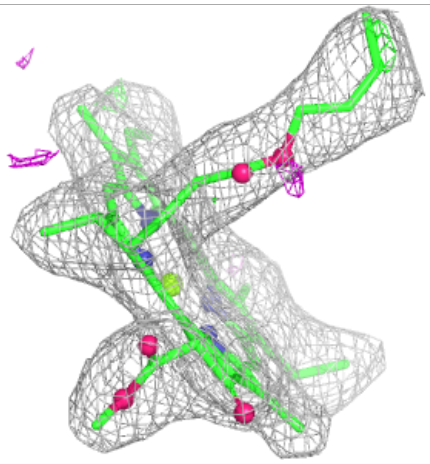


Electron density around CLA A 614:

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

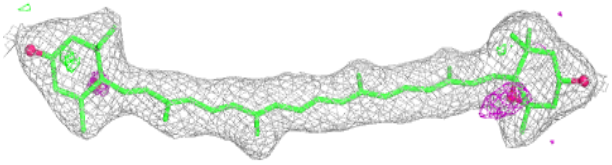


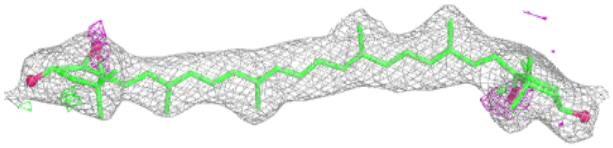


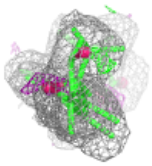


Electron density around XAT H 4622:

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

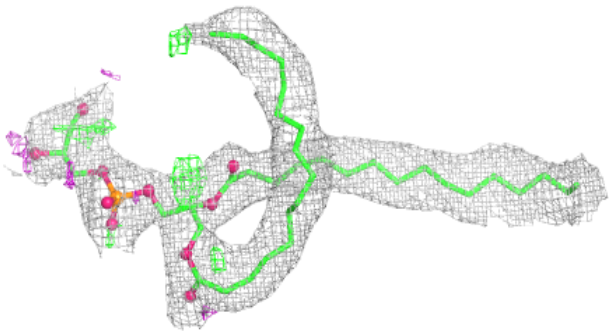


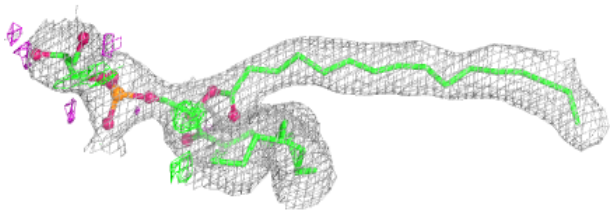


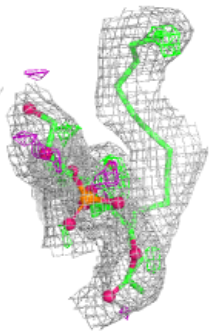


Electron density around LHG F 5630:

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

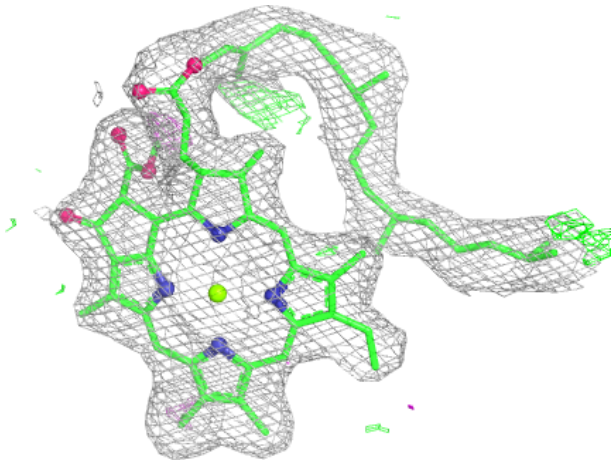


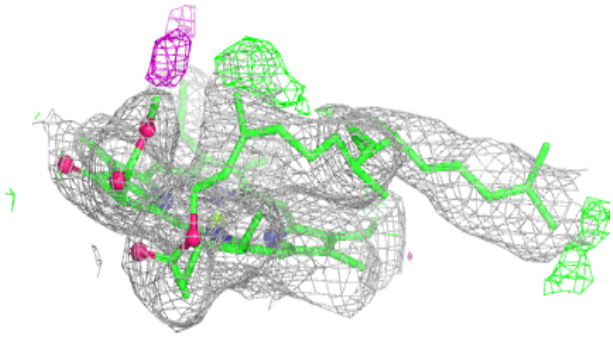


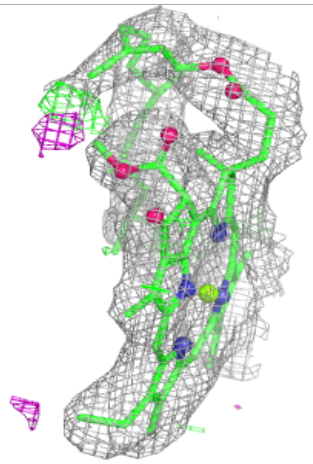


Electron density around CLA C 612:

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

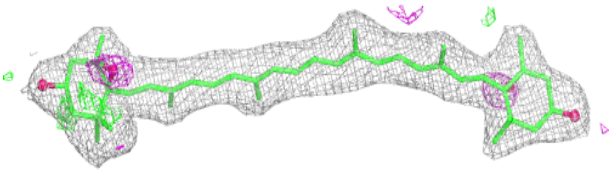


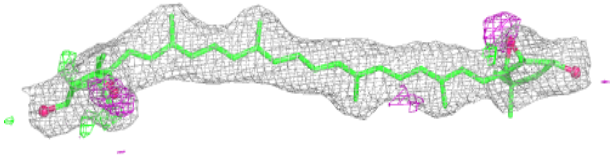


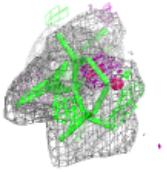


Electron density around XAT I 9622:

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

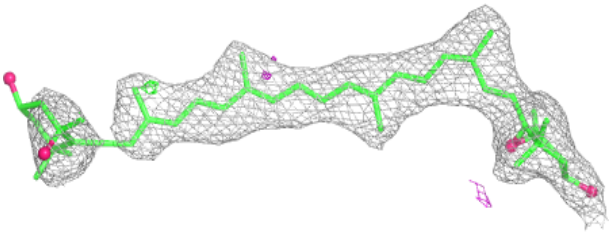


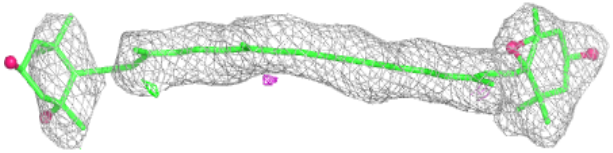


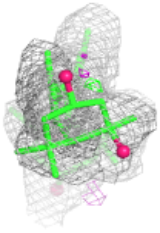


Electron density around NEX A 623:

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

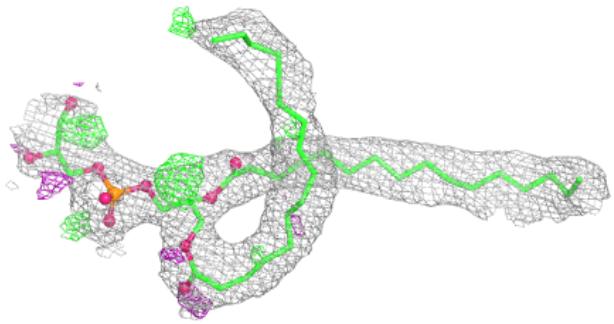


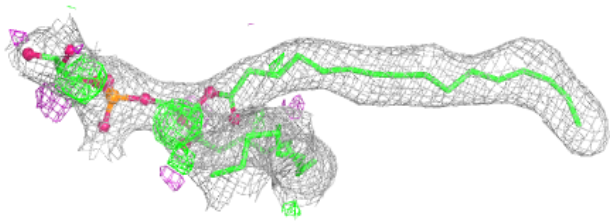


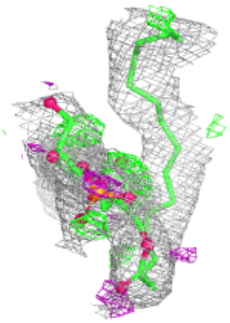


Electron density around LHG J 9630:

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

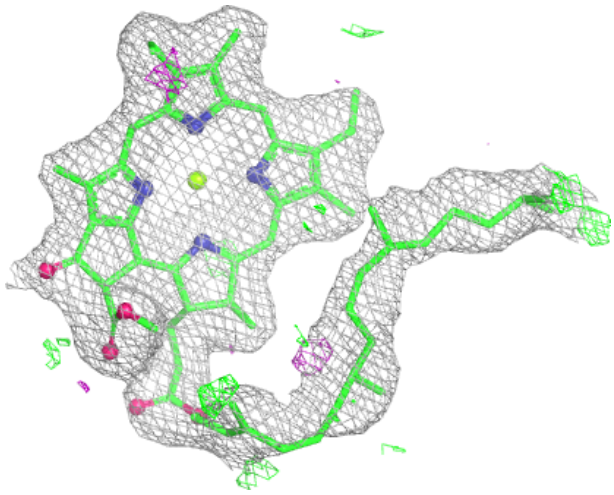


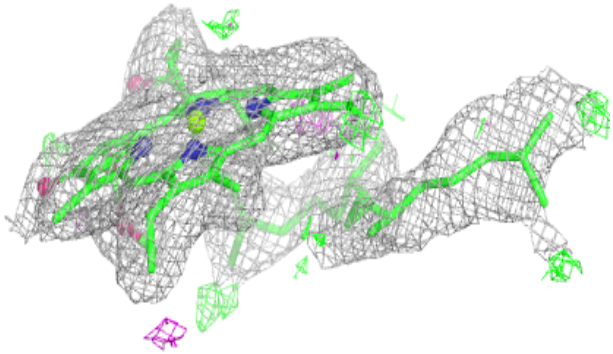




Electron density around CLA F 612:

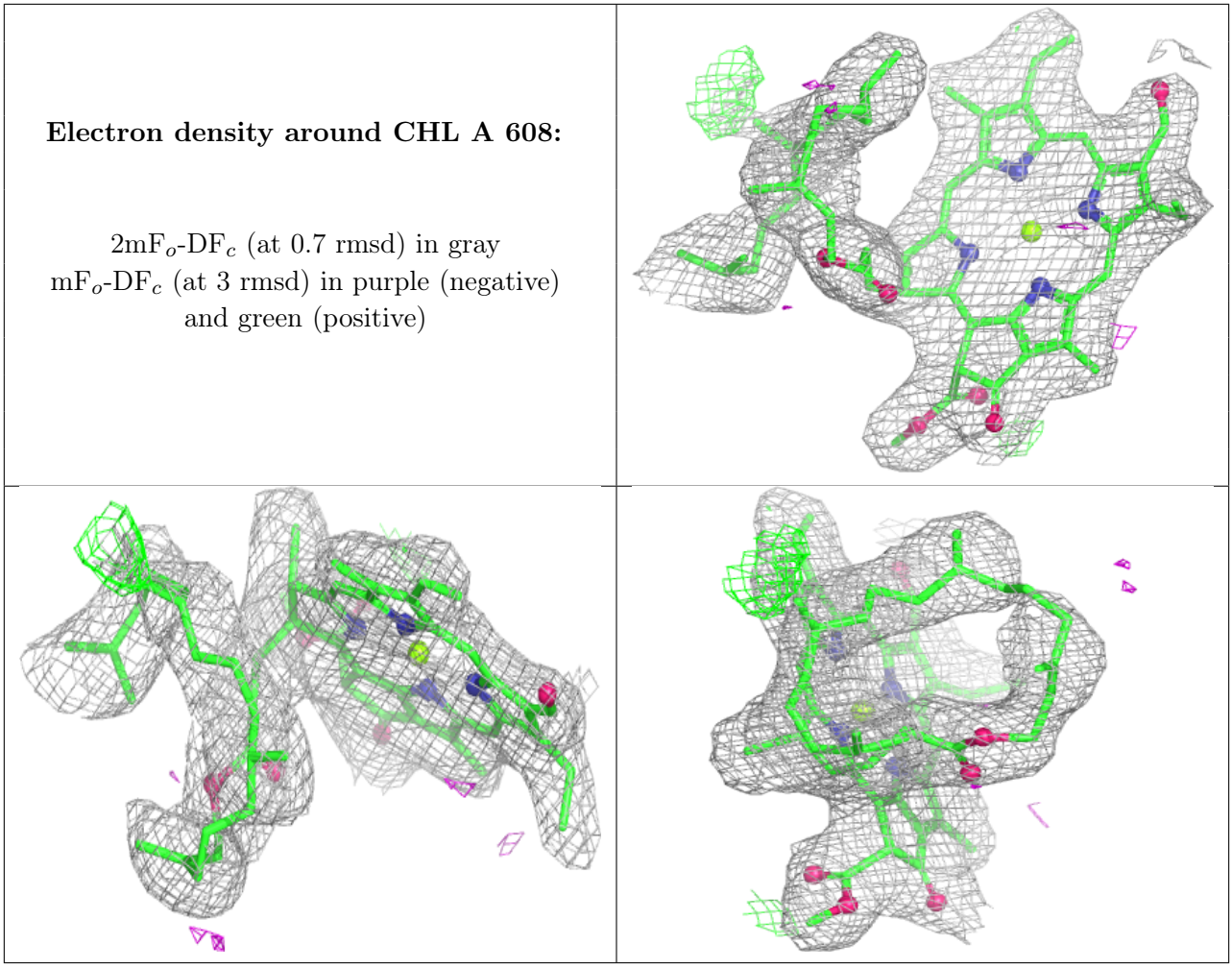
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





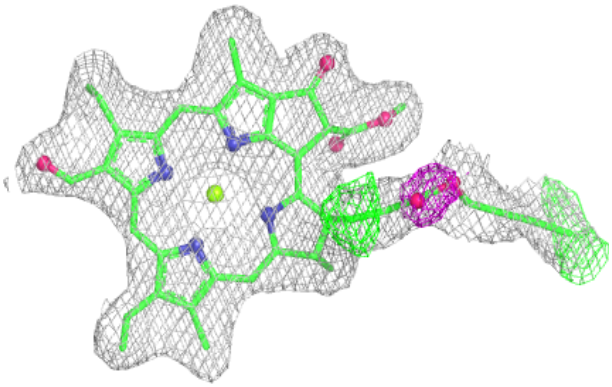
Electron density around CHL A 608:

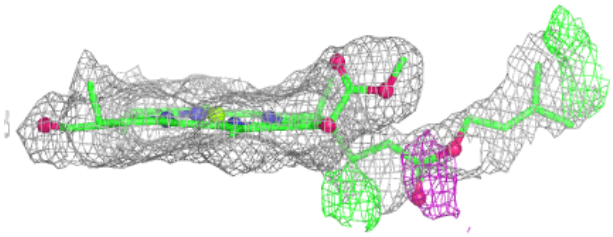
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

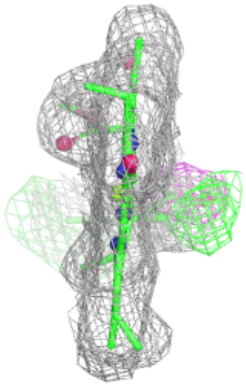


Electron density around CHL C 606:

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

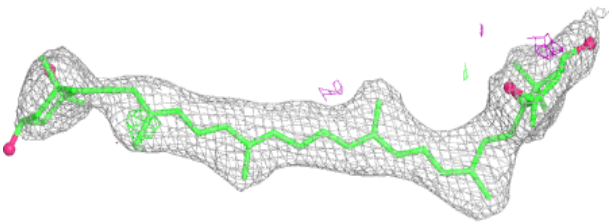


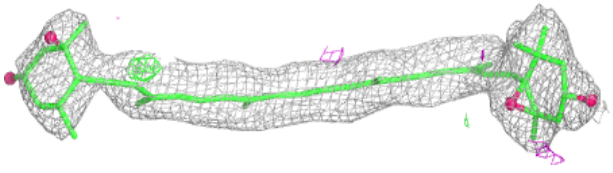




Electron density around NEX G 6623:

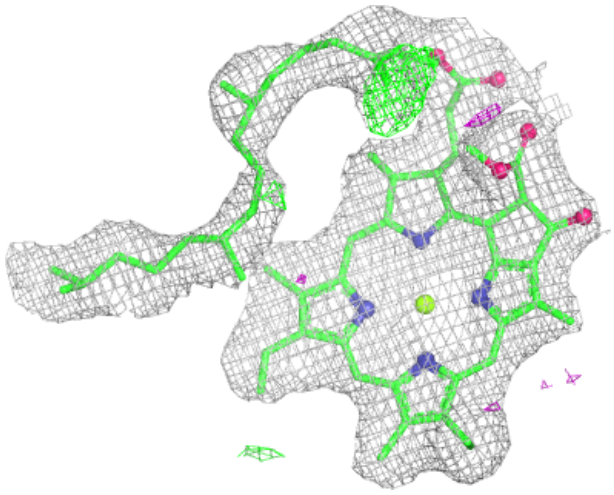
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

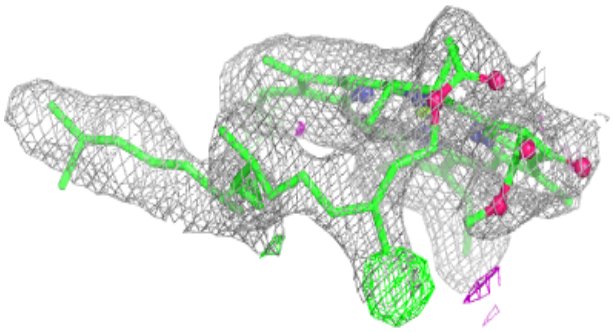


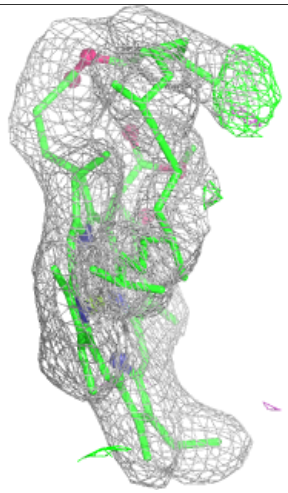


Electron density around CLA H 612:

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

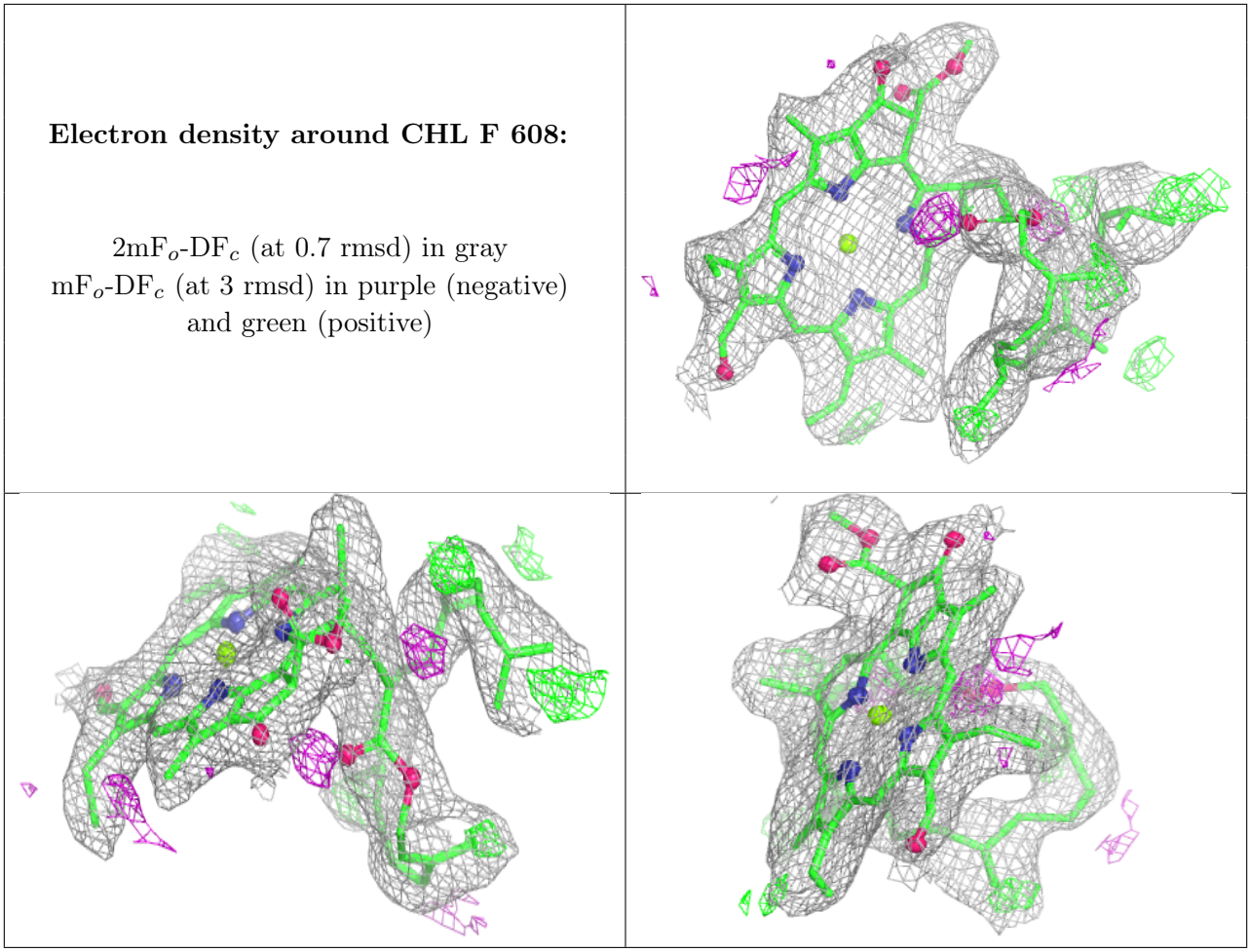






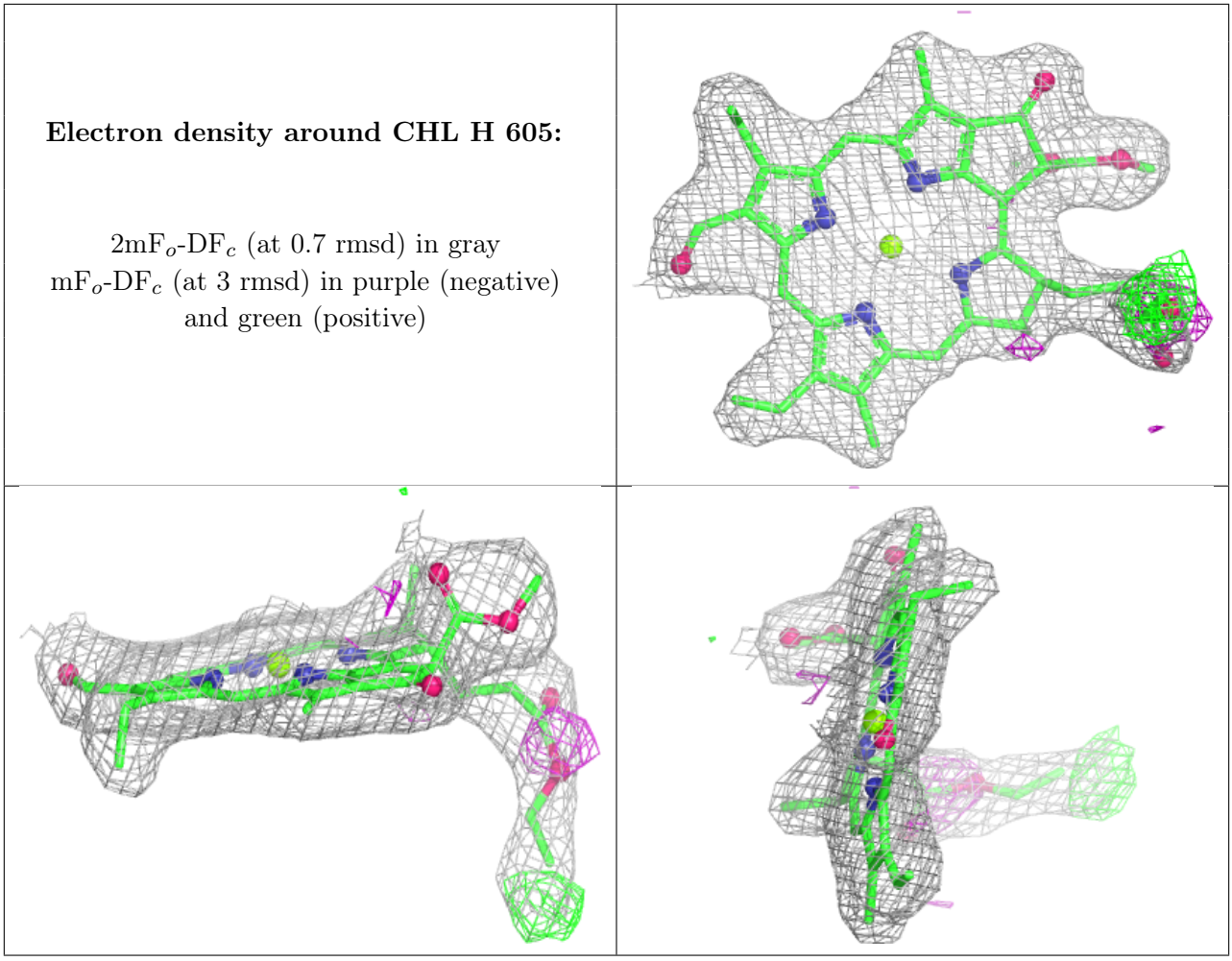
Electron density around CHL F 608:

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



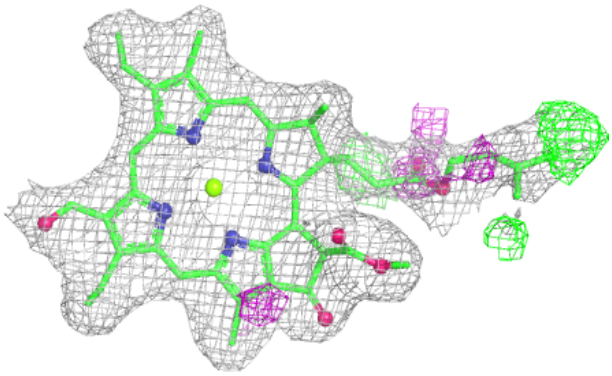
Electron density around CHL H 605:

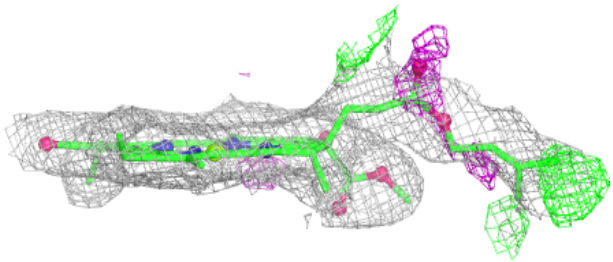
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

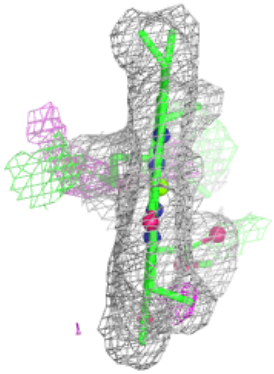


Electron density around CHL H 606:

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

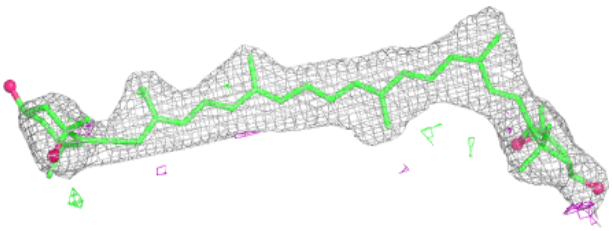


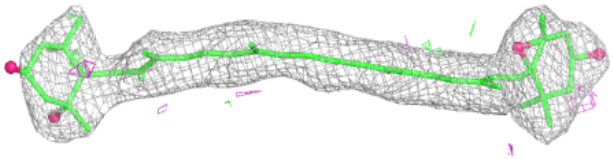


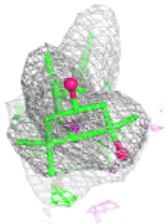


Electron density around NEX I 8623:

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

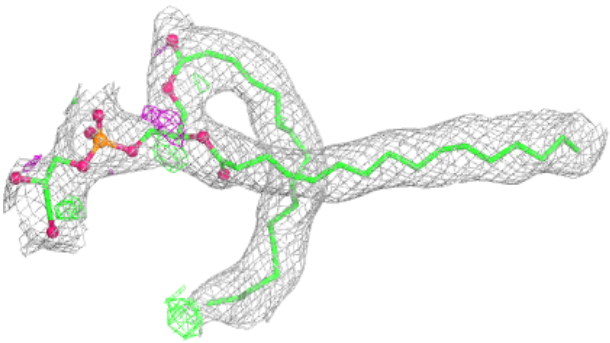


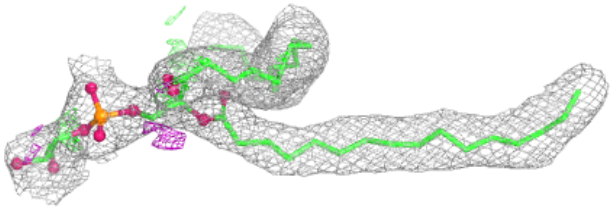


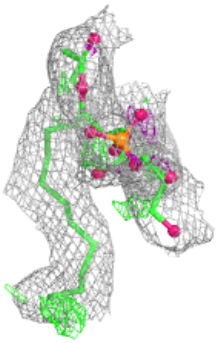


Electron density around LHG I 8630:

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

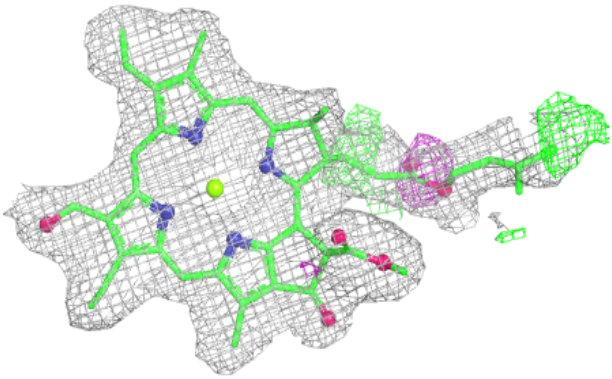


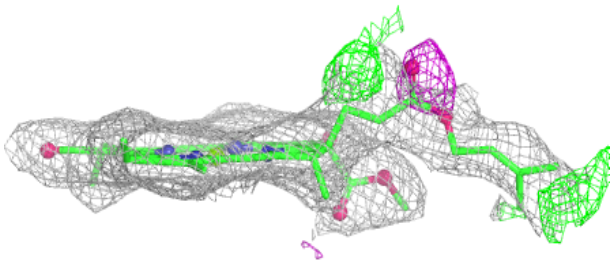


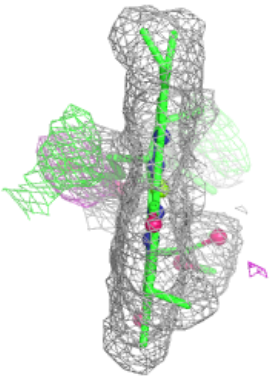


Electron density around CHL I 606:

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

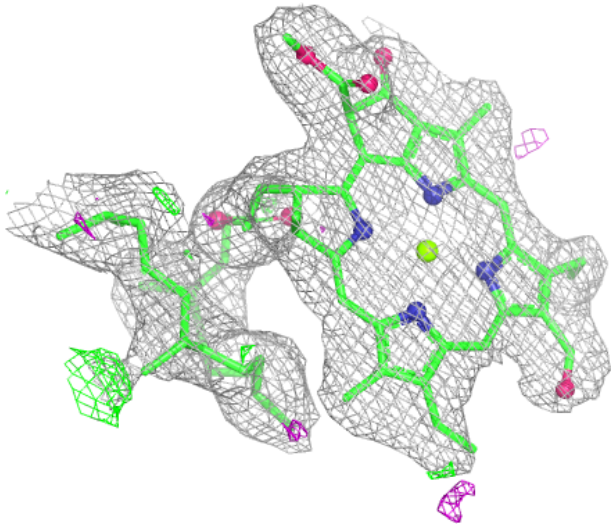


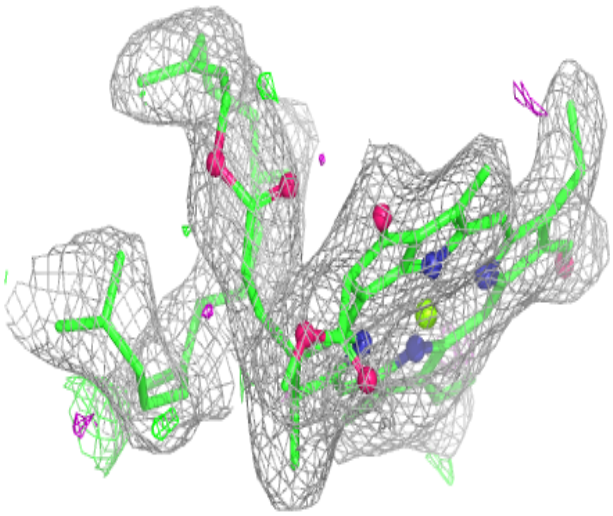


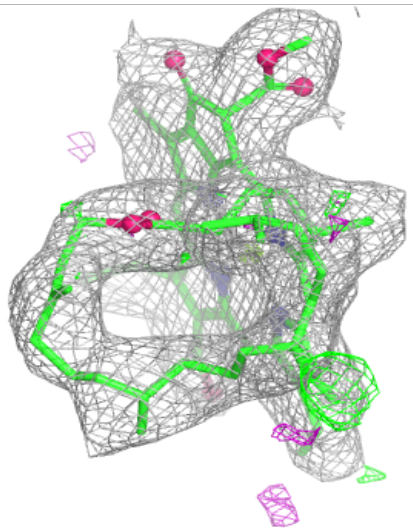


Electron density around CHL I 608:

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

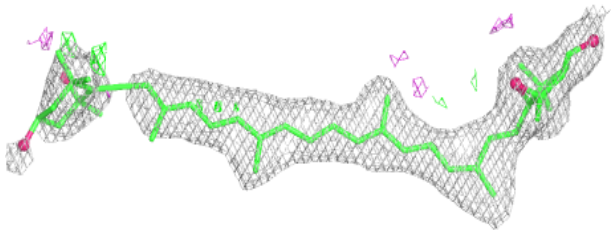


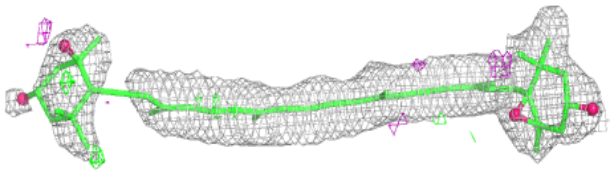


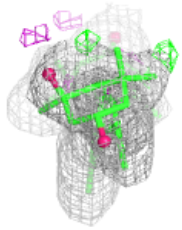


Electron density around NEX J 9623:

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

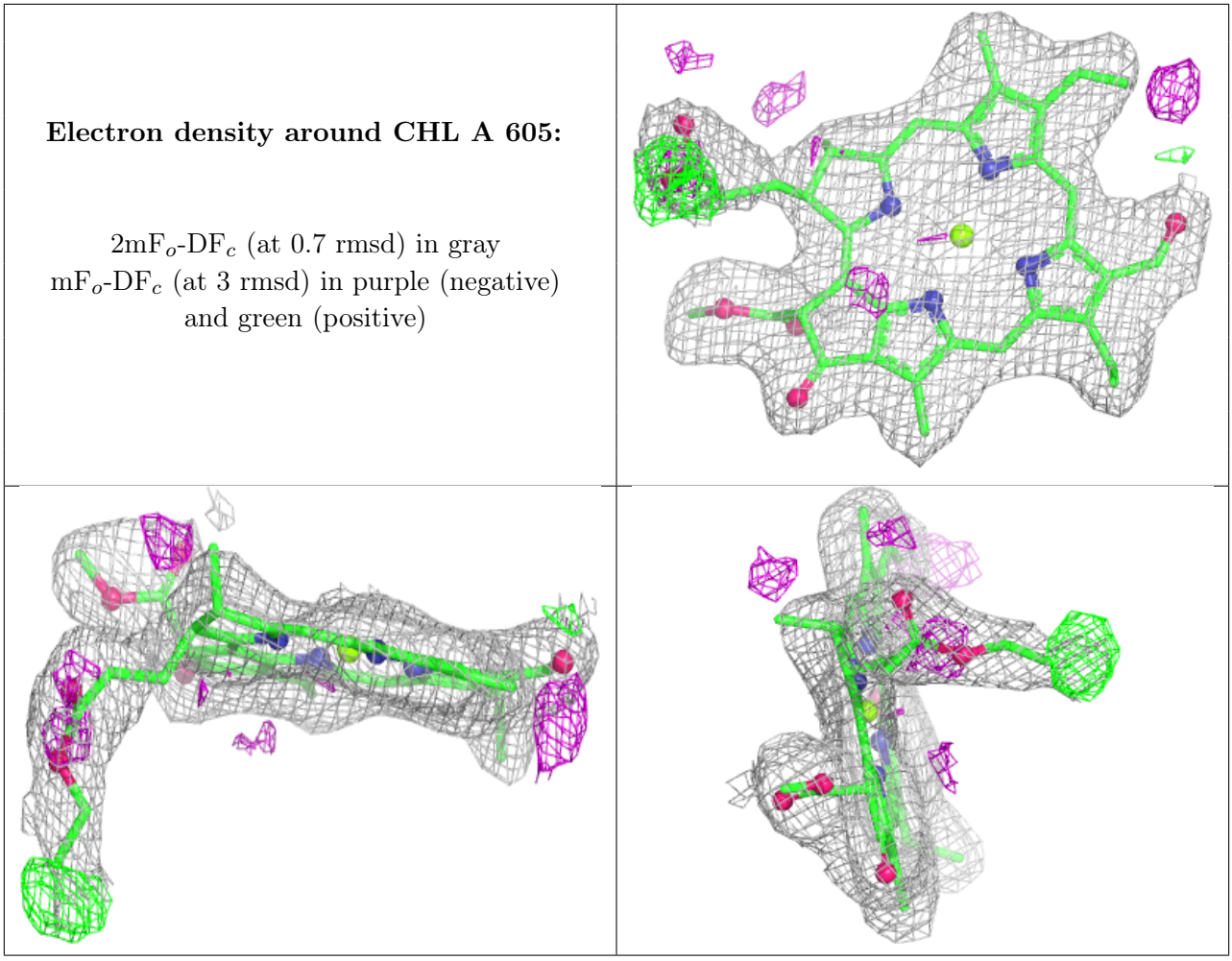






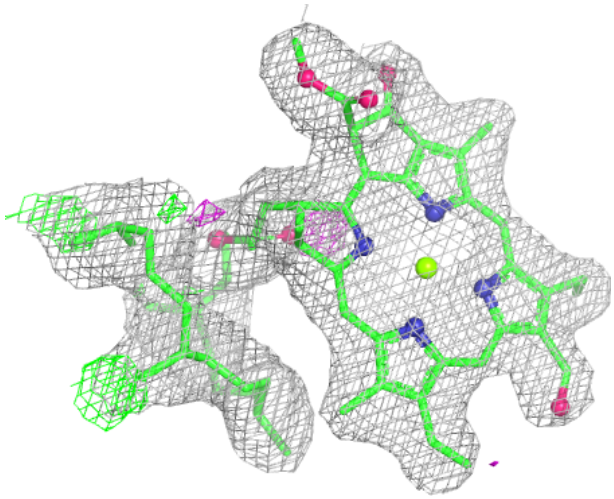
Electron density around CHL A 605:

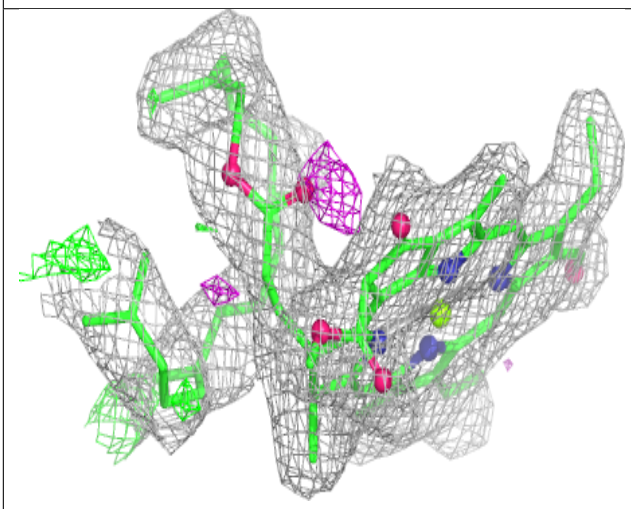
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

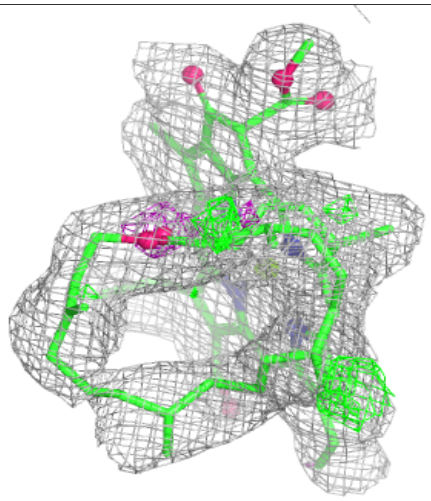


Electron density around CHL J 608:

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

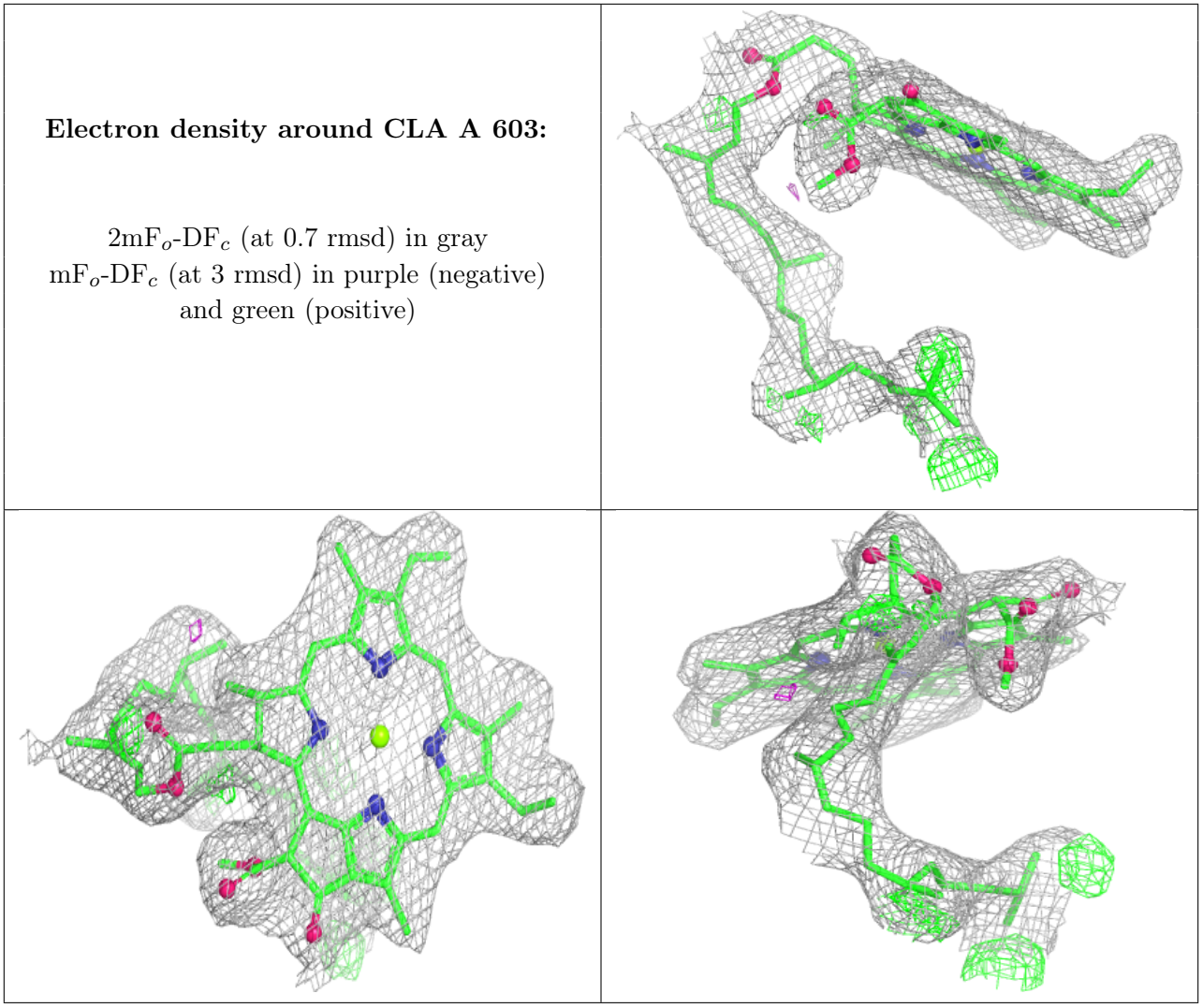






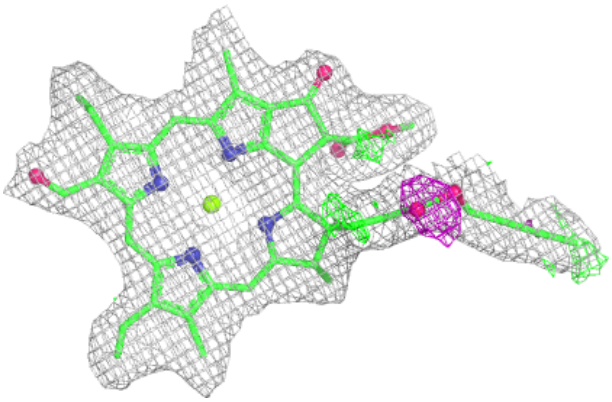
Electron density around CLA A 603:

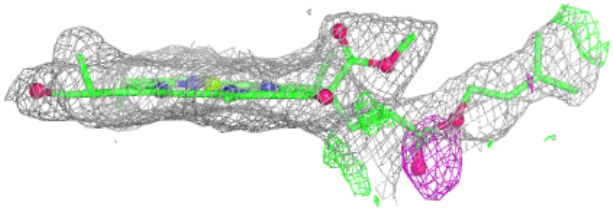
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

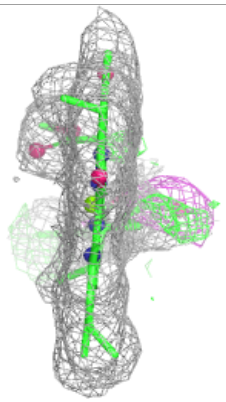


Electron density around CHL A 606:

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

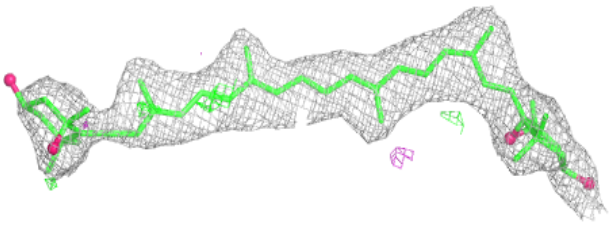


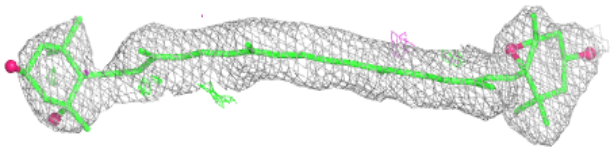


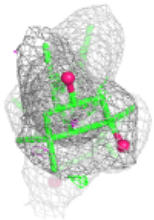


Electron density around NEX B 1623:

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

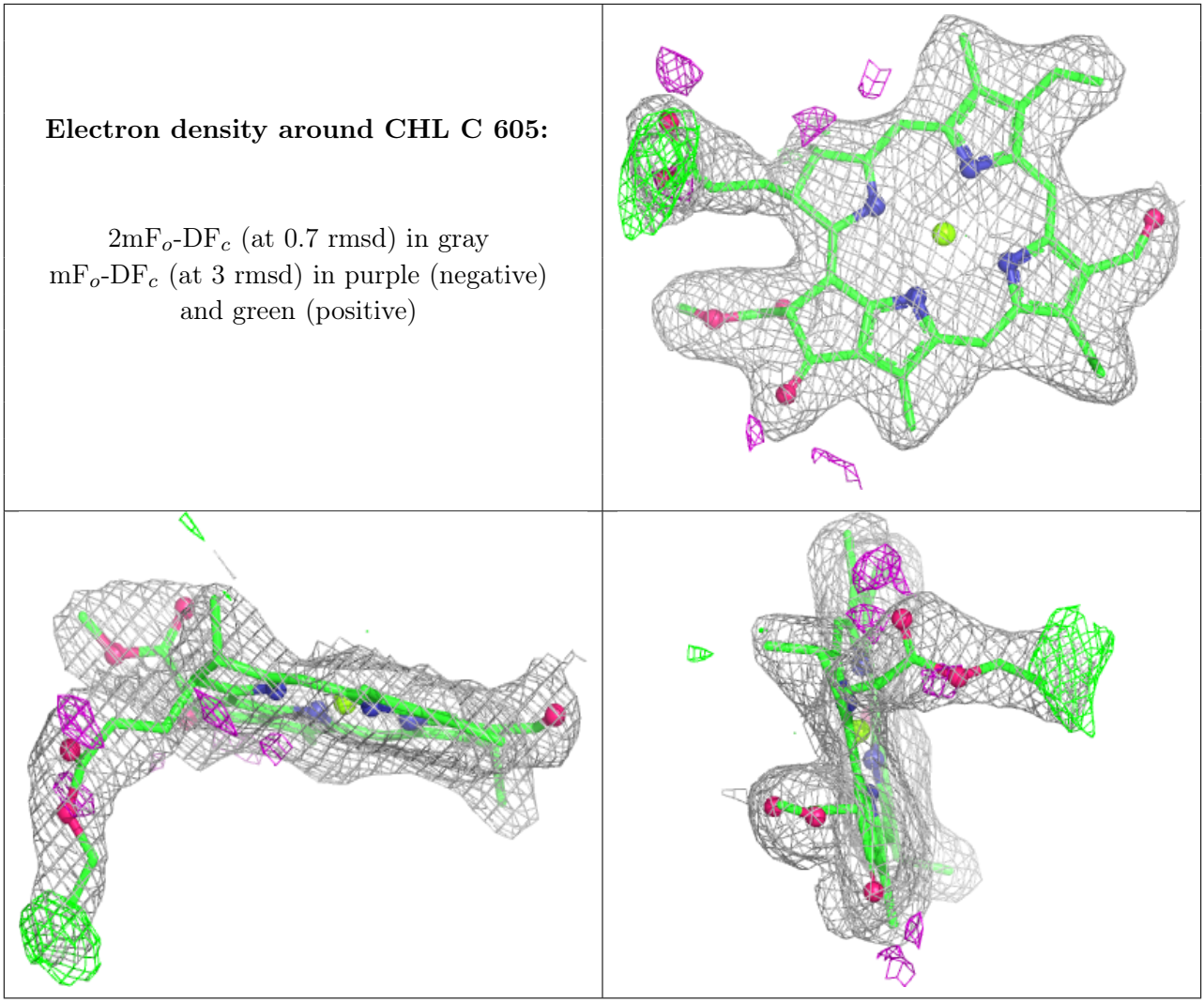






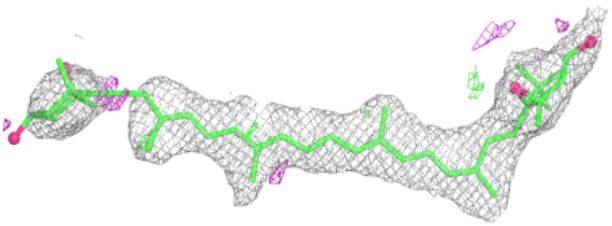
Electron density around CHL C 605:

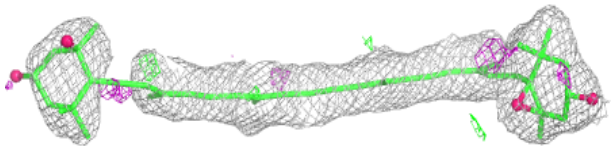
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

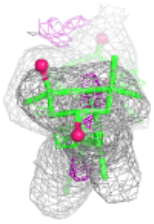


Electron density around NEX C 2623:

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

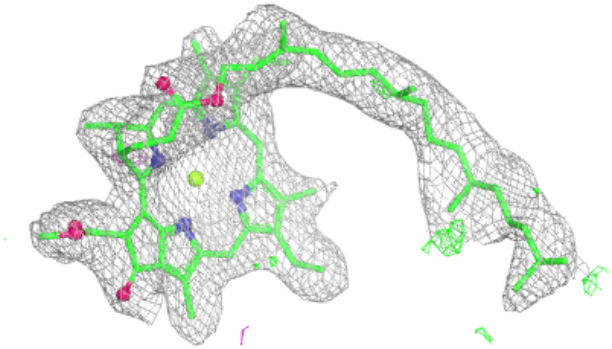


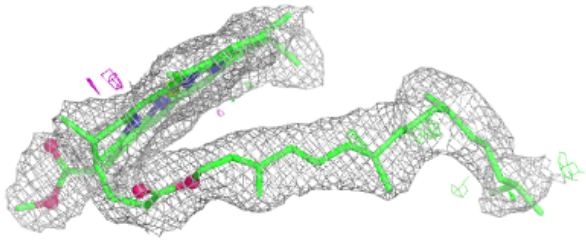


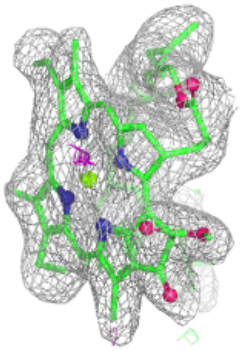


Electron density around CLA B 610:

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

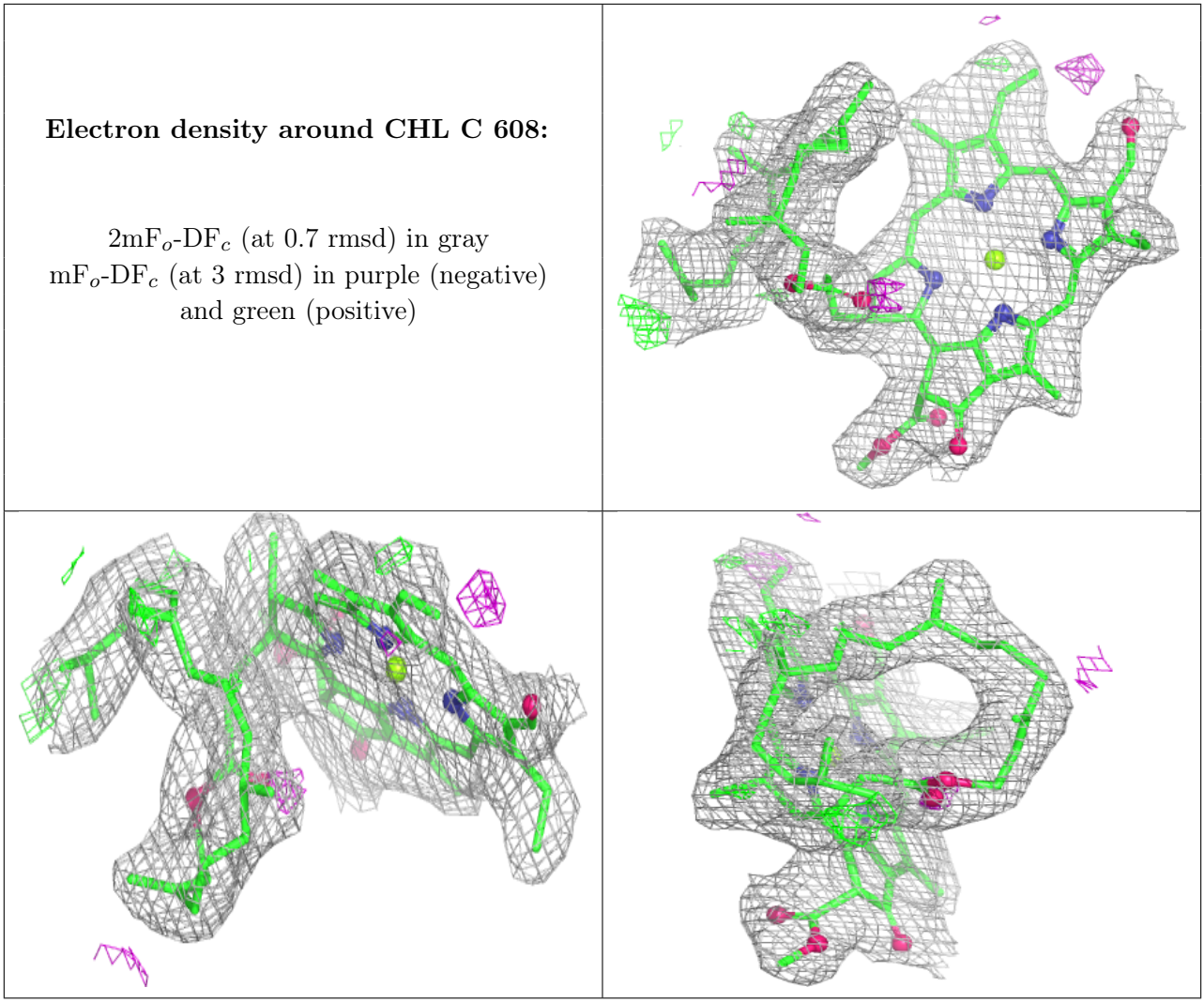






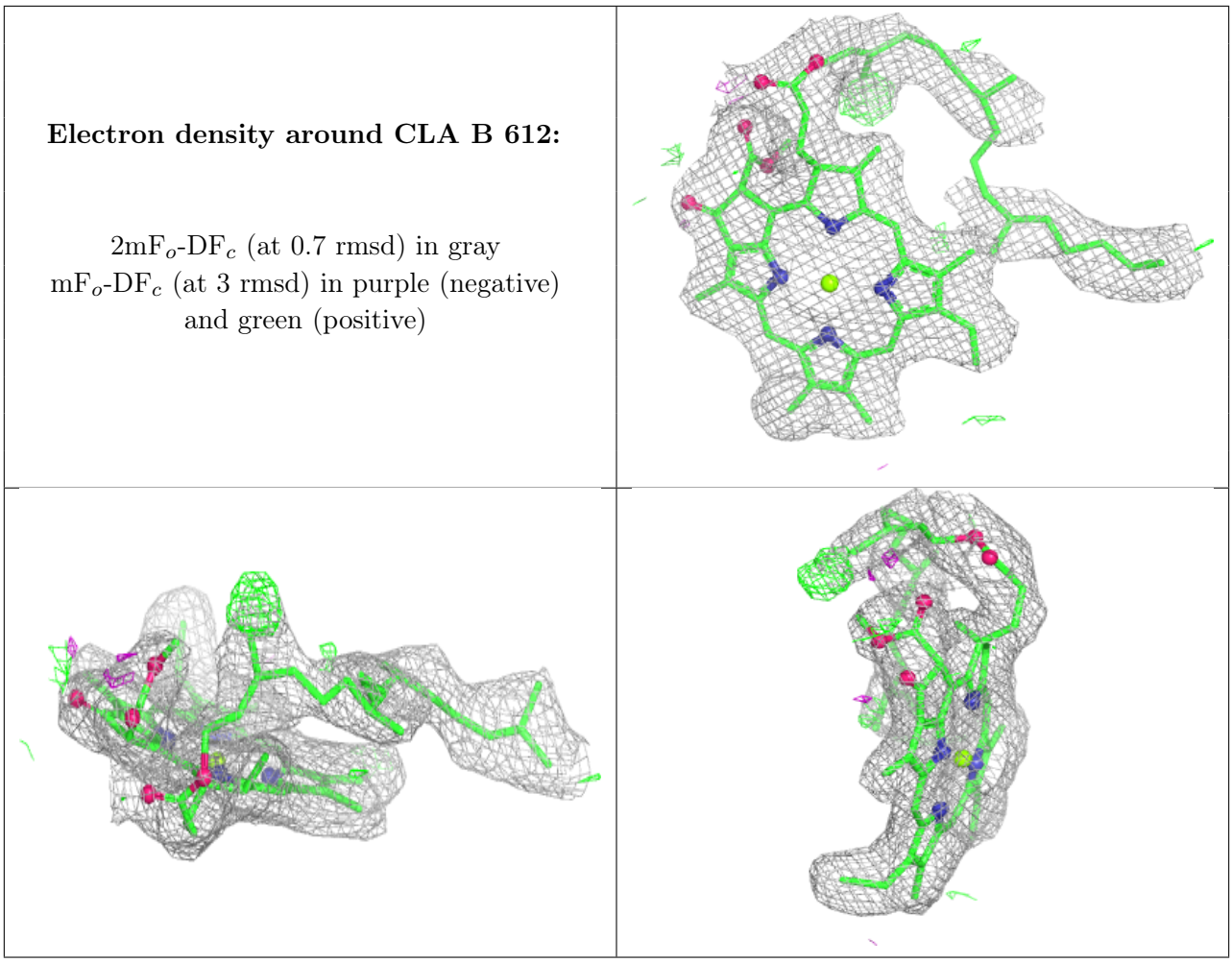
Electron density around CHL C 608:

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



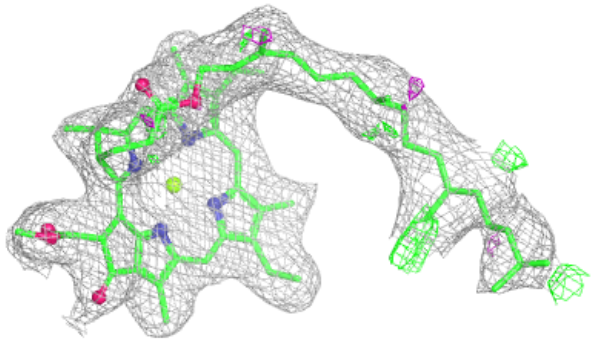
Electron density around CLA B 612:

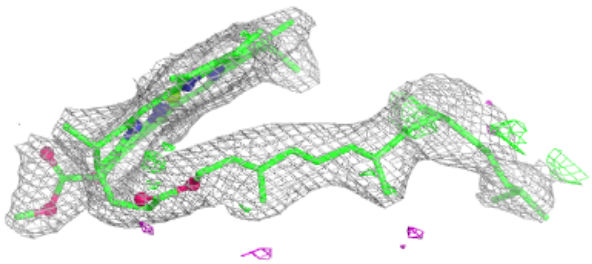
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

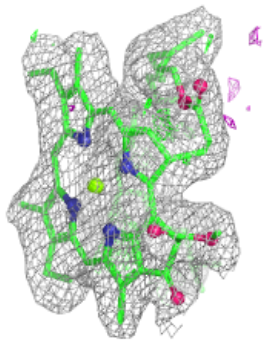


Electron density around CLA C 610:

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

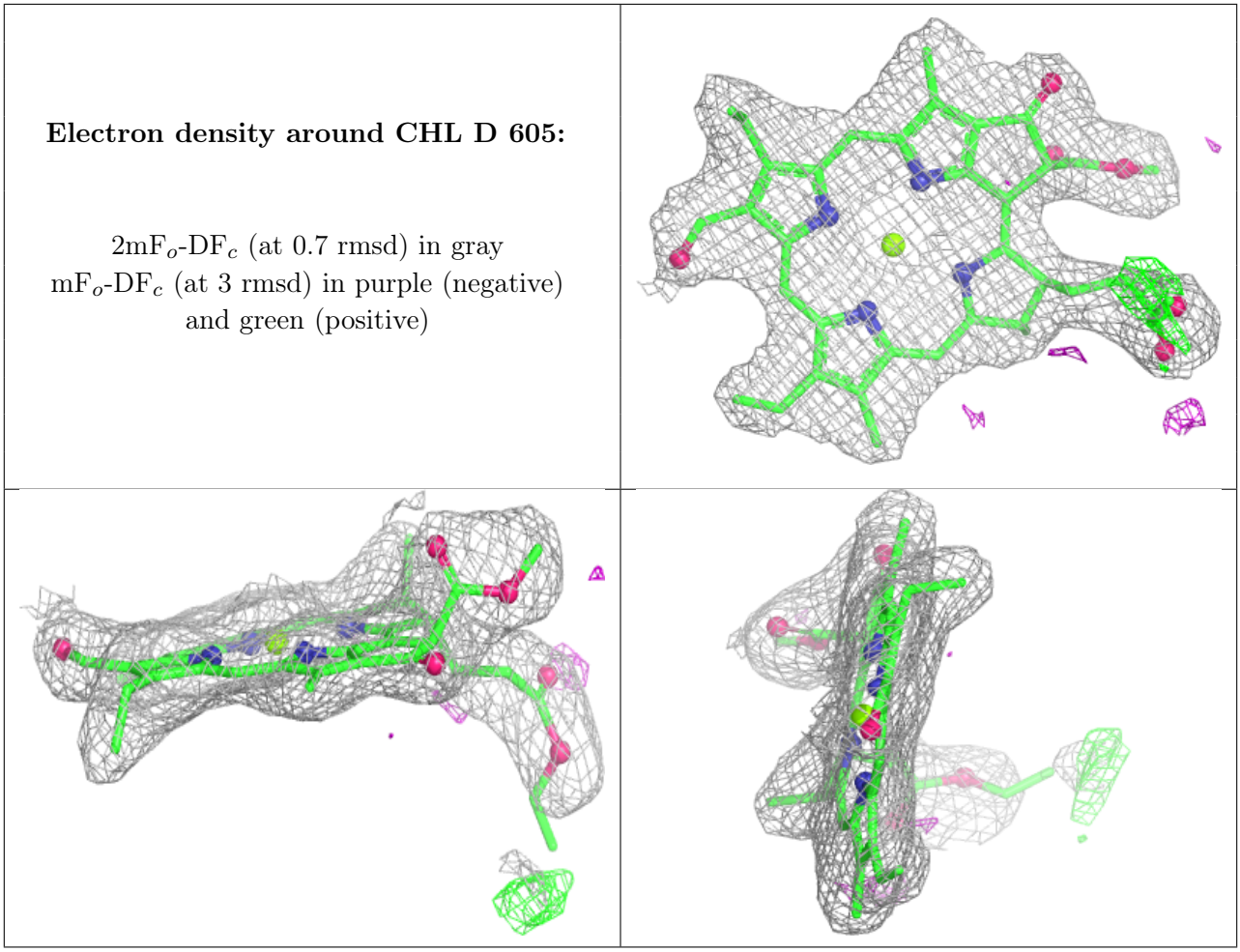






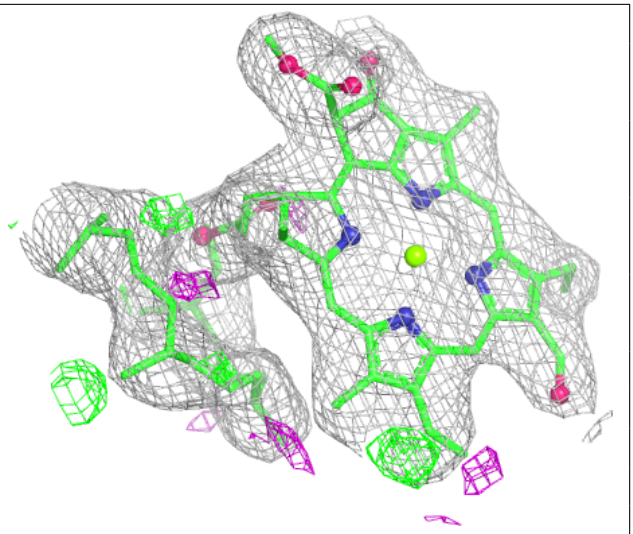
Electron density around CHL D 605:

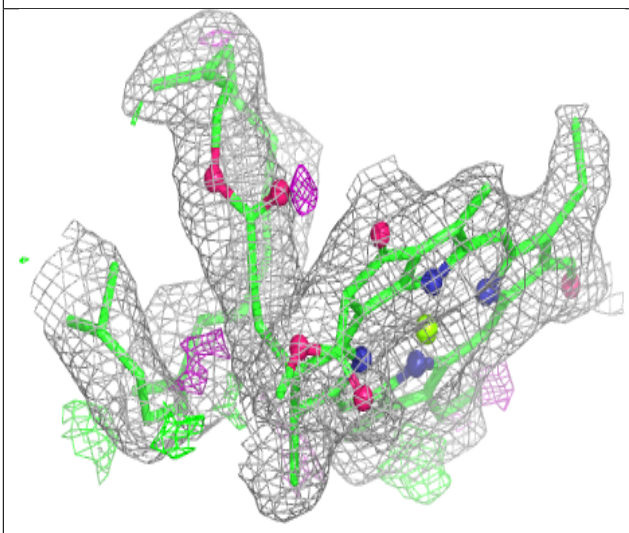
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

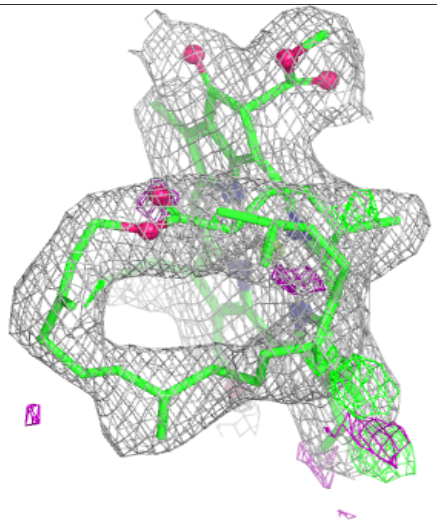


Electron density around CHL D 608:

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

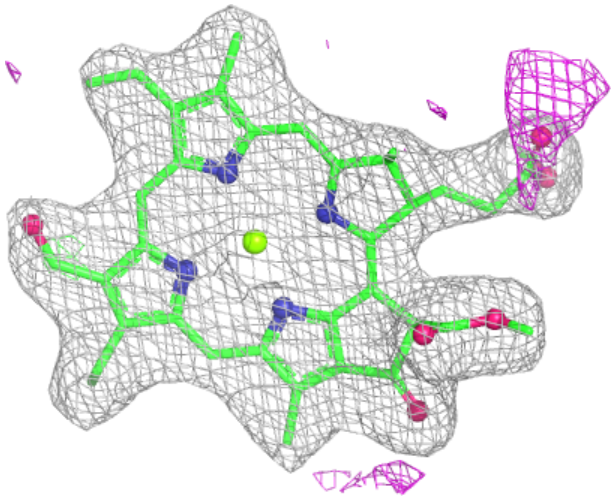


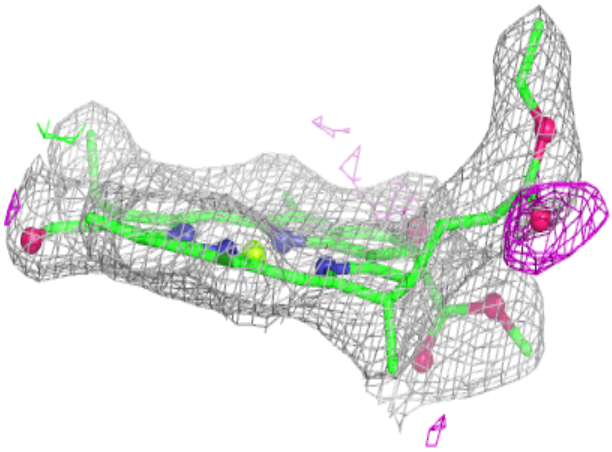


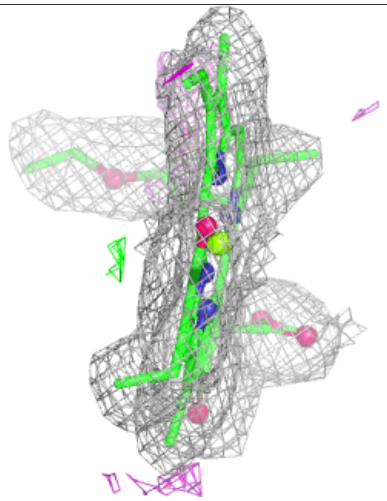


Electron density around CHL E 605:

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

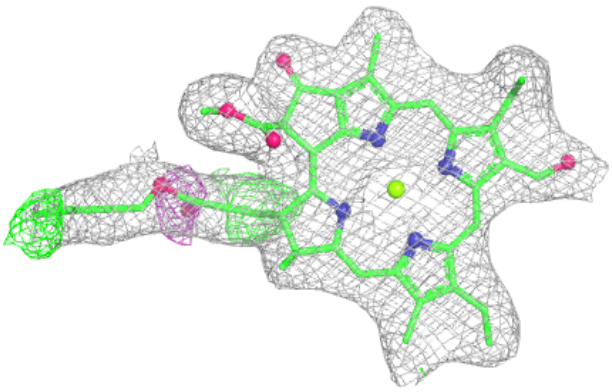


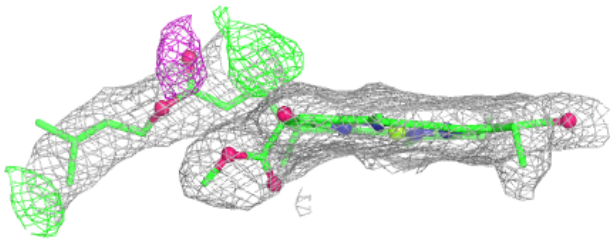


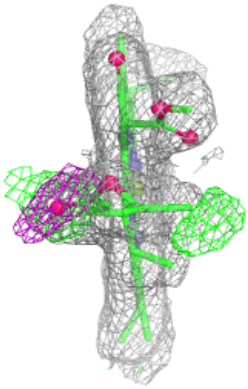


Electron density around CHL E 606:

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

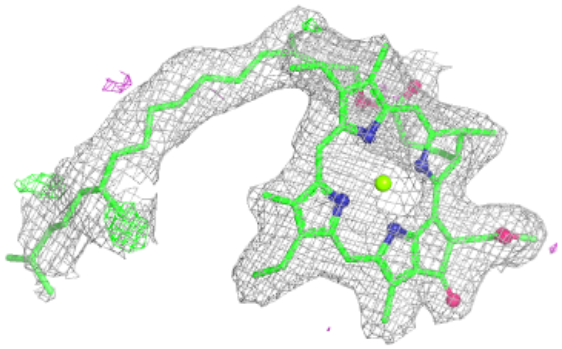


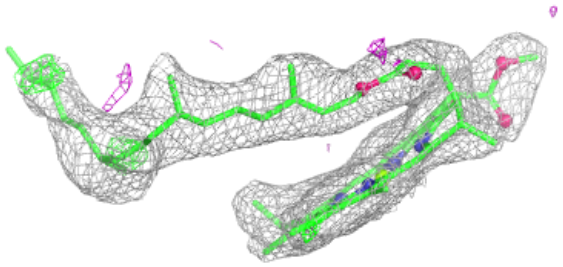




Electron density around CLA E 610:

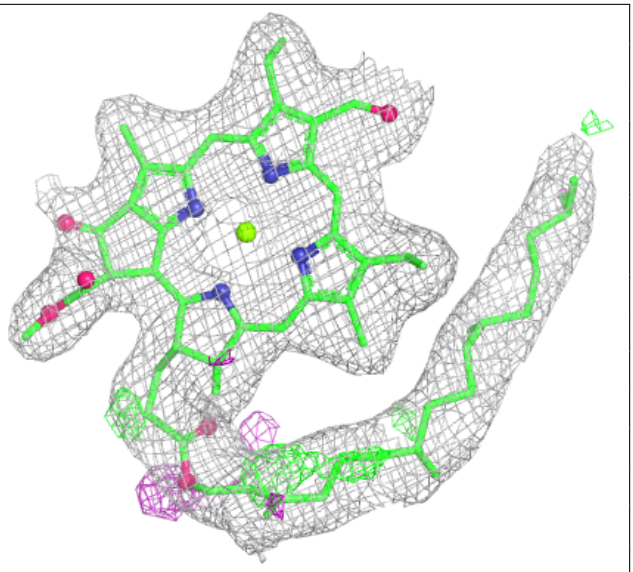
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

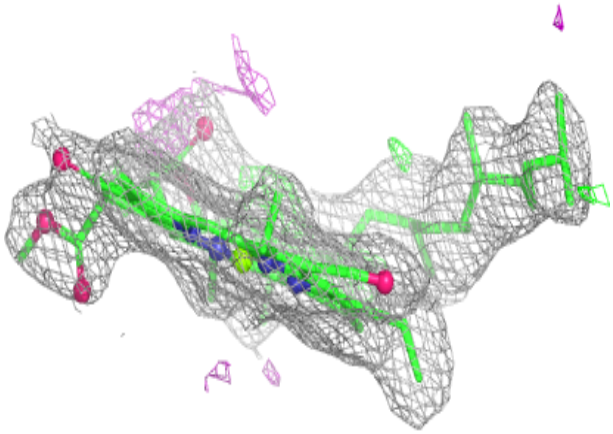




Electron density around CHL E 607:

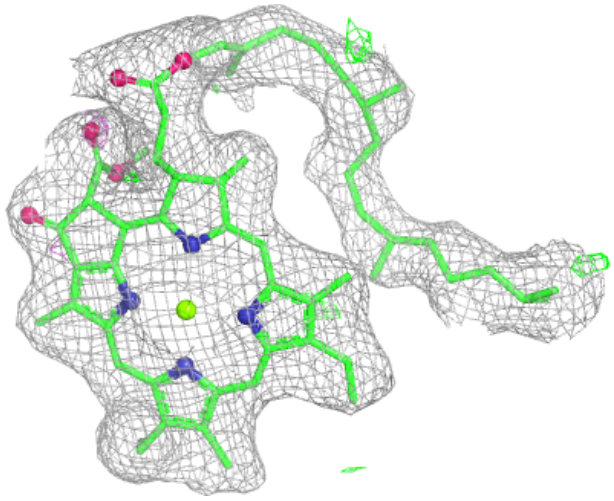
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

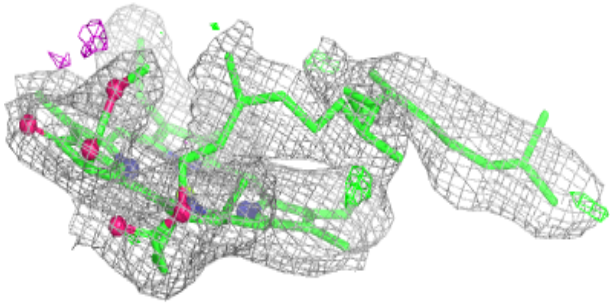


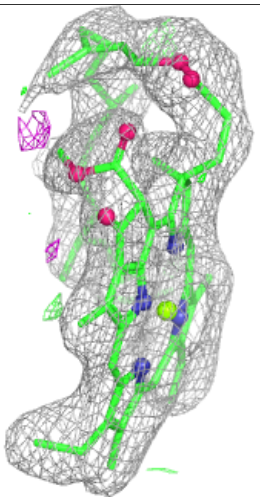


Electron density around CLA E 612:

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

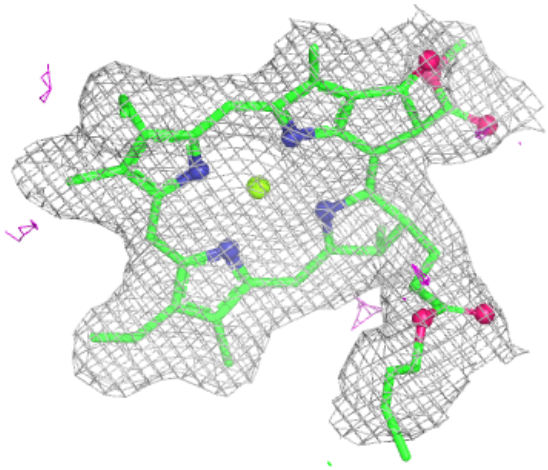


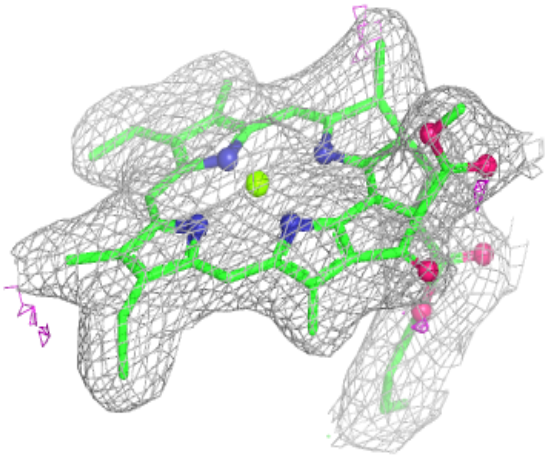


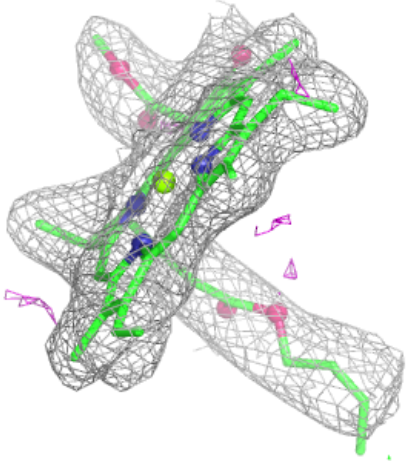


Electron density around CLA E 614:

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

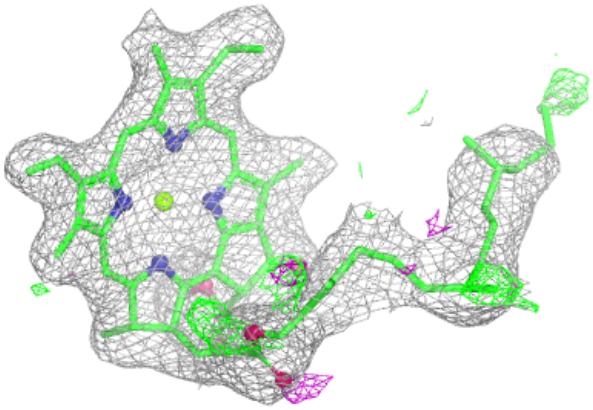


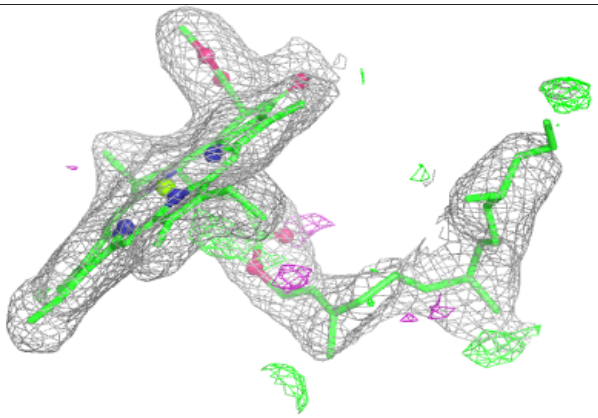


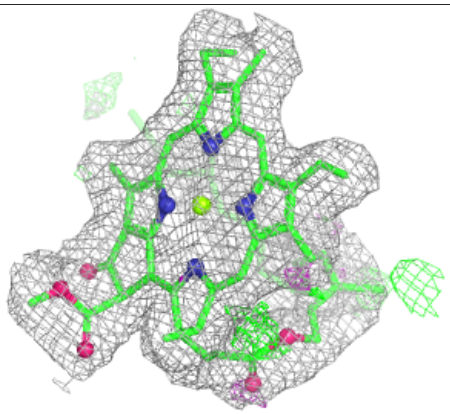


Electron density around CLA F 604:

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

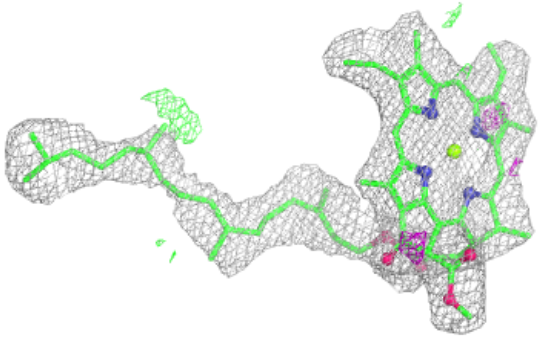


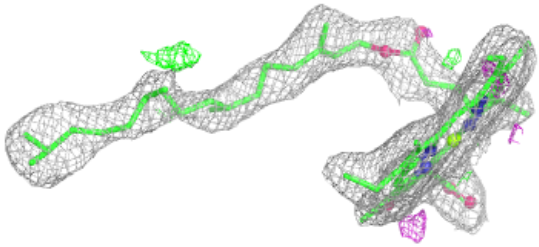


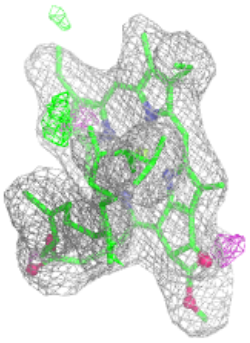


Electron density around CLA F 611:

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

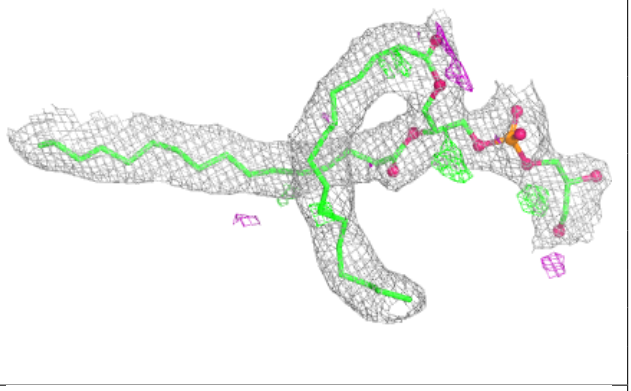


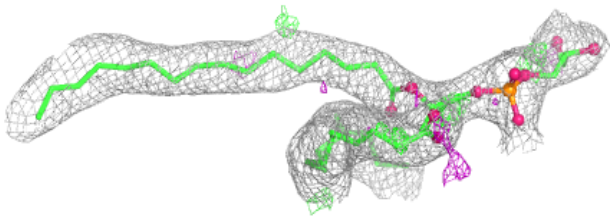


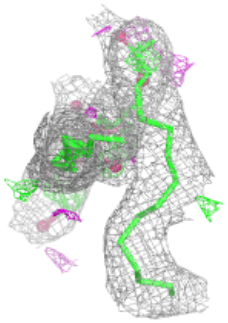


Electron density around LHG C 2630:

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

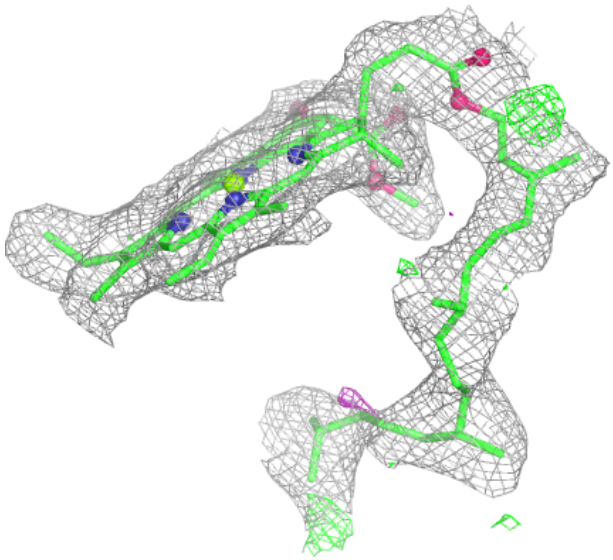


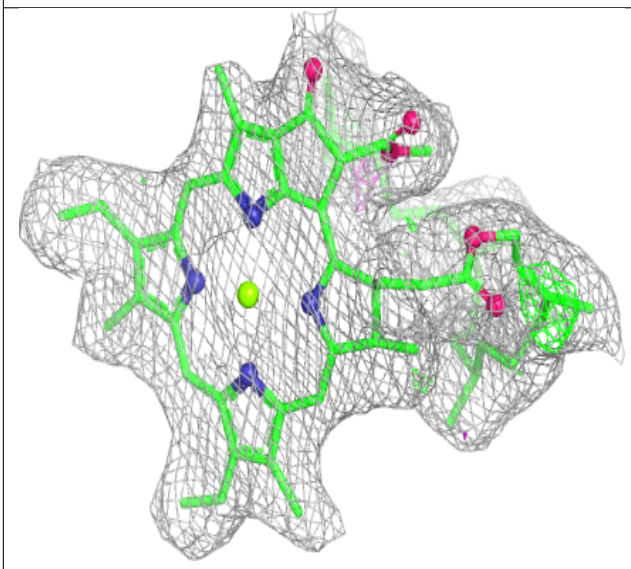


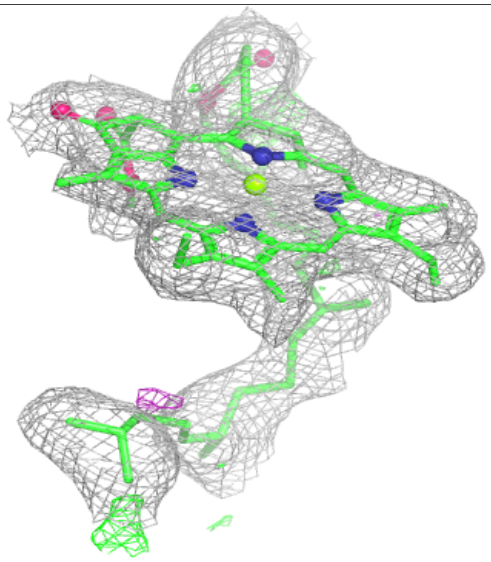


Electron density around CLA G 603:

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

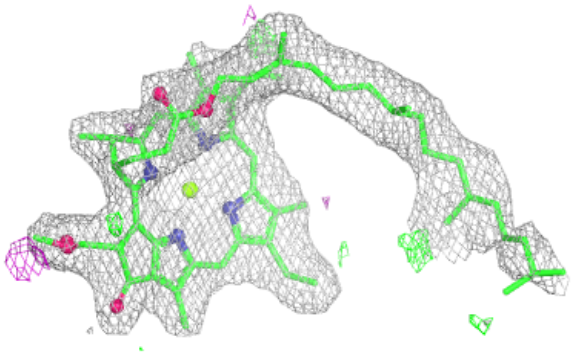


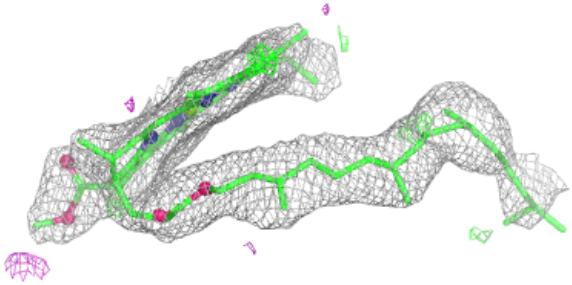


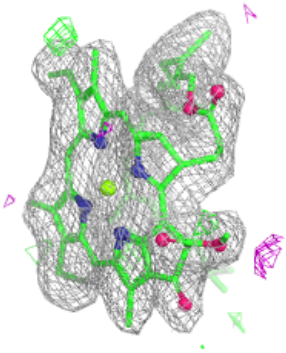


Electron density around CLA G 610:

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

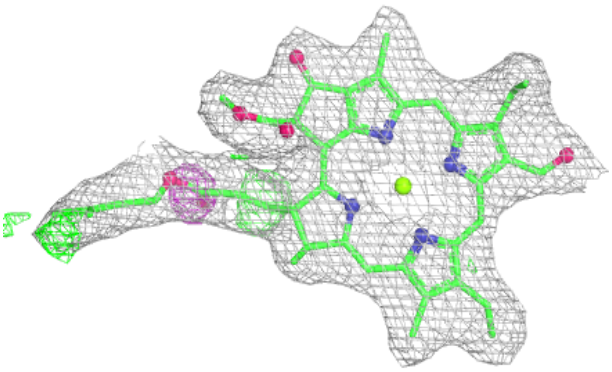


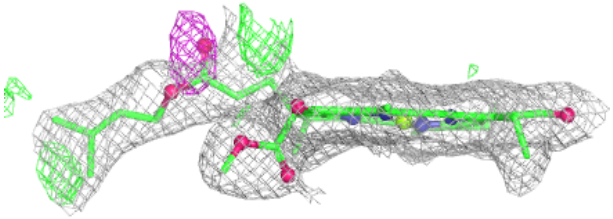


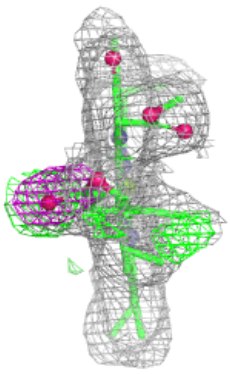


Electron density around CHL F 606:

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

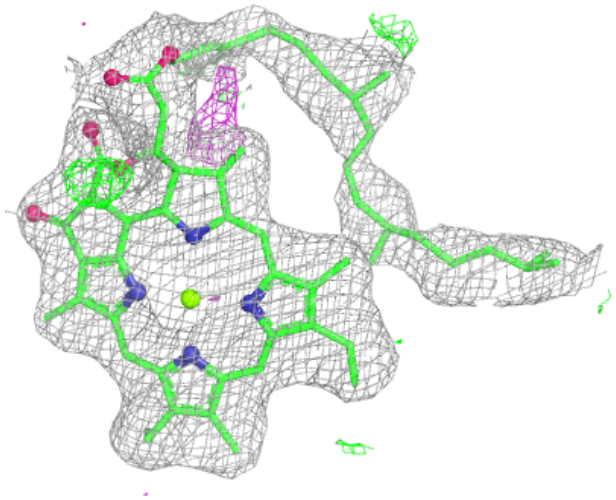


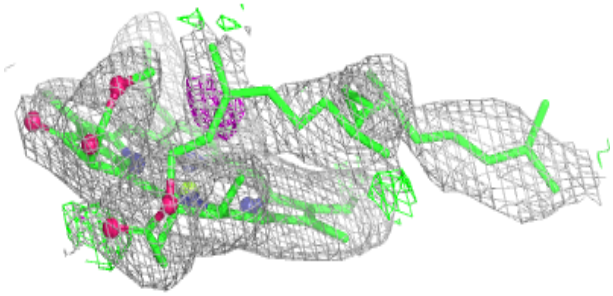


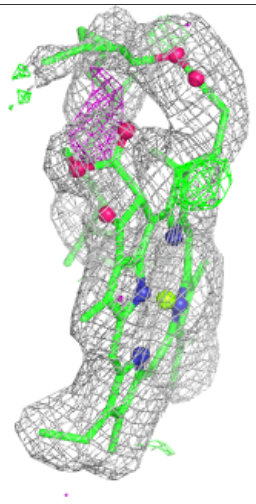


Electron density around CLA G 612:

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

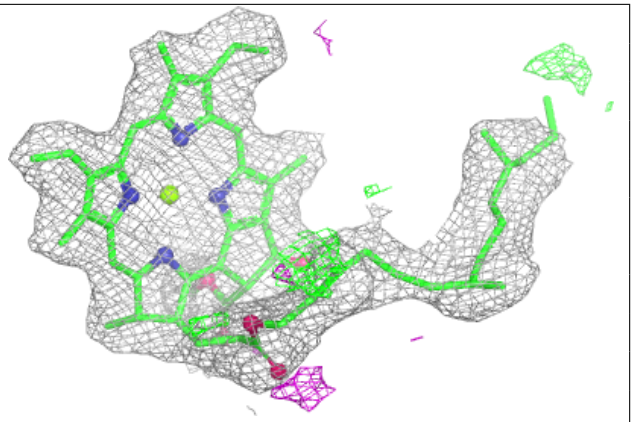


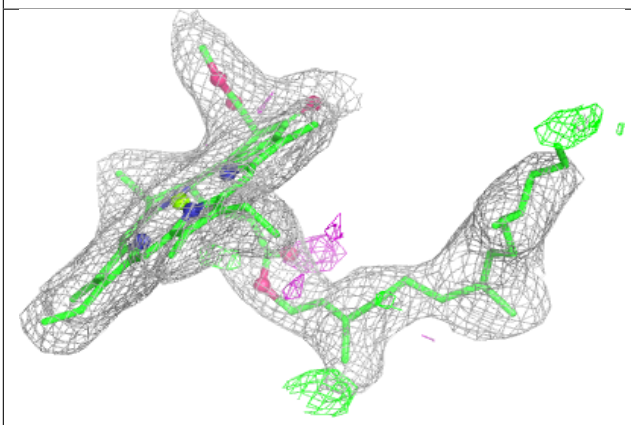


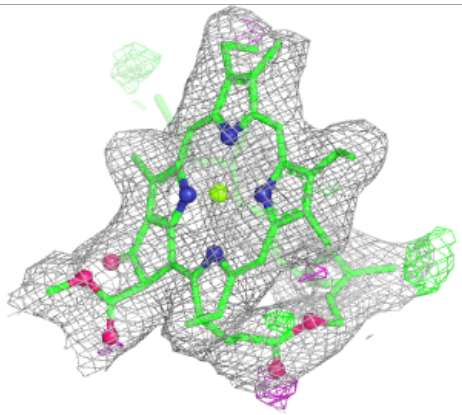


Electron density around CLA H 604:

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

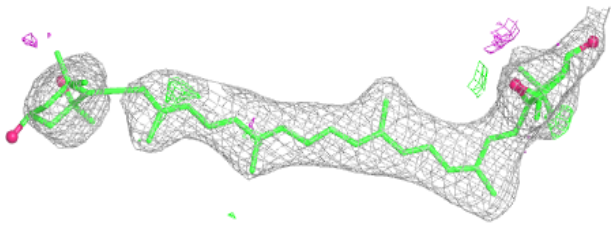


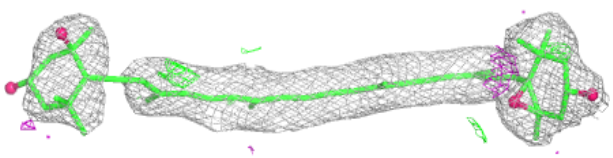


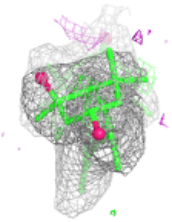


Electron density around NEX D 3623:

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

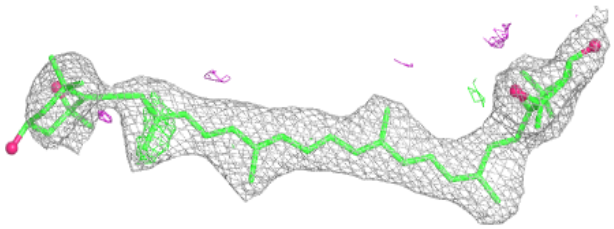


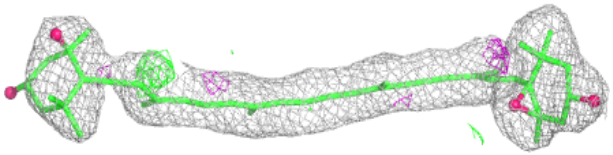


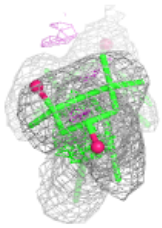


Electron density around NEX E 4623:

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

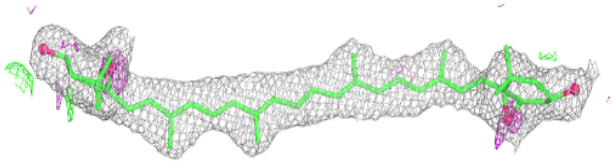


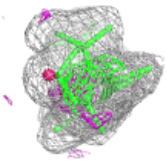




Electron density around XAT J 3622:

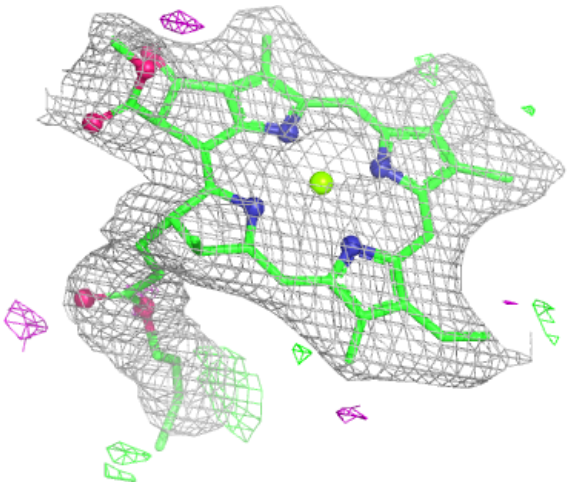
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

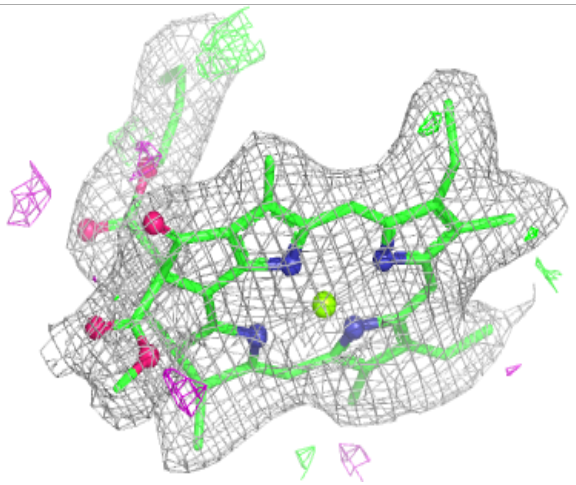


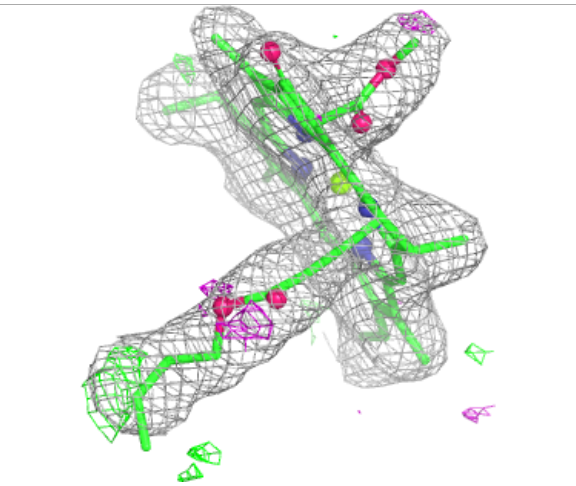


Electron density around CLA H 614:

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

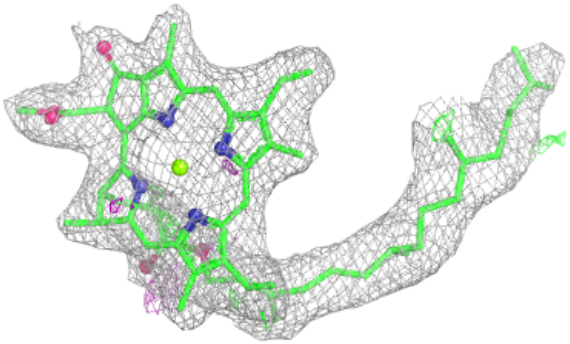


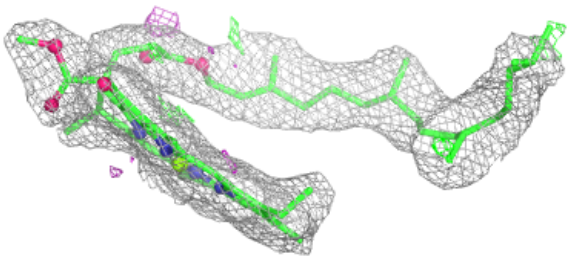




Electron density around CLA I 610:

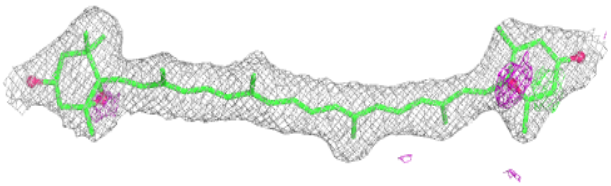
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

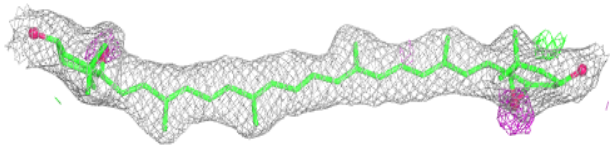


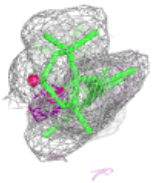


Electron density around XAT C 7622:

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

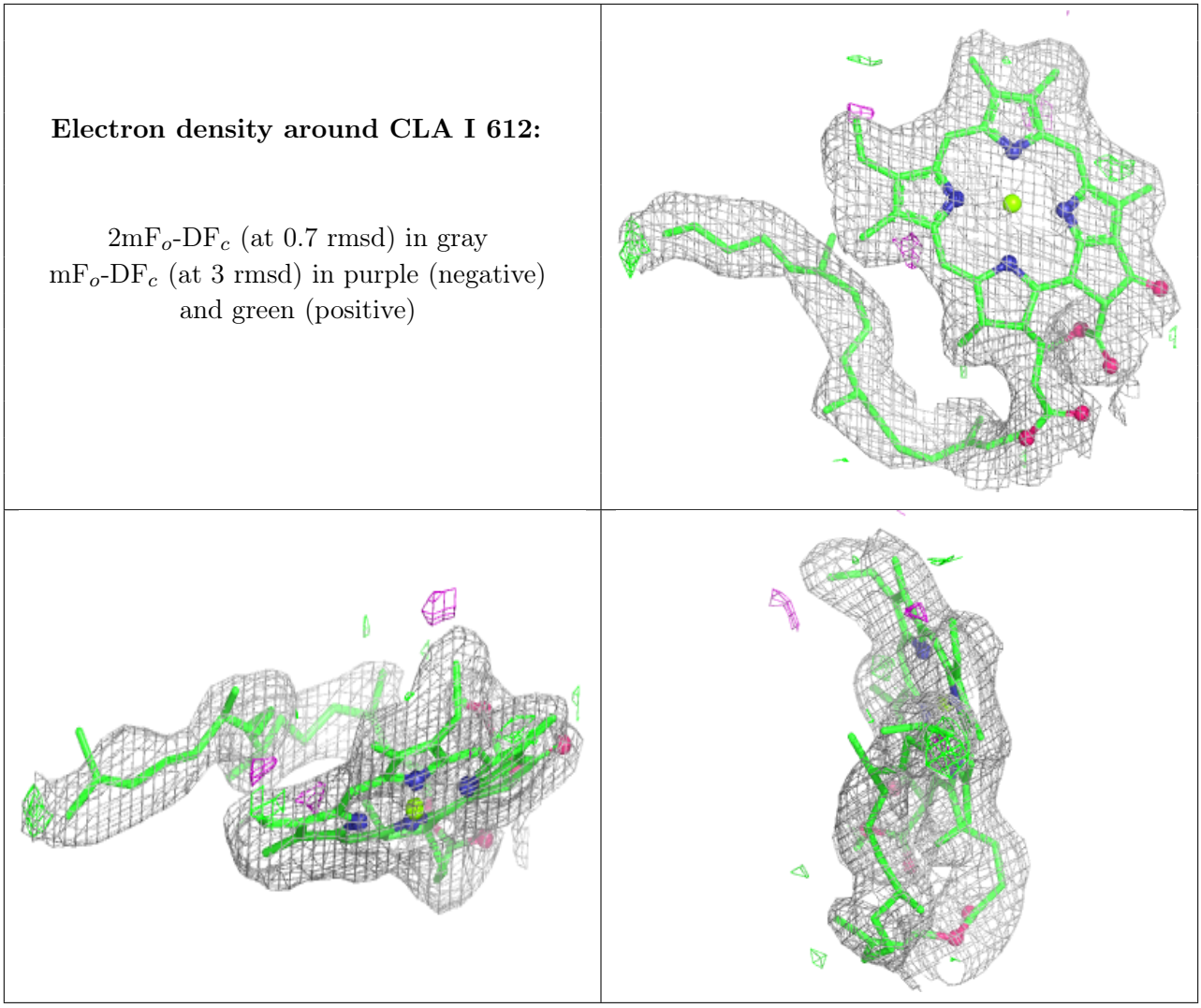






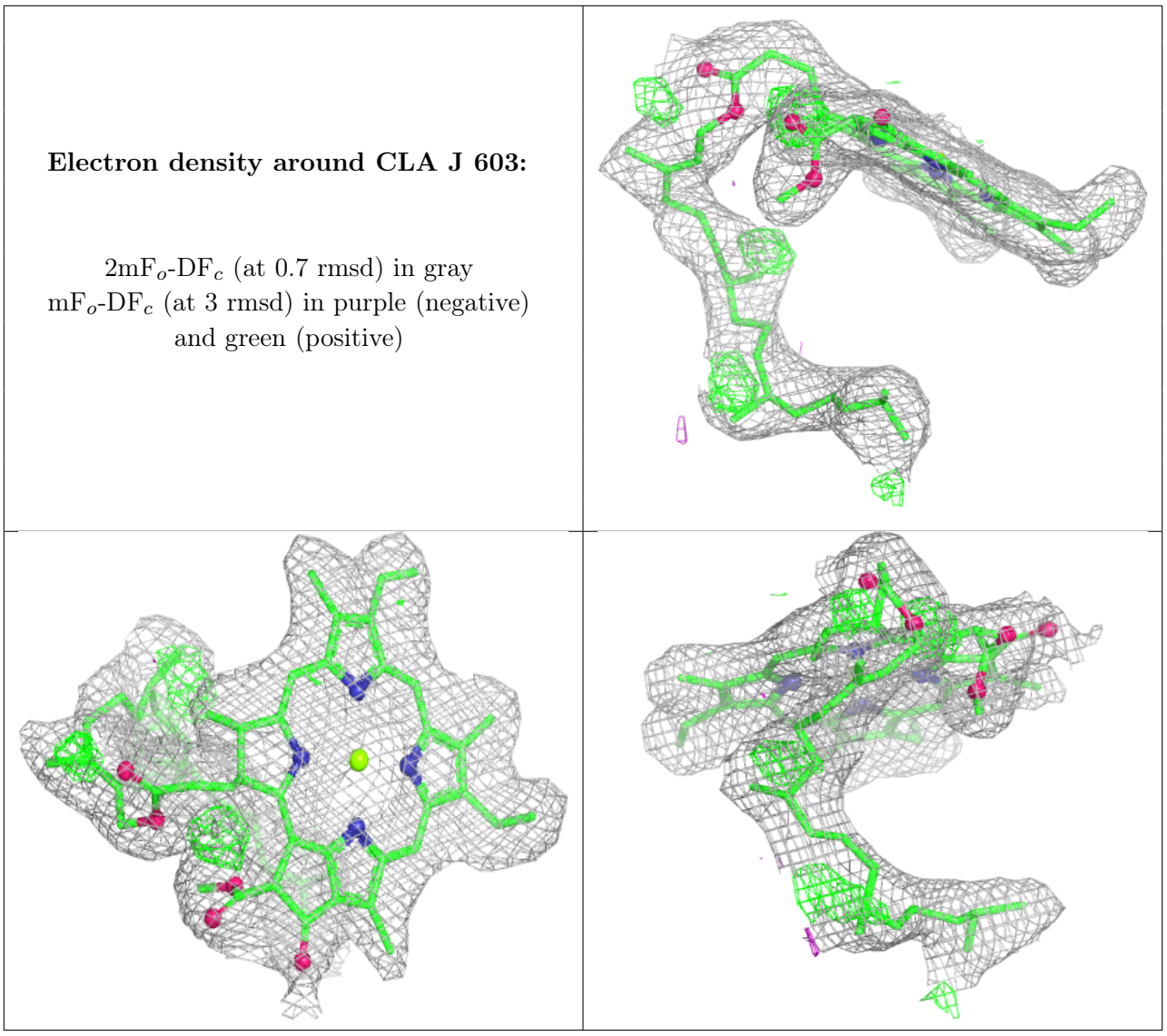
Electron density around CLA I 612:

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



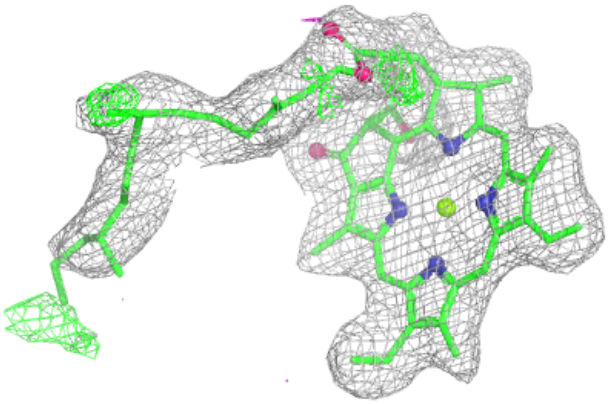
Electron density around CLA J 603:

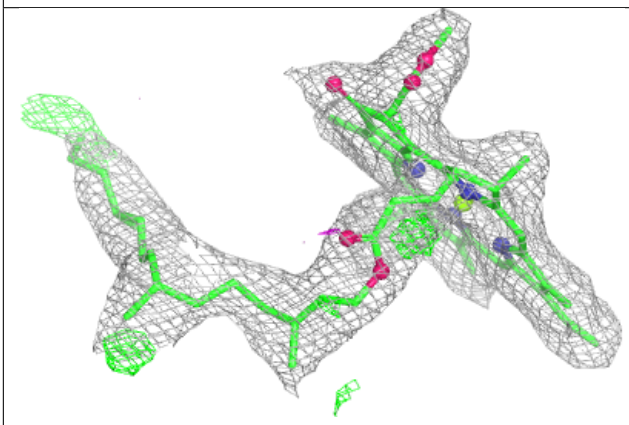
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

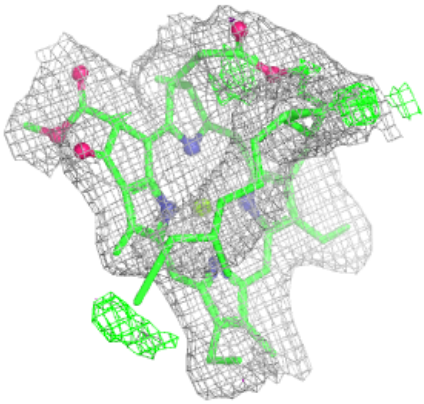


Electron density around CLA J 604:

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

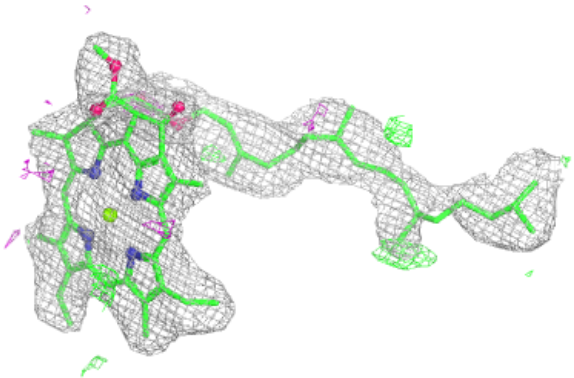


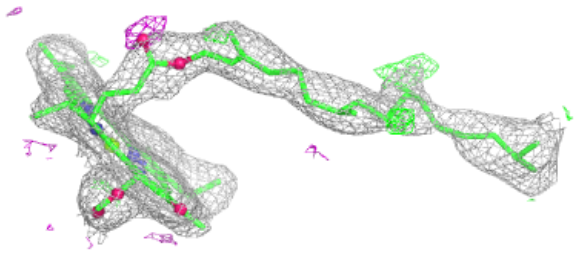


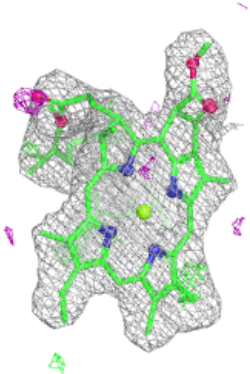


Electron density around CLA J 611:

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

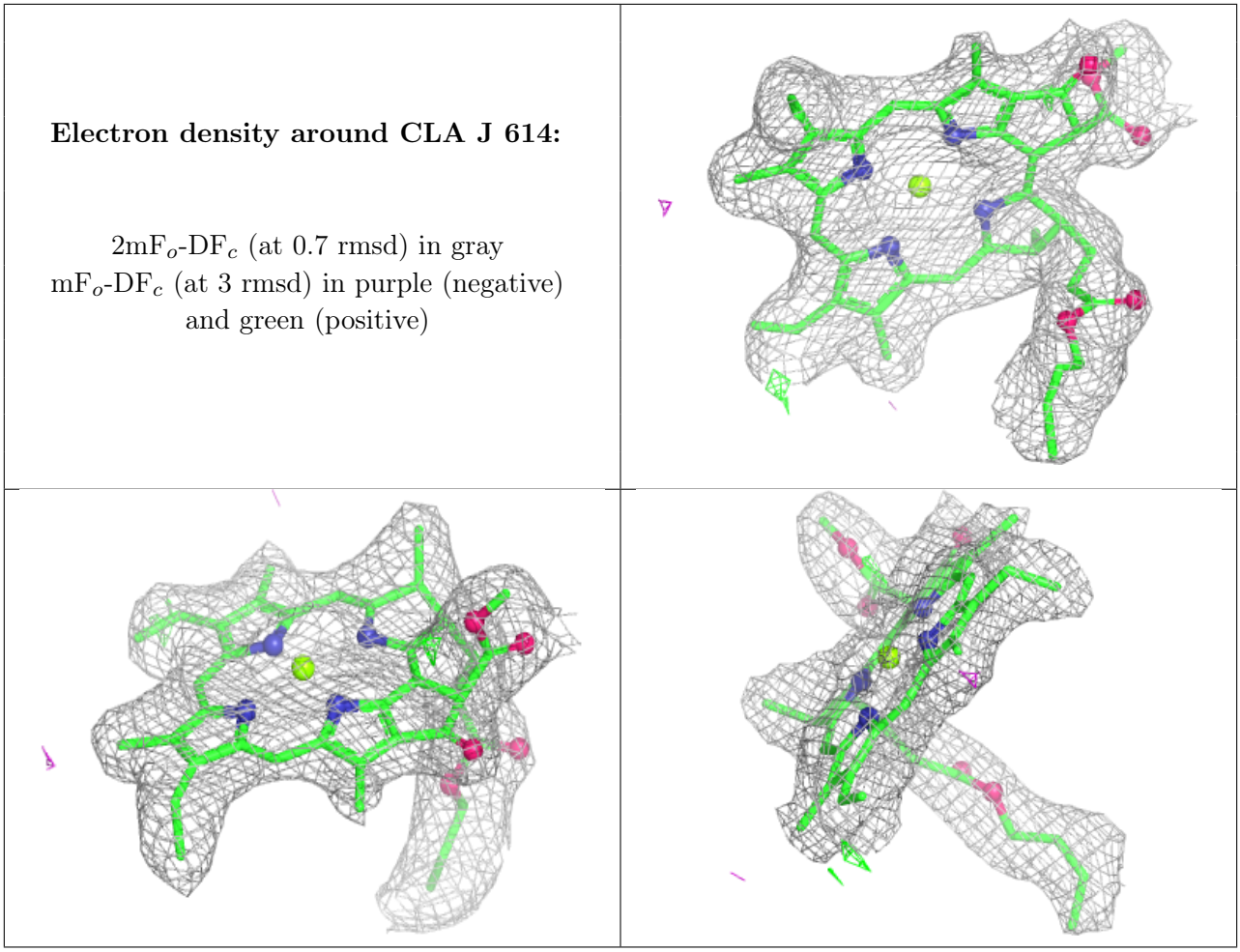






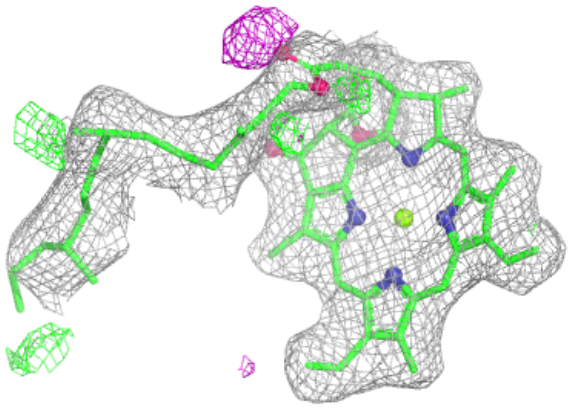
Electron density around CLA J 614:

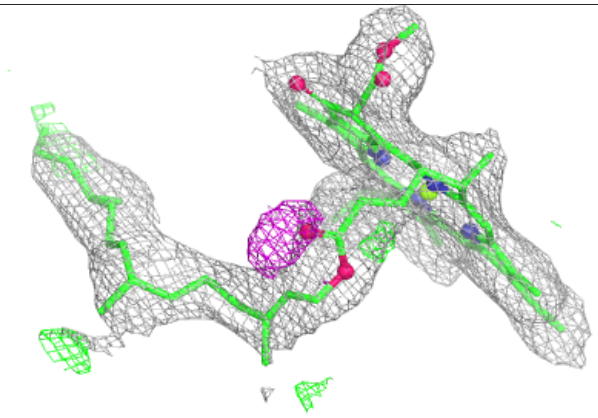
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

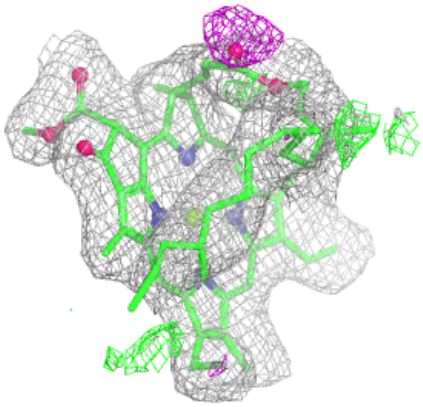


Electron density around CLA C 604:

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

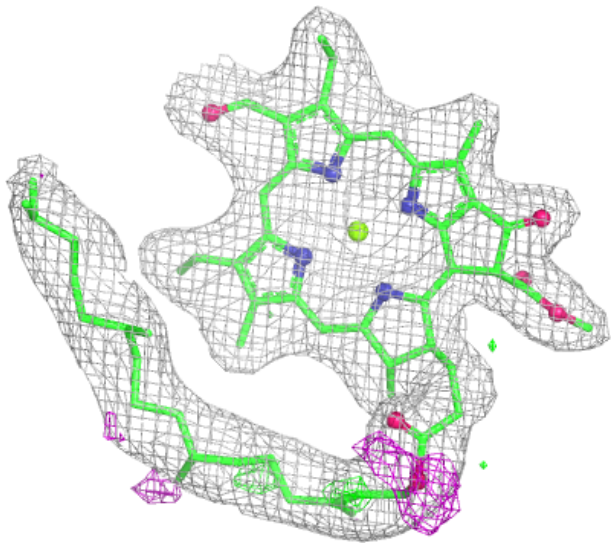


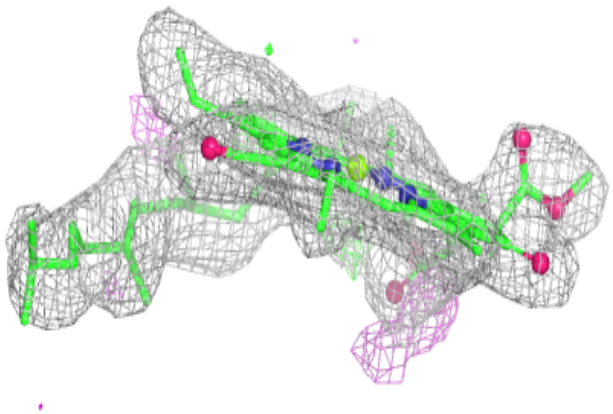




Electron density around CHL A 607:

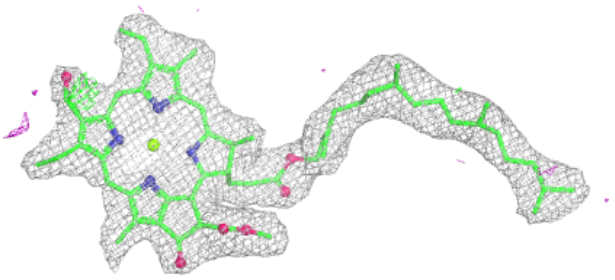
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

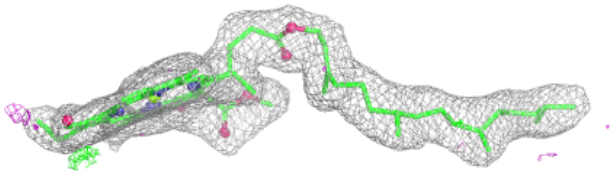




Electron density around CHL H 601:

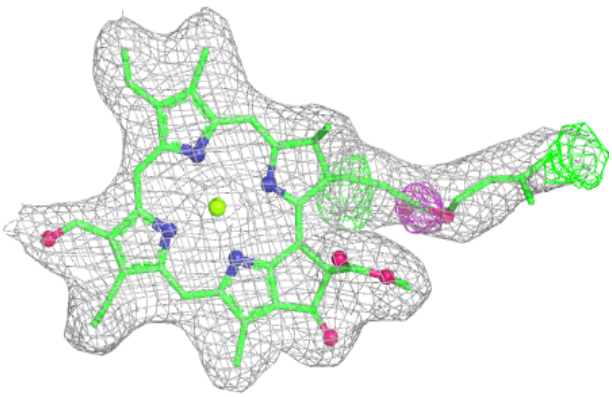
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

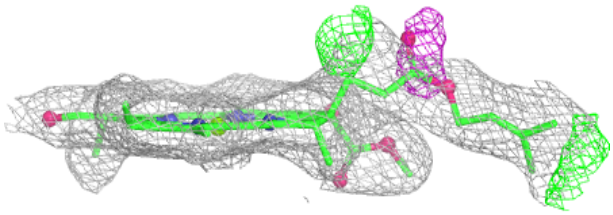


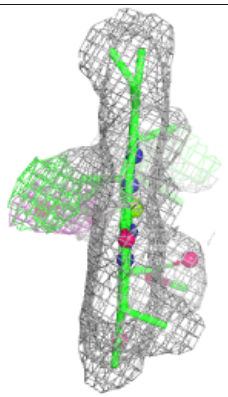


Electron density around CHL D 606:

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

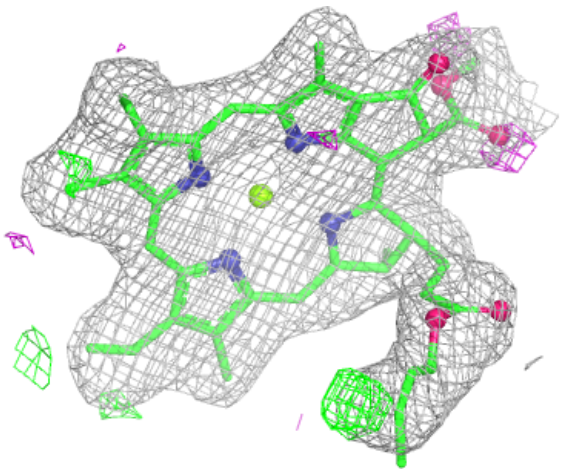


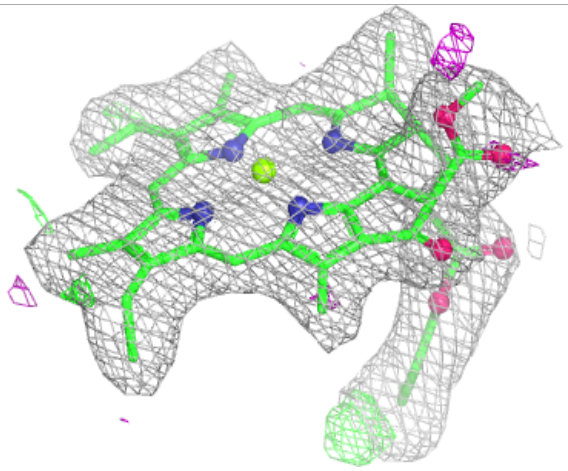


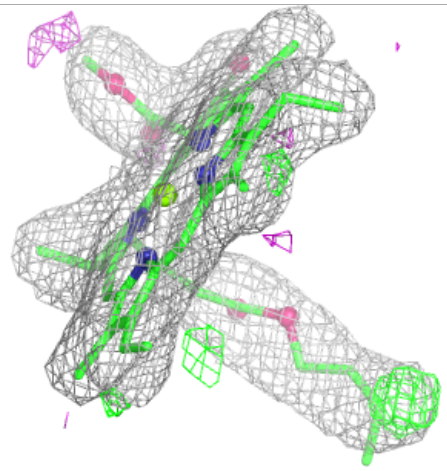


Electron density around CLA C 614:

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

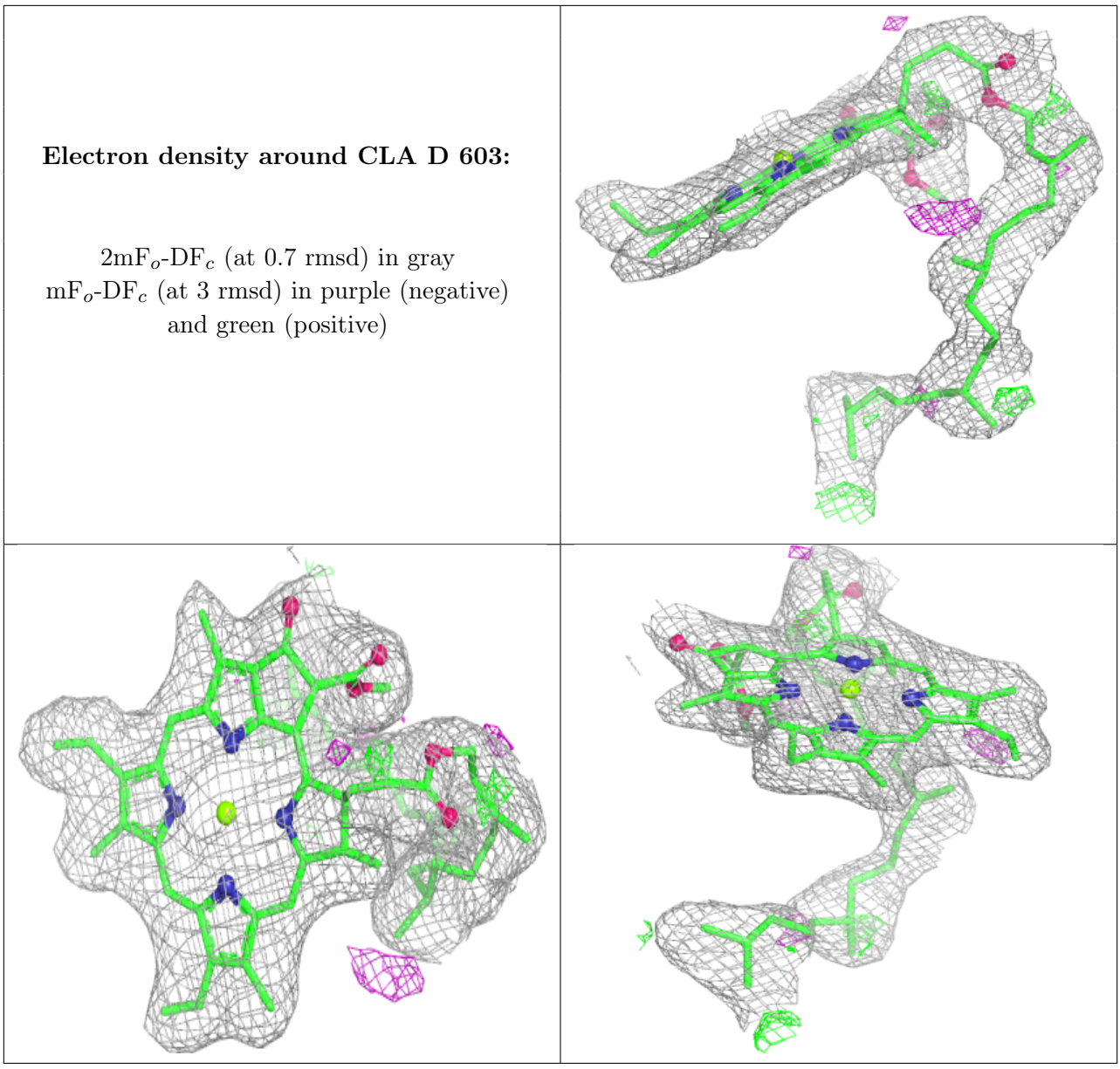






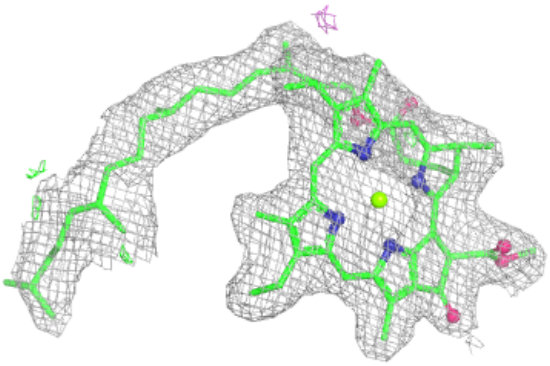
Electron density around CLA D 603:

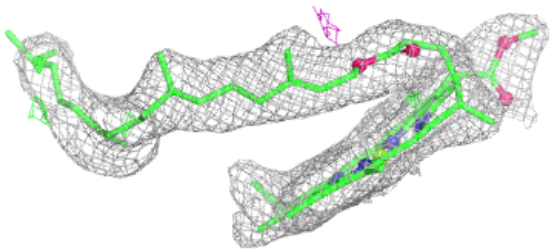
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

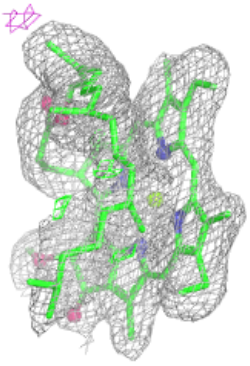


Electron density around CLA D 610:

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

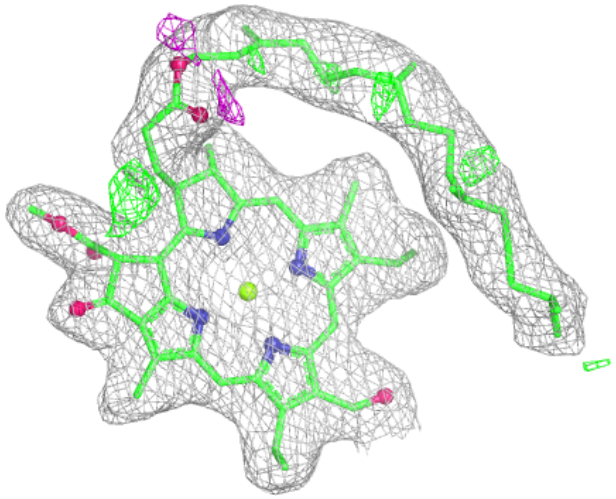


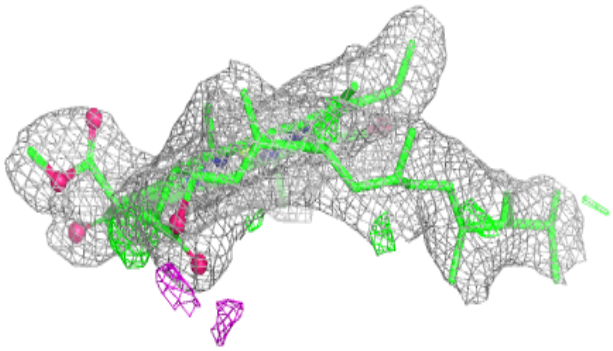




Electron density around CHL D 607:

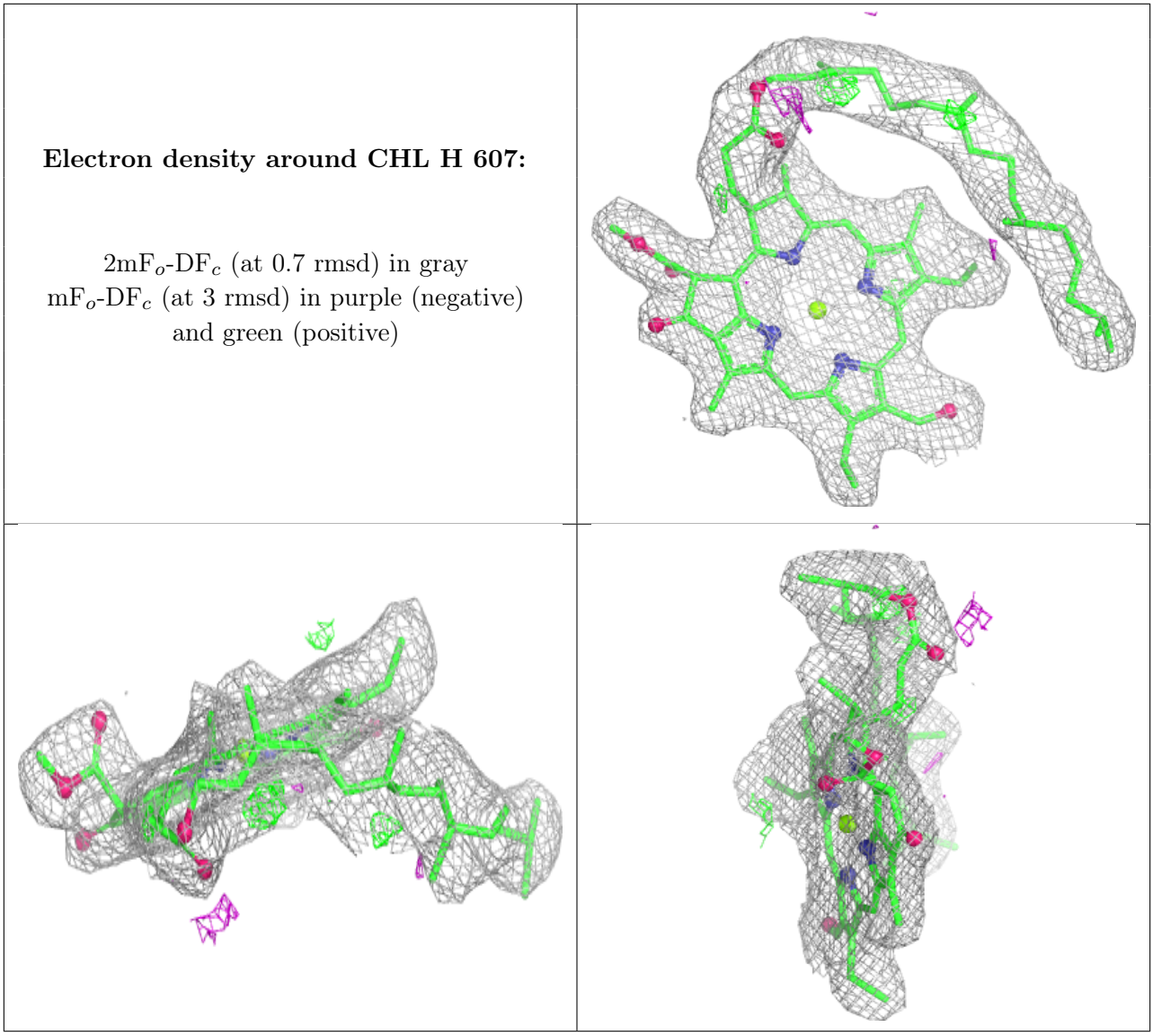
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





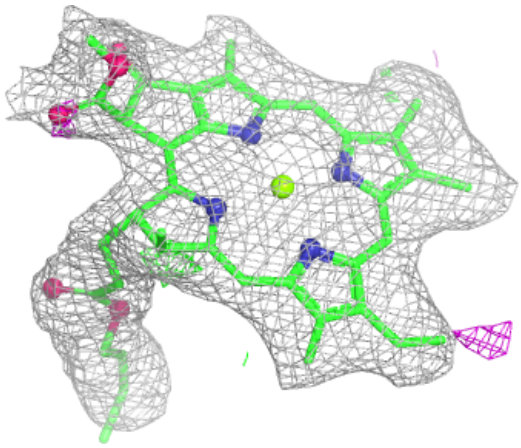
Electron density around CHL H 607:

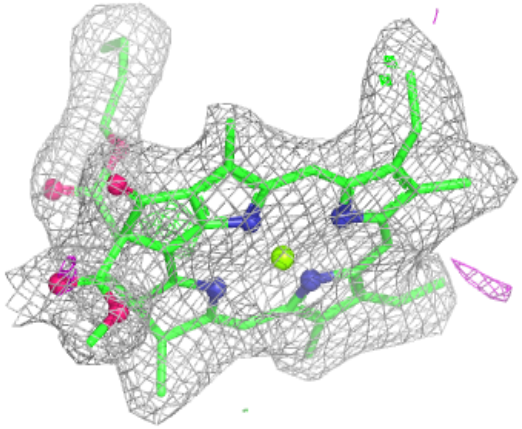
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

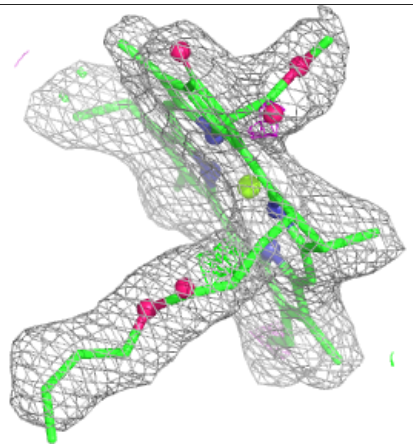


Electron density around CLA D 614:

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

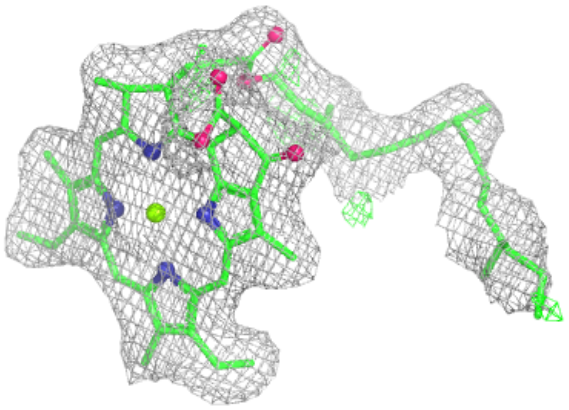


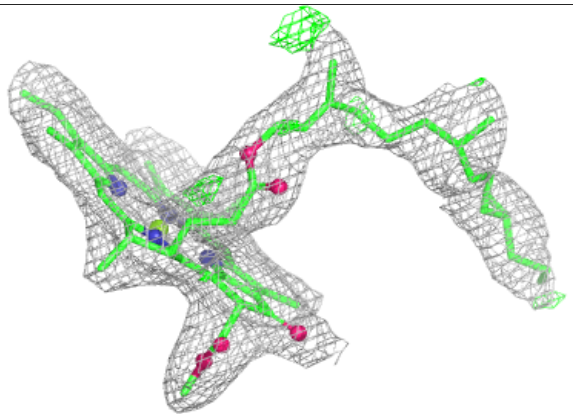


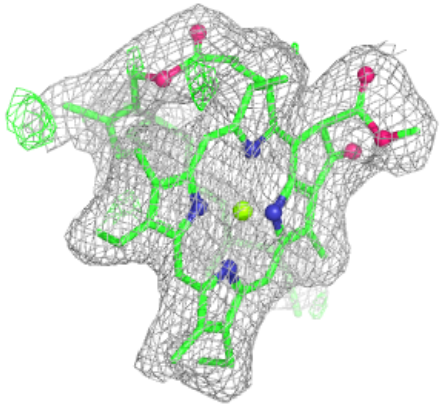


Electron density around CLA E 604:

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

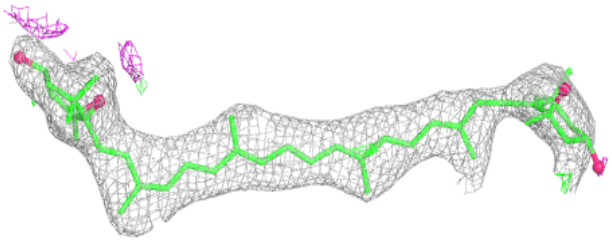


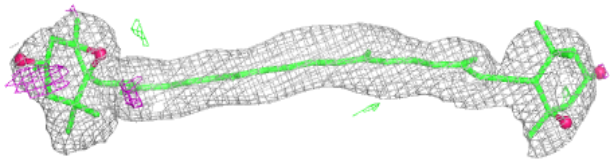


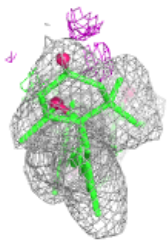


Electron density around NEX F 5623:

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

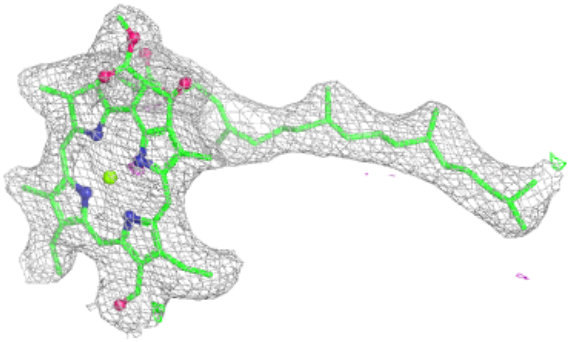


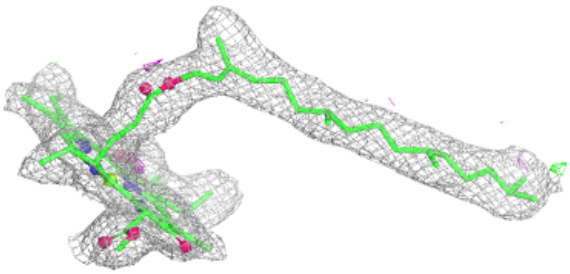


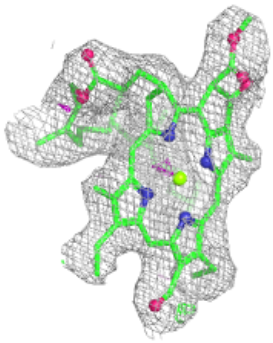


Electron density around CHL H 609:

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

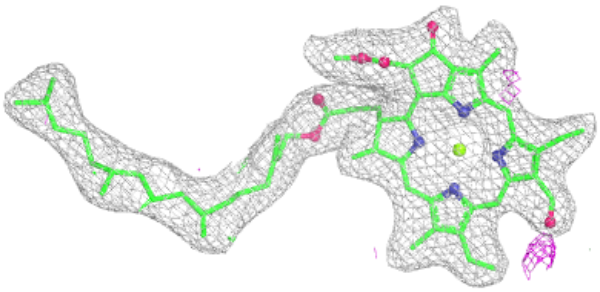


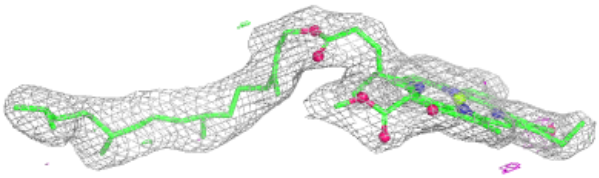


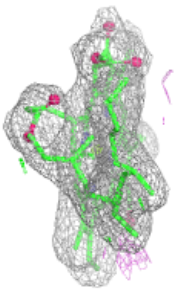


Electron density around CHL I 601:

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

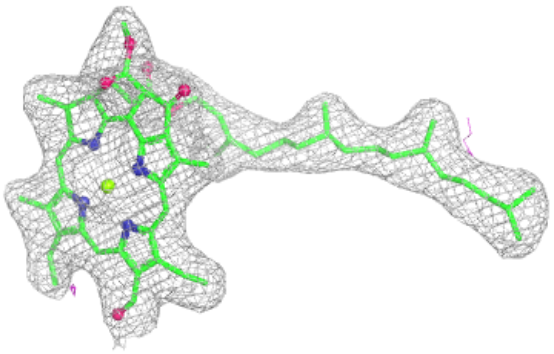


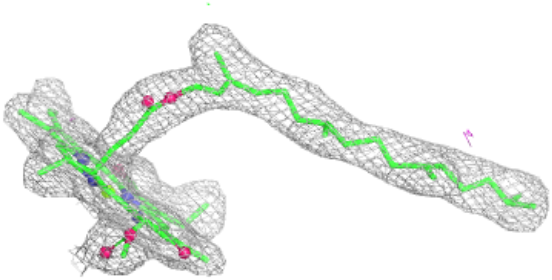


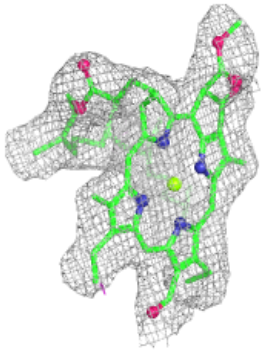


Electron density around CHL D 609:

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

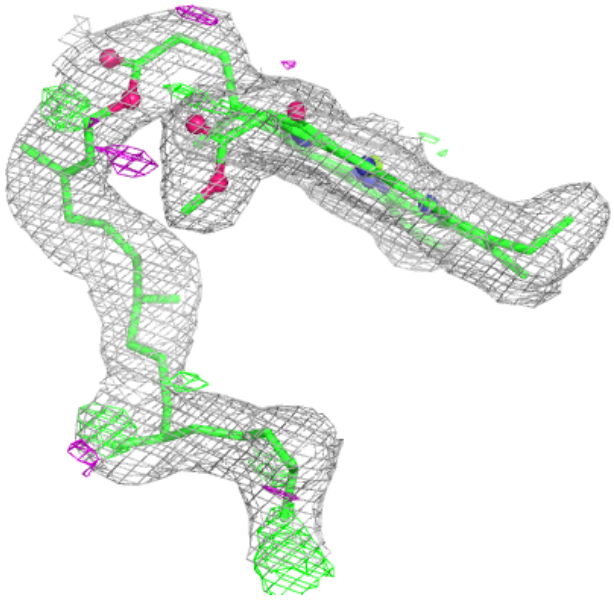


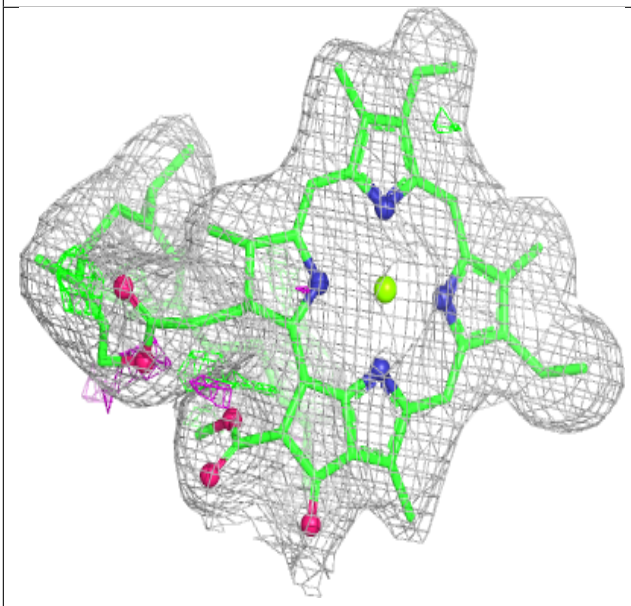


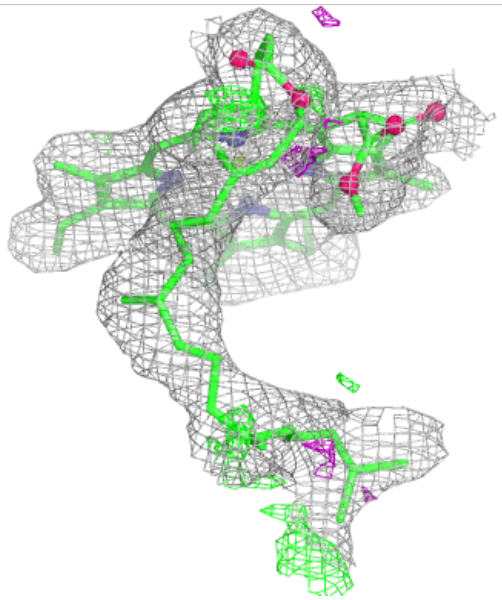


Electron density around CLA F 603:

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

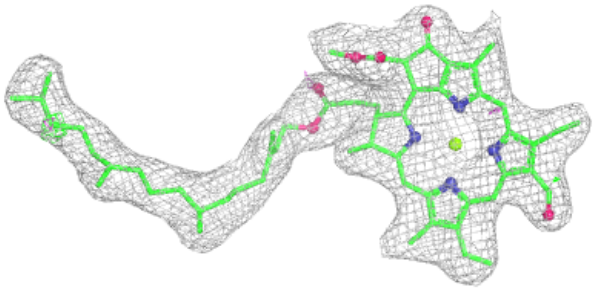


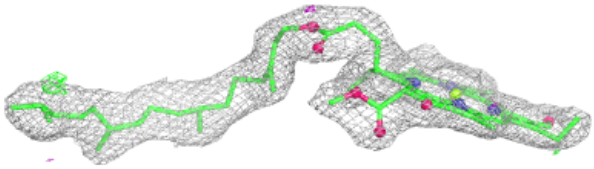


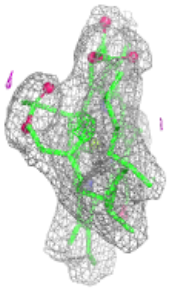


Electron density around CHL E 601:

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

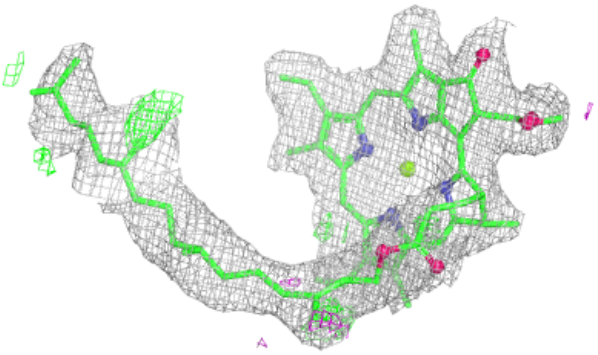


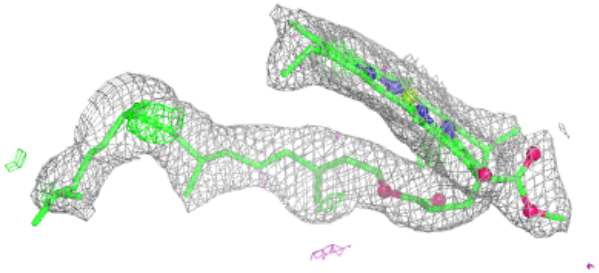


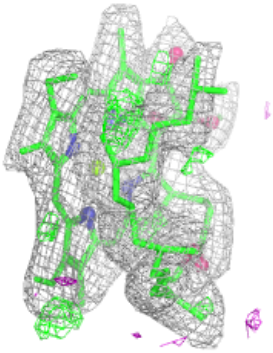


Electron density around CLA F 610:

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

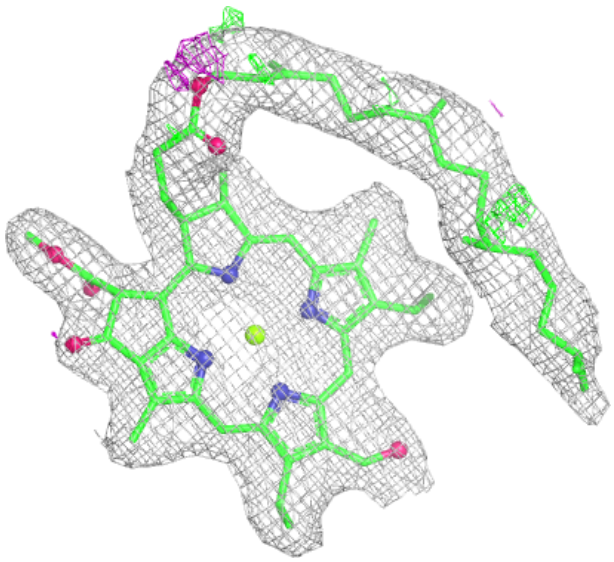


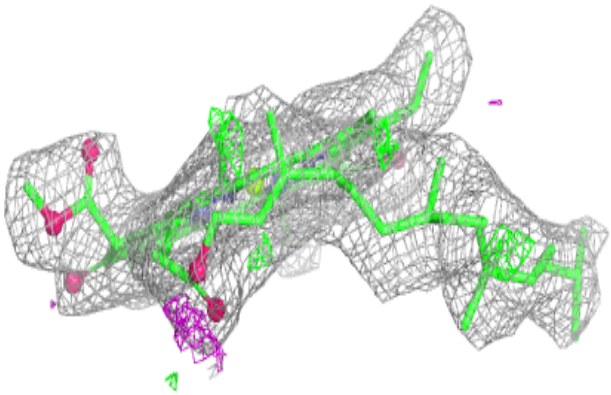


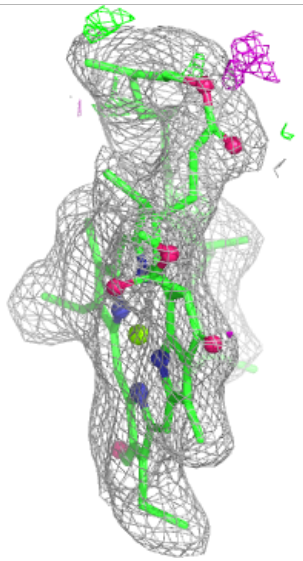


Electron density around CHL I 607:

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

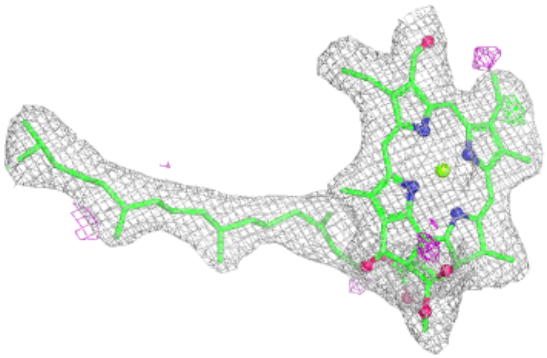


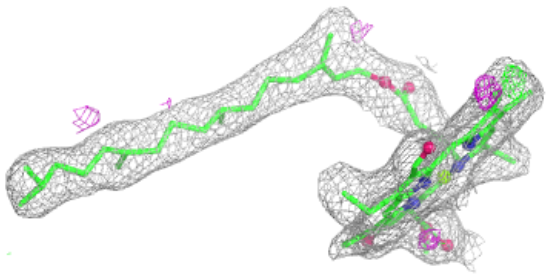


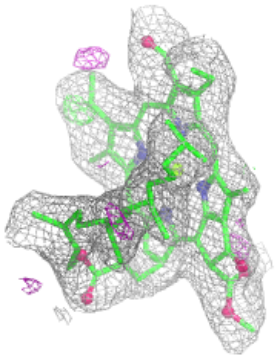


Electron density around CHL A 609:

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

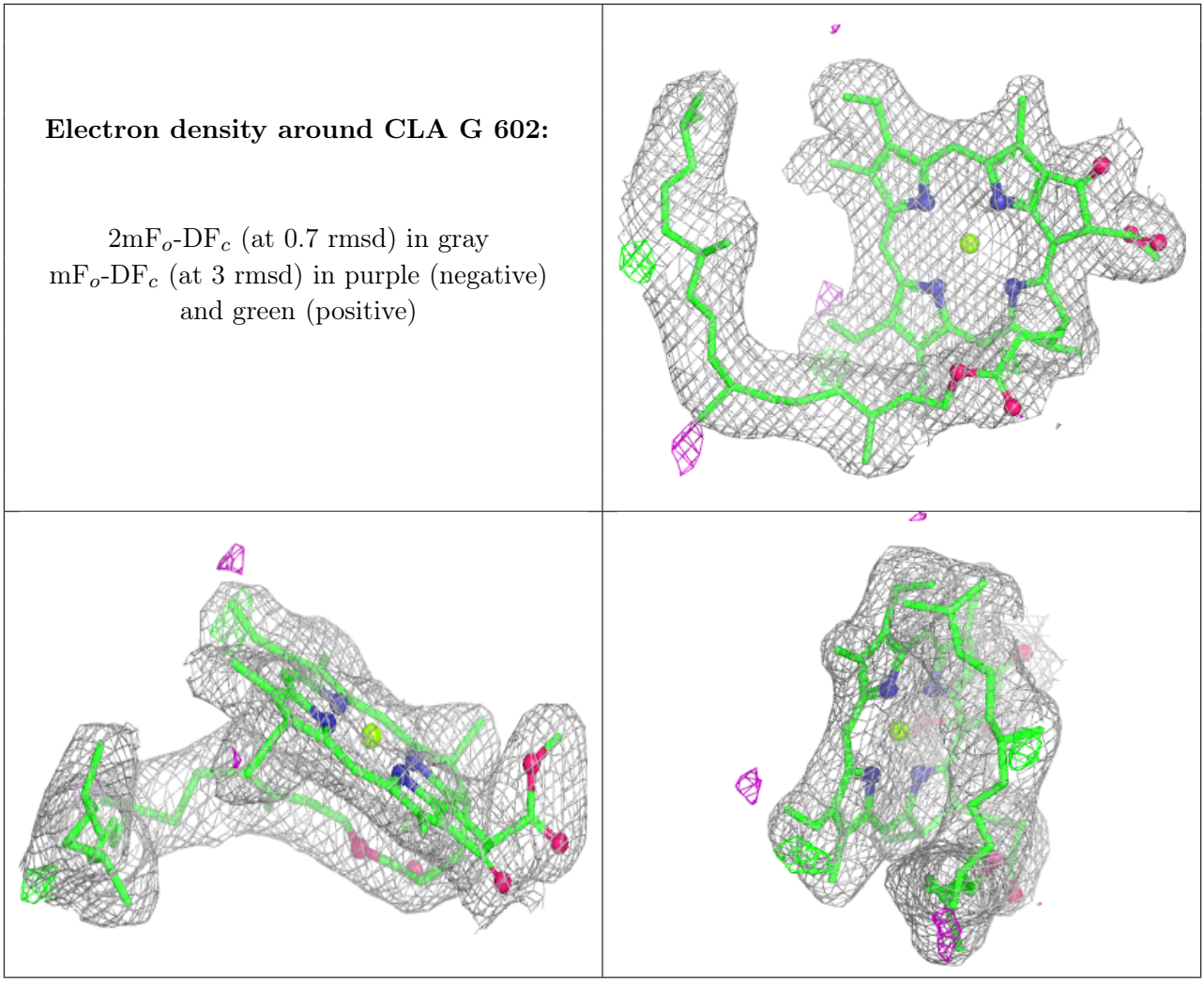






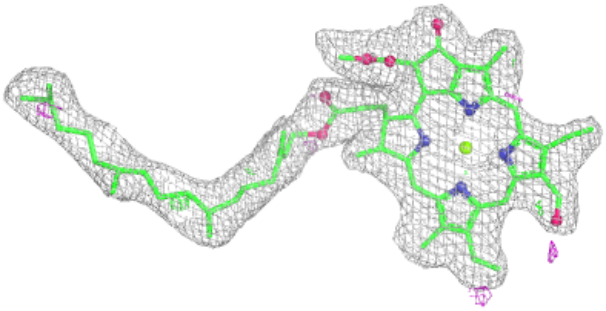
Electron density around CLA G 602:

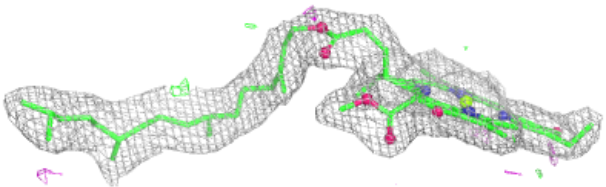
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

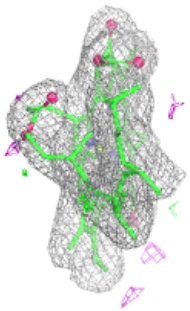


Electron density around CHL B 601:

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

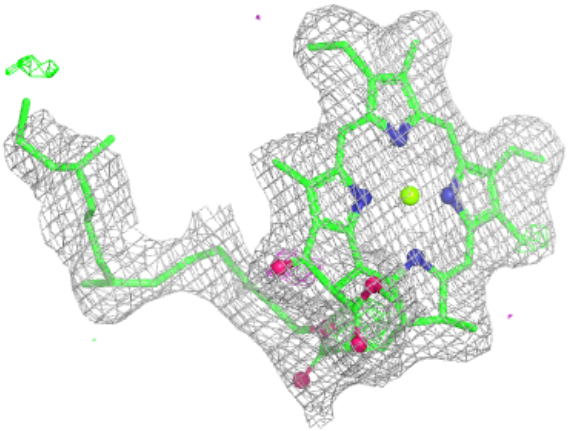


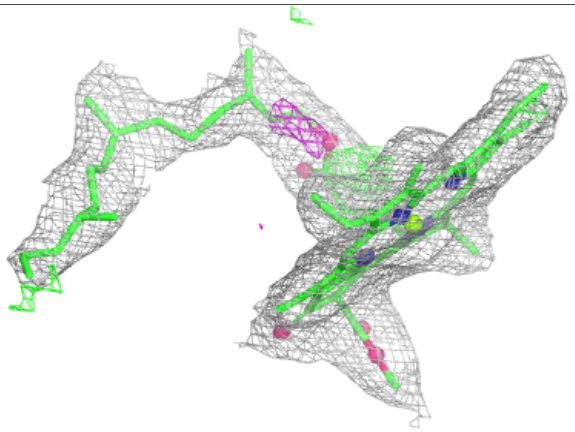


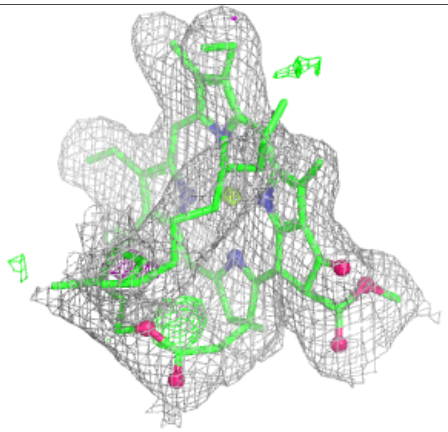


Electron density around CLA G 604:

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

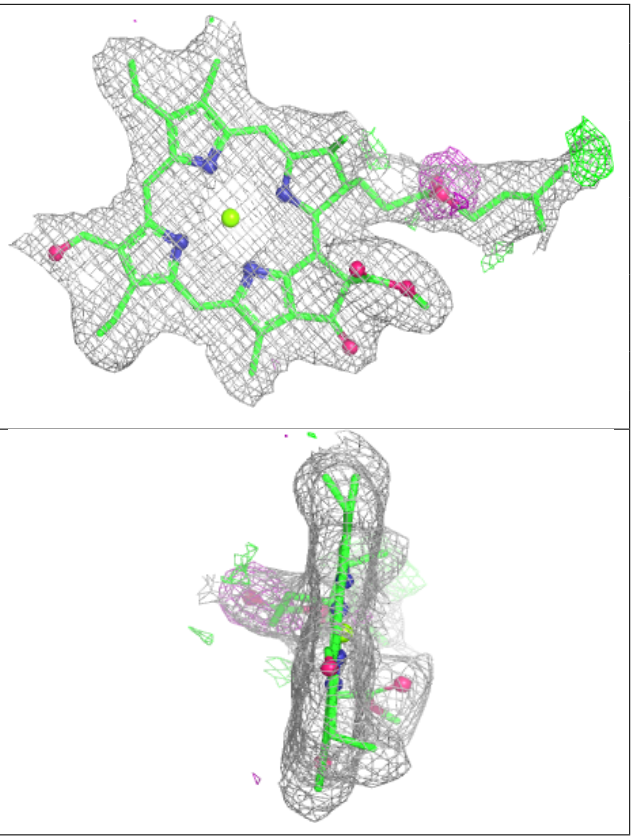


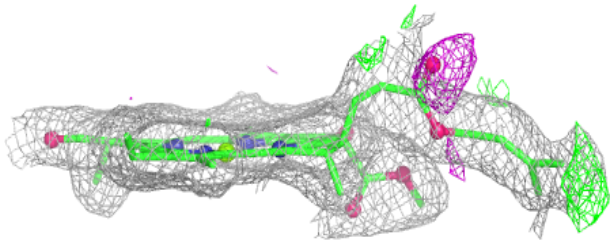




Electron density around CHL B 606:

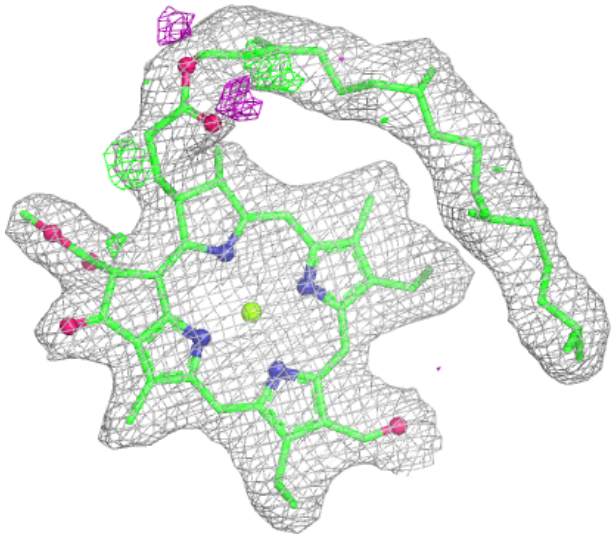
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

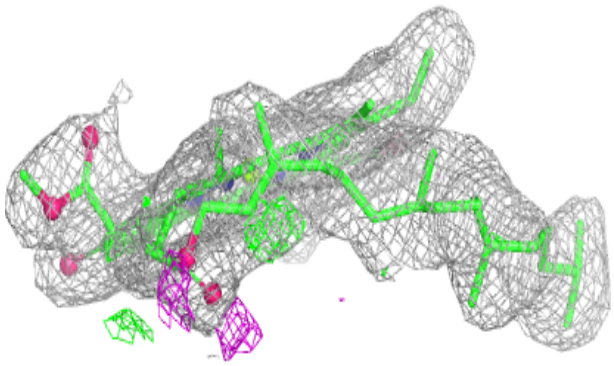




Electron density around CHL J 607:

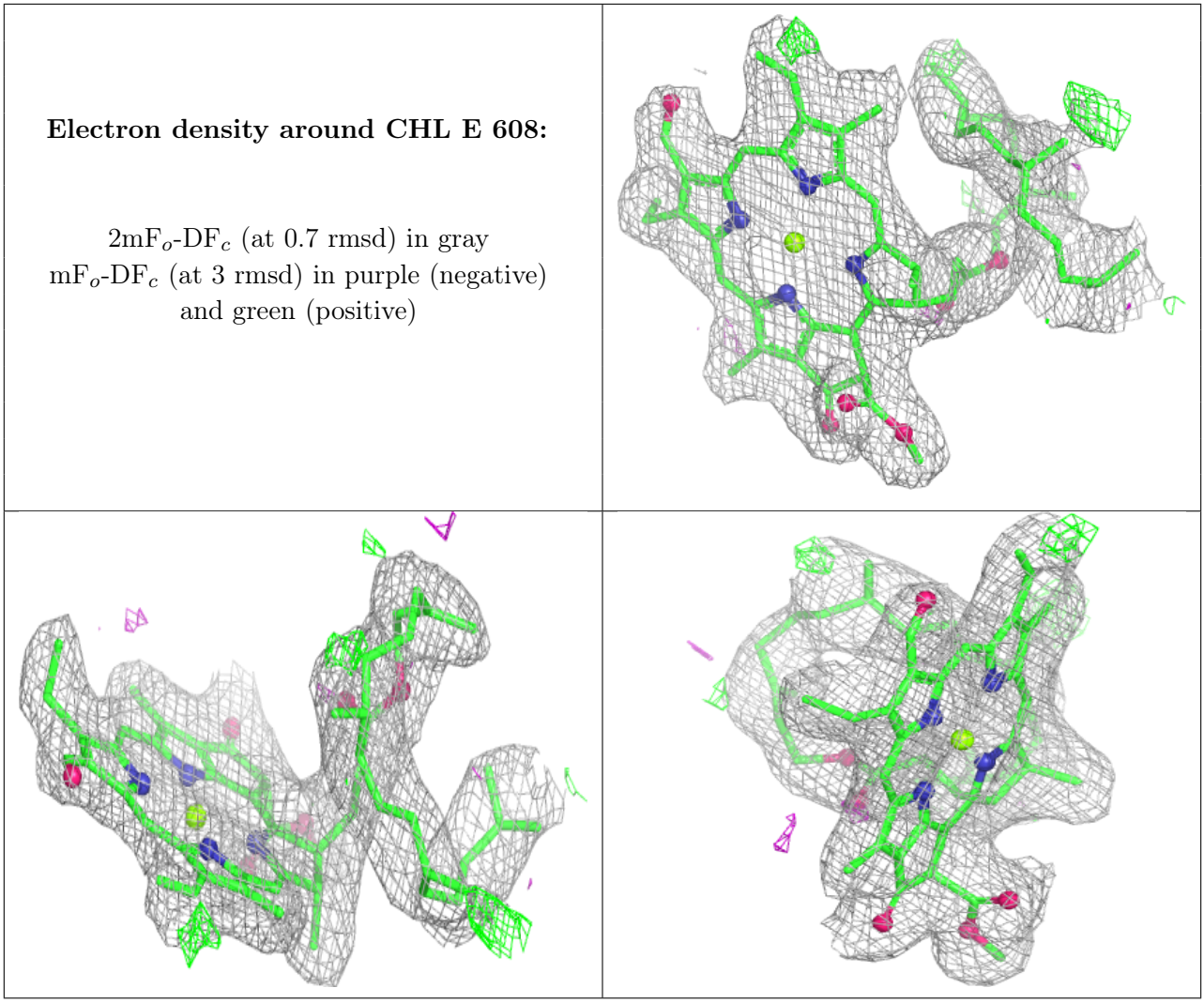
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





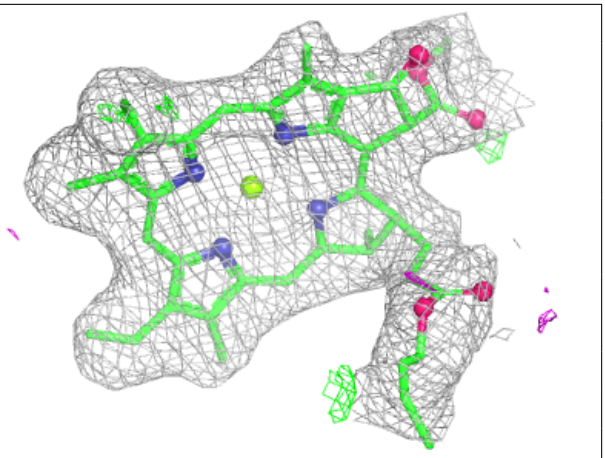
Electron density around CHL E 608:

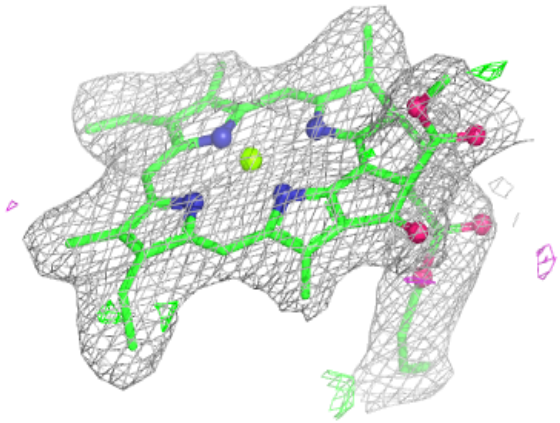
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

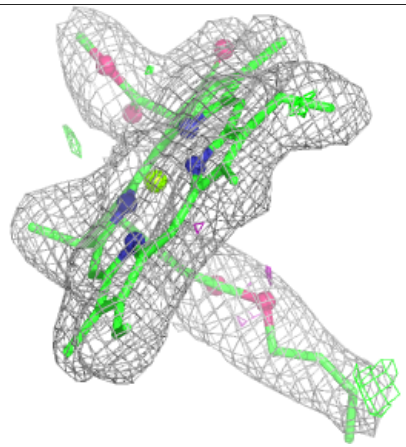


Electron density around CLA G 614:

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

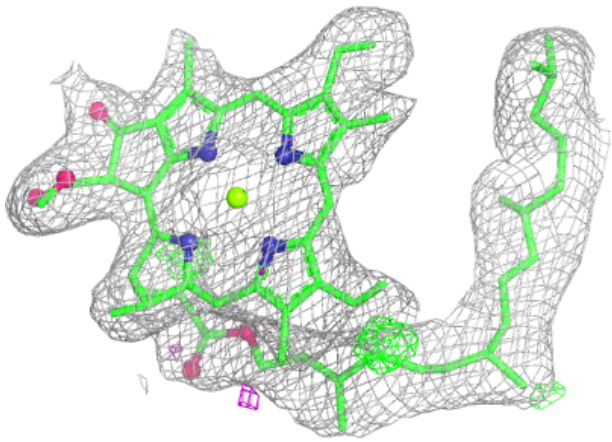


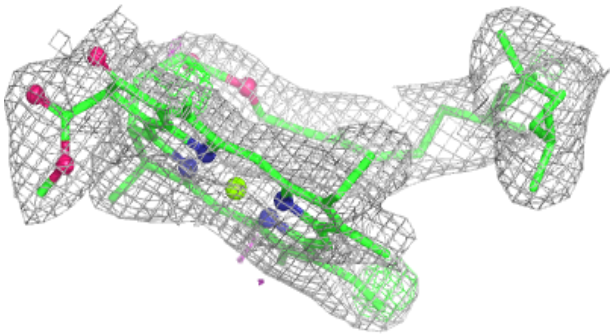


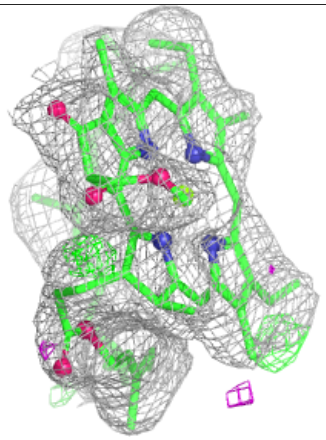


Electron density around CLA H 602:

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

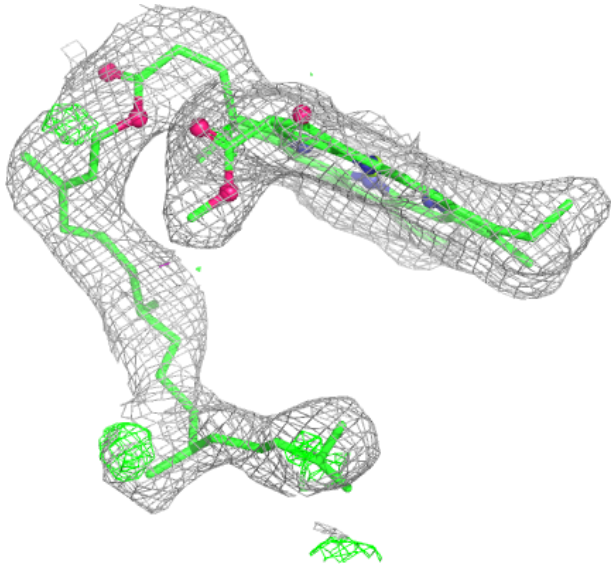


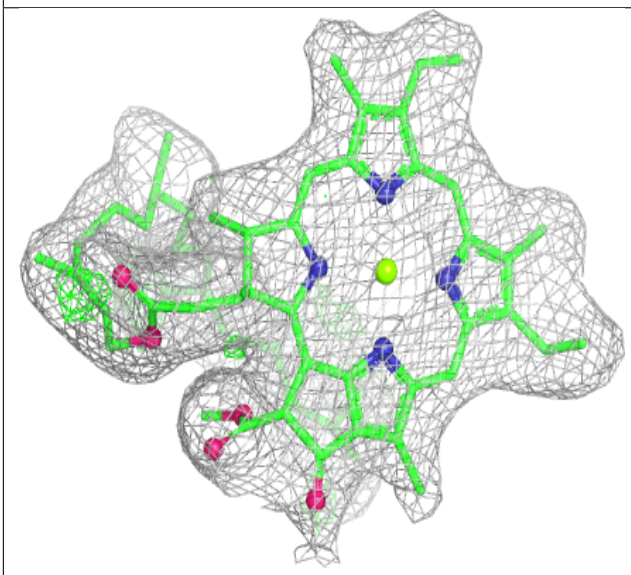


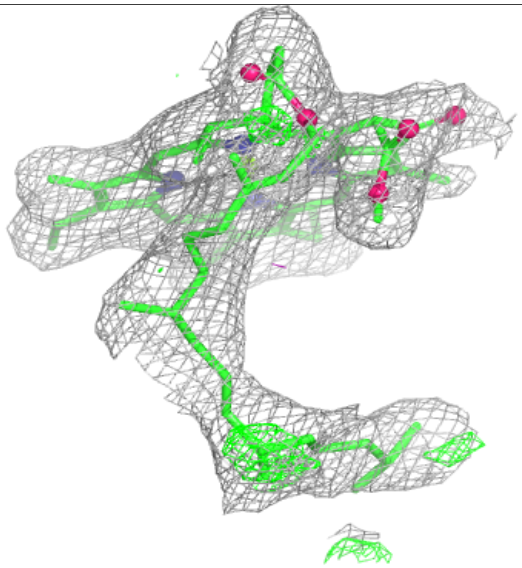


Electron density around CLA H 603:

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

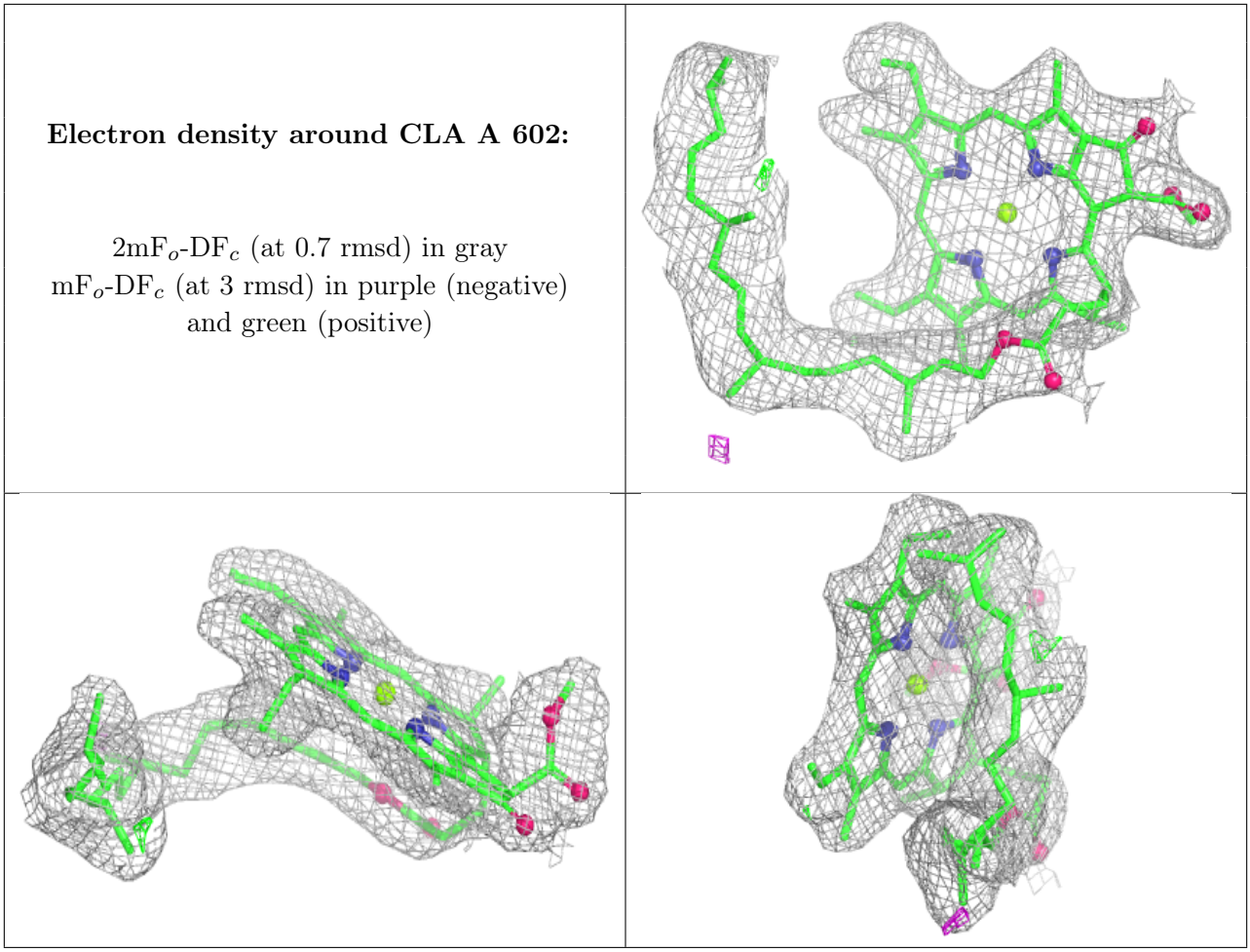






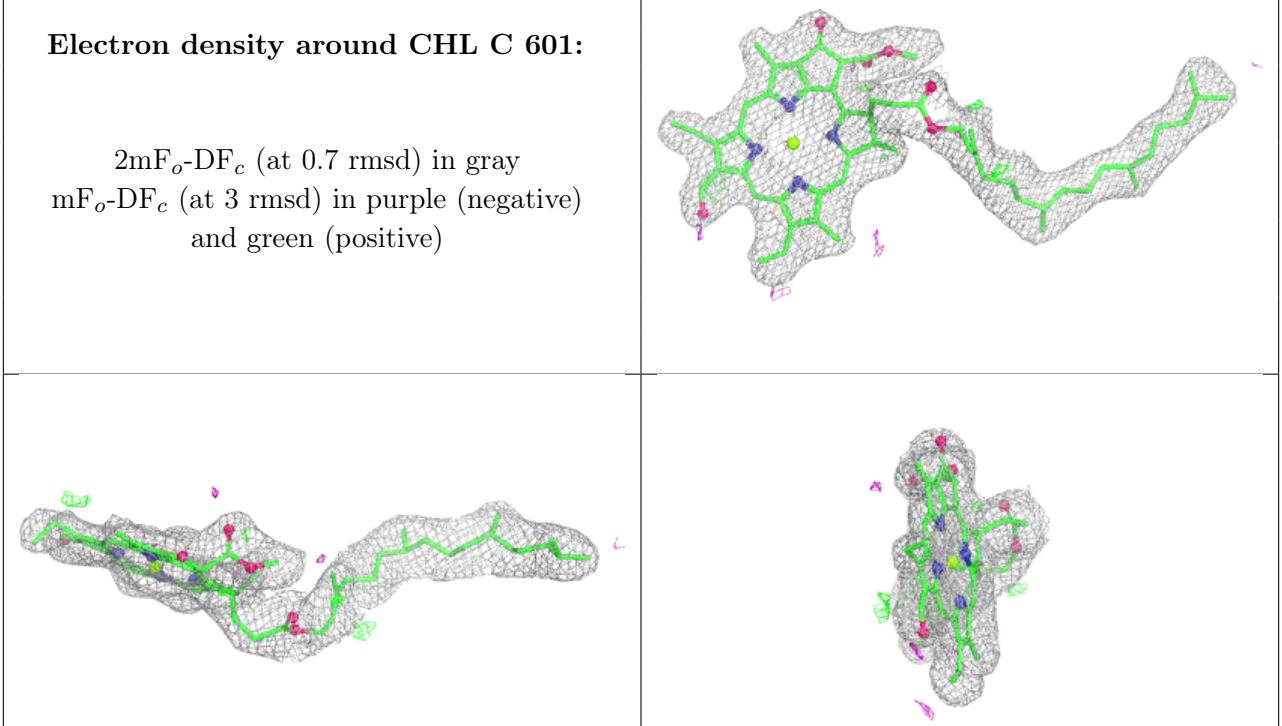
Electron density around CLA A 602:

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



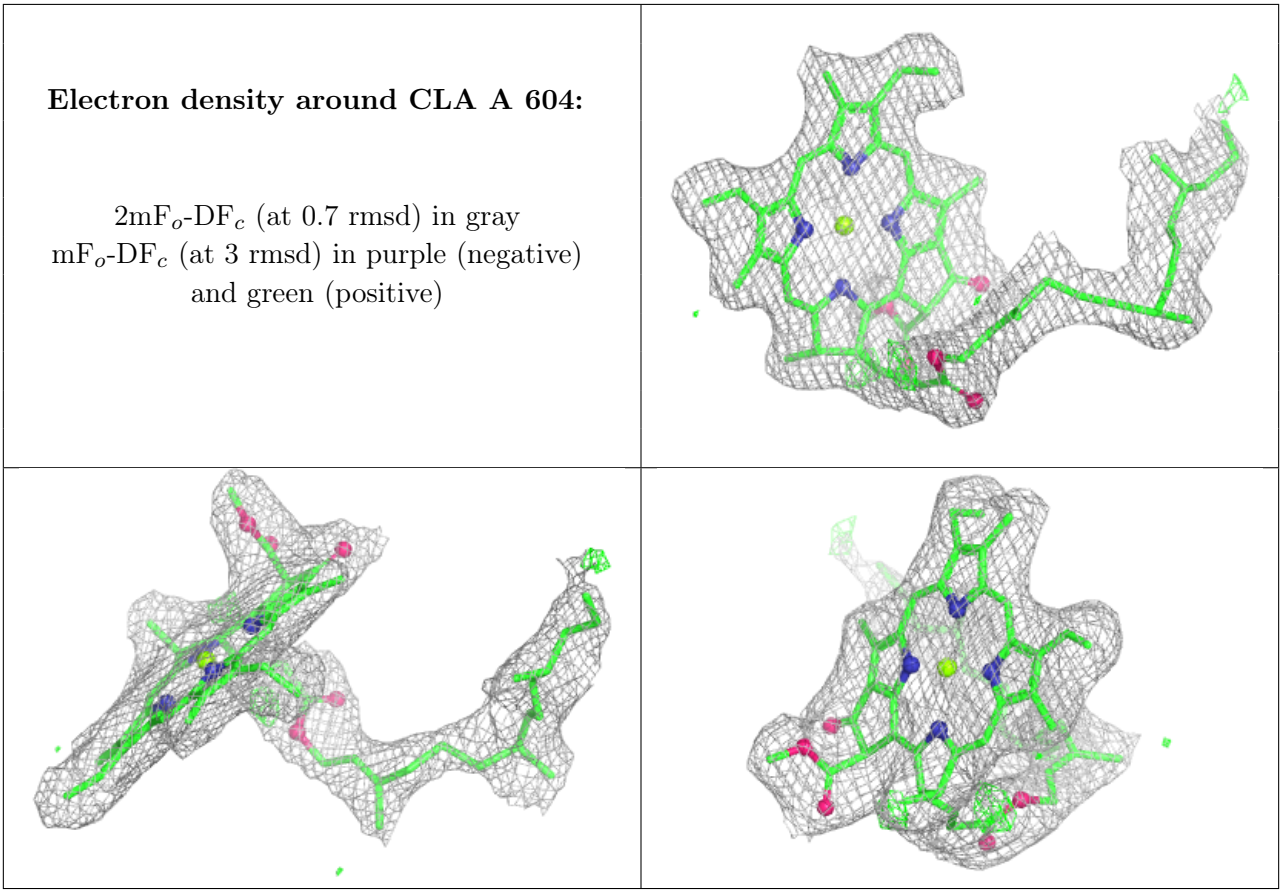
Electron density around CHL C 601:

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



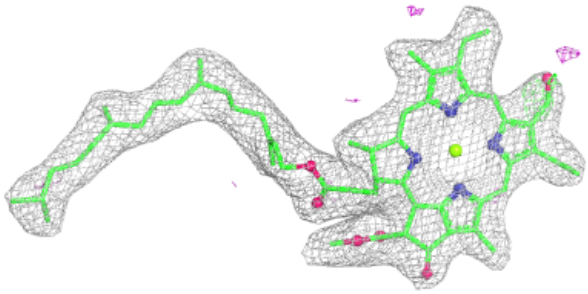
Electron density around CLA A 604:

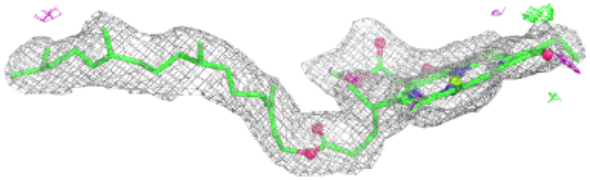
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

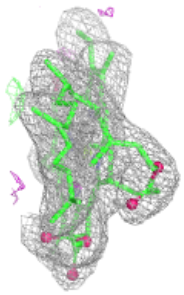


Electron density around CHL A 601:

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

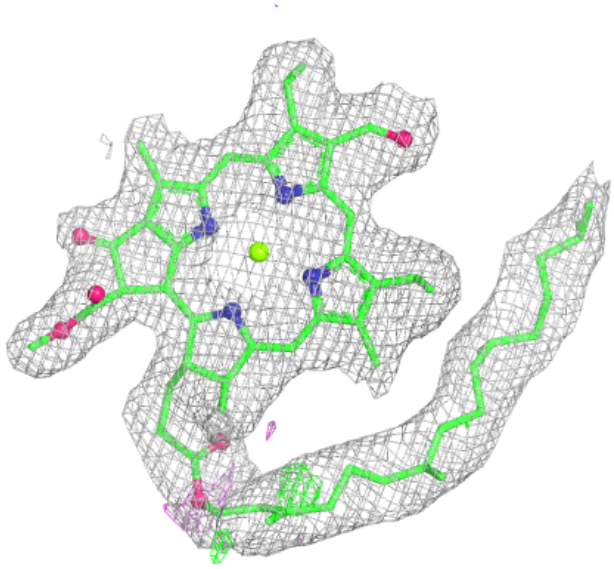


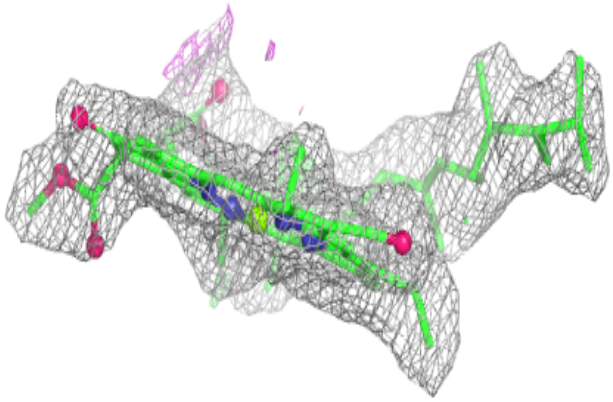


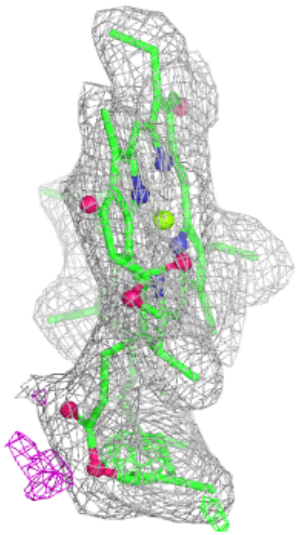


Electron density around CHL F 607:

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

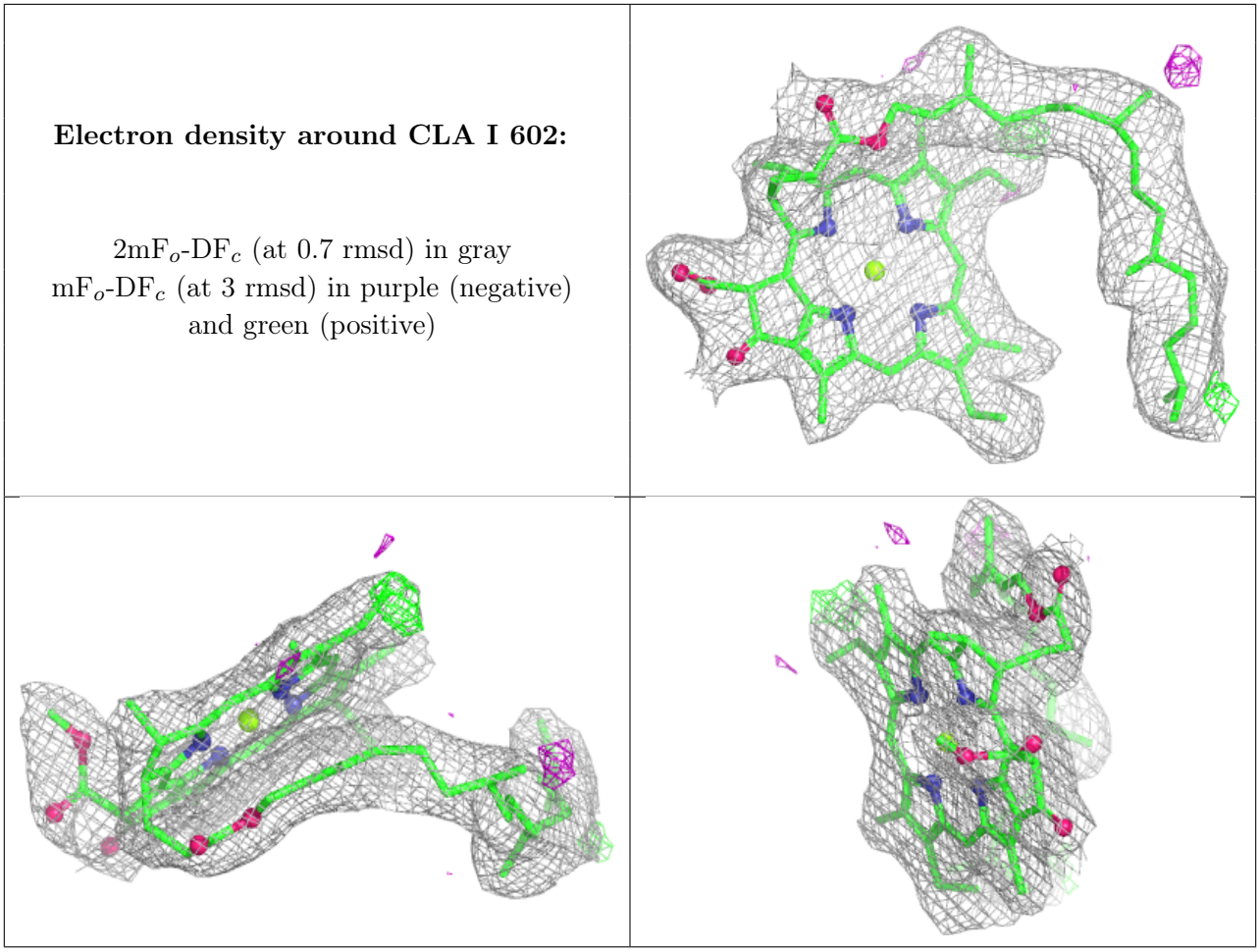






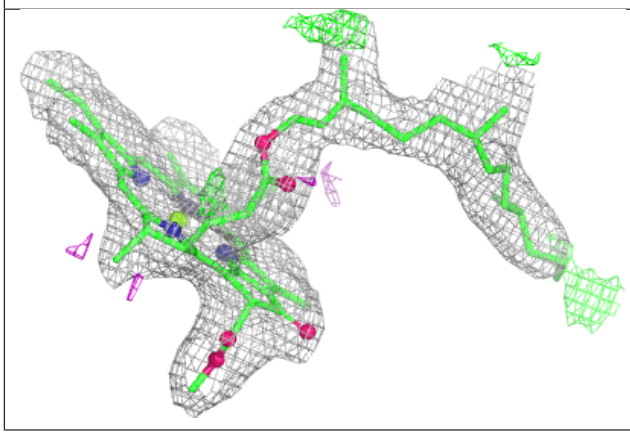
Electron density around CLA I 602:

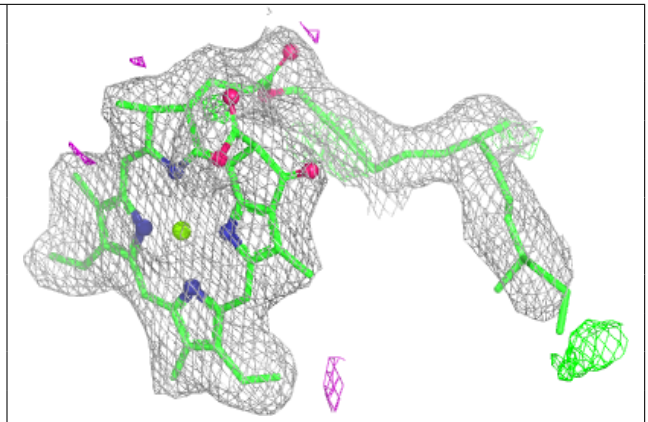
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

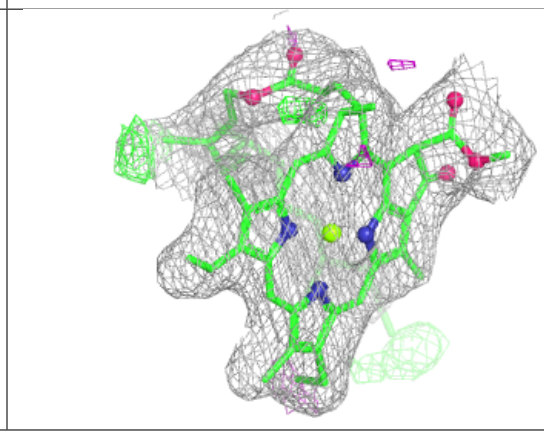


Electron density around CLA I 604:

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

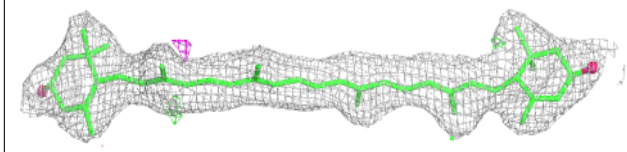


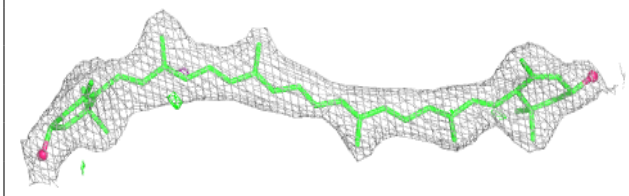


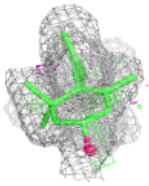


Electron density around LUT G 6621:

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

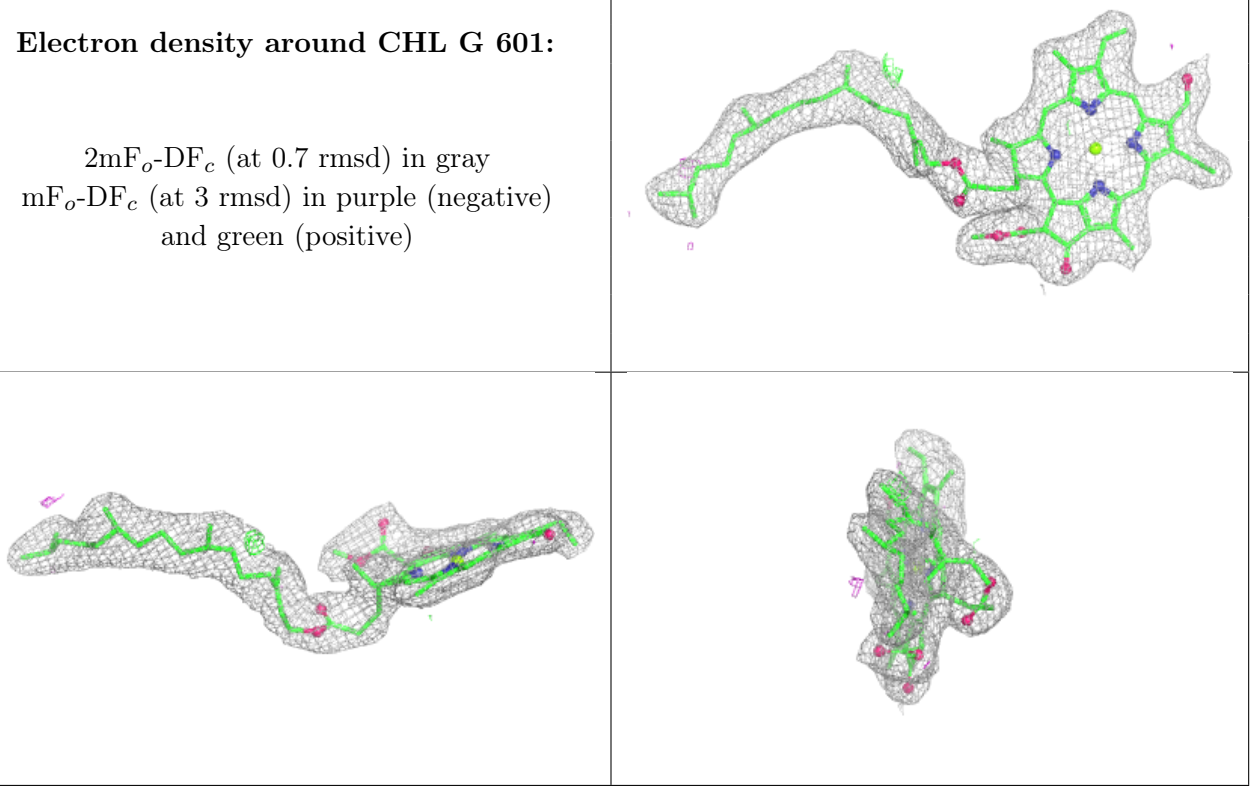






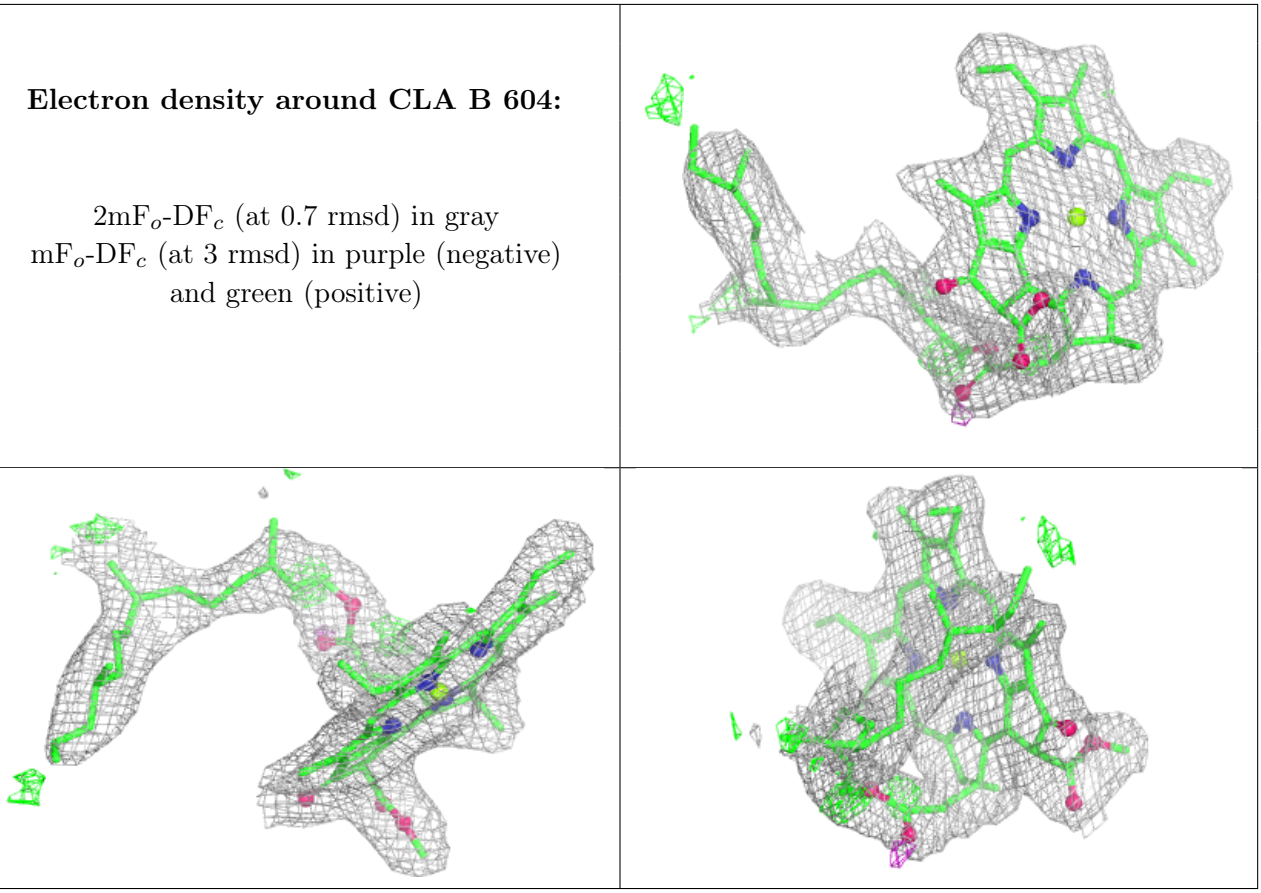
Electron density around CHL G 601:

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



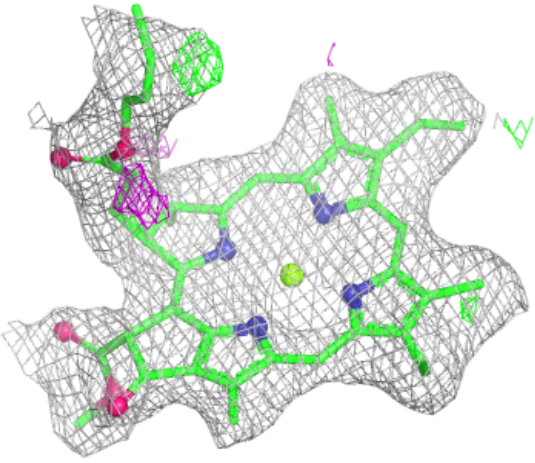
Electron density around CLA B 604:

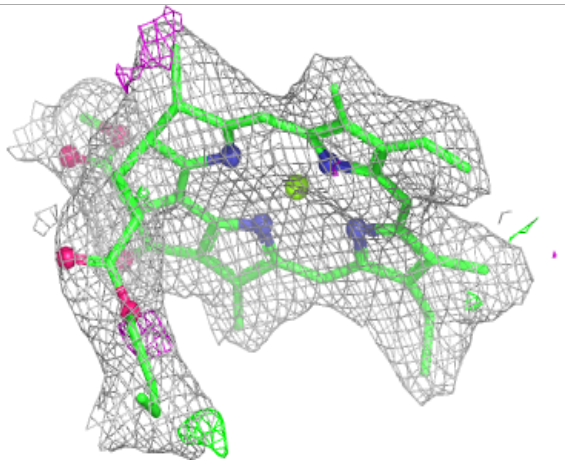
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

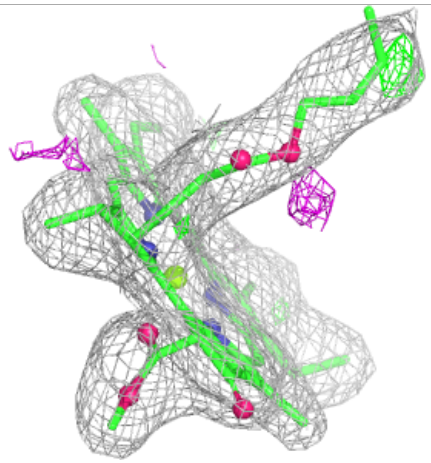


Electron density around CLA I 614:

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

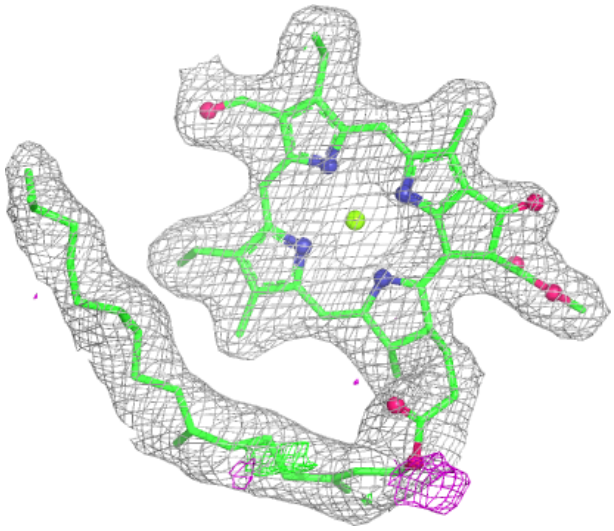


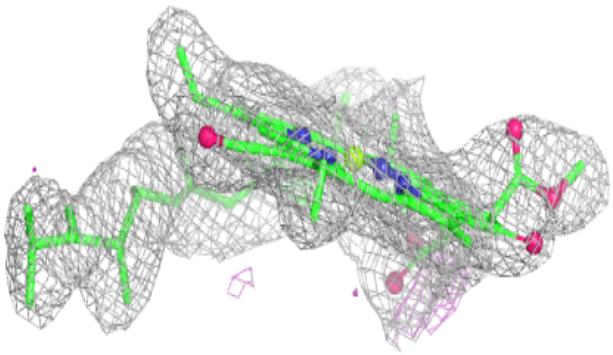


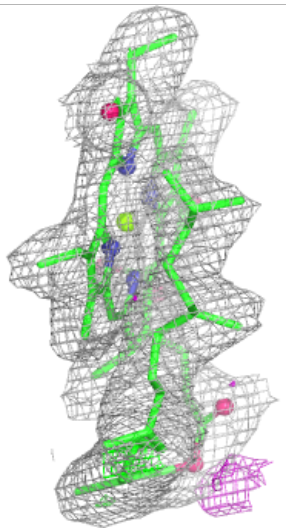


Electron density around CHL C 607:

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

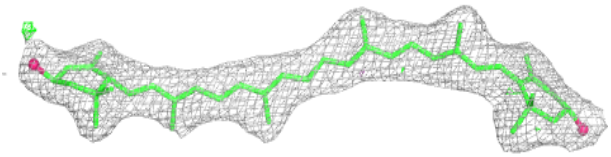


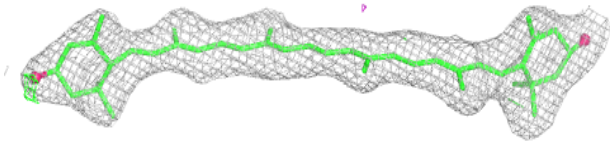


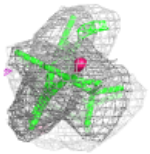


Electron density around LUT G 6620:

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

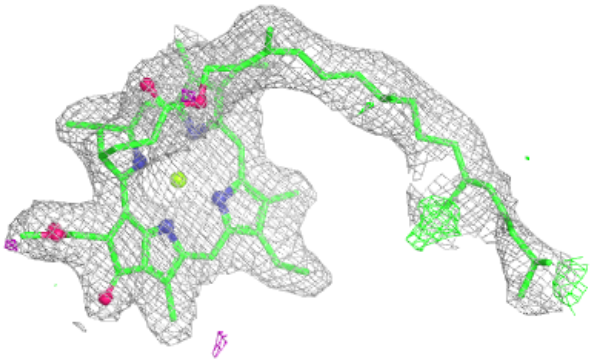


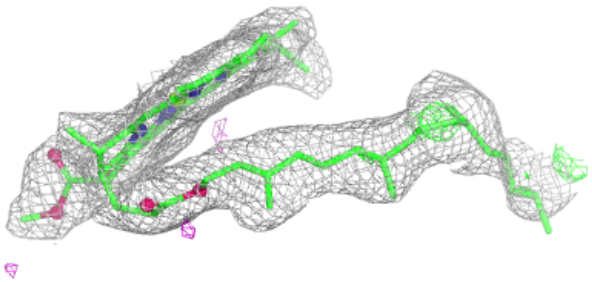


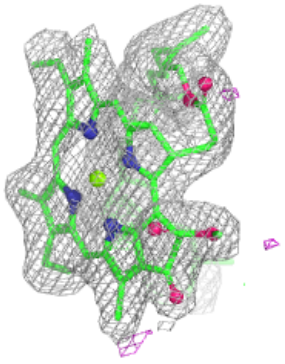


Electron density around CLA J 610:

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

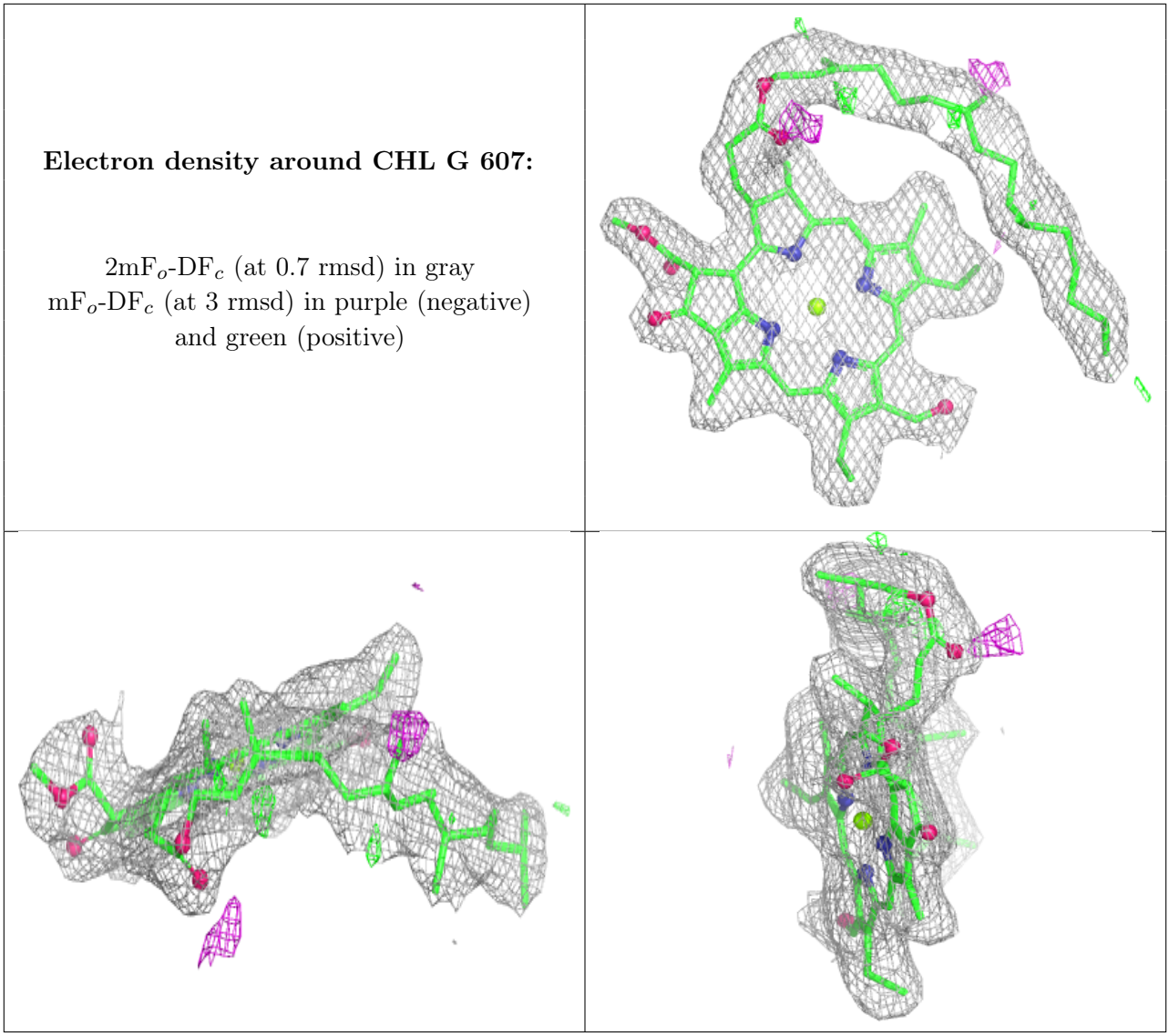






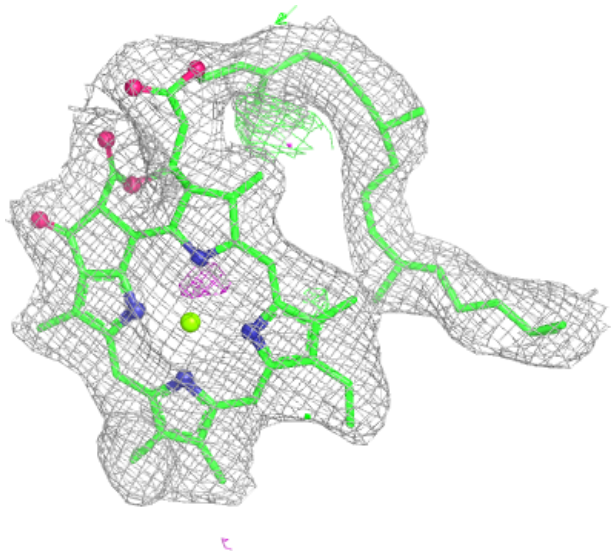
Electron density around CHL G 607:

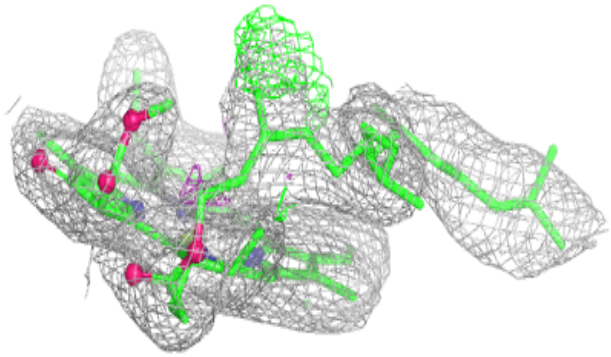
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

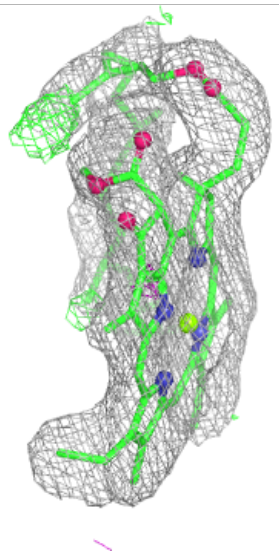


Electron density around CLA J 612:

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

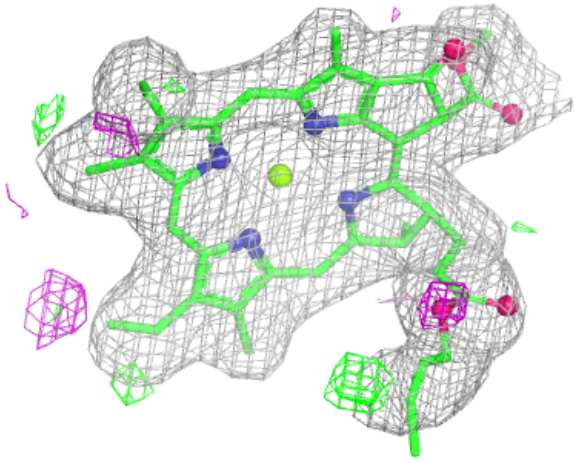


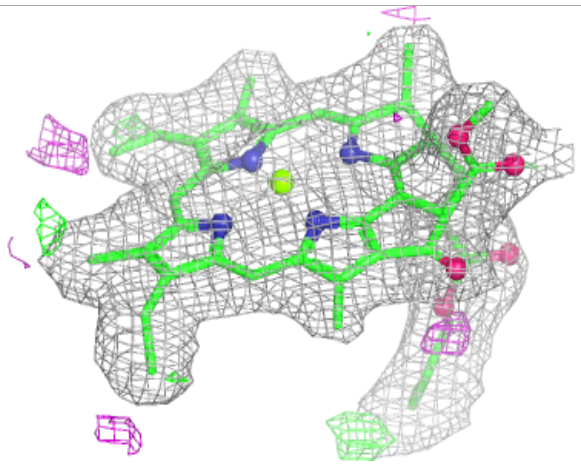


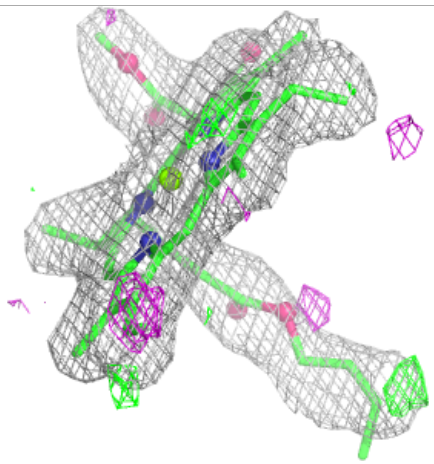


Electron density around CLA B 614:

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

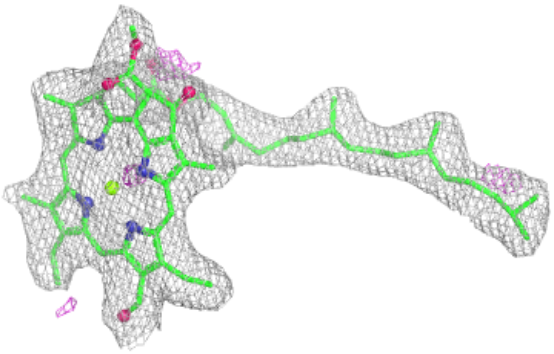


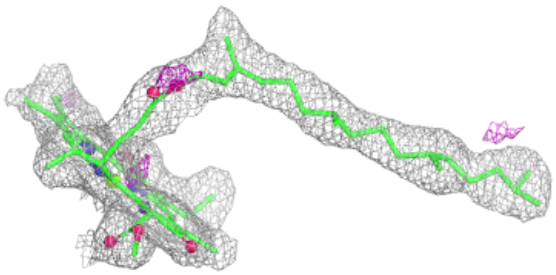


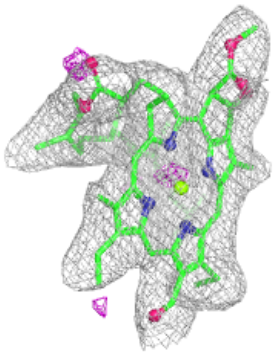


Electron density around CHL J 609:

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

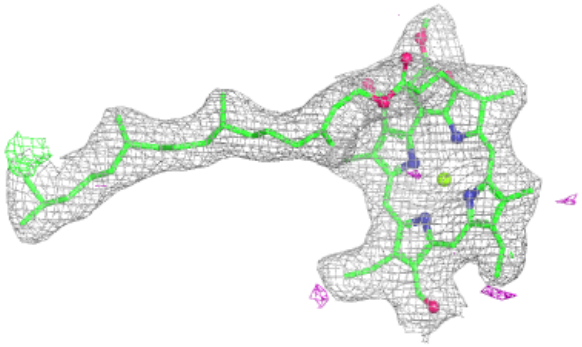


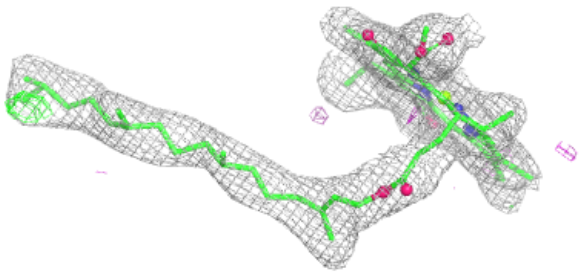




Electron density around CHL F 609:

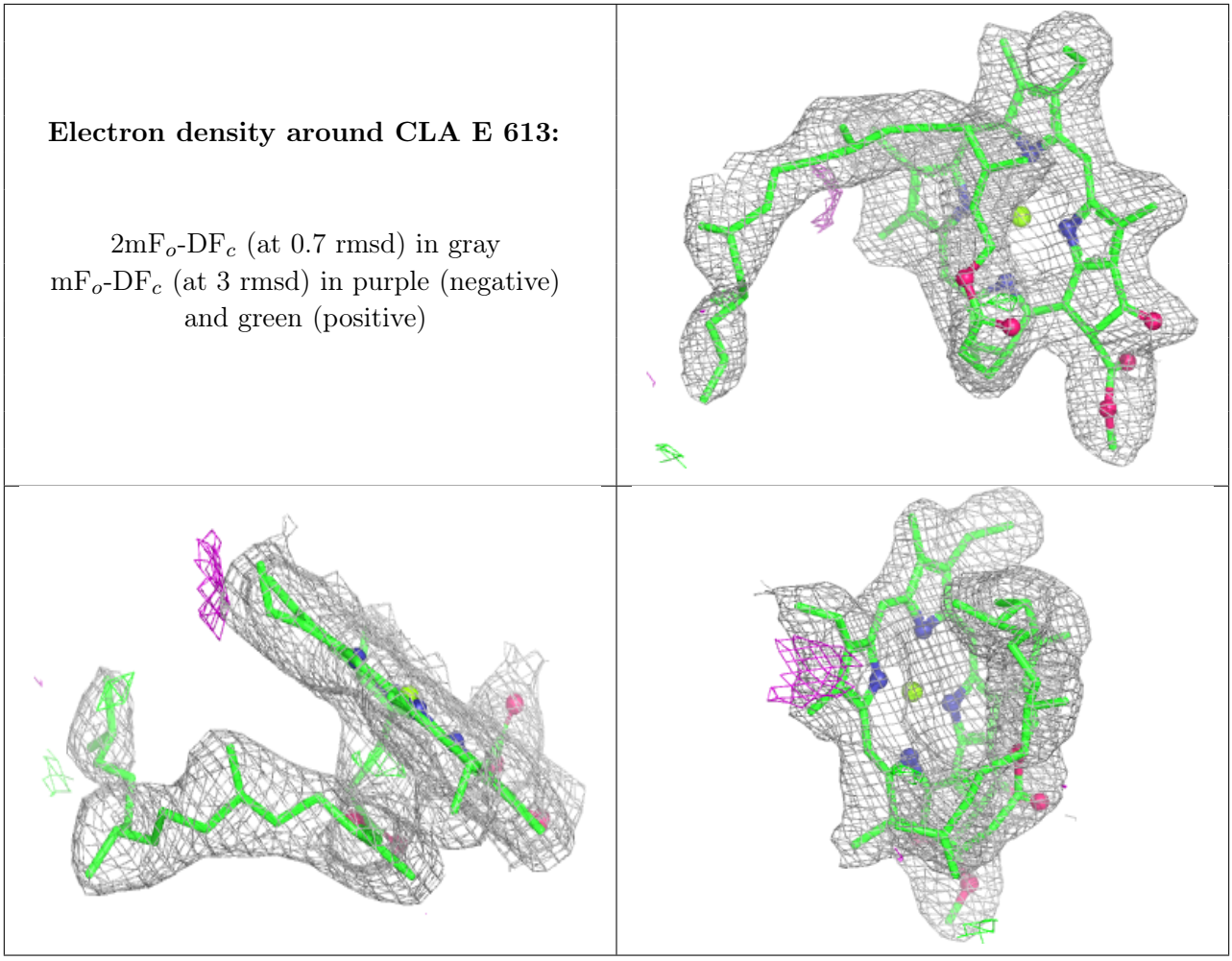
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





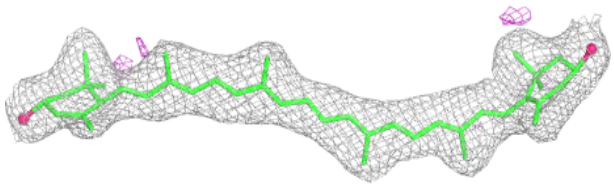
Electron density around CLA E 613:

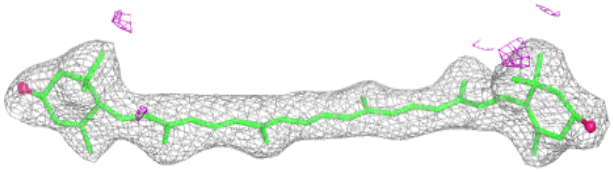
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

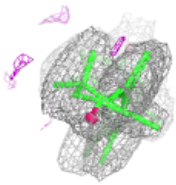


Electron density around LUT E 4620:

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

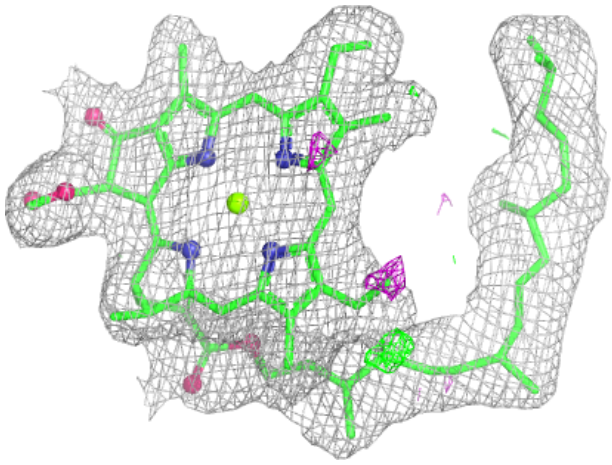


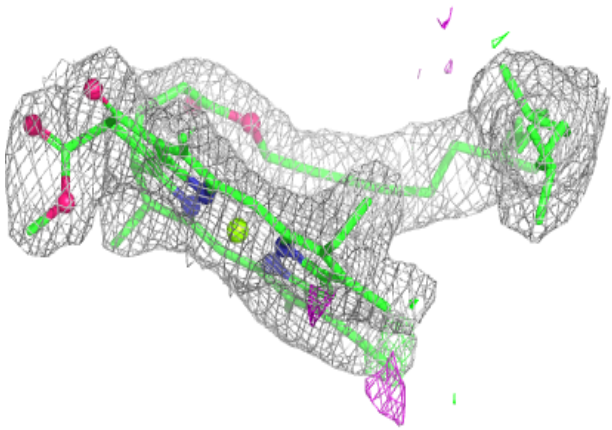


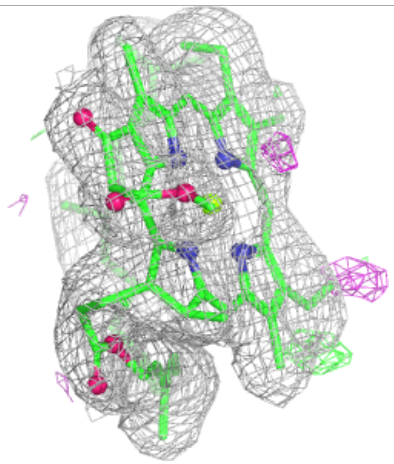


Electron density around CLA F 602:

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

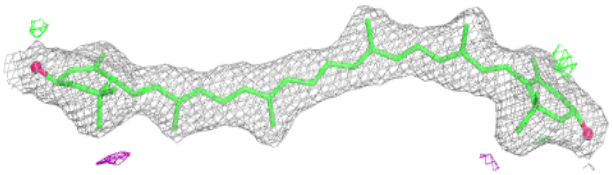


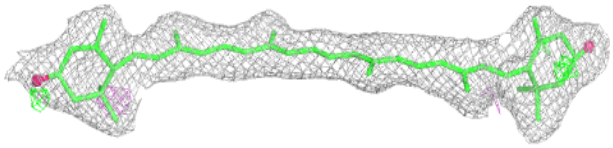


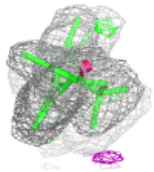


Electron density around LUT F 5620:

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

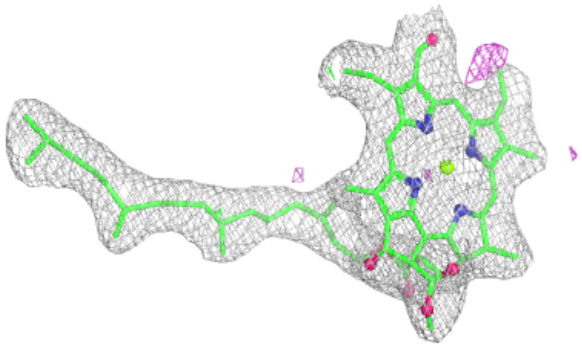


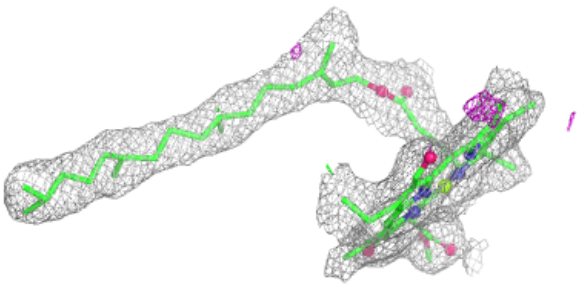


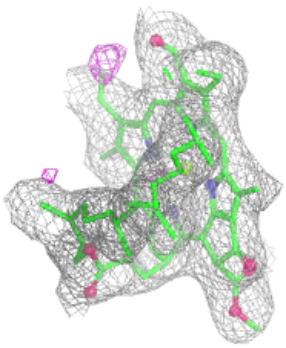


Electron density around CHL C 609:

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

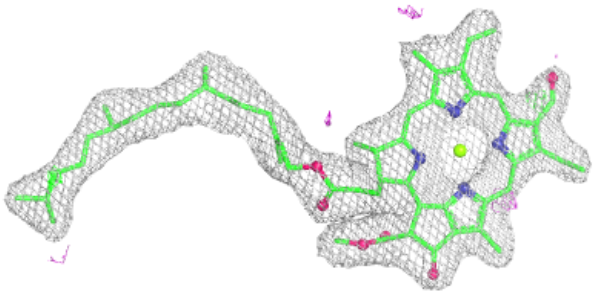


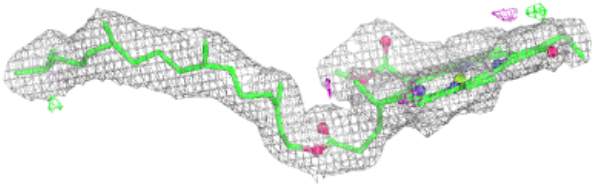


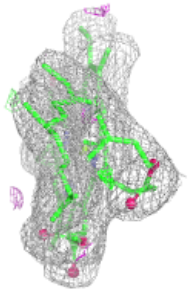


Electron density around CHL D 601:

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

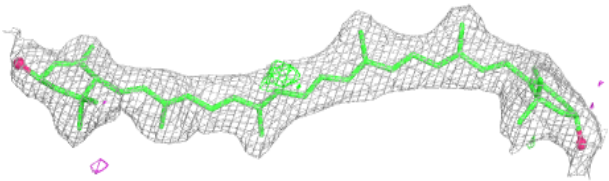


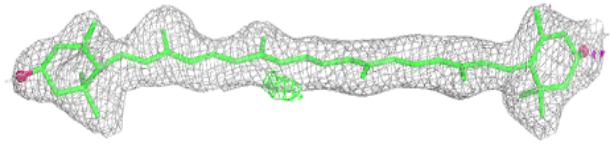


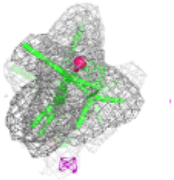


Electron density around LUT F 5621:

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

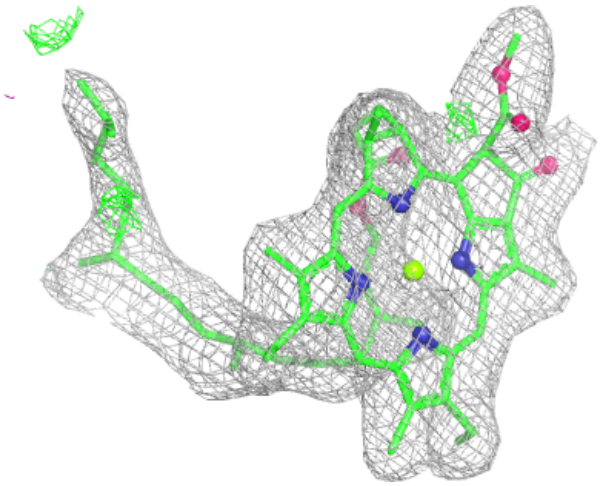


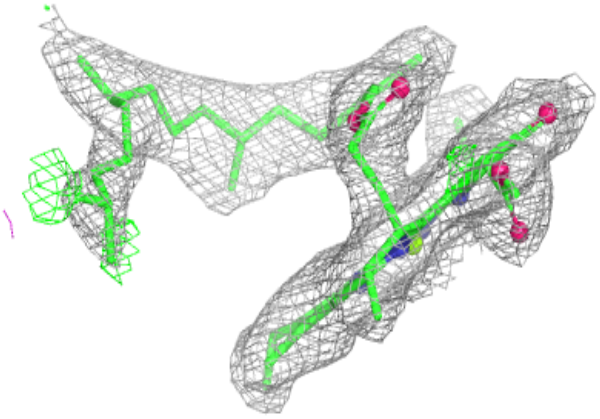


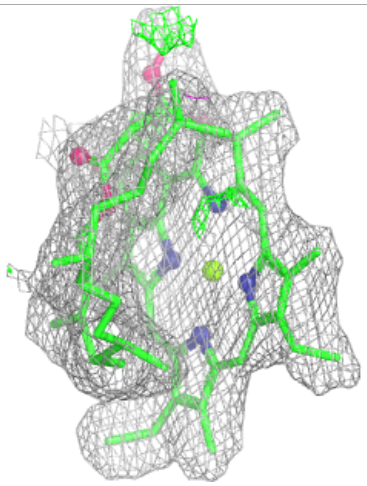


Electron density around CLA A 613:

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

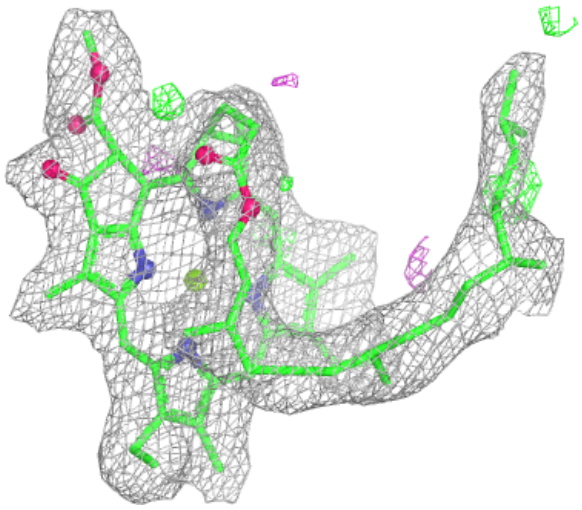


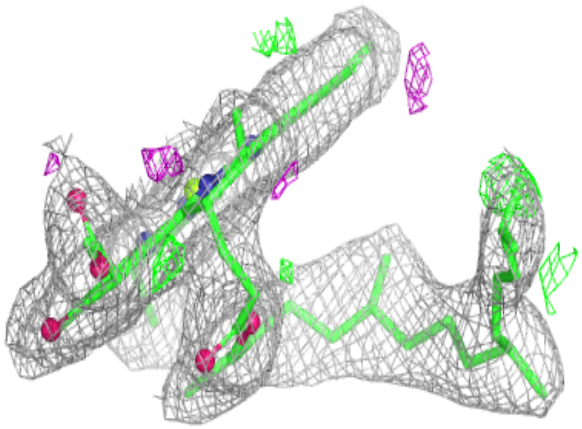


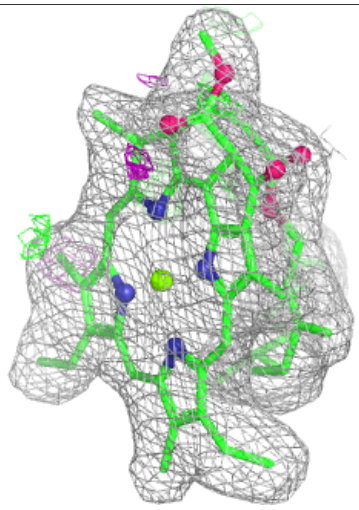


Electron density around CLA F 613:

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

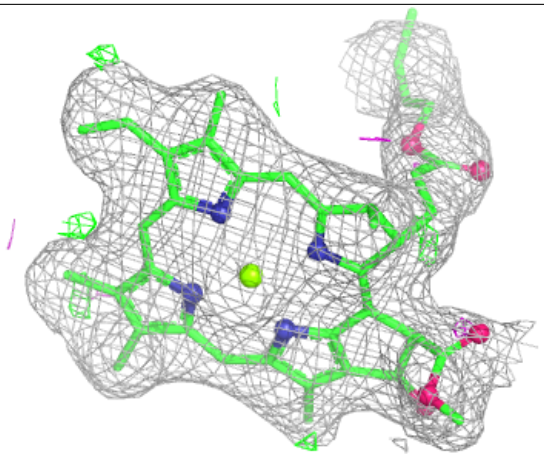


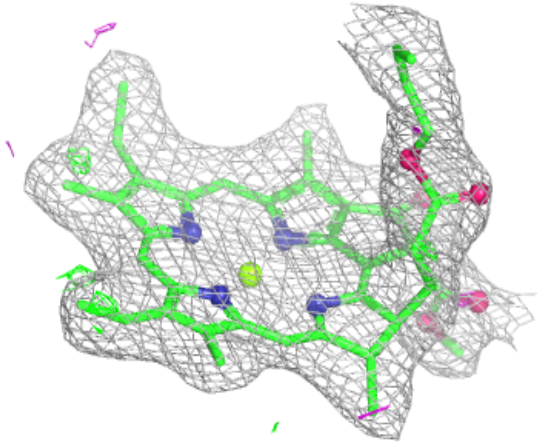


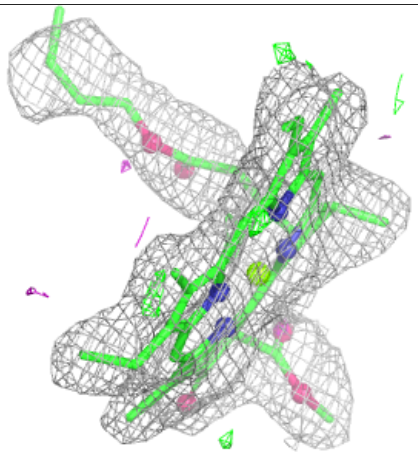


Electron density around CLA F 614:

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

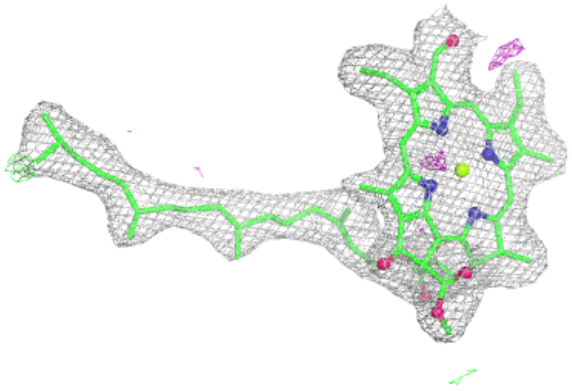


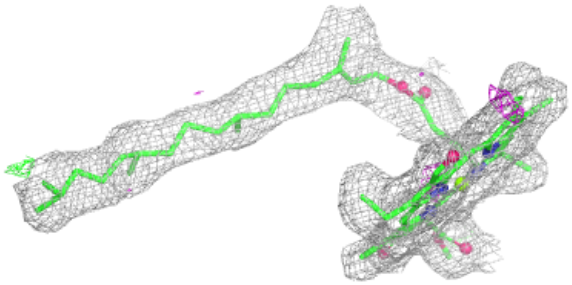




Electron density around CHL G 609:

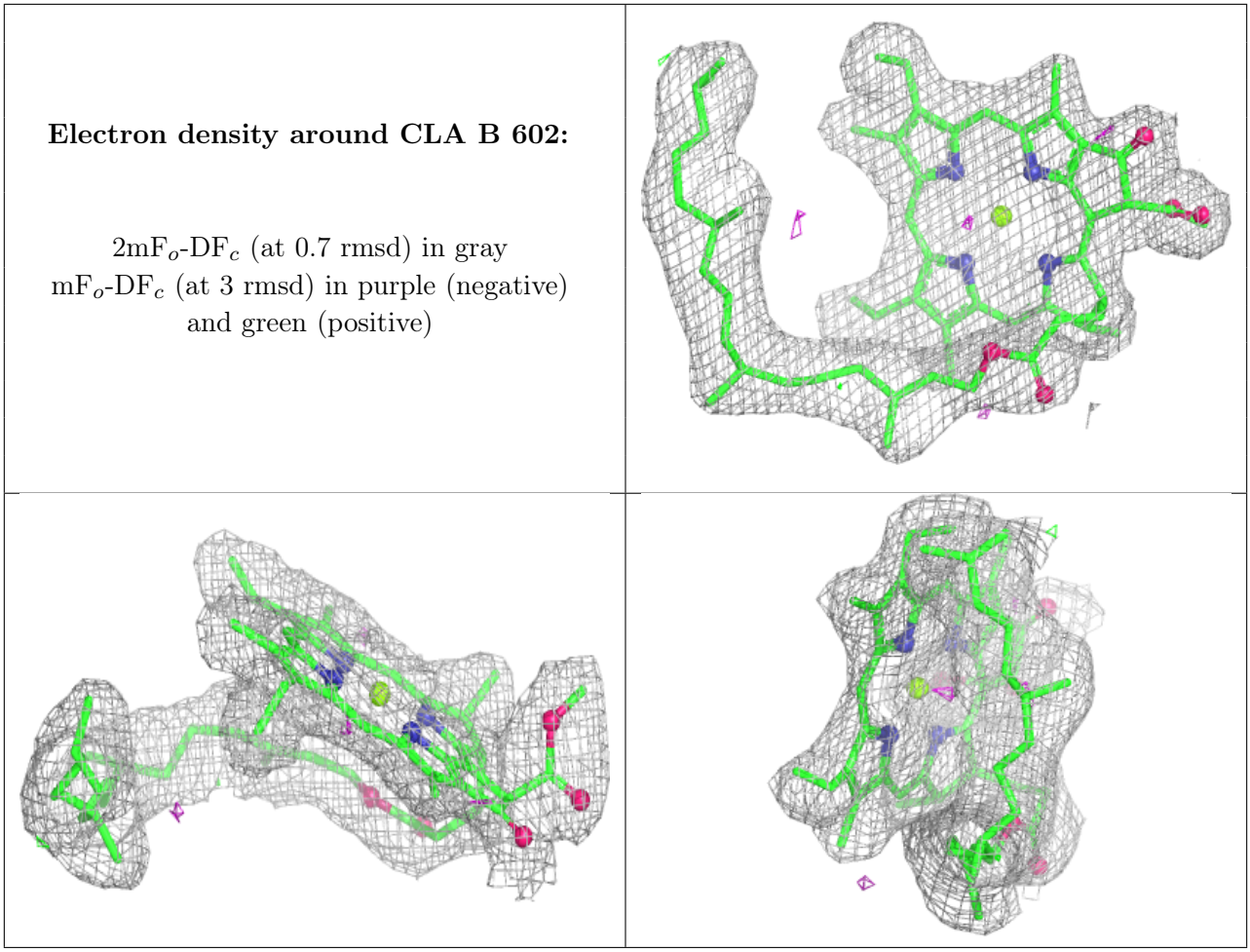
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





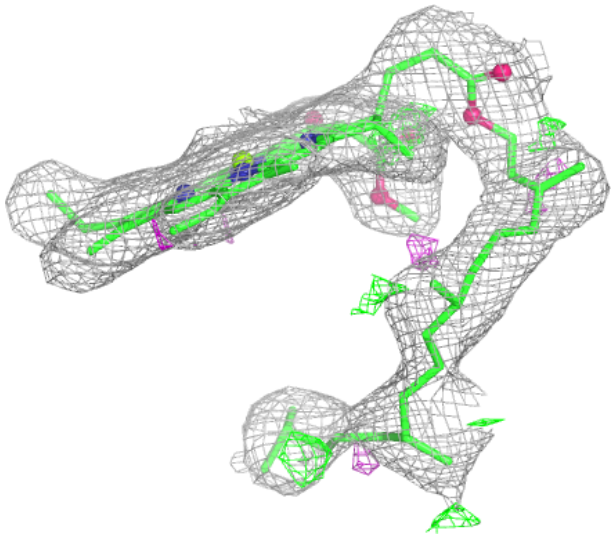
Electron density around CLA B 602:

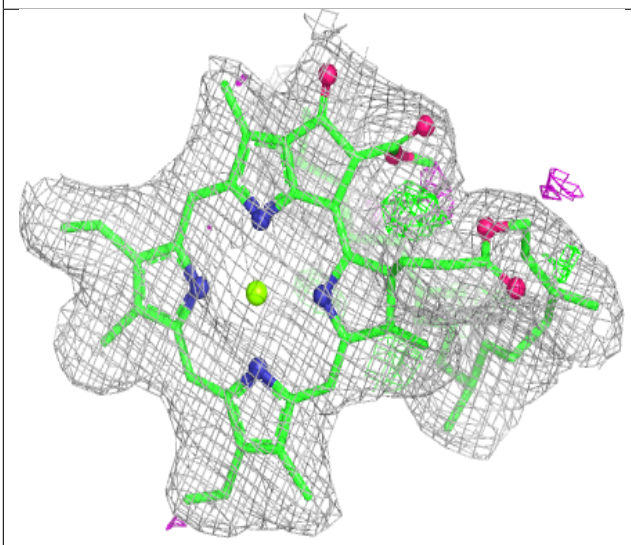
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

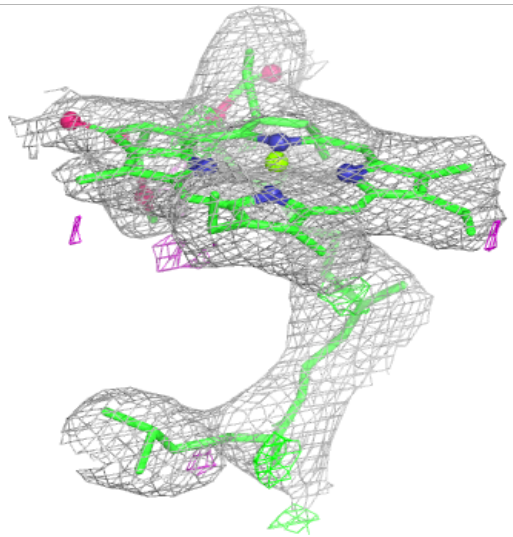


Electron density around CLA B 603:

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

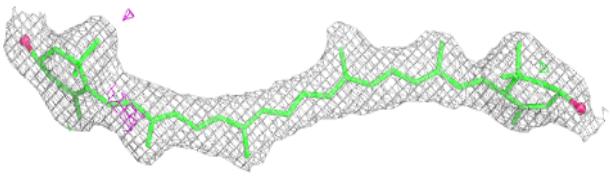


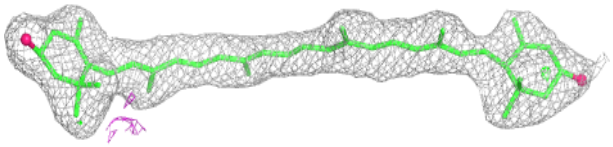


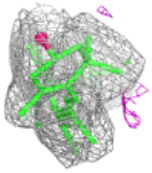


Electron density around LUT A 620:

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

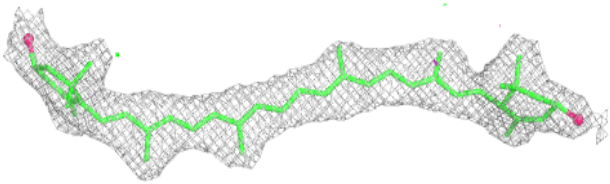


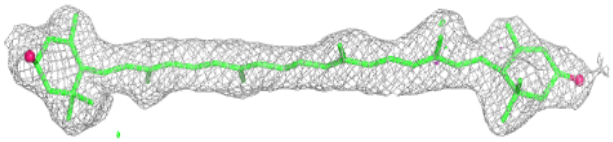


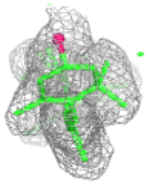


Electron density around LUT A 621:

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

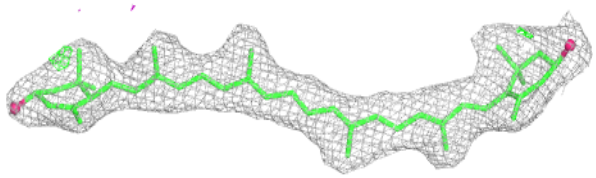


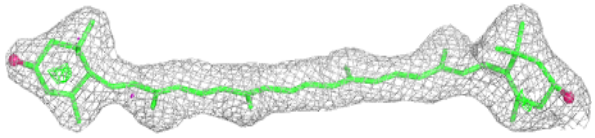


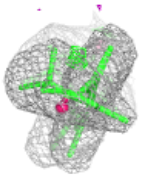


Electron density around LUT H 7620:

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

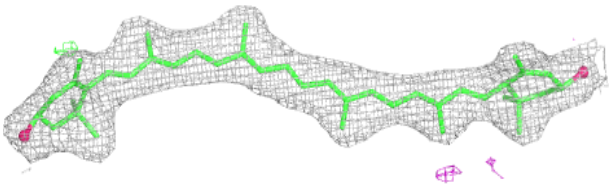


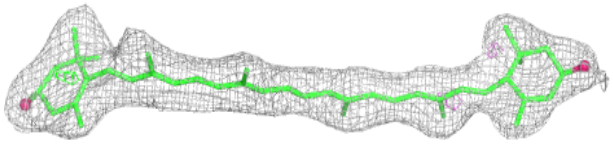


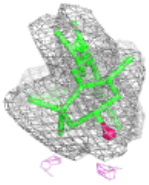


Electron density around LUT I 8620:

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

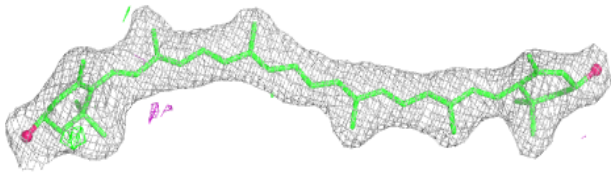


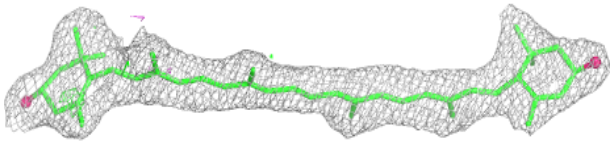


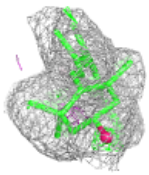


Electron density around LUT J 9620:

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

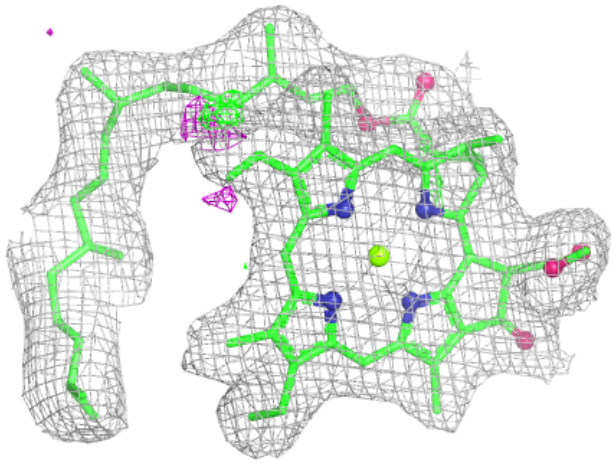


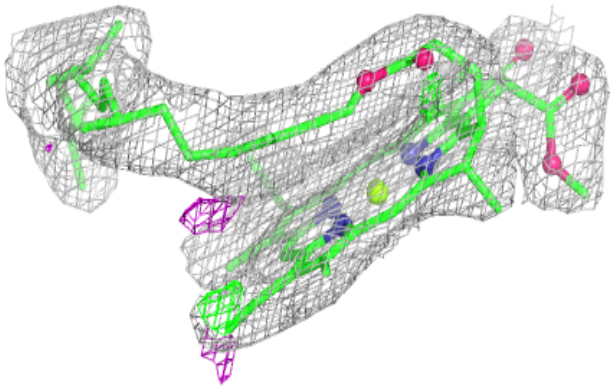


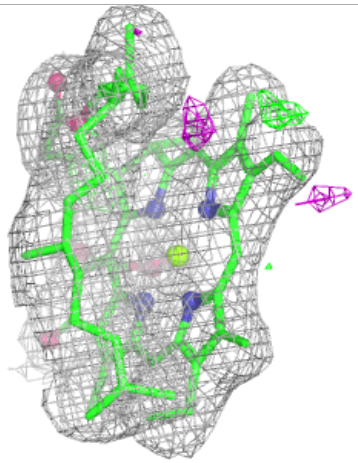


Electron density around CLA C 602:

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

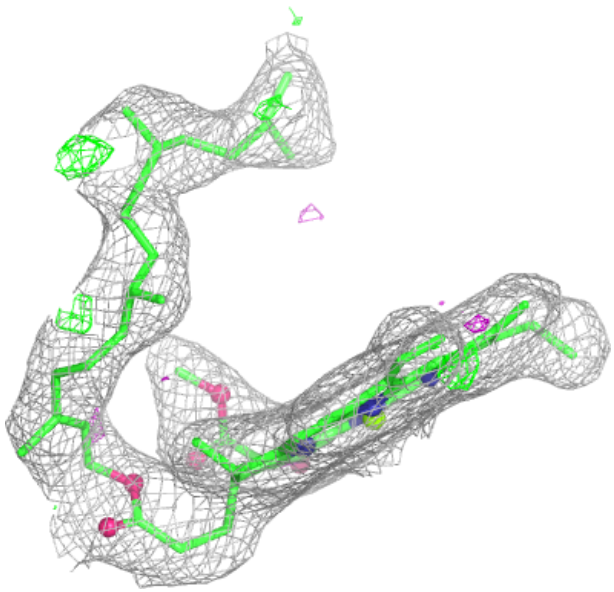


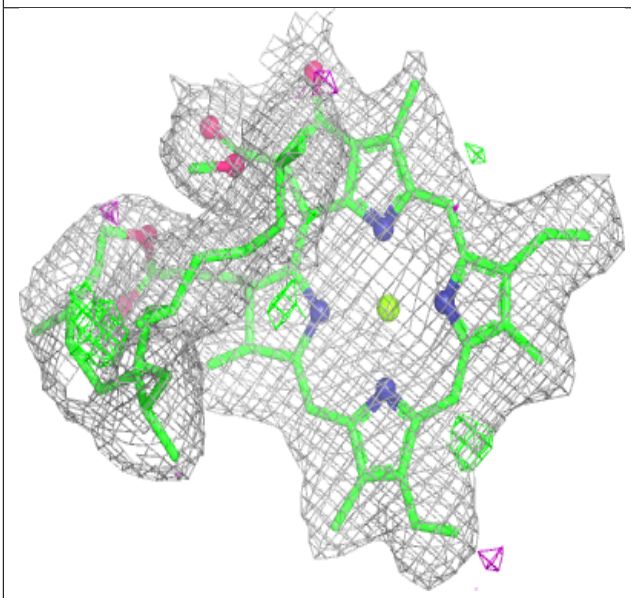


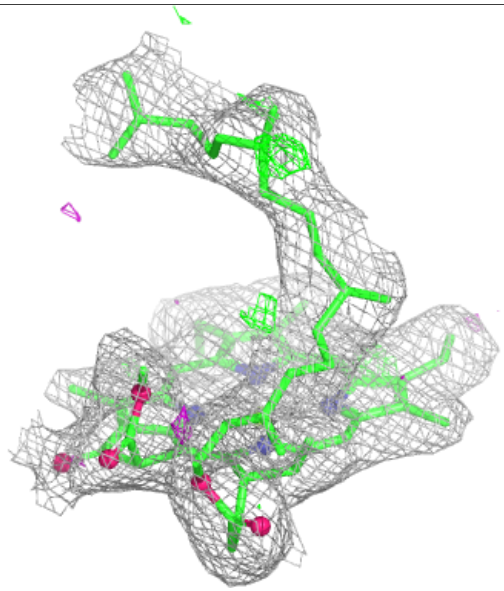


Electron density around CLA C 603:

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

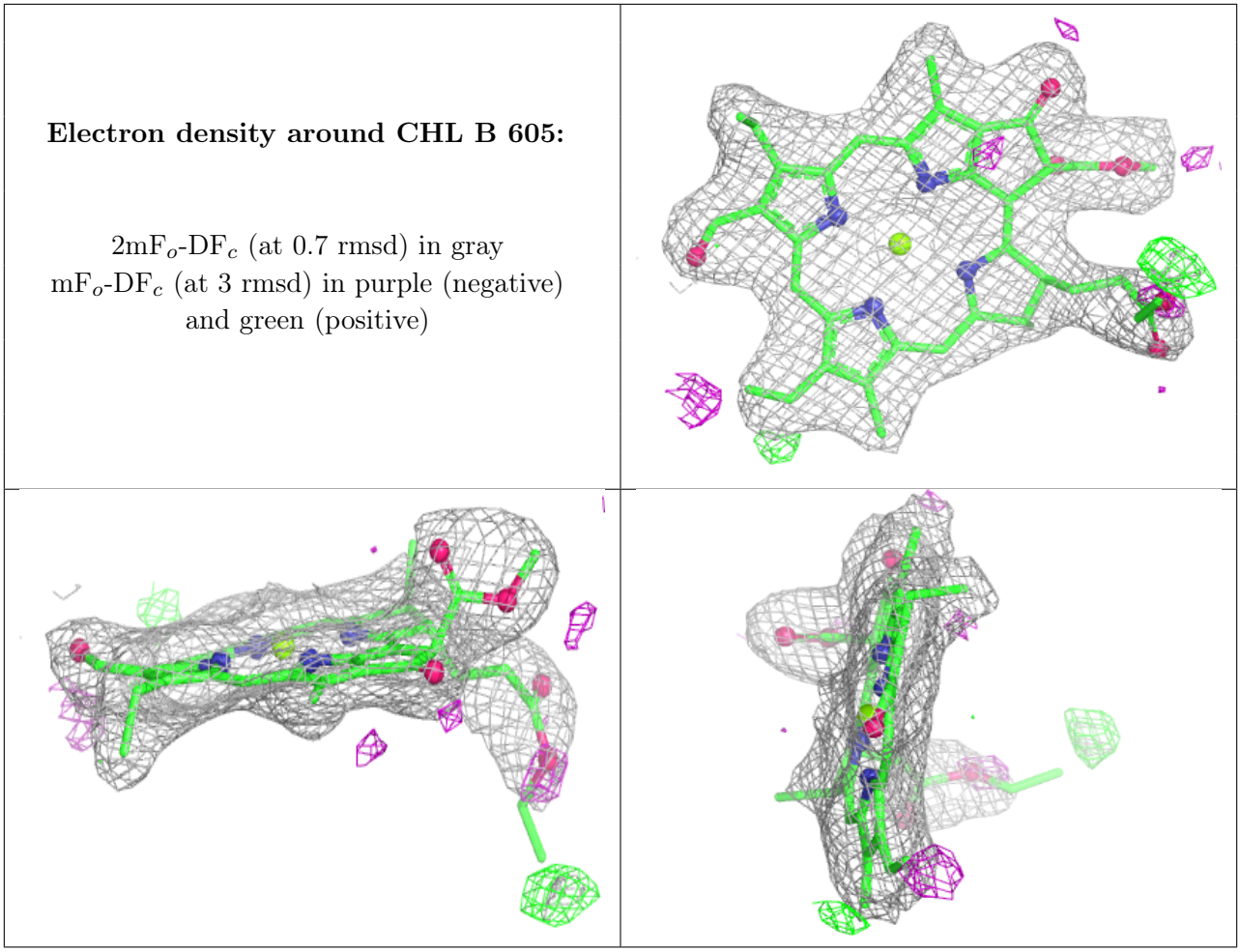






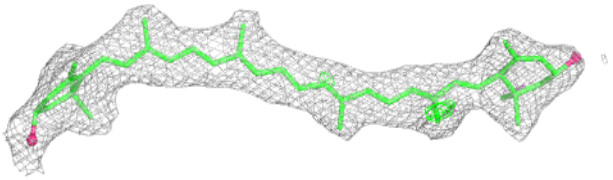
Electron density around CHL B 605:

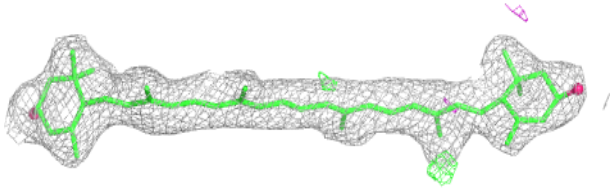
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

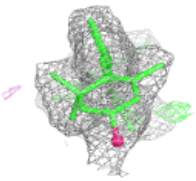


Electron density around LUT J 9621:

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

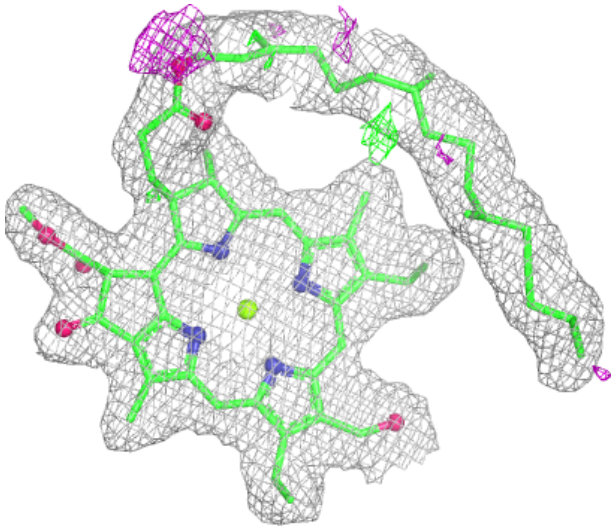


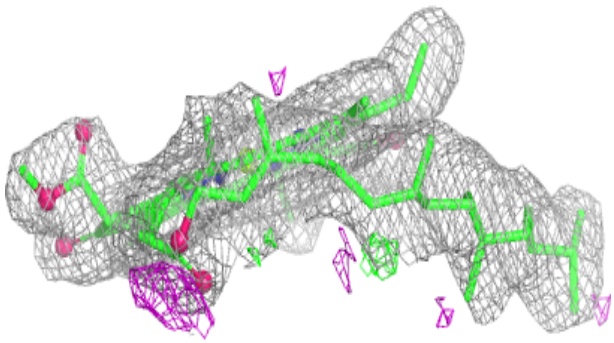


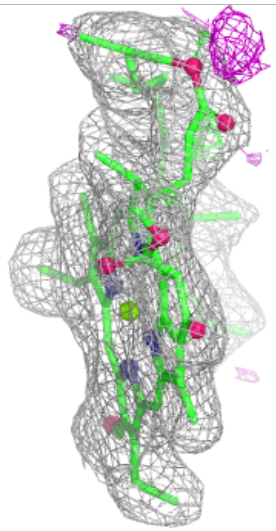


Electron density around CHL B 607:

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

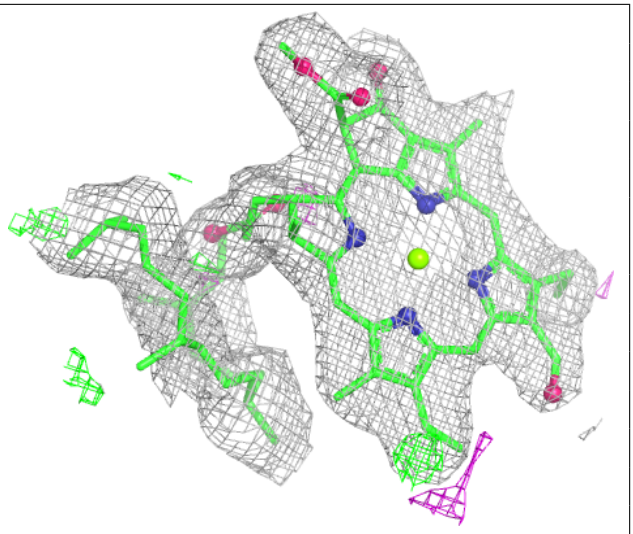


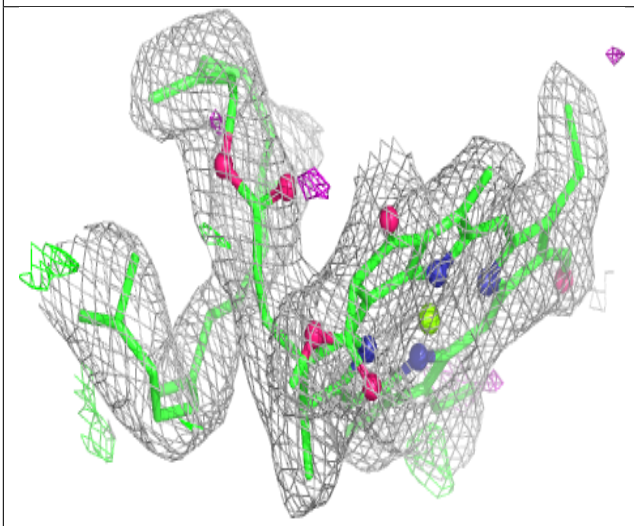


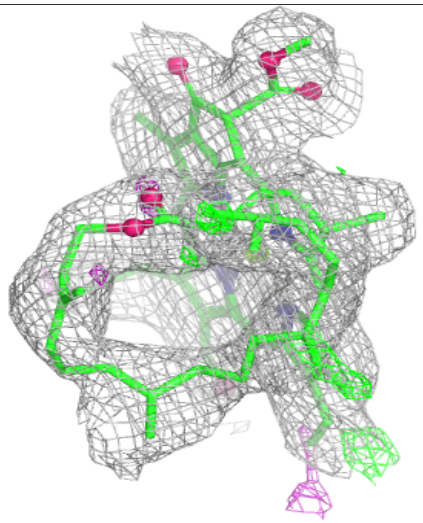


Electron density around CHL B 608:

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

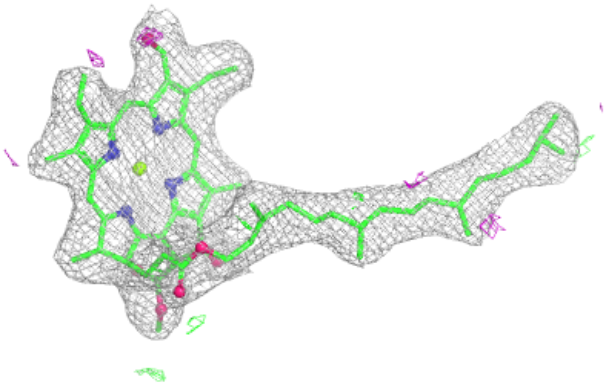


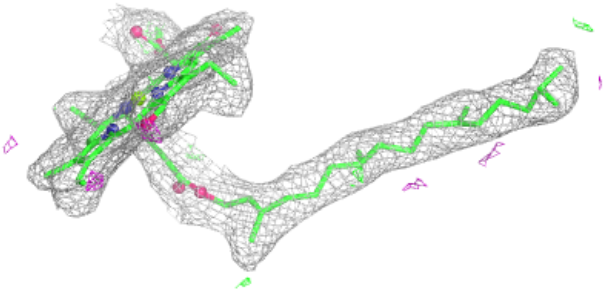


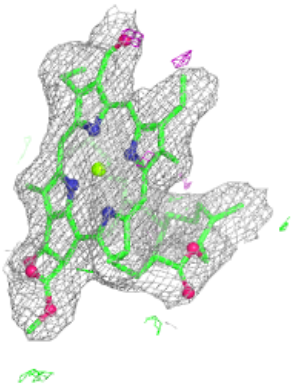


Electron density around CHL E 609:

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

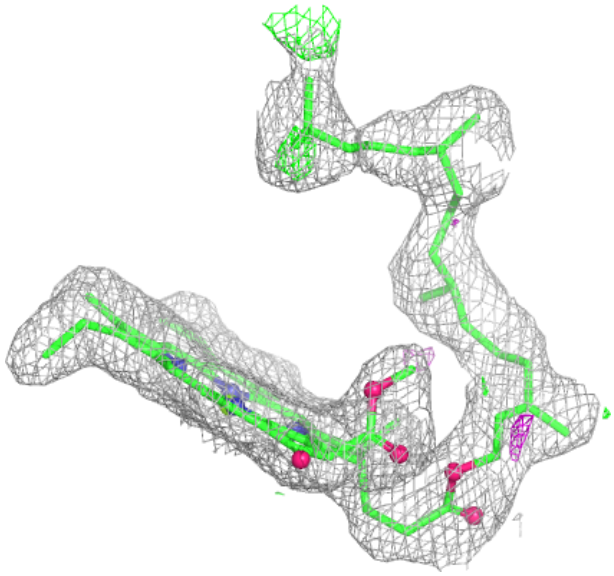


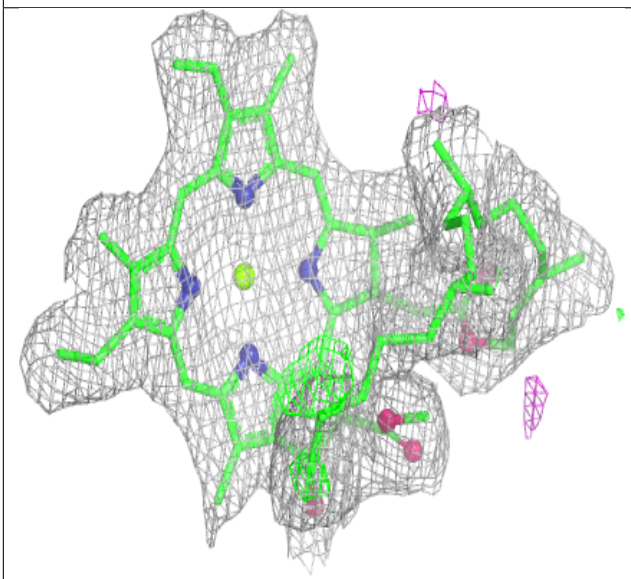


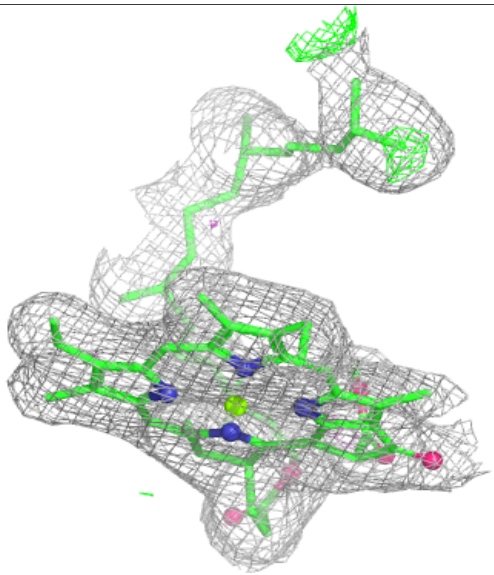


Electron density around CLA I 603:

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

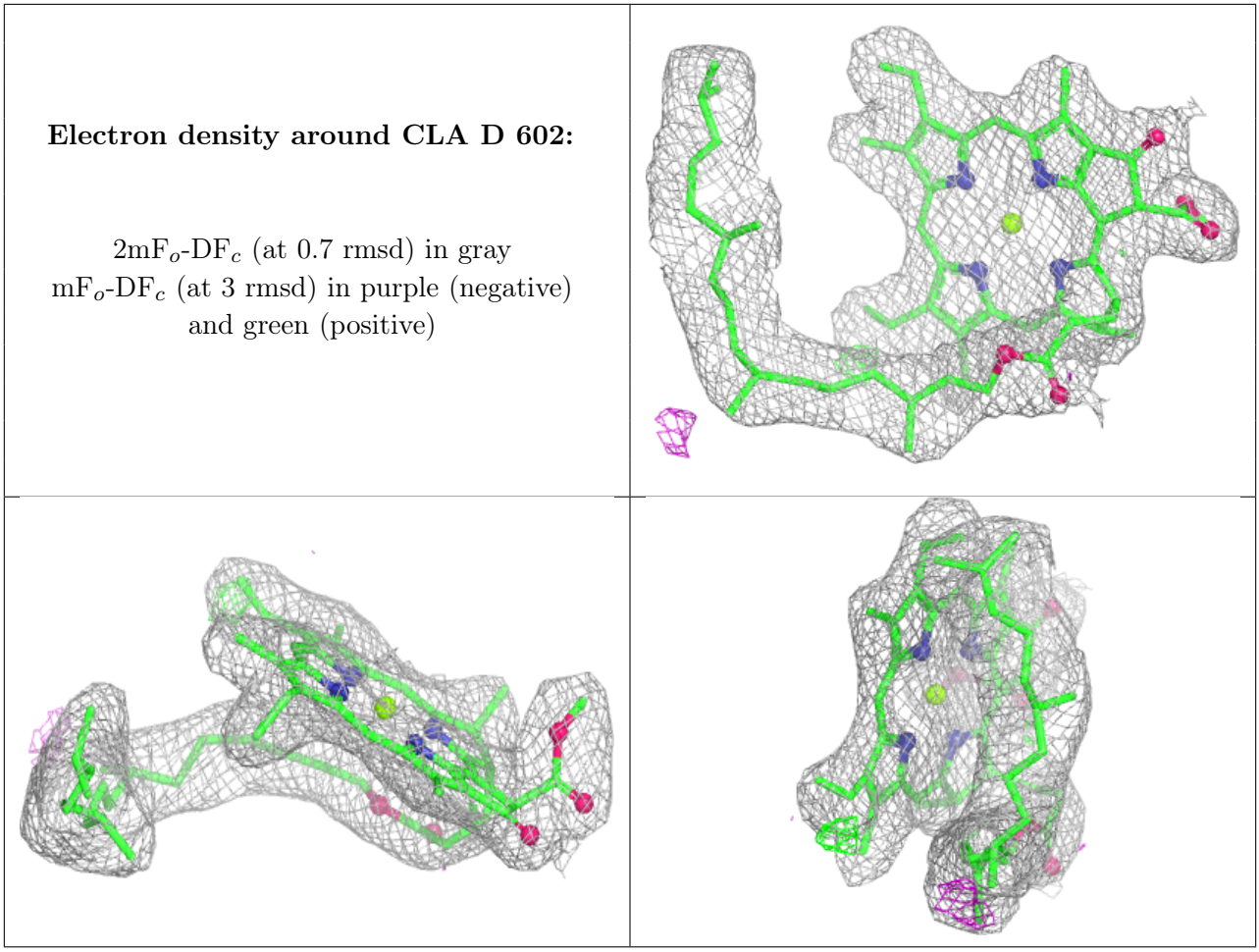






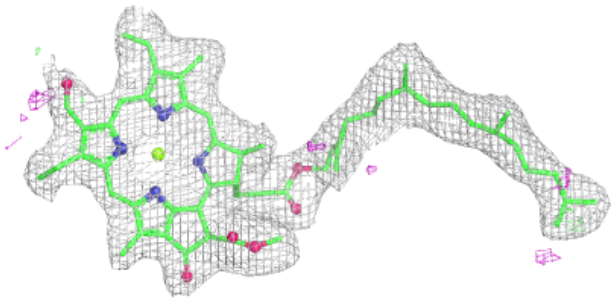
Electron density around CLA D 602:

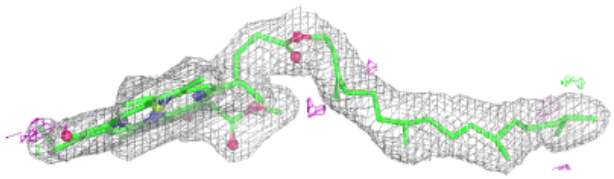
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

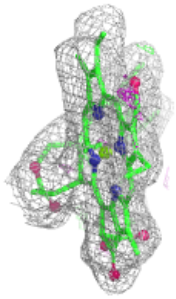


Electron density around CHL F 601:

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

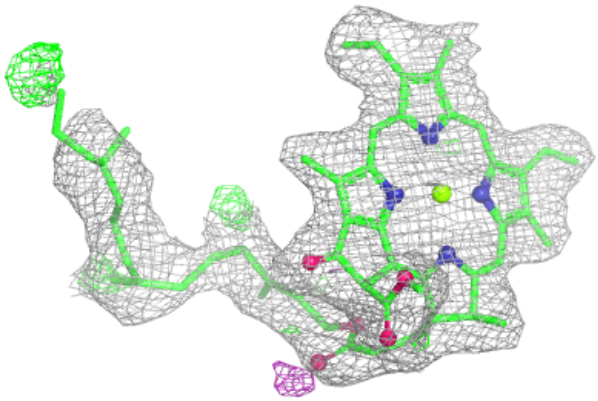


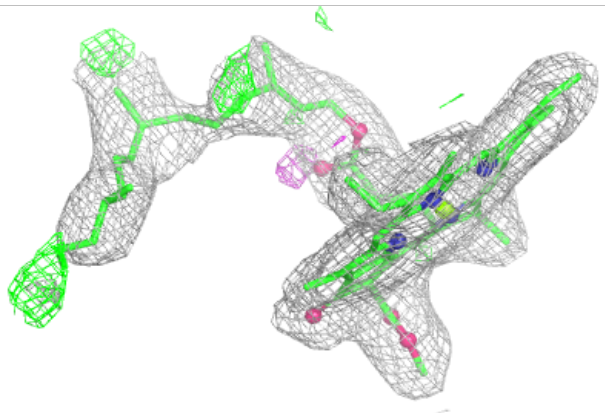


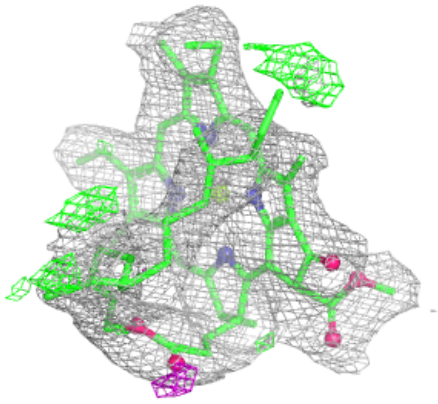


Electron density around CLA D 604:

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

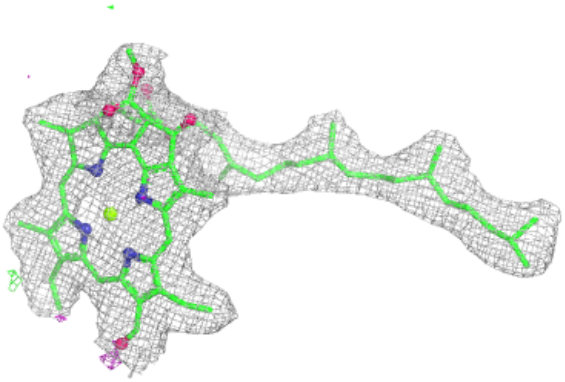


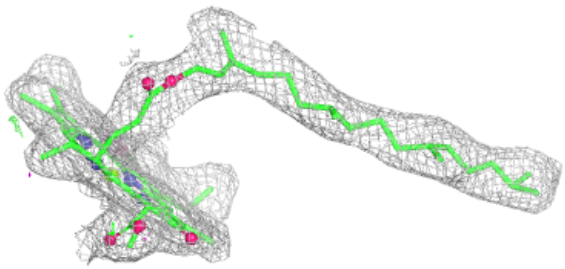


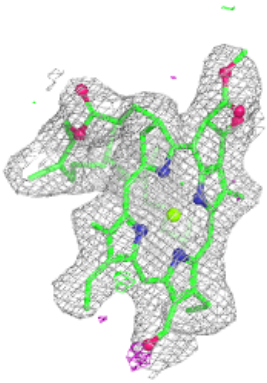


Electron density around CHL I 609:

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

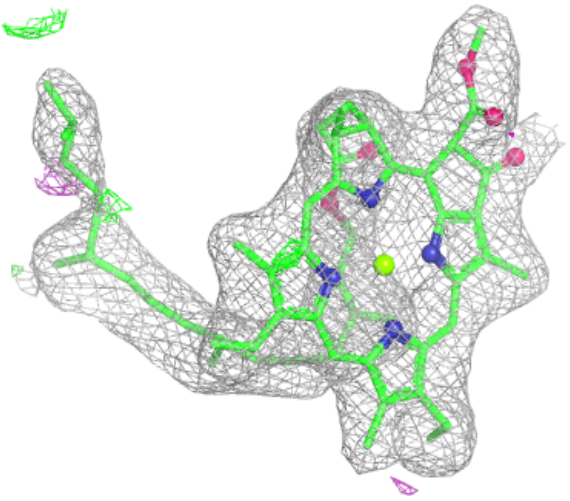


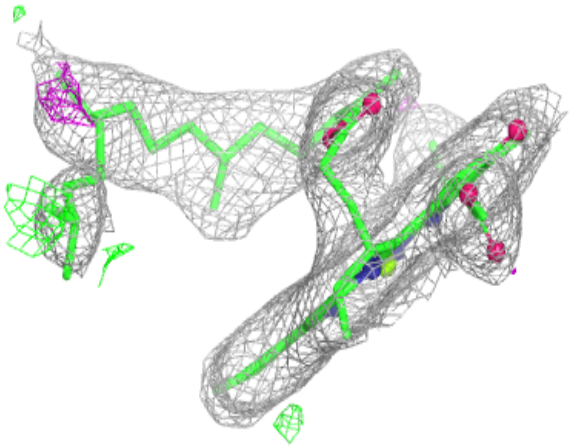


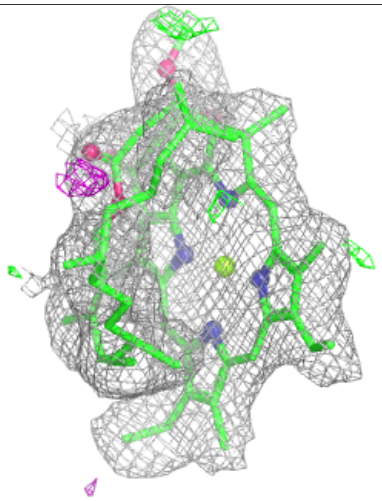


Electron density around CLA I 613:

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

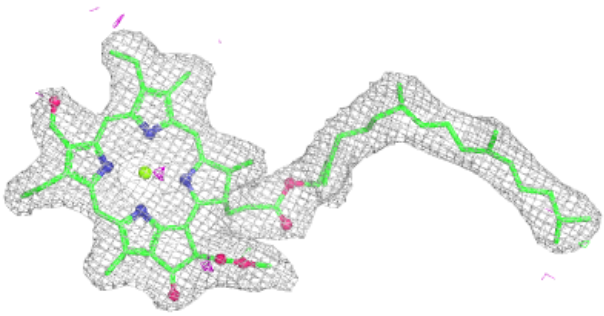


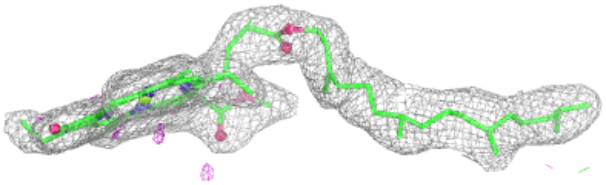


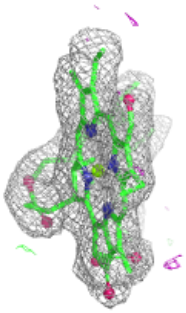


Electron density around CHL J 601:

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

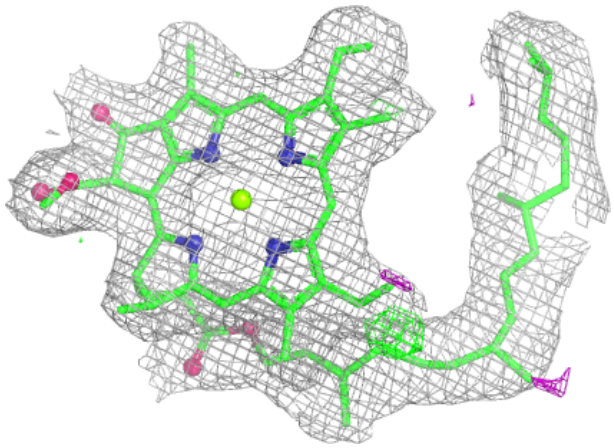


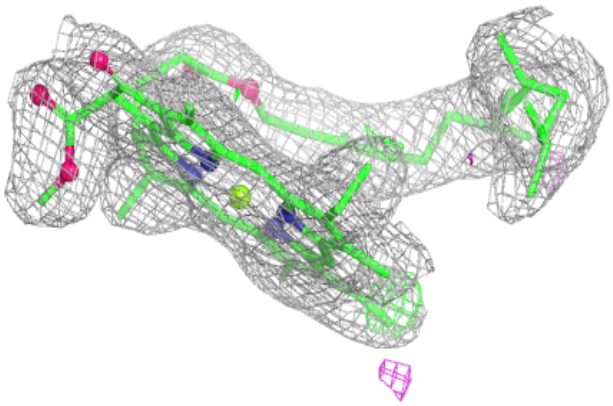


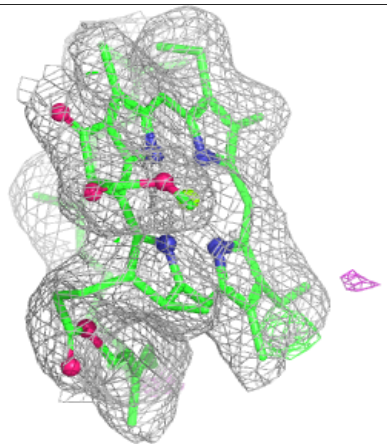


Electron density around CLA J 602:

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

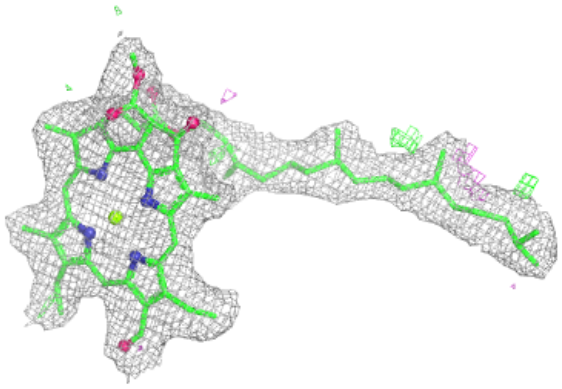


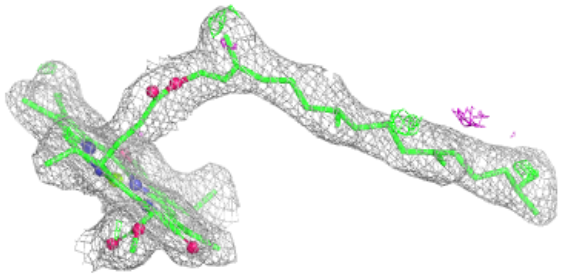


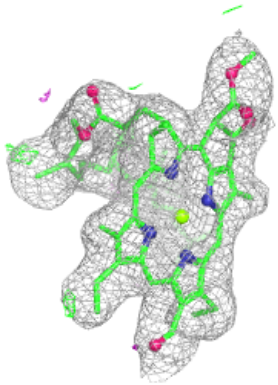


Electron density around CHL B 609:

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

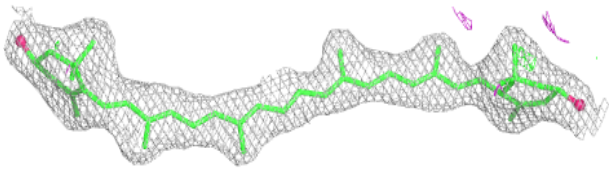


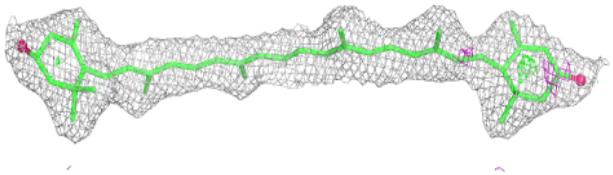


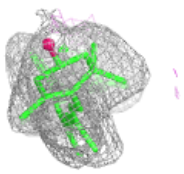


Electron density around LUT C 2620:

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

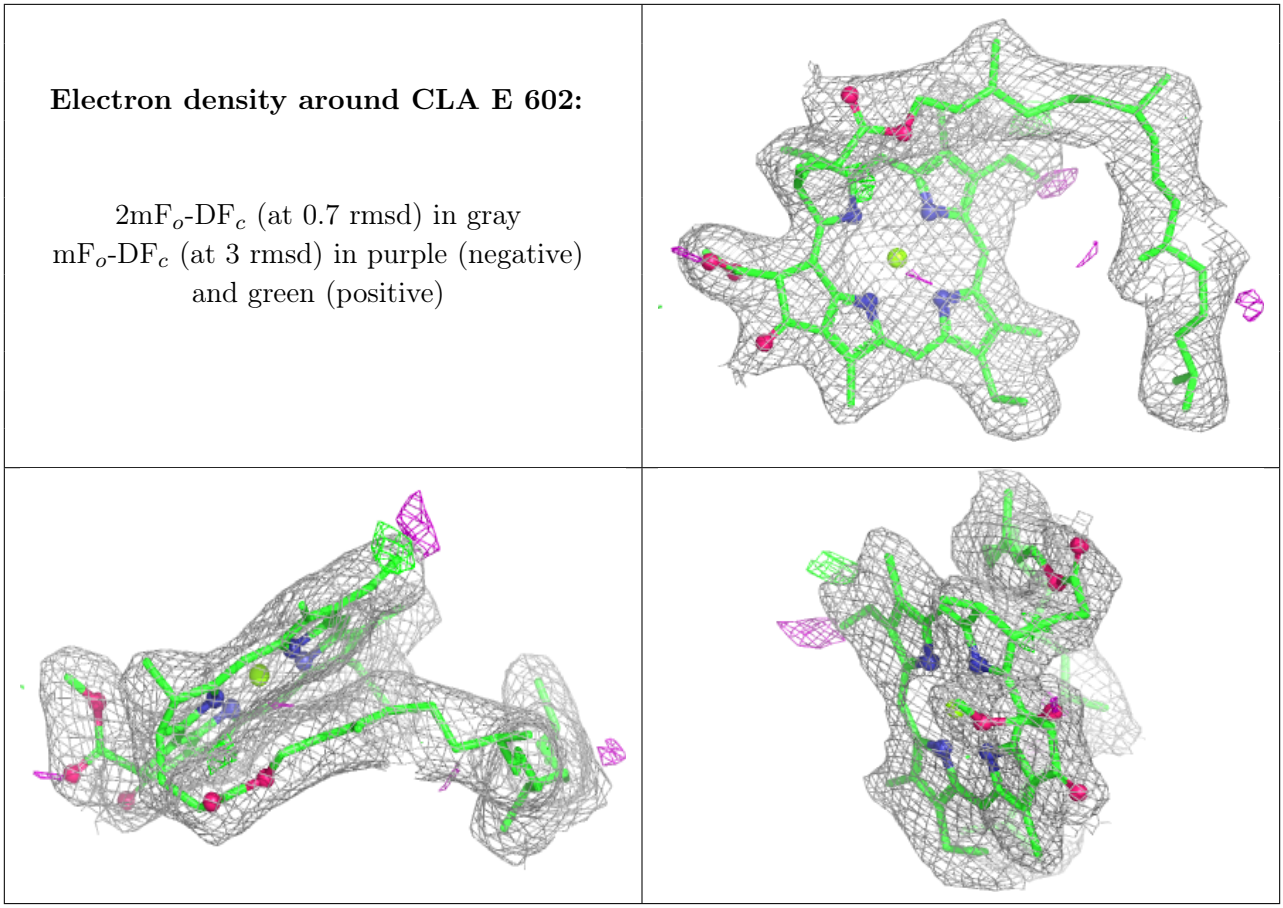






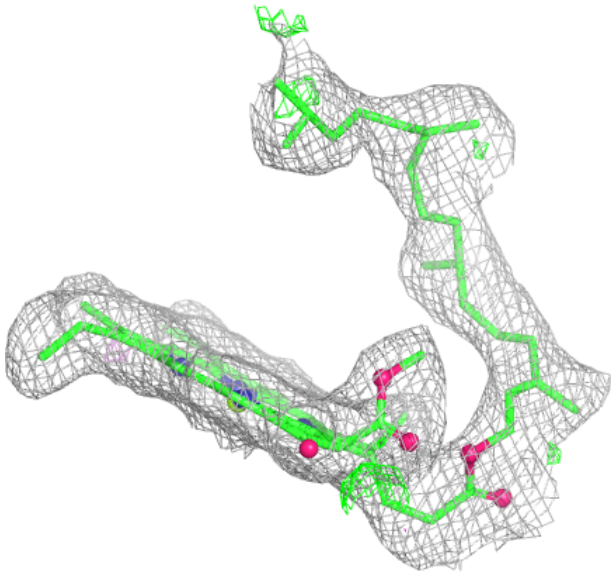
Electron density around CLA E 602:

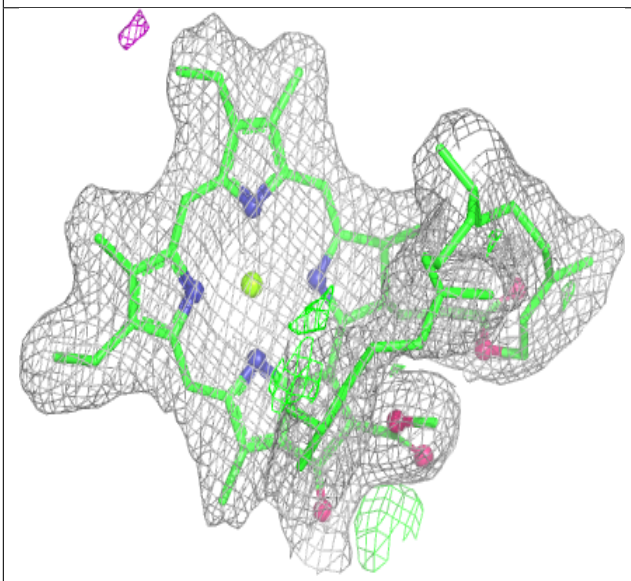
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

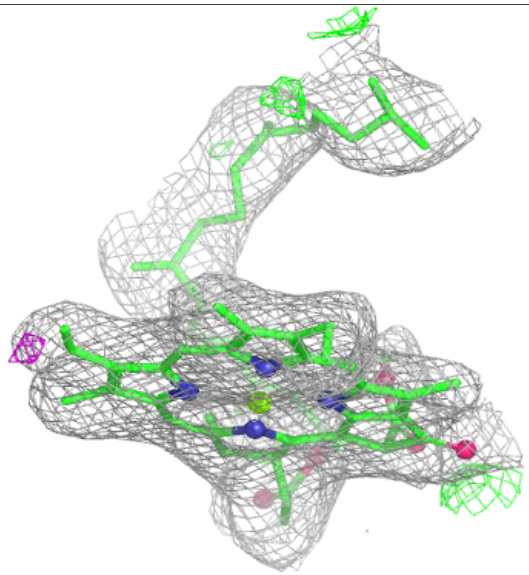


Electron density around CLA E 603:

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

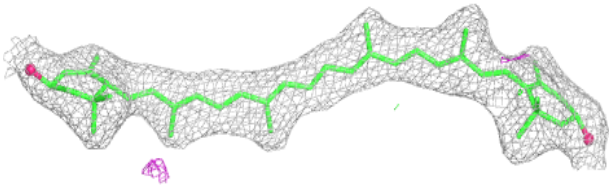


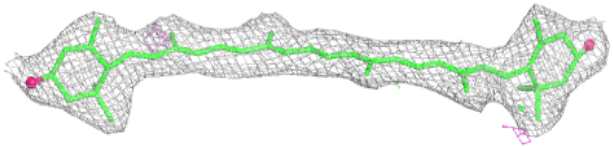


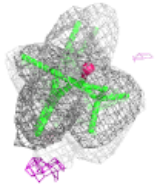


Electron density around LUT D 3620:

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

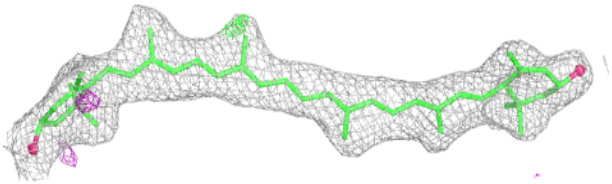


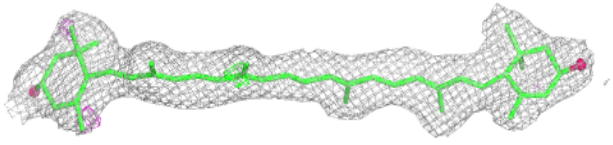


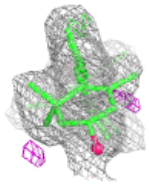


Electron density around LUT D 3621:

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

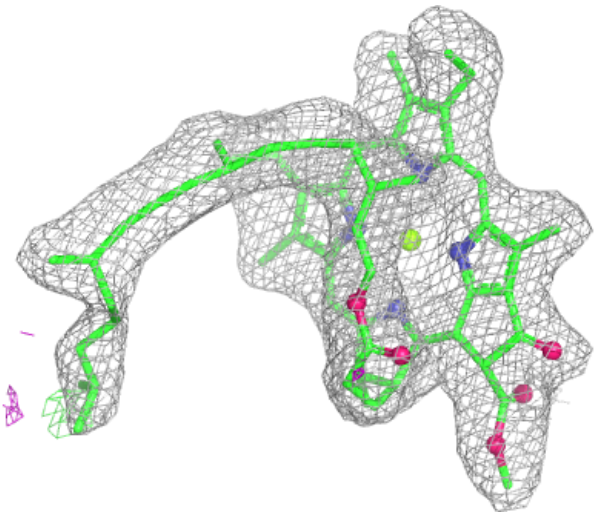


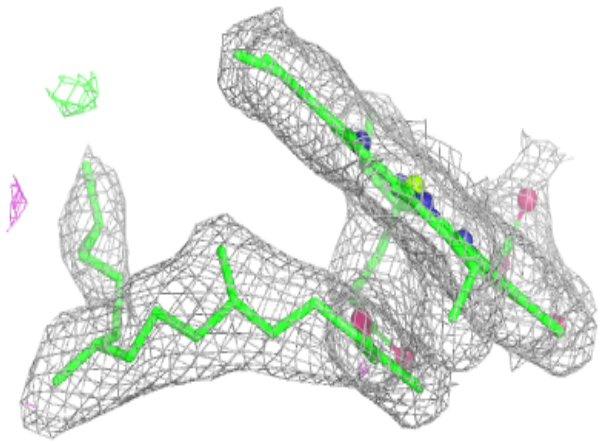


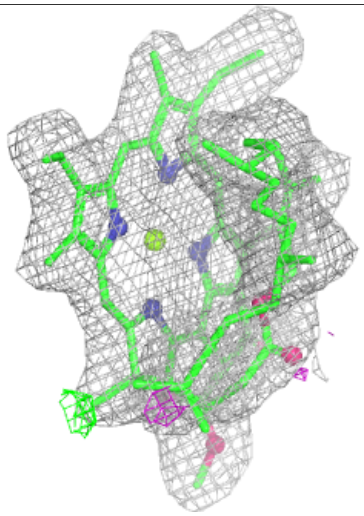


Electron density around CLA B 613:

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

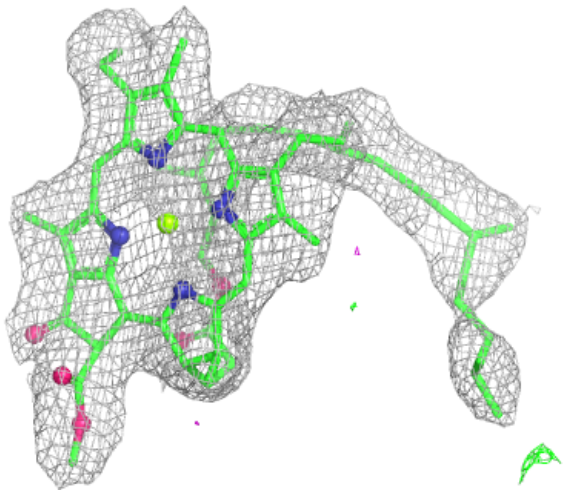


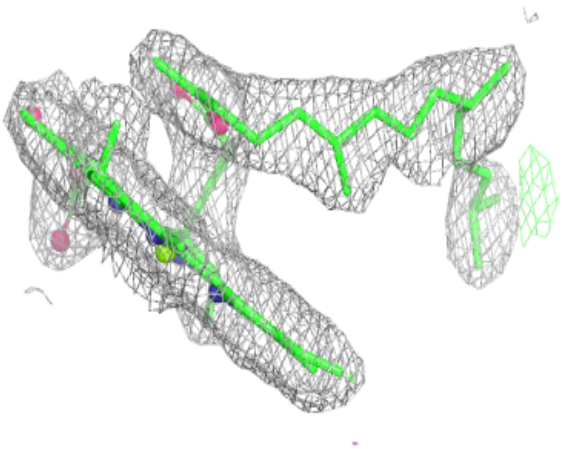


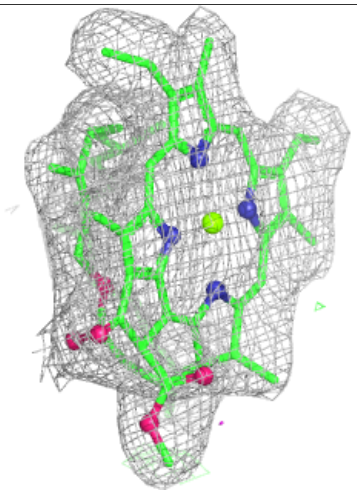


Electron density around CLA D 613:

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

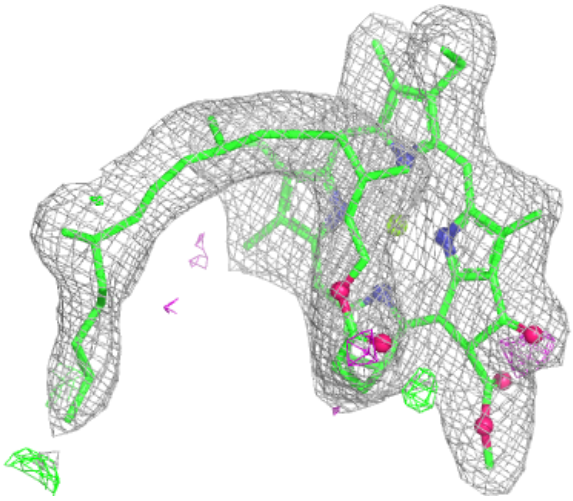


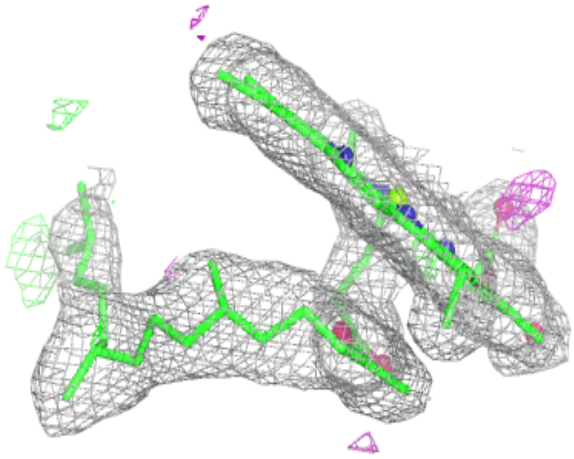


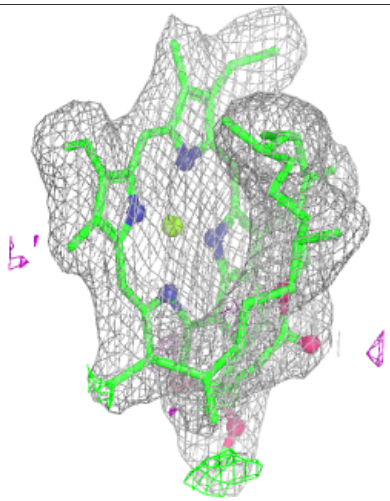


Electron density around CLA C 613:

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

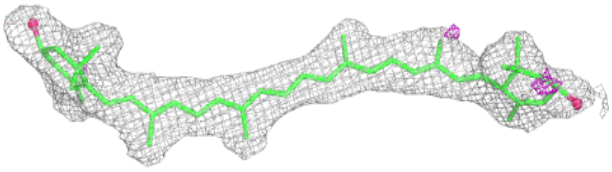


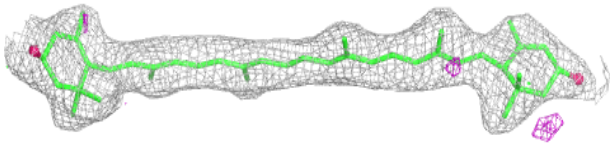




Electron density around LUT B 1621:

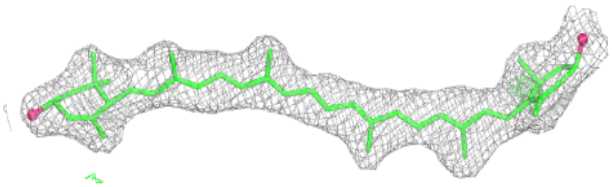
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

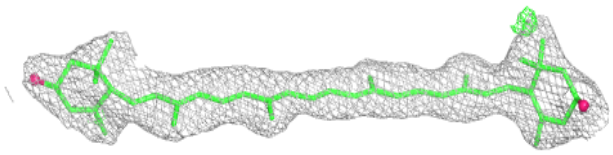


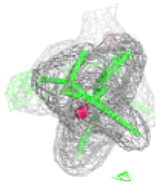


Electron density around LUT H 7621:

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

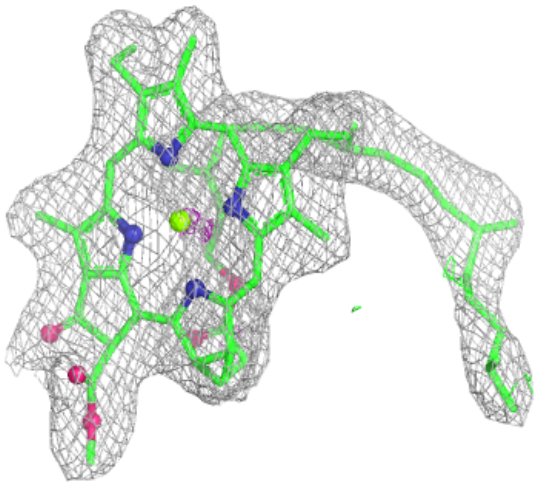


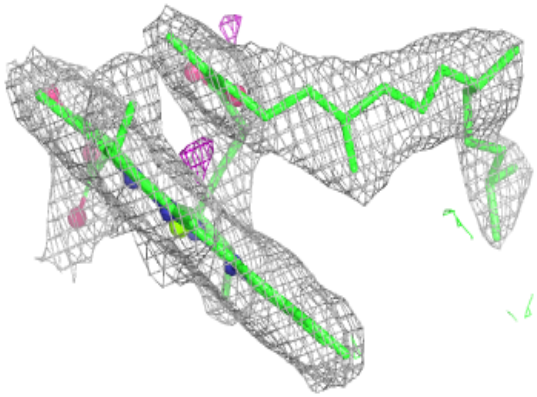


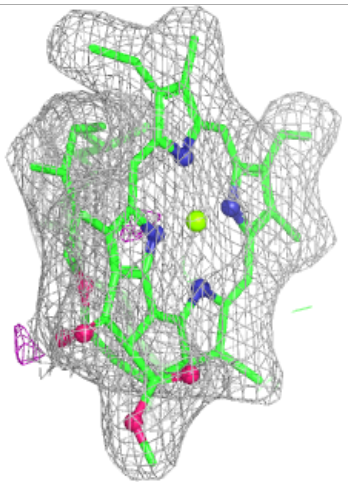


Electron density around CLA H 613:

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

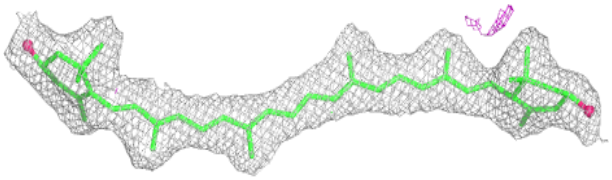


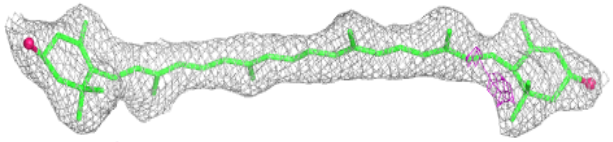


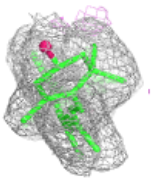


Electron density around LUT B 1620:

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

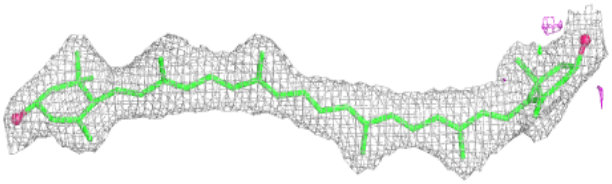


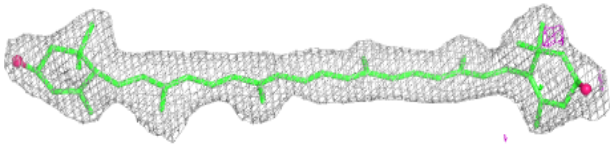


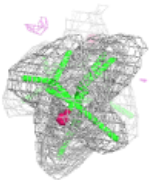


Electron density around LUT I 8621:

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

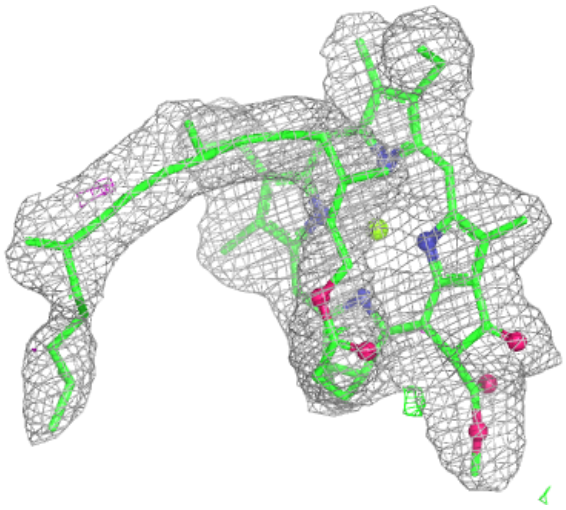


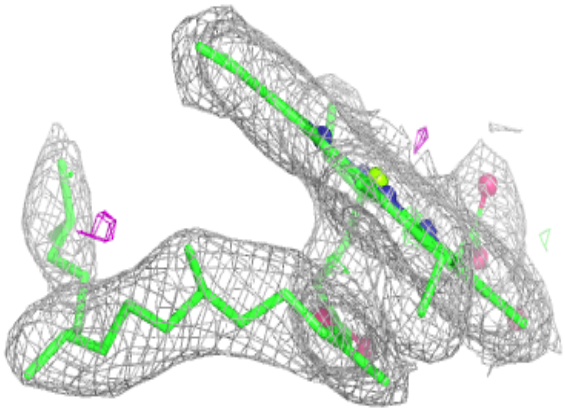


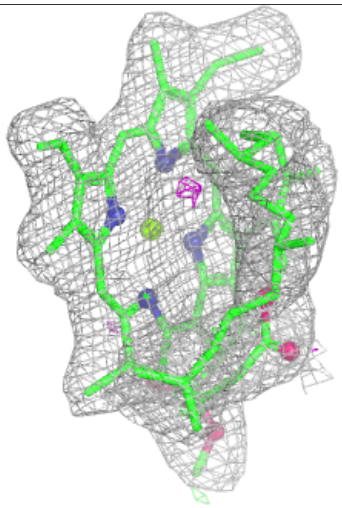


Electron density around CLA G 613:

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

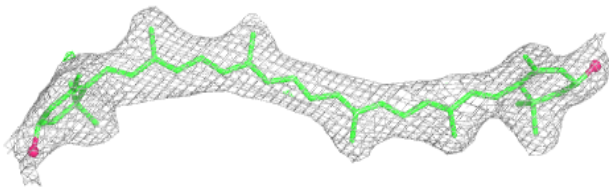


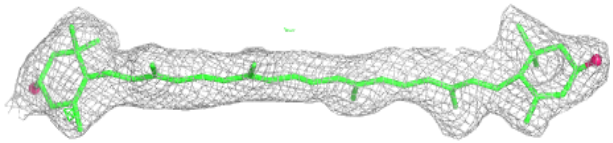


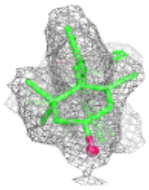


Electron density around LUT C 2621:

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

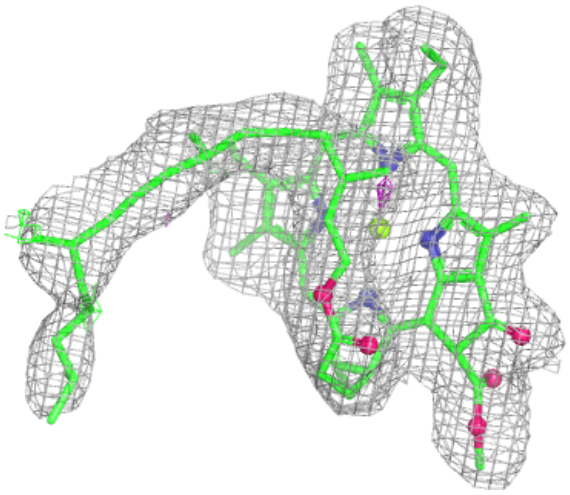


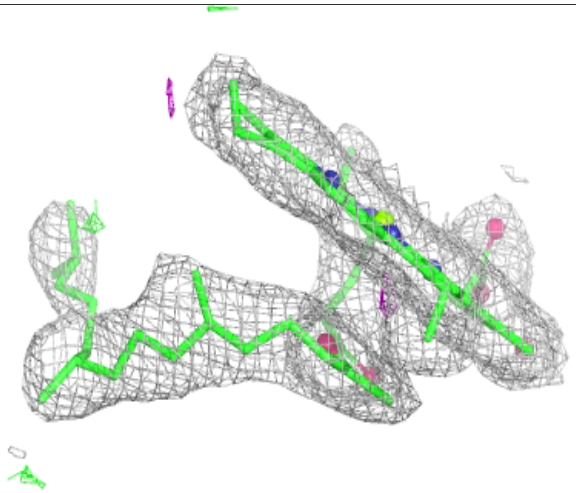


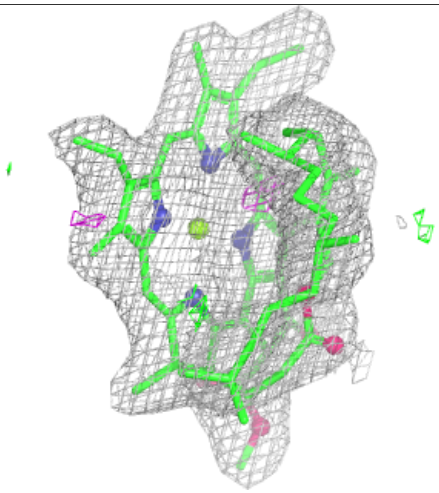


Electron density around CLA J 613:

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

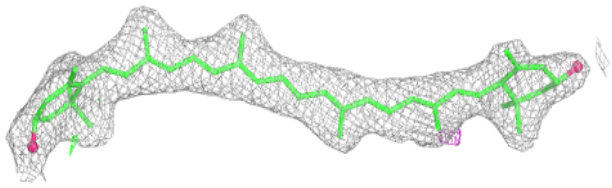


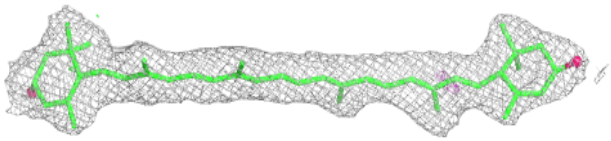


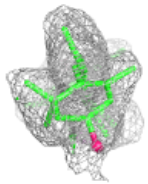


Electron density around LUT E 4621:

$2mF_o$-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.