



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:37 AM BST

PDB ID : 1RWT
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

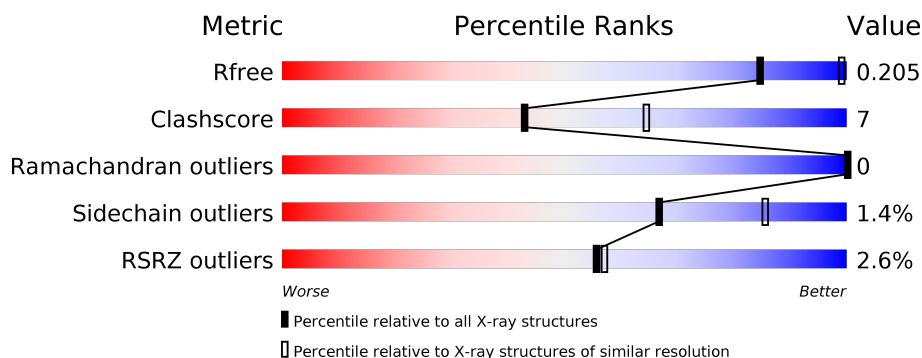
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>6%</div> </div> </div>
1	B	232	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>6%</div> </div> </div>
1	C	232	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>6%</div> </div> </div>
1	D	232	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>
1	E	232	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>6%</div> </div> </div>
1	F	232	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	232	
1	H	232	
1	I	232	
1	J	232	

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	-	-	-
10	CLA	D	611	X	-	-	-
10	CLA	D	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
10	CLA	I	613	X	-	-	-
10	CLA	I	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
2	BNG	D	3633	-	-	-	X
2	BNG	G	6633	-	-	-	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	-	-	-
9	CHL	D	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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

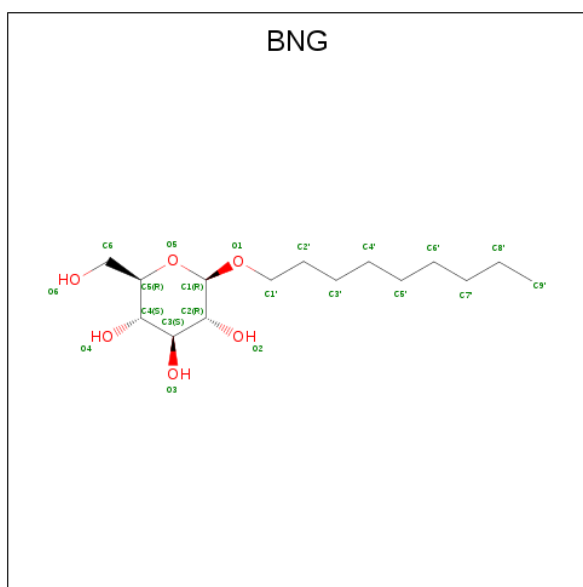
There are 11 unique types of molecules in this entry. The entry contains 29039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: BNG) (formula: C₁₅H₃₀O₆).



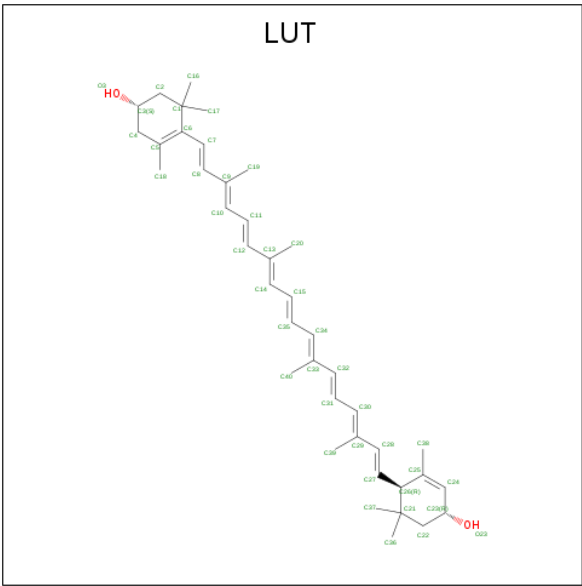
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	15	6		
2	B	1	Total	C	O	0	0
			21	15	6		
2	C	1	Total	C	O	0	0
			21	15	6		
2	D	1	Total	C	O	0	0
			21	15	6		
2	E	1	Total	C	O	0	0
			21	15	6		
2	F	1	Total	C	O	0	0
			21	15	6		
2	G	1	Total	C	O	0	0
			21	15	6		
2	H	1	Total	C	O	0	0
			21	15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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,

3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



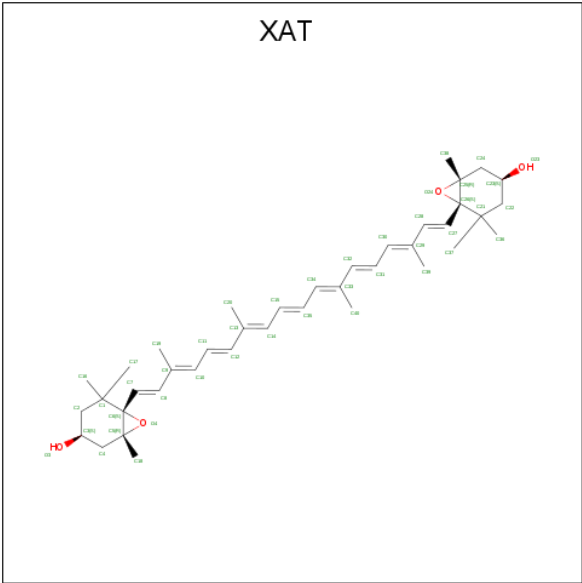
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			42	40	2		
4	A	1	Total	C	O	0	0
			42	40	2		
4	B	1	Total	C	O	0	0
			42	40	2		
4	B	1	Total	C	O	0	0
			42	40	2		
4	C	1	Total	C	O	0	0
			42	40	2		
4	C	1	Total	C	O	0	0
			42	40	2		
4	D	1	Total	C	O	0	0
			42	40	2		
4	D	1	Total	C	O	0	0
			42	40	2		
4	E	1	Total	C	O	0	0
			42	40	2		
4	E	1	Total	C	O	0	0
			42	40	2		
4	F	1	Total	C	O	0	0
			42	40	2		
4	F	1	Total	C	O	0	0
			42	40	2		
4	G	1	Total	C	O	0	0
			42	40	2		

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

- 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 (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



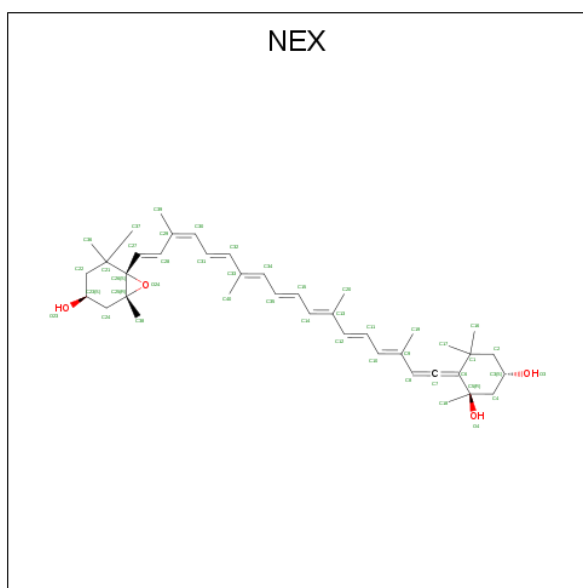
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			44	40	4		
5	B	1	Total	C	O	0	0
			44	40	4		
5	B	1	Total	C	O	0	0
			44	40	4		
5	C	1	Total	C	O	0	0
			44	40	4		

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

- 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-TETRAMETHYLOCTA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



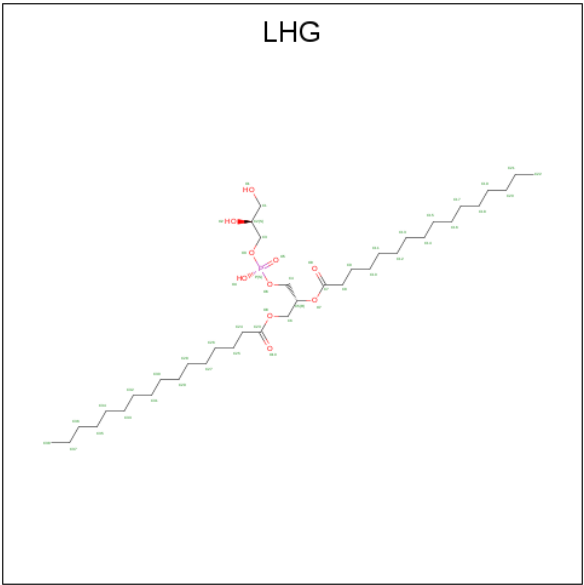
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			44	40	4		
6	B	1	Total	C	O	0	0
			44	40	4		
6	C	1	Total	C	O	0	0
			44	40	4		
6	D	1	Total	C	O	0	0
			44	40	4		

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

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



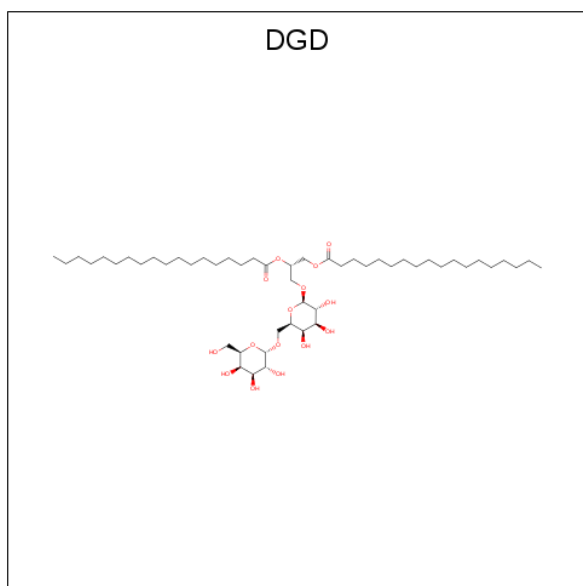
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			49	38	10	1		
7	B	1	Total	C	O	P	0	0
			49	38	10	1		
7	C	1	Total	C	O	P	0	0
			49	38	10	1		
7	D	1	Total	C	O	P	0	0
			49	38	10	1		
7	E	1	Total	C	O	P	0	0
			49	38	10	1		

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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) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



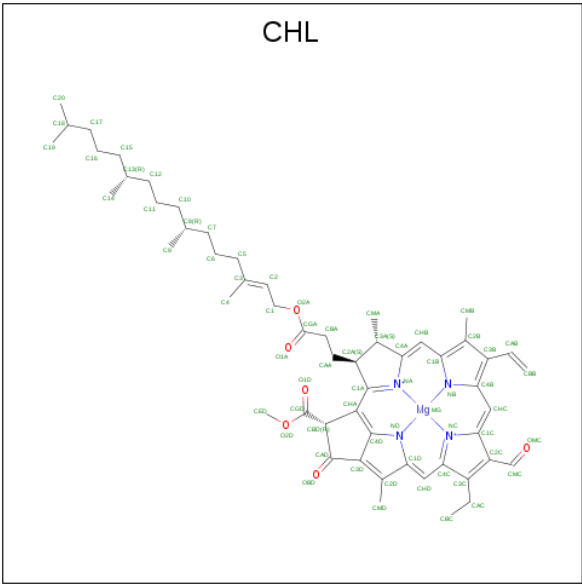
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			66	51	15		
8	B	1	Total	C	O	0	0
			66	51	15		
8	B	1	Total	C	O	0	0
			66	51	15		
8	D	1	Total	C	O	0	0
			66	51	15		
8	D	1	Total	C	O	0	0
			66	51	15		
8	E	1	Total	C	O	0	0
			66	51	15		

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

- Molecule 9 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



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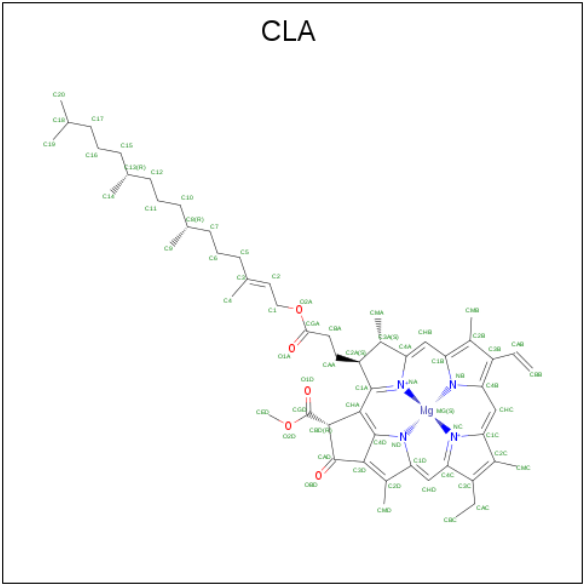
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	E	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	F	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
9	F	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
9	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	F	1	Total 66	C 55	Mg 1	N 4	O 6	0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

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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 (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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
			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 65	C 55	Mg 1	N 4	O 5	0	0
10	C	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
10	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	D	1	Total 62	C 52	Mg 1	N 4	O 5	0	0
10	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	D	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
10	E	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	E	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	E	1	Total 62	C 52	Mg 1	N 4	O 5	0	0
10	E	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	E	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	E	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	E	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
10	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
10	F	1	Total 62	C 52	Mg 1	N 4	O 5	0	0

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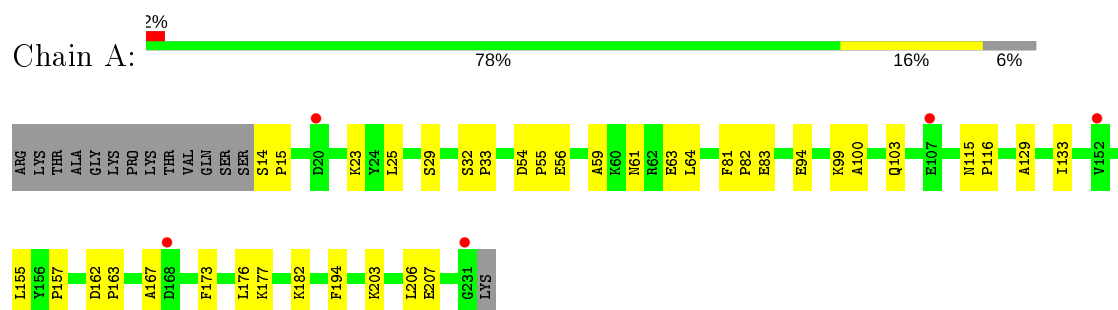
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	77	Total 77	O 77	0	0
11	E	67	Total 67	O 67	0	0
11	F	73	Total 73	O 73	0	0
11	G	71	Total 71	O 71	0	0
11	H	70	Total 70	O 70	0	0
11	I	68	Total 68	O 68	0	0
11	J	66	Total 66	O 66	0	0

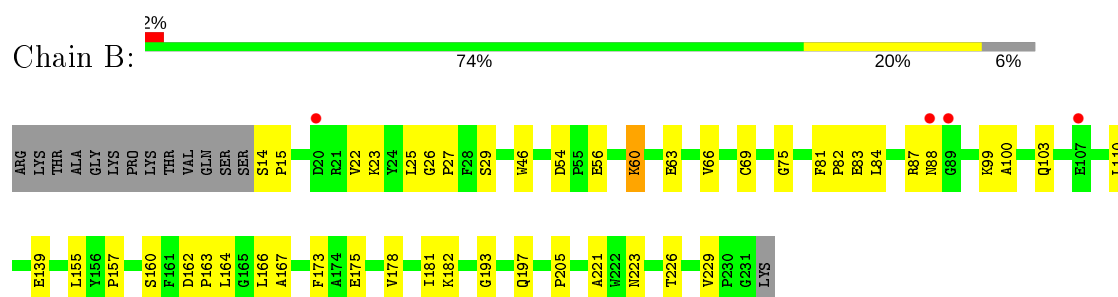
3 Residue-property plots [i](#)

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.

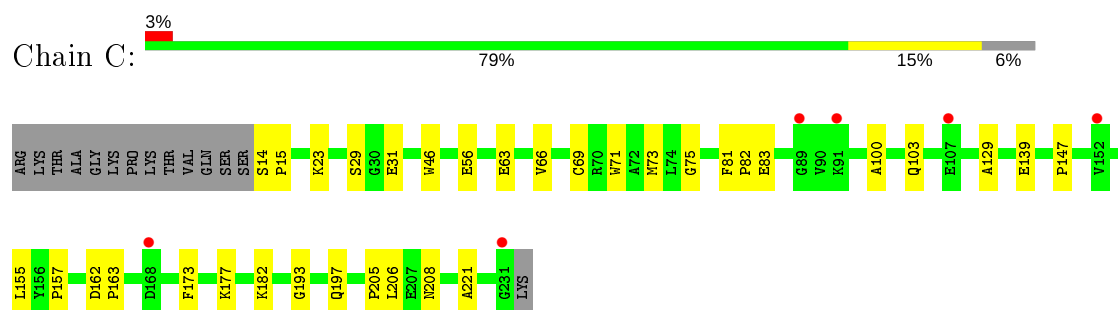
- Molecule 1: Chlorophyll A-B binding protein, chloroplast



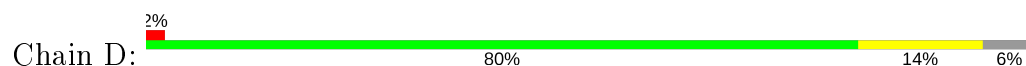
- Molecule 1: Chlorophyll A-B binding protein, chloroplast

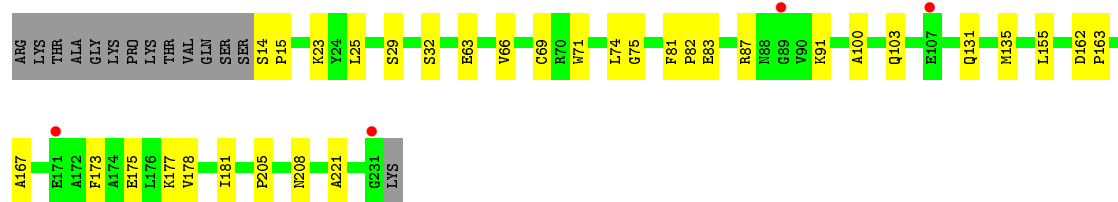


- Molecule 1: Chlorophyll A-B binding protein, chloroplast

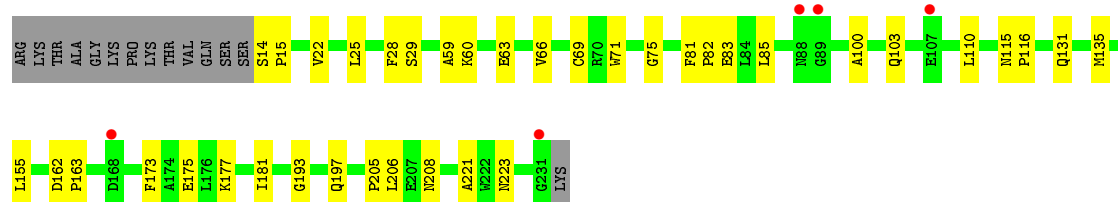
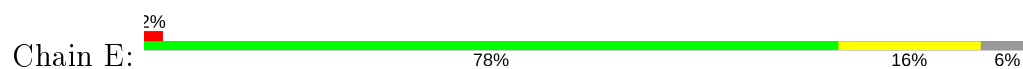


- Molecule 1: Chlorophyll A-B binding protein, chloroplast

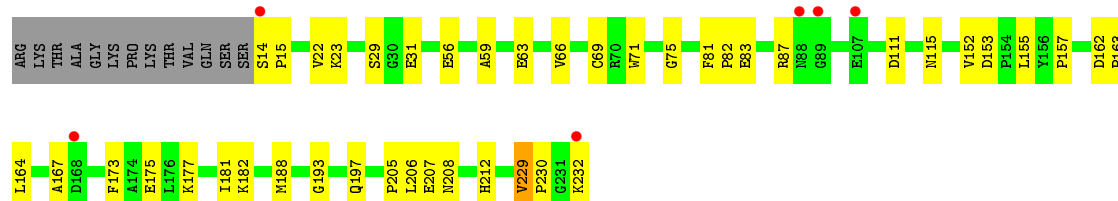
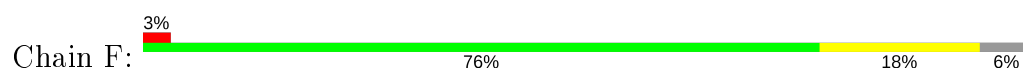




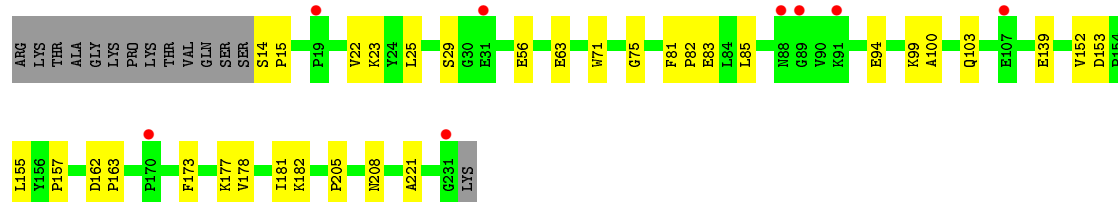
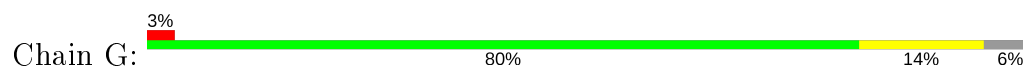
- Molecule 1: Chlorophyll A-B binding protein, chloroplast



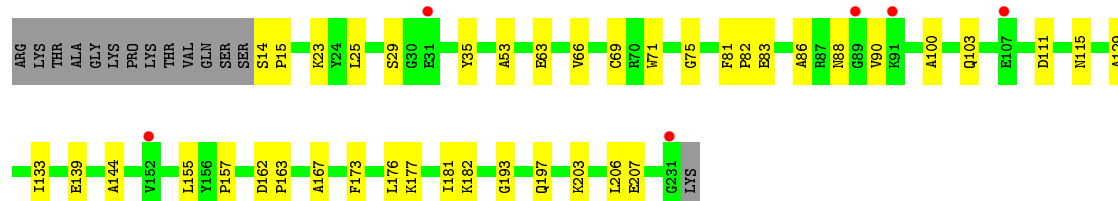
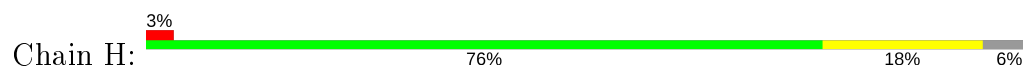
- Molecule 1: Chlorophyll A-B binding protein, chloroplast



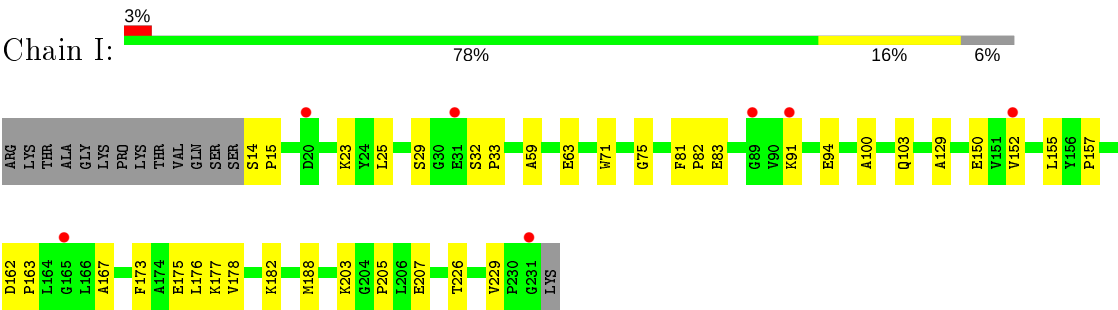
- Molecule 1: Chlorophyll A-B binding protein, chloroplast



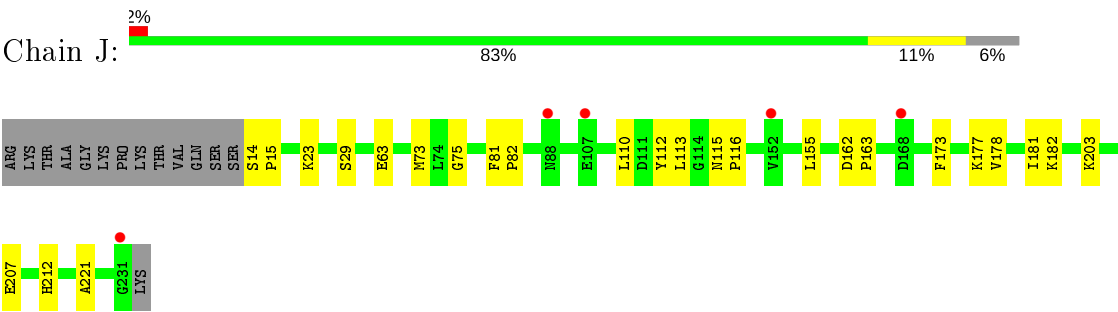
- Molecule 1: Chlorophyll A-B binding protein, chloroplast



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	261.79 Å 261.79 Å 660.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.72 25.07 – 2.71	Depositor EDS
% Data completeness (in resolution range)	83.0 (10.00-2.72) 82.8 (25.07-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.72 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.221 0.180 , 0.205	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)	0.37 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.35	0/1713	0.55	0/2333
1	B	0.37	0/1713	0.58	0/2333
1	C	0.37	0/1713	0.58	0/2333
1	D	0.37	0/1713	0.58	0/2333
1	E	0.36	0/1713	0.57	0/2333
1	F	0.37	0/1722	0.58	0/2344
1	G	0.37	0/1713	0.58	0/2333
1	H	0.36	0/1713	0.56	0/2333
1	I	0.36	0/1713	0.57	0/2333
1	J	0.36	0/1713	0.56	0/2333
All	All	0.36	0/17139	0.57	0/23341

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1661	0	1592	27	0
1	B	1661	0	1592	35	0
1	C	1661	0	1592	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1661	0	1592	21	0
1	E	1661	0	1592	26	0
1	F	1670	0	1605	30	0
1	G	1661	0	1592	27	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	3	0
4	B	84	0	112	4	0
4	C	84	0	112	2	0
4	D	84	0	112	1	0
4	E	84	0	112	3	0
4	F	84	0	112	2	0
4	G	84	0	112	1	0
4	H	84	0	112	2	0
4	I	84	0	112	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
9	A	363	0	349	4	0
9	B	363	0	349	8	0
9	C	363	0	350	5	0
9	D	363	0	349	2	0
9	E	363	0	350	3	0
9	F	363	0	350	5	0
9	G	363	0	349	9	0
9	H	363	0	350	5	0
9	I	363	0	350	5	0
9	J	363	0	350	2	0
10	A	501	0	534	12	0
10	B	501	0	532	13	0
10	C	501	0	533	14	0
10	D	501	0	532	9	0
10	E	501	0	534	10	0
10	F	501	0	534	10	0
10	G	501	0	532	12	0
10	H	501	0	534	13	0
10	I	501	0	532	10	0
10	J	501	0	533	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	388	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (388) 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
1:H:14:SER:HB2	1:H:15:PRO:HD2	1.64	0.78
1:E:60:LYS:HE2	1:E:60:LYS:HA	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
10:G:604:CLA:HBB1	10:G:604:CLA:HMB1	1.72	0.71
1:B:83:GLU:O	1:B:87:ARG:HG2	1.92	0.70
10:C:604:CLA:HBB1	10:C:604:CLA:HMB1	1.74	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
10:B:602:CLA:H93	10:B:603:CLA:HMA1	1.76	0.67
4:B:1620:LUT:H32	10:B:610:CLA:HBB1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:604:CLA:HBB1	10:J:604:CLA:HMB1	1.76	0.66
1:J:162:ASP:N	1:J:163:PRO:HD3	2.11	0.66
1:B:60:LYS:HA	1:B:60:LYS:HE3	1.78	0.65
1:G:173:PHE:CZ	1:G:177:LYS:HE3	2.31	0.65
10:H:613:CLA:HBB1	10:H:613:CLA:HMB1	1.79	0.65
10:D:604:CLA:HBB1	10:D:604:CLA:HMB1	1.79	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
10:B:604:CLA:HMB1	10:B:604:CLA:HBB1	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
10:C:613:CLA:HBB1	10:C:613:CLA:HMB1	1.79	0.63
10:F:604:CLA:HBB1	10:F:604:CLA:HMB1	1.81	0.63
10:F:613:CLA:HBB1	10:F:613:CLA:HMB1	1.79	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
10:I:602:CLA:H93	10:I:603:CLA:HMA1	1.80	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
10:G:613:CLA:HMB1	10:G:613:CLA:HBB1	1.82	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: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
10:I:604:CLA:HBB1	10:I:604:CLA:HMB1	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
10:I:613:CLA:HBB1	10:I:613:CLA:HMB1	1.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:GLU:OE1	1:D:205:PRO:HD2	2.01	0.59
10:G:602:CLA:H93	10:G:603:CLA:HMA1	1.85	0.59
1:J:182:LYS:HE2	10:J:611:CLA:O1D	2.01	0.59
10:A:602:CLA:H93	10:A:603:CLA:HMA1	1.85	0.59
10:A:604:CLA:HBB1	10:A:604:CLA:HMB1	1.85	0.59
1:J:14:SER:HB2	1:J:15:PRO:HD2	1.85	0.59
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: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
10:E:604:CLA:HMB1	10:E:604:CLA:HBB1	1.86	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:G:100:ALA:O	1:G:103:GLN:HG3	2.05	0.56
1:E:63:GLU:HA	1:E:155:LEU:HD21	1.85	0.56
10:D:613:CLA:HBB1	10:D:613:CLA:HMB1	1.87	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: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:H262	7:G:6630:LHG:HC62	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
1:H:203:LYS:HD3	1:H:207:GLU:OE2	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:602:CLA:H93	10:D:603:CLA:HMA1	1.90	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
1:C:75:GLY:HA2	4:C:2621:LUT:H181	1.91	0.53
10:E:611:CLA:HBA1	10:E:612:CLA:OBD	2.09	0.53
1:C:71:TRP:CD1	9:C:609:CHL:HMD3	2.43	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
10:F:602:CLA:H93	10:F:603:CLA:HMA1	1.91	0.53
1:J:75:GLY:HA2	4:J:9621:LUT:H181	1.91	0.53
10:E:602:CLA:H93	10:E:603:CLA:HMA1	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:E:75:GLY:HA2	4:E:4621:LUT:H181	1.91	0.52
10:H:602:CLA:H93	10:H:603:CLA:HMA1	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:D:71:TRP:CD1	9:D:609:CHL:HMD3	2.45	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
9:I:601:CHL:HBB1	9:I:601:CHL:HHC	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
1:C:182:LYS:HE2	10:C:611:CLA:O1D	2.12	0.50
10:A:603:CLA:HHC	10:A:603:CLA:HBB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:613:CLA:HBB1	10:B:613:CLA:HMB1	1.94	0.50
10:A:611:CLA:HBA1	10:A:612:CLA:OBD	2.12	0.49
1:C:14:SER:HB2	1:C:15:PRO:CD	2.42	0.49
7:I:8630:LHG:H262	7:I:8630:LHG:HC62	1.93	0.49
1:A:14:SER:HB2	1:A:15:PRO:HD2	1.95	0.49
7:A:630:LHG:HC62	7:A:630:LHG:H262	1.94	0.49
10:D:602:CLA:H92	10:J:603:CLA:H52	1.95	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:F:71:TRP:CD1	9:F:609:CHL:HMD3	2.47	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:HBB1	10:B:603:CLA:HHC	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
10:C:602:CLA:H93	10:C:603:CLA:HMA1	1.93	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:71:TRP:CD1	9:G:609:CHL:HMD3	2.49	0.48
1:G:75:GLY:HA2	4:G:6621:LUT:H181	1.95	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
1:H:129:ALA:O	1:H:133:ILE:HG12	2.13	0.47
10:J:602:CLA:H93	10:J:603:CLA:HMA1	1.96	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:HBB1	10:H:612:CLA:HHC	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
10:I:603:CLA:H52	10:J:602:CLA:H92	1.97	0.47
9:A:601:CHL:HBB1	9:A:601:CHL:HHC	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HBB1	10:H:611:CLA:HHC	1.95	0.47
1:D:100:ALA:O	1:D:103:GLN:HG3	2.14	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: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:HBB1	10:G:611:CLA:HHC	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:HBA1	9:I:606:CHL:HBD	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
1:A:59:ALA:O	1:A:63:GLU:HG3	2.16	0.45
1:E:71:TRP:CD1	9:E:609:CHL:HMD3	2.52	0.45
1:A:157:PRO:HD2	10:A:610:CLA:OBD	2.16	0.45
1:H:203:LYS:HD3	1:H:207:GLU:CD	2.36	0.45
10:B:611:CLA:HBA1	10:B:612:CLA:OBD	2.17	0.45
9:D:601:CHL:HBB1	9:D:601:CHL:HHC	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:B:157:PRO:CG	9:B:608:CHL:HMD2	2.47	0.45
1:C:100:ALA:O	1:C:103:GLN:HG3	2.17	0.45
1:E:110:LEU:HD23	1:E:110:LEU:C	2.38	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:HBB1	9:H:605:CHL:HHC	1.98	0.45
1:A:163:PRO:HD2	4:A:620:LUT:H23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1630:LHG:H262	7:B:1630:LHG:HC62	1.99	0.44
1:B:46:TRP:CE3	4:B:1621:LUT:H383	2.52	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:HBB1	9:H:601:CHL:HHC	1.98	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:182:LYS:NZ	7:B:1630:LHG:O5	2.51	0.44
1:B:167:ALA:HB1	1:B:173:PHE:CD1	2.52	0.44
1:B:26:GLY:HA3	1:B:27:PRO:HD3	1.86	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
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:HA	1:H:139:GLU:OE2	2.18	0.43
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:HBB1	10:B:611:CLA:HHC	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:110:LEU:C	1:J:110:LEU:HD23	2.39	0.43
7:F:5630:LHG:H262	7:F:5630:LHG:HC62	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:HBB1	10:J:612:CLA:HHC	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:HBB1	10:E:612:CLA:HHC	2.00	0.43
1:G:205:PRO:O	1:G:208:ASN:HB2	2.19	0.43
1:G:23:LYS:HE2	11:G:9702:HOH:O	2.18	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
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:H:100:ALA:O	1:H:103:GLN:HG3	2.19	0.43
10:A:602:CLA:HMB1	10:A:602:CLA:HAB	1.85	0.42
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:H:71:TRP:CD1	9:H:609:CHL:HMD3	2.54	0.42
9:B:605:CHL:HAB	9:B:605:CHL:HMB1	1.87	0.42
1:C:162:ASP:N	1:C:163:PRO:CD	2.81	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:I:188:MET:HB2	10:I:602:CLA:HMC3	2.02	0.42
1:H:86:ALA:C	1:H:88:ASN:H	2.22	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
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
1:H:157:PRO:CG	9:H:608:CHL:HMD2	2.50	0.42
10:C:611:CLA:HBB1	10:C:611:CLA:HHC	2.00	0.42
9:F:601:CHL:HBB1	9:F:601:CHL:HHC	2.01	0.42
1:I:71:TRP:CD1	9:I:609:CHL:HMD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:73:MET:SD	10:J:610:CLA:HBB1	2.60	0.42
7:D:3630:LHG:HC62	7:D:3630:LHG:H262	2.01	0.42
1:G:157:PRO:CG	9:G:608:CHL:HMD2	2.50	0.42
1:G:173:PHE:CE1	1:G:177:LYS:HE3	2.55	0.42
1:C:129:ALA:HB1	8:H:6632:DGD:HAE2	2.01	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: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: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:HBB1	9:E:605:CHL:HHC	2.02	0.41
1:F:155:LEU:C	1:F:157:PRO:HD3	2.40	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:111:ASP:HB3	1:H:115:ASN:O	2.20	0.41
1:H:83:GLU:HG2	1:H:206:LEU:HD12	2.03	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:162:ASP:N	1:H:163:PRO:CD	2.82	0.41
1:H:66:VAL:O	1:H:69:CYS:HB2	2.20	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
10:E:613:CLA:H8	10:E:614:CLA:HMD1	2.01	0.41
1:E:81:PHE:CE2	1:E:85:LEU:HD11	2.55	0.41
1:B:110:LEU:HD23	1:B:110:LEU:C	2.41	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:F:188:MET:HB2	10:F:602:CLA:HMC3	2.02	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:A:54:ASP:HA	1:A:55:PRO:HD3	1.94	0.41
10:B:602:CLA:H92	10:G:603:CLA:H52	2.02	0.41
1:B:166:LEU:HD12	10:B:610:CLA:CGA	2.51	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:HBB1	10:G:603:CLA:HHC	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:610:CLA:HAB	10:G:610:CLA:HMB1	1.90	0.41
9:A:608:CHL:HBB1	9:A:608:CHL:HHC	2.03	0.41
1:E:162:ASP:N	1:E:163:PRO:CD	2.84	0.41
10:F:610:CLA:HMB1	10:F:610:CLA:HAB	1.90	0.41
1:G:139:GLU:HG3	9:G:609:CHL:NB	2.36	0.41
1:G:81:PHE:CE2	1:G:85:LEU:HD11	2.56	0.41
9:J:605:CHL:HMB1	9:J:605:CHL:HAB	1.90	0.41
1:A:32:SER:HB2	1:A:33:PRO:CD	2.51	0.41
1:B:155:LEU:C	1:B:157:PRO:HD3	2.42	0.41
1:B:178:VAL:O	1:B:182:LYS:HG3	2.21	0.41
10:C:602:CLA:HAB	10:C:602:CLA:HMB1	1.90	0.41
1:D:221:ALA:CB	5:J:3622:XAT:H193	2.51	0.41
1:A:129:ALA:O	1:A:133:ILE:HG12	2.21	0.41
10:D:610:CLA:HAB	10:D:610:CLA:HMB1	1.91	0.40
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
1:C:155:LEU:C	1:C:157:PRO:HD3	2.41	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: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:226:THR:O	1:B:229:VAL:HG23	2.21	0.40
1:B:22:VAL:HB	9:B:601:CHL:CBC	2.52	0.40
10:C:612:CLA:HBB1	10:C:612:CLA:HHC	2.04	0.40
1:E:66:VAL:O	1:E:69:CYS:HB2	2.22	0.40
1:G:152:VAL:HB	1:G:153:ASP:H	1.69	0.40
10:G:611:CLA:HMB1	10:G:611:CLA:HAB	1.93	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:HA	1:I:150:GLU:OE2	2.21	0.40
1:C:73:MET:SD	10:C:610:CLA:HBB1	2.62	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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%)	167 (99%)	1 (1%)	86	94
1	B	168/180 (93%)	165 (98%)	3 (2%)	59	82
1	C	168/180 (93%)	166 (99%)	2 (1%)	71	88
1	D	168/180 (93%)	165 (98%)	3 (2%)	59	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	168/180 (93%)	165 (98%)	3 (2%)	59	82
1	F	169/180 (94%)	165 (98%)	4 (2%)	49	76
1	G	168/180 (93%)	166 (99%)	2 (1%)	71	88
1	H	168/180 (93%)	167 (99%)	1 (1%)	86	94
1	I	168/180 (93%)	165 (98%)	3 (2%)	59	82
1	J	168/180 (93%)	167 (99%)	1 (1%)	86	94
All	All	1681/1800 (93%)	1658 (99%)	23 (1%)	67	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	B	60	LYS
1	B	175	GLU
1	B	223	ASN
1	C	31	GLU
1	C	56	GLU
1	D	32	SER
1	D	91	LYS
1	D	175	GLU
1	E	175	GLU
1	E	181	ILE
1	E	223	ASN
1	F	31	GLU
1	F	56	GLU
1	F	175	GLU
1	F	229	VAL
1	G	56	GLU
1	G	181	ILE
1	H	181	ILE
1	I	91	LYS
1	I	152	VAL
1	I	175	GLU
1	J	181	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	B	611	7	59,73,73	1.55	9 (15%)	67,113,113	2.21	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CHL	G	601	1	60,74,74	1.48	9 (15%)	64,114,114	2.09	12 (18%)
4	LUT	D	3620	-	42,43,43	0.91	3 (7%)	51,60,60	1.56	7 (13%)
10	CLA	F	611	7	59,73,73	1.57	9 (15%)	67,113,113	2.06	19 (28%)
9	CHL	D	609	1	60,74,74	1.52	10 (16%)	64,114,114	2.03	13 (20%)
4	LUT	F	5620	-	42,43,43	0.86	3 (7%)	51,60,60	1.47	7 (13%)
9	CHL	H	607	11	60,74,74	1.57	9 (15%)	64,114,114	2.26	18 (28%)
10	CLA	A	610	1	59,73,73	1.60	10 (16%)	67,113,113	1.90	13 (19%)
9	CHL	J	608	11	60,74,74	1.51	11 (18%)	64,114,114	1.95	14 (21%)
10	CLA	G	614	1	43,57,73	1.86	9 (20%)	46,93,113	2.30	13 (28%)
10	CLA	F	610	1	59,73,73	1.70	10 (16%)	67,113,113	1.84	12 (17%)
6	NEX	D	3623	-	38,46,46	1.00	2 (5%)	50,70,70	1.12	5 (10%)
10	CLA	A	602	1	59,73,73	1.56	10 (16%)	67,113,113	2.18	24 (35%)
10	CLA	G	610	1	59,73,73	1.58	10 (16%)	67,113,113	1.96	15 (22%)
2	BNG	J	9633	-	21,21,21	0.52	0	26,26,26	0.80	1 (3%)
9	CHL	C	605	1	42,56,74	1.78	9 (21%)	42,92,114	2.22	13 (30%)
9	CHL	H	601	1	60,74,74	1.50	9 (15%)	64,114,114	2.06	16 (25%)
9	CHL	B	608	11	60,74,74	1.53	9 (15%)	64,114,114	2.14	19 (29%)
9	CHL	D	608	11	60,74,74	1.48	11 (18%)	64,114,114	2.05	13 (20%)
9	CHL	D	606	11	45,59,74	1.88	11 (24%)	46,96,114	2.70	18 (39%)
6	NEX	B	1623	-	38,46,46	0.90	1 (2%)	50,70,70	1.17	5 (10%)
9	CHL	F	609	1	60,74,74	1.51	11 (18%)	64,114,114	1.99	16 (25%)
10	CLA	B	603	1	59,73,73	1.57	11 (18%)	67,113,113	2.04	17 (25%)
9	CHL	I	608	11	60,74,74	1.51	9 (15%)	64,114,114	1.96	13 (20%)
10	CLA	I	604	11	56,70,73	1.49	8 (14%)	63,109,113	2.45	19 (30%)
10	CLA	C	610	1	59,73,73	1.70	11 (18%)	67,113,113	1.86	16 (23%)
8	DGD	I	8632	-	67,67,67	0.92	1 (1%)	81,81,81	1.00	8 (9%)
10	CLA	D	611	7	59,73,73	1.51	8 (13%)	67,113,113	2.16	19 (28%)
10	CLA	F	602	1	59,73,73	1.59	12 (20%)	67,113,113	2.23	23 (34%)
10	CLA	H	611	7	59,73,73	1.55	9 (15%)	67,113,113	2.09	16 (23%)
7	LHG	E	4630	10	48,48,48	0.90	3 (6%)	51,54,54	1.32	5 (9%)
6	NEX	E	4623	-	38,46,46	0.97	1 (2%)	50,70,70	1.11	4 (8%)
7	LHG	F	5630	10	48,48,48	1.02	3 (6%)	51,54,54	1.32	5 (9%)
10	CLA	C	611	7	59,73,73	1.53	10 (16%)	67,113,113	2.11	15 (22%)
10	CLA	J	612	1	59,73,73	1.60	10 (16%)	67,113,113	1.99	19 (28%)
7	LHG	H	7630	10	48,48,48	0.92	3 (6%)	51,54,54	1.33	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	G	602	1	59,73,73	1.58	13 (22%)	67,113,113	2.24	24 (35%)
9	CHL	I	601	1	60,74,74	1.42	10 (16%)	64,114,114	2.05	14 (21%)
4	LUT	E	4621	-	42,43,43	1.08	4 (9%)	51,60,60	1.41	6 (11%)
10	CLA	B	614	1	43,57,73	1.80	9 (20%)	46,93,113	2.39	12 (26%)
9	CHL	H	606	11	45,59,74	1.81	11 (24%)	46,96,114	2.52	14 (30%)
10	CLA	J	604	11	56,70,73	1.52	8 (14%)	63,109,113	2.46	19 (30%)
10	CLA	H	614	1	43,57,73	1.77	7 (16%)	46,93,113	2.38	14 (30%)
8	DGD	D	5632	-	67,67,67	0.95	1 (1%)	81,81,81	1.09	9 (11%)
10	CLA	E	604	11	56,70,73	1.52	10 (17%)	63,109,113	2.33	17 (26%)
6	NEX	F	5623	-	38,46,46	0.97	2 (5%)	50,70,70	1.20	6 (12%)
10	CLA	G	604	11	56,70,73	1.50	10 (17%)	63,109,113	2.36	19 (30%)
8	DGD	E	4632	-	67,67,67	0.97	1 (1%)	81,81,81	1.05	8 (9%)
10	CLA	F	603	1	59,73,73	1.66	11 (18%)	67,113,113	2.03	18 (26%)
2	BNG	A	633	-	21,21,21	0.56	0	26,26,26	0.79	1 (3%)
9	CHL	A	607	11	60,74,74	1.51	9 (15%)	64,114,114	2.30	17 (26%)
10	CLA	I	602	1	59,73,73	1.57	13 (22%)	67,113,113	2.34	23 (34%)
4	LUT	F	5621	-	42,43,43	1.04	4 (9%)	51,60,60	1.56	8 (15%)
9	CHL	F	607	11	60,74,74	1.60	7 (11%)	64,114,114	2.35	22 (34%)
2	BNG	G	6633	-	21,21,21	0.53	0	26,26,26	0.79	1 (3%)
10	CLA	B	602	1	59,73,73	1.59	12 (20%)	67,113,113	2.28	21 (31%)
9	CHL	C	609	1	60,74,74	1.58	11 (18%)	64,114,114	2.00	12 (18%)
2	BNG	B	1633	-	21,21,21	0.50	0	26,26,26	0.81	1 (3%)
5	XAT	H	4622	-	39,47,47	0.74	0	54,74,74	1.34	5 (9%)
10	CLA	C	612	1	59,73,73	1.57	9 (15%)	67,113,113	1.97	16 (23%)
10	CLA	A	612	1	59,73,73	1.67	10 (16%)	67,113,113	1.96	16 (23%)
4	LUT	H	7621	-	42,43,43	0.98	4 (9%)	51,60,60	1.47	6 (11%)
10	CLA	D	604	11	56,70,73	1.50	8 (14%)	63,109,113	2.54	19 (30%)
4	LUT	C	2620	-	42,43,43	0.92	3 (7%)	51,60,60	1.43	6 (11%)
10	CLA	J	602	1	59,73,73	1.55	11 (18%)	67,113,113	2.33	23 (34%)
8	DGD	G	9632	-	67,67,67	1.05	2 (2%)	81,81,81	1.07	8 (9%)
10	CLA	I	614	1	43,57,73	1.76	10 (23%)	46,93,113	2.33	12 (26%)
10	CLA	H	610	1	59,73,73	1.64	11 (18%)	67,113,113	1.91	18 (26%)
9	CHL	A	609	1	60,74,74	1.55	10 (16%)	64,114,114	1.96	13 (20%)
10	CLA	I	613	1	59,73,73	1.52	9 (15%)	67,113,113	2.20	14 (20%)
9	CHL	C	601	1	60,74,74	1.46	10 (16%)	64,114,114	2.00	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CHL	E	601	1	60,74,74	1.55	10 (16%)	64,114,114	2.04	16 (25%)
9	CHL	A	608	11	60,74,74	1.54	9 (15%)	64,114,114	2.10	16 (25%)
9	CHL	F	605	1	42,56,74	1.79	7 (16%)	42,92,114	2.19	11 (26%)
10	CLA	F	613	1	59,73,73	1.56	11 (18%)	67,113,113	2.13	14 (20%)
7	LHG	J	9630	10	48,48,48	0.97	3 (6%)	51,54,54	1.34	5 (9%)
10	CLA	E	602	1	59,73,73	1.60	12 (20%)	67,113,113	2.14	21 (31%)
9	CHL	G	609	1	60,74,74	1.50	12 (20%)	64,114,114	1.88	13 (20%)
10	CLA	E	603	1	59,73,73	1.58	11 (18%)	67,113,113	1.93	18 (26%)
10	CLA	D	610	1	59,73,73	1.68	9 (15%)	67,113,113	1.96	15 (22%)
10	CLA	J	610	1	59,73,73	1.60	10 (16%)	67,113,113	1.91	16 (23%)
5	XAT	D	8622	-	39,47,47	0.71	1 (2%)	54,74,74	1.26	6 (11%)
10	CLA	B	604	11	56,70,73	1.52	7 (12%)	63,109,113	2.55	22 (34%)
10	CLA	A	604	11	56,70,73	1.55	9 (16%)	63,109,113	2.36	15 (23%)
9	CHL	A	605	1	42,56,74	1.81	8 (19%)	42,92,114	2.14	11 (26%)
10	CLA	B	613	1	59,73,73	1.54	11 (18%)	67,113,113	2.19	16 (23%)
7	LHG	C	2630	10	48,48,48	0.94	3 (6%)	51,54,54	1.34	5 (9%)
5	XAT	C	7622	-	39,47,47	0.76	1 (2%)	54,74,74	1.26	5 (9%)
4	LUT	E	4620	-	42,43,43	1.03	4 (9%)	51,60,60	1.55	6 (11%)
10	CLA	D	613	1	59,73,73	1.62	12 (20%)	67,113,113	2.22	14 (20%)
10	CLA	I	610	1	59,73,73	1.66	11 (18%)	67,113,113	1.82	14 (20%)
4	LUT	J	9621	-	42,43,43	1.02	4 (9%)	51,60,60	1.56	7 (13%)
9	CHL	C	606	11	45,59,74	1.89	10 (22%)	46,96,114	2.59	17 (36%)
10	CLA	J	614	1	43,57,73	1.75	8 (18%)	46,93,113	2.24	12 (26%)
9	CHL	E	606	11	45,59,74	1.81	11 (24%)	46,96,114	2.64	15 (32%)
6	NEX	C	2623	-	38,46,46	1.01	2 (5%)	50,70,70	1.13	3 (6%)
10	CLA	J	611	7	59,73,73	1.52	9 (15%)	67,113,113	2.12	17 (25%)
10	CLA	A	611	7	59,73,73	1.57	10 (16%)	67,113,113	2.16	19 (28%)
10	CLA	J	613	1	59,73,73	1.60	12 (20%)	67,113,113	1.96	14 (20%)
9	CHL	F	606	11	45,59,74	1.91	10 (22%)	46,96,114	2.53	15 (32%)
10	CLA	I	603	1	59,73,73	1.59	10 (16%)	67,113,113	1.88	17 (25%)
4	LUT	J	9620	-	42,43,43	0.99	4 (9%)	51,60,60	1.52	5 (9%)
10	CLA	E	611	7	59,73,73	1.62	10 (16%)	67,113,113	2.09	17 (25%)
10	CLA	C	602	1	59,73,73	1.62	10 (16%)	67,113,113	2.19	22 (32%)
2	BNG	I	8633	-	21,21,21	0.54	0	26,26,26	0.76	1 (3%)
5	XAT	J	3622	-	39,47,47	0.72	1 (2%)	54,74,74	1.21	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	LHG	G	6630	10	48,48,48	0.98	3 (6%)	51,54,54	1.39	5 (9%)
10	CLA	G	612	1	59,73,73	1.61	11 (18%)	67,113,113	2.03	16 (23%)
4	LUT	G	6620	-	42,43,43	0.94	4 (9%)	51,60,60	1.48	8 (15%)
4	LUT	D	3621	-	42,43,43	1.08	4 (9%)	51,60,60	1.43	9 (17%)
9	CHL	I	609	1	60,74,74	1.62	10 (16%)	64,114,114	2.05	15 (23%)
9	CHL	F	608	11	60,74,74	1.50	10 (16%)	64,114,114	2.15	18 (28%)
10	CLA	H	612	1	59,73,73	1.65	12 (20%)	67,113,113	1.99	18 (26%)
10	CLA	D	603	1	59,73,73	1.51	9 (15%)	67,113,113	1.93	18 (26%)
10	CLA	I	611	7	59,73,73	1.61	9 (15%)	67,113,113	2.04	20 (29%)
7	LHG	B	1630	10	48,48,48	1.02	3 (6%)	51,54,54	1.32	5 (9%)
9	CHL	E	607	11	60,74,74	1.50	9 (15%)	64,114,114	2.33	18 (28%)
4	LUT	A	620	-	42,43,43	0.93	4 (9%)	51,60,60	1.55	7 (13%)
10	CLA	G	613	1	59,73,73	1.53	11 (18%)	67,113,113	2.21	14 (20%)
9	CHL	H	605	1	42,56,74	1.78	8 (19%)	42,92,114	2.06	12 (28%)
10	CLA	G	603	1	59,73,73	1.57	11 (18%)	67,113,113	2.04	16 (23%)
2	BNG	C	2633	-	21,21,21	0.54	0	26,26,26	0.79	1 (3%)
9	CHL	G	607	11	60,74,74	1.48	9 (15%)	64,114,114	2.31	19 (29%)
9	CHL	E	605	1	42,56,74	1.68	9 (21%)	42,92,114	2.21	11 (26%)
5	XAT	A	622	-	39,47,47	0.62	0	54,74,74	1.18	3 (5%)
10	CLA	B	610	1	59,73,73	1.59	11 (18%)	67,113,113	1.85	13 (19%)
9	CHL	C	607	11	60,74,74	1.53	9 (15%)	64,114,114	2.34	21 (32%)
10	CLA	C	614	1	43,57,73	1.81	10 (23%)	46,93,113	2.38	14 (30%)
9	CHL	E	609	1	60,74,74	1.50	11 (18%)	64,114,114	1.96	11 (17%)
10	CLA	A	614	1	43,57,73	1.78	9 (20%)	46,93,113	2.31	12 (26%)
9	CHL	G	606	11	45,59,74	1.94	10 (22%)	46,96,114	2.47	12 (26%)
5	XAT	B	5622	-	39,47,47	0.72	0	54,74,74	1.22	5 (9%)
2	BNG	F	5633	-	21,21,21	0.54	0	26,26,26	0.79	1 (3%)
9	CHL	A	601	1	60,74,74	1.43	9 (15%)	64,114,114	2.09	15 (23%)
9	CHL	B	601	1	60,74,74	1.42	8 (13%)	64,114,114	2.01	15 (23%)
10	CLA	H	602	1	59,73,73	1.65	11 (18%)	67,113,113	2.22	26 (38%)
8	DGD	H	7632	-	67,67,67	0.94	2 (2%)	81,81,81	1.00	8 (9%)
10	CLA	E	610	1	59,73,73	1.68	11 (18%)	67,113,113	1.87	13 (19%)
9	CHL	I	606	11	45,59,74	1.81	9 (20%)	46,96,114	2.59	13 (28%)
9	CHL	H	609	1	60,74,74	1.51	10 (16%)	64,114,114	1.99	14 (21%)
10	CLA	A	613	1	59,73,73	1.55	13 (22%)	67,113,113	1.94	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CHL	A	606	11	45,59,74	1.81	9 (20%)	46,96,114	2.52	17 (36%)
7	LHG	A	630	10	48,48,48	0.92	3 (6%)	51,54,54	1.41	6 (11%)
10	CLA	C	603	1	59,73,73	1.58	11 (18%)	67,113,113	2.04	17 (25%)
9	CHL	D	601	1	60,74,74	1.43	10 (16%)	64,114,114	2.07	16 (25%)
9	CHL	F	601	1	60,74,74	1.46	9 (15%)	64,114,114	2.04	14 (21%)
10	CLA	J	603	1	59,73,73	1.68	10 (16%)	67,113,113	2.02	18 (26%)
5	XAT	E	2622	-	39,47,47	0.72	0	54,74,74	1.24	6 (11%)
4	LUT	G	6621	-	42,43,43	0.94	2 (4%)	51,60,60	1.37	7 (13%)
9	CHL	J	609	1	60,74,74	1.60	10 (16%)	64,114,114	1.89	13 (20%)
6	NEX	A	623	-	38,46,46	1.03	2 (5%)	50,70,70	1.25	5 (10%)
4	LUT	B	1621	-	42,43,43	1.03	5 (11%)	51,60,60	1.36	4 (7%)
10	CLA	I	612	1	59,73,73	1.62	10 (16%)	67,113,113	2.00	17 (25%)
10	CLA	H	604	11	56,70,73	1.46	8 (14%)	63,109,113	2.44	22 (34%)
8	DGD	B	2632	-	67,67,67	0.92	1 (1%)	81,81,81	1.05	8 (9%)
4	LUT	H	7620	-	42,43,43	0.88	2 (4%)	51,60,60	1.52	6 (11%)
9	CHL	G	605	1	42,56,74	1.77	9 (21%)	42,92,114	2.09	11 (26%)
9	CHL	B	605	1	42,56,74	1.69	9 (21%)	42,92,114	2.14	12 (28%)
9	CHL	D	605	1	42,56,74	1.81	8 (19%)	42,92,114	2.25	11 (26%)
2	BNG	E	4633	-	21,21,21	0.53	0	26,26,26	0.75	1 (3%)
9	CHL	J	607	11	60,74,74	1.41	8 (13%)	64,114,114	2.23	18 (28%)
9	CHL	B	606	11	45,59,74	1.82	10 (22%)	46,96,114	2.47	14 (30%)
8	DGD	B	1632	-	67,67,67	0.96	2 (2%)	81,81,81	1.04	8 (9%)
10	CLA	F	614	1	43,57,73	1.81	7 (16%)	46,93,113	2.27	13 (28%)
2	BNG	D	3633	-	21,21,21	0.51	0	26,26,26	0.84	1 (3%)
7	LHG	I	8630	10	48,48,48	1.02	3 (6%)	51,54,54	1.38	5 (9%)
6	NEX	H	7623	-	38,46,46	0.96	2 (5%)	50,70,70	1.20	5 (10%)
9	CHL	I	607	11	60,74,74	1.61	9 (15%)	64,114,114	2.30	20 (31%)
8	DGD	A	632	-	67,67,67	0.95	2 (2%)	81,81,81	0.97	8 (9%)
4	LUT	I	8620	-	42,43,43	0.87	4 (9%)	51,60,60	1.51	7 (13%)
9	CHL	I	605	1	42,56,74	1.79	8 (19%)	42,92,114	2.17	12 (28%)
9	CHL	J	606	11	45,59,74	1.89	10 (22%)	46,96,114	2.46	12 (26%)
10	CLA	D	612	1	59,73,73	1.64	11 (18%)	67,113,113	2.02	18 (26%)
4	LUT	I	8621	-	42,43,43	0.96	4 (9%)	51,60,60	1.53	7 (13%)
10	CLA	F	612	1	59,73,73	1.72	10 (16%)	67,113,113	2.00	16 (23%)
10	CLA	E	612	1	59,73,73	1.70	10 (16%)	67,113,113	1.91	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	C	604	11	56,70,73	1.51	10 (17%)	63,109,113	2.48	17 (26%)
10	CLA	D	602	1	59,73,73	1.61	12 (20%)	67,113,113	2.20	23 (34%)
5	XAT	B	1622	-	39,47,47	0.67	0	54,74,74	1.36	4 (7%)
6	NEX	I	8623	-	38,46,46	0.98	2 (5%)	50,70,70	1.13	4 (8%)
9	CHL	H	608	11	60,74,74	1.53	10 (16%)	64,114,114	2.09	16 (25%)
6	NEX	G	6623	-	38,46,46	0.99	2 (5%)	50,70,70	1.27	6 (12%)
2	BNG	H	7633	-	21,21,21	0.52	0	26,26,26	0.79	1 (3%)
9	CHL	J	605	1	42,56,74	1.80	9 (21%)	42,92,114	2.23	11 (26%)
5	XAT	I	9622	-	39,47,47	0.75	1 (2%)	54,74,74	1.21	4 (7%)
10	CLA	F	604	11	56,70,73	1.47	8 (14%)	63,109,113	2.42	21 (33%)
10	CLA	B	612	1	59,73,73	1.66	12 (20%)	67,113,113	1.93	16 (23%)
4	LUT	C	2621	-	42,43,43	1.20	5 (11%)	51,60,60	1.43	8 (15%)
10	CLA	H	603	1	59,73,73	1.59	10 (16%)	67,113,113	1.94	15 (22%)
9	CHL	C	608	11	60,74,74	1.53	11 (18%)	64,114,114	2.14	17 (26%)
6	NEX	J	9623	-	38,46,46	1.02	2 (5%)	50,70,70	1.17	4 (8%)
10	CLA	D	614	1	43,57,73	1.80	9 (20%)	46,93,113	2.29	12 (26%)
10	CLA	G	611	7	59,73,73	1.56	10 (16%)	67,113,113	2.15	17 (25%)
8	DGD	H	6632	-	67,67,67	0.85	1 (1%)	81,81,81	1.01	7 (8%)
10	CLA	H	613	1	59,73,73	1.50	8 (13%)	67,113,113	2.23	16 (23%)
4	LUT	B	1620	-	42,43,43	0.95	3 (7%)	51,60,60	1.42	7 (13%)
8	DGD	D	3632	-	67,67,67	0.97	2 (2%)	81,81,81	1.00	8 (9%)
10	CLA	C	613	1	59,73,73	1.50	12 (20%)	67,113,113	2.16	15 (22%)
5	XAT	F	6622	-	39,47,47	0.67	0	54,74,74	1.21	6 (11%)
10	CLA	E	613	1	59,73,73	1.60	10 (16%)	67,113,113	2.08	16 (23%)
9	CHL	J	601	1	60,74,74	1.49	12 (20%)	64,114,114	1.91	12 (18%)
9	CHL	E	608	11	60,74,74	1.53	10 (16%)	64,114,114	2.08	18 (28%)
9	CHL	G	608	11	60,74,74	1.56	10 (16%)	64,114,114	1.94	12 (18%)
10	CLA	A	603	1	59,73,73	1.58	10 (16%)	67,113,113	2.04	19 (28%)
9	CHL	D	607	11	60,74,74	1.42	10 (16%)	64,114,114	2.17	16 (25%)
10	CLA	E	614	1	43,57,73	1.81	8 (18%)	46,93,113	2.36	14 (30%)
9	CHL	B	609	1	60,74,74	1.58	12 (20%)	64,114,114	1.88	13 (20%)
9	CHL	B	607	11	60,74,74	1.52	9 (15%)	64,114,114	2.33	20 (31%)
4	LUT	A	621	-	42,43,43	1.15	5 (11%)	51,60,60	1.55	8 (15%)
7	LHG	D	3630	10	48,48,48	0.85	3 (6%)	51,54,54	1.26	5 (9%)

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	B	611	7	3/3/20/25	19/37/135/135	-
9	CHL	G	601	1	4/4/20/26	13/39/137/137	-
10	CLA	G	613	1	3/3/20/25	12/37/135/135	-
10	CLA	F	611	7	3/3/20/25	20/37/135/135	-
9	CHL	D	609	1	5/5/20/26	17/39/137/137	-
4	LUT	F	5620	-	-	1/29/67/67	0/2/2/2
9	CHL	H	607	11	3/3/20/26	13/39/137/137	-
10	CLA	A	610	1	3/3/20/25	5/37/135/135	-
10	CLA	G	614	1	3/3/16/25	5/18/116/135	-
10	CLA	F	610	1	3/3/20/25	7/37/135/135	-
6	NEX	D	3623	-	-	2/27/83/83	0/3/3/3
10	CLA	A	602	1	4/4/20/25	18/37/135/135	-
10	CLA	G	610	1	3/3/20/25	7/37/135/135	-
9	CHL	I	605	1	3/3/16/26	9/18/116/137	-
9	CHL	C	605	1	3/3/16/26	8/18/116/137	-
9	CHL	H	601	1	4/4/20/26	8/39/137/137	-
9	CHL	B	608	11	4/4/20/26	21/39/137/137	-
9	CHL	D	608	11	4/4/20/26	14/39/137/137	-
9	CHL	D	606	11	3/3/17/26	7/21/119/137	-
6	NEX	B	1623	-	-	3/27/83/83	0/3/3/3
9	CHL	F	609	1	5/5/20/26	15/39/137/137	-
10	CLA	B	603	1	4/4/20/25	15/37/135/135	-
9	CHL	I	608	11	4/4/20/26	17/39/137/137	-
10	CLA	I	604	11	3/3/19/25	11/34/132/135	-
10	CLA	C	610	1	3/3/20/25	4/37/135/135	-
8	DGD	I	8632	-	2/2/13/13	26/55/95/95	0/2/2/2
10	CLA	D	611	7	3/3/20/25	18/37/135/135	-
10	CLA	H	611	7	3/3/20/25	16/37/135/135	-
7	LHG	E	4630	10	-	35/53/53/53	-
6	NEX	E	4623	-	-	3/27/83/83	0/3/3/3
7	LHG	F	5630	10	-	32/53/53/53	-
10	CLA	C	611	7	3/3/20/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	J	612	1	3/3/20/25	14/37/135/135	-
7	LHG	H	7630	10	-	34/53/53/53	-
10	CLA	G	602	1	4/4/20/25	14/37/135/135	-
7	LHG	A	630	10	-	39/53/53/53	-
4	LUT	E	4621	-	-	2/29/67/67	0/2/2/2
10	CLA	B	614	1	3/3/16/25	5/18/116/135	-
9	CHL	H	606	11	3/3/17/26	6/21/119/137	-
6	NEX	I	8623	-	-	2/27/83/83	0/3/3/3
10	CLA	H	614	1	3/3/16/25	5/18/116/135	-
2	BNG	I	8633	-	-	9/12/32/32	0/1/1/1
8	DGD	D	5632	-	2/2/13/13	27/55/95/95	0/2/2/2
10	CLA	E	604	11	3/3/19/25	6/34/132/135	-
6	NEX	F	5623	-	-	2/27/83/83	0/3/3/3
10	CLA	G	604	11	3/3/19/25	16/34/132/135	-
8	DGD	E	4632	-	2/2/13/13	23/55/95/95	0/2/2/2
10	CLA	F	603	1	4/4/20/25	15/37/135/135	-
2	BNG	A	633	-	-	11/12/32/32	0/1/1/1
9	CHL	A	607	11	3/3/20/26	14/39/137/137	-
10	CLA	I	602	1	4/4/20/25	13/37/135/135	-
4	LUT	F	5621	-	-	2/29/67/67	0/2/2/2
9	CHL	F	607	11	3/3/20/26	16/39/137/137	-
2	BNG	G	6633	-	-	9/12/32/32	0/1/1/1
10	CLA	B	602	1	4/4/20/25	17/37/135/135	-
9	CHL	C	609	1	5/5/20/26	14/39/137/137	-
2	BNG	B	1633	-	-	11/12/32/32	0/1/1/1
5	XAT	H	4622	-	-	1/31/93/93	0/4/4/4
10	CLA	C	612	1	3/3/20/25	11/37/135/135	-
5	XAT	D	8622	-	-	1/31/93/93	0/4/4/4
10	CLA	A	612	1	3/3/20/25	15/37/135/135	-
4	LUT	H	7621	-	-	2/29/67/67	0/2/2/2
10	CLA	D	604	11	3/3/19/25	15/34/132/135	-
4	LUT	C	2620	-	-	1/29/67/67	0/2/2/2
10	CLA	J	602	1	4/4/20/25	14/37/135/135	-
4	LUT	D	3620	-	-	1/29/67/67	0/2/2/2
8	DGD	G	9632	-	2/2/13/13	28/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	I	614	1	3/3/16/25	7/18/116/135	-
10	CLA	H	610	1	4/4/20/25	9/37/135/135	-
9	CHL	A	609	1	5/5/20/26	18/39/137/137	-
10	CLA	I	613	1	3/3/20/25	11/37/135/135	-
9	CHL	C	601	1	4/4/20/26	17/39/137/137	-
9	CHL	E	601	1	4/4/20/26	14/39/137/137	-
9	CHL	A	608	11	4/4/20/26	17/39/137/137	-
9	CHL	F	605	1	3/3/16/26	6/18/116/137	-
10	CLA	F	613	1	3/3/20/25	7/37/135/135	-
7	LHG	J	9630	10	-	32/53/53/53	-
10	CLA	E	602	1	4/4/20/25	15/37/135/135	-
9	CHL	G	609	1	5/5/20/26	17/39/137/137	-
10	CLA	E	603	1	4/4/20/25	13/37/135/135	-
10	CLA	D	610	1	3/3/20/25	9/37/135/135	-
10	CLA	J	610	1	3/3/20/25	5/37/135/135	-
2	BNG	J	9633	-	-	10/12/32/32	0/1/1/1
10	CLA	B	604	11	3/3/19/25	9/34/132/135	-
10	CLA	A	604	11	3/3/19/25	11/34/132/135	-
9	CHL	A	605	1	3/3/16/26	6/18/116/137	-
10	CLA	B	613	1	3/3/20/25	8/37/135/135	-
7	LHG	C	2630	10	-	35/53/53/53	-
5	XAT	C	7622	-	-	0/31/93/93	0/4/4/4
4	LUT	E	4620	-	-	1/29/67/67	0/2/2/2
10	CLA	D	613	1	3/3/20/25	10/37/135/135	-
10	CLA	I	610	1	4/4/20/25	8/37/135/135	-
9	CHL	G	607	11	3/3/20/26	14/39/137/137	-
9	CHL	C	606	11	3/3/17/26	7/21/119/137	-
10	CLA	J	614	1	3/3/16/25	8/18/116/135	-
9	CHL	E	606	11	3/3/17/26	5/21/119/137	-
6	NEX	C	2623	-	-	2/27/83/83	0/3/3/3
10	CLA	J	611	7	3/3/20/25	18/37/135/135	-
4	LUT	G	6620	-	-	1/29/67/67	0/2/2/2
10	CLA	A	611	7	3/3/20/25	19/37/135/135	-
10	CLA	J	613	1	3/3/20/25	13/37/135/135	-
9	CHL	F	606	11	3/3/17/26	7/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	I	603	1	4/4/20/25	16/37/135/135	-
10	CLA	D	614	1	3/3/16/25	5/18/116/135	-
8	DGD	H	6632	-	2/2/13/13	33/55/95/95	0/2/2/2
10	CLA	C	602	1	4/4/20/25	14/37/135/135	-
10	CLA	E	611	7	3/3/20/25	19/37/135/135	-
5	XAT	J	3622	-	-	0/31/93/93	0/4/4/4
7	LHG	G	6630	10	-	38/53/53/53	-
10	CLA	G	612	1	3/3/20/25	13/37/135/135	-
10	CLA	C	604	11	3/3/19/25	16/34/132/135	-
4	LUT	D	3621	-	-	2/29/67/67	0/2/2/2
9	CHL	I	609	1	5/5/20/26	16/39/137/137	-
9	CHL	F	608	11	4/4/20/26	17/39/137/137	-
10	CLA	H	612	1	3/3/20/25	14/37/135/135	-
10	CLA	D	603	1	4/4/20/25	17/37/135/135	-
4	LUT	B	1620	-	-	1/29/67/67	0/2/2/2
7	LHG	B	1630	10	-	35/53/53/53	-
9	CHL	E	607	11	3/3/20/26	13/39/137/137	-
10	CLA	F	602	1	4/4/20/25	16/37/135/135	-
9	CHL	H	605	1	3/3/16/26	7/18/116/137	-
10	CLA	G	603	1	4/4/20/25	14/37/135/135	-
2	BNG	C	2633	-	-	9/12/32/32	0/1/1/1
9	CHL	E	605	1	3/3/16/26	8/18/116/137	-
5	XAT	A	622	-	-	0/31/93/93	0/4/4/4
10	CLA	B	610	1	3/3/20/25	3/37/135/135	-
9	CHL	C	607	11	3/3/20/26	15/39/137/137	-
10	CLA	C	614	1	3/3/16/25	5/18/116/135	-
9	CHL	E	609	1	5/5/20/26	17/39/137/137	-
9	CHL	G	606	11	3/3/17/26	5/21/119/137	-
5	XAT	B	5622	-	-	1/31/93/93	0/4/4/4
2	BNG	F	5633	-	-	9/12/32/32	0/1/1/1
9	CHL	A	601	1	5/5/20/26	14/39/137/137	-
9	CHL	B	601	1	4/4/20/26	13/39/137/137	-
10	CLA	H	602	1	4/4/20/25	18/37/135/135	-
8	DGD	H	7632	-	2/2/13/13	30/55/95/95	0/2/2/2
10	CLA	E	610	1	3/3/20/25	3/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CHL	I	606	11	3/3/17/26	6/21/119/137	-
9	CHL	H	609	1	5/5/20/26	15/39/137/137	-
10	CLA	A	613	1	3/3/20/25	7/37/135/135	-
4	LUT	C	2621	-	-	2/29/67/67	0/2/2/2
9	CHL	A	606	11	3/3/17/26	5/21/119/137	-
9	CHL	I	601	1	4/4/20/26	15/39/137/137	-
10	CLA	C	603	1	4/4/20/25	15/37/135/135	-
9	CHL	D	601	1	4/4/20/26	17/39/137/137	-
9	CHL	F	601	1	4/4/20/26	15/39/137/137	-
10	CLA	J	603	1	4/4/20/25	13/37/135/135	-
5	XAT	E	2622	-	-	1/31/93/93	0/4/4/4
4	LUT	G	6621	-	-	2/29/67/67	0/2/2/2
4	LUT	A	620	-	-	1/29/67/67	0/2/2/2
9	CHL	J	609	1	5/5/20/26	21/39/137/137	-
6	NEX	A	623	-	-	3/27/83/83	0/3/3/3
4	LUT	B	1621	-	-	2/29/67/67	0/2/2/2
10	CLA	I	612	1	3/3/20/25	14/37/135/135	-
10	CLA	H	604	11	3/3/19/25	18/34/132/135	-
8	DGD	B	2632	-	2/2/13/13	29/55/95/95	0/2/2/2
4	LUT	H	7620	-	-	1/29/67/67	0/2/2/2
9	CHL	G	605	1	3/3/16/26	6/18/116/137	-
9	CHL	B	605	1	3/3/16/26	7/18/116/137	-
9	CHL	D	605	1	3/3/16/26	7/18/116/137	-
2	BNG	E	4633	-	-	10/12/32/32	0/1/1/1
9	CHL	J	607	11	3/3/20/26	11/39/137/137	-
9	CHL	B	606	11	3/3/17/26	7/21/119/137	-
8	DGD	B	1632	-	2/2/13/13	30/55/95/95	0/2/2/2
10	CLA	F	614	1	3/3/16/25	5/18/116/135	-
2	BNG	D	3633	-	-	10/12/32/32	0/1/1/1
7	LHG	I	8630	10	-	38/53/53/53	-
6	NEX	H	7623	-	-	2/27/83/83	0/3/3/3
9	CHL	I	607	11	3/3/20/26	13/39/137/137	-
8	DGD	A	632	-	2/2/13/13	26/55/95/95	0/2/2/2
4	LUT	I	8620	-	-	1/29/67/67	0/2/2/2
9	CHL	J	606	11	3/3/17/26	7/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	D	612	1	3/3/20/25	13/37/135/135	-
4	LUT	I	8621	-	-	2/29/67/67	0/2/2/2
10	CLA	F	612	1	3/3/20/25	15/37/135/135	-
10	CLA	E	612	1	3/3/20/25	15/37/135/135	-
9	CHL	J	608	11	4/4/20/26	21/39/137/137	-
10	CLA	D	602	1	4/4/20/25	17/37/135/135	-
5	XAT	B	1622	-	-	1/31/93/93	0/4/4/4
10	CLA	J	604	11	3/3/19/25	9/34/132/135	-
4	LUT	J	9621	-	-	2/29/67/67	0/2/2/2
6	NEX	G	6623	-	-	2/27/83/83	0/3/3/3
2	BNG	H	7633	-	-	10/12/32/32	0/1/1/1
9	CHL	J	605	1	3/3/16/26	8/18/116/137	-
5	XAT	I	9622	-	-	0/31/93/93	0/4/4/4
10	CLA	F	604	11	3/3/19/25	15/34/132/135	-
10	CLA	B	612	1	3/3/20/25	15/37/135/135	-
10	CLA	A	614	1	3/3/16/25	7/18/116/135	-
10	CLA	H	603	1	4/4/20/25	14/37/135/135	-
9	CHL	C	608	11	4/4/20/26	17/39/137/137	-
6	NEX	J	9623	-	-	2/27/83/83	0/3/3/3
4	LUT	J	9620	-	-	2/29/67/67	0/2/2/2
10	CLA	G	611	7	3/3/20/25	17/37/135/135	-
9	CHL	H	608	11	4/4/20/26	22/39/137/137	-
10	CLA	H	613	1	3/3/20/25	13/37/135/135	-
10	CLA	I	611	7	3/3/20/25	20/37/135/135	-
8	DGD	D	3632	-	2/2/13/13	27/55/95/95	0/2/2/2
10	CLA	C	613	1	3/3/20/25	10/37/135/135	-
5	XAT	F	6622	-	-	1/31/93/93	0/4/4/4
10	CLA	E	613	1	3/3/20/25	11/37/135/135	-
9	CHL	J	601	1	4/4/20/26	18/39/137/137	-
9	CHL	E	608	11	4/4/20/26	17/39/137/137	-
9	CHL	G	608	11	4/4/20/26	18/39/137/137	-
10	CLA	A	603	1	4/4/20/25	18/37/135/135	-
7	LHG	D	3630	10	-	32/53/53/53	-
10	CLA	E	614	1	3/3/16/25	5/18/116/135	-
9	CHL	B	609	1	5/5/20/26	16/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CHL	B	607	11	3/3/20/26	15/39/137/137	-
4	LUT	A	621	-	-	2/29/67/67	0/2/2/2
9	CHL	D	607	11	3/3/20/26	14/39/137/137	-

All (1521) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	612	CLA	MG-NA	7.23	2.23	2.06
8	G	9632	DGD	O2G-C1B	7.13	1.54	1.34
10	A	612	CLA	MG-NA	6.66	2.22	2.06
8	E	4632	DGD	O2G-C1B	6.64	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	6.53	1.52	1.33
10	J	612	CLA	MG-NA	6.35	2.21	2.06
10	H	612	CLA	MG-NA	6.34	2.21	2.06
8	D	5632	DGD	O2G-C1B	6.33	1.52	1.34
9	C	606	CHL	O2A-CGA	6.32	1.51	1.33
9	D	606	CHL	O2A-CGA	6.32	1.51	1.33
8	D	3632	DGD	O2G-C1B	6.29	1.52	1.34
8	H	7632	DGD	O2G-C1B	6.28	1.52	1.34
8	B	1632	DGD	O2G-C1B	6.23	1.51	1.34
9	A	606	CHL	O2A-CGA	6.23	1.51	1.33
9	F	606	CHL	O2A-CGA	6.19	1.51	1.33
8	B	2632	DGD	O2G-C1B	6.19	1.51	1.34
10	H	603	CLA	MG-NA	6.18	2.21	2.06
8	A	632	DGD	O2G-C1B	6.12	1.51	1.34
9	J	606	CHL	O2A-CGA	6.11	1.51	1.33
10	F	603	CLA	MG-NA	6.06	2.20	2.06
8	I	8632	DGD	O2G-C1B	6.03	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
10	C	614	CLA	MG-NA	5.93	2.20	2.06
9	I	606	CHL	O2A-CGA	5.90	1.50	1.33
10	G	612	CLA	MG-NA	5.84	2.20	2.06
10	I	611	CLA	MG-NA	5.83	2.20	2.06
10	B	612	CLA	MG-NA	5.80	2.20	2.06
10	B	614	CLA	MG-NA	5.79	2.20	2.06
10	E	613	CLA	MG-NA	5.78	2.20	2.06
9	I	607	CHL	MG-NA	5.76	2.19	2.06
10	E	614	CLA	MG-NA	5.74	2.19	2.06
9	F	607	CHL	MG-NA	5.74	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	612	CLA	MG-NA	5.73	2.19	2.06
9	A	607	CHL	MG-NA	5.71	2.19	2.06
10	G	614	CLA	MG-NA	5.70	2.19	2.06
10	D	612	CLA	MG-NA	5.70	2.19	2.06
10	H	614	CLA	MG-NA	5.69	2.19	2.06
10	J	603	CLA	MG-NA	5.61	2.19	2.06
10	D	614	CLA	MG-NA	5.59	2.19	2.06
9	I	609	CHL	MG-NA	5.58	2.19	2.06
10	D	603	CLA	MG-NA	5.58	2.19	2.06
9	F	606	CHL	MG-NA	5.58	2.19	2.06
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	H	607	CHL	MG-NA	5.49	2.19	2.06
10	B	603	CLA	MG-NA	5.47	2.19	2.06
9	D	606	CHL	MG-NA	5.47	2.19	2.06
9	C	607	CHL	MG-NA	5.46	2.19	2.06
9	I	606	CHL	MG-NA	5.46	2.19	2.06
9	B	607	CHL	MG-NA	5.45	2.19	2.06
9	J	606	CHL	MG-NA	5.42	2.19	2.06
10	D	610	CLA	MG-NA	5.41	2.19	2.06
10	E	603	CLA	MG-NA	5.41	2.19	2.06
9	E	606	CHL	MG-NA	5.40	2.19	2.06
9	J	605	CHL	MG-NA	5.39	2.19	2.06
9	B	606	CHL	MG-NA	5.38	2.19	2.06
10	D	611	CLA	MG-NA	5.37	2.19	2.06
10	H	610	CLA	O2D-CGD	5.36	1.46	1.33
10	F	614	CLA	MG-NA	5.35	2.19	2.06
10	I	610	CLA	O2D-CGD	5.35	1.46	1.33
10	J	610	CLA	O2A-CGA	5.35	1.49	1.33
10	G	611	CLA	MG-NA	5.33	2.18	2.06
9	H	605	CHL	O2A-CGA	5.33	1.48	1.33
10	H	602	CLA	O2D-CGD	5.32	1.46	1.33
10	G	603	CLA	MG-NA	5.31	2.18	2.06
9	B	609	CHL	MG-NA	5.31	2.18	2.06
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
10	H	602	CLA	MG-NA	5.30	2.18	2.06
9	I	607	CHL	O2D-CGD	5.29	1.46	1.33
9	J	609	CHL	MG-NA	5.29	2.18	2.06
10	A	614	CLA	MG-NA	5.28	2.18	2.06
9	F	607	CHL	O2D-CGD	5.26	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	608	CHL	MG-NA	5.25	2.18	2.06
9	H	601	CHL	MG-NA	5.25	2.18	2.06
9	A	609	CHL	MG-NA	5.25	2.18	2.06
10	F	610	CLA	O2A-CGA	5.23	1.48	1.33
9	I	605	CHL	MG-NA	5.22	2.18	2.06
9	G	606	CHL	MG-NA	5.20	2.18	2.06
9	C	609	CHL	MG-NA	5.19	2.18	2.06
10	F	611	CLA	MG-NA	5.19	2.18	2.06
10	C	602	CLA	MG-NA	5.18	2.18	2.06
10	C	611	CLA	MG-NA	5.17	2.18	2.06
10	J	613	CLA	MG-NA	5.15	2.18	2.06
9	B	606	CHL	O2A-CGA	5.15	1.48	1.33
9	H	609	CHL	MG-NA	5.13	2.18	2.06
10	H	613	CLA	O2D-CGD	5.13	1.45	1.33
9	E	607	CHL	MG-NA	5.11	2.18	2.06
9	C	605	CHL	MG-NA	5.10	2.18	2.06
10	A	604	CLA	O2A-CGA	5.09	1.48	1.33
9	A	605	CHL	MG-NA	5.08	2.18	2.06
10	E	610	CLA	O2D-CGD	5.07	1.45	1.33
9	F	601	CHL	MG-NA	5.07	2.18	2.06
10	A	611	CLA	MG-NA	5.07	2.18	2.06
9	C	606	CHL	MG-NA	5.07	2.18	2.06
10	H	611	CLA	MG-NA	5.06	2.18	2.06
9	F	605	CHL	MG-NA	5.05	2.18	2.06
10	E	604	CLA	O2D-CGD	5.04	1.45	1.33
9	I	608	CHL	MG-NA	5.04	2.18	2.06
10	D	610	CLA	O2D-CGD	5.03	1.45	1.33
9	G	607	CHL	MG-NA	5.03	2.18	2.06
10	F	613	CLA	O2D-CGD	5.02	1.45	1.33
9	A	606	CHL	MG-NA	5.02	2.18	2.06
10	C	610	CLA	O2D-CGD	5.01	1.45	1.33
10	E	610	CLA	O2A-CGA	5.00	1.48	1.33
9	A	605	CHL	O2A-CGA	4.98	1.47	1.33
9	C	608	CHL	MG-NA	4.98	2.18	2.06
9	D	605	CHL	O2D-CGD	4.98	1.45	1.33
9	G	601	CHL	MG-NA	4.98	2.18	2.06
9	I	605	CHL	O2A-CGA	4.97	1.47	1.33
9	B	601	CHL	MG-NA	4.97	2.18	2.06
10	B	602	CLA	MG-NA	4.97	2.18	2.06
10	I	614	CLA	MG-NA	4.96	2.18	2.06
10	E	602	CLA	MG-NA	4.95	2.18	2.06
10	B	613	CLA	O2D-CGD	4.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	608	CHL	O2D-CGD	4.94	1.45	1.33
10	J	614	CLA	MG-NA	4.93	2.18	2.06
10	A	602	CLA	O2D-CGD	4.93	1.45	1.33
10	I	613	CLA	MG-NA	4.92	2.18	2.06
10	D	610	CLA	O2A-CGA	4.92	1.47	1.33
10	C	610	CLA	O2A-CGA	4.91	1.47	1.33
10	A	610	CLA	O2A-CGA	4.90	1.47	1.33
9	I	609	CHL	O2A-CGA	4.90	1.47	1.33
9	F	605	CHL	O2D-CGD	4.90	1.45	1.33
9	E	606	CHL	O2A-CGA	4.89	1.47	1.33
9	D	605	CHL	MG-NA	4.89	2.17	2.06
10	B	610	CLA	O2A-CGA	4.88	1.47	1.33
10	I	602	CLA	MG-NA	4.88	2.17	2.06
10	F	613	CLA	MG-NA	4.87	2.17	2.06
9	H	606	CHL	O2A-CGA	4.85	1.47	1.33
9	C	605	CHL	O2A-CGA	4.84	1.47	1.33
9	A	608	CHL	MG-NA	4.84	2.17	2.06
9	E	601	CHL	O2A-CGA	4.84	1.47	1.33
9	G	605	CHL	MG-NA	4.84	2.17	2.06
10	H	613	CLA	MG-NA	4.83	2.17	2.06
10	C	613	CLA	MG-NA	4.83	2.17	2.06
10	E	612	CLA	O2D-CGD	4.82	1.45	1.33
9	B	608	CHL	MG-NA	4.82	2.17	2.06
9	C	607	CHL	O2D-CGD	4.82	1.44	1.33
9	F	605	CHL	O2A-CGA	4.81	1.47	1.33
10	D	613	CLA	O2D-CGD	4.80	1.44	1.33
10	A	610	CLA	O2D-CGD	4.79	1.44	1.33
10	G	610	CLA	O2D-CGD	4.79	1.44	1.33
10	E	610	CLA	MG-NA	4.79	2.17	2.06
7	B	1630	LHG	O8-C23	4.78	1.47	1.33
10	G	613	CLA	MG-NA	4.78	2.17	2.06
10	D	613	CLA	MG-NA	4.77	2.17	2.06
10	E	613	CLA	O2D-CGD	4.77	1.44	1.33
10	J	604	CLA	O2D-CGD	4.77	1.44	1.33
9	H	607	CHL	O2D-CGD	4.76	1.44	1.33
10	F	610	CLA	MG-NA	4.76	2.17	2.06
9	E	601	CHL	MG-NA	4.74	2.17	2.06
9	G	608	CHL	MG-NA	4.73	2.17	2.06
10	I	610	CLA	O2A-CGA	4.73	1.47	1.33
10	F	602	CLA	MG-NA	4.72	2.17	2.06
10	D	602	CLA	MG-NA	4.72	2.17	2.06
10	A	613	CLA	MG-NA	4.71	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	613	CLA	O2A-CGA	4.71	1.47	1.33
9	H	608	CHL	MG-NA	4.71	2.17	2.06
9	D	609	CHL	MG-NA	4.70	2.17	2.06
9	H	606	CHL	MG-NA	4.69	2.17	2.06
10	D	604	CLA	O2A-CGA	4.69	1.47	1.33
9	D	605	CHL	O2A-CGA	4.69	1.47	1.33
9	E	605	CHL	MG-NA	4.68	2.17	2.06
10	J	603	CLA	O2A-CGA	4.68	1.47	1.33
9	F	609	CHL	MG-NA	4.68	2.17	2.06
10	H	610	CLA	O2A-CGA	4.67	1.47	1.33
10	B	602	CLA	O2D-CGD	4.66	1.44	1.33
10	E	602	CLA	O2D-CGD	4.65	1.44	1.33
9	E	609	CHL	MG-NA	4.63	2.17	2.06
7	I	8630	LHG	O8-C23	4.63	1.46	1.33
10	G	610	CLA	O2A-CGA	4.62	1.46	1.33
10	D	602	CLA	O2D-CGD	4.60	1.44	1.33
10	G	604	CLA	MG-NA	4.59	2.17	2.06
9	E	608	CHL	MG-NA	4.59	2.17	2.06
10	F	610	CLA	O2D-CGD	4.58	1.44	1.33
10	H	611	CLA	O2D-CGD	4.57	1.44	1.33
10	A	602	CLA	MG-NA	4.56	2.17	2.06
10	J	602	CLA	MG-NA	4.56	2.17	2.06
10	B	610	CLA	MG-NA	4.56	2.17	2.06
10	I	611	CLA	O2A-CGA	4.55	1.46	1.33
6	D	3623	NEX	C7-C8	4.55	1.39	1.32
10	C	610	CLA	MG-NA	4.55	2.17	2.06
9	F	608	CHL	MG-NA	4.55	2.17	2.06
9	G	608	CHL	O2A-CGA	4.54	1.46	1.33
10	A	614	CLA	O2A-CGA	4.54	1.46	1.33
10	G	602	CLA	MG-NA	4.53	2.17	2.06
10	J	602	CLA	O2D-CGD	4.53	1.44	1.33
10	C	602	CLA	O2D-CGD	4.53	1.44	1.33
9	I	601	CHL	MG-NA	4.52	2.17	2.06
10	G	602	CLA	O2D-CGD	4.52	1.44	1.33
9	F	609	CHL	O2A-CGA	4.51	1.46	1.33
9	J	605	CHL	O2A-CGA	4.51	1.46	1.33
9	J	607	CHL	MG-NA	4.49	2.16	2.06
9	H	605	CHL	MG-NA	4.48	2.16	2.06
9	G	605	CHL	O2D-CGD	4.47	1.44	1.33
10	B	610	CLA	O2D-CGD	4.47	1.44	1.33
10	I	614	CLA	O2A-CGA	4.47	1.46	1.33
9	A	601	CHL	MG-NA	4.47	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	613	CLA	O2D-CGD	4.46	1.44	1.33
9	J	609	CHL	O2A-CGA	4.46	1.46	1.33
9	A	605	CHL	O2D-CGD	4.45	1.44	1.33
10	I	610	CLA	MG-NA	4.45	2.16	2.06
10	C	604	CLA	O2A-CGA	4.42	1.46	1.33
9	B	605	CHL	MG-NA	4.41	2.16	2.06
9	A	609	CHL	O2A-CGA	4.41	1.46	1.33
10	H	604	CLA	MG-NA	4.41	2.16	2.06
10	B	604	CLA	O2A-CGA	4.41	1.46	1.33
9	J	608	CHL	MG-NA	4.40	2.16	2.06
6	A	623	NEX	C7-C8	4.40	1.39	1.32
10	I	604	CLA	O2D-CGD	4.40	1.43	1.33
10	E	602	CLA	O2A-CGA	4.39	1.46	1.33
9	C	601	CHL	MG-NA	4.39	2.16	2.06
10	I	602	CLA	O2D-CGD	4.38	1.43	1.33
9	J	608	CHL	O2A-CGA	4.37	1.46	1.33
10	B	613	CLA	MG-NA	4.37	2.16	2.06
10	A	604	CLA	MG-NA	4.35	2.16	2.06
10	B	603	CLA	O2A-CGA	4.35	1.46	1.33
10	J	604	CLA	MG-NA	4.34	2.16	2.06
9	B	601	CHL	O2A-CGA	4.34	1.46	1.33
9	E	601	CHL	O2D-CGD	4.34	1.43	1.33
10	F	602	CLA	O2D-CGD	4.34	1.43	1.33
9	J	601	CHL	MG-NA	4.33	2.16	2.06
10	H	614	CLA	O2A-CGA	4.33	1.46	1.33
10	I	604	CLA	MG-NA	4.32	2.16	2.06
9	D	609	CHL	O2A-CGA	4.32	1.46	1.33
10	B	604	CLA	O2D-CGD	4.31	1.43	1.33
10	E	611	CLA	O2D-CGD	4.31	1.43	1.33
9	H	605	CHL	O2D-CGD	4.31	1.43	1.33
10	C	603	CLA	O2A-CGA	4.29	1.45	1.33
10	A	603	CLA	O2D-CGD	4.29	1.43	1.33
7	F	5630	LHG	O7-C7	4.28	1.46	1.34
9	G	605	CHL	O2A-CGA	4.28	1.45	1.33
10	F	604	CLA	MG-NA	4.27	2.16	2.06
10	J	614	CLA	O2A-CGA	4.27	1.45	1.33
9	H	606	CHL	O2D-CGD	4.27	1.43	1.33
10	F	614	CLA	O2D-CGD	4.26	1.43	1.33
9	H	601	CHL	O2A-CGA	4.26	1.45	1.33
10	B	612	CLA	O2D-CGD	4.26	1.43	1.33
7	G	6630	LHG	O8-C23	4.26	1.45	1.33
10	G	614	CLA	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	611	CLA	O2D-CGD	4.25	1.43	1.33
9	A	608	CHL	O2D-CGD	4.25	1.43	1.33
9	B	609	CHL	O2A-CGA	4.25	1.45	1.33
9	B	605	CHL	O2A-CGA	4.24	1.45	1.33
10	D	604	CLA	O2D-CGD	4.23	1.43	1.33
9	H	608	CHL	O2A-CGA	4.22	1.45	1.33
10	J	610	CLA	MG-NA	4.22	2.16	2.06
6	E	4623	NEX	C7-C8	4.21	1.39	1.32
10	J	603	CLA	O2D-CGD	4.21	1.43	1.33
10	C	614	CLA	O2D-CGD	4.20	1.43	1.33
10	D	604	CLA	MG-NA	4.20	2.16	2.06
10	J	610	CLA	O2D-CGD	4.20	1.43	1.33
9	E	606	CHL	O2D-CGD	4.20	1.43	1.33
10	E	614	CLA	O2A-CGA	4.20	1.45	1.33
7	J	9630	LHG	O7-C7	4.19	1.46	1.34
9	C	605	CHL	O2D-CGD	4.19	1.43	1.33
9	F	608	CHL	O2A-CGA	4.19	1.45	1.33
10	B	614	CLA	O2A-CGA	4.18	1.45	1.33
9	B	608	CHL	O2D-CGD	4.18	1.43	1.33
6	I	8623	NEX	C7-C8	4.18	1.38	1.32
6	J	9623	NEX	C7-C8	4.17	1.38	1.32
10	D	602	CLA	O2A-CGA	4.16	1.45	1.33
10	A	610	CLA	MG-NA	4.16	2.16	2.06
10	F	611	CLA	C1B-NB	4.16	1.38	1.35
10	G	613	CLA	O2D-CGD	4.15	1.43	1.33
9	J	607	CHL	O2D-CGD	4.15	1.43	1.33
10	F	614	CLA	O2A-CGA	4.15	1.45	1.33
10	D	610	CLA	C1B-NB	4.15	1.38	1.35
9	D	607	CHL	MG-NA	4.15	2.16	2.06
10	F	610	CLA	C1B-NB	4.14	1.38	1.35
9	E	605	CHL	O2D-CGD	4.14	1.43	1.33
9	H	609	CHL	O2A-CGA	4.13	1.45	1.33
10	I	613	CLA	O2D-CGD	4.13	1.43	1.33
9	C	601	CHL	O2D-CGD	4.13	1.43	1.33
10	G	611	CLA	O2A-CGA	4.12	1.45	1.33
10	H	604	CLA	O2A-CGA	4.11	1.45	1.33
10	A	604	CLA	O2D-CGD	4.11	1.43	1.33
7	C	2630	LHG	O8-C23	4.10	1.45	1.33
10	B	611	CLA	O2D-CGD	4.10	1.43	1.33
10	H	604	CLA	O2D-CGD	4.09	1.43	1.33
10	A	611	CLA	O2A-CGA	4.09	1.45	1.33
10	F	612	CLA	O2D-CGD	4.09	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	612	CLA	O2D-CGD	4.09	1.43	1.33
9	G	608	CHL	O2D-CGD	4.09	1.43	1.33
9	E	607	CHL	O2D-CGD	4.08	1.43	1.33
6	H	7623	NEX	C7-C8	4.08	1.38	1.32
9	E	609	CHL	O2A-CGA	4.07	1.45	1.33
10	G	612	CLA	O2D-CGD	4.07	1.43	1.33
10	D	614	CLA	O2D-CGD	4.07	1.43	1.33
10	D	603	CLA	O2A-CGA	4.07	1.45	1.33
6	F	5623	NEX	C7-C8	4.06	1.38	1.32
9	C	608	CHL	O2A-CGA	4.06	1.45	1.33
10	F	610	CLA	C4B-NB	4.06	1.38	1.35
10	B	611	CLA	O2A-CGA	4.06	1.45	1.33
9	C	606	CHL	O2D-CGD	4.06	1.43	1.33
9	D	601	CHL	O2A-CGA	4.05	1.45	1.33
10	D	611	CLA	O2D-CGD	4.05	1.43	1.33
10	F	603	CLA	O2A-CGA	4.05	1.45	1.33
10	C	613	CLA	O2D-CGD	4.05	1.43	1.33
9	I	607	CHL	O2A-CGA	4.04	1.45	1.33
10	E	603	CLA	O2A-CGA	4.04	1.45	1.33
10	J	604	CLA	O2A-CGA	4.04	1.45	1.33
10	A	611	CLA	O2D-CGD	4.04	1.43	1.33
10	H	612	CLA	O2A-CGA	4.03	1.45	1.33
9	G	607	CHL	O2D-CGD	4.03	1.43	1.33
10	D	612	CLA	O2D-CGD	4.02	1.43	1.33
10	F	602	CLA	C1B-NB	4.02	1.38	1.35
9	I	609	CHL	O2D-CGD	4.01	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	D	601	CHL	O2D-CGD	4.01	1.43	1.33
10	H	614	CLA	C4B-NB	4.00	1.38	1.35
6	C	2623	NEX	C7-C8	4.00	1.38	1.32
10	F	603	CLA	O2D-CGD	4.00	1.43	1.33
9	I	609	CHL	C4B-NB	4.00	1.38	1.35
10	J	614	CLA	O2D-CGD	4.00	1.43	1.33
10	C	603	CLA	C4B-NB	4.00	1.38	1.35
9	J	601	CHL	O2A-CGA	3.99	1.45	1.33
9	B	606	CHL	C1B-NB	3.99	1.38	1.35
10	F	611	CLA	O2A-CGA	3.99	1.45	1.33
10	A	612	CLA	C1B-NB	3.99	1.38	1.35
10	C	602	CLA	C1B-NB	3.99	1.38	1.35
10	G	614	CLA	O2D-CGD	3.99	1.42	1.33
10	B	604	CLA	MG-NA	3.99	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	605	CHL	O2D-CGD	3.99	1.42	1.33
10	A	602	CLA	O2A-CGA	3.98	1.45	1.33
10	A	613	CLA	O2D-CGD	3.98	1.42	1.33
10	I	604	CLA	O2A-CGA	3.98	1.45	1.33
10	I	603	CLA	O2A-CGA	3.97	1.45	1.33
10	D	612	CLA	O2A-CGA	3.97	1.44	1.33
6	G	6623	NEX	C7-C8	3.97	1.38	1.32
9	J	605	CHL	C1B-NB	3.96	1.38	1.35
10	D	603	CLA	C4B-NB	3.96	1.38	1.35
10	I	610	CLA	C1B-NB	3.95	1.38	1.35
9	J	605	CHL	O2D-CGD	3.95	1.42	1.33
10	J	603	CLA	C1B-NB	3.95	1.38	1.35
10	C	604	CLA	O2D-CGD	3.95	1.42	1.33
9	G	609	CHL	MG-NA	3.94	2.15	2.06
10	J	611	CLA	O2D-CGD	3.94	1.42	1.33
10	E	604	CLA	MG-NA	3.93	2.15	2.06
9	A	601	CHL	O2A-CGA	3.93	1.44	1.33
9	H	607	CHL	O2A-CGA	3.92	1.44	1.33
10	C	612	CLA	C1B-NB	3.92	1.38	1.35
9	C	609	CHL	O2A-CGA	3.92	1.44	1.33
10	G	614	CLA	C1B-NB	3.92	1.38	1.35
9	G	606	CHL	O2D-CGD	3.92	1.42	1.33
9	F	601	CHL	C1B-NB	3.91	1.38	1.35
10	A	614	CLA	C4B-NB	3.91	1.38	1.35
10	H	602	CLA	C1B-NB	3.91	1.38	1.35
10	B	612	CLA	O2A-CGA	3.91	1.44	1.33
10	E	611	CLA	C1B-NB	3.90	1.38	1.35
9	B	607	CHL	O2D-CGD	3.90	1.42	1.33
10	J	612	CLA	O2D-CGD	3.90	1.42	1.33
10	D	611	CLA	O2A-CGA	3.90	1.44	1.33
9	I	601	CHL	O2A-CGA	3.90	1.44	1.33
9	A	605	CHL	C1B-NB	3.90	1.38	1.35
10	G	603	CLA	O2D-CGD	3.89	1.42	1.33
9	F	607	CHL	O2A-CGA	3.89	1.44	1.33
10	I	611	CLA	O2D-CGD	3.89	1.42	1.33
10	G	612	CLA	C4B-NB	3.89	1.38	1.35
10	E	612	CLA	O2A-CGA	3.89	1.44	1.33
10	B	613	CLA	O2A-CGA	3.88	1.44	1.33
9	A	608	CHL	O2A-CGA	3.88	1.44	1.33
10	D	612	CLA	C4B-NB	3.88	1.38	1.35
9	J	605	CHL	C4B-NB	3.87	1.38	1.35
10	D	614	CLA	C4B-NB	3.87	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	606	CHL	C1B-NB	3.86	1.38	1.35
9	I	605	CHL	C1B-NB	3.86	1.38	1.35
10	H	603	CLA	O2D-CGD	3.86	1.42	1.33
9	G	609	CHL	C4B-NB	3.86	1.38	1.35
10	J	613	CLA	O2A-CGA	3.85	1.44	1.33
10	G	603	CLA	C4B-NB	3.85	1.38	1.35
9	D	601	CHL	MG-NA	3.85	2.15	2.06
10	F	612	CLA	O2A-CGA	3.85	1.44	1.33
10	C	610	CLA	C4B-NB	3.85	1.38	1.35
10	G	602	CLA	C1B-NB	3.85	1.38	1.35
10	I	613	CLA	O2A-CGA	3.85	1.44	1.33
10	G	614	CLA	C4B-NB	3.84	1.38	1.35
10	E	610	CLA	C1B-NB	3.84	1.38	1.35
9	A	607	CHL	O2A-CGA	3.84	1.44	1.33
10	F	603	CLA	C4B-NB	3.84	1.38	1.35
9	G	601	CHL	O2A-CGA	3.84	1.44	1.33
10	J	614	CLA	C4B-NB	3.84	1.38	1.35
10	F	613	CLA	C1B-NB	3.83	1.38	1.35
10	G	604	CLA	O2D-CGD	3.83	1.42	1.33
10	C	602	CLA	O2A-CGA	3.83	1.44	1.33
10	E	614	CLA	C1B-NB	3.83	1.38	1.35
9	D	609	CHL	O2D-CGD	3.83	1.42	1.33
10	B	612	CLA	C4B-NB	3.83	1.38	1.35
9	G	607	CHL	O2A-CGA	3.82	1.44	1.33
7	F	5630	LHG	O8-C23	3.82	1.44	1.33
9	F	605	CHL	C1B-NB	3.82	1.38	1.35
10	I	614	CLA	C4B-NB	3.82	1.38	1.35
10	A	612	CLA	C4B-NB	3.82	1.38	1.35
9	B	608	CHL	C4B-NB	3.81	1.38	1.35
10	G	603	CLA	O2A-CGA	3.81	1.44	1.33
10	C	612	CLA	O2D-CGD	3.81	1.42	1.33
10	F	614	CLA	C1B-NB	3.80	1.38	1.35
10	H	610	CLA	MG-NA	3.80	2.15	2.06
9	F	606	CHL	C1B-NB	3.80	1.38	1.35
10	G	610	CLA	MG-NA	3.80	2.15	2.06
10	A	602	CLA	C4B-NB	3.79	1.38	1.35
10	I	614	CLA	O2D-CGD	3.79	1.42	1.33
9	C	609	CHL	O2D-CGD	3.79	1.42	1.33
10	D	614	CLA	O2A-CGA	3.79	1.44	1.33
10	C	611	CLA	O2D-CGD	3.79	1.42	1.33
10	G	610	CLA	C4B-NB	3.79	1.38	1.35
9	D	606	CHL	C1B-NB	3.78	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	609	CHL	O2D-CGD	3.78	1.42	1.33
10	J	602	CLA	C4B-NB	3.78	1.38	1.35
9	D	608	CHL	O2A-CGA	3.77	1.44	1.33
9	I	608	CHL	C1B-NB	3.77	1.38	1.35
4	C	2621	LUT	C23-C24	3.77	1.55	1.50
9	C	605	CHL	C1B-NB	3.77	1.38	1.35
9	E	605	CHL	O2A-CGA	3.76	1.44	1.33
10	B	614	CLA	C4B-NB	3.76	1.38	1.35
10	C	611	CLA	C1B-NB	3.76	1.38	1.35
10	J	613	CLA	C1B-NB	3.76	1.38	1.35
9	J	609	CHL	C4B-NB	3.76	1.38	1.35
7	A	630	LHG	O8-C23	3.76	1.44	1.33
10	C	610	CLA	C1B-NB	3.75	1.38	1.35
10	A	603	CLA	O2A-CGA	3.75	1.44	1.33
10	C	602	CLA	C4B-NB	3.75	1.38	1.35
10	F	612	CLA	C1B-NB	3.74	1.38	1.35
10	H	612	CLA	C4B-NB	3.74	1.38	1.35
9	H	601	CHL	C1B-NB	3.74	1.38	1.35
9	E	605	CHL	C4B-NB	3.74	1.38	1.35
10	A	611	CLA	C1B-NB	3.73	1.38	1.35
9	C	601	CHL	C1B-NB	3.73	1.38	1.35
9	E	606	CHL	C1B-NB	3.73	1.38	1.35
9	D	605	CHL	C4B-NB	3.73	1.38	1.35
10	D	614	CLA	C1B-NB	3.73	1.38	1.35
10	C	614	CLA	C4B-NB	3.73	1.38	1.35
10	E	613	CLA	O2A-CGA	3.72	1.44	1.33
10	H	603	CLA	C4B-NB	3.72	1.38	1.35
9	H	606	CHL	C4B-NB	3.72	1.38	1.35
9	F	609	CHL	C4B-NB	3.72	1.38	1.35
9	H	608	CHL	C1B-NB	3.72	1.38	1.35
9	H	605	CHL	C1B-NB	3.72	1.38	1.35
10	H	603	CLA	C1B-NB	3.72	1.38	1.35
9	G	605	CHL	C1B-NB	3.71	1.38	1.35
9	B	606	CHL	O2D-CGD	3.71	1.42	1.33
10	H	612	CLA	C1B-NB	3.71	1.38	1.35
10	F	614	CLA	C4B-NB	3.71	1.38	1.35
9	B	607	CHL	C1B-NB	3.71	1.38	1.35
9	E	605	CHL	C1B-NB	3.70	1.38	1.35
9	I	606	CHL	C1B-NB	3.70	1.38	1.35
10	F	611	CLA	C4B-NB	3.70	1.38	1.35
9	D	601	CHL	C4B-NB	3.70	1.38	1.35
10	G	611	CLA	C4B-NB	3.69	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	603	CLA	C4B-NB	3.69	1.38	1.35
9	I	605	CHL	O2D-CGD	3.69	1.42	1.33
9	H	608	CHL	C4B-NB	3.69	1.38	1.35
9	F	606	CHL	O2D-CGD	3.69	1.42	1.33
9	E	607	CHL	O2A-CGA	3.69	1.44	1.33
10	F	613	CLA	O2A-CGA	3.69	1.44	1.33
9	J	609	CHL	O2D-CGD	3.69	1.42	1.33
9	G	601	CHL	C1B-NB	3.69	1.38	1.35
10	H	611	CLA	C1B-NB	3.69	1.38	1.35
9	D	605	CHL	C1B-NB	3.69	1.38	1.35
10	E	614	CLA	O2D-CGD	3.69	1.42	1.33
10	A	610	CLA	C4B-NB	3.68	1.38	1.35
10	E	611	CLA	C4B-NB	3.68	1.38	1.35
9	J	606	CHL	O2D-CGD	3.68	1.42	1.33
10	A	613	CLA	O2A-CGA	3.68	1.44	1.33
10	D	612	CLA	C1B-NB	3.68	1.38	1.35
10	D	602	CLA	C1B-NB	3.68	1.38	1.35
10	E	603	CLA	O2D-CGD	3.67	1.42	1.33
9	H	601	CHL	O2D-CGD	3.67	1.42	1.33
9	C	609	CHL	C1B-NB	3.67	1.38	1.35
10	J	614	CLA	C1B-NB	3.67	1.38	1.35
10	H	603	CLA	O2A-CGA	3.67	1.44	1.33
9	F	608	CHL	O2D-CGD	3.67	1.42	1.33
10	J	610	CLA	C1B-NB	3.66	1.38	1.35
10	F	612	CLA	C4B-NB	3.66	1.38	1.35
9	A	607	CHL	O2D-CGD	3.66	1.42	1.33
10	C	614	CLA	C1B-NB	3.66	1.38	1.35
10	G	611	CLA	C1B-NB	3.66	1.38	1.35
10	I	612	CLA	C1B-NB	3.66	1.38	1.35
10	J	603	CLA	C4B-NB	3.64	1.38	1.35
10	J	602	CLA	C1B-NB	3.64	1.38	1.35
9	E	601	CHL	C1B-NB	3.64	1.38	1.35
10	A	603	CLA	C1B-NB	3.64	1.38	1.35
10	H	614	CLA	C1B-NB	3.63	1.38	1.35
10	F	602	CLA	C4B-NB	3.63	1.38	1.35
9	B	605	CHL	C4B-NB	3.63	1.38	1.35
9	C	608	CHL	O2D-CGD	3.63	1.42	1.33
10	B	602	CLA	C4B-NB	3.63	1.38	1.35
9	G	609	CHL	O2A-CGA	3.63	1.43	1.33
10	G	611	CLA	O2D-CGD	3.63	1.42	1.33
9	C	607	CHL	O2A-CGA	3.63	1.43	1.33
10	J	610	CLA	C4B-NB	3.63	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	606	CHL	C1B-NB	3.62	1.38	1.35
10	I	603	CLA	C1B-NB	3.62	1.38	1.35
9	B	601	CHL	O2D-CGD	3.62	1.42	1.33
10	E	612	CLA	C4B-NB	3.62	1.38	1.35
10	B	612	CLA	C1B-NB	3.62	1.38	1.35
10	H	611	CLA	C4B-NB	3.62	1.38	1.35
10	B	611	CLA	C4B-NB	3.61	1.38	1.35
9	A	601	CHL	O2D-CGD	3.61	1.42	1.33
10	D	613	CLA	C1B-NB	3.61	1.38	1.35
10	E	612	CLA	C1B-NB	3.60	1.38	1.35
10	H	611	CLA	O2A-CGA	3.60	1.43	1.33
10	C	612	CLA	C4B-NB	3.60	1.38	1.35
10	J	611	CLA	C1B-NB	3.60	1.38	1.35
10	G	613	CLA	O2A-CGA	3.60	1.43	1.33
9	B	608	CHL	C1B-NB	3.60	1.38	1.35
9	B	607	CHL	O2A-CGA	3.60	1.43	1.33
10	B	602	CLA	O2A-CGA	3.60	1.43	1.33
9	J	601	CHL	O2D-CGD	3.60	1.42	1.33
9	C	609	CHL	C4B-NB	3.59	1.38	1.35
10	J	612	CLA	C1B-NB	3.59	1.38	1.35
10	B	613	CLA	C1B-NB	3.58	1.38	1.35
9	C	601	CHL	C4B-NB	3.57	1.38	1.35
7	H	7630	LHG	O8-C23	3.57	1.43	1.33
9	G	605	CHL	C4B-NB	3.57	1.38	1.35
9	J	601	CHL	C4B-NB	3.57	1.38	1.35
10	D	611	CLA	C1B-NB	3.57	1.38	1.35
10	B	602	CLA	C1B-NB	3.57	1.38	1.35
10	J	612	CLA	C4B-NB	3.56	1.38	1.35
9	H	609	CHL	C4B-NB	3.56	1.38	1.35
9	G	609	CHL	O2D-CGD	3.56	1.41	1.33
10	F	604	CLA	O2A-CGA	3.56	1.43	1.33
10	B	614	CLA	C1B-NB	3.56	1.38	1.35
10	I	612	CLA	O2D-CED	-3.56	1.36	1.45
9	A	608	CHL	C4B-NB	3.56	1.38	1.35
10	E	602	CLA	C1B-NB	3.56	1.38	1.35
9	A	607	CHL	C4B-NB	3.55	1.38	1.35
10	I	610	CLA	C4B-NB	3.55	1.38	1.35
10	B	614	CLA	O2D-CGD	3.55	1.41	1.33
9	H	606	CHL	C1B-NB	3.55	1.38	1.35
9	E	608	CHL	C4B-NB	3.55	1.38	1.35
10	E	603	CLA	C4B-NB	3.54	1.38	1.35
10	G	612	CLA	C1B-NB	3.54	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	611	CLA	O2A-CGA	3.54	1.43	1.33
10	H	610	CLA	C1B-NB	3.54	1.38	1.35
9	A	601	CHL	C4B-NB	3.54	1.38	1.35
10	J	611	CLA	O2A-CGA	3.54	1.43	1.33
10	B	604	CLA	C1B-NB	3.54	1.38	1.35
9	H	605	CHL	C4B-NB	3.54	1.38	1.35
10	F	604	CLA	C1B-NB	3.53	1.38	1.35
9	E	601	CHL	C4B-NB	3.53	1.38	1.35
10	E	610	CLA	C4B-NB	3.53	1.38	1.35
10	E	613	CLA	C1B-NB	3.53	1.38	1.35
10	D	603	CLA	C1B-NB	3.53	1.38	1.35
10	H	602	CLA	O2A-CGA	3.53	1.43	1.33
9	I	601	CHL	C1B-NB	3.52	1.38	1.35
9	A	606	CHL	C1B-NB	3.52	1.38	1.35
10	A	614	CLA	C1B-NB	3.52	1.38	1.35
9	G	601	CHL	O2D-CED	-3.51	1.37	1.45
9	A	609	CHL	O2D-CGD	3.51	1.41	1.33
9	I	607	CHL	CMB-C2B	3.51	1.58	1.51
9	B	601	CHL	C1B-NB	3.51	1.38	1.35
10	G	604	CLA	C1B-NB	3.50	1.38	1.35
9	A	607	CHL	C1B-NB	3.50	1.38	1.35
9	F	601	CHL	O2A-CGA	3.50	1.43	1.33
10	E	614	CLA	C4B-NB	3.50	1.38	1.35
9	D	606	CHL	O2D-CGD	3.50	1.41	1.33
10	J	611	CLA	C4B-NB	3.50	1.38	1.35
10	B	611	CLA	C1B-NB	3.50	1.38	1.35
9	I	609	CHL	C1B-NB	3.50	1.38	1.35
10	C	614	CLA	O2A-CGA	3.49	1.43	1.33
10	A	602	CLA	C1B-NB	3.49	1.38	1.35
10	A	603	CLA	C4B-NB	3.49	1.38	1.35
9	J	608	CHL	C1B-NB	3.49	1.38	1.35
9	E	608	CHL	O2A-CGA	3.48	1.43	1.33
7	E	4630	LHG	O8-C23	3.48	1.43	1.33
9	F	601	CHL	C4B-NB	3.48	1.38	1.35
9	I	601	CHL	O2D-CGD	3.48	1.41	1.33
9	C	606	CHL	C4B-NB	3.48	1.38	1.35
9	H	609	CHL	C1B-NB	3.48	1.38	1.35
10	F	603	CLA	C1B-NB	3.48	1.38	1.35
10	G	603	CLA	C1B-NB	3.48	1.38	1.35
10	B	610	CLA	C1B-NB	3.48	1.38	1.35
9	H	608	CHL	O2D-CED	-3.47	1.37	1.45
10	H	610	CLA	C4B-NB	3.47	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	CHL	C1B-NB	3.47	1.38	1.35
10	A	613	CLA	C4B-NB	3.47	1.38	1.35
10	C	613	CLA	C1B-NB	3.47	1.38	1.35
6	B	1623	NEX	C7-C8	3.47	1.37	1.32
9	I	608	CHL	O2D-CGD	3.47	1.41	1.33
9	H	607	CHL	C4B-NB	3.47	1.38	1.35
9	I	607	CHL	C1B-NB	3.47	1.38	1.35
9	E	609	CHL	C1B-NB	3.47	1.38	1.35
10	H	613	CLA	C1B-NB	3.46	1.38	1.35
10	I	602	CLA	O2A-CGA	3.46	1.43	1.33
10	C	604	CLA	MG-NA	3.46	2.14	2.06
10	G	604	CLA	O2A-CGA	3.46	1.43	1.33
10	D	610	CLA	C4B-NB	3.45	1.38	1.35
9	B	601	CHL	C4B-NB	3.45	1.38	1.35
10	C	613	CLA	C4B-NB	3.45	1.38	1.35
9	A	609	CHL	C1B-NB	3.45	1.38	1.35
10	I	611	CLA	C1B-NB	3.45	1.38	1.35
9	F	608	CHL	C4B-NB	3.45	1.38	1.35
9	G	608	CHL	C1B-NB	3.45	1.38	1.35
10	H	612	CLA	O2D-CGD	3.45	1.41	1.33
9	A	605	CHL	C4B-NB	3.44	1.38	1.35
10	F	603	CLA	O2D-CED	-3.44	1.37	1.45
10	I	613	CLA	C1B-NB	3.44	1.38	1.35
10	A	610	CLA	C1B-NB	3.44	1.38	1.35
9	H	607	CHL	C1B-NB	3.44	1.38	1.35
9	J	609	CHL	C1B-NB	3.43	1.38	1.35
10	I	612	CLA	O2A-CGA	3.43	1.43	1.33
10	I	612	CLA	O2D-CGD	3.43	1.41	1.33
10	I	614	CLA	C1B-NB	3.43	1.38	1.35
9	I	601	CHL	C4B-NB	3.43	1.38	1.35
10	E	604	CLA	O2A-CGA	3.43	1.43	1.33
10	I	611	CLA	C4B-NB	3.42	1.38	1.35
9	J	608	CHL	C4B-NB	3.42	1.38	1.35
10	C	604	CLA	C1B-NB	3.42	1.38	1.35
10	A	612	CLA	O2D-CED	-3.42	1.37	1.45
9	G	606	CHL	C4B-NB	3.42	1.38	1.35
10	C	611	CLA	C4B-NB	3.42	1.38	1.35
9	B	609	CHL	C4B-NB	3.42	1.38	1.35
10	G	612	CLA	O2A-CGA	3.42	1.43	1.33
10	G	613	CLA	C1B-NB	3.42	1.38	1.35
10	G	602	CLA	C4B-NB	3.41	1.38	1.35
9	D	607	CHL	O2D-CGD	3.41	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	605	CHL	C1B-NB	3.41	1.38	1.35
9	C	608	CHL	C1B-NB	3.41	1.38	1.35
10	G	610	CLA	C1B-NB	3.40	1.38	1.35
9	G	601	CHL	O2D-CGD	3.40	1.41	1.33
10	F	602	CLA	O2A-CGA	3.40	1.43	1.33
9	B	607	CHL	C4B-NB	3.39	1.38	1.35
10	I	603	CLA	O2D-CGD	3.39	1.41	1.33
10	J	604	CLA	C4B-NB	3.39	1.38	1.35
10	F	604	CLA	O2D-CGD	3.38	1.41	1.33
10	I	613	CLA	C4B-NB	3.38	1.38	1.35
9	F	605	CHL	C4B-NB	3.38	1.38	1.35
9	F	608	CHL	C1B-NB	3.38	1.38	1.35
9	E	609	CHL	C4B-NB	3.38	1.38	1.35
9	C	606	CHL	C1B-NB	3.38	1.38	1.35
9	F	607	CHL	C4B-NB	3.37	1.38	1.35
9	B	609	CHL	C1B-NB	3.37	1.38	1.35
9	E	608	CHL	C1B-NB	3.37	1.38	1.35
10	B	603	CLA	O2D-CGD	3.37	1.41	1.33
10	I	602	CLA	C1B-NB	3.37	1.38	1.35
9	C	607	CHL	C4B-NB	3.36	1.38	1.35
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	601	CHL	C1B-NB	3.36	1.38	1.35
9	F	606	CHL	C4B-NB	3.35	1.38	1.35
9	E	607	CHL	C4B-NB	3.35	1.38	1.35
10	F	604	CLA	C4B-NB	3.35	1.38	1.35
10	E	613	CLA	C4B-NB	3.35	1.38	1.35
10	E	603	CLA	C1B-NB	3.34	1.38	1.35
9	G	608	CHL	C4B-NB	3.34	1.38	1.35
10	A	614	CLA	O2D-CGD	3.34	1.41	1.33
9	G	601	CHL	C4B-NB	3.34	1.38	1.35
9	D	608	CHL	O2D-CGD	3.34	1.41	1.33
9	A	608	CHL	C1B-NB	3.34	1.38	1.35
4	A	621	LUT	C1-C6	3.34	1.58	1.53
9	I	606	CHL	O2D-CGD	3.33	1.41	1.33
9	C	605	CHL	C4B-NB	3.33	1.38	1.35
10	B	610	CLA	C4B-NB	3.32	1.38	1.35
9	E	607	CHL	C1B-NB	3.32	1.38	1.35
10	C	604	CLA	O2D-CED	-3.32	1.37	1.45
9	G	608	CHL	O2D-CED	-3.32	1.37	1.45
9	A	609	CHL	C4B-NB	3.31	1.38	1.35
9	D	609	CHL	C4B-NB	3.31	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	604	CLA	C4B-NB	3.31	1.38	1.35
9	H	601	CHL	C4B-NB	3.31	1.38	1.35
10	I	612	CLA	C4B-NB	3.30	1.38	1.35
10	E	602	CLA	C4B-NB	3.30	1.38	1.35
10	J	612	CLA	O2A-CGA	3.30	1.43	1.33
10	B	604	CLA	C4B-NB	3.29	1.38	1.35
9	I	608	CHL	C4B-NB	3.29	1.38	1.35
10	H	602	CLA	C4B-NB	3.28	1.38	1.35
10	A	611	CLA	C4B-NB	3.28	1.38	1.35
9	I	608	CHL	O2D-CED	-3.28	1.37	1.45
9	J	607	CHL	C4B-NB	3.27	1.38	1.35
9	J	607	CHL	CMB-C2B	3.27	1.58	1.51
10	G	613	CLA	C4B-NB	3.27	1.38	1.35
10	J	613	CLA	C4B-NB	3.27	1.38	1.35
9	G	607	CHL	C4B-NB	3.26	1.38	1.35
9	D	608	CHL	C4B-NB	3.26	1.38	1.35
9	D	607	CHL	C4B-NB	3.25	1.38	1.35
10	I	604	CLA	C1B-NB	3.24	1.38	1.35
10	H	613	CLA	C4B-NB	3.24	1.38	1.35
10	D	611	CLA	C4B-NB	3.24	1.38	1.35
10	D	602	CLA	C4B-NB	3.24	1.38	1.35
9	D	608	CHL	C1B-NB	3.24	1.38	1.35
9	D	609	CHL	C1B-NB	3.23	1.38	1.35
9	D	607	CHL	C1B-NB	3.23	1.38	1.35
4	E	4621	LUT	C23-C24	3.22	1.54	1.50
9	D	601	CHL	C1B-NB	3.22	1.38	1.35
9	F	609	CHL	C1B-NB	3.21	1.38	1.35
9	J	606	CHL	C4B-NB	3.21	1.38	1.35
10	B	603	CLA	C1B-NB	3.20	1.38	1.35
9	A	606	CHL	O2D-CGD	3.19	1.41	1.33
10	C	612	CLA	O2A-CGA	3.19	1.42	1.33
10	A	613	CLA	C1B-NB	3.18	1.38	1.35
10	A	604	CLA	C1B-NB	3.18	1.38	1.35
9	C	607	CHL	C1B-NB	3.17	1.38	1.35
10	D	612	CLA	O2D-CED	-3.17	1.37	1.45
10	E	604	CLA	C4B-NB	3.17	1.38	1.35
10	I	602	CLA	C4B-NB	3.17	1.38	1.35
10	G	612	CLA	O2D-CED	-3.17	1.37	1.45
9	G	607	CHL	C1B-NB	3.16	1.38	1.35
10	I	604	CLA	C4B-NB	3.16	1.38	1.35
10	A	612	CLA	O2A-CGA	3.16	1.42	1.33
9	F	607	CHL	CMB-C2B	3.16	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	613	CLA	C4B-NB	3.15	1.38	1.35
9	G	609	CHL	C1B-NB	3.15	1.38	1.35
9	H	608	CHL	O2D-CGD	3.13	1.40	1.33
7	I	8630	LHG	O7-C7	3.13	1.43	1.34
9	I	605	CHL	C4B-NB	3.13	1.38	1.35
10	D	603	CLA	O2D-CGD	3.13	1.40	1.33
9	I	607	CHL	C4B-NB	3.13	1.38	1.35
10	F	612	CLA	C2-C3	3.12	1.40	1.33
10	B	603	CLA	O2D-CED	-3.12	1.38	1.45
10	J	602	CLA	O2A-CGA	3.12	1.42	1.33
9	C	608	CHL	C4B-NB	3.11	1.38	1.35
10	B	603	CLA	C4B-NB	3.11	1.38	1.35
7	G	6630	LHG	O7-C7	3.11	1.43	1.34
9	F	601	CHL	O2D-CGD	3.11	1.40	1.33
10	E	611	CLA	O2D-CED	-3.10	1.38	1.45
10	F	612	CLA	O2D-CED	-3.10	1.38	1.45
10	H	612	CLA	C2-C3	3.10	1.40	1.33
9	F	607	CHL	C1B-NB	3.10	1.38	1.35
9	J	608	CHL	O2D-CED	-3.10	1.38	1.45
7	D	3630	LHG	O8-C23	3.09	1.42	1.33
10	G	613	CLA	C2-C3	3.09	1.40	1.33
10	G	604	CLA	C4B-NB	3.09	1.38	1.35
4	J	9621	LUT	C1-C6	3.09	1.58	1.53
7	C	2630	LHG	O7-C7	3.09	1.43	1.34
10	C	612	CLA	O2D-CED	-3.08	1.38	1.45
10	B	612	CLA	C2-C3	3.07	1.40	1.33
9	D	607	CHL	CMB-C2B	3.07	1.58	1.51
10	C	613	CLA	O2A-CGA	3.07	1.42	1.33
10	G	602	CLA	O2A-CGA	3.07	1.42	1.33
4	D	3621	LUT	C23-C24	3.07	1.54	1.50
7	J	9630	LHG	O8-C23	3.07	1.42	1.33
10	C	603	CLA	C1B-NB	3.06	1.37	1.35
9	J	607	CHL	C1B-NB	3.06	1.37	1.35
9	B	606	CHL	C4B-NB	3.06	1.37	1.35
9	H	609	CHL	O2D-CGD	3.06	1.40	1.33
10	C	603	CLA	O2D-CGD	3.06	1.40	1.33
9	B	608	CHL	O2D-CED	-3.04	1.38	1.45
10	B	613	CLA	C4B-NB	3.04	1.37	1.35
10	J	602	CLA	CHC-C1C	3.04	1.42	1.35
9	C	608	CHL	O2D-CED	-3.04	1.38	1.45
9	A	608	CHL	O2D-CED	-3.03	1.38	1.45
10	I	604	CLA	O2D-CED	-3.03	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	602	CLA	CHC-C1C	3.03	1.42	1.35
9	D	606	CHL	C4B-NB	3.03	1.37	1.35
9	G	607	CHL	CMB-C2B	3.03	1.57	1.51
10	F	613	CLA	C4B-NB	3.02	1.37	1.35
9	F	606	CHL	C2-C3	3.02	1.41	1.32
10	F	604	CLA	O2D-CED	-3.02	1.38	1.45
9	J	608	CHL	O2D-CGD	3.02	1.40	1.33
10	H	613	CLA	O2A-CGA	3.02	1.42	1.33
9	B	608	CHL	C2-C3	3.01	1.40	1.33
10	H	612	CLA	O2D-CED	-3.01	1.38	1.45
10	J	612	CLA	C2-C3	3.01	1.40	1.33
4	G	6621	LUT	C23-C24	3.01	1.54	1.50
9	A	606	CHL	C4B-NB	3.01	1.37	1.35
10	G	602	CLA	C1-C2	-3.01	1.40	1.49
10	I	602	CLA	C1-C2	-3.00	1.40	1.49
4	E	4620	LUT	C23-C24	2.99	1.54	1.50
9	B	606	CHL	O2D-CED	-2.99	1.38	1.45
9	F	608	CHL	O2D-CED	-2.98	1.38	1.45
10	G	612	CLA	C2-C3	2.98	1.40	1.33
10	D	602	CLA	C1-C2	-2.98	1.40	1.49
10	A	604	CLA	C4B-NB	2.98	1.37	1.35
10	E	610	CLA	CHC-C1C	2.97	1.42	1.35
10	F	610	CLA	CHC-C1C	2.97	1.42	1.35
10	I	610	CLA	CHC-C1C	2.97	1.42	1.35
9	C	601	CHL	O2A-CGA	2.96	1.42	1.33
7	A	630	LHG	O7-C7	2.96	1.42	1.34
4	A	621	LUT	C23-C24	2.96	1.54	1.50
10	I	612	CLA	C2-C3	2.96	1.40	1.33
10	F	602	CLA	CHC-C1C	2.96	1.42	1.35
10	F	613	CLA	C2-C3	2.95	1.40	1.33
4	B	1620	LUT	C23-C24	2.95	1.54	1.50
9	G	606	CHL	C2-C3	2.95	1.40	1.32
10	B	603	CLA	C3B-C2B	-2.95	1.36	1.40
10	D	612	CLA	C2-C3	2.95	1.40	1.33
9	C	606	CHL	C2-C3	2.94	1.40	1.32
10	H	602	CLA	O2D-CED	-2.94	1.38	1.45
10	H	613	CLA	C2-C3	2.94	1.40	1.33
10	G	602	CLA	O2D-CED	-2.94	1.38	1.45
10	H	611	CLA	C2-C3	2.94	1.40	1.33
10	A	602	CLA	CHC-C1C	2.93	1.42	1.35
9	A	606	CHL	CMB-C2B	2.93	1.57	1.51
10	E	604	CLA	C1B-NB	2.93	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	604	CLA	C2-C3	2.93	1.40	1.33
10	D	604	CLA	C1B-NB	2.92	1.37	1.35
9	A	606	CHL	C2-C3	2.92	1.40	1.32
9	F	606	CHL	CMB-C2B	2.92	1.57	1.51
10	E	612	CLA	C2-C3	2.92	1.40	1.33
9	B	607	CHL	C2-C3	2.92	1.40	1.33
9	I	605	CHL	O2D-CED	-2.92	1.38	1.45
9	J	607	CHL	O2A-CGA	2.92	1.41	1.33
10	C	611	CLA	C2-C3	2.92	1.40	1.33
10	D	613	CLA	CMB-C2B	2.91	1.57	1.51
9	E	609	CHL	CHC-C1C	2.91	1.42	1.35
10	A	613	CLA	C2-C3	2.91	1.40	1.33
10	F	603	CLA	C2-C3	2.91	1.40	1.33
10	I	602	CLA	CHC-C1C	2.91	1.42	1.35
9	F	608	CHL	C2-C3	2.91	1.40	1.33
9	C	609	CHL	O2D-CED	-2.91	1.38	1.45
9	J	606	CHL	CMB-C2B	2.91	1.57	1.51
9	J	609	CHL	CHC-C1C	2.91	1.42	1.35
10	D	604	CLA	O2D-CED	-2.90	1.38	1.45
9	D	609	CHL	O2D-CED	-2.90	1.38	1.45
9	I	608	CHL	C2-C3	2.90	1.39	1.33
4	J	9620	LUT	C5-C6	2.90	1.39	1.34
9	I	606	CHL	C4B-NB	2.90	1.37	1.35
4	F	5621	LUT	C23-C24	2.90	1.54	1.50
10	H	604	CLA	C2-C3	2.90	1.39	1.33
9	E	606	CHL	CMB-C2B	2.89	1.57	1.51
10	G	610	CLA	C2-C3	2.89	1.39	1.33
10	H	610	CLA	O2D-CED	-2.89	1.38	1.45
7	B	1630	LHG	O7-C7	2.89	1.42	1.34
10	C	602	CLA	C1-C2	-2.89	1.40	1.49
10	H	604	CLA	C4B-NB	2.89	1.37	1.35
10	F	610	CLA	C2-C3	2.89	1.39	1.33
10	J	613	CLA	C2-C3	2.88	1.39	1.33
10	I	613	CLA	C2-C3	2.88	1.39	1.33
10	C	610	CLA	CHC-C1C	2.88	1.42	1.35
9	H	608	CHL	C2-C3	2.88	1.39	1.33
4	H	7621	LUT	C23-C24	2.88	1.54	1.50
10	D	604	CLA	C4B-NB	2.88	1.37	1.35
10	H	602	CLA	CHC-C1C	2.87	1.42	1.35
9	H	606	CHL	C2-C3	2.87	1.40	1.32
10	E	602	CLA	CHC-C1C	2.87	1.42	1.35
10	G	611	CLA	C2-C3	2.87	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	607	CHL	O2D-CED	-2.87	1.38	1.45
10	A	611	CLA	C2-C3	2.86	1.39	1.33
10	B	613	CLA	C2-C3	2.86	1.39	1.33
10	J	611	CLA	C2-C3	2.86	1.39	1.33
10	J	603	CLA	CMB-C2B	2.86	1.57	1.51
10	J	603	CLA	O2D-CED	-2.86	1.38	1.45
10	B	604	CLA	C2-C3	2.86	1.39	1.33
4	G	6620	LUT	C5-C6	2.86	1.39	1.34
10	A	604	CLA	C2-C3	2.86	1.39	1.33
10	E	610	CLA	C2-C3	2.86	1.39	1.33
10	A	612	CLA	C2-C3	2.85	1.39	1.33
9	G	609	CHL	O2D-CED	-2.85	1.38	1.45
9	D	606	CHL	C2-C3	2.85	1.40	1.32
9	C	605	CHL	O2D-CED	-2.85	1.38	1.45
10	B	604	CLA	O2D-CED	-2.85	1.38	1.45
10	C	602	CLA	CHC-C1C	2.85	1.42	1.35
10	E	604	CLA	O2D-CED	-2.85	1.38	1.45
10	J	610	CLA	C2-C3	2.85	1.39	1.33
10	E	611	CLA	C2-C3	2.85	1.39	1.33
10	G	604	CLA	C2-C3	2.84	1.39	1.33
10	D	611	CLA	C2-C3	2.84	1.39	1.33
9	B	609	CHL	O2D-CED	-2.84	1.38	1.45
10	I	604	CLA	C2-C3	2.84	1.39	1.33
9	J	608	CHL	C2-C3	2.84	1.39	1.33
10	A	603	CLA	O2D-CED	-2.84	1.38	1.45
10	J	604	CLA	C1B-NB	2.84	1.37	1.35
9	H	609	CHL	C2-C3	2.83	1.39	1.33
9	H	607	CHL	C2-C3	2.83	1.39	1.33
9	A	608	CHL	C2-C3	2.83	1.39	1.33
9	F	607	CHL	C2-C3	2.83	1.39	1.33
9	E	606	CHL	C4B-NB	2.83	1.37	1.35
10	E	613	CLA	C2-C3	2.83	1.39	1.33
9	J	609	CHL	O2D-CED	-2.83	1.38	1.45
9	E	606	CHL	C2-C3	2.83	1.40	1.32
9	I	606	CHL	C2-C3	2.83	1.40	1.32
10	G	603	CLA	CMB-C2B	2.83	1.57	1.51
10	B	611	CLA	C2-C3	2.83	1.39	1.33
10	A	604	CLA	O2D-CED	-2.83	1.38	1.45
9	E	609	CHL	O2D-CGD	2.82	1.40	1.33
10	C	610	CLA	C2-C3	2.82	1.39	1.33
10	D	613	CLA	C2-C3	2.82	1.39	1.33
10	G	610	CLA	CHC-C1C	2.81	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	601	CHL	C2-C3	2.81	1.39	1.33
9	J	608	CHL	CHC-C1C	2.81	1.42	1.35
9	E	609	CHL	C2-C3	2.81	1.39	1.33
10	B	610	CLA	CHC-C1C	2.81	1.42	1.35
9	B	609	CHL	C2-C3	2.81	1.39	1.33
9	J	606	CHL	C2-C3	2.81	1.40	1.32
10	H	610	CLA	C2-C3	2.81	1.39	1.33
10	J	603	CLA	C2-C3	2.81	1.39	1.33
10	F	604	CLA	C2-C3	2.80	1.39	1.33
10	D	610	CLA	C2-C3	2.80	1.39	1.33
10	E	612	CLA	C3B-C2B	-2.80	1.36	1.40
10	C	604	CLA	C2-C3	2.80	1.39	1.33
9	E	608	CHL	C2-C3	2.80	1.39	1.33
10	E	610	CLA	O2D-CED	-2.80	1.38	1.45
9	I	607	CHL	C2-C3	2.80	1.39	1.33
10	J	612	CLA	O2D-CED	-2.80	1.38	1.45
9	B	606	CHL	C2-C3	2.80	1.40	1.32
10	H	604	CLA	C1B-NB	2.80	1.37	1.35
9	G	607	CHL	C2-C3	2.80	1.39	1.33
10	C	612	CLA	C2-C3	2.79	1.39	1.33
10	B	602	CLA	CHC-C1C	2.79	1.42	1.35
9	A	609	CHL	C3B-C2B	-2.79	1.36	1.40
9	G	605	CHL	CMB-C2B	2.79	1.57	1.51
10	D	612	CLA	CMB-C2B	2.78	1.57	1.51
9	A	607	CHL	C2-C3	2.78	1.39	1.33
10	D	602	CLA	O2D-CED	-2.78	1.38	1.45
8	B	1632	DGD	O1G-C1A	2.77	1.41	1.33
9	E	601	CHL	C2-C3	2.77	1.39	1.33
4	E	4620	LUT	C5-C6	2.76	1.39	1.34
10	A	610	CLA	CHC-C1C	2.76	1.42	1.35
10	H	614	CLA	CHC-C1C	2.76	1.42	1.35
9	J	601	CHL	C2-C3	2.76	1.39	1.33
7	D	3630	LHG	O7-C7	2.76	1.42	1.34
9	C	606	CHL	CMB-C2B	2.76	1.57	1.51
9	D	608	CHL	O2D-CED	-2.76	1.38	1.45
10	E	602	CLA	C2-C3	2.76	1.39	1.33
9	A	601	CHL	O2D-CED	-2.75	1.38	1.45
10	F	611	CLA	C2-C3	2.75	1.39	1.33
10	I	611	CLA	C2-C3	2.75	1.39	1.33
10	E	603	CLA	O2D-CED	-2.75	1.38	1.45
9	A	609	CHL	O2D-CED	-2.75	1.38	1.45
9	D	607	CHL	C2-C3	2.75	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	4630	LHG	O7-C7	2.75	1.42	1.34
9	G	609	CHL	C2-C3	2.74	1.39	1.33
9	F	609	CHL	C2-C3	2.74	1.39	1.33
10	E	603	CLA	C2-C3	2.74	1.39	1.33
10	H	610	CLA	CHC-C1C	2.74	1.42	1.35
9	F	609	CHL	O2D-CGD	2.74	1.39	1.33
10	B	612	CLA	CMB-C2B	2.74	1.57	1.51
10	J	610	CLA	CHC-C1C	2.74	1.42	1.35
9	J	607	CHL	C2-C3	2.74	1.39	1.33
9	C	609	CHL	C2-C3	2.73	1.39	1.33
9	C	607	CHL	C2-C3	2.73	1.39	1.33
10	E	604	CLA	C2-C3	2.73	1.39	1.33
9	I	609	CHL	C2-C3	2.73	1.39	1.33
10	C	603	CLA	C2-C3	2.73	1.39	1.33
4	C	2621	LUT	C24-C25	2.73	1.36	1.33
9	A	609	CHL	CHC-C1C	2.73	1.42	1.35
10	J	604	CLA	O2D-CED	-2.73	1.38	1.45
10	J	604	CLA	C2-C3	2.73	1.39	1.33
9	G	601	CHL	C2-C3	2.73	1.39	1.33
10	D	610	CLA	CHC-C1C	2.72	1.42	1.35
10	G	613	CLA	O2D-CED	-2.72	1.38	1.45
10	H	603	CLA	C2-C3	2.72	1.39	1.33
9	I	609	CHL	CHC-C1C	2.72	1.41	1.35
4	A	621	LUT	C24-C25	2.71	1.36	1.33
4	C	2620	LUT	C23-C24	2.71	1.54	1.50
10	I	603	CLA	C2-C3	2.71	1.39	1.33
10	D	603	CLA	O2D-CED	-2.71	1.38	1.45
10	J	613	CLA	O2D-CED	-2.71	1.38	1.45
9	H	607	CHL	O2D-CED	-2.71	1.38	1.45
10	J	602	CLA	O2D-CED	-2.70	1.39	1.45
9	G	608	CHL	C2-C3	2.70	1.39	1.33
9	D	609	CHL	C2-C3	2.70	1.39	1.33
9	J	601	CHL	O2D-CED	-2.70	1.39	1.45
9	C	609	CHL	CHC-C1C	2.69	1.41	1.35
10	G	604	CLA	O2D-CED	-2.69	1.39	1.45
9	B	609	CHL	CHC-C1C	2.69	1.41	1.35
9	I	608	CHL	CHC-C1C	2.69	1.41	1.35
9	C	601	CHL	CHC-C1C	2.69	1.41	1.35
9	I	609	CHL	C3B-C2B	-2.68	1.36	1.40
9	D	607	CHL	O2A-CGA	2.68	1.41	1.33
9	J	609	CHL	C3B-C2B	-2.68	1.36	1.40
10	C	613	CLA	C2-C3	2.68	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	603	CLA	C2-C3	2.68	1.39	1.33
9	A	608	CHL	CHC-C1C	2.67	1.41	1.35
9	E	608	CHL	CHC-C1C	2.67	1.41	1.35
9	D	607	CHL	O2D-CED	-2.67	1.39	1.45
10	I	610	CLA	C2-C3	2.67	1.39	1.33
4	B	1621	LUT	C23-C24	2.67	1.54	1.50
7	B	1630	LHG	C26-C25	-2.67	1.36	1.51
9	D	609	CHL	CHC-C1C	2.67	1.41	1.35
10	I	612	CLA	C3B-C2B	-2.67	1.36	1.40
10	I	603	CLA	O2D-CED	-2.67	1.39	1.45
9	A	608	CHL	C3B-C2B	-2.66	1.36	1.40
9	F	609	CHL	O2D-CED	-2.66	1.39	1.45
4	E	4621	LUT	C24-C25	2.66	1.36	1.33
9	E	607	CHL	C2-C3	2.66	1.39	1.33
10	B	612	CLA	O2D-CED	-2.66	1.39	1.45
10	D	602	CLA	CHC-C1C	2.66	1.41	1.35
10	I	602	CLA	C3B-C2B	-2.66	1.36	1.40
10	I	613	CLA	O2D-CED	-2.66	1.39	1.45
10	D	603	CLA	C2-C3	2.66	1.39	1.33
10	G	603	CLA	C2-C3	2.65	1.39	1.33
9	B	601	CHL	C2-C3	2.65	1.39	1.33
9	C	601	CHL	C2-C3	2.65	1.39	1.33
9	G	609	CHL	CHC-C1C	2.65	1.41	1.35
7	I	8630	LHG	C26-C25	-2.65	1.36	1.51
10	A	611	CLA	O2D-CED	-2.65	1.39	1.45
9	E	607	CHL	CMB-C2B	2.65	1.57	1.51
4	C	2621	LUT	C1-C6	2.65	1.57	1.53
7	J	9630	LHG	C26-C25	-2.64	1.36	1.51
10	A	610	CLA	C2-C3	2.64	1.39	1.33
9	C	609	CHL	C3B-C2B	-2.64	1.36	1.40
9	D	608	CHL	C2-C3	2.64	1.39	1.33
9	I	601	CHL	C2-C3	2.64	1.39	1.33
10	J	602	CLA	C1-C2	-2.64	1.41	1.49
9	D	601	CHL	C2-C3	2.63	1.39	1.33
9	D	606	CHL	CMB-C2B	2.63	1.57	1.51
10	H	610	CLA	C3B-C2B	-2.63	1.36	1.40
9	A	601	CHL	C2-C3	2.63	1.39	1.33
9	F	609	CHL	CHC-C1C	2.63	1.41	1.35
10	D	614	CLA	CHC-C1C	2.63	1.41	1.35
9	J	605	CHL	O2D-CED	-2.62	1.39	1.45
10	B	610	CLA	C2-C3	2.62	1.39	1.33
9	F	601	CHL	O2D-CED	-2.62	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	608	CHL	O2D-CED	-2.62	1.39	1.45
9	A	605	CHL	CHC-C1C	2.61	1.41	1.35
9	J	609	CHL	C2-C3	2.61	1.39	1.33
10	G	614	CLA	CHC-C1C	2.61	1.41	1.35
9	E	609	CHL	C3B-C2B	-2.61	1.36	1.40
4	I	8620	LUT	C23-C24	2.61	1.53	1.50
9	I	601	CHL	O2D-CED	-2.61	1.39	1.45
10	E	614	CLA	CHC-C1C	2.61	1.41	1.35
10	E	602	CLA	C3B-C2B	-2.61	1.36	1.40
10	F	614	CLA	CHC-C1C	2.61	1.41	1.35
9	D	609	CHL	C3B-C2B	-2.61	1.36	1.40
7	D	3630	LHG	C26-C25	-2.60	1.37	1.51
9	F	601	CHL	C2-C3	2.60	1.39	1.33
9	H	601	CHL	O2D-CED	-2.60	1.39	1.45
10	F	603	CLA	C3B-C2B	-2.60	1.36	1.40
10	A	602	CLA	C2-C3	2.60	1.39	1.33
9	G	601	CHL	CHC-C1C	2.60	1.41	1.35
10	B	610	CLA	CMB-C2B	2.60	1.57	1.51
10	B	610	CLA	C3B-C2B	-2.59	1.36	1.40
10	C	613	CLA	CMC-C2C	2.59	1.56	1.50
9	D	605	CHL	CHC-C1C	2.59	1.41	1.35
10	A	603	CLA	C2-C3	2.59	1.39	1.33
9	C	608	CHL	C2-C3	2.59	1.39	1.33
9	E	609	CHL	C1-C2	-2.59	1.41	1.49
10	H	602	CLA	C3B-C2B	-2.59	1.36	1.40
10	A	602	CLA	O2D-CED	-2.58	1.39	1.45
10	H	612	CLA	C3B-C2B	-2.58	1.36	1.40
8	G	9632	DGD	O1G-C1A	2.57	1.40	1.33
9	H	605	CHL	CMB-C2B	2.57	1.57	1.51
7	G	6630	LHG	C26-C25	-2.57	1.37	1.51
10	H	602	CLA	C1-C2	-2.57	1.41	1.49
7	E	4630	LHG	C26-C25	-2.57	1.37	1.51
10	I	602	CLA	O2D-CED	-2.57	1.39	1.45
10	C	611	CLA	O2D-CED	-2.57	1.39	1.45
10	C	602	CLA	C2-C3	2.57	1.39	1.33
9	B	601	CHL	CHC-C1C	2.56	1.41	1.35
10	B	602	CLA	O2D-CED	-2.56	1.39	1.45
10	E	603	CLA	C3B-C2B	-2.56	1.36	1.40
4	E	4620	LUT	C24-C25	2.56	1.36	1.33
10	D	602	CLA	C3B-C2B	-2.55	1.36	1.40
9	F	605	CHL	CHC-C1C	2.55	1.41	1.35
9	E	609	CHL	O2D-CED	-2.55	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	602	CLA	C3B-C2B	-2.55	1.36	1.40
9	H	609	CHL	CHC-C1C	2.55	1.41	1.35
9	J	608	CHL	C3B-C2B	-2.55	1.36	1.40
9	A	609	CHL	C2-C3	2.55	1.39	1.33
9	F	601	CHL	CHC-C1C	2.55	1.41	1.35
9	I	608	CHL	C3B-C2B	-2.55	1.36	1.40
10	C	610	CLA	O2D-CED	-2.54	1.39	1.45
10	A	610	CLA	C3B-C2B	-2.54	1.36	1.40
10	I	614	CLA	CHC-C1C	2.54	1.41	1.35
10	J	613	CLA	CHC-C1C	2.54	1.41	1.35
10	G	612	CLA	C3B-C2B	-2.54	1.36	1.40
9	H	601	CHL	CHC-C1C	2.53	1.41	1.35
4	E	4621	LUT	C1-C6	2.53	1.57	1.53
9	D	605	CHL	O2D-CED	-2.53	1.39	1.45
10	H	603	CLA	O2D-CED	-2.53	1.39	1.45
10	I	612	CLA	CMB-C2B	2.53	1.56	1.51
4	A	620	LUT	C23-C24	2.53	1.53	1.50
9	C	606	CHL	CHC-C1C	2.52	1.41	1.35
9	E	609	CHL	CMB-C2B	2.52	1.56	1.51
9	H	608	CHL	CHC-C1C	2.52	1.41	1.35
9	E	607	CHL	O2D-CED	-2.51	1.39	1.45
10	B	614	CLA	CHC-C1C	2.51	1.41	1.35
4	J	9621	LUT	C23-C24	2.51	1.53	1.50
9	I	606	CHL	CHC-C1C	2.51	1.41	1.35
10	B	602	CLA	C1-C2	-2.51	1.41	1.49
9	F	609	CHL	C3B-C2B	-2.51	1.36	1.40
4	G	6621	LUT	C24-C25	2.50	1.36	1.33
9	F	608	CHL	CHC-C1C	2.50	1.41	1.35
10	F	602	CLA	C1-C2	-2.50	1.41	1.49
9	I	607	CHL	O2D-CED	-2.50	1.39	1.45
9	B	606	CHL	CMB-C2B	2.50	1.56	1.51
4	J	9620	LUT	C26-C27	2.50	1.54	1.50
10	I	611	CLA	CHC-C1C	2.50	1.41	1.35
9	J	601	CHL	CHC-C1C	2.50	1.41	1.35
9	H	606	CHL	CMB-C2B	2.49	1.56	1.51
4	G	6620	LUT	C23-C24	2.49	1.53	1.50
9	C	608	CHL	CHC-C1C	2.49	1.41	1.35
9	E	601	CHL	CHC-C1C	2.49	1.41	1.35
9	G	608	CHL	CHC-C1C	2.49	1.41	1.35
10	J	614	CLA	CMB-C2B	2.49	1.56	1.51
10	G	604	CLA	C4-C3	2.49	1.57	1.50
9	D	608	CHL	C3B-C2B	-2.49	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	605	CHL	O2D-CED	-2.49	1.39	1.45
10	F	612	CLA	C3B-C2B	-2.48	1.36	1.40
10	B	614	CLA	CMB-C2B	2.48	1.56	1.51
9	E	606	CHL	O2D-CED	-2.48	1.39	1.45
10	H	604	CLA	O2D-CED	-2.48	1.39	1.45
10	I	603	CLA	C3B-C2B	-2.48	1.36	1.40
10	B	613	CLA	C5-C3	2.48	1.56	1.51
9	E	601	CHL	CMB-C2B	2.48	1.56	1.51
10	B	602	CLA	C2-C3	2.48	1.38	1.33
10	F	612	CLA	CHC-C1C	2.47	1.41	1.35
10	C	614	CLA	CMB-C2B	2.47	1.56	1.51
10	E	613	CLA	CHC-C1C	2.47	1.41	1.35
9	H	606	CHL	O2D-CED	-2.47	1.39	1.45
4	D	3621	LUT	C24-C25	2.47	1.36	1.33
10	H	614	CLA	C3B-C2B	-2.47	1.36	1.40
10	I	611	CLA	C3B-C2B	-2.47	1.36	1.40
10	D	603	CLA	CHC-C1C	2.47	1.41	1.35
9	G	606	CHL	CHC-C1C	2.46	1.41	1.35
9	I	605	CHL	CMB-C2B	2.46	1.56	1.51
9	G	609	CHL	C3B-C2B	-2.46	1.37	1.40
9	C	601	CHL	O2D-CED	-2.45	1.39	1.45
4	D	3620	LUT	C5-C6	2.45	1.38	1.34
7	F	5630	LHG	C26-C25	-2.45	1.37	1.51
4	D	3620	LUT	C23-C24	2.45	1.53	1.50
9	C	608	CHL	C1-C2	-2.45	1.41	1.49
10	I	603	CLA	CMB-C2B	2.45	1.56	1.51
9	J	609	CHL	C1-C2	-2.45	1.41	1.49
10	C	612	CLA	C3B-C2B	-2.45	1.37	1.40
10	C	603	CLA	C3B-C2B	-2.45	1.37	1.40
10	D	613	CLA	O2D-CED	-2.45	1.39	1.45
7	C	2630	LHG	C26-C25	-2.45	1.37	1.51
10	E	614	CLA	CMB-C2B	2.45	1.56	1.51
10	D	612	CLA	C3B-C2B	-2.45	1.37	1.40
9	B	608	CHL	CHC-C1C	2.45	1.41	1.35
10	E	611	CLA	CHC-C1C	2.44	1.41	1.35
10	G	610	CLA	C3B-C2B	-2.44	1.37	1.40
9	G	605	CHL	CHC-C1C	2.44	1.41	1.35
9	H	609	CHL	O2D-CED	-2.44	1.39	1.45
9	I	606	CHL	O2D-CED	-2.44	1.39	1.45
9	A	607	CHL	CHC-C1C	2.44	1.41	1.35
10	D	602	CLA	CMC-C2C	2.44	1.56	1.50
10	E	602	CLA	CMC-C2C	2.44	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	603	CLA	C3B-C2B	-2.44	1.37	1.40
10	D	614	CLA	C3B-C2B	-2.44	1.37	1.40
9	C	605	CHL	CHC-C1C	2.43	1.41	1.35
9	B	606	CHL	CHC-C1C	2.43	1.41	1.35
4	F	5621	LUT	C5-C6	2.43	1.38	1.34
10	I	611	CLA	CMB-C2B	2.43	1.56	1.51
9	G	608	CHL	C3B-C2B	-2.43	1.37	1.40
9	E	605	CHL	CHC-C1C	2.43	1.41	1.35
9	H	608	CHL	C3B-C2B	-2.42	1.37	1.40
9	J	605	CHL	CHC-C1C	2.42	1.41	1.35
9	C	608	CHL	C3B-C2B	-2.42	1.37	1.40
4	B	1621	LUT	C5-C6	2.42	1.38	1.34
10	D	602	CLA	C2-C3	2.42	1.38	1.33
9	F	608	CHL	C3B-C2B	-2.41	1.37	1.40
10	B	603	CLA	CMC-C2C	2.41	1.55	1.50
9	H	607	CHL	CHC-C1C	2.41	1.41	1.35
10	F	603	CLA	CHC-C1C	2.41	1.41	1.35
9	A	606	CHL	CHC-C1C	2.41	1.41	1.35
4	F	5621	LUT	C24-C25	2.41	1.36	1.33
4	B	1621	LUT	C24-C25	2.41	1.36	1.33
9	I	601	CHL	CHC-C1C	2.41	1.41	1.35
10	D	613	CLA	CMC-C2C	2.41	1.55	1.50
10	H	603	CLA	C3B-C2B	-2.41	1.37	1.40
10	C	613	CLA	CMB-C2B	2.41	1.56	1.51
9	F	606	CHL	CHC-C1C	2.40	1.41	1.35
9	B	609	CHL	C3B-C2B	-2.40	1.37	1.40
10	C	602	CLA	C3B-C2B	-2.40	1.37	1.40
10	J	603	CLA	C3B-C2B	-2.40	1.37	1.40
9	D	606	CHL	CHC-C1C	2.40	1.41	1.35
9	B	605	CHL	CHC-C1C	2.40	1.41	1.35
4	F	5620	LUT	C23-C24	2.40	1.53	1.50
9	D	601	CHL	CHC-C1C	2.40	1.41	1.35
10	H	611	CLA	C3B-C2B	-2.39	1.37	1.40
9	I	605	CHL	CHC-C1C	2.39	1.41	1.35
4	I	8621	LUT	C23-C24	2.39	1.53	1.50
4	E	4621	LUT	C26-C27	2.39	1.53	1.50
10	D	603	CLA	C3B-C2B	-2.39	1.37	1.40
10	A	613	CLA	CMC-C2C	2.39	1.55	1.50
4	B	1620	LUT	C5-C6	2.39	1.38	1.34
4	I	8621	LUT	C1-C6	2.39	1.57	1.53
10	G	613	CLA	CMB-C2B	2.39	1.56	1.51
10	G	614	CLA	CMB-C2B	2.38	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	614	CLA	CHC-C1C	2.38	1.41	1.35
10	J	610	CLA	C3B-C2B	-2.38	1.37	1.40
4	D	3621	LUT	C26-C27	2.38	1.53	1.50
9	H	606	CHL	CHC-C1C	2.38	1.41	1.35
4	D	3621	LUT	C5-C6	2.38	1.38	1.34
10	A	613	CLA	CHC-C1C	2.38	1.41	1.35
7	A	630	LHG	C26-C25	-2.38	1.38	1.51
9	H	608	CHL	CMB-C2B	2.38	1.56	1.51
10	D	610	CLA	O2D-CED	-2.37	1.39	1.45
9	J	606	CHL	CHC-C1C	2.37	1.41	1.35
9	D	607	CHL	CHC-C1C	2.37	1.41	1.35
9	G	607	CHL	O2D-CED	-2.37	1.39	1.45
9	A	607	CHL	O2D-CED	-2.37	1.39	1.45
10	F	611	CLA	CHC-C1C	2.37	1.41	1.35
9	E	608	CHL	C3B-C2B	-2.37	1.37	1.40
9	C	607	CHL	CMB-C2B	2.37	1.56	1.51
4	J	9621	LUT	C24-C25	2.37	1.36	1.33
10	J	612	CLA	C3B-C2B	-2.36	1.37	1.40
9	B	605	CHL	C3B-C2B	-2.36	1.37	1.40
10	E	612	CLA	CMB-C2B	2.36	1.56	1.51
9	B	608	CHL	C3B-C2B	-2.36	1.37	1.40
10	G	613	CLA	CMC-C2C	2.36	1.55	1.50
10	G	602	CLA	C2-C3	2.36	1.38	1.33
10	D	610	CLA	C3B-C2B	-2.36	1.37	1.40
10	F	614	CLA	C3B-C2B	-2.36	1.37	1.40
7	H	7630	LHG	C26-C25	-2.36	1.38	1.51
10	C	611	CLA	C3B-C2B	-2.36	1.37	1.40
4	F	5620	LUT	C5-C6	2.36	1.38	1.34
9	J	601	CHL	C3B-C2B	-2.35	1.37	1.40
10	I	604	CLA	C4-C3	2.35	1.56	1.50
10	F	602	CLA	C2-C3	2.35	1.38	1.33
8	A	632	DGD	O1G-C1A	2.35	1.40	1.33
10	H	602	CLA	C2-C3	2.35	1.38	1.33
9	C	608	CHL	CMB-C2B	2.35	1.56	1.51
10	G	604	CLA	CMC-C2C	2.35	1.55	1.50
10	B	602	CLA	C3B-C2B	-2.35	1.37	1.40
9	D	609	CHL	C4-C3	2.35	1.56	1.50
10	B	612	CLA	CBD-CGD	2.35	1.59	1.52
9	A	605	CHL	C3B-C2B	-2.35	1.37	1.40
9	D	605	CHL	CMB-C2B	2.34	1.56	1.51
10	F	603	CLA	CBD-CGD	2.34	1.59	1.52
10	B	603	CLA	CMB-C2B	2.34	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	602	CLA	CMC-C2C	2.34	1.55	1.50
10	C	614	CLA	CHC-C1C	2.34	1.41	1.35
8	D	3632	DGD	O1G-C1A	2.34	1.40	1.33
10	B	611	CLA	O2D-CED	-2.33	1.39	1.45
10	B	610	CLA	O2D-CED	-2.33	1.39	1.45
10	D	611	CLA	C3B-C2B	-2.33	1.37	1.40
10	J	611	CLA	CHC-C1C	2.33	1.40	1.35
10	G	603	CLA	O2D-CED	-2.33	1.39	1.45
4	C	2621	LUT	C26-C27	2.33	1.53	1.50
9	B	609	CHL	C1-C2	-2.33	1.42	1.49
10	A	613	CLA	CMB-C2B	2.33	1.56	1.51
10	I	602	CLA	C2-C3	2.33	1.38	1.33
10	C	610	CLA	CBD-CGD	2.33	1.59	1.52
9	A	605	CHL	O2D-CED	-2.32	1.39	1.45
9	J	601	CHL	CMB-C2B	2.32	1.56	1.51
9	G	609	CHL	MG-NC	2.32	2.11	2.06
4	A	621	LUT	C5-C6	2.32	1.38	1.34
10	F	604	CLA	C5-C3	2.32	1.56	1.51
10	A	603	CLA	CMB-C2B	2.32	1.56	1.51
9	A	601	CHL	CHC-C1C	2.32	1.40	1.35
9	C	605	CHL	CMB-C2B	2.32	1.56	1.51
10	G	610	CLA	CAC-C3C	2.32	1.57	1.51
9	B	607	CHL	CMB-C2B	2.32	1.56	1.51
10	G	613	CLA	C5-C3	2.31	1.56	1.51
10	H	613	CLA	CMB-C2B	2.31	1.56	1.51
9	B	605	CHL	CMB-C2B	2.31	1.56	1.51
10	G	614	CLA	C3B-C2B	-2.31	1.37	1.40
10	A	612	CLA	CHC-C1C	2.31	1.40	1.35
9	D	608	CHL	CHC-C1C	2.31	1.40	1.35
9	C	609	CHL	C4-C3	2.31	1.56	1.50
10	B	611	CLA	CMB-C2B	2.31	1.56	1.51
10	F	613	CLA	O2D-CED	-2.31	1.39	1.45
10	J	602	CLA	C2-C3	2.31	1.38	1.33
4	B	1620	LUT	C24-C25	2.31	1.36	1.33
10	E	603	CLA	CMB-C2B	2.31	1.56	1.51
10	E	603	CLA	CHC-C1C	2.31	1.40	1.35
10	J	610	CLA	O2D-CED	-2.30	1.39	1.45
10	J	611	CLA	O2D-CED	-2.30	1.39	1.45
10	J	610	CLA	CMB-C2B	2.30	1.56	1.51
10	C	603	CLA	CHC-C1C	2.30	1.40	1.35
10	B	614	CLA	O2D-CED	-2.30	1.39	1.45
9	H	605	CHL	CHC-C1C	2.30	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	612	CLA	C3B-C2B	-2.30	1.37	1.40
6	I	8623	NEX	C1-C6	2.30	1.58	1.54
10	J	603	CLA	CHC-C1C	2.30	1.40	1.35
9	E	601	CHL	C3B-C2B	-2.29	1.37	1.40
4	H	7621	LUT	C24-C25	2.29	1.36	1.33
10	F	610	CLA	O2D-CED	-2.29	1.39	1.45
10	A	611	CLA	CHC-C1C	2.29	1.40	1.35
4	A	620	LUT	C5-C6	2.29	1.38	1.34
8	H	7632	DGD	O1G-C1A	2.29	1.40	1.33
9	H	601	CHL	C3B-C2B	-2.29	1.37	1.40
10	G	603	CLA	C3B-C2B	-2.29	1.37	1.40
9	E	607	CHL	CHC-C1C	2.29	1.40	1.35
10	I	614	CLA	C3B-C2B	-2.29	1.37	1.40
6	C	2623	NEX	C1-C6	2.29	1.58	1.54
9	C	607	CHL	O2D-CED	-2.29	1.39	1.45
10	J	614	CLA	CHC-C1C	2.29	1.40	1.35
9	B	609	CHL	C4-C3	2.28	1.56	1.50
10	D	611	CLA	CHC-C1C	2.28	1.40	1.35
10	F	602	CLA	CMB-C2B	2.28	1.56	1.51
10	J	613	CLA	C3B-C2B	-2.28	1.37	1.40
9	H	607	CHL	CMB-C2B	2.28	1.56	1.51
9	H	609	CHL	C3B-C2B	-2.28	1.37	1.40
10	C	612	CLA	CHC-C1C	2.28	1.40	1.35
10	C	610	CLA	C3B-C2B	-2.28	1.37	1.40
4	E	4620	LUT	C1-C6	2.28	1.56	1.53
4	I	8621	LUT	C5-C6	2.28	1.38	1.34
9	I	606	CHL	C4-C3	2.28	1.56	1.50
10	E	610	CLA	C3B-C2B	-2.27	1.37	1.40
4	H	7620	LUT	C5-C6	2.27	1.38	1.34
10	G	612	CLA	CHC-C1C	2.27	1.40	1.35
10	G	602	CLA	C3B-C2B	-2.27	1.37	1.40
10	I	610	CLA	CMB-C2B	2.27	1.56	1.51
9	J	605	CHL	C3B-C2B	-2.27	1.37	1.40
9	G	606	CHL	C4-C3	2.27	1.56	1.50
9	C	601	CHL	C3B-C2B	-2.27	1.37	1.40
10	G	610	CLA	O2D-CED	-2.27	1.40	1.45
9	J	601	CHL	C4-C3	2.27	1.56	1.50
10	I	602	CLA	CMB-C2B	2.27	1.56	1.51
10	H	610	CLA	CMB-C2B	2.27	1.56	1.51
10	J	602	CLA	C3B-C2B	-2.27	1.37	1.40
10	D	612	CLA	CHC-C1C	2.26	1.40	1.35
9	F	606	CHL	C5-C3	2.26	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	610	CLA	CMB-C2B	2.26	1.56	1.51
10	G	611	CLA	O2D-CED	-2.26	1.40	1.45
10	H	614	CLA	O2D-CGD	2.26	1.38	1.33
9	E	608	CHL	CMB-C2B	2.26	1.56	1.51
9	J	606	CHL	C4-C3	2.26	1.56	1.50
10	C	613	CLA	C1-C2	-2.26	1.42	1.49
5	C	7622	XAT	C28-C27	2.26	1.37	1.32
10	H	603	CLA	CHC-C1C	2.26	1.40	1.35
9	D	601	CHL	C3B-C2B	-2.25	1.37	1.40
10	F	602	CLA	C3B-C2B	-2.25	1.37	1.40
9	I	601	CHL	CMB-C2B	2.25	1.56	1.51
9	G	608	CHL	CMB-C2B	2.25	1.56	1.51
9	E	605	CHL	O2D-CED	-2.25	1.40	1.45
10	J	611	CLA	C3B-C2B	-2.25	1.37	1.40
10	I	612	CLA	CHC-C1C	2.24	1.40	1.35
10	G	611	CLA	CHC-C1C	2.24	1.40	1.35
10	C	611	CLA	CHC-C1C	2.24	1.40	1.35
9	E	601	CHL	O2D-CED	-2.24	1.40	1.45
9	I	607	CHL	CHC-C1C	2.24	1.40	1.35
10	E	611	CLA	C3B-C2B	-2.23	1.37	1.40
10	G	603	CLA	CHC-C1C	2.23	1.40	1.35
5	D	8622	XAT	C28-C27	2.23	1.37	1.32
10	E	603	CLA	CAC-C3C	2.23	1.56	1.51
9	G	606	CHL	C5-C3	2.23	1.56	1.50
10	H	612	CLA	CMB-C2B	2.23	1.56	1.51
10	E	610	CLA	CMB-C2B	2.23	1.56	1.51
10	G	604	CLA	C5-C3	2.23	1.55	1.51
9	D	606	CHL	C5-C3	2.23	1.56	1.50
6	J	9623	NEX	C1-C6	2.23	1.58	1.54
10	F	610	CLA	C3B-C2B	-2.23	1.37	1.40
9	J	605	CHL	CMB-C2B	2.23	1.56	1.51
10	E	613	CLA	CMC-C2C	2.22	1.55	1.50
10	D	613	CLA	CHC-C1C	2.22	1.40	1.35
9	J	606	CHL	C5-C3	2.22	1.56	1.50
9	B	605	CHL	CBD-CGD	2.22	1.59	1.52
10	G	611	CLA	C3B-C2B	-2.22	1.37	1.40
10	E	604	CLA	C4-C3	2.22	1.56	1.50
10	E	612	CLA	O2D-CED	-2.22	1.40	1.45
9	B	601	CHL	C3B-C2B	-2.21	1.37	1.40
10	G	614	CLA	CAC-C3C	2.21	1.56	1.51
4	B	1621	LUT	C1-C6	2.21	1.56	1.53
10	B	602	CLA	CMB-C2B	2.21	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	612	CLA	CHC-C1C	2.21	1.40	1.35
9	D	607	CHL	C4-C3	2.21	1.56	1.50
9	E	606	CHL	C4-C3	2.20	1.56	1.50
4	H	7621	LUT	C1-C6	2.20	1.56	1.53
10	C	611	CLA	CMB-C2B	2.20	1.56	1.51
10	J	602	CLA	CMB-C2B	2.20	1.56	1.51
10	F	610	CLA	C4-C3	2.20	1.56	1.50
9	G	605	CHL	C3B-C2B	-2.19	1.37	1.40
10	A	610	CLA	CAC-C3C	2.19	1.56	1.51
4	F	5621	LUT	C1-C6	2.19	1.56	1.53
10	F	613	CLA	C1-C2	-2.19	1.42	1.49
10	C	614	CLA	O2D-CED	-2.19	1.40	1.45
10	I	610	CLA	C4-C3	2.19	1.56	1.50
9	D	601	CHL	CMB-C2B	2.19	1.56	1.51
10	A	612	CLA	C3B-C2B	-2.19	1.37	1.40
4	A	620	LUT	C26-C27	2.19	1.53	1.50
6	A	623	NEX	C1-C6	2.18	1.58	1.54
10	A	614	CLA	C3B-C2B	-2.18	1.37	1.40
4	I	8621	LUT	C24-C25	2.18	1.35	1.33
10	G	602	CLA	C4-C3	2.18	1.56	1.50
9	D	606	CHL	C4-C3	2.18	1.56	1.50
10	A	613	CLA	C1-C2	-2.18	1.42	1.49
5	I	9622	XAT	C28-C27	2.18	1.37	1.32
10	E	612	CLA	CHC-C1C	2.18	1.40	1.35
10	C	614	CLA	C3B-C2B	-2.17	1.37	1.40
10	F	603	CLA	CAC-C3C	2.17	1.56	1.51
10	B	603	CLA	CHC-C1C	2.17	1.40	1.35
9	G	601	CHL	C3B-C2B	-2.17	1.37	1.40
10	E	611	CLA	CMB-C2B	2.17	1.56	1.51
10	E	604	CLA	C5-C3	2.17	1.55	1.51
9	C	605	CHL	C3B-C2B	-2.17	1.37	1.40
10	B	613	CLA	O2D-CED	-2.17	1.40	1.45
10	C	613	CLA	CBD-CGD	2.17	1.59	1.52
10	B	613	CLA	CHC-C1C	2.17	1.40	1.35
10	E	604	CLA	C1-C2	-2.17	1.42	1.49
9	H	606	CHL	C4-C3	2.16	1.56	1.50
9	C	606	CHL	C5-C3	2.16	1.56	1.50
10	G	613	CLA	CHC-C1C	2.16	1.40	1.35
4	C	2621	LUT	C5-C6	2.16	1.38	1.34
10	B	611	CLA	CHC-C1C	2.16	1.40	1.35
10	B	614	CLA	C3B-C2B	-2.16	1.37	1.40
9	A	606	CHL	C5-C3	2.16	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	613	CLA	C4-C3	2.16	1.56	1.50
9	I	609	CHL	O2D-CED	-2.15	1.40	1.45
10	H	604	CLA	C4-C3	2.15	1.56	1.50
10	I	614	CLA	O2D-CED	-2.15	1.40	1.45
9	A	601	CHL	C3B-C2B	-2.15	1.37	1.40
9	D	606	CHL	O2D-CED	-2.15	1.40	1.45
4	H	7621	LUT	C5-C6	2.15	1.38	1.34
4	J	9620	LUT	C23-C24	2.15	1.53	1.50
10	E	613	CLA	C3B-C2B	-2.15	1.37	1.40
10	H	612	CLA	CHC-C1C	2.15	1.40	1.35
9	F	605	CHL	C3B-C2B	-2.15	1.37	1.40
9	B	607	CHL	CHC-C1C	2.15	1.40	1.35
10	F	602	CLA	O2D-CED	-2.15	1.40	1.45
9	H	605	CHL	O2D-CED	-2.15	1.40	1.45
10	C	604	CLA	CBD-CGD	2.14	1.59	1.52
9	E	605	CHL	CMB-C2B	2.14	1.56	1.51
10	G	603	CLA	CMC-C2C	2.14	1.55	1.50
9	E	606	CHL	CHC-C1C	2.14	1.40	1.35
9	J	601	CHL	C1-C2	-2.14	1.42	1.49
9	G	606	CHL	CMB-C2B	2.14	1.56	1.51
9	G	609	CHL	C4-C3	2.14	1.56	1.50
10	F	611	CLA	O2D-CED	-2.14	1.40	1.45
9	E	606	CHL	C5-C3	2.13	1.56	1.50
10	E	602	CLA	CMB-C2B	2.13	1.56	1.51
4	F	5620	LUT	C1-C6	2.13	1.56	1.53
10	B	602	CLA	C4-C3	2.13	1.56	1.50
10	E	610	CLA	CAC-C3C	2.13	1.56	1.51
10	C	603	CLA	CBD-CGD	2.13	1.59	1.52
10	B	613	CLA	CMB-C2B	2.13	1.56	1.51
10	I	613	CLA	C1-C2	-2.13	1.42	1.49
9	B	606	CHL	C4-C3	2.13	1.56	1.50
9	J	608	CHL	CMB-C2B	2.12	1.56	1.51
10	D	614	CLA	CAC-C3C	2.12	1.56	1.51
10	A	603	CLA	CMC-C2C	2.12	1.55	1.50
10	I	614	CLA	CMB-C2B	2.12	1.56	1.51
10	J	614	CLA	C3B-C2B	-2.12	1.37	1.40
10	D	614	CLA	CMB-C2B	2.12	1.56	1.51
4	C	2620	LUT	C1-C6	2.11	1.56	1.53
9	F	601	CHL	C3B-C2B	-2.11	1.37	1.40
10	B	613	CLA	C4-C3	2.11	1.56	1.50
10	I	602	CLA	CAC-C3C	2.11	1.56	1.51
4	J	9621	LUT	C5-C6	2.10	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	613	CLA	C4-C3	2.10	1.56	1.50
10	D	613	CLA	C1-C2	-2.10	1.42	1.49
9	J	607	CHL	CHC-C1C	2.10	1.40	1.35
10	H	612	CLA	C4-C3	2.10	1.56	1.50
10	E	614	CLA	CMC-C2C	2.10	1.55	1.50
10	A	611	CLA	C3B-C2B	-2.10	1.37	1.40
6	G	6623	NEX	C1-C6	2.10	1.58	1.54
10	F	611	CLA	C3B-C2B	-2.10	1.37	1.40
10	H	611	CLA	O2D-CED	-2.09	1.40	1.45
9	A	607	CHL	CMB-C2B	2.09	1.56	1.51
10	G	602	CLA	CAC-C3C	2.09	1.56	1.51
10	A	611	CLA	CMB-C2B	2.09	1.56	1.51
10	J	604	CLA	CMC-C2C	2.09	1.55	1.50
4	D	3620	LUT	C24-C25	2.09	1.35	1.33
10	F	612	CLA	C4-C3	2.09	1.56	1.50
10	H	613	CLA	CHC-C1C	2.09	1.40	1.35
10	C	613	CLA	CHC-C1C	2.09	1.40	1.35
9	H	609	CHL	CMB-C2B	2.09	1.56	1.51
10	C	603	CLA	CMB-C2B	2.09	1.56	1.51
10	B	612	CLA	CHC-C1C	2.09	1.40	1.35
9	D	608	CHL	CMB-C2B	2.09	1.56	1.51
10	A	614	CLA	CMB-C2B	2.09	1.56	1.51
4	G	6620	LUT	C24-C25	2.08	1.35	1.33
10	H	611	CLA	CHC-C1C	2.08	1.40	1.35
10	C	610	CLA	CMC-C2C	2.08	1.55	1.50
10	A	612	CLA	CMB-C2B	2.08	1.56	1.51
4	A	621	LUT	C26-C27	2.08	1.53	1.50
10	C	602	CLA	C1D-C2D	2.08	1.47	1.42
10	F	613	CLA	CMB-C2B	2.08	1.56	1.51
10	I	602	CLA	CMC-C2C	2.08	1.55	1.50
10	A	602	CLA	CAC-C3C	2.07	1.56	1.51
4	I	8620	LUT	C1-C6	2.07	1.56	1.53
10	D	604	CLA	C4-C3	2.07	1.56	1.50
4	I	8620	LUT	C24-C25	2.07	1.35	1.33
10	F	613	CLA	CHC-C1C	2.07	1.40	1.35
10	C	604	CLA	C4-C3	2.07	1.56	1.50
4	B	1621	LUT	C26-C27	2.07	1.53	1.50
10	I	613	CLA	CHC-C1C	2.07	1.40	1.35
10	D	612	CLA	C4-C3	2.07	1.56	1.50
10	H	610	CLA	CAC-C3C	2.06	1.56	1.51
4	C	2620	LUT	C5-C6	2.06	1.38	1.34
9	G	607	CHL	CHC-C1C	2.06	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	609	CHL	C4-C3	2.06	1.56	1.50
10	G	602	CLA	CMB-C2B	2.06	1.55	1.51
10	G	612	CLA	CMB-C2B	2.06	1.55	1.51
10	H	603	CLA	CMB-C2B	2.06	1.55	1.51
10	A	604	CLA	C4-C3	2.06	1.56	1.50
4	A	620	LUT	C1-C6	2.06	1.56	1.53
10	A	604	CLA	C5-C3	2.06	1.55	1.51
9	C	607	CHL	CHC-C1C	2.05	1.40	1.35
9	B	609	CHL	CMB-C2B	2.05	1.55	1.51
10	H	602	CLA	CAC-C3C	2.05	1.56	1.51
10	F	613	CLA	CMC-C2C	2.05	1.55	1.50
10	I	610	CLA	O2D-CED	-2.05	1.40	1.45
10	A	614	CLA	CMC-C2C	2.05	1.55	1.50
9	C	606	CHL	C4-C3	2.05	1.55	1.50
6	D	3623	NEX	C1-C6	2.05	1.58	1.54
4	I	8620	LUT	C5-C6	2.05	1.38	1.34
10	C	614	CLA	CMC-C2C	2.04	1.55	1.50
9	A	609	CHL	C1-C2	-2.04	1.43	1.49
10	D	613	CLA	C5-C3	2.04	1.55	1.51
10	J	612	CLA	C4-C3	2.04	1.55	1.50
10	J	613	CLA	CMC-C2C	2.04	1.55	1.50
10	B	610	CLA	C1D-C2D	2.04	1.47	1.42
9	D	608	CHL	C4-C3	2.04	1.55	1.50
10	A	613	CLA	O2D-CED	-2.04	1.40	1.45
10	H	612	CLA	CAC-C3C	2.04	1.56	1.51
10	E	602	CLA	C4-C3	2.04	1.55	1.50
10	I	614	CLA	CMC-C2C	2.04	1.55	1.50
9	C	601	CHL	CMB-C2B	2.04	1.55	1.51
9	F	606	CHL	C4-C3	2.03	1.55	1.50
10	A	613	CLA	C5-C3	2.03	1.55	1.51
9	C	609	CHL	C1-C2	-2.03	1.43	1.49
9	H	606	CHL	MG-NC	2.03	2.11	2.06
6	F	5623	NEX	C1-C6	2.03	1.57	1.54
9	G	609	CHL	C1-C2	-2.03	1.43	1.49
9	F	609	CHL	CMB-C2B	2.03	1.55	1.51
10	E	602	CLA	O2D-CED	-2.03	1.40	1.45
6	H	7623	NEX	C1-C6	2.03	1.57	1.54
10	J	613	CLA	CAC-C3C	2.03	1.56	1.51
10	B	612	CLA	C4-C3	2.03	1.55	1.50
10	G	612	CLA	C4-C3	2.03	1.55	1.50
9	F	608	CHL	CMB-C2B	2.02	1.55	1.51
4	J	9620	LUT	C1-C6	2.02	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	609	CHL	C1-C2	-2.02	1.43	1.49
5	J	3622	XAT	C28-C27	2.02	1.37	1.32
9	I	601	CHL	C3B-C2B	-2.02	1.37	1.40
4	G	6620	LUT	C1-C6	2.02	1.56	1.53
9	J	608	CHL	C4-C3	2.01	1.55	1.50
9	D	601	CHL	O2D-CED	-2.01	1.40	1.45
10	C	613	CLA	O2D-CED	-2.01	1.40	1.45
9	E	605	CHL	C3B-C2B	-2.01	1.37	1.40
10	I	603	CLA	CHC-C1C	2.01	1.40	1.35
4	H	7620	LUT	C23-C24	2.01	1.53	1.50
10	I	610	CLA	C3B-C2B	-2.01	1.37	1.40
10	D	602	CLA	CMB-C2B	2.00	1.55	1.51
10	C	604	CLA	C5-C3	2.00	1.55	1.51
10	E	613	CLA	CMB-C2B	2.00	1.55	1.51
10	C	603	CLA	O2D-CED	-2.00	1.40	1.45
10	G	611	CLA	CMC-C2C	2.00	1.55	1.50

All (2618) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	607	CHL	C4A-NA-C1A	9.29	110.88	106.71
9	F	607	CHL	C4A-NA-C1A	9.14	110.82	106.71
9	A	607	CHL	C4A-NA-C1A	9.00	110.75	106.71
9	B	607	CHL	C4A-NA-C1A	8.99	110.75	106.71
9	F	606	CHL	C4A-NA-C1A	8.96	110.74	106.71
9	C	607	CHL	C4A-NA-C1A	8.86	110.69	106.71
9	J	606	CHL	C4A-NA-C1A	8.76	110.64	106.71
9	J	607	CHL	C4A-NA-C1A	8.71	110.62	106.71
9	D	607	CHL	C4A-NA-C1A	8.67	110.61	106.71
9	H	606	CHL	C4A-NA-C1A	8.59	110.57	106.71
9	A	606	CHL	C4A-NA-C1A	8.53	110.54	106.71
9	G	606	CHL	C4A-NA-C1A	8.51	110.53	106.71
10	F	613	CLA	C4A-NA-C1A	8.49	110.52	106.71
9	I	606	CHL	C4A-NA-C1A	8.49	110.52	106.71
9	H	607	CHL	C4A-NA-C1A	8.46	110.51	106.71
10	C	613	CLA	C4A-NA-C1A	8.43	110.50	106.71
9	I	607	CHL	C4A-NA-C1A	8.41	110.49	106.71
9	E	606	CHL	C4A-NA-C1A	8.39	110.48	106.71
9	I	601	CHL	C4A-NA-C1A	8.33	110.45	106.71
9	E	607	CHL	C4A-NA-C1A	8.33	110.45	106.71
10	I	604	CLA	C4A-NA-C1A	8.30	110.44	106.71
10	G	613	CLA	C4A-NA-C1A	8.29	110.44	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	613	CLA	C4A-NA-C1A	8.26	110.42	106.71
10	D	613	CLA	C4A-NA-C1A	8.26	110.42	106.71
9	D	606	CHL	C4A-NA-C1A	8.17	110.38	106.71
10	H	613	CLA	C4A-NA-C1A	8.17	110.38	106.71
9	C	601	CHL	C4A-NA-C1A	8.15	110.37	106.71
10	I	613	CLA	C4A-NA-C1A	8.14	110.37	106.71
9	D	601	CHL	C4A-NA-C1A	8.13	110.36	106.71
9	B	606	CHL	C4A-NA-C1A	8.11	110.35	106.71
9	G	601	CHL	C4A-NA-C1A	8.08	110.34	106.71
9	H	601	CHL	C4A-NA-C1A	8.05	110.33	106.71
9	A	601	CHL	C4A-NA-C1A	8.04	110.32	106.71
9	B	601	CHL	C4A-NA-C1A	7.97	110.29	106.71
10	A	613	CLA	C4A-NA-C1A	7.95	110.28	106.71
9	C	606	CHL	C4A-NA-C1A	7.94	110.27	106.71
9	D	609	CHL	C4A-NA-C1A	7.91	110.26	106.71
10	H	603	CLA	C4A-NA-C1A	7.88	110.25	106.71
9	F	601	CHL	C4A-NA-C1A	7.87	110.24	106.71
10	G	610	CLA	C4A-NA-C1A	7.87	110.24	106.71
10	I	610	CLA	C4A-NA-C1A	7.86	110.24	106.71
10	F	604	CLA	C4A-NA-C1A	7.85	110.23	106.71
10	D	604	CLA	CMB-C2B-C1B	-7.83	116.43	128.46
9	E	605	CHL	C4A-NA-C1A	7.82	110.22	106.71
10	G	613	CLA	CMB-C2B-C1B	-7.81	116.45	128.46
10	C	604	CLA	CMB-C2B-C1B	-7.81	116.46	128.46
10	A	604	CLA	C4A-NA-C1A	7.81	110.22	106.71
10	H	610	CLA	C4A-NA-C1A	7.80	110.21	106.71
9	D	605	CHL	C4A-NA-C1A	7.80	110.21	106.71
10	J	604	CLA	C4A-NA-C1A	7.78	110.20	106.71
9	B	605	CHL	C4A-NA-C1A	7.76	110.20	106.71
10	E	611	CLA	C4A-NA-C1A	7.76	110.19	106.71
9	J	601	CHL	C4A-NA-C1A	7.76	110.19	106.71
10	J	610	CLA	C4A-NA-C1A	7.75	110.19	106.71
10	A	604	CLA	CMB-C2B-C1B	-7.74	116.57	128.46
9	D	608	CHL	C4A-NA-C1A	7.73	110.18	106.71
9	E	601	CHL	C4A-NA-C1A	7.73	110.18	106.71
9	I	605	CHL	C4A-NA-C1A	7.72	110.17	106.71
10	I	613	CLA	CMB-C2B-C1B	-7.71	116.62	128.46
10	J	603	CLA	C4A-NA-C1A	7.70	110.17	106.71
10	E	604	CLA	C4A-NA-C1A	7.69	110.17	106.71
10	B	613	CLA	C4A-NA-C1A	7.69	110.16	106.71
9	C	605	CHL	C4A-NA-C1A	7.68	110.16	106.71
10	J	611	CLA	C4A-NA-C1A	7.68	110.16	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	613	CLA	CMB-C2B-C1B	-7.67	116.67	128.46
9	F	605	CHL	C4A-NA-C1A	7.64	110.14	106.71
9	F	608	CHL	C4A-NA-C1A	7.64	110.14	106.71
10	G	604	CLA	C4A-NA-C1A	7.62	110.13	106.71
9	A	608	CHL	C4A-NA-C1A	7.61	110.13	106.71
9	J	605	CHL	C4A-NA-C1A	7.61	110.13	106.71
10	F	610	CLA	C4A-NA-C1A	7.57	110.11	106.71
10	C	611	CLA	C4A-NA-C1A	7.56	110.10	106.71
9	C	608	CHL	C4A-NA-C1A	7.54	110.10	106.71
9	A	605	CHL	C4A-NA-C1A	7.54	110.09	106.71
10	D	602	CLA	C4A-NA-C1A	7.54	110.09	106.71
9	G	609	CHL	C4A-NA-C1A	7.53	110.09	106.71
10	A	603	CLA	C4A-NA-C1A	7.53	110.09	106.71
10	H	604	CLA	C4A-NA-C1A	7.53	110.09	106.71
9	E	608	CHL	C4A-NA-C1A	7.53	110.09	106.71
9	H	605	CHL	C4A-NA-C1A	7.52	110.09	106.71
10	E	610	CLA	C4A-NA-C1A	7.52	110.09	106.71
10	J	602	CLA	C4A-NA-C1A	7.51	110.08	106.71
10	C	613	CLA	CMB-C2B-C1B	-7.50	116.93	128.46
10	C	614	CLA	O2D-CGD-CBD	7.47	124.54	111.27
10	J	613	CLA	C4A-NA-C1A	7.45	110.06	106.71
10	B	604	CLA	C4A-NA-C1A	7.45	110.06	106.71
10	F	604	CLA	CMB-C2B-C1B	-7.45	117.02	128.46
10	B	613	CLA	CMB-C2B-C1B	-7.45	117.02	128.46
9	I	609	CHL	C4A-NA-C1A	7.44	110.05	106.71
10	H	613	CLA	CMB-C2B-C1B	-7.44	117.03	128.46
10	G	611	CLA	C4A-NA-C1A	7.44	110.05	106.71
10	B	602	CLA	C4A-NA-C1A	7.42	110.04	106.71
10	E	604	CLA	CMB-C2B-C1B	-7.42	117.06	128.46
10	D	604	CLA	C4A-NA-C1A	7.39	110.03	106.71
10	G	614	CLA	C4A-NA-C1A	7.38	110.02	106.71
10	G	603	CLA	C4A-NA-C1A	7.38	110.02	106.71
10	I	603	CLA	C4A-NA-C1A	7.37	110.02	106.71
10	B	614	CLA	O2D-CGD-CBD	7.35	124.34	111.27
10	E	614	CLA	C4A-NA-C1A	7.34	110.01	106.71
9	J	608	CHL	C4A-NA-C1A	7.34	110.01	106.71
10	D	612	CLA	C4A-NA-C1A	7.33	110.00	106.71
10	A	611	CLA	C4A-NA-C1A	7.32	110.00	106.71
10	A	610	CLA	C4A-NA-C1A	7.32	110.00	106.71
10	D	610	CLA	C4A-NA-C1A	7.30	109.99	106.71
10	I	614	CLA	C4A-NA-C1A	7.30	109.99	106.71
10	B	610	CLA	C4A-NA-C1A	7.29	109.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	604	CLA	C4A-NA-C1A	7.29	109.98	106.71
10	I	602	CLA	C4A-NA-C1A	7.27	109.97	106.71
10	B	604	CLA	CMB-C2B-C1B	-7.27	117.29	128.46
10	G	612	CLA	C4A-NA-C1A	7.26	109.97	106.71
10	F	602	CLA	C4A-NA-C1A	7.25	109.97	106.71
9	I	608	CHL	C4A-NA-C1A	7.22	109.95	106.71
9	H	609	CHL	C4A-NA-C1A	7.22	109.95	106.71
10	E	612	CLA	C4A-NA-C1A	7.21	109.95	106.71
10	D	611	CLA	C4A-NA-C1A	7.20	109.94	106.71
9	B	608	CHL	C4A-NA-C1A	7.19	109.94	106.71
9	B	609	CHL	C4A-NA-C1A	7.18	109.93	106.71
10	J	612	CLA	C4A-NA-C1A	7.17	109.93	106.71
10	I	612	CLA	C4A-NA-C1A	7.17	109.93	106.71
10	F	613	CLA	CMB-C2B-C1B	-7.16	117.45	128.46
10	A	602	CLA	C4A-NA-C1A	7.16	109.92	106.71
10	G	604	CLA	CMB-C2B-C1B	-7.15	117.47	128.46
10	F	612	CLA	C4A-NA-C1A	7.14	109.92	106.71
9	G	605	CHL	C4A-NA-C1A	7.13	109.91	106.71
9	C	609	CHL	C4A-NA-C1A	7.12	109.91	106.71
10	D	603	CLA	C4A-NA-C1A	7.11	109.90	106.71
9	E	609	CHL	C4A-NA-C1A	7.11	109.90	106.71
10	E	602	CLA	C4A-NA-C1A	7.10	109.90	106.71
10	I	604	CLA	CMB-C2B-C1B	-7.08	117.59	128.46
10	E	614	CLA	O2D-CGD-CBD	7.05	123.80	111.27
10	F	603	CLA	C4A-NA-C1A	7.04	109.87	106.71
10	E	603	CLA	C4A-NA-C1A	7.03	109.87	106.71
10	J	614	CLA	C4A-NA-C1A	7.03	109.87	106.71
10	H	612	CLA	C4A-NA-C1A	7.02	109.86	106.71
10	B	603	CLA	C4A-NA-C1A	7.02	109.86	106.71
10	A	612	CLA	C4A-NA-C1A	7.01	109.86	106.71
10	C	602	CLA	C4A-NA-C1A	7.01	109.86	106.71
9	A	609	CHL	C4A-NA-C1A	7.00	109.86	106.71
10	C	603	CLA	C4A-NA-C1A	7.00	109.85	106.71
10	D	614	CLA	C4A-NA-C1A	6.98	109.84	106.71
10	H	614	CLA	O2D-CGD-CBD	6.97	123.66	111.27
10	B	612	CLA	C4A-NA-C1A	6.97	109.84	106.71
10	A	614	CLA	O2D-CGD-CBD	6.96	123.63	111.27
10	H	614	CLA	C4A-NA-C1A	6.94	109.83	106.71
10	H	602	CLA	C4A-NA-C1A	6.94	109.83	106.71
10	J	604	CLA	CMB-C2B-C1B	-6.92	117.83	128.46
10	B	614	CLA	C4A-NA-C1A	6.90	109.81	106.71
10	I	611	CLA	C4A-NA-C1A	6.90	109.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	614	CLA	O2D-CGD-CBD	6.88	123.49	111.27
9	I	606	CHL	CMB-C2B-C1B	-6.87	117.90	128.46
9	F	609	CHL	C4A-NA-C1A	6.86	109.79	106.71
9	H	608	CHL	C4A-NA-C1A	6.82	109.77	106.71
10	B	611	CLA	C4A-NA-C1A	6.82	109.77	106.71
9	J	609	CHL	C4A-NA-C1A	6.80	109.77	106.71
10	A	614	CLA	C4A-NA-C1A	6.78	109.75	106.71
10	G	602	CLA	C4A-NA-C1A	6.78	109.75	106.71
10	H	611	CLA	C4A-NA-C1A	6.77	109.75	106.71
10	C	612	CLA	C4A-NA-C1A	6.72	109.73	106.71
9	G	608	CHL	C4A-NA-C1A	6.68	109.71	106.71
10	F	611	CLA	C4A-NA-C1A	6.68	109.71	106.71
9	E	606	CHL	CBA-CAA-C2A	-6.63	94.28	113.86
10	C	610	CLA	C4A-NA-C1A	6.61	109.68	106.71
9	C	607	CHL	OMC-CMC-C2C	6.60	140.62	125.69
10	C	614	CLA	C4A-NA-C1A	6.60	109.67	106.71
10	D	614	CLA	O2D-CGD-CBD	6.57	122.95	111.27
10	J	611	CLA	CAA-C2A-C3A	-6.56	94.83	112.78
9	E	607	CHL	CMB-C2B-C1B	-6.55	118.40	128.46
10	F	614	CLA	C4A-NA-C1A	6.53	109.64	106.71
9	D	606	CHL	CMB-C2B-C1B	-6.51	118.46	128.46
10	H	604	CLA	CMB-C2B-C1B	-6.48	118.51	128.46
10	C	604	CLA	O2A-CGA-CBA	6.46	132.17	111.91
10	D	604	CLA	O2A-CGA-CBA	6.45	132.14	111.91
10	B	604	CLA	O2A-CGA-CBA	6.44	132.13	111.91
9	A	607	CHL	OMC-CMC-C2C	6.43	140.22	125.69
9	A	609	CHL	OMC-CMC-C2C	6.35	140.05	125.69
9	C	608	CHL	OMC-CMC-C2C	6.35	140.03	125.69
10	C	614	CLA	O1D-CGD-CBD	-6.34	111.51	124.48
10	G	611	CLA	CBA-CAA-C2A	6.33	132.55	113.86
10	G	613	CLA	CMB-C2B-C3B	6.30	136.47	124.68
10	I	613	CLA	CMB-C2B-C3B	6.25	136.38	124.68
9	I	607	CHL	CMB-C2B-C1B	-6.24	118.88	128.46
10	C	604	CLA	CMB-C2B-C3B	6.19	136.26	124.68
10	D	613	CLA	CMB-C2B-C3B	6.18	136.24	124.68
10	F	614	CLA	O2D-CGD-CBD	6.18	122.25	111.27
9	H	607	CHL	CMB-C2B-C1B	-6.13	119.04	128.46
9	G	607	CHL	CMB-C2B-C1B	-6.11	119.07	128.46
10	D	604	CLA	CMB-C2B-C3B	6.11	136.11	124.68
9	B	606	CHL	CMB-C2B-C1B	-6.11	119.08	128.46
10	G	614	CLA	O2D-CGD-CBD	6.10	122.11	111.27
9	B	607	CHL	OMC-CMC-C2C	6.09	139.45	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	609	CHL	OMC-CMC-C2C	6.08	139.42	125.69
10	C	611	CLA	CAA-C2A-C3A	-6.07	96.16	112.78
10	A	604	CLA	CMB-C2B-C3B	6.07	136.03	124.68
9	J	607	CHL	CMB-C2B-C1B	-6.06	119.15	128.46
10	C	613	CLA	CMB-C2B-C3B	6.05	136.00	124.68
9	E	607	CHL	OMC-CMC-C2C	6.02	139.30	125.69
4	E	4620	LUT	C18-C5-C6	6.01	131.28	124.53
10	H	613	CLA	CMB-C2B-C3B	6.01	135.92	124.68
10	B	614	CLA	O1D-CGD-CBD	-6.00	112.20	124.48
10	B	613	CLA	CMB-C2B-C3B	6.00	135.90	124.68
5	B	1622	XAT	C24-C23-C22	5.99	122.34	110.77
10	D	611	CLA	CBA-CAA-C2A	5.99	131.54	113.86
10	J	614	CLA	O2D-CGD-CBD	5.98	121.89	111.27
10	E	611	CLA	CBA-CAA-C2A	5.96	131.45	113.86
9	A	607	CHL	CMB-C2B-C1B	-5.92	119.36	128.46
9	C	606	CHL	CMB-C2B-C1B	-5.92	119.37	128.46
10	F	604	CLA	CMB-C2B-C3B	5.91	135.74	124.68
10	A	611	CLA	CBA-CAA-C2A	5.91	131.31	113.86
9	I	609	CHL	OMC-CMC-C2C	5.89	139.01	125.69
10	C	611	CLA	CBA-CAA-C2A	5.88	131.22	113.86
10	E	604	CLA	CMB-C2B-C3B	5.83	135.59	124.68
10	H	611	CLA	CBA-CAA-C2A	5.81	131.02	113.86
9	D	606	CHL	CBA-CAA-C2A	-5.77	96.84	113.86
10	F	611	CLA	CAA-C2A-C3A	-5.76	97.00	112.78
5	H	4622	XAT	C24-C23-C22	5.76	121.89	110.77
9	H	606	CHL	CAA-CBA-CGA	5.76	130.08	113.25
10	B	604	CLA	CMB-C2B-C3B	5.76	135.45	124.68
10	F	613	CLA	CMB-C2B-C3B	5.75	135.44	124.68
10	B	613	CLA	CED-O2D-CGD	5.74	128.93	115.94
9	E	606	CHL	CMB-C2B-C1B	-5.74	119.64	128.46
10	E	604	CLA	O2A-CGA-CBA	5.74	129.91	111.91
10	D	613	CLA	CBA-CAA-C2A	5.73	130.78	113.86
10	I	614	CLA	O1D-CGD-CBD	-5.71	112.79	124.48
10	H	614	CLA	O1D-CGD-CBD	-5.71	112.80	124.48
10	E	614	CLA	O1D-CGD-CBD	-5.70	112.82	124.48
9	I	606	CHL	CBA-CAA-C2A	-5.67	97.12	113.86
10	G	604	CLA	CMB-C2B-C3B	5.66	135.27	124.68
5	C	7622	XAT	C24-C23-C22	5.66	121.69	110.77
10	A	614	CLA	O1D-CGD-CBD	-5.64	112.94	124.48
9	G	606	CHL	CMB-C2B-C1B	-5.64	119.79	128.46
10	E	604	CLA	CAA-C2A-C3A	-5.63	97.37	112.78
10	J	604	CLA	O2A-CGA-CBA	5.62	129.56	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	604	CLA	CMB-C2B-C3B	5.61	135.17	124.68
10	E	613	CLA	CMB-C2B-C1B	-5.60	119.86	128.46
9	H	606	CHL	CMB-C2B-C1B	-5.58	119.89	128.46
9	G	601	CHL	CBA-CAA-C2A	5.55	130.25	113.86
10	F	604	CLA	O2A-CGA-CBA	5.52	129.22	111.91
9	F	607	CHL	OMC-CMC-C2C	5.50	138.13	125.69
10	J	604	CLA	CMB-C2B-C3B	5.50	134.97	124.68
7	I	8630	LHG	O8-C23-C24	5.49	129.13	111.91
9	F	601	CHL	OMC-CMC-C2C	5.48	138.07	125.69
9	D	609	CHL	OMC-CMC-C2C	5.47	138.04	125.69
10	I	611	CLA	CAA-CBA-CGA	5.46	129.21	113.25
9	A	608	CHL	CED-O2D-CGD	5.45	128.26	115.94
9	D	607	CHL	OMC-CMC-C2C	5.44	137.99	125.69
9	F	606	CHL	CMB-C2B-C1B	-5.42	120.13	128.46
10	H	604	CLA	O2A-CGA-CBA	5.42	128.93	111.91
9	J	609	CHL	OMC-CMC-C2C	5.42	137.94	125.69
9	D	608	CHL	OMC-CMC-C2C	5.40	137.89	125.69
9	I	606	CHL	CMB-C2B-C3B	5.39	134.77	124.68
10	I	602	CLA	C1-C2-C3	5.38	135.34	126.04
9	F	608	CHL	OMC-CMC-C2C	5.36	137.80	125.69
9	B	606	CHL	O2A-CGA-CBA	5.36	128.72	111.91
4	H	7620	LUT	C38-C25-C24	-5.35	112.12	123.56
10	G	612	CLA	C1-C2-C3	5.35	135.29	126.04
10	D	614	CLA	O1D-CGD-CBD	-5.34	113.56	124.48
4	J	9620	LUT	C38-C25-C24	-5.33	112.15	123.56
10	I	604	CLA	O2A-CGA-CBA	5.31	128.57	111.91
9	E	608	CHL	CED-O2D-CGD	5.30	127.92	115.94
10	B	602	CLA	CED-O2D-CGD	5.28	127.87	115.94
4	E	4621	LUT	C3-C4-C5	5.27	122.35	111.85
9	H	607	CHL	OMC-CMC-C2C	5.27	137.59	125.69
10	D	604	CLA	CAA-C2A-C3A	-5.26	98.36	112.78
10	F	614	CLA	O1D-CGD-CBD	-5.26	113.72	124.48
9	J	606	CHL	CMB-C2B-C1B	-5.26	120.38	128.46
9	C	607	CHL	CMB-C2B-C1B	-5.25	120.40	128.46
10	B	604	CLA	CED-O2D-CGD	5.24	127.79	115.94
10	D	602	CLA	C1-C2-C3	5.24	135.11	126.04
10	J	614	CLA	O1D-CGD-CBD	-5.24	113.76	124.48
9	E	607	CHL	CMB-C2B-C3B	5.24	134.48	124.68
10	C	603	CLA	O2D-CGD-CBD	5.23	120.56	111.27
10	J	613	CLA	CMB-C2B-C1B	-5.21	120.46	128.46
9	B	607	CHL	CMB-C2B-C1B	-5.20	120.47	128.46
9	D	606	CHL	CMB-C2B-C3B	5.19	134.40	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	601	CHL	OMC-CMC-C2C	5.19	137.43	125.69
10	H	613	CLA	CED-O2D-CGD	5.17	127.62	115.94
9	D	601	CHL	CBA-CAA-C2A	5.15	129.07	113.86
9	D	607	CHL	CMB-C2B-C1B	-5.15	120.55	128.46
9	C	609	CHL	CMB-C2B-C1B	-5.14	120.56	128.46
9	F	609	CHL	OMC-CMC-C2C	5.13	137.29	125.69
10	B	611	CLA	CBA-CAA-C2A	5.13	129.00	113.86
10	H	611	CLA	C1-C2-C3	5.11	134.88	126.04
9	A	606	CHL	CMB-C2B-C1B	-5.11	120.62	128.46
5	D	8622	XAT	C24-C23-C22	5.10	120.63	110.77
10	C	604	CLA	CAA-C2A-C3A	-5.10	98.82	112.78
10	B	611	CLA	CAA-C2A-C3A	-5.09	98.83	112.78
10	D	611	CLA	C1-C2-C3	5.09	134.85	126.04
4	J	9621	LUT	C3-C4-C5	5.09	121.99	111.85
9	G	609	CHL	OMC-CMC-C2C	5.09	137.18	125.69
9	C	601	CHL	CED-O2D-CGD	5.08	127.42	115.94
10	C	613	CLA	CED-O2D-CGD	5.07	127.41	115.94
4	J	9620	LUT	C18-C5-C6	5.07	130.22	124.53
9	J	607	CHL	OMC-CMC-C2C	5.05	137.11	125.69
9	G	606	CHL	C1-C2-C3	5.04	134.91	126.75
10	A	612	CLA	C1-C2-C3	5.04	134.76	126.04
10	H	604	CLA	CMB-C2B-C3B	5.04	134.10	124.68
10	G	604	CLA	O2A-CGA-CBA	5.03	127.70	111.91
10	G	614	CLA	O1D-CGD-CBD	-5.03	114.19	124.48
9	J	606	CHL	O2A-CGA-CBA	5.02	127.67	111.91
10	I	602	CLA	O2D-CGD-CBD	5.02	120.19	111.27
9	J	601	CHL	CED-O2D-CGD	5.01	127.27	115.94
10	A	611	CLA	C1-C2-C3	5.01	134.70	126.04
10	F	602	CLA	C1-C2-C3	4.99	134.68	126.04
9	H	608	CHL	C7-C6-C5	4.99	126.90	113.36
9	J	607	CHL	CMB-C2B-C3B	4.97	133.97	124.68
5	I	9622	XAT	C24-C23-C22	4.97	120.36	110.77
5	F	6622	XAT	C24-C23-C22	4.96	120.35	110.77
9	I	607	CHL	CMB-C2B-C3B	4.96	133.95	124.68
9	D	605	CHL	OMC-CMC-C2C	4.96	136.89	125.69
9	G	607	CHL	CMB-C2B-C3B	4.95	133.94	124.68
9	H	609	CHL	C1-C2-C3	4.94	134.58	126.04
4	I	8620	LUT	C18-C5-C6	4.94	130.07	124.53
6	A	623	NEX	C5-C4-C3	4.93	117.59	111.75
10	B	602	CLA	C1-C2-C3	4.93	134.58	126.04
4	A	620	LUT	C18-C5-C6	4.93	130.06	124.53
10	A	613	CLA	CBA-CAA-C2A	4.92	128.39	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	612	CLA	O2D-CGD-CBD	4.92	120.00	111.27
4	F	5621	LUT	C38-C25-C24	-4.91	113.06	123.56
7	A	630	LHG	O8-C23-C24	4.91	127.30	111.91
10	I	604	CLA	CED-O2D-CGD	4.90	127.03	115.94
9	C	606	CHL	C1-C2-C3	4.90	134.68	126.75
9	A	606	CHL	CBA-CAA-C2A	-4.90	99.40	113.86
9	F	606	CHL	O2A-CGA-CBA	4.89	127.25	111.91
9	J	606	CHL	CAA-CBA-CGA	4.88	127.53	113.25
4	A	621	LUT	C3-C4-C5	4.87	121.56	111.85
4	D	3620	LUT	C18-C5-C6	4.87	130.00	124.53
10	E	602	CLA	C1-C2-C3	4.87	134.46	126.04
10	H	613	CLA	CBA-CAA-C2A	4.85	128.19	113.86
4	I	8620	LUT	C38-C25-C24	-4.85	113.18	123.56
10	A	604	CLA	O2A-CGA-CBA	4.85	127.13	111.91
10	A	603	CLA	O2D-CGD-CBD	4.84	119.88	111.27
9	D	606	CHL	O2A-CGA-CBA	4.84	127.11	111.91
4	B	1621	LUT	C38-C25-C24	-4.84	113.20	123.56
9	I	606	CHL	CAA-CBA-CGA	4.84	127.40	113.25
4	C	2620	LUT	C18-C5-C6	4.83	129.96	124.53
9	D	601	CHL	OMC-CMC-C2C	4.82	136.59	125.69
9	A	601	CHL	CBA-CAA-C2A	4.82	128.09	113.86
7	E	4630	LHG	O8-C23-C24	4.82	127.03	111.91
9	J	601	CHL	CBA-CAA-C2A	4.82	128.08	113.86
9	H	607	CHL	CMB-C2B-C3B	4.81	133.68	124.68
9	C	608	CHL	CED-O2D-CGD	4.81	126.81	115.94
6	G	6623	NEX	C5-C4-C3	4.80	117.43	111.75
9	B	606	CHL	CMB-C2B-C3B	4.80	133.66	124.68
9	H	606	CHL	C1-C2-C3	4.79	134.51	126.75
7	G	6630	LHG	O8-C23-C24	4.79	126.95	111.91
9	C	606	CHL	CBA-CAA-C2A	-4.79	99.73	113.86
10	H	604	CLA	O2D-CGD-CBD	4.78	119.77	111.27
9	E	605	CHL	OMC-CMC-C2C	4.78	136.49	125.69
7	C	2630	LHG	O8-C23-C24	4.78	126.90	111.91
4	F	5621	LUT	C3-C4-C5	4.77	121.36	111.85
10	F	602	CLA	C4-C3-C5	4.77	123.30	115.27
9	D	609	CHL	CMB-C2B-C1B	-4.77	121.13	128.46
9	G	601	CHL	CED-O2D-CGD	4.77	126.73	115.94
5	B	5622	XAT	C24-C23-C22	4.77	119.98	110.77
10	J	613	CLA	CED-O2D-CGD	4.76	126.71	115.94
5	A	622	XAT	C24-C23-C22	4.76	119.96	110.77
10	G	613	CLA	C4-C3-C5	-4.76	107.27	115.27
9	J	609	CHL	CMB-C2B-C1B	-4.75	121.16	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	604	CLA	CAA-C2A-C3A	-4.75	99.77	112.78
7	A	630	LHG	O8-C6-C5	4.75	122.26	108.43
4	G	6621	LUT	C3-C4-C5	4.74	121.30	111.85
9	A	607	CHL	CMB-C2B-C3B	4.74	133.55	124.68
9	D	606	CHL	C1-C2-C3	4.74	134.42	126.75
7	B	1630	LHG	O8-C23-C24	4.74	126.77	111.91
9	J	605	CHL	OMC-CMC-C2C	4.73	136.38	125.69
9	C	606	CHL	CMB-C2B-C3B	4.72	133.52	124.68
9	H	601	CHL	CBA-CAA-C2A	4.72	127.81	113.86
4	C	2621	LUT	C3-C4-C5	4.72	121.26	111.85
9	B	609	CHL	OMC-CMC-C2C	4.72	136.36	125.69
9	F	609	CHL	CMB-C2B-C1B	-4.72	121.21	128.46
7	G	6630	LHG	O8-C6-C5	4.71	122.15	108.43
10	H	614	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
10	B	611	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
6	B	1623	NEX	C5-C4-C3	4.70	117.31	111.75
10	J	612	CLA	C1-C2-C3	4.69	134.16	126.04
10	C	602	CLA	C1-C2-C3	4.69	134.15	126.04
10	B	603	CLA	O2D-CGD-CBD	4.69	119.60	111.27
10	A	614	CLA	CMB-C2B-C1B	-4.68	121.26	128.46
7	J	9630	LHG	O8-C23-C24	4.68	126.59	111.91
9	F	605	CHL	OMC-CMC-C2C	4.67	136.25	125.69
10	J	604	CLA	CAA-C2A-C3A	-4.67	99.99	112.78
9	E	607	CHL	C7-C6-C5	-4.66	100.72	113.36
9	I	608	CHL	C1-C2-C3	4.65	134.09	126.04
4	G	6620	LUT	C18-C5-C6	4.64	129.74	124.53
4	A	620	LUT	C38-C25-C24	-4.64	113.62	123.56
10	H	610	CLA	CBA-CAA-C2A	4.64	127.57	113.86
4	I	8621	LUT	C38-C25-C24	-4.64	113.63	123.56
10	E	613	CLA	CMB-C2B-C3B	4.62	133.31	124.68
10	B	612	CLA	C1-C2-C3	4.61	134.02	126.04
6	H	7623	NEX	C5-C4-C3	4.61	117.20	111.75
4	G	6620	LUT	C38-C25-C24	-4.60	113.71	123.56
9	B	608	CHL	C7-C6-C5	4.60	125.85	113.36
10	A	610	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
10	F	603	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
4	B	1620	LUT	C18-C5-C6	4.60	129.69	124.53
10	G	602	CLA	C1-C2-C3	4.59	133.99	126.04
7	H	7630	LHG	O8-C6-C5	4.59	121.80	108.43
9	F	607	CHL	O2A-CGA-CBA	4.59	126.31	111.91
9	I	601	CHL	OMC-CMC-C2C	4.59	136.06	125.69
10	B	611	CLA	O2A-CGA-CBA	4.59	126.30	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	606	CHL	C1-C2-C3	4.58	134.16	126.75
9	F	606	CHL	C1-C2-C3	4.58	134.16	126.75
9	F	608	CHL	C7-C6-C5	4.58	125.79	113.36
10	B	603	CLA	CBA-CAA-C2A	4.57	127.34	113.86
10	J	602	CLA	C1-C2-C3	4.56	133.93	126.04
4	F	5620	LUT	C18-C5-C6	4.56	129.65	124.53
9	F	607	CHL	CMB-C2B-C1B	-4.55	121.47	128.46
10	E	603	CLA	CBA-CAA-C2A	4.55	127.29	113.86
10	E	613	CLA	CED-O2D-CGD	4.54	126.22	115.94
9	I	607	CHL	OMC-CMC-C2C	4.54	135.94	125.69
10	D	613	CLA	CED-O2D-CGD	4.53	126.18	115.94
5	J	3622	XAT	C24-C23-C22	4.52	119.51	110.77
4	D	3621	LUT	C3-C4-C5	4.52	120.86	111.85
10	H	612	CLA	C1-C2-C3	4.52	133.86	126.04
9	E	606	CHL	CMB-C2B-C3B	4.51	133.12	124.68
10	J	610	CLA	O2A-CGA-CBA	4.51	126.08	111.91
9	B	601	CHL	CBA-CAA-C2A	4.51	127.18	113.86
9	F	601	CHL	CBA-CAA-C2A	4.51	127.18	113.86
10	J	603	CLA	O2D-CGD-CBD	4.51	119.28	111.27
10	I	602	CLA	O1D-CGD-CBD	-4.51	115.26	124.48
10	G	604	CLA	CAA-C2A-C3A	-4.51	100.44	112.78
10	G	610	CLA	CBA-CAA-C2A	4.50	127.16	113.86
4	D	3620	LUT	C38-C25-C24	-4.50	113.94	123.56
10	G	613	CLA	CED-O2D-CGD	4.50	126.11	115.94
10	G	611	CLA	C1-C2-C3	4.49	133.81	126.04
9	C	606	CHL	O2A-CGA-CBA	4.49	126.00	111.91
9	B	605	CHL	OMC-CMC-C2C	4.49	135.83	125.69
10	J	602	CLA	C4-C3-C5	4.49	122.82	115.27
10	H	603	CLA	CBA-CAA-C2A	4.48	127.09	113.86
10	F	614	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
9	A	601	CHL	OMC-CMC-C2C	4.48	135.81	125.69
10	H	610	CLA	O2A-CGA-CBA	4.48	125.95	111.91
10	G	614	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
10	B	614	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
9	G	606	CHL	CMB-C2B-C3B	4.47	133.03	124.68
4	H	7620	LUT	C18-C5-C6	4.46	129.54	124.53
9	H	601	CHL	CED-O2D-CGD	4.46	126.03	115.94
9	I	601	CHL	CMB-C2B-C1B	-4.46	121.60	128.46
9	A	606	CHL	O2A-CGA-CBA	4.44	125.83	111.91
10	F	610	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
9	H	609	CHL	CMB-C2B-C1B	-4.44	121.65	128.46
10	C	612	CLA	O2D-CGD-CBD	4.44	119.15	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	601	CHL	OMC-CMC-C2C	4.43	135.71	125.69
10	G	611	CLA	CAA-C2A-C3A	-4.43	100.64	112.78
10	C	603	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
10	B	611	CLA	C1-C2-C3	4.43	133.70	126.04
9	I	601	CHL	CBA-CAA-C2A	4.42	126.92	113.86
10	A	603	CLA	CBA-CAA-C2A	4.42	126.90	113.86
9	C	609	CHL	C1-C2-C3	4.41	133.67	126.04
10	A	613	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
4	I	8621	LUT	C3-C4-C5	4.40	120.62	111.85
10	A	604	CLA	CAA-C2A-C3A	-4.40	100.73	112.78
4	F	5620	LUT	C38-C25-C24	-4.40	114.15	123.56
10	D	611	CLA	CMB-C2B-C1B	-4.39	121.71	128.46
10	G	602	CLA	C4-C3-C5	4.39	122.65	115.27
4	H	7621	LUT	C38-C25-C24	-4.39	114.18	123.56
9	G	606	CHL	CAA-CBA-CGA	4.39	126.07	113.25
10	G	603	CLA	C6-C5-C3	4.39	124.95	113.45
10	J	604	CLA	C1-C2-C3	4.38	133.62	126.04
10	I	612	CLA	OBD-CAD-CBD	-4.38	119.64	125.89
7	H	7630	LHG	O8-C23-C24	4.37	125.63	111.91
10	I	613	CLA	CED-O2D-CGD	4.37	125.82	115.94
9	A	601	CHL	CMB-C2B-C1B	-4.37	121.75	128.46
10	I	613	CLA	CBA-CAA-C2A	4.36	126.74	113.86
10	J	611	CLA	C1-C2-C3	4.36	133.58	126.04
9	E	609	CHL	CMB-C2B-C1B	-4.36	121.77	128.46
10	H	604	CLA	CAA-C2A-C3A	-4.36	100.85	112.78
9	I	605	CHL	OMC-CMC-C2C	4.35	135.52	125.69
10	B	610	CLA	CBA-CAA-C2A	4.34	126.68	113.86
9	B	608	CHL	CMB-C2B-C1B	-4.34	121.79	128.46
10	E	602	CLA	O2D-CGD-CBD	4.34	118.97	111.27
10	J	610	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
10	J	614	CLA	CMB-C2B-C1B	-4.33	121.80	128.46
10	E	611	CLA	O2A-CGA-CBA	4.33	125.51	111.91
10	J	611	CLA	CBA-CAA-C2A	4.33	126.66	113.86
9	H	608	CHL	OMC-CMC-C2C	4.33	135.48	125.69
4	J	9621	LUT	C38-C25-C24	-4.33	114.29	123.56
6	J	9623	NEX	C5-C4-C3	4.33	116.87	111.75
9	B	608	CHL	CED-O2D-CGD	4.32	125.71	115.94
10	D	604	CLA	O2D-CGD-CBD	4.32	118.95	111.27
9	C	605	CHL	CED-O2D-CGD	4.32	125.71	115.94
10	F	612	CLA	C1-C2-C3	4.32	133.51	126.04
10	B	602	CLA	C6-C5-C3	4.32	124.78	113.45
10	D	614	CLA	CMB-C2B-C1B	-4.32	121.83	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	602	CLA	C4-C3-C5	4.31	122.52	115.27
6	C	2623	NEX	C5-C4-C3	4.31	116.85	111.75
10	A	610	CLA	CBA-CAA-C2A	4.31	126.58	113.86
6	I	8623	NEX	C5-C4-C3	4.31	116.84	111.75
4	B	1620	LUT	C38-C25-C24	-4.31	114.35	123.56
10	F	612	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
9	H	601	CHL	CMB-C2B-C1B	-4.30	121.86	128.46
9	F	607	CHL	C4-C3-C5	-4.30	108.04	115.27
10	I	603	CLA	O2D-CGD-CBD	4.30	118.91	111.27
10	H	604	CLA	C1-C2-C3	4.30	133.48	126.04
10	F	602	CLA	C5-C3-C2	-4.30	112.42	121.12
9	C	609	CHL	OMC-CMC-C2C	4.30	135.40	125.69
10	H	602	CLA	C1-C2-C3	4.30	133.47	126.04
10	G	603	CLA	CED-O2D-CGD	4.29	125.64	115.94
6	F	5623	NEX	C5-C4-C3	4.29	116.82	111.75
4	B	1621	LUT	C3-C4-C5	4.29	120.39	111.85
9	H	606	CHL	CMB-C2B-C3B	4.28	132.68	124.68
10	F	611	CLA	CBA-CAA-C2A	4.28	126.48	113.86
9	J	605	CHL	O2A-CGA-CBA	4.27	125.31	111.91
4	E	4620	LUT	C38-C25-C24	-4.25	114.47	123.56
10	G	612	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
9	H	608	CHL	CMB-C2B-C1B	-4.25	121.93	128.46
9	I	609	CHL	CMB-C2B-C1B	-4.25	121.94	128.46
9	G	607	CHL	O2A-CGA-CBA	4.25	125.23	111.91
10	D	610	CLA	CBA-CAA-C2A	4.25	126.40	113.86
6	D	3623	NEX	C5-C4-C3	4.24	116.77	111.75
10	D	610	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
10	A	602	CLA	C6-C5-C3	4.24	124.57	113.45
10	A	602	CLA	CMC-C2C-C1C	4.24	131.49	125.04
10	B	602	CLA	O2D-CGD-CBD	4.24	118.80	111.27
4	C	2620	LUT	C38-C25-C24	-4.23	114.50	123.56
9	A	609	CHL	CMB-C2B-C1B	-4.23	121.97	128.46
7	D	3630	LHG	O8-C6-C5	4.23	120.73	108.43
4	A	621	LUT	C38-C25-C24	-4.23	114.52	123.56
9	D	601	CHL	CED-O2D-CGD	4.22	125.49	115.94
9	I	601	CHL	CED-O2D-CGD	4.22	125.48	115.94
9	B	607	CHL	C7-C6-C5	-4.21	101.92	113.36
7	F	5630	LHG	O8-C6-C5	4.21	120.69	108.43
10	C	614	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
10	E	603	CLA	O2D-CGD-CBD	4.20	118.73	111.27
4	J	9621	LUT	C2-C3-C4	4.20	116.05	110.30
10	J	602	CLA	O2D-CGD-CBD	4.19	118.72	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	606	CHL	O2A-CGA-CBA	4.19	125.06	111.91
9	F	601	CHL	CMB-C2B-C1B	-4.19	122.02	128.46
7	C	2630	LHG	O8-C6-C5	4.18	120.61	108.43
4	H	7621	LUT	C2-C3-C4	4.18	116.03	110.30
10	G	612	CLA	O1D-CGD-CBD	-4.18	115.94	124.48
10	F	613	CLA	CED-O2D-CGD	4.18	125.38	115.94
10	F	611	CLA	C1-C2-C3	4.18	133.26	126.04
10	E	602	CLA	C6-C5-C3	4.17	124.39	113.45
9	D	607	CHL	CMB-C2B-C3B	4.16	132.47	124.68
9	I	609	CHL	CED-O2D-CGD	4.16	125.36	115.94
9	G	605	CHL	OMC-CMC-C2C	4.16	135.10	125.69
5	E	2622	XAT	O24-C25-C24	4.16	116.50	113.38
10	D	603	CLA	CBA-CAA-C2A	4.16	126.13	113.86
10	H	603	CLA	O2D-CGD-CBD	4.15	118.65	111.27
9	F	606	CHL	CMB-C2B-C3B	4.15	132.45	124.68
9	H	606	CHL	O2A-CGA-CBA	4.15	124.93	111.91
10	D	612	CLA	C16-C15-C13	4.15	129.33	115.92
9	H	609	CHL	OMC-CMC-C2C	4.14	135.05	125.69
10	J	602	CLA	CMC-C2C-C1C	4.14	131.35	125.04
9	C	607	CHL	CMB-C2B-C3B	4.14	132.43	124.68
7	F	5630	LHG	O8-C23-C24	4.14	124.91	111.91
9	E	609	CHL	C1-C2-C3	4.14	133.21	126.04
6	E	4623	NEX	C5-C4-C3	4.14	116.65	111.75
9	B	607	CHL	CMB-C2B-C3B	4.14	132.42	124.68
9	G	608	CHL	CMB-C2B-C1B	-4.14	122.11	128.46
9	C	607	CHL	O2A-CGA-CBA	4.14	124.89	111.91
9	J	606	CHL	CMB-C2B-C3B	4.13	132.41	124.68
10	E	610	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
10	E	610	CLA	CBA-CAA-C2A	4.13	126.06	113.86
4	H	7621	LUT	C3-C4-C5	4.13	120.08	111.85
10	C	611	CLA	C1-C2-C3	4.13	133.19	126.04
10	J	602	CLA	C5-C3-C2	-4.13	112.76	121.12
9	I	609	CHL	C1-C2-C3	4.13	133.19	126.04
10	J	611	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
9	F	606	CHL	CAA-CBA-CGA	4.13	125.31	113.25
9	C	608	CHL	C16-C15-C13	4.13	129.25	115.92
9	G	608	CHL	OMC-CMC-C2C	4.12	135.01	125.69
9	A	601	CHL	CED-O2D-CGD	4.12	125.26	115.94
9	A	608	CHL	OMC-CMC-C2C	4.12	135.00	125.69
9	E	601	CHL	CBA-CAA-C2A	4.12	126.03	113.86
10	D	612	CLA	O2D-CGD-CBD	4.12	118.59	111.27
9	C	601	CHL	CMB-C2B-C1B	-4.11	122.14	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	610	CLA	O2A-CGA-CBA	4.11	124.81	111.91
9	G	607	CHL	CBA-CAA-C2A	4.10	125.98	113.86
9	F	601	CHL	CED-O2D-CGD	4.10	125.22	115.94
10	D	610	CLA	CED-O2D-CGD	4.10	125.21	115.94
5	E	2622	XAT	C24-C23-C22	4.10	118.69	110.77
10	A	611	CLA	O2A-CGA-CBA	4.10	124.77	111.91
7	J	9630	LHG	O8-C6-C5	4.10	120.36	108.43
10	F	611	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
10	J	610	CLA	CBA-CAA-C2A	4.09	125.95	113.86
10	J	613	CLA	CMB-C2B-C3B	4.08	132.32	124.68
9	A	605	CHL	CED-O2D-CGD	4.08	125.17	115.94
10	I	604	CLA	CAA-CBA-CGA	4.08	125.18	113.25
9	E	606	CHL	O2A-CGA-CBA	4.08	124.71	111.91
10	I	602	CLA	C5-C3-C2	-4.08	112.86	121.12
9	D	608	CHL	CED-O2D-CGD	4.08	125.16	115.94
9	B	606	CHL	C1-C2-C3	4.08	133.35	126.75
9	C	606	CHL	CAA-CBA-CGA	4.07	125.16	113.25
10	H	611	CLA	O2A-CGA-CBA	4.07	124.68	111.91
9	A	606	CHL	C1-C2-C3	4.06	133.33	126.75
10	I	614	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
10	A	612	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
10	H	612	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
10	E	612	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
9	I	605	CHL	O2A-CGA-CBA	4.05	124.62	111.91
10	C	612	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
4	J	9620	LUT	C18-C5-C4	-4.04	106.86	114.36
9	E	608	CHL	CBA-CAA-C2A	4.04	125.80	113.86
10	J	613	CLA	C4-C3-C5	-4.04	108.48	115.27
10	C	611	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
9	E	601	CHL	CED-O2D-CGD	4.03	125.06	115.94
8	D	5632	DGD	O2G-C1B-C2B	4.03	120.19	111.50
10	C	603	CLA	O1D-CGD-CBD	-4.03	116.24	124.48
9	A	606	CHL	CMB-C2B-C3B	4.03	132.22	124.68
9	A	608	CHL	CBA-CAA-C2A	4.03	125.75	113.86
9	J	606	CHL	CED-O2D-CGD	4.03	125.04	115.94
4	E	4621	LUT	C2-C3-C4	4.03	115.81	110.30
10	I	602	CLA	CED-O2D-CGD	4.02	125.03	115.94
10	G	603	CLA	O2D-CGD-CBD	4.02	118.41	111.27
9	C	601	CHL	CBA-CAA-C2A	4.02	125.73	113.86
10	E	614	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
9	H	607	CHL	O2A-CGA-CBA	4.02	124.52	111.91
10	I	611	CLA	CMB-C2B-C1B	-4.01	122.30	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	602	CLA	O2D-CGD-CBD	4.01	118.40	111.27
10	C	612	CLA	C1-C2-C3	4.01	132.97	126.04
10	H	604	CLA	O1D-CGD-CBD	-4.00	116.30	124.48
9	H	601	CHL	OMC-CMC-C2C	4.00	134.73	125.69
10	G	602	CLA	C5-C3-C2	-4.00	113.02	121.12
4	F	5621	LUT	C2-C3-C4	4.00	115.78	110.30
10	D	612	CLA	C1-C2-C3	4.00	132.96	126.04
10	H	612	CLA	OBD-CAD-CBD	-3.99	120.19	125.89
4	J	9621	LUT	C18-C5-C6	3.99	129.01	124.53
9	F	605	CHL	CMB-C2B-C1B	-3.99	122.33	128.46
10	C	604	CLA	CED-O2D-CGD	3.99	124.95	115.94
4	E	4620	LUT	C18-C5-C4	-3.99	106.97	114.36
10	E	611	CLA	C1-C2-C3	3.98	132.93	126.04
4	I	8621	LUT	C2-C3-C4	3.98	115.75	110.30
10	G	602	CLA	O2D-CGD-CBD	3.98	118.34	111.27
10	J	603	CLA	CBA-CAA-C2A	3.98	125.61	113.86
9	I	607	CHL	O2A-CGA-CBA	3.98	124.39	111.91
9	B	609	CHL	CMB-C2B-C1B	-3.98	122.35	128.46
10	A	603	CLA	O1D-CGD-CBD	-3.97	116.35	124.48
9	I	607	CHL	C4-C3-C5	-3.97	108.59	115.27
9	C	609	CHL	CED-O2D-CGD	3.97	124.92	115.94
9	E	606	CHL	CAA-CBA-CGA	3.97	124.86	113.25
9	D	605	CHL	CED-O2D-CGD	3.97	124.92	115.94
9	C	605	CHL	OMC-CMC-C2C	3.97	134.66	125.69
10	G	602	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
10	D	603	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
10	A	602	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
10	C	602	CLA	C6-C5-C3	3.96	123.84	113.45
9	G	607	CHL	OMC-CMC-C2C	3.96	134.64	125.69
10	I	610	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
9	G	606	CHL	CED-O2D-CGD	3.96	124.89	115.94
9	C	605	CHL	O2A-CGA-CBA	3.95	124.32	111.91
9	H	605	CHL	O2A-CGA-CBA	3.95	124.31	111.91
10	I	604	CLA	O2D-CGD-CBD	3.95	118.29	111.27
9	C	601	CHL	OMC-CMC-C2C	3.95	134.61	125.69
9	D	605	CHL	CMB-C2B-C1B	-3.94	122.40	128.46
9	B	601	CHL	C11-C12-C13	3.94	128.66	115.92
10	C	610	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
10	D	612	CLA	O2A-CGA-CBA	3.94	124.27	111.91
10	J	612	CLA	O2D-CGD-CBD	3.94	118.27	111.27
9	B	606	CHL	CAA-C2A-C3A	-3.94	102.00	112.78
10	B	613	CLA	CBA-CAA-C2A	3.93	125.48	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	602	CLA	C5-C3-C2	-3.93	113.16	121.12
9	E	608	CHL	OMC-CMC-C2C	3.93	134.58	125.69
10	B	603	CLA	OBD-CAD-CBD	-3.93	120.28	125.89
10	A	611	CLA	CAA-C2A-C3A	-3.93	102.02	112.78
10	G	602	CLA	CMC-C2C-C1C	3.93	131.02	125.04
9	G	608	CHL	CED-O2D-CGD	3.93	124.82	115.94
10	D	611	CLA	O2A-CGA-CBA	3.93	124.24	111.91
10	H	610	CLA	CED-O2D-CGD	3.93	124.82	115.94
10	J	612	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
10	J	602	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
10	I	610	CLA	CBA-CAA-C2A	3.92	125.43	113.86
10	F	603	CLA	O2D-CGD-CBD	3.92	118.22	111.27
9	H	608	CHL	CBA-CAA-C2A	3.91	125.42	113.86
10	B	612	CLA	OBD-CAD-CBD	-3.91	120.30	125.89
10	E	613	CLA	C4-C3-C5	-3.91	108.69	115.27
9	I	605	CHL	CMB-C2B-C1B	-3.91	122.45	128.46
10	B	610	CLA	O2A-CGA-CBA	3.91	124.17	111.91
10	C	611	CLA	O2A-CGA-CBA	3.91	124.16	111.91
10	D	602	CLA	O2D-CGD-CBD	3.90	118.21	111.27
10	I	612	CLA	O2D-CGD-CBD	3.90	118.20	111.27
10	E	610	CLA	O2A-CGA-CBA	3.90	124.14	111.91
10	H	611	CLA	CAA-C2A-C3A	-3.90	102.11	112.78
9	H	609	CHL	CED-O2D-CGD	3.89	124.75	115.94
10	A	610	CLA	O2A-CGA-CBA	3.89	124.12	111.91
10	C	602	CLA	OBD-CAD-CBD	-3.89	120.34	125.89
10	F	610	CLA	CBA-CAA-C2A	3.89	125.33	113.86
10	C	610	CLA	C14-C13-C15	3.88	125.36	111.29
10	H	611	CLA	CED-O2D-CGD	3.88	124.72	115.94
10	F	611	CLA	CAA-CBA-CGA	3.88	124.60	113.25
10	I	612	CLA	O2A-CGA-CBA	3.88	124.09	111.91
10	B	602	CLA	C5-C3-C2	-3.88	113.26	121.12
9	D	608	CHL	CMB-C2B-C1B	-3.88	122.51	128.46
9	J	608	CHL	CED-O2D-CGD	3.88	124.70	115.94
7	F	5630	LHG	O7-C7-C8	3.87	119.85	111.50
9	A	605	CHL	O2A-CGA-CBA	3.87	124.05	111.91
9	G	601	CHL	CMB-C2B-C1B	-3.87	122.52	128.46
10	D	610	CLA	C1-C2-C3	3.86	132.73	126.04
4	C	2621	LUT	C2-C3-C4	3.86	115.59	110.30
10	H	613	CLA	C4-C3-C5	-3.86	108.78	115.27
9	C	607	CHL	OBD-CAD-CBD	-3.86	120.38	125.89
10	G	604	CLA	O2D-CGD-CBD	3.86	118.12	111.27
4	D	3621	LUT	C38-C25-C24	-3.86	115.31	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1630	LHG	O8-C6-C5	3.85	119.65	108.43
10	I	611	CLA	OBD-CAD-CBD	-3.85	120.39	125.89
10	G	603	CLA	CAA-CBA-CGA	3.85	124.51	113.25
4	H	7620	LUT	C18-C5-C4	-3.85	107.22	114.36
7	E	4630	LHG	O8-C6-C5	3.85	119.64	108.43
4	D	3620	LUT	C3-C4-C5	3.84	119.51	111.85
9	J	605	CHL	CMB-C2B-C1B	-3.84	122.56	128.46
4	G	6620	LUT	C18-C5-C4	-3.84	107.25	114.36
10	A	613	CLA	CED-O2D-CGD	3.84	124.62	115.94
9	E	605	CHL	CMB-C2B-C1B	-3.83	122.58	128.46
9	G	609	CHL	C1-C2-C3	3.83	132.67	126.04
10	F	604	CLA	O2D-CGD-CBD	3.83	118.07	111.27
10	J	602	CLA	OBD-CAD-CBD	-3.83	120.43	125.89
10	F	610	CLA	O2A-CGA-CBA	3.82	123.90	111.91
10	G	613	CLA	CBA-CAA-C2A	3.82	125.13	113.86
10	B	602	CLA	C4-C3-C5	3.82	121.69	115.27
9	C	609	CHL	CMB-C2B-C3B	3.82	131.82	124.68
10	E	612	CLA	OBD-CAD-CBD	-3.81	120.45	125.89
9	F	609	CHL	CAA-CBA-CGA	3.81	124.39	113.25
4	G	6621	LUT	C38-C25-C24	-3.81	115.41	123.56
10	H	602	CLA	O2D-CGD-CBD	3.81	118.04	111.27
9	D	606	CHL	CAA-CBA-CGA	3.81	124.39	113.25
10	B	604	CLA	C1-C2-C3	3.81	132.63	126.04
10	J	611	CLA	O2A-CGA-CBA	3.81	123.85	111.91
9	D	605	CHL	O2A-CGA-CBA	3.80	123.83	111.91
9	E	608	CHL	O2A-CGA-CBA	3.80	123.83	111.91
10	B	611	CLA	CED-O2D-CGD	3.80	124.52	115.94
9	J	606	CHL	C1-C2-C3	3.80	132.89	126.75
10	G	610	CLA	CED-O2D-CGD	3.79	124.52	115.94
10	B	610	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
9	E	601	CHL	CMB-C2B-C1B	-3.79	122.64	128.46
9	B	601	CHL	CED-O2D-CGD	3.79	124.51	115.94
10	B	612	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
10	D	603	CLA	CED-O2D-CGD	3.79	124.50	115.94
10	G	610	CLA	CMB-C2B-C1B	-3.79	122.65	128.46
10	J	603	CLA	C6-C5-C3	3.78	123.38	113.45
9	B	601	CHL	OMC-CMC-C2C	3.78	134.24	125.69
9	D	608	CHL	C16-C15-C13	3.78	128.15	115.92
9	I	608	CHL	CBA-CAA-C2A	3.78	125.03	113.86
10	A	610	CLA	CED-O2D-CGD	3.78	124.48	115.94
10	A	612	CLA	OBD-CAD-CBD	-3.77	120.50	125.89
10	D	612	CLA	O1D-CGD-CBD	-3.77	116.78	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5620	LUT	C2-C3-C4	3.77	115.46	110.30
10	D	603	CLA	OBD-CAD-CBD	-3.77	120.51	125.89
10	G	602	CLA	CBA-CAA-C2A	3.77	124.98	113.86
9	B	608	CHL	OMC-CMC-C2C	3.77	134.20	125.69
9	A	607	CHL	CBA-CAA-C2A	3.77	124.98	113.86
9	D	606	CHL	OBD-CAD-CBD	-3.76	120.52	125.89
9	G	605	CHL	CMB-C2B-C1B	-3.76	122.68	128.46
10	H	612	CLA	C4-C3-C5	-3.76	108.95	115.27
9	H	609	CHL	C1D-CHD-C4C	3.76	127.52	122.56
9	A	606	CHL	CAA-CBA-CGA	3.76	124.24	113.25
10	C	612	CLA	OBD-CAD-CBD	-3.76	120.53	125.89
10	A	604	CLA	C1-C2-C3	3.75	132.53	126.04
7	I	8630	LHG	O10-C23-C24	-3.75	109.09	123.73
10	E	612	CLA	C1-C2-C3	3.75	132.53	126.04
10	J	602	CLA	C6-C5-C3	3.75	123.28	113.45
10	A	612	CLA	O2D-CGD-CBD	3.75	117.93	111.27
10	C	604	CLA	O2D-CGD-CBD	3.74	117.92	111.27
4	A	621	LUT	C2-C3-C4	3.74	115.42	110.30
9	I	609	CHL	CAA-CBA-CGA	3.74	124.17	113.25
4	J	9620	LUT	C21-C26-C27	3.73	117.42	112.70
10	A	611	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
10	E	602	CLA	O1D-CGD-CBD	-3.73	116.85	124.48
7	I	8630	LHG	O8-C6-C5	3.73	119.29	108.43
4	D	3620	LUT	C18-C5-C4	-3.73	107.45	114.36
9	I	609	CHL	CAA-C2A-C3A	-3.73	102.57	112.78
10	F	603	CLA	OBD-CAD-CBD	-3.73	120.57	125.89
10	C	602	CLA	C5-C3-C2	-3.73	113.58	121.12
10	I	612	CLA	O1D-CGD-CBD	-3.72	116.86	124.48
10	H	611	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
10	E	612	CLA	O2D-CGD-CBD	3.72	117.88	111.27
10	H	612	CLA	O2A-CGA-CBA	3.72	123.58	111.91
10	C	604	CLA	O1A-CGA-CBA	-3.72	109.22	123.73
10	H	602	CLA	C4D-C3D-CAD	-3.72	106.40	108.47
9	J	608	CHL	O2A-CGA-CBA	3.72	123.58	111.91
10	A	604	CLA	O2D-CGD-CBD	3.72	117.88	111.27
10	F	612	CLA	O2D-CGD-CBD	3.72	117.87	111.27
9	A	609	CHL	C1-C2-C3	3.71	132.47	126.04
10	I	604	CLA	CAA-C2A-C3A	-3.71	102.61	112.78
10	F	602	CLA	C6-C5-C3	3.71	123.18	113.45
10	I	603	CLA	CBA-CAA-C2A	3.71	124.81	113.86
10	J	603	CLA	O1D-CGD-CBD	-3.71	116.90	124.48
10	A	602	CLA	C1-C2-C3	3.71	132.45	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	604	CLA	C4D-C3D-CAD	-3.70	106.41	108.47
10	D	602	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
10	F	612	CLA	OBD-CAD-CBD	-3.69	120.62	125.89
4	A	620	LUT	C18-C5-C4	-3.69	107.51	114.36
9	A	608	CHL	C1-C2-C3	3.69	132.43	126.04
10	D	603	CLA	O2D-CGD-CBD	3.69	117.82	111.27
9	I	606	CHL	O2A-CGA-CBA	3.68	123.46	111.91
4	D	3620	LUT	C2-C3-C4	3.68	115.34	110.30
10	H	602	CLA	OBD-CAD-CBD	-3.68	120.64	125.89
9	E	608	CHL	CMB-C2B-C1B	-3.68	122.81	128.46
7	D	3630	LHG	O8-C23-C24	3.68	123.45	111.91
10	D	604	CLA	O1A-CGA-CBA	-3.68	109.39	123.73
9	H	608	CHL	CED-O2D-CGD	3.67	124.25	115.94
10	B	604	CLA	O1A-CGA-CBA	-3.67	109.40	123.73
10	G	614	CLA	C1D-CHD-C4C	3.67	127.41	122.56
10	B	610	CLA	CED-O2D-CGD	3.67	124.24	115.94
10	I	613	CLA	C4-C3-C5	-3.67	109.10	115.27
10	I	603	CLA	OBD-CAD-CBD	-3.67	120.65	125.89
10	A	603	CLA	OBD-CAD-CBD	-3.67	120.65	125.89
9	D	605	CHL	OBD-CAD-CBD	-3.67	120.66	125.89
9	C	608	CHL	OBD-CAD-CBD	-3.67	120.66	125.89
10	A	602	CLA	CED-O2D-CGD	3.67	124.23	115.94
10	B	603	CLA	O1D-CGD-CBD	-3.67	116.98	124.48
10	E	602	CLA	OBD-CAD-CBD	-3.66	120.66	125.89
9	B	606	CHL	OBD-CAD-CBD	-3.66	120.66	125.89
10	J	604	CLA	CED-O2D-CGD	3.66	124.21	115.94
10	E	612	CLA	C16-C15-C13	3.66	127.75	115.92
10	G	610	CLA	O2A-CGA-CBA	3.66	123.39	111.91
9	C	607	CHL	CBA-CAA-C2A	3.66	124.66	113.86
9	H	608	CHL	C6-C5-C3	3.65	123.03	113.45
10	B	603	CLA	C4D-C3D-CAD	-3.65	106.43	108.47
10	F	603	CLA	C4D-C3D-CAD	-3.65	106.43	108.47
10	F	612	CLA	CED-O2D-CGD	3.65	124.20	115.94
10	B	602	CLA	O1D-CGD-CBD	-3.65	117.01	124.48
9	A	607	CHL	O2A-CGA-CBA	3.65	123.37	111.91
10	J	602	CLA	C4D-C3D-CAD	-3.65	106.43	108.47
10	A	602	CLA	O2D-CGD-CBD	3.65	117.75	111.27
10	E	611	CLA	CAA-C2A-C3A	-3.65	102.79	112.78
10	D	602	CLA	CBA-CAA-C2A	3.65	124.63	113.86
10	G	611	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
10	C	610	CLA	CBA-CAA-C2A	3.64	124.62	113.86
10	B	602	CLA	OBD-CAD-CBD	-3.64	120.69	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	605	CHL	O2A-CGA-CBA	3.64	123.34	111.91
8	G	9632	DGD	O2G-C1B-C2B	3.64	119.34	111.50
10	F	612	CLA	C16-C15-C13	3.64	127.68	115.92
9	B	608	CHL	CBA-CAA-C2A	3.64	124.60	113.86
10	J	602	CLA	O2A-CGA-CBA	3.64	123.32	111.91
9	F	608	CHL	C1-C2-C3	3.63	132.33	126.04
10	G	611	CLA	C1D-CHD-C4C	3.63	127.35	122.56
9	H	606	CHL	CED-O2D-CGD	3.63	124.15	115.94
10	J	610	CLA	CED-O2D-CGD	3.63	124.14	115.94
9	I	608	CHL	CMB-C2B-C1B	-3.63	122.89	128.46
10	C	602	CLA	C4-C3-C5	3.63	121.37	115.27
9	G	605	CHL	OBD-CAD-CBD	-3.63	120.71	125.89
10	I	611	CLA	C1D-CHD-C4C	3.63	127.34	122.56
10	H	602	CLA	C6-C7-C8	-3.62	104.20	115.92
4	E	4621	LUT	C38-C25-C24	-3.62	115.81	123.56
10	F	604	CLA	CAA-C2A-C3A	-3.62	102.86	112.78
10	B	611	CLA	CAA-C2A-C1A	3.62	123.84	111.97
9	A	606	CHL	CED-O2D-CGD	3.62	124.12	115.94
10	B	611	CLA	OBD-CAD-CBD	-3.62	120.72	125.89
9	A	608	CHL	C16-C15-C13	3.62	127.62	115.92
9	D	609	CHL	C1D-CHD-C4C	3.62	127.33	122.56
8	B	1632	DGD	O2G-C1B-C2B	3.61	119.29	111.50
9	E	608	CHL	OBD-CAD-CBD	-3.61	120.73	125.89
9	E	609	CHL	CED-O2D-CGD	3.61	124.10	115.94
10	D	603	CLA	C4D-C3D-CAD	-3.61	106.46	108.47
10	H	612	CLA	O2D-CGD-CBD	3.61	117.68	111.27
10	C	603	CLA	CED-O2D-CGD	3.61	124.09	115.94
9	J	608	CHL	OBD-CAD-CBD	-3.61	120.74	125.89
10	I	612	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
10	F	611	CLA	OBD-CAD-CBD	-3.60	120.75	125.89
10	B	613	CLA	C4D-C3D-CAD	-3.60	106.46	108.47
10	B	604	CLA	CAA-CBA-CGA	3.60	123.77	113.25
10	C	610	CLA	CMC-C2C-C1C	3.60	130.52	125.04
10	G	603	CLA	OBD-CAD-CBD	-3.60	120.76	125.89
10	I	611	CLA	C1-C2-C3	3.60	132.26	126.04
10	A	613	CLA	C4-C3-C5	-3.60	109.22	115.27
9	B	605	CHL	O2A-CGA-CBA	3.59	123.18	111.91
10	J	613	CLA	CBA-CAA-C2A	3.59	124.47	113.86
10	I	602	CLA	C6-C5-C3	3.59	122.87	113.45
9	J	609	CHL	C1D-CHD-C4C	3.59	127.30	122.56
10	D	602	CLA	C6-C5-C3	3.59	122.87	113.45
9	B	608	CHL	O2A-CGA-CBA	3.58	123.16	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1622	XAT	O24-C25-C24	3.58	116.07	113.38
9	C	609	CHL	CAA-CBA-CGA	3.58	123.72	113.25
10	G	603	CLA	CBA-CAA-C2A	3.58	124.43	113.86
10	I	612	CLA	C4-C3-C5	-3.58	109.25	115.27
9	E	609	CHL	C1D-CHD-C4C	3.58	127.28	122.56
9	G	609	CHL	CMB-C2B-C1B	-3.58	122.97	128.46
10	G	602	CLA	C4D-C3D-CAD	-3.58	106.48	108.47
9	I	607	CHL	OBD-CAD-CBD	-3.58	120.79	125.89
9	E	606	CHL	OBD-CAD-CBD	-3.57	120.79	125.89
10	J	602	CLA	CBA-CAA-C2A	3.57	124.41	113.86
10	I	604	CLA	OBD-CAD-CBD	-3.57	120.80	125.89
10	D	612	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
10	C	610	CLA	O2A-CGA-CBA	3.57	123.11	111.91
10	I	602	CLA	C4D-C3D-CAD	-3.57	106.48	108.47
10	C	603	CLA	OBD-CAD-CBD	-3.57	120.80	125.89
10	I	602	CLA	OBD-CAD-CBD	-3.57	120.80	125.89
10	A	603	CLA	C6-C5-C3	3.56	122.80	113.45
8	B	2632	DGD	O2G-C1B-C2B	3.56	119.18	111.50
10	G	611	CLA	CED-O2D-CGD	3.56	124.00	115.94
10	H	603	CLA	CED-O2D-CGD	3.56	123.99	115.94
10	I	610	CLA	O2A-CGA-CBA	3.56	123.08	111.91
10	E	602	CLA	C4D-C3D-CAD	-3.56	106.49	108.47
10	J	604	CLA	CBA-CAA-C2A	3.56	124.36	113.86
10	H	611	CLA	OBD-CAD-CBD	-3.56	120.81	125.89
10	E	604	CLA	CED-O2D-CGD	3.55	123.98	115.94
10	E	602	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
10	B	610	CLA	C14-C13-C15	3.55	124.16	111.29
9	F	608	CHL	OBD-CAD-CBD	-3.55	120.82	125.89
10	C	610	CLA	C1D-CHD-C4C	3.55	127.24	122.56
10	G	611	CLA	OBD-CAD-CBD	-3.55	120.82	125.89
9	F	605	CHL	OBD-CAD-CBD	-3.55	120.82	125.89
10	J	602	CLA	C12-C11-C10	-3.55	96.94	113.24
10	I	613	CLA	C4D-C3D-CAD	-3.55	106.49	108.47
10	G	602	CLA	OBD-CAD-CBD	-3.55	120.83	125.89
10	G	611	CLA	O2A-CGA-CBA	3.55	123.03	111.91
10	A	613	CLA	CMB-C2B-C3B	3.55	131.31	124.68
10	J	612	CLA	C16-C15-C13	3.54	127.38	115.92
9	B	609	CHL	CED-O2D-CGD	3.54	123.95	115.94
10	D	602	CLA	OBD-CAD-CBD	-3.54	120.84	125.89
9	F	609	CHL	C1D-CHD-C4C	3.54	127.23	122.56
10	F	614	CLA	OBD-CAD-CBD	-3.54	120.84	125.89
10	C	612	CLA	C1D-CHD-C4C	3.54	127.23	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5620	LUT	C3-C4-C5	3.54	118.90	111.85
10	C	612	CLA	O1D-CGD-CBD	-3.53	117.25	124.48
10	H	611	CLA	C1D-CHD-C4C	3.53	127.22	122.56
9	B	607	CHL	O2A-CGA-CBA	3.53	122.99	111.91
9	F	608	CHL	C1D-CHD-C4C	3.53	127.22	122.56
10	J	603	CLA	C4-C3-C5	-3.53	109.34	115.27
10	B	603	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
10	J	604	CLA	O2D-CGD-CBD	3.53	117.53	111.27
10	D	612	CLA	OBD-CAD-CBD	-3.53	120.86	125.89
9	B	609	CHL	C1D-CHD-C4C	3.52	127.21	122.56
9	F	607	CHL	CMB-C2B-C3B	3.52	131.27	124.68
10	G	603	CLA	O2A-CGA-CBA	3.52	122.96	111.91
9	F	608	CHL	CMB-C2B-C1B	-3.52	123.05	128.46
9	I	609	CHL	C1D-CHD-C4C	3.52	127.20	122.56
10	F	602	CLA	CBA-CAA-C2A	3.52	124.26	113.86
9	C	605	CHL	OBD-CAD-CBD	-3.52	120.87	125.89
9	A	608	CHL	OBD-CAD-CBD	-3.52	120.87	125.89
10	A	602	CLA	C11-C10-C8	-3.52	104.55	115.92
10	H	610	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
10	F	613	CLA	CBA-CAA-C2A	3.52	124.24	113.86
10	A	611	CLA	CAA-C2A-C1A	3.52	123.50	111.97
10	C	604	CLA	OBD-CAD-CBD	-3.51	120.87	125.89
10	G	610	CLA	C14-C13-C15	3.51	124.02	111.29
9	J	606	CHL	C1D-CHD-C4C	3.51	127.19	122.56
9	B	607	CHL	C4-C3-C5	-3.51	109.37	115.27
10	C	602	CLA	C14-C13-C15	3.51	123.99	111.29
4	A	620	LUT	C3-C4-C5	3.51	118.84	111.85
10	C	604	CLA	C4D-C3D-CAD	-3.51	106.52	108.47
10	B	611	CLA	CMB-C2B-C3B	3.51	131.24	124.68
10	E	602	CLA	CBA-CAA-C2A	3.51	124.21	113.86
9	J	608	CHL	C16-C15-C13	3.50	127.25	115.92
10	A	603	CLA	C4D-C3D-CAD	-3.50	106.52	108.47
10	D	602	CLA	C4-C3-C5	3.50	121.16	115.27
10	F	611	CLA	C4D-C3D-CAD	-3.50	106.52	108.47
10	I	602	CLA	C14-C13-C15	3.50	123.97	111.29
5	J	3622	XAT	O24-C25-C24	3.50	116.01	113.38
10	H	602	CLA	C14-C13-C15	3.50	123.97	111.29
9	F	606	CHL	C5-C3-C4	-3.50	106.87	114.60
10	J	611	CLA	CAA-C2A-C1A	3.50	123.44	111.97
10	E	604	CLA	C4D-C3D-CAD	-3.50	106.52	108.47
9	J	607	CHL	O2A-CGA-CBA	3.49	122.87	111.91
9	E	605	CHL	O2A-CGA-CBA	3.49	122.87	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	607	CHL	OBD-CAD-CBD	-3.49	120.91	125.89
10	G	612	CLA	OBD-CAD-CBD	-3.49	120.91	125.89
10	D	604	CLA	O1D-CGD-CBD	-3.49	117.34	124.48
8	D	5632	DGD	C6D-O5D-C1E	3.48	120.54	113.74
10	E	613	CLA	C4D-C3D-CAD	-3.48	106.53	108.47
10	F	604	CLA	CBA-CAA-C2A	3.48	124.13	113.86
10	J	614	CLA	C1D-CHD-C4C	3.48	127.15	122.56
9	B	601	CHL	CMB-C2B-C1B	-3.48	123.12	128.46
9	C	608	CHL	CMB-C2B-C1B	-3.48	123.12	128.46
10	G	612	CLA	O2A-CGA-CBA	3.48	122.82	111.91
9	D	601	CHL	OBD-CAD-CBD	-3.48	120.93	125.89
10	A	603	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
10	B	612	CLA	O2A-CGA-CBA	3.47	122.81	111.91
10	I	611	CLA	C4D-C3D-CAD	-3.47	106.53	108.47
10	I	610	CLA	C1D-CHD-C4C	3.47	127.14	122.56
9	H	605	CHL	OMC-CMC-C2C	3.47	133.53	125.69
9	D	601	CHL	C1D-CHD-C4C	3.47	127.14	122.56
9	C	605	CHL	CMB-C2B-C1B	-3.47	123.13	128.46
9	H	607	CHL	OBD-CAD-CBD	-3.47	120.94	125.89
10	E	604	CLA	OBD-CAD-CBD	-3.47	120.94	125.89
10	D	610	CLA	C14-C13-C15	3.47	123.86	111.29
9	B	606	CHL	C4D-C3D-CAD	-3.47	106.54	108.47
10	F	602	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
9	C	609	CHL	C1D-CHD-C4C	3.46	127.13	122.56
9	A	605	CHL	OBD-CAD-CBD	-3.46	120.95	125.89
10	A	611	CLA	OBD-CAD-CBD	-3.46	120.95	125.89
9	F	601	CHL	OBD-CAD-CBD	-3.46	120.95	125.89
9	F	608	CHL	C4D-C3D-CAD	-3.46	106.54	108.47
4	H	7621	LUT	C18-C5-C4	-3.46	107.95	114.36
10	G	614	CLA	CBA-CAA-C2A	3.46	124.07	113.86
10	G	603	CLA	C1-C2-C3	3.46	132.02	126.04
4	I	8621	LUT	C18-C5-C6	3.46	128.41	124.53
9	F	609	CHL	CMB-C2B-C3B	3.46	131.14	124.68
9	H	608	CHL	C1D-CHD-C4C	3.45	127.11	122.56
10	B	614	CLA	CAA-CBA-CGA	3.45	123.34	113.25
9	D	609	CHL	CMB-C2B-C3B	3.45	131.14	124.68
10	C	602	CLA	C4D-C3D-CAD	-3.45	106.55	108.47
10	D	611	CLA	OBD-CAD-CBD	-3.45	120.96	125.89
10	A	602	CLA	C1D-CHD-C4C	3.45	127.11	122.56
9	F	607	CHL	C5-C3-C2	3.45	128.10	121.12
10	G	611	CLA	CAA-C2A-C1A	3.45	123.28	111.97
10	F	602	CLA	O2D-CGD-CBD	3.45	117.39	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	608	CHL	C4D-C3D-CAD	-3.45	106.55	108.47
9	I	605	CHL	OBD-CAD-CBD	-3.45	120.97	125.89
10	D	604	CLA	CBA-CAA-C2A	3.45	124.03	113.86
10	D	604	CLA	C4D-C3D-CAD	-3.44	106.55	108.47
10	G	610	CLA	C1D-CHD-C4C	3.44	127.10	122.56
10	F	613	CLA	C4-C3-C5	-3.44	109.48	115.27
4	B	1620	LUT	C18-C5-C4	-3.44	107.97	114.36
10	D	610	CLA	C4D-C3D-CAD	-3.44	106.55	108.47
10	I	602	CLA	CBA-CAA-C2A	3.44	124.03	113.86
10	A	602	CLA	OBD-CAD-CBD	-3.44	120.98	125.89
9	B	609	CHL	C14-C13-C15	3.44	123.76	111.29
10	J	612	CLA	OBD-CAD-CBD	-3.44	120.98	125.89
5	B	5622	XAT	O24-C25-C24	3.44	115.97	113.38
10	I	604	CLA	C4D-C3D-CAD	-3.44	106.55	108.47
10	H	603	CLA	OBD-CAD-CBD	-3.44	120.99	125.89
10	A	611	CLA	C1D-CHD-C4C	3.44	127.09	122.56
10	C	602	CLA	CMC-C2C-C1C	3.43	130.27	125.04
9	F	607	CHL	CBA-CAA-C2A	3.43	124.00	113.86
9	G	606	CHL	C1D-CHD-C4C	3.43	127.09	122.56
9	J	608	CHL	CMB-C2B-C1B	-3.43	123.19	128.46
10	B	611	CLA	C1D-CHD-C4C	3.43	127.09	122.56
9	E	607	CHL	C1D-CHD-C4C	3.43	127.09	122.56
10	J	602	CLA	O1D-CGD-CBD	-3.43	117.47	124.48
10	F	614	CLA	C1D-CHD-C4C	3.43	127.08	122.56
10	F	603	CLA	CBA-CAA-C2A	3.42	123.97	113.86
10	H	602	CLA	C4-C3-C5	3.42	121.03	115.27
10	D	604	CLA	OBD-CAD-CBD	-3.42	121.01	125.89
10	J	611	CLA	OBD-CAD-CBD	-3.42	121.01	125.89
10	H	604	CLA	OBD-CAD-CBD	-3.42	121.01	125.89
7	A	630	LHG	O10-C23-C24	-3.42	110.39	123.73
9	J	608	CHL	CBA-CAA-C2A	3.42	123.96	113.86
10	C	611	CLA	C1D-CHD-C4C	3.42	127.07	122.56
9	G	609	CHL	C1D-CHD-C4C	3.42	127.07	122.56
10	H	602	CLA	CMC-C2C-C1C	3.42	130.24	125.04
9	J	608	CHL	OMC-CMC-C2C	3.42	133.41	125.69
9	A	607	CHL	C12-C11-C10	-3.42	97.54	113.24
9	D	609	CHL	C14-C13-C15	3.41	123.66	111.29
10	F	603	CLA	CMB-C2B-C3B	3.41	131.07	124.68
9	G	606	CHL	OBD-CAD-CBD	-3.41	121.02	125.89
10	I	612	CLA	C4D-C3D-CAD	-3.41	106.57	108.47
10	D	602	CLA	C4D-C3D-CAD	-3.41	106.57	108.47
10	C	612	CLA	O2A-CGA-CBA	3.41	122.61	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	602	CLA	CBA-CAA-C2A	3.41	123.93	113.86
9	G	601	CHL	C1D-CHD-C4C	3.41	127.06	122.56
4	C	2621	LUT	C38-C25-C24	-3.41	116.27	123.56
9	I	608	CHL	OMC-CMC-C2C	3.41	133.39	125.69
9	G	605	CHL	O2A-CGA-CBA	3.41	122.61	111.91
10	F	602	CLA	CMC-C2C-C1C	3.41	130.23	125.04
9	B	608	CHL	C6-C5-C3	3.41	122.39	113.45
10	F	612	CLA	C1D-CHD-C4C	3.41	127.05	122.56
10	F	604	CLA	CAA-CBA-CGA	3.41	123.20	113.25
7	A	630	LHG	O7-C7-C8	3.41	118.84	111.50
10	J	604	CLA	OBD-CAD-CBD	-3.41	121.03	125.89
9	B	608	CHL	OBD-CAD-CBD	-3.40	121.04	125.89
9	J	609	CHL	CMB-C2B-C3B	3.40	131.04	124.68
10	D	614	CLA	OBD-CAD-CBD	-3.40	121.04	125.89
10	F	602	CLA	C11-C10-C8	-3.40	104.93	115.92
10	A	614	CLA	C1D-CHD-C4C	3.40	127.04	122.56
9	J	605	CHL	OBD-CAD-CBD	-3.40	121.04	125.89
10	F	610	CLA	C4D-C3D-CAD	-3.40	106.58	108.47
4	A	621	LUT	C18-C5-C6	3.40	128.34	124.53
10	A	604	CLA	OBD-CAD-CBD	-3.39	121.05	125.89
10	D	602	CLA	CED-O2D-CGD	3.39	123.61	115.94
5	D	8622	XAT	O24-C25-C24	3.39	115.93	113.38
10	F	602	CLA	OBD-CAD-CBD	-3.39	121.05	125.89
9	D	608	CHL	OBD-CAD-CBD	-3.39	121.05	125.89
10	A	602	CLA	C4D-C3D-CAD	-3.39	106.58	108.47
10	F	613	CLA	C4D-C3D-CAD	-3.39	106.58	108.47
10	C	602	CLA	CBA-CAA-C2A	3.39	123.86	113.86
9	C	607	CHL	C4D-C3D-CAD	-3.38	106.58	108.47
9	I	606	CHL	OBD-CAD-CBD	-3.38	121.06	125.89
10	H	612	CLA	C16-C15-C13	3.38	126.86	115.92
10	B	602	CLA	C11-C10-C8	-3.38	104.98	115.92
10	E	610	CLA	C4D-C3D-CAD	-3.38	106.58	108.47
9	I	608	CHL	CED-O2D-CGD	3.38	123.59	115.94
10	H	614	CLA	C1D-CHD-C4C	3.38	127.02	122.56
9	I	607	CHL	C12-C11-C10	-3.38	97.70	113.24
10	D	611	CLA	CAA-C2A-C1A	3.38	123.06	111.97
10	I	613	CLA	OBD-CAD-CBD	-3.38	121.06	125.89
9	D	607	CHL	O2A-CGA-CBA	3.38	122.52	111.91
9	A	605	CHL	CMB-C2B-C1B	-3.38	123.27	128.46
10	C	602	CLA	C1D-CHD-C4C	3.38	127.02	122.56
10	E	602	CLA	CED-O2D-CGD	3.38	123.58	115.94
10	C	612	CLA	CED-O2D-CGD	3.38	123.58	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	607	CHL	CBA-CAA-C2A	3.38	123.83	113.86
9	E	605	CHL	OBD-CAD-CBD	-3.37	121.07	125.89
9	D	607	CHL	OBD-CAD-CBD	-3.37	121.08	125.89
10	J	602	CLA	C11-C10-C8	-3.37	105.02	115.92
9	E	607	CHL	OBD-CAD-CBD	-3.37	121.08	125.89
10	E	612	CLA	CED-O2D-CGD	3.37	123.56	115.94
10	H	610	CLA	C1D-CHD-C4C	3.37	127.01	122.56
10	H	602	CLA	CBA-CAA-C2A	3.37	123.81	113.86
10	E	611	CLA	OBD-CAD-CBD	-3.37	121.08	125.89
10	H	603	CLA	O1D-CGD-CBD	-3.37	117.59	124.48
10	I	612	CLA	C1-C2-C3	3.37	131.87	126.04
9	C	601	CHL	C1D-CHD-C4C	3.37	127.00	122.56
9	A	605	CHL	C1D-CHD-C4C	3.37	127.00	122.56
10	B	611	CLA	C4D-C3D-CAD	-3.37	106.59	108.47
10	C	614	CLA	C1D-CHD-C4C	3.37	127.00	122.56
10	F	602	CLA	C4D-C3D-CAD	-3.37	106.59	108.47
10	A	614	CLA	CMB-C2B-C3B	3.37	130.97	124.68
10	I	604	CLA	O1D-CGD-CBD	-3.37	117.60	124.48
10	G	602	CLA	C6-C5-C3	3.36	122.27	113.45
10	B	604	CLA	C4-C3-C5	-3.36	109.62	115.27
10	F	612	CLA	O2A-CGA-CBA	3.36	122.45	111.91
10	D	604	CLA	CED-O2D-CGD	3.36	123.53	115.94
10	B	610	CLA	C4D-C3D-CAD	-3.36	106.60	108.47
10	I	612	CLA	C1D-CHD-C4C	3.36	126.99	122.56
9	J	601	CHL	OMC-CMC-C2C	3.36	133.27	125.69
9	J	601	CHL	CMB-C2B-C1B	-3.35	123.31	128.46
4	B	1621	LUT	C2-C3-C4	3.35	114.89	110.30
9	B	601	CHL	C4D-C3D-CAD	-3.35	106.60	108.47
10	H	614	CLA	CMB-C2B-C3B	3.35	130.95	124.68
9	A	601	CHL	C1D-CHD-C4C	3.35	126.98	122.56
9	G	608	CHL	OBD-CAD-CBD	-3.35	121.11	125.89
10	J	614	CLA	CAA-CBA-CGA	3.35	123.04	113.25
9	F	608	CHL	CED-O2D-CGD	3.35	123.51	115.94
9	F	607	CHL	C1D-CHD-C4C	3.35	126.97	122.56
10	G	612	CLA	C1D-CHD-C4C	3.35	126.97	122.56
9	E	605	CHL	C1D-CHD-C4C	3.35	126.97	122.56
10	B	612	CLA	O2D-CGD-CBD	3.34	117.21	111.27
2	D	3633	BNG	C1'-O1-C1	3.34	119.38	113.84
10	E	614	CLA	CBA-CAA-C2A	3.34	123.72	113.86
9	H	605	CHL	C1D-CHD-C4C	3.34	126.97	122.56
10	C	602	CLA	O1D-CGD-CBD	-3.34	117.65	124.48
10	D	611	CLA	CAA-CBA-CGA	3.34	123.01	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	605	CHL	C4D-C3D-CAD	-3.34	106.61	108.47
10	E	614	CLA	O2A-CGA-CBA	3.34	122.38	111.91
10	C	610	CLA	CED-O2D-CGD	3.34	123.48	115.94
10	E	611	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
9	A	608	CHL	CMB-C2B-C1B	-3.33	123.34	128.46
9	G	607	CHL	OBD-CAD-CBD	-3.33	121.13	125.89
9	I	601	CHL	CMB-C2B-C3B	3.33	130.91	124.68
10	D	611	CLA	O2D-CGD-CBD	3.33	117.18	111.27
10	J	603	CLA	CED-O2D-CGD	3.33	123.46	115.94
10	A	610	CLA	C1D-CHD-C4C	3.33	126.95	122.56
10	B	604	CLA	OBD-CAD-CBD	-3.33	121.14	125.89
10	A	612	CLA	C16-C15-C13	3.32	126.67	115.92
7	G	6630	LHG	O10-C23-C24	-3.32	110.76	123.73
10	D	611	CLA	C1D-CHD-C4C	3.32	126.94	122.56
10	A	611	CLA	CED-O2D-CGD	3.32	123.45	115.94
10	F	613	CLA	OBD-CAD-CBD	-3.32	121.15	125.89
9	B	605	CHL	C1D-CHD-C4C	3.32	126.94	122.56
10	J	603	CLA	C5-C3-C2	3.32	127.83	121.12
9	F	601	CHL	C1D-CHD-C4C	3.32	126.94	122.56
9	G	601	CHL	OBD-CAD-CBD	-3.32	121.16	125.89
10	J	613	CLA	OBD-CAD-CBD	-3.31	121.16	125.89
9	C	606	CHL	OBD-CAD-CBD	-3.31	121.17	125.89
9	B	601	CHL	OBD-CAD-CBD	-3.31	121.17	125.89
10	C	603	CLA	CMB-C2B-C3B	3.31	130.87	124.68
10	F	604	CLA	C1-C2-C3	3.31	131.76	126.04
9	A	608	CHL	C1D-CHD-C4C	3.31	126.92	122.56
9	H	607	CHL	C7-C6-C5	-3.31	104.38	113.36
10	A	614	CLA	CBA-CAA-C2A	3.31	123.62	113.86
10	C	613	CLA	C4D-C3D-CAD	-3.31	106.63	108.47
10	B	602	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
9	E	601	CHL	C4-C3-C5	-3.30	109.71	115.27
4	H	7621	LUT	C18-C5-C6	3.30	128.24	124.53
10	G	604	CLA	OBD-CAD-CBD	-3.30	121.18	125.89
10	B	602	CLA	C4D-C3D-CAD	-3.30	106.63	108.47
9	J	605	CHL	CED-O2D-CGD	3.30	123.40	115.94
10	A	610	CLA	CMB-C2B-C3B	3.30	130.85	124.68
10	E	603	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
10	B	610	CLA	OBD-CAD-CBD	-3.30	121.18	125.89
9	D	606	CHL	C4D-C3D-CAD	-3.30	106.63	108.47
9	A	606	CHL	C5-C3-C4	-3.30	107.32	114.60
10	F	602	CLA	C1D-CHD-C4C	3.30	126.91	122.56
10	J	612	CLA	O1D-CGD-CBD	-3.30	117.74	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	603	CLA	O1D-CGD-CBD	-3.30	117.74	124.48
10	D	602	CLA	CMC-C2C-C1C	3.29	130.05	125.04
9	J	607	CHL	CBA-CAA-C2A	3.29	123.58	113.86
9	D	607	CHL	C7-C6-C5	-3.29	104.42	113.36
10	C	610	CLA	OBD-CAD-CBD	-3.29	121.19	125.89
10	E	612	CLA	C1D-CHD-C4C	3.29	126.90	122.56
9	C	608	CHL	C1D-CHD-C4C	3.29	126.90	122.56
10	I	614	CLA	C4D-C3D-CAD	-3.29	106.64	108.47
9	E	609	CHL	CMB-C2B-C3B	3.29	130.83	124.68
10	E	602	CLA	O2A-CGA-CBA	3.29	122.22	111.91
9	D	609	CHL	C7-C6-C5	-3.29	104.44	113.36
10	B	602	CLA	CBA-CAA-C2A	3.28	123.56	113.86
9	G	608	CHL	C1D-CHD-C4C	3.28	126.89	122.56
10	G	604	CLA	O1D-CGD-CBD	-3.28	117.77	124.48
9	E	608	CHL	C16-C15-C13	3.28	126.53	115.92
10	G	611	CLA	C4D-C3D-CAD	-3.28	106.64	108.47
10	H	613	CLA	C4D-C3D-CAD	-3.28	106.64	108.47
10	I	612	CLA	C16-C15-C13	3.28	126.53	115.92
10	A	612	CLA	O1D-CGD-CBD	-3.28	117.77	124.48
10	H	612	CLA	C1D-CHD-C4C	3.28	126.89	122.56
9	I	606	CHL	C4D-C3D-CAD	-3.28	106.64	108.47
9	J	606	CHL	OBD-CAD-CBD	-3.28	121.21	125.89
10	G	604	CLA	C6-C7-C8	3.28	126.52	115.92
8	I	8632	DGD	O2G-C1B-C2B	3.28	118.57	111.50
10	F	602	CLA	C12-C11-C10	-3.28	98.17	113.24
10	E	603	CLA	OBD-CAD-CBD	-3.28	121.21	125.89
9	G	609	CHL	CED-O2D-CGD	3.28	123.35	115.94
9	I	608	CHL	OBD-CAD-CBD	-3.28	121.21	125.89
10	H	611	CLA	C4D-C3D-CAD	-3.28	106.64	108.47
9	I	608	CHL	C1D-CHD-C4C	3.28	126.88	122.56
10	B	614	CLA	OBD-CAD-CBD	-3.27	121.22	125.89
9	B	608	CHL	C4-C3-C5	-3.27	109.76	115.27
10	I	602	CLA	C11-C10-C8	-3.27	105.33	115.92
10	C	610	CLA	C4D-C3D-CAD	-3.27	106.64	108.47
10	C	603	CLA	C4D-C3D-CAD	-3.27	106.64	108.47
10	B	602	CLA	C1D-CHD-C4C	3.27	126.88	122.56
4	I	8620	LUT	C18-C5-C4	-3.27	108.30	114.36
9	D	601	CHL	C16-C15-C13	3.27	126.49	115.92
9	F	609	CHL	OBD-CAD-CBD	-3.27	121.22	125.89
9	H	606	CHL	C1D-CHD-C4C	3.27	126.87	122.56
10	H	602	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
9	A	609	CHL	OBD-CAD-CBD	-3.27	121.23	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	3630	LHG	O7-C7-C8	3.27	118.54	111.50
4	B	1620	LUT	C3-C4-C5	3.27	118.36	111.85
10	F	612	CLA	O1D-CGD-CBD	-3.27	117.80	124.48
9	A	608	CHL	C4D-C3D-CAD	-3.27	106.65	108.47
10	H	602	CLA	C12-C11-C10	-3.26	98.25	113.24
9	H	606	CHL	OBD-CAD-CBD	-3.26	121.23	125.89
9	F	605	CHL	C4D-C3D-CAD	-3.26	106.65	108.47
10	J	610	CLA	C4D-C3D-CAD	-3.26	106.65	108.47
10	H	602	CLA	O1D-CGD-CBD	-3.26	117.81	124.48
10	I	614	CLA	C1D-CHD-C4C	3.26	126.86	122.56
9	A	609	CHL	C1D-CHD-C4C	3.26	126.86	122.56
10	I	611	CLA	CAA-C2A-C3A	-3.26	103.85	112.78
10	B	604	CLA	C1D-CHD-C4C	3.26	126.86	122.56
4	A	621	LUT	C18-C5-C4	-3.26	108.32	114.36
10	F	610	CLA	C1D-CHD-C4C	3.26	126.86	122.56
10	J	611	CLA	C1D-CHD-C4C	3.26	126.86	122.56
9	C	607	CHL	C1D-CHD-C4C	3.26	126.86	122.56
10	E	611	CLA	C1D-CHD-C4C	3.26	126.86	122.56
9	B	607	CHL	C1D-CHD-C4C	3.26	126.86	122.56
9	F	601	CHL	C4D-C3D-CAD	-3.26	106.65	108.47
5	H	4622	XAT	O24-C25-C24	3.26	115.83	113.38
10	D	610	CLA	OBD-CAD-CBD	-3.26	121.24	125.89
10	C	612	CLA	C16-C15-C13	3.26	126.44	115.92
10	C	604	CLA	C1-C2-C3	3.25	131.67	126.04
10	B	612	CLA	C16-C15-C13	3.25	126.43	115.92
9	F	608	CHL	C6-C5-C3	3.25	121.98	113.45
10	B	602	CLA	C14-C13-C15	3.25	123.07	111.29
7	B	1630	LHG	O10-C23-C24	-3.25	111.05	123.73
4	E	4620	LUT	C21-C26-C27	3.25	116.81	112.70
9	D	601	CHL	CMB-C2B-C1B	-3.25	123.47	128.46
9	A	601	CHL	CMB-C2B-C3B	3.25	130.75	124.68
9	C	605	CHL	C4D-C3D-CAD	-3.25	106.66	108.47
9	I	608	CHL	C4D-C3D-CAD	-3.24	106.66	108.47
9	G	605	CHL	C4D-C3D-CAD	-3.24	106.66	108.47
9	G	608	CHL	O2A-CGA-CBA	3.24	122.09	111.91
10	A	612	CLA	C1D-CHD-C4C	3.24	126.84	122.56
9	J	607	CHL	C4-C3-C5	-3.24	109.82	115.27
10	J	602	CLA	C1D-CHD-C4C	3.24	126.84	122.56
9	D	609	CHL	C4D-C3D-CAD	-3.24	106.66	108.47
10	C	612	CLA	C4D-C3D-CAD	-3.24	106.66	108.47
10	B	604	CLA	C4D-C3D-CAD	-3.24	106.66	108.47
9	F	606	CHL	CBA-CAA-C2A	-3.24	104.30	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	602	CLA	CED-O2D-CGD	3.24	123.27	115.94
10	H	603	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
10	B	602	CLA	CMC-C2C-C1C	3.24	129.97	125.04
9	C	605	CHL	C1D-CHD-C4C	3.24	126.83	122.56
9	B	601	CHL	C1D-CHD-C4C	3.24	126.83	122.56
9	J	605	CHL	C1D-CHD-C4C	3.24	126.83	122.56
10	E	611	CLA	CAA-C2A-C1A	3.24	122.58	111.97
10	D	602	CLA	C11-C10-C8	-3.24	105.46	115.92
10	I	603	CLA	C4D-C3D-CAD	-3.24	106.67	108.47
10	D	602	CLA	O1D-CGD-CBD	-3.23	117.87	124.48
10	G	603	CLA	C4D-C3D-CAD	-3.23	106.67	108.47
10	D	612	CLA	C1D-CHD-C4C	3.23	126.83	122.56
10	H	612	CLA	C4D-C3D-CAD	-3.23	106.67	108.47
9	D	609	CHL	OBD-CAD-CBD	-3.23	121.28	125.89
10	F	603	CLA	CAA-CBA-CGA	3.23	122.69	113.25
10	I	611	CLA	O2A-CGA-CBA	3.23	122.03	111.91
9	B	608	CHL	C4D-C3D-CAD	-3.23	106.67	108.47
10	C	613	CLA	OBD-CAD-CBD	-3.23	121.29	125.89
10	B	614	CLA	CMB-C2B-C3B	3.23	130.71	124.68
9	H	605	CHL	CMB-C2B-C1B	-3.22	123.51	128.46
8	E	4632	DGD	O2G-C1B-C2B	3.22	118.45	111.50
9	J	609	CHL	C4D-C3D-CAD	-3.22	106.67	108.47
7	C	2630	LHG	O10-C23-C24	-3.22	111.16	123.73
10	D	611	CLA	C4D-C3D-CAD	-3.22	106.67	108.47
9	H	607	CHL	C4D-C3D-CAD	-3.22	106.67	108.47
10	G	604	CLA	C4D-C3D-CAD	-3.22	106.67	108.47
9	B	609	CHL	C1-C2-C3	3.22	131.61	126.04
9	F	605	CHL	C1D-CHD-C4C	3.22	126.81	122.56
9	H	608	CHL	C4-C3-C5	-3.22	109.86	115.27
10	H	603	CLA	C4D-C3D-CAD	-3.22	106.68	108.47
9	F	606	CHL	OBD-CAD-CBD	-3.22	121.30	125.89
10	E	603	CLA	O1D-CGD-CBD	-3.22	117.90	124.48
9	J	608	CHL	C1-C2-C3	3.22	131.60	126.04
10	E	610	CLA	C1D-CHD-C4C	3.22	126.80	122.56
10	J	614	CLA	CMB-C2B-C3B	3.21	130.69	124.68
9	F	606	CHL	C1D-CHD-C4C	3.21	126.80	122.56
9	G	601	CHL	C4D-C3D-CAD	-3.21	106.68	108.47
9	D	605	CHL	C1D-CHD-C4C	3.21	126.80	122.56
10	C	602	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
10	I	603	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
10	E	604	CLA	C1D-CHD-C4C	3.21	126.80	122.56
10	J	610	CLA	C1D-CHD-C4C	3.21	126.80	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	614	CLA	OBD-CAD-CBD	-3.21	121.31	125.89
9	E	601	CHL	OBD-CAD-CBD	-3.21	121.31	125.89
10	C	614	CLA	CBA-CAA-C2A	3.21	123.33	113.86
9	B	608	CHL	CMB-C2B-C3B	3.21	130.68	124.68
10	H	611	CLA	CAA-C2A-C1A	3.21	122.48	111.97
9	B	607	CHL	C14-C13-C12	3.21	122.90	111.29
9	E	607	CHL	CBA-CAA-C2A	3.20	123.32	113.86
10	C	614	CLA	OBD-CAD-CBD	-3.20	121.32	125.89
9	D	608	CHL	C4D-C3D-CAD	-3.20	106.68	108.47
9	A	606	CHL	OBD-CAD-CBD	-3.20	121.32	125.89
10	E	612	CLA	O1D-CGD-CBD	-3.20	117.94	124.48
9	I	601	CHL	C1D-CHD-C4C	3.20	126.78	122.56
10	I	614	CLA	O2A-CGA-CBA	3.20	121.95	111.91
10	F	614	CLA	CBA-CAA-C2A	3.20	123.31	113.86
9	I	601	CHL	C4D-C3D-CAD	-3.20	106.69	108.47
10	D	610	CLA	C1D-CHD-C4C	3.20	126.78	122.56
9	G	605	CHL	C1D-CHD-C4C	3.20	126.78	122.56
9	C	609	CHL	OBD-CAD-CBD	-3.20	121.33	125.89
9	H	609	CHL	CMB-C2B-C3B	3.20	130.66	124.68
9	D	606	CHL	CED-O2D-CGD	3.20	123.17	115.94
9	I	601	CHL	C11-C12-C13	3.20	126.26	115.92
10	J	604	CLA	C4D-C3D-CAD	-3.20	106.69	108.47
9	B	607	CHL	CBA-CAA-C2A	3.20	123.30	113.86
10	I	603	CLA	O1D-CGD-CBD	-3.20	117.95	124.48
10	D	614	CLA	O2A-CGA-CBA	3.19	121.93	111.91
10	A	602	CLA	C7-C6-C5	3.19	122.03	113.36
9	C	606	CHL	C1D-CHD-C4C	3.19	126.77	122.56
9	H	608	CHL	CMB-C2B-C3B	3.19	130.65	124.68
9	H	601	CHL	C1-C2-C3	3.19	131.56	126.04
10	F	611	CLA	C1D-CHD-C4C	3.19	126.77	122.56
10	H	612	CLA	O1D-CGD-CBD	-3.19	117.96	124.48
10	J	603	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
9	E	608	CHL	C1D-CHD-C4C	3.19	126.76	122.56
9	F	609	CHL	C4D-C3D-CAD	-3.19	106.69	108.47
9	I	605	CHL	C4D-C3D-CAD	-3.19	106.69	108.47
10	F	611	CLA	O2A-CGA-CBA	3.19	121.91	111.91
4	G	6621	LUT	C2-C3-C4	3.19	114.67	110.30
9	E	606	CHL	CED-O2D-CGD	3.19	123.14	115.94
10	D	614	CLA	C1D-CHD-C4C	3.18	126.76	122.56
10	B	612	CLA	C1D-CHD-C4C	3.18	126.76	122.56
9	D	608	CHL	C1D-CHD-C4C	3.18	126.75	122.56
4	H	7621	LUT	C1-C2-C3	3.18	120.82	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	9633	BNG	C1'-O1-C1	3.18	119.11	113.84
9	H	601	CHL	OBD-CAD-CBD	-3.18	121.36	125.89
7	I	8630	LHG	C27-C26-C25	3.18	130.55	114.42
10	D	613	CLA	C6-C5-C3	3.17	121.78	113.45
10	J	613	CLA	C4D-C3D-CAD	-3.17	106.70	108.47
9	E	605	CHL	C4D-C3D-CAD	-3.17	106.70	108.47
4	F	5621	LUT	C18-C5-C6	3.17	128.09	124.53
10	G	602	CLA	O1D-CGD-CBD	-3.17	118.00	124.48
9	J	608	CHL	C4D-C3D-CAD	-3.17	106.70	108.47
9	E	607	CHL	O2A-CGA-CBA	3.17	121.84	111.91
10	E	613	CLA	OBD-CAD-CBD	-3.17	121.37	125.89
8	H	6632	DGD	C3G-O3G-C1D	3.16	119.92	113.74
9	I	606	CHL	C1D-CHD-C4C	3.16	126.73	122.56
10	E	614	CLA	C1D-CHD-C4C	3.16	126.73	122.56
10	H	614	CLA	CBA-CAA-C2A	3.16	123.20	113.86
7	E	4630	LHG	C27-C26-C25	3.16	130.48	114.42
10	H	614	CLA	OBD-CAD-CBD	-3.16	121.38	125.89
10	D	611	CLA	CMB-C2B-C3B	3.16	130.59	124.68
9	H	601	CHL	CMB-C2B-C3B	3.16	130.59	124.68
10	G	613	CLA	C1D-CHD-C4C	3.16	126.73	122.56
9	J	601	CHL	C1D-CHD-C4C	3.16	126.73	122.56
9	H	601	CHL	C12-C11-C10	-3.16	98.73	113.24
10	G	610	CLA	C4D-C3D-CAD	-3.16	106.71	108.47
10	A	604	CLA	CBA-CAA-C2A	3.16	123.18	113.86
10	E	610	CLA	OBD-CAD-CBD	-3.16	121.39	125.89
9	D	601	CHL	C4D-C3D-CAD	-3.16	106.71	108.47
9	D	606	CHL	C1D-CHD-C4C	3.16	126.72	122.56
9	G	606	CHL	CBA-CAA-C2A	3.16	123.18	113.86
9	B	607	CHL	CED-O2D-CGD	3.15	123.07	115.94
10	A	614	CLA	OBD-CAD-CBD	-3.15	121.39	125.89
9	G	608	CHL	C4D-C3D-CAD	-3.15	106.71	108.47
10	C	602	CLA	O2A-CGA-CBA	3.15	121.79	111.91
10	D	602	CLA	C1D-CHD-C4C	3.15	126.72	122.56
10	E	613	CLA	C1D-CHD-C4C	3.15	126.72	122.56
10	F	604	CLA	OBD-CAD-CBD	-3.15	121.40	125.89
10	G	614	CLA	CMB-C2B-C3B	3.15	130.57	124.68
10	D	613	CLA	C4D-C3D-CAD	-3.15	106.72	108.47
4	I	8620	LUT	C2-C3-C4	3.15	114.61	110.30
10	A	613	CLA	C4D-C3D-CAD	-3.14	106.72	108.47
9	J	609	CHL	C1-C2-C3	3.14	131.48	126.04
4	I	8620	LUT	C3-C4-C5	3.14	118.11	111.85
2	C	2633	BNG	C1'-O1-C1	3.14	119.05	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	608	CHL	C1D-CHD-C4C	3.14	126.70	122.56
9	J	607	CHL	C12-C11-C10	-3.14	98.80	113.24
10	B	610	CLA	C1D-CHD-C4C	3.14	126.70	122.56
9	G	608	CHL	C16-C15-C13	3.14	126.07	115.92
4	C	2621	LUT	C1-C2-C3	3.14	120.73	113.64
9	D	609	CHL	CED-O2D-CGD	3.14	123.04	115.94
10	J	610	CLA	CMB-C2B-C3B	3.14	130.55	124.68
10	F	614	CLA	CMB-C2B-C3B	3.14	130.55	124.68
4	C	2620	LUT	C18-C5-C4	-3.14	108.54	114.36
7	E	4630	LHG	O10-C23-C24	-3.14	111.49	123.73
9	A	601	CHL	C14-C13-C15	3.14	122.65	111.29
10	E	602	CLA	C1D-CHD-C4C	3.14	126.70	122.56
9	G	608	CHL	CMB-C2B-C3B	3.14	130.54	124.68
10	D	613	CLA	C4-C3-C5	-3.14	110.00	115.27
10	A	602	CLA	O1D-CGD-CBD	-3.13	118.07	124.48
10	G	613	CLA	C5-C3-C2	3.13	127.46	121.12
10	A	604	CLA	C4D-C3D-CAD	-3.13	106.72	108.47
8	G	9632	DGD	C3G-O3G-C1D	3.13	119.85	113.74
9	A	606	CHL	C1D-CHD-C4C	3.13	126.68	122.56
9	H	609	CHL	CAA-C2A-C3A	-3.12	104.22	112.78
9	C	608	CHL	C4D-C3D-CAD	-3.12	106.73	108.47
10	I	603	CLA	C6-C5-C3	3.12	121.64	113.45
10	H	602	CLA	CED-O2D-CGD	3.12	122.99	115.94
10	A	604	CLA	C1D-CHD-C4C	3.12	126.67	122.56
9	A	605	CHL	C4D-C3D-CAD	-3.12	106.73	108.47
9	E	609	CHL	C14-C13-C15	3.12	122.58	111.29
10	D	613	CLA	C1D-CHD-C4C	3.12	126.67	122.56
8	H	6632	DGD	C3D-C4D-C5D	3.11	115.80	110.24
10	D	611	CLA	CED-O2D-CGD	3.11	122.98	115.94
10	G	612	CLA	CMB-C2B-C3B	3.11	130.50	124.68
10	E	611	CLA	CAA-CBA-CGA	3.11	122.35	113.25
9	C	601	CHL	OBD-CAD-CBD	-3.11	121.45	125.89
10	I	610	CLA	CED-O2D-CGD	3.11	122.97	115.94
10	G	613	CLA	O2A-CGA-CBA	3.11	121.67	111.91
9	I	606	CHL	C1-C2-C3	3.11	131.78	126.75
9	E	601	CHL	C1D-CHD-C4C	3.11	126.66	122.56
10	A	611	CLA	C4D-C3D-CAD	-3.11	106.74	108.47
9	B	608	CHL	C1-C2-C3	3.11	131.42	126.04
10	F	610	CLA	CMB-C2B-C3B	3.11	130.49	124.68
9	E	605	CHL	CED-O2D-CGD	3.11	122.96	115.94
9	J	601	CHL	C11-C12-C13	3.11	125.96	115.92
10	G	613	CLA	C4D-C3D-CAD	-3.10	106.74	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	613	CLA	OBD-CAD-CBD	-3.10	121.46	125.89
10	C	603	CLA	C6-C5-C3	3.10	121.59	113.45
10	F	610	CLA	CED-O2D-CGD	3.10	122.96	115.94
10	F	604	CLA	C1D-CHD-C4C	3.10	126.65	122.56
10	C	613	CLA	C1D-CHD-C4C	3.10	126.65	122.56
10	D	602	CLA	O2A-CGA-CBA	3.10	121.64	111.91
9	A	601	CHL	C16-C15-C13	3.10	125.95	115.92
10	A	611	CLA	CAA-CBA-CGA	3.10	122.31	113.25
10	A	604	CLA	CED-O2D-CGD	3.10	122.94	115.94
9	A	607	CHL	C1D-CHD-C4C	3.10	126.65	122.56
10	I	613	CLA	C1D-CHD-C4C	3.10	126.65	122.56
8	E	4632	DGD	C3D-C4D-C5D	3.10	115.76	110.24
9	J	605	CHL	C4D-C3D-CAD	-3.10	106.74	108.47
9	G	608	CHL	CBA-CAA-C2A	3.10	123.00	113.86
4	C	2620	LUT	C2-C3-C4	3.09	114.54	110.30
10	I	610	CLA	C4D-C3D-CAD	-3.09	106.75	108.47
10	J	612	CLA	C1D-CHD-C4C	3.09	126.64	122.56
9	F	608	CHL	C4-C3-C5	-3.09	110.07	115.27
10	B	614	CLA	C1D-CHD-C4C	3.09	126.64	122.56
9	B	608	CHL	C1D-CHD-C4C	3.09	126.64	122.56
4	F	5621	LUT	C18-C5-C4	-3.09	108.63	114.36
9	H	609	CHL	C4D-C3D-CAD	-3.09	106.75	108.47
9	I	607	CHL	CBA-CAA-C2A	3.09	122.98	113.86
10	B	612	CLA	C4D-C3D-CAD	-3.09	106.75	108.47
10	J	603	CLA	OBD-CAD-CBD	-3.09	121.49	125.89
10	E	604	CLA	O1A-CGA-CBA	-3.09	111.70	123.73
10	F	613	CLA	C1D-CHD-C4C	3.08	126.63	122.56
2	B	1633	BNG	C1'-O1-C1	3.08	118.95	113.84
7	J	9630	LHG	O10-C23-C24	-3.08	111.72	123.73
9	D	609	CHL	C1-C2-C3	3.08	131.37	126.04
9	I	609	CHL	CMB-C2B-C3B	3.08	130.43	124.68
10	C	603	CLA	CAA-CBA-CGA	3.08	122.24	113.25
10	D	614	CLA	CMB-C2B-C3B	3.08	130.43	124.68
10	H	610	CLA	C4D-C3D-CAD	-3.07	106.76	108.47
9	A	605	CHL	OMC-CMC-C2C	3.07	132.63	125.69
10	F	614	CLA	C4D-C3D-CAD	-3.07	106.76	108.47
10	A	610	CLA	C14-C13-C15	3.07	122.41	111.29
5	E	2622	XAT	C7-C8-C9	3.07	130.29	125.53
8	A	632	DGD	O2G-C1B-C2B	3.07	118.11	111.50
10	B	613	CLA	C1D-CHD-C4C	3.06	126.60	122.56
10	H	602	CLA	C1D-CHD-C4C	3.06	126.60	122.56
4	E	4620	LUT	C3-C4-C5	3.06	117.95	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	605	CHL	CED-O2D-CGD	3.06	122.86	115.94
9	A	609	CHL	C4D-C3D-CAD	-3.06	106.76	108.47
9	F	607	CHL	C7-C6-C5	-3.06	105.05	113.36
9	A	609	CHL	CMB-C2B-C3B	3.06	130.40	124.68
10	J	610	CLA	C14-C13-C15	3.06	122.36	111.29
10	J	604	CLA	C1D-CHD-C4C	3.06	126.59	122.56
10	H	610	CLA	OBD-CAD-CBD	-3.05	121.53	125.89
10	F	604	CLA	C4D-C3D-CAD	-3.05	106.77	108.47
9	B	609	CHL	C4D-C3D-CAD	-3.05	106.77	108.47
9	E	606	CHL	C4D-C3D-CAD	-3.05	106.77	108.47
10	B	612	CLA	C14-C13-C15	3.05	122.34	111.29
9	I	605	CHL	C1D-CHD-C4C	3.05	126.58	122.56
10	H	603	CLA	C1D-CHD-C4C	3.05	126.58	122.56
10	D	602	CLA	C14-C13-C15	3.05	122.34	111.29
9	A	606	CHL	C4D-C3D-CAD	-3.05	106.77	108.47
10	D	604	CLA	C1D-CHD-C4C	3.05	126.58	122.56
9	F	607	CHL	OBD-CAD-CBD	-3.05	121.54	125.89
10	J	613	CLA	C1D-CHD-C4C	3.05	126.58	122.56
10	F	602	CLA	C14-C13-C15	3.05	122.33	111.29
10	H	602	CLA	C6-C5-C3	3.05	121.44	113.45
10	I	604	CLA	C1D-CHD-C4C	3.05	126.58	122.56
10	H	604	CLA	C1D-CHD-C4C	3.05	126.58	122.56
10	F	612	CLA	CMB-C2B-C3B	3.05	130.38	124.68
2	F	5633	BNG	C1'-O1-C1	3.05	118.89	113.84
10	C	611	CLA	OBD-CAD-CBD	-3.05	121.54	125.89
10	F	603	CLA	C1D-CHD-C4C	3.04	126.58	122.56
10	I	602	CLA	C1D-CHD-C4C	3.04	126.58	122.56
10	I	604	CLA	C1-C2-C3	3.04	131.31	126.04
9	A	601	CHL	C4D-C3D-CAD	-3.04	106.77	108.47
10	A	603	CLA	C4-C3-C5	-3.04	110.16	115.27
9	H	608	CHL	O2A-CGA-CBA	3.04	121.44	111.91
10	H	613	CLA	C1D-CHD-C4C	3.04	126.56	122.56
10	E	603	CLA	C4D-C3D-CAD	-3.04	106.78	108.47
10	I	602	CLA	C7-C6-C5	3.03	121.60	113.36
2	H	7633	BNG	C1'-O1-C1	3.03	118.87	113.84
9	C	608	CHL	CBA-CAA-C2A	3.03	122.82	113.86
10	J	604	CLA	O1A-CGA-CBA	-3.03	111.90	123.73
4	D	3621	LUT	C1-C2-C3	3.03	120.49	113.64
8	G	9632	DGD	C3D-C4D-C5D	3.03	115.65	110.24
8	G	9632	DGD	C6D-O5D-C1E	3.03	119.67	113.74
10	I	602	CLA	CMC-C2C-C1C	3.03	129.66	125.04
9	F	609	CHL	CED-O2D-CGD	3.03	122.80	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	609	CHL	C4D-C3D-CAD	-3.03	106.78	108.47
9	E	609	CHL	CAA-CBA-CGA	3.03	122.11	113.25
10	G	602	CLA	C1D-CHD-C4C	3.03	126.56	122.56
10	J	611	CLA	CMB-C2B-C3B	3.03	130.35	124.68
10	J	603	CLA	CAA-CBA-CGA	3.03	122.11	113.25
9	H	601	CHL	C4D-C3D-CAD	-3.03	106.78	108.47
9	H	607	CHL	C4-C3-C5	-3.03	110.18	115.27
10	C	613	CLA	C4-C3-C5	-3.03	110.18	115.27
9	C	609	CHL	C4D-C3D-CAD	-3.03	106.78	108.47
9	H	608	CHL	C16-C15-C13	3.03	125.70	115.92
9	I	607	CHL	C5-C3-C2	3.03	127.24	121.12
10	E	613	CLA	CBA-CAA-C2A	3.03	122.79	113.86
10	C	614	CLA	CMB-C2B-C3B	3.03	130.34	124.68
8	E	4632	DGD	C6D-O5D-C1E	3.02	119.65	113.74
9	F	605	CHL	CED-O2D-CGD	3.02	122.77	115.94
10	C	602	CLA	C12-C11-C10	-3.02	99.35	113.24
2	G	6633	BNG	C1'-O1-C1	3.02	118.85	113.84
9	H	605	CHL	OBD-CAD-CBD	-3.02	121.58	125.89
9	F	601	CHL	CMB-C2B-C3B	3.02	130.33	124.68
10	A	613	CLA	C1D-CHD-C4C	3.02	126.54	122.56
9	F	608	CHL	O2A-CGA-CBA	3.02	121.38	111.91
10	G	610	CLA	OBD-CAD-CBD	-3.02	121.58	125.89
9	H	601	CHL	C1D-CHD-C4C	3.02	126.54	122.56
2	A	633	BNG	C1'-O1-C1	3.02	118.84	113.84
10	E	603	CLA	C6-C5-C3	3.01	121.36	113.45
9	J	609	CHL	OBD-CAD-CBD	-3.01	121.59	125.89
10	F	604	CLA	O1D-CGD-CBD	-3.01	118.32	124.48
7	B	1630	LHG	C27-C26-C25	3.01	129.71	114.42
9	G	607	CHL	C1D-CHD-C4C	3.01	126.53	122.56
8	I	8632	DGD	C3G-O3G-C1D	3.01	119.62	113.74
10	J	614	CLA	OBD-CAD-CBD	-3.01	121.60	125.89
10	C	604	CLA	C1D-CHD-C4C	3.01	126.53	122.56
7	J	9630	LHG	O7-C7-C8	3.01	117.98	111.50
10	F	610	CLA	CMC-C2C-C1C	3.01	129.62	125.04
10	G	602	CLA	C11-C12-C13	-3.01	106.20	115.92
9	H	608	CHL	C4D-C3D-CAD	-3.01	106.79	108.47
9	D	608	CHL	C5-C3-C2	-3.00	115.05	121.12
9	E	601	CHL	C11-C12-C13	3.00	125.61	115.92
4	H	7620	LUT	C3-C4-C5	3.00	117.83	111.85
9	B	606	CHL	C1D-CHD-C4C	3.00	126.51	122.56
10	I	610	CLA	C14-C13-C15	2.99	122.13	111.29
10	F	602	CLA	C11-C12-C13	-2.99	106.24	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	609	CHL	C1-C2-C3	2.99	131.22	126.04
9	I	601	CHL	OBD-CAD-CBD	-2.99	121.62	125.89
10	E	613	CLA	O2A-CGA-CBA	2.99	121.29	111.91
10	E	603	CLA	CED-O2D-CGD	2.99	122.70	115.94
10	A	603	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
7	H	7630	LHG	O7-C7-C8	2.99	117.94	111.50
10	C	603	CLA	CBA-CAA-C2A	2.99	122.68	113.86
10	A	612	CLA	CMB-C2B-C3B	2.99	130.27	124.68
8	I	8632	DGD	C6D-O5D-C1E	2.99	119.57	113.74
9	C	606	CHL	C4D-C3D-CAD	-2.98	106.81	108.47
10	G	612	CLA	C4D-C3D-CAD	-2.98	106.81	108.47
10	B	603	CLA	O2A-CGA-CBA	2.98	121.27	111.91
10	J	614	CLA	CBA-CAA-C2A	2.98	122.67	113.86
9	B	607	CHL	C12-C11-C10	-2.98	99.53	113.24
10	E	611	CLA	C4D-C3D-CAD	-2.98	106.81	108.47
10	H	613	CLA	OBD-CAD-CBD	-2.98	121.64	125.89
10	D	614	CLA	CBA-CAA-C2A	2.98	122.66	113.86
9	D	607	CHL	C1D-CHD-C4C	2.98	126.49	122.56
9	C	601	CHL	C11-C12-C13	2.98	125.55	115.92
9	B	605	CHL	C4D-C3D-CAD	-2.98	106.81	108.47
10	G	604	CLA	CED-O2D-CGD	2.98	122.67	115.94
10	J	604	CLA	CAA-CBA-CGA	2.98	121.96	113.25
9	A	601	CHL	OBD-CAD-CBD	-2.98	121.64	125.89
4	C	2620	LUT	C3-C4-C5	2.98	117.79	111.85
9	D	607	CHL	C6-C5-C3	2.98	121.26	113.45
10	H	604	CLA	O1A-CGA-CBA	-2.98	112.12	123.73
10	E	612	CLA	CMB-C2B-C3B	2.97	130.24	124.68
9	B	605	CHL	OBD-CAD-CBD	-2.97	121.65	125.89
10	D	610	CLA	CMB-C2B-C3B	2.97	130.24	124.68
9	B	607	CHL	C5-C3-C2	2.97	127.13	121.12
9	C	601	CHL	C4D-C3D-CAD	-2.97	106.81	108.47
10	D	603	CLA	O1D-CGD-CBD	-2.97	118.41	124.48
9	C	608	CHL	O2A-CGA-CBA	2.97	121.22	111.91
10	G	613	CLA	OBD-CAD-CBD	-2.97	121.66	125.89
4	J	9621	LUT	C18-C5-C4	-2.97	108.86	114.36
9	J	607	CHL	OBD-CAD-CBD	-2.97	121.66	125.89
10	E	613	CLA	C12-C11-C10	-2.96	99.62	113.24
8	B	1632	DGD	C6D-O5D-C1E	2.96	119.53	113.74
9	B	609	CHL	CMB-C2B-C3B	2.96	130.22	124.68
9	I	608	CHL	O2A-CGA-CBA	2.96	121.20	111.91
10	C	613	CLA	CBA-CAA-C2A	2.96	122.60	113.86
4	F	5620	LUT	C18-C5-C4	-2.96	108.87	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	611	CLA	CMB-C2B-C3B	2.96	130.22	124.68
4	I	8620	LUT	C21-C26-C27	2.96	116.44	112.70
9	G	609	CHL	C4D-C3D-CAD	-2.96	106.82	108.47
9	G	607	CHL	C4D-C3D-CAD	-2.96	106.82	108.47
9	I	607	CHL	C1D-CHD-C4C	2.96	126.47	122.56
10	J	602	CLA	CED-O2D-CGD	2.96	122.63	115.94
4	F	5621	LUT	C1-C2-C3	2.96	120.33	113.64
7	H	7630	LHG	O10-C23-C24	-2.96	112.19	123.73
10	B	604	CLA	O2D-CGD-CBD	2.96	116.52	111.27
8	H	7632	DGD	C3D-C4D-C5D	2.95	115.51	110.24
10	G	604	CLA	C1D-CHD-C4C	2.95	126.46	122.56
10	E	614	CLA	OBD-CAD-CBD	-2.95	121.67	125.89
8	H	6632	DGD	O2G-C1B-C2B	2.95	117.86	111.50
10	B	604	CLA	CBA-CAA-C2A	2.95	122.58	113.86
9	H	609	CHL	OBD-CAD-CBD	-2.95	121.68	125.89
9	B	607	CHL	OBD-CAD-CBD	-2.95	121.68	125.89
10	H	613	CLA	C5-C3-C2	2.95	127.09	121.12
8	A	632	DGD	C6D-O5D-C1E	2.95	119.50	113.74
8	D	3632	DGD	C6D-O5D-C1E	2.95	119.50	113.74
10	J	614	CLA	C4D-C3D-CAD	-2.95	106.83	108.47
9	C	606	CHL	C5-C3-C4	-2.95	108.09	114.60
9	E	601	CHL	C4D-C3D-CAD	-2.95	106.83	108.47
10	A	613	CLA	OBD-CAD-CBD	-2.95	121.69	125.89
10	A	610	CLA	C4D-C3D-CAD	-2.94	106.83	108.47
9	I	607	CHL	C4D-C3D-CAD	-2.94	106.83	108.47
9	G	607	CHL	C4-C3-C5	-2.94	110.32	115.27
10	D	614	CLA	C4D-C3D-CAD	-2.94	106.83	108.47
9	J	601	CHL	OBD-CAD-CBD	-2.94	121.70	125.89
10	H	610	CLA	C14-C13-C15	2.94	121.93	111.29
7	B	1630	LHG	O7-C7-C8	2.94	117.83	111.50
10	J	613	CLA	C5-C3-C2	2.94	127.06	121.12
10	J	604	CLA	O1D-CGD-CBD	-2.94	118.48	124.48
9	J	606	CHL	C4D-C3D-CAD	-2.94	106.83	108.47
8	E	4632	DGD	C3G-O3G-C1D	2.94	119.47	113.74
10	D	604	CLA	C1-C2-C3	2.94	131.12	126.04
9	I	605	CHL	CMB-C2B-C3B	2.94	130.17	124.68
7	C	2630	LHG	C27-C26-C25	2.93	129.32	114.42
9	J	607	CHL	C4D-C3D-CAD	-2.93	106.83	108.47
4	A	621	LUT	C1-C2-C3	2.93	120.26	113.64
10	C	612	CLA	CMB-C2B-C3B	2.93	130.16	124.68
10	H	612	CLA	CMB-C2B-C3B	2.93	130.16	124.68
10	C	611	CLA	CMB-C2B-C3B	2.93	130.16	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	614	CLA	OBD-CAD-CBD	-2.93	121.71	125.89
10	C	613	CLA	C1-C2-C3	2.93	131.10	126.04
10	F	610	CLA	OBD-CAD-CBD	-2.93	121.72	125.89
10	I	614	CLA	CBA-CAA-C2A	2.92	122.50	113.86
8	A	632	DGD	C3G-O3G-C1D	2.92	119.45	113.74
10	J	611	CLA	C4D-C3D-CAD	-2.92	106.84	108.47
9	D	607	CHL	C4D-C3D-CAD	-2.92	106.84	108.47
9	E	607	CHL	C12-C11-C10	-2.92	99.82	113.24
10	D	604	CLA	C4-C3-C5	-2.92	110.36	115.27
9	J	607	CHL	C1D-CHD-C4C	2.92	126.41	122.56
9	F	605	CHL	CMB-C2B-C3B	2.92	130.14	124.68
9	H	605	CHL	C4D-C3D-CAD	-2.92	106.84	108.47
9	H	609	CHL	C16-C15-C13	2.92	125.35	115.92
2	I	8633	BNG	C1'-O1-C1	2.92	118.67	113.84
9	B	606	CHL	O1A-CGA-CBA	-2.91	112.36	123.73
8	D	3632	DGD	C3G-O3G-C1D	2.91	119.43	113.74
10	C	603	CLA	C1D-CHD-C4C	2.91	126.40	122.56
8	H	6632	DGD	C6D-O5D-C1E	2.91	119.43	113.74
10	J	612	CLA	CED-O2D-CGD	2.91	122.52	115.94
10	F	602	CLA	C9-C8-C7	2.91	121.83	111.29
10	F	612	CLA	C4D-C3D-CAD	-2.91	106.85	108.47
10	D	613	CLA	OBD-CAD-CBD	-2.91	121.74	125.89
10	D	611	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
10	F	603	CLA	CED-O2D-CGD	2.91	122.52	115.94
10	H	604	CLA	CBA-CAA-C2A	2.91	122.44	113.86
4	G	6621	LUT	C1-C2-C3	2.91	120.21	113.64
4	I	8621	LUT	C18-C5-C4	-2.91	108.97	114.36
8	B	2632	DGD	C3G-O3G-C1D	2.90	119.41	113.74
9	E	607	CHL	C4D-C3D-CAD	-2.90	106.85	108.47
10	I	614	CLA	CMB-C2B-C3B	2.90	130.11	124.68
9	H	601	CHL	C11-C12-C13	2.90	125.30	115.92
10	A	613	CLA	C6-C5-C3	2.90	121.07	113.45
9	H	607	CHL	C1D-CHD-C4C	2.90	126.39	122.56
10	I	610	CLA	CMB-C2B-C3B	2.90	130.10	124.68
7	G	6630	LHG	C27-C26-C25	2.90	129.14	114.42
10	I	611	CLA	CMB-C2B-C3B	2.90	130.10	124.68
9	B	609	CHL	OBD-CAD-CBD	-2.90	121.76	125.89
7	G	6630	LHG	O7-C7-C8	2.89	117.74	111.50
10	I	603	CLA	CED-O2D-CGD	2.89	122.48	115.94
7	C	2630	LHG	O7-C7-C8	2.89	117.73	111.50
10	F	611	CLA	CAA-C2A-C1A	2.89	121.45	111.97
5	C	7622	XAT	C38-C25-C24	-2.89	111.03	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	610	CLA	CMB-C2B-C3B	2.89	130.09	124.68
10	A	612	CLA	C14-C13-C15	2.89	121.76	111.29
9	C	601	CHL	CMB-C2B-C3B	2.89	130.09	124.68
9	H	608	CHL	OBD-CAD-CBD	-2.89	121.77	125.89
10	F	603	CLA	O1D-CGD-CBD	-2.89	118.57	124.48
10	F	604	CLA	O1A-CGA-CBA	-2.89	112.46	123.73
10	D	602	CLA	C5-C3-C2	-2.89	115.27	121.12
4	I	8621	LUT	C1-C2-C3	2.89	120.16	113.64
10	G	602	CLA	C12-C11-C10	-2.89	99.97	113.24
9	B	605	CHL	CMB-C2B-C1B	-2.89	124.03	128.46
10	E	612	CLA	C4D-C3D-CAD	-2.89	106.86	108.47
9	B	607	CHL	C4D-C3D-CAD	-2.89	106.86	108.47
10	A	604	CLA	O1D-CGD-CBD	-2.88	118.58	124.48
8	B	1632	DGD	C3D-C4D-C5D	2.88	115.38	110.24
9	D	608	CHL	CBA-CAA-C2A	2.88	122.37	113.86
6	H	7623	NEX	C24-C23-C22	2.88	116.34	110.77
7	D	3630	LHG	C27-C26-C25	2.88	129.04	114.42
9	C	606	CHL	O2D-CGD-CBD	2.88	116.38	111.27
10	C	614	CLA	C4D-C3D-CAD	-2.87	106.87	108.47
10	B	613	CLA	C6-C5-C3	2.87	120.98	113.45
4	E	4621	LUT	C1-C2-C3	2.87	120.12	113.64
9	G	601	CHL	CMB-C2B-C3B	2.87	130.04	124.68
9	A	608	CHL	C14-C13-C15	2.86	121.67	111.29
10	D	603	CLA	C1-C2-C3	2.86	131.00	126.04
10	H	604	CLA	CAA-CBA-CGA	2.86	121.61	113.25
10	H	602	CLA	C11-C10-C8	-2.86	106.67	115.92
10	D	612	CLA	C4D-C3D-CAD	-2.86	106.88	108.47
10	E	602	CLA	CMC-C2C-C1C	2.86	129.39	125.04
10	G	612	CLA	CED-O2D-CGD	2.86	122.40	115.94
10	I	603	CLA	C1D-CHD-C4C	2.86	126.33	122.56
10	C	611	CLA	C4D-C3D-CAD	-2.85	106.88	108.47
10	E	614	CLA	CMB-C2B-C3B	2.85	130.02	124.68
10	G	604	CLA	CBA-CAA-C2A	2.85	122.28	113.86
10	B	612	CLA	CED-O2D-CGD	2.85	122.38	115.94
10	F	614	CLA	CAA-CBA-CGA	2.85	121.58	113.25
9	C	606	CHL	CED-O2D-CGD	2.85	122.38	115.94
9	J	609	CHL	CED-O2D-CGD	2.85	122.38	115.94
10	E	610	CLA	C1-C2-C3	2.85	130.97	126.04
8	E	4632	DGD	C4D-C3D-C2D	2.85	115.79	110.82
10	H	602	CLA	O2A-CGA-CBA	2.85	120.84	111.91
10	J	602	CLA	C6-C7-C8	-2.85	106.72	115.92
10	I	602	CLA	C12-C11-C10	-2.84	100.17	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	5630	LHG	C27-C26-C25	2.84	128.85	114.42
10	G	602	CLA	CMB-C2B-C3B	2.84	129.99	124.68
10	I	604	CLA	O1A-CGA-CBA	-2.84	112.65	123.73
10	A	610	CLA	CMC-C2C-C1C	2.84	129.36	125.04
10	E	610	CLA	CED-O2D-CGD	2.84	122.35	115.94
10	G	603	CLA	C1D-CHD-C4C	2.84	126.30	122.56
10	F	602	CLA	C6-C7-C8	-2.84	106.75	115.92
5	J	3622	XAT	C38-C25-C24	-2.84	111.09	114.28
10	B	612	CLA	CMB-C2B-C3B	2.83	129.98	124.68
10	D	603	CLA	CMB-C2B-C3B	2.83	129.98	124.68
9	C	607	CHL	CAC-C3C-C4C	2.83	128.49	124.81
9	C	607	CHL	C14-C13-C12	2.83	121.55	111.29
10	A	602	CLA	CMB-C2B-C3B	2.83	129.98	124.68
8	H	7632	DGD	C6D-O5D-C1E	2.83	119.27	113.74
5	A	622	XAT	O24-C25-C24	2.83	115.51	113.38
9	D	608	CHL	O2A-CGA-CBA	2.83	120.78	111.91
9	E	607	CHL	C4-C3-C5	-2.83	110.51	115.27
10	B	614	CLA	C4D-C3D-CAD	-2.83	106.89	108.47
10	G	604	CLA	C1-C2-C3	2.83	130.93	126.04
10	A	612	CLA	O2A-CGA-CBA	2.83	120.78	111.91
7	H	7630	LHG	C27-C26-C25	2.83	128.77	114.42
9	G	609	CHL	OBD-CAD-CBD	-2.83	121.86	125.89
10	H	604	CLA	C6-C7-C8	2.82	125.05	115.92
9	J	609	CHL	C16-C15-C13	2.82	125.04	115.92
9	D	605	CHL	CMB-C2B-C3B	2.82	129.95	124.68
10	G	614	CLA	O2A-CGA-CBA	2.82	120.75	111.91
9	E	606	CHL	C1D-CHD-C4C	2.82	126.28	122.56
8	B	1632	DGD	C3G-O3G-C1D	2.82	119.24	113.74
10	J	612	CLA	CMB-C2B-C3B	2.82	129.95	124.68
10	J	613	CLA	C6-C5-C3	2.82	120.84	113.45
9	H	606	CHL	C4D-C3D-CAD	-2.82	106.90	108.47
4	G	6620	LUT	C2-C3-C4	2.81	114.16	110.30
10	H	614	CLA	O2A-CGA-CBA	2.81	120.73	111.91
10	J	612	CLA	C4D-C3D-CAD	-2.81	106.90	108.47
10	A	612	CLA	C4D-C3D-CAD	-2.81	106.90	108.47
10	E	614	CLA	CAA-CBA-CGA	2.81	121.46	113.25
10	D	603	CLA	C1D-CHD-C4C	2.81	126.27	122.56
10	G	602	CLA	C14-C13-C15	2.81	121.46	111.29
9	F	601	CHL	C9-C8-C10	2.81	121.46	111.29
10	H	614	CLA	C4D-C3D-CAD	-2.81	106.91	108.47
10	C	610	CLA	CMB-C2B-C3B	2.80	129.92	124.68
9	E	609	CHL	OBD-CAD-CBD	-2.80	121.89	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	608	CHL	CMB-C2B-C3B	2.80	129.92	124.68
9	F	606	CHL	C4D-C3D-CAD	-2.80	106.91	108.47
2	E	4633	BNG	C1'-O1-C1	2.80	118.48	113.84
9	E	601	CHL	C12-C11-C10	-2.80	100.37	113.24
8	B	2632	DGD	C6D-O5D-C1E	2.80	119.21	113.74
9	C	609	CHL	C14-C13-C15	2.80	121.42	111.29
9	I	609	CHL	OBD-CAD-CBD	-2.79	121.90	125.89
10	J	603	CLA	C4D-C3D-CAD	-2.79	106.91	108.47
10	C	602	CLA	C6-C7-C8	-2.79	106.89	115.92
9	F	607	CHL	CED-O2D-CGD	2.79	122.25	115.94
10	D	612	CLA	C4-C3-C5	-2.79	110.58	115.27
10	C	611	CLA	C4-C3-C5	-2.79	110.58	115.27
8	H	7632	DGD	C3G-O3G-C1D	2.79	119.19	113.74
8	D	5632	DGD	C3G-C2G-C1G	-2.79	105.19	111.79
10	J	612	CLA	O2A-CGA-CBA	2.79	120.66	111.91
9	J	601	CHL	C4D-C3D-CAD	-2.79	106.92	108.47
10	J	612	CLA	C14-C13-C15	2.79	121.39	111.29
4	D	3621	LUT	C18-C5-C4	-2.79	109.19	114.36
9	A	608	CHL	O2A-CGA-CBA	2.79	120.65	111.91
10	I	602	CLA	O2A-CGA-CBA	2.79	120.65	111.91
8	B	2632	DGD	C3D-C4D-C5D	2.78	115.21	110.24
5	F	6622	XAT	C7-C8-C9	2.78	129.85	125.53
6	E	4623	NEX	O24-C25-C24	2.78	115.47	113.38
9	F	608	CHL	CBA-CAA-C2A	2.78	122.07	113.86
10	C	610	CLA	C14-C13-C12	2.78	121.36	111.29
9	E	601	CHL	C6-C5-C3	2.78	120.74	113.45
4	D	3621	LUT	C2-C3-C4	2.78	114.11	110.30
10	F	603	CLA	C6-C5-C3	2.78	120.73	113.45
10	G	610	CLA	CMC-C2C-C1C	2.78	129.27	125.04
10	G	602	CLA	O2A-CGA-CBA	2.77	120.61	111.91
10	D	612	CLA	C11-C10-C8	2.77	124.89	115.92
4	J	9621	LUT	C1-C2-C3	2.77	119.91	113.64
10	J	612	CLA	C7-C6-C5	-2.77	105.83	113.36
10	G	603	CLA	C16-C15-C13	2.77	124.87	115.92
10	B	613	CLA	C4-C3-C5	-2.77	110.61	115.27
8	D	3632	DGD	O2G-C1B-C2B	2.77	117.47	111.50
10	E	603	CLA	C1D-CHD-C4C	2.77	126.21	122.56
9	G	609	CHL	C16-C15-C13	2.77	124.87	115.92
8	D	3632	DGD	C4D-C3D-C2D	2.77	115.66	110.82
9	E	608	CHL	CMB-C2B-C3B	2.77	129.85	124.68
9	E	605	CHL	CMB-C2B-C3B	2.76	129.85	124.68
10	J	602	CLA	CMB-C2B-C3B	2.76	129.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	602	CLA	CED-O2D-CGD	2.76	122.19	115.94
10	A	612	CLA	CED-O2D-CGD	2.76	122.19	115.94
4	A	620	LUT	C2-C3-C4	2.76	114.08	110.30
10	E	602	CLA	C14-C13-C15	2.76	121.29	111.29
9	E	605	CHL	CAA-C2A-C3A	-2.76	105.22	112.78
10	J	610	CLA	OBD-CAD-CBD	-2.76	121.95	125.89
10	A	611	CLA	CMB-C2B-C3B	2.76	129.84	124.68
10	D	602	CLA	C9-C8-C10	-2.76	101.30	111.29
10	C	613	CLA	C6-C5-C3	2.76	120.69	113.45
9	A	607	CHL	C4-C3-C5	-2.76	110.63	115.27
10	H	604	CLA	CMD-C2D-C3D	2.76	129.84	124.68
9	G	605	CHL	CMB-C2B-C3B	2.76	129.84	124.68
10	G	610	CLA	C1-C2-C3	2.76	130.81	126.04
10	B	602	CLA	O2A-CGA-CBA	2.76	120.56	111.91
10	F	603	CLA	O2A-CGA-CBA	2.75	120.55	111.91
10	E	602	CLA	C12-C11-C10	-2.75	100.59	113.24
9	F	607	CHL	O2A-CGA-O1A	-2.75	116.65	123.59
10	D	604	CLA	C9-C8-C10	2.75	121.25	111.29
8	D	5632	DGD	C3G-O3G-C1D	2.75	119.11	113.74
10	H	604	CLA	CED-O2D-CGD	2.75	122.15	115.94
10	A	603	CLA	C1D-CHD-C4C	2.75	126.18	122.56
6	C	2623	NEX	C26-C27-C28	2.75	131.80	125.99
9	A	607	CHL	C4D-C3D-CAD	-2.74	106.94	108.47
10	A	614	CLA	C4D-C3D-CAD	-2.74	106.94	108.47
10	G	603	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
7	A	630	LHG	C27-C26-C25	2.74	128.34	114.42
4	H	7620	LUT	C21-C26-C27	2.74	116.17	112.70
10	B	603	CLA	C9-C8-C10	-2.74	101.37	111.29
10	C	614	CLA	O2A-CGA-CBA	2.74	120.51	111.91
10	J	611	CLA	CED-O2D-CGD	2.74	122.14	115.94
9	E	601	CHL	CMB-C2B-C3B	2.74	129.80	124.68
9	C	607	CHL	O2A-CGA-O1A	-2.74	116.68	123.59
10	F	602	CLA	CED-O2D-CGD	2.74	122.12	115.94
10	B	611	CLA	O2D-CGD-CBD	2.74	116.13	111.27
4	B	1621	LUT	C1-C2-C3	2.73	119.82	113.64
9	G	607	CHL	C7-C6-C5	-2.73	105.93	113.36
9	I	608	CHL	C16-C15-C13	2.73	124.76	115.92
8	H	7632	DGD	C3G-C2G-C1G	-2.73	105.33	111.79
8	H	7632	DGD	C4D-C3D-C2D	2.73	115.59	110.82
10	H	614	CLA	CED-O2D-CGD	2.73	122.11	115.94
4	G	6620	LUT	C21-C26-C27	2.73	116.15	112.70
5	F	6622	XAT	C37-C21-C22	-2.73	104.24	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	607	CHL	C14-C13-C12	2.73	121.17	111.29
10	G	611	CLA	C4-C3-C5	-2.73	110.68	115.27
9	D	601	CHL	C9-C8-C10	2.72	121.16	111.29
10	F	603	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
10	B	612	CLA	C4-C3-C5	-2.72	110.69	115.27
9	H	609	CHL	CAA-CBA-CGA	2.72	121.21	113.25
10	G	610	CLA	C16-C15-C13	2.72	124.72	115.92
10	E	602	CLA	C5-C3-C2	-2.72	115.61	121.12
10	F	610	CLA	C14-C13-C15	2.72	121.15	111.29
10	I	611	CLA	C9-C8-C10	2.72	121.14	111.29
9	D	607	CHL	O2A-CGA-O1A	-2.72	116.73	123.59
5	C	7622	XAT	O24-C25-C24	2.72	115.42	113.38
10	G	602	CLA	C6-C7-C8	-2.72	107.14	115.92
10	F	603	CLA	C4-C3-C5	-2.71	110.71	115.27
10	E	614	CLA	C4D-C3D-CAD	-2.71	106.96	108.47
10	J	603	CLA	C16-C15-C13	2.71	124.69	115.92
5	A	622	XAT	C7-C8-C9	2.71	129.74	125.53
10	C	604	CLA	O1D-CGD-CBD	-2.71	118.94	124.48
9	A	609	CHL	CAA-CBA-CGA	2.71	121.16	113.25
10	J	603	CLA	C1D-CHD-C4C	2.71	126.13	122.56
9	E	607	CHL	O2A-CGA-O1A	-2.70	116.78	123.59
9	J	605	CHL	CMB-C2B-C3B	2.70	129.73	124.68
10	E	603	CLA	CAA-CBA-CGA	2.70	121.13	113.25
10	A	614	CLA	O2A-CGA-CBA	2.69	120.36	111.91
9	B	608	CHL	C16-C15-C13	2.69	124.63	115.92
10	D	612	CLA	CED-O2D-CGD	2.69	122.03	115.94
9	D	607	CHL	CED-O2D-CGD	2.69	122.02	115.94
4	A	621	LUT	C7-C8-C9	2.69	130.30	126.23
9	F	607	CHL	C4D-C3D-CAD	-2.69	106.97	108.47
9	G	601	CHL	C7-C6-C5	-2.69	106.05	113.36
7	F	5630	LHG	O10-C23-C24	-2.69	113.25	123.73
10	B	613	CLA	C1-C2-C3	2.69	130.69	126.04
10	H	602	CLA	C7-C6-C5	2.68	120.65	113.36
9	E	607	CHL	CAA-C2A-C1A	2.68	120.77	111.97
10	I	603	CLA	C7-C6-C5	-2.68	106.07	113.36
9	A	609	CHL	C14-C13-C15	2.68	121.00	111.29
10	A	610	CLA	OBD-CAD-CBD	-2.68	122.07	125.89
7	J	9630	LHG	C27-C26-C25	2.68	128.01	114.42
10	B	610	CLA	CMB-C2B-C3B	2.67	129.68	124.68
9	H	606	CHL	C5-C3-C4	-2.67	108.70	114.60
8	E	4632	DGD	C3G-C2G-C1G	-2.67	105.47	111.79
9	H	608	CHL	C1-C2-C3	2.67	130.66	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	609	CHL	C4D-C3D-CAD	-2.67	106.98	108.47
10	I	603	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
9	E	607	CHL	CED-O2D-CGD	2.67	121.97	115.94
10	J	613	CLA	O2A-CGA-CBA	2.67	120.28	111.91
10	G	612	CLA	C16-C15-C13	2.67	124.53	115.92
8	B	2632	DGD	C4D-C3D-C2D	2.66	115.47	110.82
10	G	614	CLA	C4D-C3D-CAD	-2.66	106.98	108.47
8	A	632	DGD	C3G-C2G-C1G	-2.66	105.49	111.79
10	E	612	CLA	C14-C13-C15	2.66	120.93	111.29
8	B	2632	DGD	C3G-C2G-C1G	-2.66	105.50	111.79
6	G	6623	NEX	C16-C1-C6	2.66	112.85	110.47
9	J	601	CHL	C14-C13-C12	2.65	120.91	111.29
10	C	610	CLA	C1-C2-C3	2.65	130.63	126.04
9	G	606	CHL	C4D-C3D-CAD	-2.65	106.99	108.47
10	I	602	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
9	J	606	CHL	O1A-CGA-CBA	-2.65	113.38	123.73
10	B	612	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
8	D	3632	DGD	C3D-C4D-C5D	2.65	114.97	110.24
8	I	8632	DGD	C3G-C2G-C1G	-2.65	105.52	111.79
10	H	611	CLA	CMB-C2B-C3B	2.65	129.64	124.68
10	D	612	CLA	C14-C13-C15	2.65	120.88	111.29
9	G	601	CHL	C1-C2-C3	2.65	130.62	126.04
10	H	604	CLA	C11-C10-C8	2.65	124.48	115.92
10	I	611	CLA	CAA-C2A-C1A	2.65	120.64	111.97
9	J	607	CHL	C5-C3-C2	2.64	126.47	121.12
10	G	611	CLA	CAA-CBA-CGA	2.64	120.98	113.25
8	B	1632	DGD	C3G-C2G-C1G	-2.64	105.55	111.79
9	D	606	CHL	C5-C3-C4	-2.64	108.78	114.60
9	H	607	CHL	CMD-C2D-C3D	2.64	129.61	124.68
10	E	602	CLA	C4-C3-C5	2.64	119.71	115.27
9	D	601	CHL	CAC-C3C-C4C	2.64	128.23	124.81
9	A	607	CHL	CED-O2D-CGD	2.63	121.89	115.94
9	J	607	CHL	CED-O2D-CGD	2.63	121.89	115.94
6	F	5623	NEX	C16-C1-C6	2.63	112.83	110.47
9	C	607	CHL	CMD-C2D-C3D	2.63	129.60	124.68
10	E	610	CLA	C14-C13-C15	2.63	120.82	111.29
10	I	610	CLA	OBD-CAD-CBD	-2.63	122.14	125.89
9	D	601	CHL	C14-C13-C15	-2.63	101.77	111.29
6	A	623	NEX	C16-C1-C6	2.63	112.82	110.47
10	C	603	CLA	O2A-CGA-CBA	2.63	120.15	111.91
10	F	604	CLA	C6-C7-C8	2.62	124.40	115.92
10	G	604	CLA	O1A-CGA-CBA	-2.62	113.50	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	607	CHL	O2A-CGA-O1A	-2.62	116.97	123.59
10	B	603	CLA	C1D-CHD-C4C	2.62	126.02	122.56
10	F	614	CLA	O2A-CGA-CBA	2.62	120.13	111.91
10	E	613	CLA	C5-C3-C2	2.62	126.41	121.12
10	B	603	CLA	CMB-C2B-C3B	2.62	129.57	124.68
10	G	610	CLA	CMB-C2B-C3B	2.61	129.56	124.68
10	F	612	CLA	C4-C3-C5	-2.61	110.88	115.27
10	H	614	CLA	CAA-CBA-CGA	2.61	120.88	113.25
10	B	603	CLA	C6-C5-C3	2.61	120.29	113.45
10	C	603	CLA	C1-C2-C3	2.61	130.55	126.04
10	E	612	CLA	O2A-CGA-CBA	2.61	120.08	111.91
10	D	602	CLA	CMB-C2B-C3B	2.60	129.55	124.68
4	D	3620	LUT	C1-C2-C3	2.60	119.52	113.64
9	I	606	CHL	C5-C3-C4	-2.60	108.86	114.60
9	G	601	CHL	C9-C8-C10	2.60	120.71	111.29
9	A	609	CHL	CAA-C2A-C3A	-2.60	105.66	112.78
6	J	9623	NEX	C24-C23-C22	2.60	115.80	110.77
9	F	607	CHL	C6-C5-C3	2.60	120.27	113.45
10	J	603	CLA	O2A-CGA-CBA	2.60	120.07	111.91
4	C	2621	LUT	C18-C5-C4	-2.60	109.54	114.36
10	C	604	CLA	C6-C7-C8	2.60	124.31	115.92
9	A	607	CHL	O2A-CGA-O1A	-2.60	117.04	123.59
10	I	612	CLA	C11-C12-C13	2.60	124.31	115.92
9	A	601	CHL	C1-C2-C3	2.60	130.53	126.04
10	I	610	CLA	C11-C10-C8	-2.60	107.53	115.92
10	B	611	CLA	C4-C3-C5	-2.59	110.91	115.27
10	C	602	CLA	C11-C12-C13	-2.59	107.54	115.92
10	G	611	CLA	CMB-C2B-C3B	2.59	129.53	124.68
10	D	610	CLA	CMC-C2C-C1C	2.59	128.98	125.04
5	H	4622	XAT	C7-C8-C9	2.59	129.54	125.53
9	J	607	CHL	O2A-CGA-O1A	-2.59	117.06	123.59
6	I	8623	NEX	C16-C1-C6	2.58	112.78	110.47
9	D	607	CHL	C14-C13-C12	2.58	120.64	111.29
10	E	603	CLA	O2A-CGA-CBA	2.58	120.00	111.91
9	D	607	CHL	CBA-CAA-C2A	2.58	121.47	113.86
10	J	602	CLA	C14-C13-C15	2.58	120.62	111.29
10	E	610	CLA	CMC-C2C-C1C	2.58	128.96	125.04
8	H	7632	DGD	O2G-C1B-C2B	2.57	117.05	111.50
10	I	604	CLA	CBA-CAA-C2A	2.57	121.46	113.86
10	I	612	CLA	CMB-C2B-C3B	2.57	129.49	124.68
10	C	611	CLA	CED-O2D-CGD	2.57	121.75	115.94
8	D	3632	DGD	C3G-C2G-C1G	-2.57	105.71	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	603	CLA	C1-C2-C3	2.57	130.49	126.04
6	G	6623	NEX	C24-C23-C22	2.57	115.73	110.77
9	I	608	CHL	CMB-C2B-C3B	2.57	129.48	124.68
9	C	607	CHL	CAA-C2A-C1A	2.57	120.38	111.97
9	I	607	CHL	CAC-C3C-C4C	2.57	128.14	124.81
9	G	606	CHL	C5-C3-C4	-2.56	108.94	114.60
10	J	610	CLA	CMC-C2C-C1C	2.56	128.94	125.04
4	H	7620	LUT	C2-C3-C4	2.56	113.81	110.30
9	B	601	CHL	CMD-C2D-C3D	2.56	129.47	124.68
10	D	612	CLA	CMB-C2B-C3B	2.56	129.47	124.68
5	D	8622	XAT	C37-C21-C22	-2.56	104.54	108.98
10	G	602	CLA	C11-C10-C8	-2.56	107.65	115.92
9	H	609	CHL	C14-C13-C15	2.56	120.56	111.29
10	I	614	CLA	CAA-CBA-CGA	2.56	120.73	113.25
10	D	604	CLA	CMD-C2D-C3D	2.56	129.46	124.68
10	F	602	CLA	O1D-CGD-CBD	-2.56	119.26	124.48
4	D	3621	LUT	C7-C8-C9	2.55	130.09	126.23
10	B	614	CLA	O2A-CGA-CBA	2.55	119.92	111.91
10	A	603	CLA	CMB-C2B-C3B	2.55	129.45	124.68
10	B	603	CLA	C20-C18-C19	-2.55	98.75	110.51
9	F	609	CHL	C14-C13-C15	2.55	120.52	111.29
9	C	601	CHL	C7-C6-C5	-2.55	106.44	113.36
9	H	607	CHL	CAA-C2A-C1A	2.55	120.33	111.97
9	C	605	CHL	CMB-C2B-C3B	2.55	129.44	124.68
9	F	608	CHL	C16-C15-C13	2.54	124.14	115.92
4	D	3621	LUT	C1-C6-C5	-2.54	119.03	122.61
9	C	608	CHL	CMB-C2B-C3B	2.54	129.43	124.68
4	G	6620	LUT	C3-C4-C5	2.54	116.91	111.85
10	H	614	CLA	CMC-C2C-C1C	2.54	128.91	125.04
9	G	609	CHL	C14-C13-C15	2.54	120.48	111.29
9	G	607	CHL	O2A-CGA-O1A	-2.54	117.19	123.59
10	D	604	CLA	C6-C7-C8	2.53	124.11	115.92
10	A	604	CLA	O1A-CGA-CBA	-2.53	113.84	123.73
9	I	607	CHL	O2A-CGA-O1A	-2.53	117.20	123.59
4	E	4621	LUT	C18-C5-C6	2.53	127.37	124.53
8	B	1632	DGD	C6D-C5D-C4D	2.53	117.38	112.09
10	H	610	CLA	C11-C10-C8	-2.53	107.74	115.92
9	I	607	CHL	CAA-C2A-C1A	2.53	120.27	111.97
10	A	602	CLA	C12-C11-C10	-2.53	101.61	113.24
9	J	608	CHL	CMB-C2B-C3B	2.53	129.41	124.68
9	G	609	CHL	CMB-C2B-C3B	2.53	129.41	124.68
9	B	607	CHL	O2A-CGA-O1A	-2.53	117.21	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	608	CHL	CMB-C2B-C3B	2.53	129.41	124.68
10	C	602	CLA	C11-C10-C8	-2.52	107.76	115.92
9	B	606	CHL	CMD-C2D-C3D	2.52	129.40	124.68
5	C	7622	XAT	C37-C21-C22	-2.52	104.60	108.98
5	I	9622	XAT	C7-C8-C9	2.52	129.44	125.53
10	H	602	CLA	C11-C12-C13	-2.52	107.77	115.92
10	D	611	CLA	C6-C7-C8	2.52	124.06	115.92
8	D	5632	DGD	C3D-C4D-C5D	2.52	114.73	110.24
10	A	602	CLA	C9-C8-C10	-2.52	102.18	111.29
8	G	9632	DGD	C3G-C2G-C1G	-2.52	105.84	111.79
10	C	614	CLA	CAA-CBA-CGA	2.51	120.60	113.25
9	B	601	CHL	CMB-C2B-C3B	2.51	129.37	124.68
10	E	602	CLA	CMB-C2B-C3B	2.51	129.37	124.68
8	E	4632	DGD	C6D-C5D-C4D	2.50	117.32	112.09
6	H	7623	NEX	C16-C1-C6	2.50	112.71	110.47
9	E	607	CHL	C14-C13-C12	2.50	120.35	111.29
10	C	604	CLA	CBA-CAA-C2A	2.50	121.25	113.86
9	D	609	CHL	C6-C5-C3	2.50	120.01	113.45
4	C	2620	LUT	C21-C26-C27	2.50	115.86	112.70
9	C	601	CHL	C16-C15-C13	2.50	124.00	115.92
10	H	610	CLA	CMB-C2B-C3B	2.50	129.35	124.68
9	H	601	CHL	C6-C5-C3	2.50	120.00	113.45
9	A	609	CHL	CED-O2D-CGD	2.50	121.58	115.94
10	B	604	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
10	G	602	CLA	C9-C8-C10	-2.50	102.25	111.29
6	B	1623	NEX	C16-C1-C6	2.49	112.70	110.47
5	F	6622	XAT	C38-C25-C24	-2.49	111.47	114.28
10	E	611	CLA	CED-O2D-CGD	2.49	121.56	115.94
10	C	603	CLA	CAC-C3C-C4C	2.48	128.03	124.81
10	A	603	CLA	C16-C15-C13	2.48	123.94	115.92
10	F	613	CLA	O2A-CGA-CBA	2.48	119.69	111.91
8	G	9632	DGD	C4D-C3D-C2D	2.48	115.15	110.82
9	F	607	CHL	C12-C11-C10	-2.48	101.86	113.24
10	E	602	CLA	C11-C10-C8	-2.47	107.93	115.92
9	F	608	CHL	C14-C13-C15	2.47	120.23	111.29
4	G	6621	LUT	C18-C5-C4	-2.47	109.78	114.36
10	A	602	CLA	C14-C13-C15	2.46	120.21	111.29
10	H	603	CLA	O2A-CGA-CBA	2.46	119.64	111.91
9	C	608	CHL	C6-C7-C8	-2.46	107.96	115.92
9	D	607	CHL	C12-C11-C10	-2.46	101.92	113.24
10	I	610	CLA	C2A-C1A-CHA	2.46	128.16	123.86
8	H	7632	DGD	O3G-C1D-C2D	2.46	112.14	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	602	CLA	C9-C8-C10	-2.46	102.39	111.29
6	I	8623	NEX	C24-C23-C22	2.46	115.52	110.77
9	E	606	CHL	C5-C3-C4	-2.46	109.18	114.60
10	B	604	CLA	C6-C7-C8	2.45	123.85	115.92
10	B	603	CLA	C1-C2-C3	2.45	130.29	126.04
6	J	9623	NEX	C16-C1-C6	2.45	112.67	110.47
4	F	5620	LUT	C21-C26-C27	2.45	115.80	112.70
5	I	9622	XAT	C27-C28-C29	-2.45	121.72	125.53
9	F	607	CHL	CAA-C2A-C1A	2.45	120.01	111.97
9	I	609	CHL	C14-C13-C15	2.45	120.17	111.29
10	I	611	CLA	CED-O2D-CGD	2.45	121.48	115.94
8	H	6632	DGD	C4D-C3D-C2D	2.45	115.10	110.82
9	E	608	CHL	C1-C2-C3	2.45	130.28	126.04
7	E	4630	LHG	O7-C7-C8	2.45	116.78	111.50
5	D	8622	XAT	C15-C35-C34	-2.45	118.46	123.47
10	G	613	CLA	C1-C2-C3	2.45	130.28	126.04
10	F	613	CLA	C6-C5-C3	2.45	119.87	113.45
10	F	602	CLA	CMB-C2B-C3B	2.45	129.25	124.68
10	A	603	CLA	C1-C2-C3	2.45	130.27	126.04
10	I	604	CLA	CAA-C2A-C1A	2.44	119.99	111.97
10	A	610	CLA	C2A-C1A-CHA	2.44	128.13	123.86
9	A	605	CHL	CMB-C2B-C3B	2.44	129.25	124.68
10	F	604	CLA	CAA-C2A-C1A	2.44	119.97	111.97
9	B	607	CHL	C16-C15-C13	-2.44	108.04	115.92
10	H	612	CLA	C14-C13-C15	2.44	120.11	111.29
9	H	605	CHL	CED-O2D-CGD	2.44	121.45	115.94
6	E	4623	NEX	C16-C1-C6	2.44	112.65	110.47
10	I	613	CLA	C6-C5-C3	2.43	119.84	113.45
10	D	602	CLA	C11-C12-C13	-2.43	108.05	115.92
10	A	611	CLA	C11-C12-C13	2.43	123.79	115.92
6	F	5623	NEX	C24-C23-C22	2.43	115.47	110.77
9	I	606	CHL	CED-O2D-CGD	2.43	121.44	115.94
9	J	609	CHL	C14-C13-C15	2.43	120.10	111.29
10	B	614	CLA	CED-O2D-CGD	2.43	121.43	115.94
10	H	610	CLA	C1-C2-C3	2.43	130.24	126.04
10	I	604	CLA	CMD-C2D-C3D	2.42	129.21	124.68
10	A	602	CLA	C4-C3-C5	2.42	119.34	115.27
10	I	613	CLA	O2A-CGA-CBA	2.42	119.49	111.91
9	A	608	CHL	CMB-C2B-C3B	2.41	129.19	124.68
9	C	607	CHL	C12-C11-C10	-2.41	102.16	113.24
10	A	613	CLA	O2A-CGA-CBA	2.41	119.47	111.91
9	I	606	CHL	CMD-C2D-C3D	2.41	129.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	613	CLA	O2A-CGA-CBA	2.41	119.47	111.91
5	F	6622	XAT	O24-C25-C24	2.40	115.19	113.38
10	I	613	CLA	C5-C3-C2	2.40	125.98	121.12
10	H	602	CLA	C9-C8-C7	2.40	119.99	111.29
7	D	3630	LHG	O10-C23-C24	-2.40	114.36	123.73
10	H	603	CLA	C1-C2-C3	2.40	130.19	126.04
9	G	605	CHL	CED-O2D-CGD	2.40	121.36	115.94
10	C	612	CLA	C11-C12-C13	2.40	123.68	115.92
9	J	601	CHL	CMB-C2B-C3B	2.40	129.17	124.68
9	G	607	CHL	C6-C5-C3	2.40	119.74	113.45
6	A	623	NEX	C24-C23-C22	2.39	115.40	110.77
8	E	4632	DGD	O3G-C1D-C2D	2.39	112.04	108.30
4	A	621	LUT	C1-C6-C5	-2.39	119.24	122.61
10	G	602	CLA	C7-C6-C5	2.39	119.85	113.36
10	I	611	CLA	C4-C3-C5	-2.39	111.25	115.27
9	J	601	CHL	C7-C6-C5	-2.39	106.88	113.36
10	B	604	CLA	C9-C8-C10	2.39	119.93	111.29
10	F	604	CLA	C6-C5-C3	2.39	119.71	113.45
10	I	602	CLA	C6-C7-C8	-2.38	108.21	115.92
5	B	1622	XAT	C27-C28-C29	-2.38	121.83	125.53
10	F	611	CLA	C4-C3-C5	-2.38	111.26	115.27
7	I	8630	LHG	O7-C7-C8	2.38	116.64	111.50
10	D	611	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
10	I	602	CLA	C11-C12-C13	-2.38	108.22	115.92
10	B	611	CLA	C9-C8-C10	2.38	119.91	111.29
10	J	614	CLA	O2A-CGA-CBA	2.38	119.37	111.91
8	H	6632	DGD	C3G-C2G-C1G	-2.38	106.16	111.79
10	E	611	CLA	C9-C8-C10	2.38	119.90	111.29
10	D	613	CLA	C5-C3-C2	2.37	125.92	121.12
10	E	603	CLA	CMB-C2B-C3B	2.37	129.11	124.68
10	C	613	CLA	CMD-C2D-C3D	2.37	129.11	124.68
9	G	607	CHL	CED-O2D-CGD	2.37	121.29	115.94
10	B	602	CLA	C12-C11-C10	-2.37	102.36	113.24
5	B	5622	XAT	C37-C21-C22	-2.37	104.87	108.98
9	H	607	CHL	CED-O2D-CGD	2.36	121.29	115.94
9	F	609	CHL	C16-C15-C13	2.36	123.56	115.92
9	C	606	CHL	CMD-C2D-C3D	2.36	129.10	124.68
10	H	602	CLA	CMD-C2D-C3D	2.36	129.10	124.68
9	I	605	CHL	CAA-C2A-C3A	-2.36	106.30	112.78
10	H	612	CLA	CED-O2D-CGD	2.36	121.28	115.94
10	F	610	CLA	C2A-C1A-CHA	2.36	127.99	123.86
10	A	614	CLA	CAA-CBA-CGA	2.36	120.16	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	613	CLA	O2A-CGA-CBA	2.36	119.32	111.91
9	A	601	CHL	C6-C5-C3	2.36	119.65	113.45
8	G	9632	DGD	O3G-C1D-C2D	2.36	111.99	108.30
10	A	610	CLA	O2D-CGD-CBD	2.36	115.46	111.27
10	I	612	CLA	CMD-C2D-C3D	2.36	129.09	124.68
4	G	6621	LUT	C1-C6-C5	-2.35	119.30	122.61
9	B	601	CHL	CAC-C3C-C4C	2.35	127.86	124.81
10	G	610	CLA	C2A-C1A-CHA	2.35	127.98	123.86
10	I	611	CLA	C16-C15-C13	2.35	123.52	115.92
10	B	614	CLA	CBA-CAA-C2A	2.35	120.80	113.86
9	H	605	CHL	CMB-C2B-C3B	2.35	129.08	124.68
10	I	611	CLA	C11-C12-C13	2.35	123.51	115.92
5	B	1622	XAT	C38-C25-C24	-2.35	111.64	114.28
10	I	603	CLA	CMB-C2B-C3B	2.35	129.07	124.68
9	D	609	CHL	CAA-CBA-CGA	2.34	120.09	113.25
8	H	6632	DGD	O3G-C1D-C2D	2.34	111.95	108.30
8	D	5632	DGD	C6D-C5D-C4D	2.34	116.97	112.09
9	H	601	CHL	C4-C3-C5	-2.34	111.34	115.27
6	G	6623	NEX	C38-C25-C24	-2.34	111.65	114.28
9	F	606	CHL	CAA-C2A-C1A	2.33	119.61	111.97
10	B	602	CLA	CMB-C2B-C3B	2.33	129.04	124.68
10	E	603	CLA	C11-C12-C13	2.33	123.45	115.92
10	F	604	CLA	CED-O2D-CGD	2.33	121.20	115.94
10	H	603	CLA	CMB-C2B-C3B	2.33	129.03	124.68
10	E	611	CLA	C4-C3-C5	-2.33	111.36	115.27
10	D	610	CLA	C2A-C1A-CHA	2.33	127.92	123.86
10	C	602	CLA	OBD-CAD-C3D	2.32	131.84	127.98
10	H	610	CLA	C2A-C1A-CHA	2.32	127.92	123.86
9	C	601	CHL	C14-C13-C12	2.32	119.71	111.29
10	I	612	CLA	OBD-CAD-C3D	2.32	131.84	127.98
6	F	5623	NEX	C1-C2-C3	2.32	118.88	113.64
10	J	610	CLA	C2A-C1A-CHA	2.32	127.91	123.86
9	E	606	CHL	OMC-CMC-C2C	2.32	130.93	125.69
6	C	2623	NEX	C16-C1-C6	2.32	112.55	110.47
9	C	608	CHL	C14-C13-C15	2.32	119.68	111.29
10	H	613	CLA	C1-C2-C3	2.32	130.05	126.04
10	E	611	CLA	CMB-C2B-C3B	2.32	129.01	124.68
9	F	607	CHL	C2A-C1A-CHA	2.31	127.90	123.86
10	B	610	CLA	C2A-C1A-CHA	2.31	127.90	123.86
5	H	4622	XAT	C37-C21-C22	-2.31	104.96	108.98
9	B	601	CHL	C4-C3-C5	-2.31	111.38	115.27
4	F	5621	LUT	C1-C6-C5	-2.31	119.36	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	603	CLA	C4-C3-C5	-2.31	111.38	115.27
10	E	603	CLA	C12-C11-C10	-2.31	102.61	113.24
10	J	611	CLA	C12-C11-C10	-2.31	102.62	113.24
10	J	603	CLA	CMB-C2B-C3B	2.31	129.00	124.68
9	F	606	CHL	O1A-CGA-CBA	-2.31	114.72	123.73
4	A	620	LUT	C1-C2-C3	2.31	118.86	113.64
9	C	607	CHL	CED-O2D-CGD	2.31	121.16	115.94
8	B	2632	DGD	O3G-C1D-C2D	2.31	111.91	108.30
4	D	3621	LUT	C22-C23-C24	2.31	114.37	111.74
4	I	8621	LUT	C22-C23-C24	2.31	114.37	111.74
10	C	611	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
10	F	612	CLA	CBA-CAA-C2A	2.30	120.67	113.86
9	H	607	CHL	C14-C13-C12	2.30	119.64	111.29
9	E	605	CHL	O2A-CGA-O1A	-2.30	117.78	123.59
9	G	605	CHL	O2A-CGA-O1A	-2.30	117.78	123.59
10	B	603	CLA	OBD-CAD-C3D	2.30	131.80	127.98
9	F	609	CHL	CAA-C2A-C3A	-2.30	106.48	112.78
10	G	610	CLA	C14-C13-C12	2.30	119.61	111.29
8	D	5632	DGD	C4D-C3D-C2D	2.30	114.83	110.82
9	B	609	CHL	CAA-CBA-CGA	2.29	119.96	113.25
10	E	613	CLA	C11-C10-C8	2.29	123.33	115.92
9	J	605	CHL	O2A-CGA-O1A	-2.29	117.81	123.59
6	I	8623	NEX	C1-C2-C3	2.29	118.82	113.64
5	C	7622	XAT	C37-C21-C36	2.29	110.75	107.37
10	H	613	CLA	CAA-CBA-CGA	2.29	119.94	113.25
10	B	611	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
10	I	604	CLA	C11-C10-C8	2.29	123.31	115.92
9	F	601	CHL	CAC-C3C-C4C	2.29	127.78	124.81
9	J	605	CHL	CAA-C2A-C3A	-2.29	106.52	112.78
10	F	613	CLA	CMD-C2D-C3D	2.28	128.95	124.68
10	A	611	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
10	I	612	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
10	D	603	CLA	O2A-CGA-CBA	2.28	119.07	111.91
10	H	611	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
10	G	603	CLA	C7-C6-C5	-2.28	107.16	113.36
9	I	607	CHL	C7-C6-C5	-2.28	107.16	113.36
10	G	614	CLA	CMC-C2C-C1C	2.28	128.51	125.04
9	A	606	CHL	CMD-C2D-C3D	2.28	128.95	124.68
4	E	4621	LUT	C18-C5-C4	-2.28	110.13	114.36
10	E	610	CLA	C2A-C1A-CHA	2.28	127.85	123.86
9	D	607	CHL	CAC-C3C-C4C	2.28	127.77	124.81
10	H	611	CLA	O2D-CGD-CBD	2.28	115.32	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	607	CHL	C7-C6-C5	-2.28	107.17	113.36
9	D	606	CHL	O2A-CGA-O1A	-2.28	117.84	123.59
6	H	7623	NEX	C1-C2-C3	2.28	118.78	113.64
10	A	612	CLA	CBA-CAA-C2A	2.28	120.58	113.86
9	D	601	CHL	C6-C5-C3	2.28	119.42	113.45
8	A	632	DGD	C6D-C5D-C4D	2.28	116.84	112.09
10	C	614	CLA	CAA-C2A-C3A	-2.28	106.55	112.78
9	I	601	CHL	C12-C11-C10	-2.27	102.79	113.24
4	B	1620	LUT	C1-C2-C3	2.27	118.78	113.64
9	D	601	CHL	CMB-C2B-C3B	2.27	128.93	124.68
9	B	601	CHL	C16-C15-C13	2.27	123.26	115.92
10	J	602	CLA	C9-C8-C10	-2.27	103.07	111.29
10	E	603	CLA	CAA-C2A-C1A	2.27	119.41	111.97
10	J	602	CLA	OBD-CAD-C3D	2.27	131.75	127.98
9	A	607	CHL	CMD-C2D-C3D	2.27	128.92	124.68
5	I	9622	XAT	O24-C25-C24	2.27	115.08	113.38
10	F	603	CLA	CAA-C2A-C1A	2.27	119.40	111.97
10	H	602	CLA	C9-C8-C10	-2.27	103.09	111.29
9	J	607	CHL	C14-C13-C12	2.26	119.49	111.29
9	B	607	CHL	CMD-C2D-C3D	2.26	128.91	124.68
4	F	5620	LUT	C1-C2-C3	2.26	118.75	113.64
10	B	602	CLA	C11-C12-C13	-2.26	108.61	115.92
10	C	610	CLA	C11-C10-C8	-2.26	108.62	115.92
10	C	613	CLA	O2A-CGA-CBA	2.26	118.99	111.91
10	D	602	CLA	C12-C11-C10	-2.26	102.87	113.24
9	C	605	CHL	O2A-CGA-O1A	-2.25	117.90	123.59
10	D	612	CLA	C11-C12-C13	2.25	123.19	115.92
8	D	5632	DGD	O3G-C1D-C2D	2.25	111.82	108.30
10	E	604	CLA	O2D-CGD-CBD	2.25	115.27	111.27
9	E	607	CHL	C2A-C1A-CHA	2.25	127.79	123.86
6	A	623	NEX	C1-C2-C3	2.25	118.72	113.64
9	J	609	CHL	O2D-CGD-CBD	2.25	115.26	111.27
9	E	608	CHL	C14-C13-C15	2.25	119.42	111.29
9	E	608	CHL	CAC-C3C-C4C	2.25	127.72	124.81
9	F	608	CHL	CMD-C2D-C3D	2.24	128.87	124.68
10	J	612	CLA	C4-C3-C5	-2.24	111.50	115.27
10	I	612	CLA	C14-C13-C15	2.24	119.40	111.29
10	C	603	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
10	A	611	CLA	C9-C8-C10	2.24	119.40	111.29
6	D	3623	NEX	C24-C23-C22	2.24	115.10	110.77
9	A	606	CHL	O2D-CGD-CBD	2.24	115.24	111.27
10	F	604	CLA	C9-C8-C10	2.24	119.39	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3621	LUT	C18-C5-C6	2.24	127.04	124.53
10	E	614	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
5	J	3622	XAT	C36-C21-C22	-2.23	105.10	108.98
9	A	605	CHL	CAA-C2A-C3A	-2.23	106.67	112.78
9	E	601	CHL	C14-C13-C15	2.23	119.38	111.29
10	C	602	CLA	CMB-C2B-C3B	2.23	128.85	124.68
10	H	613	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
9	I	607	CHL	C2A-C1A-CHA	2.23	127.76	123.86
9	D	606	CHL	O1A-CGA-CBA	-2.23	115.03	123.73
9	H	608	CHL	C14-C13-C15	2.23	119.36	111.29
10	F	614	CLA	OBD-CAD-C3D	2.23	131.68	127.98
10	G	614	CLA	CAA-CBA-CGA	2.23	119.76	113.25
9	J	609	CHL	CAA-CBA-CGA	2.23	119.76	113.25
9	H	606	CHL	CMD-C2D-C3D	2.23	128.84	124.68
10	C	611	CLA	C12-C11-C10	-2.22	103.02	113.24
9	E	601	CHL	C5-C3-C2	2.22	125.62	121.12
10	F	613	CLA	C5-C3-C2	2.22	125.62	121.12
6	B	1623	NEX	O24-C25-C24	2.22	115.05	113.38
10	J	611	CLA	C6-C7-C8	2.22	123.11	115.92
10	C	604	CLA	CMD-C2D-C3D	2.22	128.84	124.68
9	G	608	CHL	C14-C13-C15	2.22	119.34	111.29
9	F	609	CHL	C6-C5-C3	2.22	119.28	113.45
4	G	6620	LUT	C1-C2-C3	2.22	118.66	113.64
10	I	611	CLA	CBA-CAA-C2A	2.22	120.42	113.86
10	E	611	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
9	C	606	CHL	O2A-CGA-O1A	-2.22	117.99	123.59
10	G	612	CLA	C4-C3-C5	-2.22	111.54	115.27
10	E	612	CLA	CMC-C2C-C1C	2.22	128.41	125.04
9	A	608	CHL	O2D-CGD-CBD	2.21	115.20	111.27
9	F	607	CHL	CAC-C3C-C4C	2.21	127.68	124.81
10	F	603	CLA	C1-C2-C3	2.21	129.87	126.04
10	F	611	CLA	C9-C8-C10	2.21	119.31	111.29
9	J	608	CHL	C14-C13-C15	2.21	119.30	111.29
8	I	8632	DGD	O3G-C1D-C2D	2.21	111.75	108.30
10	D	610	CLA	C11-C10-C8	-2.21	108.78	115.92
10	A	613	CLA	C5-C3-C2	2.21	125.59	121.12
10	B	602	CLA	OBD-CAD-C3D	2.21	131.65	127.98
9	F	606	CHL	O2A-CGA-O1A	-2.20	118.03	123.59
5	F	6622	XAT	C37-C21-C36	2.20	110.62	107.37
5	E	2622	XAT	C27-C28-C29	-2.20	122.11	125.53
9	G	607	CHL	CMD-C2D-C3D	2.20	128.79	124.68
10	J	611	CLA	CAA-CBA-CGA	2.20	119.68	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	6623	NEX	C1-C2-C3	2.20	118.61	113.64
9	D	606	CHL	CMD-C2D-C3D	2.20	128.79	124.68
10	E	611	CLA	C6-C7-C8	2.20	123.02	115.92
10	E	604	CLA	C1-C2-C3	2.19	129.84	126.04
10	D	602	CLA	CMD-C2D-C3D	2.19	128.78	124.68
10	F	612	CLA	C11-C12-C13	2.19	123.01	115.92
9	I	608	CHL	C14-C13-C15	2.19	119.23	111.29
10	J	611	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
10	B	611	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
8	I	8632	DGD	C6D-C5D-C4D	2.19	116.67	112.09
10	E	604	CLA	CMD-C2D-C3D	2.19	128.77	124.68
10	F	611	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
10	C	610	CLA	C2A-C1A-CHA	2.19	127.69	123.86
4	B	1620	LUT	C2-C3-C4	2.19	113.30	110.30
10	E	613	CLA	CAA-C2A-C1A	2.19	119.14	111.97
10	G	604	CLA	C12-C11-C10	-2.19	103.19	113.24
10	H	602	CLA	CMB-C2B-C3B	2.19	128.77	124.68
10	A	611	CLA	C16-C15-C13	2.18	122.98	115.92
9	F	607	CHL	CMD-C2D-C3D	2.18	128.76	124.68
8	H	7632	DGD	C6D-C5D-C4D	2.18	116.65	112.09
9	A	606	CHL	C3A-C2A-C1A	2.18	104.61	101.34
10	F	602	CLA	O2A-CGA-CBA	2.18	118.75	111.91
10	J	610	CLA	O1A-CGA-CBA	-2.18	115.23	123.73
9	D	605	CHL	O2A-CGA-O1A	-2.18	118.09	123.59
10	B	613	CLA	C5-C3-C2	2.18	125.53	121.12
10	H	614	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
9	D	606	CHL	OBD-CAD-C3D	2.18	131.60	127.98
5	E	2622	XAT	C37-C21-C22	-2.18	105.20	108.98
9	H	605	CHL	CAA-C2A-C3A	-2.18	106.82	112.78
10	A	602	CLA	C11-C12-C13	-2.18	108.89	115.92
10	A	613	CLA	C12-C11-C10	-2.17	103.25	113.24
4	B	1620	LUT	C21-C26-C27	2.17	115.45	112.70
10	H	604	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
5	B	5622	XAT	C27-C28-C29	-2.17	122.16	125.53
4	D	3620	LUT	C21-C26-C27	2.17	115.44	112.70
9	F	605	CHL	O2A-CGA-O1A	-2.17	118.12	123.59
10	B	603	CLA	C11-C12-C13	2.17	122.92	115.92
9	J	607	CHL	C6-C5-C3	2.17	119.14	113.45
10	A	612	CLA	C4-C3-C5	-2.17	111.63	115.27
10	A	602	CLA	C9-C8-C7	2.16	119.13	111.29
6	B	1623	NEX	C24-C23-C22	2.16	114.95	110.77
9	G	609	CHL	CAA-C2A-C3A	-2.16	106.85	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	602	CLA	OBD-CAD-C3D	2.16	131.57	127.98
10	G	611	CLA	O2D-CGD-CBD	2.16	115.11	111.27
9	C	607	CHL	C2A-C1A-CHA	2.16	127.64	123.86
10	D	611	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
10	G	612	CLA	CMD-C2D-C3D	2.16	128.72	124.68
9	I	605	CHL	O2A-CGA-O1A	-2.16	118.14	123.59
10	E	602	CLA	C9-C8-C10	-2.16	103.48	111.29
9	A	607	CHL	C2A-C1A-CHA	2.16	127.63	123.86
10	H	602	CLA	OBD-CAD-C3D	2.16	131.56	127.98
9	C	608	CHL	C5-C3-C2	-2.16	116.75	121.12
9	B	605	CHL	O2D-CGD-CBD	2.16	115.10	111.27
10	J	604	CLA	CAA-C2A-C1A	2.15	119.03	111.97
10	I	602	CLA	OBD-CAD-C3D	2.15	131.56	127.98
10	H	604	CLA	CAA-C2A-C1A	2.15	119.03	111.97
4	E	4620	LUT	C2-C3-C4	2.15	113.25	110.30
10	D	611	CLA	CMD-C2D-C3D	2.15	128.71	124.68
9	I	601	CHL	CMD-C2D-C3D	2.15	128.71	124.68
10	J	612	CLA	CBA-CAA-C2A	2.15	120.21	113.86
4	J	9621	LUT	C22-C23-C24	2.15	114.19	111.74
8	B	1632	DGD	O3G-C1D-C2D	2.15	111.66	108.30
9	I	607	CHL	C6-C5-C3	2.15	119.09	113.45
4	I	8620	LUT	C1-C2-C3	2.15	118.49	113.64
10	C	612	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
10	A	611	CLA	C11-C10-C8	2.15	122.86	115.92
6	F	5623	NEX	C38-C25-C24	-2.15	111.86	114.28
10	I	611	CLA	O2D-CGD-CBD	2.15	115.08	111.27
10	J	610	CLA	C16-C15-C13	2.15	122.86	115.92
10	G	612	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
9	B	608	CHL	C14-C13-C15	2.14	119.06	111.29
5	B	5622	XAT	C37-C21-C36	2.14	110.53	107.37
9	I	601	CHL	C16-C15-C13	2.14	122.85	115.92
10	C	614	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
10	F	611	CLA	CED-O2D-CGD	2.14	120.78	115.94
10	D	603	CLA	OBD-CAD-C3D	2.14	131.54	127.98
10	B	604	CLA	CMD-C2D-C3D	2.14	128.69	124.68
9	F	607	CHL	C14-C13-C12	2.14	119.05	111.29
9	B	605	CHL	O2A-CGA-O1A	-2.14	118.19	123.59
10	B	613	CLA	CAA-C2A-C1A	2.14	118.99	111.97
8	I	8632	DGD	C4D-C3D-C2D	2.14	114.56	110.82
9	B	605	CHL	CAA-C2A-C3A	-2.14	106.92	112.78
10	G	604	CLA	CAA-C2A-C1A	2.14	118.99	111.97
10	C	613	CLA	C5-C3-C2	2.14	125.45	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	613	CLA	C1-C2-C3	2.14	129.74	126.04
9	C	607	CHL	C5-C3-C2	2.14	125.44	121.12
9	E	606	CHL	O2D-CGD-CBD	2.14	115.07	111.27
4	A	620	LUT	C35-C15-C14	-2.14	119.10	123.47
9	B	606	CHL	CED-O2D-CGD	2.14	120.77	115.94
10	H	603	CLA	C9-C8-C10	-2.14	103.56	111.29
10	D	613	CLA	CAA-C2A-C1A	2.13	118.97	111.97
9	F	601	CHL	C11-C10-C8	2.13	122.82	115.92
9	D	601	CHL	C7-C6-C5	-2.13	107.56	113.36
9	H	607	CHL	C2A-C1A-CHA	2.13	127.59	123.86
9	C	606	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
9	C	605	CHL	O2D-CGD-CBD	2.13	115.06	111.27
8	D	5632	DGD	O1B-C1B-C2B	-2.13	115.42	123.73
5	D	8622	XAT	C37-C21-C36	2.13	110.51	107.37
9	B	609	CHL	O2A-CGA-CBA	2.13	118.59	111.91
8	I	8632	DGD	C3D-C4D-C5D	2.13	114.03	110.24
10	H	610	CLA	CAA-CBA-CGA	2.13	119.47	113.25
10	A	602	CLA	C6-C7-C8	-2.13	109.05	115.92
10	I	614	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
4	C	2621	LUT	C1-C6-C5	-2.13	119.62	122.61
9	F	605	CHL	O2D-CGD-CBD	2.13	115.05	111.27
10	D	603	CLA	CAA-CBA-CGA	2.12	119.46	113.25
10	G	614	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
10	G	611	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
10	F	614	CLA	CED-O2D-CGD	2.12	120.74	115.94
9	G	607	CHL	C5-C3-C2	2.12	125.41	121.12
10	C	611	CLA	CAA-C2A-C1A	2.12	118.93	111.97
10	B	604	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
10	A	613	CLA	CAA-CBA-CGA	2.12	119.45	113.25
6	E	4623	NEX	C1-C2-C3	2.12	118.43	113.64
10	B	613	CLA	C3A-C2A-C1A	2.12	104.52	101.34
4	G	6621	LUT	C18-C5-C6	2.12	126.91	124.53
10	G	612	CLA	CMC-C2C-C1C	2.12	128.26	125.04
9	G	607	CHL	C2A-C1A-CHA	2.12	127.56	123.86
10	D	603	CLA	C16-C17-C18	2.12	125.96	115.98
9	C	607	CHL	C4-C3-C5	-2.12	111.71	115.27
6	J	9623	NEX	C1-C2-C3	2.12	118.42	113.64
10	J	612	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
9	G	607	CHL	CAA-C2A-C1A	2.12	118.91	111.97
10	A	604	CLA	C2A-C1A-CHA	2.11	127.56	123.86
9	H	606	CHL	O2A-CGA-O1A	-2.11	118.26	123.59
10	B	611	CLA	CMD-C2D-C3D	2.11	128.63	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	603	CLA	OBD-CAD-C3D	2.11	131.49	127.98
9	B	607	CHL	C1-C2-C3	-2.11	122.39	126.04
10	H	611	CLA	C6-C7-C8	2.11	122.74	115.92
10	E	612	CLA	C11-C12-C13	2.11	122.74	115.92
10	H	610	CLA	O1A-CGA-CBA	-2.11	115.50	123.73
9	F	601	CHL	C6-C5-C3	2.11	118.99	113.45
10	H	612	CLA	C4-C3-C2	2.11	129.09	123.68
8	B	1632	DGD	C4D-C3D-C2D	2.11	114.50	110.82
9	I	605	CHL	CED-O2D-CGD	2.11	120.70	115.94
4	G	6620	LUT	C1-C6-C5	-2.11	119.65	122.61
10	J	610	CLA	C11-C10-C8	-2.11	109.11	115.92
9	C	607	CHL	OBD-CAD-C3D	2.11	131.48	127.98
10	B	604	CLA	C2A-C1A-CHA	2.11	127.54	123.86
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	B	606	CHL	O2D-CGD-CBD	2.10	115.01	111.27
9	B	609	CHL	C7-C6-C5	-2.10	107.64	113.36
9	A	606	CHL	O2A-CGA-O1A	-2.10	118.28	123.59
9	B	606	CHL	OBD-CAD-C3D	2.10	131.47	127.98
10	J	603	CLA	CAA-C2A-C1A	2.10	118.86	111.97
10	F	604	CLA	C11-C10-C8	2.10	122.72	115.92
10	J	610	CLA	C14-C13-C12	2.10	118.91	111.29
9	H	609	CHL	CBA-CAA-C2A	2.10	120.07	113.86
10	A	612	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
9	C	608	CHL	C11-C12-C13	2.10	122.71	115.92
10	I	603	CLA	O2A-CGA-CBA	2.10	118.50	111.91
10	I	611	CLA	OBD-CAD-C3D	2.10	131.47	127.98
10	B	610	CLA	C11-C10-C8	-2.10	109.13	115.92
10	J	613	CLA	CAA-CBA-CGA	2.10	119.39	113.25
6	H	7623	NEX	C27-C28-C29	2.10	128.79	125.53
9	F	607	CHL	C1-C2-C3	-2.10	122.41	126.04
10	D	611	CLA	C4-C3-C5	-2.10	111.74	115.27
10	H	603	CLA	CMD-C2D-C3D	2.10	128.60	124.68
10	F	613	CLA	C1-C2-C3	2.10	129.67	126.04
10	J	603	CLA	C1-C2-C3	2.10	129.67	126.04
9	C	605	CHL	C2A-C1A-CHA	2.10	127.53	123.86
10	I	603	CLA	C16-C15-C13	2.10	122.69	115.92
10	J	604	CLA	CMD-C2D-C3D	2.10	128.60	124.68
10	J	604	CLA	C6-C7-C8	2.10	122.69	115.92
10	D	602	CLA	OBD-CAD-C3D	2.09	131.46	127.98
10	C	612	CLA	C11-C10-C8	2.09	122.69	115.92
10	H	613	CLA	CMA-C3A-C4A	2.09	117.40	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	606	CHL	CAA-C2A-C1A	2.09	118.83	111.97
10	F	604	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
9	J	608	CHL	OBD-CAD-C3D	2.09	131.45	127.98
9	C	608	CHL	OBD-CAD-C3D	2.09	131.45	127.98
10	G	613	CLA	C6-C5-C3	2.09	118.94	113.45
6	G	6623	NEX	O24-C25-C24	2.09	114.95	113.38
10	I	613	CLA	C3A-C2A-C1A	2.09	104.46	101.34
9	A	608	CHL	C2A-C1A-CHA	2.08	127.50	123.86
6	B	1623	NEX	C1-C2-C3	2.08	118.35	113.64
6	A	623	NEX	C38-C25-C24	-2.08	111.94	114.28
9	E	606	CHL	O2A-CGA-O1A	-2.08	118.33	123.59
8	B	2632	DGD	C6D-C5D-C4D	2.08	116.44	112.09
10	B	612	CLA	OBD-CAD-C3D	2.08	131.43	127.98
10	H	612	CLA	CMD-C2D-C3D	2.08	128.57	124.68
10	G	611	CLA	C16-C15-C13	2.08	122.64	115.92
10	A	603	CLA	CAA-CBA-CGA	2.08	119.33	113.25
9	H	607	CHL	C12-C11-C10	-2.08	103.69	113.24
9	H	605	CHL	O2A-CGA-O1A	-2.08	118.35	123.59
10	E	613	CLA	C6-C5-C3	2.08	118.90	113.45
9	F	609	CHL	O2D-CGD-CBD	2.08	114.96	111.27
6	F	5623	NEX	O24-C25-C24	2.08	114.94	113.38
9	E	608	CHL	OBD-CAD-C3D	2.07	131.43	127.98
10	E	604	CLA	CBA-CAA-C2A	2.07	119.98	113.86
10	D	612	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
9	D	601	CHL	OBD-CAD-C3D	2.07	131.42	127.98
10	B	613	CLA	CMD-C2D-C3D	2.07	128.55	124.68
10	F	612	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
9	B	607	CHL	C2A-C1A-CHA	2.07	127.47	123.86
10	J	613	CLA	C3A-C2A-C1A	2.07	104.44	101.34
10	H	612	CLA	OBD-CAD-C3D	2.07	131.41	127.98
10	D	603	CLA	C9-C8-C10	-2.07	103.81	111.29
10	H	604	CLA	C12-C11-C10	-2.07	103.75	113.24
10	A	603	CLA	CED-O2D-CGD	2.07	120.61	115.94
9	B	608	CHL	O2A-CGA-O1A	-2.06	118.38	123.59
10	D	603	CLA	C16-C15-C13	2.06	122.59	115.92
10	F	611	CLA	O2D-CGD-CBD	2.06	114.94	111.27
4	C	2621	LUT	C22-C23-C24	2.06	114.09	111.74
9	D	608	CHL	C1-C2-C3	2.06	129.61	126.04
9	E	607	CHL	C6-C7-C8	2.06	122.58	115.92
8	A	632	DGD	O3G-C1D-C2D	2.06	111.52	108.30
10	E	604	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
10	J	612	CLA	C4-C3-C2	2.06	128.96	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	606	CHL	O2D-CGD-CBD	2.06	114.92	111.27
8	G	9632	DGD	C6D-C5D-C4D	2.06	116.39	112.09
10	D	603	CLA	C4-C3-C5	-2.06	111.81	115.27
6	D	3623	NEX	C4-C3-C2	-2.06	106.80	110.77
10	B	611	CLA	OBD-CAD-C3D	2.05	131.39	127.98
10	G	604	CLA	C9-C8-C10	2.05	118.73	111.29
10	D	610	CLA	C16-C15-C13	2.05	122.56	115.92
9	G	609	CHL	CAA-CBA-CGA	2.05	119.25	113.25
8	D	3632	DGD	O3G-C1D-C2D	2.05	111.51	108.30
10	I	611	CLA	CMD-C2D-C3D	2.05	128.52	124.68
9	D	605	CHL	OBD-CAD-C3D	2.05	131.39	127.98
9	C	605	CHL	CMD-C2D-C3D	2.05	128.52	124.68
9	F	609	CHL	C12-C11-C10	-2.05	103.82	113.24
10	E	603	CLA	C11-C10-C8	2.05	122.55	115.92
10	H	604	CLA	OBD-CAD-C3D	2.05	131.38	127.98
9	I	609	CHL	C6-C5-C3	2.05	118.83	113.45
10	J	602	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
10	C	603	CLA	OBD-CAD-C3D	2.05	131.38	127.98
9	E	601	CHL	C7-C6-C5	-2.05	107.80	113.36
10	A	603	CLA	C16-C17-C18	2.05	125.62	115.98
9	I	607	CHL	CMD-C2D-C3D	2.05	128.51	124.68
9	B	601	CHL	CAA-CBA-CGA	2.04	119.23	113.25
10	D	612	CLA	C3A-C2A-C1A	2.04	104.40	101.34
10	E	604	CLA	C2A-C1A-CHA	2.04	127.43	123.86
9	E	608	CHL	C2A-C1A-CHA	2.04	127.43	123.86
9	E	608	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
10	H	610	CLA	C9-C8-C7	2.04	118.69	111.29
10	C	604	CLA	OBD-CAD-C3D	2.04	131.37	127.98
10	A	614	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
9	J	607	CHL	C6-C7-C8	2.04	122.52	115.92
7	H	7630	LHG	C26-C25-C24	2.04	120.53	113.19
10	A	602	CLA	OBD-CAD-C3D	2.04	131.37	127.98
9	A	601	CHL	CAC-C3C-C4C	2.04	127.46	124.81
9	H	601	CHL	CAA-CBA-CGA	2.04	119.21	113.25
10	H	611	CLA	CAA-CBA-CGA	2.04	119.21	113.25
9	I	609	CHL	CAA-C2A-C1A	2.04	118.65	111.97
10	G	602	CLA	OBD-CAD-C3D	2.04	131.37	127.98
10	C	614	CLA	C2A-C1A-CHA	2.04	127.42	123.86
10	E	614	CLA	C2A-C1A-CHA	2.04	127.42	123.86
9	B	608	CHL	C2A-C1A-CHA	2.04	127.42	123.86
10	H	613	CLA	C3A-C2A-C1A	2.04	104.39	101.34
10	B	610	CLA	OBD-CAD-C3D	2.04	131.36	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	613	CLA	C3A-C2A-C1A	2.03	104.39	101.34
9	C	606	CHL	CAA-C2A-C1A	2.03	118.64	111.97
9	I	609	CHL	C16-C15-C13	2.03	122.50	115.92
9	F	608	CHL	C6-C7-C8	2.03	122.49	115.92
10	A	602	CLA	O2A-CGA-CBA	2.03	118.29	111.91
9	A	607	CHL	C14-C13-C12	2.03	118.66	111.29
10	F	611	CLA	CMD-C2D-C3D	2.03	128.48	124.68
5	D	8622	XAT	C31-C30-C29	-2.03	124.41	127.31
10	B	612	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
9	D	606	CHL	OMC-CMC-C2C	2.03	130.28	125.69
10	D	604	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
10	B	604	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
10	B	611	CLA	CAA-CBA-CGA	2.03	119.18	113.25
10	I	613	CLA	OBD-CAD-C3D	2.03	131.35	127.98
5	E	2622	XAT	C37-C21-C36	2.03	110.36	107.37
4	C	2621	LUT	C18-C5-C6	2.03	126.81	124.53
9	F	606	CHL	O2D-CGD-CBD	2.03	114.87	111.27
9	F	601	CHL	CMD-C2D-C3D	2.03	128.47	124.68
9	A	601	CHL	CMD-C2D-C3D	2.02	128.47	124.68
9	A	607	CHL	C11-C12-C13	2.02	122.46	115.92
9	I	607	CHL	C14-C13-C12	2.02	118.62	111.29
10	H	612	CLA	CBA-CAA-C2A	2.02	119.83	113.86
10	A	613	CLA	C3A-C2A-C1A	2.02	104.37	101.34
10	A	603	CLA	CMD-C2D-C3D	2.02	128.46	124.68
10	F	611	CLA	OBD-CAD-C3D	2.02	131.34	127.98
9	A	605	CHL	O2D-CGD-CBD	2.02	114.86	111.27
10	I	604	CLA	OBD-CAD-C3D	2.02	131.34	127.98
10	E	604	CLA	OBD-CAD-C3D	2.02	131.34	127.98
4	F	5621	LUT	C7-C8-C9	2.02	129.29	126.23
9	H	605	CHL	C2A-C1A-CHA	2.02	127.39	123.86
10	I	610	CLA	C1-C2-C3	2.02	129.53	126.04
4	J	9620	LUT	C3-C4-C5	2.02	115.87	111.85
10	E	613	CLA	C3A-C2A-C1A	2.02	104.36	101.34
9	I	601	CHL	C1-C2-C3	2.02	129.53	126.04
10	D	614	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
10	G	603	CLA	OBD-CAD-C3D	2.02	131.33	127.98
10	A	603	CLA	O2A-CGA-CBA	2.02	118.23	111.91
10	I	603	CLA	OBD-CAD-C3D	2.02	131.33	127.98
9	A	606	CHL	O1A-CGA-CBA	-2.01	115.87	123.73
9	E	608	CHL	CAA-C2A-C3A	-2.01	107.26	112.78
10	J	612	CLA	C3A-C2A-C1A	2.01	104.35	101.34
10	C	612	CLA	CMD-C2D-C3D	2.01	128.44	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	605	CHL	CMD-C2D-C3D	2.01	128.44	124.68
8	A	632	DGD	C4D-C3D-C2D	2.01	114.33	110.82
10	I	610	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
10	B	611	CLA	O1A-CGA-CBA	-2.01	115.89	123.73
7	A	630	LHG	C26-C25-C24	2.01	120.42	113.19
10	J	614	CLA	C2A-C1A-CHA	2.01	127.37	123.86
10	E	614	CLA	CMC-C2C-C1C	2.01	128.10	125.04
10	C	610	CLA	OBD-CAD-C3D	2.01	131.32	127.98
10	E	612	CLA	OBD-CAD-C3D	2.01	131.32	127.98
10	F	602	CLA	OBD-CAD-C3D	2.01	131.31	127.98
9	I	605	CHL	OBD-CAD-C3D	2.01	131.31	127.98
9	C	609	CHL	C7-C6-C5	-2.01	107.91	113.36
9	B	605	CHL	CMD-C2D-C3D	2.01	128.43	124.68
9	A	608	CHL	O1D-CGD-CBD	-2.01	120.38	124.48
10	H	603	CLA	C16-C17-C18	2.01	125.44	115.98
10	J	604	CLA	C2A-C1A-CHA	2.01	127.37	123.86
10	I	603	CLA	C3A-C2A-C1A	2.01	104.34	101.34
6	D	3623	NEX	O24-C25-C24	2.01	114.89	113.38
8	A	632	DGD	C3D-C4D-C5D	2.01	113.82	110.24
10	J	611	CLA	C2A-C1A-CHA	2.01	127.36	123.86
10	H	610	CLA	C16-C15-C13	2.00	122.40	115.92
10	H	610	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
9	H	601	CHL	O2A-CGA-CBA	2.00	118.19	111.91
9	A	609	CHL	CBA-CAA-C2A	2.00	119.78	113.86
8	D	3632	DGD	C6D-C5D-C4D	2.00	116.28	112.09
10	D	614	CLA	C2A-C1A-CHA	2.00	127.36	123.86
9	C	607	CHL	C10-C8-C7	2.00	122.66	112.13
10	G	604	CLA	CMD-C2D-C3D	2.00	128.42	124.68
9	C	608	CHL	C16-C17-C18	2.00	125.41	115.98
9	J	606	CHL	CAA-C2A-C1A	2.00	118.53	111.97
5	H	4622	XAT	C31-C30-C29	-2.00	124.45	127.31
10	A	611	CLA	C6-C7-C8	2.00	122.39	115.92
9	B	608	CHL	C16-C17-C18	2.00	125.41	115.98
10	C	613	CLA	C3A-C2A-C1A	2.00	104.34	101.34

All (503) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	611	CLA	NC
10	B	611	CLA	ND
10	B	611	CLA	NA
9	G	601	CHL	C8

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Mol	Chain	Res	Type	Atom
9	G	601	CHL	NC
9	G	601	CHL	ND
9	G	601	CHL	NA
10	F	611	CLA	NC
10	F	611	CLA	ND
10	F	611	CLA	NA
9	D	609	CHL	C8
9	D	609	CHL	C13
9	D	609	CHL	NC
9	D	609	CHL	NA
9	D	609	CHL	ND
9	H	607	CHL	NC
9	H	607	CHL	ND
9	H	607	CHL	NA
10	A	610	CLA	NC
10	A	610	CLA	NA
10	A	610	CLA	ND
10	G	613	CLA	NC
10	G	613	CLA	ND
10	G	613	CLA	NA
10	F	610	CLA	NC
10	F	610	CLA	ND
10	F	610	CLA	NA
10	A	602	CLA	C8
10	A	602	CLA	NC
10	A	602	CLA	ND
10	A	602	CLA	NA
10	G	610	CLA	NC
10	G	610	CLA	NA
10	G	610	CLA	ND
9	C	605	CHL	NC
9	C	605	CHL	ND
9	C	605	CHL	NA
9	H	601	CHL	C8
9	H	601	CHL	NC
9	H	601	CHL	ND
9	H	601	CHL	NA
9	B	608	CHL	C8
9	B	608	CHL	NC
9	B	608	CHL	ND
9	B	608	CHL	NA
9	D	608	CHL	C8

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Mol	Chain	Res	Type	Atom
9	D	608	CHL	NC
9	D	608	CHL	ND
9	D	608	CHL	NA
9	D	606	CHL	NC
9	D	606	CHL	ND
9	D	606	CHL	NA
9	F	609	CHL	C8
9	F	609	CHL	C13
9	F	609	CHL	NC
9	F	609	CHL	ND
9	F	609	CHL	NA
10	B	603	CLA	C8
10	B	603	CLA	NC
10	B	603	CLA	ND
10	B	603	CLA	NA
9	I	608	CHL	C8
9	I	608	CHL	NC
9	I	608	CHL	ND
9	I	608	CHL	NA
10	I	604	CLA	NC
10	I	604	CLA	ND
10	I	604	CLA	NA
10	C	610	CLA	NC
10	C	610	CLA	NA
10	C	610	CLA	ND
8	I	8632	DGD	C2D
8	I	8632	DGD	C5D
10	D	611	CLA	NC
10	D	611	CLA	ND
10	D	611	CLA	NA
10	F	602	CLA	C8
10	F	602	CLA	NC
10	F	602	CLA	ND
10	F	602	CLA	NA
10	H	611	CLA	NC
10	H	611	CLA	NA
10	H	611	CLA	ND
10	C	611	CLA	NC
10	C	611	CLA	ND
10	C	611	CLA	NA
10	J	612	CLA	NC
10	J	612	CLA	ND

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Mol	Chain	Res	Type	Atom
10	J	612	CLA	NA
10	G	602	CLA	C8
10	G	602	CLA	NC
10	G	602	CLA	ND
10	G	602	CLA	NA
9	I	601	CHL	C8
9	I	601	CHL	NC
9	I	601	CHL	ND
9	I	601	CHL	NA
10	B	614	CLA	NC
10	B	614	CLA	ND
10	B	614	CLA	NA
9	H	606	CHL	NC
9	H	606	CHL	ND
9	H	606	CHL	NA
10	J	604	CLA	NC
10	J	604	CLA	ND
10	J	604	CLA	NA
10	H	614	CLA	NC
10	H	614	CLA	ND
10	H	614	CLA	NA
8	D	5632	DGD	C2D
8	D	5632	DGD	C5D
10	E	604	CLA	NC
10	E	604	CLA	ND
10	E	604	CLA	NA
8	A	632	DGD	C2D
8	A	632	DGD	C5D
8	E	4632	DGD	C2D
8	E	4632	DGD	C5D
10	F	603	CLA	C8
10	F	603	CLA	NC
10	F	603	CLA	ND
10	F	603	CLA	NA
9	A	607	CHL	NC
9	A	607	CHL	ND
9	A	607	CHL	NA
10	I	602	CLA	C8
10	I	602	CLA	NC
10	I	602	CLA	ND
10	I	602	CLA	NA
10	I	614	CLA	NC

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Mol	Chain	Res	Type	Atom
10	I	614	CLA	ND
10	I	614	CLA	NA
10	B	602	CLA	C8
10	B	602	CLA	NC
10	B	602	CLA	ND
10	B	602	CLA	NA
9	C	609	CHL	C8
9	C	609	CHL	C13
9	C	609	CHL	NC
9	C	609	CHL	ND
9	C	609	CHL	NA
10	C	612	CLA	NC
10	C	612	CLA	ND
10	C	612	CLA	NA
10	A	612	CLA	NC
10	A	612	CLA	ND
10	A	612	CLA	NA
10	C	604	CLA	NC
10	C	604	CLA	ND
10	C	604	CLA	NA
10	D	604	CLA	NC
10	D	604	CLA	ND
10	D	604	CLA	NA
10	J	602	CLA	C8
10	J	602	CLA	NC
10	J	602	CLA	ND
10	J	602	CLA	NA
10	G	614	CLA	NC
10	G	614	CLA	NA
10	G	614	CLA	ND
8	G	9632	DGD	C2D
8	G	9632	DGD	C5D
10	H	610	CLA	C13
10	H	610	CLA	NC
10	H	610	CLA	NA
10	H	610	CLA	ND
9	A	609	CHL	C8
9	A	609	CHL	C13
9	A	609	CHL	NC
9	A	609	CHL	ND
9	A	609	CHL	NA
10	I	613	CLA	NC

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Mol	Chain	Res	Type	Atom
10	I	613	CLA	ND
10	I	613	CLA	NA
9	C	601	CHL	C8
9	C	601	CHL	NC
9	C	601	CHL	ND
9	C	601	CHL	NA
9	E	601	CHL	C8
9	E	601	CHL	NC
9	E	601	CHL	ND
9	E	601	CHL	NA
9	A	608	CHL	C8
9	A	608	CHL	NC
9	A	608	CHL	ND
9	A	608	CHL	NA
9	F	605	CHL	NC
9	F	605	CHL	ND
9	F	605	CHL	NA
10	F	613	CLA	NC
10	F	613	CLA	ND
10	F	613	CLA	NA
10	E	602	CLA	C8
10	E	602	CLA	NC
10	E	602	CLA	ND
10	E	602	CLA	NA
9	G	609	CHL	C8
9	G	609	CHL	C13
9	G	609	CHL	NC
9	G	609	CHL	NA
9	G	609	CHL	ND
10	E	603	CLA	C8
10	E	603	CLA	NC
10	E	603	CLA	ND
10	E	603	CLA	NA
10	D	610	CLA	NC
10	D	610	CLA	ND
10	D	610	CLA	NA
10	J	610	CLA	NC
10	J	610	CLA	NA
10	J	610	CLA	ND
10	B	604	CLA	NC
10	B	604	CLA	ND
10	B	604	CLA	NA

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Mol	Chain	Res	Type	Atom
10	G	604	CLA	NC
10	G	604	CLA	ND
10	G	604	CLA	NA
10	A	604	CLA	NC
10	A	604	CLA	ND
10	A	604	CLA	NA
9	A	605	CHL	NC
9	A	605	CHL	ND
9	A	605	CHL	NA
10	B	613	CLA	NC
10	B	613	CLA	ND
10	B	613	CLA	NA
10	D	613	CLA	NC
10	D	613	CLA	ND
10	D	613	CLA	NA
10	I	610	CLA	C13
10	I	610	CLA	NC
10	I	610	CLA	NA
10	I	610	CLA	ND
9	G	607	CHL	NC
9	G	607	CHL	ND
9	G	607	CHL	NA
9	C	606	CHL	NC
9	C	606	CHL	ND
9	C	606	CHL	NA
10	J	614	CLA	NC
10	J	614	CLA	ND
10	J	614	CLA	NA
9	F	607	CHL	NC
9	F	607	CHL	ND
9	F	607	CHL	NA
9	E	606	CHL	NC
9	E	606	CHL	ND
9	E	606	CHL	NA
10	I	603	CLA	C8
10	I	603	CLA	NC
10	I	603	CLA	ND
10	I	603	CLA	NA
10	J	611	CLA	NC
10	J	611	CLA	ND
10	J	611	CLA	NA
10	A	611	CLA	NC

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Mol	Chain	Res	Type	Atom
10	A	611	CLA	NA
10	A	611	CLA	ND
10	J	613	CLA	NC
10	J	613	CLA	ND
10	J	613	CLA	NA
9	F	606	CHL	NC
9	F	606	CHL	ND
9	F	606	CHL	NA
10	C	602	CLA	C8
10	C	602	CLA	NC
10	C	602	CLA	ND
10	C	602	CLA	NA
10	G	612	CLA	NC
10	G	612	CLA	ND
10	G	612	CLA	NA
9	I	609	CHL	C8
9	I	609	CHL	C13
9	I	609	CHL	NC
9	I	609	CHL	ND
9	I	609	CHL	NA
9	F	608	CHL	C8
9	F	608	CHL	NC
9	F	608	CHL	ND
9	F	608	CHL	NA
10	H	612	CLA	NC
10	H	612	CLA	ND
10	H	612	CLA	NA
10	D	603	CLA	C8
10	D	603	CLA	NC
10	D	603	CLA	ND
10	D	603	CLA	NA
10	I	611	CLA	NC
10	I	611	CLA	NA
10	I	611	CLA	ND
9	E	607	CHL	NC
9	E	607	CHL	ND
9	E	607	CHL	NA
9	H	605	CHL	NC
9	H	605	CHL	ND
9	H	605	CHL	NA
10	G	603	CLA	C8
10	G	603	CLA	NC

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Mol	Chain	Res	Type	Atom
10	G	603	CLA	ND
10	G	603	CLA	NA
9	E	605	CHL	NC
9	E	605	CHL	ND
9	E	605	CHL	NA
10	B	610	CLA	NC
10	B	610	CLA	NA
10	B	610	CLA	ND
10	D	612	CLA	NC
10	D	612	CLA	ND
10	D	612	CLA	NA
9	C	607	CHL	NC
9	C	607	CHL	ND
9	C	607	CHL	NA
10	C	614	CLA	NC
10	C	614	CLA	ND
10	C	614	CLA	NA
9	E	609	CHL	C8
9	E	609	CHL	C13
9	E	609	CHL	NC
9	E	609	CHL	ND
9	E	609	CHL	NA
9	G	606	CHL	NC
9	G	606	CHL	ND
9	G	606	CHL	NA
9	A	601	CHL	C8
9	A	601	CHL	C13
9	A	601	CHL	NC
9	A	601	CHL	ND
9	A	601	CHL	NA
9	B	601	CHL	C8
9	B	601	CHL	NC
9	B	601	CHL	ND
9	B	601	CHL	NA
10	H	602	CLA	C8
10	H	602	CLA	NC
10	H	602	CLA	ND
10	H	602	CLA	NA
8	H	7632	DGD	C2D
8	H	7632	DGD	C5D
10	E	610	CLA	NC
10	E	610	CLA	NA

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Mol	Chain	Res	Type	Atom
10	E	610	CLA	ND
9	I	606	CHL	NC
9	I	606	CHL	ND
9	I	606	CHL	NA
9	H	609	CHL	C8
9	H	609	CHL	C13
9	H	609	CHL	NC
9	H	609	CHL	NA
9	H	609	CHL	ND
10	A	613	CLA	NC
10	A	613	CLA	ND
10	A	613	CLA	NA
9	A	606	CHL	NC
9	A	606	CHL	ND
9	A	606	CHL	NA
10	C	603	CLA	C8
10	C	603	CLA	NC
10	C	603	CLA	ND
10	C	603	CLA	NA
9	D	601	CHL	C8
9	D	601	CHL	NC
9	D	601	CHL	ND
9	D	601	CHL	NA
9	F	601	CHL	C8
9	F	601	CHL	NC
9	F	601	CHL	ND
9	F	601	CHL	NA
10	J	603	CLA	C8
10	J	603	CLA	NC
10	J	603	CLA	ND
10	J	603	CLA	NA
9	J	609	CHL	C8
9	J	609	CHL	C13
9	J	609	CHL	NC
9	J	609	CHL	NA
9	J	609	CHL	ND
10	I	612	CLA	NC
10	I	612	CLA	ND
10	I	612	CLA	NA
10	H	604	CLA	NC
10	H	604	CLA	ND
10	H	604	CLA	NA

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Mol	Chain	Res	Type	Atom
8	B	2632	DGD	C2D
8	B	2632	DGD	C5D
9	G	605	CHL	NC
9	G	605	CHL	ND
9	G	605	CHL	NA
9	B	605	CHL	NC
9	B	605	CHL	ND
9	B	605	CHL	NA
9	D	605	CHL	NC
9	D	605	CHL	ND
9	D	605	CHL	NA
10	E	611	CLA	NC
10	E	611	CLA	ND
10	E	611	CLA	NA
9	J	607	CHL	NC
9	J	607	CHL	ND
9	J	607	CHL	NA
9	B	606	CHL	NC
9	B	606	CHL	ND
9	B	606	CHL	NA
8	B	1632	DGD	C2D
8	B	1632	DGD	C5D
10	F	614	CLA	NC
10	F	614	CLA	NA
10	F	614	CLA	ND
9	I	605	CHL	NC
9	I	605	CHL	ND
9	I	605	CHL	NA
9	J	606	CHL	NC
9	J	606	CHL	ND
9	J	606	CHL	NA
9	I	607	CHL	NC
9	I	607	CHL	ND
9	I	607	CHL	NA
10	F	612	CLA	NC
10	F	612	CLA	ND
10	F	612	CLA	NA
10	E	612	CLA	NC
10	E	612	CLA	ND
10	E	612	CLA	NA
9	J	608	CHL	C8
9	J	608	CHL	NC

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Mol	Chain	Res	Type	Atom
9	J	608	CHL	ND
9	J	608	CHL	NA
10	D	602	CLA	C8
10	D	602	CLA	NC
10	D	602	CLA	ND
10	D	602	CLA	NA
9	H	608	CHL	C8
9	H	608	CHL	NC
9	H	608	CHL	ND
9	H	608	CHL	NA
9	J	605	CHL	NC
9	J	605	CHL	ND
9	J	605	CHL	NA
10	F	604	CLA	NC
10	F	604	CLA	ND
10	F	604	CLA	NA
10	B	612	CLA	NC
10	B	612	CLA	ND
10	B	612	CLA	NA
10	A	614	CLA	NC
10	A	614	CLA	ND
10	A	614	CLA	NA
10	H	603	CLA	C8
10	H	603	CLA	NC
10	H	603	CLA	ND
10	H	603	CLA	NA
9	C	608	CHL	C8
9	C	608	CHL	NC
9	C	608	CHL	ND
9	C	608	CHL	NA
10	D	614	CLA	NC
10	D	614	CLA	ND
10	D	614	CLA	NA
10	G	611	CLA	NC
10	G	611	CLA	NA
10	G	611	CLA	ND
8	H	6632	DGD	C2D
8	H	6632	DGD	C5D
10	H	613	CLA	NC
10	H	613	CLA	ND
10	H	613	CLA	NA
8	D	3632	DGD	C2D

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Mol	Chain	Res	Type	Atom
8	D	3632	DGD	C5D
10	C	613	CLA	NC
10	C	613	CLA	ND
10	C	613	CLA	NA
10	E	613	CLA	NC
10	E	613	CLA	ND
10	E	613	CLA	NA
9	J	601	CHL	C8
9	J	601	CHL	NC
9	J	601	CHL	ND
9	J	601	CHL	NA
9	E	608	CHL	C8
9	E	608	CHL	NC
9	E	608	CHL	ND
9	E	608	CHL	NA
9	G	608	CHL	C8
9	G	608	CHL	NC
9	G	608	CHL	ND
9	G	608	CHL	NA
10	A	603	CLA	C8
10	A	603	CLA	NC
10	A	603	CLA	ND
10	A	603	CLA	NA
9	D	607	CHL	NC
9	D	607	CHL	ND
9	D	607	CHL	NA
10	E	614	CLA	NC
10	E	614	CLA	ND
10	E	614	CLA	NA
9	B	609	CHL	C8
9	B	609	CHL	C13
9	B	609	CHL	NC
9	B	609	CHL	ND
9	B	609	CHL	NA
9	B	607	CHL	NC
9	B	607	CHL	ND
9	B	607	CHL	NA

All (2523) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	602	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	G	610	CLA	C14-C13-C15-C16
2	J	9633	BNG	C2-C1-O1-C1'
2	J	9633	BNG	O5-C1-O1-C1'
9	C	605	CHL	C3A-C2A-CAA-CBA
9	H	601	CHL	CHA-CBD-CGD-O1D
9	H	601	CHL	CHA-CBD-CGD-O2D
9	D	608	CHL	C2A-CAA-CBA-CGA
9	D	606	CHL	CBA-CGA-O2A-C1
9	D	606	CHL	O1A-CGA-O2A-C1
10	I	604	CLA	C1A-C2A-CAA-CBA
10	D	611	CLA	C1A-C2A-CAA-CBA
7	E	4630	LHG	O1-C1-C2-C3
7	E	4630	LHG	C1-C2-C3-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
10	C	611	CLA	C6-C7-C8-C10
10	J	612	CLA	CBD-CGD-O2D-CED
7	H	7630	LHG	O1-C1-C2-C3
10	G	602	CLA	C2-C3-C5-C6
10	G	602	CLA	C4-C3-C5-C6
9	I	601	CHL	CHA-CBD-CGD-O1D
9	H	606	CHL	C1A-C2A-CAA-CBA
10	F	603	CLA	C1A-C2A-CAA-CBA
10	I	602	CLA	C2-C3-C5-C6
10	I	602	CLA	C4-C3-C5-C6
5	H	4622	XAT	O24-C26-C27-C28
10	D	604	CLA	C1A-C2A-CAA-CBA
9	E	601	CHL	CHA-CBD-CGD-O1D
9	E	601	CHL	CHA-CBD-CGD-O2D
9	F	605	CHL	C3A-C2A-CAA-CBA
7	J	9630	LHG	O1-C1-C2-O2
7	J	9630	LHG	O1-C1-C2-C3
7	J	9630	LHG	C4-O6-P-O3
10	E	602	CLA	C4-C3-C5-C6
5	D	8622	XAT	O24-C26-C27-C28
10	B	604	CLA	C6-C7-C8-C10
10	A	604	CLA	C1A-C2A-CAA-CBA
7	C	2630	LHG	O1-C1-C2-C3
9	E	606	CHL	C3A-C2A-CAA-CBA
10	I	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
10	I	603	CLA	C3A-C2A-CAA-CBA
10	A	611	CLA	C1A-C2A-CAA-CBA
10	C	602	CLA	C4-C3-C5-C6
10	G	612	CLA	CBD-CGD-O2D-CED
9	I	609	CHL	C1A-C2A-CAA-CBA
9	F	608	CHL	C1A-C2A-CAA-CBA
10	I	611	CLA	C1A-C2A-CAA-CBA
7	B	1630	LHG	O1-C1-C2-C3
7	B	1630	LHG	C1-C2-C3-O3
9	E	605	CHL	C1A-C2A-CAA-CBA
10	D	612	CLA	CBD-CGD-O2D-CED
9	G	606	CHL	C1A-C2A-CAA-CBA
9	A	601	CHL	CHA-CBD-CGD-O1D
9	A	601	CHL	CHA-CBD-CGD-O2D
9	B	601	CHL	CHA-CBD-CGD-O2D
10	H	602	CLA	C2-C3-C5-C6
10	H	602	CLA	C4-C3-C5-C6
9	I	606	CHL	C1A-C2A-CAA-CBA
9	I	606	CHL	O1A-CGA-O2A-C1
7	A	630	LHG	O1-C1-C2-O2
7	A	630	LHG	O1-C1-C2-C3
7	A	630	LHG	C4-O6-P-O5
10	I	612	CLA	CBD-CGD-O2D-CED
9	G	605	CHL	C1A-C2A-CAA-CBA
9	G	605	CHL	C3A-C2A-CAA-CBA
10	E	611	CLA	C1A-C2A-CAA-CBA
9	B	606	CHL	C1A-C2A-CAA-CBA
7	I	8630	LHG	C4-O6-P-O4
7	I	8630	LHG	C4-O6-P-O5
7	G	6630	LHG	O1-C1-C2-O2
7	G	6630	LHG	O1-C1-C2-C3
7	G	6630	LHG	C4-O6-P-O5
7	G	6630	LHG	O10-C23-O8-C6
9	J	606	CHL	C1A-C2A-CAA-CBA
10	D	602	CLA	C2-C3-C5-C6
10	D	602	CLA	C4-C3-C5-C6
10	B	612	CLA	C14-C13-C15-C16
9	J	601	CHL	CHA-CBD-CGD-O1D
7	D	3630	LHG	O1-C1-C2-C3
7	D	3630	LHG	C4-O6-P-O3
10	A	602	CLA	CBD-CGD-O2D-CED
10	A	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	A	609	CHL	CBD-CGD-O2D-CED
10	H	612	CLA	CBD-CGD-O2D-CED
10	H	602	CLA	CBD-CGD-O2D-CED
9	I	605	CHL	CBD-CGD-O2D-CED
10	F	612	CLA	CBD-CGD-O2D-CED
10	E	612	CLA	CBD-CGD-O2D-CED
9	G	608	CHL	CBD-CGD-O2D-CED
9	A	607	CHL	O1A-CGA-O2A-C1
9	G	607	CHL	O1A-CGA-O2A-C1
9	C	606	CHL	O1A-CGA-O2A-C1
9	E	606	CHL	O1A-CGA-O2A-C1
9	C	607	CHL	O1A-CGA-O2A-C1
9	A	606	CHL	O1A-CGA-O2A-C1
7	A	630	LHG	O10-C23-O8-C6
7	I	8630	LHG	O10-C23-O8-C6
10	I	612	CLA	O1D-CGD-O2D-CED
10	J	612	CLA	O1D-CGD-O2D-CED
10	H	612	CLA	O1D-CGD-O2D-CED
10	D	612	CLA	O1D-CGD-O2D-CED
7	J	9630	LHG	C24-C23-O8-C6
9	G	607	CHL	CBA-CGA-O2A-C1
9	C	606	CHL	CBA-CGA-O2A-C1
9	E	606	CHL	CBA-CGA-O2A-C1
9	A	606	CHL	CBA-CGA-O2A-C1
7	A	630	LHG	C24-C23-O8-C6
7	I	8630	LHG	C24-C23-O8-C6
10	G	613	CLA	CBD-CGD-O2D-CED
10	G	602	CLA	CBD-CGD-O2D-CED
10	I	614	CLA	CBD-CGD-O2D-CED
9	C	609	CHL	CBD-CGD-O2D-CED
10	J	602	CLA	CBD-CGD-O2D-CED
9	F	605	CHL	CBD-CGD-O2D-CED
9	E	609	CHL	CBD-CGD-O2D-CED
9	F	601	CHL	CBD-CGD-O2D-CED
9	J	609	CHL	CBD-CGD-O2D-CED
9	B	606	CHL	CBD-CGD-O2D-CED
10	D	602	CLA	CBD-CGD-O2D-CED
9	H	607	CHL	O1A-CGA-O2A-C1
7	E	4630	LHG	O10-C23-O8-C6
7	F	5630	LHG	O10-C23-O8-C6
7	H	7630	LHG	O10-C23-O8-C6
9	H	606	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	D	5632	DGD	O1A-C1A-O1G-C1G
8	A	632	DGD	O1A-C1A-O1G-C1G
7	J	9630	LHG	O10-C23-O8-C6
7	C	2630	LHG	O10-C23-O8-C6
9	F	607	CHL	O1A-CGA-O2A-C1
9	F	606	CHL	O1A-CGA-O2A-C1
7	B	1630	LHG	O10-C23-O8-C6
9	E	607	CHL	O1A-CGA-O2A-C1
9	H	605	CHL	O1A-CGA-O2A-C1
8	B	2632	DGD	O1A-C1A-O1G-C1G
9	J	607	CHL	O1A-CGA-O2A-C1
9	I	605	CHL	O1A-CGA-O2A-C1
9	I	607	CHL	O1A-CGA-O2A-C1
9	D	607	CHL	O1A-CGA-O2A-C1
9	B	607	CHL	O1A-CGA-O2A-C1
7	D	3630	LHG	O10-C23-O8-C6
10	G	612	CLA	O1D-CGD-O2D-CED
9	F	609	CHL	CBD-CGD-O2D-CED
10	B	611	CLA	C3-C5-C6-C7
9	G	601	CHL	C3-C5-C6-C7
9	H	607	CHL	C3-C5-C6-C7
10	D	611	CLA	C3-C5-C6-C7
10	H	611	CLA	C3-C5-C6-C7
10	C	611	CLA	C3-C5-C6-C7
9	I	601	CHL	C3-C5-C6-C7
10	F	603	CLA	C3-C5-C6-C7
9	E	601	CHL	C3-C5-C6-C7
10	E	603	CLA	C3-C5-C6-C7
9	G	607	CHL	C3-C5-C6-C7
9	F	607	CHL	C3-C5-C6-C7
10	J	611	CLA	C3-C5-C6-C7
9	I	609	CHL	C3-C5-C6-C7
10	H	612	CLA	C3-C5-C6-C7
10	D	603	CLA	C3-C5-C6-C7
10	I	611	CLA	C3-C5-C6-C7
10	G	603	CLA	C3-C5-C6-C7
9	H	609	CHL	C3-C5-C6-C7
9	J	609	CHL	C3-C5-C6-C7
9	J	607	CHL	C3-C5-C6-C7
9	I	607	CHL	C3-C5-C6-C7
10	H	603	CLA	C3-C5-C6-C7
10	G	611	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
10	A	603	CLA	C3-C5-C6-C7
9	H	607	CHL	CBA-CGA-O2A-C1
7	E	4630	LHG	C24-C23-O8-C6
7	F	5630	LHG	C24-C23-O8-C6
7	H	7630	LHG	C24-C23-O8-C6
9	A	607	CHL	CBA-CGA-O2A-C1
10	G	614	CLA	CBA-CGA-O2A-C1
7	C	2630	LHG	C24-C23-O8-C6
9	F	606	CHL	CBA-CGA-O2A-C1
7	B	1630	LHG	C24-C23-O8-C6
9	C	607	CHL	CBA-CGA-O2A-C1
10	C	614	CLA	CBA-CGA-O2A-C1
9	I	606	CHL	CBA-CGA-O2A-C1
7	G	6630	LHG	C24-C23-O8-C6
9	I	607	CHL	CBA-CGA-O2A-C1
9	D	607	CHL	CBA-CGA-O2A-C1
7	D	3630	LHG	C24-C23-O8-C6
9	F	606	CHL	CBD-CGD-O2D-CED
10	A	602	CLA	C2-C3-C5-C6
10	E	602	CLA	C2-C3-C5-C6
10	C	602	CLA	C2-C3-C5-C6
9	G	601	CHL	C2A-CAA-CBA-CGA
9	H	601	CHL	C2A-CAA-CBA-CGA
9	B	608	CHL	C2A-CAA-CBA-CGA
10	B	603	CLA	C2A-CAA-CBA-CGA
9	I	608	CHL	C2A-CAA-CBA-CGA
10	H	611	CLA	C2A-CAA-CBA-CGA
9	I	601	CHL	C2A-CAA-CBA-CGA
10	F	603	CLA	C2A-CAA-CBA-CGA
9	E	601	CHL	C2A-CAA-CBA-CGA
9	A	608	CHL	C2A-CAA-CBA-CGA
10	E	603	CLA	C2A-CAA-CBA-CGA
10	I	603	CLA	C2A-CAA-CBA-CGA
10	J	611	CLA	C2A-CAA-CBA-CGA
10	D	603	CLA	C2A-CAA-CBA-CGA
10	G	603	CLA	C2A-CAA-CBA-CGA
9	A	601	CHL	C2A-CAA-CBA-CGA
9	B	601	CHL	C2A-CAA-CBA-CGA
10	C	603	CLA	C2A-CAA-CBA-CGA
9	F	601	CHL	C2A-CAA-CBA-CGA
10	J	603	CLA	C2A-CAA-CBA-CGA
9	J	606	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	J	608	CHL	C2A-CAA-CBA-CGA
9	H	608	CHL	C2A-CAA-CBA-CGA
10	H	603	CLA	C2A-CAA-CBA-CGA
9	C	608	CHL	C2A-CAA-CBA-CGA
9	E	608	CHL	C2A-CAA-CBA-CGA
9	G	608	CHL	C2A-CAA-CBA-CGA
10	A	603	CLA	C2A-CAA-CBA-CGA
10	F	612	CLA	O1D-CGD-O2D-CED
10	F	611	CLA	C3-C5-C6-C7
10	B	603	CLA	C3-C5-C6-C7
9	A	607	CHL	C3-C5-C6-C7
10	A	611	CLA	C3-C5-C6-C7
9	D	601	CHL	C3-C5-C6-C7
10	E	611	CLA	C3-C5-C6-C7
9	C	605	CHL	CBA-CGA-O2A-C1
10	J	612	CLA	CBA-CGA-O2A-C1
9	H	606	CHL	CBA-CGA-O2A-C1
10	H	614	CLA	CBA-CGA-O2A-C1
8	D	5632	DGD	C2A-C1A-O1G-C1G
8	A	632	DGD	C2A-C1A-O1G-C1G
9	F	605	CHL	CBA-CGA-O2A-C1
9	F	607	CHL	CBA-CGA-O2A-C1
10	G	612	CLA	CBA-CGA-O2A-C1
9	E	607	CHL	CBA-CGA-O2A-C1
9	H	605	CHL	CBA-CGA-O2A-C1
9	E	605	CHL	CBA-CGA-O2A-C1
8	B	2632	DGD	C2A-C1A-O1G-C1G
9	G	605	CHL	CBA-CGA-O2A-C1
9	B	605	CHL	CBA-CGA-O2A-C1
9	J	607	CHL	CBA-CGA-O2A-C1
9	I	605	CHL	CBA-CGA-O2A-C1
10	E	614	CLA	CBA-CGA-O2A-C1
9	B	607	CHL	CBA-CGA-O2A-C1
2	H	7633	BNG	O5-C5-C6-O6
10	C	604	CLA	CBD-CGD-O2D-CED
10	A	612	CLA	O1D-CGD-O2D-CED
9	A	609	CHL	O1D-CGD-O2D-CED
9	E	609	CHL	O1D-CGD-O2D-CED
10	E	612	CLA	O1D-CGD-O2D-CED
9	G	608	CHL	O1D-CGD-O2D-CED
9	C	605	CHL	O1A-CGA-O2A-C1
10	H	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	E	4632	DGD	O1A-C1A-O1G-C1G
10	G	614	CLA	O1A-CGA-O2A-C1
9	A	605	CHL	O1A-CGA-O2A-C1
9	E	605	CHL	O1A-CGA-O2A-C1
10	C	614	CLA	O1A-CGA-O2A-C1
9	G	605	CHL	O1A-CGA-O2A-C1
9	B	605	CHL	O1A-CGA-O2A-C1
9	D	605	CHL	O1A-CGA-O2A-C1
9	J	605	CHL	O1A-CGA-O2A-C1
9	C	601	CHL	CBD-CGD-O2D-CED
9	C	606	CHL	CBD-CGD-O2D-CED
10	E	614	CLA	CBD-CGD-O2D-CED
9	B	609	CHL	CBD-CGD-O2D-CED
7	A	630	LHG	O2-C2-C3-O3
9	H	601	CHL	C3-C5-C6-C7
10	I	603	CLA	C3-C5-C6-C7
10	C	603	CLA	C3-C5-C6-C7
9	D	607	CHL	C3-C5-C6-C7
10	B	611	CLA	CBA-CGA-O2A-C1
8	E	4632	DGD	C2A-C1A-O1G-C1G
10	I	614	CLA	CBA-CGA-O2A-C1
8	G	9632	DGD	C2A-C1A-O1G-C1G
9	A	605	CHL	CBA-CGA-O2A-C1
10	E	611	CLA	CBA-CGA-O2A-C1
9	J	605	CHL	CBA-CGA-O2A-C1
8	H	6632	DGD	C2A-C1A-O1G-C1G
10	J	612	CLA	O1A-CGA-O2A-C1
9	F	605	CHL	O1A-CGA-O2A-C1
10	E	614	CLA	O1A-CGA-O2A-C1
10	B	603	CLA	CBD-CGD-O2D-CED
10	E	602	CLA	CBD-CGD-O2D-CED
2	A	633	BNG	O5-C5-C6-O6
2	H	7633	BNG	C4-C5-C6-O6
9	A	608	CHL	CBD-CGD-O2D-CED
10	H	613	CLA	CBD-CGD-O2D-CED
10	I	604	CLA	C3-C5-C6-C7
9	E	607	CHL	C3-C5-C6-C7
10	I	612	CLA	CBA-CGA-O2A-C1
9	D	605	CHL	CBA-CGA-O2A-C1
9	I	605	CHL	O1D-CGD-O2D-CED
2	C	2633	BNG	O5-C5-C6-O6
8	G	9632	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
10	G	612	CLA	O1A-CGA-O2A-C1
10	E	611	CLA	O1A-CGA-O2A-C1
8	H	6632	DGD	O1A-C1A-O1G-C1G
10	F	602	CLA	C4-C3-C5-C6
10	B	602	CLA	C4-C3-C5-C6
10	J	602	CLA	C4-C3-C5-C6
10	F	602	CLA	C2-C3-C5-C6
10	B	602	CLA	C2-C3-C5-C6
10	J	602	CLA	C2-C3-C5-C6
9	D	609	CHL	CBD-CGD-O2D-CED
10	A	602	CLA	O1D-CGD-O2D-CED
9	J	609	CHL	O1D-CGD-O2D-CED
2	J	9633	BNG	O5-C5-C6-O6
10	B	611	CLA	O1A-CGA-O2A-C1
10	I	614	CLA	O1A-CGA-O2A-C1
10	H	612	CLA	O1A-CGA-O2A-C1
9	B	606	CHL	O1A-CGA-O2A-C1
8	A	632	DGD	O6D-C1D-O3G-C3G
8	G	9632	DGD	O6D-C1D-O3G-C3G
8	B	2632	DGD	O6D-C1D-O3G-C3G
8	D	3632	DGD	O6D-C1D-O3G-C3G
10	H	612	CLA	CBA-CGA-O2A-C1
9	B	606	CHL	CBA-CGA-O2A-C1
10	B	612	CLA	CBA-CGA-O2A-C1
9	C	609	CHL	O1D-CGD-O2D-CED
10	I	612	CLA	O1A-CGA-O2A-C1
10	B	612	CLA	O1A-CGA-O2A-C1
10	G	613	CLA	O1D-CGD-O2D-CED
10	J	602	CLA	O1D-CGD-O2D-CED
9	F	605	CHL	O1D-CGD-O2D-CED
9	F	601	CHL	O1D-CGD-O2D-CED
7	A	630	LHG	C1-C2-C3-O3
10	A	612	CLA	O1A-CGA-O2A-C1
10	A	614	CLA	O1A-CGA-O2A-C1
9	D	609	CHL	C3-C5-C6-C7
10	A	612	CLA	C3-C5-C6-C7
9	J	601	CHL	C3-C5-C6-C7
9	F	609	CHL	O1D-CGD-O2D-CED
10	F	611	CLA	CBA-CGA-O2A-C1
8	I	8632	DGD	C2A-C1A-O1G-C1G
10	D	611	CLA	CBA-CGA-O2A-C1
10	H	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	C	611	CLA	CBA-CGA-O2A-C1
10	C	612	CLA	CBA-CGA-O2A-C1
10	A	612	CLA	CBA-CGA-O2A-C1
10	J	611	CLA	CBA-CGA-O2A-C1
10	A	611	CLA	CBA-CGA-O2A-C1
10	D	612	CLA	CBA-CGA-O2A-C1
8	H	7632	DGD	C2A-C1A-O1G-C1G
8	B	1632	DGD	C2A-C1A-O1G-C1G
10	E	612	CLA	CBA-CGA-O2A-C1
10	A	614	CLA	CBA-CGA-O2A-C1
10	D	614	CLA	CBA-CGA-O2A-C1
10	G	611	CLA	CBA-CGA-O2A-C1
8	D	3632	DGD	C2A-C1A-O1G-C1G
2	J	9633	BNG	C4-C5-C6-O6
10	F	603	CLA	C5-C6-C7-C8
9	A	607	CHL	C10-C11-C12-C13
10	E	611	CLA	C13-C15-C16-C17
9	I	607	CHL	C5-C6-C7-C8
9	D	607	CHL	C10-C11-C12-C13
2	D	3633	BNG	O5-C5-C6-O6
9	B	608	CHL	C8-C10-C11-C12
10	C	612	CLA	C8-C10-C11-C12
10	E	603	CLA	C5-C6-C7-C8
10	D	613	CLA	C13-C15-C16-C17
10	G	612	CLA	C8-C10-C11-C12
10	H	612	CLA	C8-C10-C11-C12
10	I	611	CLA	C10-C11-C12-C13
9	J	608	CHL	C13-C15-C16-C17
10	G	611	CLA	C5-C6-C7-C8
9	E	608	CHL	C8-C10-C11-C12
9	B	607	CHL	C10-C11-C12-C13
7	B	1630	LHG	O2-C2-C3-O3
8	G	9632	DGD	C1B-C2B-C3B-C4B
8	I	8632	DGD	C2D-C1D-O3G-C3G
8	D	5632	DGD	C2D-C1D-O3G-C3G
8	A	632	DGD	C2D-C1D-O3G-C3G
8	E	4632	DGD	C2D-C1D-O3G-C3G
2	A	633	BNG	C2-C1-O1-C1'
2	B	1633	BNG	C2-C1-O1-C1'
8	G	9632	DGD	C2D-C1D-O3G-C3G
2	G	6633	BNG	C2-C1-O1-C1'
2	I	8633	BNG	C2-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
2	C	2633	BNG	C2-C1-O1-C1'
2	F	5633	BNG	C2-C1-O1-C1'
8	H	7632	DGD	C2D-C1D-O3G-C3G
8	B	2632	DGD	C2D-C1D-O3G-C3G
2	E	4633	BNG	C2-C1-O1-C1'
8	B	1632	DGD	C2D-C1D-O3G-C3G
2	D	3633	BNG	C2-C1-O1-C1'
2	H	7633	BNG	C2-C1-O1-C1'
8	H	6632	DGD	C2D-C1D-O3G-C3G
8	D	3632	DGD	C2D-C1D-O3G-C3G
10	F	612	CLA	CBA-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
10	D	612	CLA	O1A-CGA-O2A-C1
2	B	1633	BNG	O5-C5-C6-O6
9	G	601	CHL	C11-C10-C8-C9
10	A	610	CLA	C14-C13-C15-C16
10	F	610	CLA	C14-C13-C15-C16
9	D	608	CHL	C14-C13-C15-C16
9	F	609	CHL	C14-C13-C15-C16
9	I	608	CHL	C14-C13-C15-C16
10	C	610	CLA	C14-C13-C15-C16
10	J	612	CLA	C14-C13-C15-C16
10	A	612	CLA	C14-C13-C15-C16
9	A	608	CHL	C14-C13-C15-C16
9	G	609	CHL	C14-C13-C15-C16
10	D	610	CLA	C14-C13-C15-C16
9	G	607	CHL	C11-C10-C8-C9
9	F	607	CHL	C11-C10-C8-C9
9	I	609	CHL	C14-C13-C15-C16
9	F	608	CHL	C14-C13-C15-C16
10	I	611	CLA	C11-C10-C8-C9
10	B	610	CLA	C14-C13-C15-C16
10	D	612	CLA	C14-C13-C15-C16
9	E	609	CHL	C14-C13-C15-C16
9	B	601	CHL	C11-C12-C13-C14
9	H	609	CHL	C14-C13-C15-C16
9	D	601	CHL	C11-C10-C8-C9
9	F	601	CHL	C11-C10-C8-C9
9	F	601	CHL	C11-C12-C13-C14
9	J	609	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
10	I	612	CLA	C14-C13-C15-C16
10	F	612	CLA	C14-C13-C15-C16
10	E	612	CLA	C14-C13-C15-C16
9	J	608	CHL	C14-C13-C15-C16
9	H	608	CHL	C14-C13-C15-C16
9	C	608	CHL	C14-C13-C15-C16
10	E	613	CLA	C11-C10-C8-C9
9	J	601	CHL	C11-C12-C13-C14
9	G	608	CHL	C14-C13-C15-C16
10	I	614	CLA	O1D-CGD-O2D-CED
9	F	608	CHL	C2A-CAA-CBA-CGA
10	G	611	CLA	C2A-CAA-CBA-CGA
8	I	8632	DGD	C1B-C2B-C3B-C4B
8	B	2632	DGD	C1B-C2B-C3B-C4B
8	I	8632	DGD	O1A-C1A-O1G-C1G
10	A	611	CLA	O1A-CGA-O2A-C1
8	D	3632	DGD	O1A-C1A-O1G-C1G
10	D	611	CLA	C5-C6-C7-C8
10	J	612	CLA	C8-C10-C11-C12
9	C	601	CHL	C10-C11-C12-C13
10	A	611	CLA	C5-C6-C7-C8
9	H	608	CHL	C15-C16-C17-C18
10	J	613	CLA	CBD-CGD-O2D-CED
9	D	601	CHL	CBD-CGD-O2D-CED
9	H	608	CHL	CBD-CGD-O2D-CED
2	C	2633	BNG	C4-C5-C6-O6
10	I	604	CLA	C13-C15-C16-C17
10	D	604	CLA	C13-C15-C16-C17
10	A	604	CLA	C13-C15-C16-C17
10	H	604	CLA	C13-C15-C16-C17
10	F	604	CLA	C13-C15-C16-C17
10	B	614	CLA	CBA-CGA-O2A-C1
10	J	614	CLA	CBA-CGA-O2A-C1
10	B	611	CLA	C5-C6-C7-C8
9	H	607	CHL	C15-C16-C17-C18
10	H	611	CLA	C5-C6-C7-C8
10	H	611	CLA	C13-C15-C16-C17
9	A	607	CHL	C5-C6-C7-C8
10	A	612	CLA	C8-C10-C11-C12
10	H	610	CLA	C13-C15-C16-C17
10	I	613	CLA	C13-C15-C16-C17
10	I	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
9	J	607	CHL	C5-C6-C7-C8
9	J	607	CHL	C10-C11-C12-C13
9	I	607	CHL	C10-C11-C12-C13
10	F	612	CLA	C8-C10-C11-C12
2	F	5633	BNG	O5-C5-C6-O6
2	E	4633	BNG	O5-C5-C6-O6
8	E	4632	DGD	C1A-C2A-C3A-C4A
8	E	4632	DGD	C1B-C2B-C3B-C4B
8	G	9632	DGD	C1A-C2A-C3A-C4A
8	B	1632	DGD	C1A-C2A-C3A-C4A
2	G	6633	BNG	O5-C5-C6-O6
9	H	607	CHL	C10-C11-C12-C13
10	G	613	CLA	C13-C15-C16-C17
9	H	601	CHL	C13-C15-C16-C17
9	B	608	CHL	C15-C16-C17-C18
9	I	608	CHL	C13-C15-C16-C17
9	I	608	CHL	C15-C16-C17-C18
10	C	611	CLA	C13-C15-C16-C17
9	I	601	CHL	C13-C15-C16-C17
10	F	603	CLA	C15-C16-C17-C18
9	A	607	CHL	C15-C16-C17-C18
9	F	607	CHL	C15-C16-C17-C18
10	J	611	CLA	C13-C15-C16-C17
10	A	611	CLA	C13-C15-C16-C17
10	J	613	CLA	C13-C15-C16-C17
9	F	608	CHL	C5-C6-C7-C8
10	I	611	CLA	C13-C15-C16-C17
9	E	607	CHL	C10-C11-C12-C13
9	E	607	CHL	C15-C16-C17-C18
10	G	603	CLA	C8-C10-C11-C12
9	C	607	CHL	C5-C6-C7-C8
10	E	612	CLA	C8-C10-C11-C12
9	H	608	CHL	C13-C15-C16-C17
10	H	603	CLA	C5-C6-C7-C8
10	H	613	CLA	C13-C15-C16-C17
9	J	601	CHL	C10-C11-C12-C13
9	G	608	CHL	C15-C16-C17-C18
9	B	606	CHL	O1D-CGD-O2D-CED
7	F	5630	LHG	O1-C1-C2-O2
10	C	612	CLA	O1A-CGA-O2A-C1
10	E	612	CLA	O1A-CGA-O2A-C1
8	I	8632	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
8	A	632	DGD	C1A-C2A-C3A-C4A
8	A	632	DGD	C1B-C2B-C3B-C4B
8	H	7632	DGD	C1B-C2B-C3B-C4B
8	B	2632	DGD	C1A-C2A-C3A-C4A
7	I	8630	LHG	C23-C24-C25-C26
8	H	6632	DGD	C1A-C2A-C3A-C4A
8	H	6632	DGD	C1B-C2B-C3B-C4B
8	D	3632	DGD	C1B-C2B-C3B-C4B
10	F	611	CLA	C5-C6-C7-C8
10	C	611	CLA	C5-C6-C7-C8
9	E	601	CHL	C13-C15-C16-C17
10	E	603	CLA	C15-C16-C17-C18
9	G	607	CHL	C15-C16-C17-C18
10	A	611	CLA	C10-C11-C12-C13
9	E	607	CHL	C5-C6-C7-C8
9	A	601	CHL	C10-C11-C12-C13
9	G	608	CHL	C13-C15-C16-C17
9	H	607	CHL	C5-C6-C7-C8
9	C	601	CHL	C13-C15-C16-C17
9	F	607	CHL	C5-C6-C7-C8
10	I	603	CLA	C10-C11-C12-C13
10	J	611	CLA	C10-C11-C12-C13
9	F	608	CHL	C13-C15-C16-C17
10	A	613	CLA	C13-C15-C16-C17
8	H	7632	DGD	C1A-C2A-C3A-C4A
10	J	614	CLA	CBD-CGD-O2D-CED
10	E	604	CLA	C13-C15-C16-C17
9	G	601	CHL	C13-C15-C16-C17
10	G	603	CLA	C5-C6-C7-C8
10	C	603	CLA	C5-C6-C7-C8
9	A	608	CHL	O1D-CGD-O2D-CED
10	A	602	CLA	C11-C10-C8-C7
9	H	601	CHL	C12-C13-C15-C16
9	I	601	CHL	C11-C12-C13-C15
10	B	602	CLA	C11-C10-C8-C7
10	C	604	CLA	C6-C7-C8-C10
10	G	604	CLA	C6-C7-C8-C10
10	H	604	CLA	C6-C7-C8-C10
10	F	604	CLA	C6-C7-C8-C10
9	B	607	CHL	C12-C13-C15-C16
10	J	604	CLA	C3-C5-C6-C7
10	G	612	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	F	608	CHL	C3-C5-C6-C7
9	H	608	CHL	C3-C5-C6-C7
9	B	607	CHL	C3-C5-C6-C7
10	C	611	CLA	O1A-CGA-O2A-C1
10	B	614	CLA	O1A-CGA-O2A-C1
8	H	7632	DGD	O1A-C1A-O1G-C1G
10	G	611	CLA	O1A-CGA-O2A-C1
9	H	606	CHL	C2A-CAA-CBA-CGA
10	J	604	CLA	C2A-CAA-CBA-CGA
10	E	611	CLA	C2A-CAA-CBA-CGA
9	B	609	CHL	O1D-CGD-O2D-CED
10	F	611	CLA	C10-C11-C12-C13
9	A	608	CHL	C13-C15-C16-C17
10	I	611	CLA	C5-C6-C7-C8
9	A	601	CHL	C15-C16-C17-C18
10	E	611	CLA	C5-C6-C7-C8
9	I	607	CHL	C15-C16-C17-C18
9	C	608	CHL	C8-C10-C11-C12
8	B	2632	DGD	O6E-C5E-C6E-O5E
10	J	614	CLA	O1A-CGA-O2A-C1
8	B	1632	DGD	O1A-C1A-O1G-C1G
10	F	612	CLA	O1A-CGA-O2A-C1
8	I	8632	DGD	O6D-C1D-O3G-C3G
8	D	5632	DGD	O6D-C1D-O3G-C3G
8	E	4632	DGD	O6D-C1D-O3G-C3G
2	I	8633	BNG	O5-C1-O1-C1'
2	F	5633	BNG	O5-C1-O1-C1'
8	B	1632	DGD	O6D-C1D-O3G-C3G
9	G	607	CHL	C10-C11-C12-C13
8	D	5632	DGD	C1A-C2A-C3A-C4A
8	D	5632	DGD	C1B-C2B-C3B-C4B
9	F	609	CHL	C3-C5-C6-C7
10	J	604	CLA	C13-C15-C16-C17
10	B	604	CLA	C13-C15-C16-C17
10	B	611	CLA	C13-C15-C16-C17
9	A	608	CHL	C8-C10-C11-C12
9	F	608	CHL	C15-C16-C17-C18
10	E	611	CLA	C10-C11-C12-C13
10	B	612	CLA	C8-C10-C11-C12
9	C	608	CHL	C15-C16-C17-C18
9	E	608	CHL	C15-C16-C17-C18
9	G	608	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
9	B	607	CHL	C5-C6-C7-C8
10	D	611	CLA	O1A-CGA-O2A-C1
10	D	614	CLA	O1A-CGA-O2A-C1
7	E	4630	LHG	C23-C24-C25-C26
7	J	9630	LHG	C23-C24-C25-C26
7	A	630	LHG	C23-C24-C25-C26
10	A	603	CLA	O1D-CGD-O2D-CED
9	B	608	CHL	C13-C15-C16-C17
9	D	608	CHL	C13-C15-C16-C17
9	D	608	CHL	C15-C16-C17-C18
9	I	608	CHL	C8-C10-C11-C12
10	A	612	CLA	C10-C11-C12-C13
10	E	603	CLA	C10-C11-C12-C13
10	I	610	CLA	C13-C15-C16-C17
9	C	607	CHL	C10-C11-C12-C13
9	C	607	CHL	C15-C16-C17-C18
9	B	601	CHL	C10-C11-C12-C13
9	J	608	CHL	C15-C16-C17-C18
10	E	613	CLA	C13-C15-C16-C17
9	E	608	CHL	C13-C15-C16-C17
10	A	603	CLA	C13-C15-C16-C17
9	D	609	CHL	O1D-CGD-O2D-CED
10	B	612	CLA	CBD-CGD-O2D-CED
10	F	611	CLA	C13-C15-C16-C17
9	F	607	CHL	C10-C11-C12-C13
10	C	603	CLA	C10-C11-C12-C13
10	G	611	CLA	C13-C15-C16-C17
9	D	607	CHL	C15-C16-C17-C18
7	E	4630	LHG	C4-O6-P-O3
7	H	7630	LHG	C4-O6-P-O3
7	A	630	LHG	C4-O6-P-O3
7	I	8630	LHG	C4-O6-P-O3
9	C	607	CHL	C3-C5-C6-C7
10	I	611	CLA	CBA-CGA-O2A-C1
10	F	614	CLA	CBA-CGA-O2A-C1
10	B	603	CLA	O1D-CGD-O2D-CED
10	D	611	CLA	C13-C15-C16-C17
9	F	608	CHL	C8-C10-C11-C12
10	D	603	CLA	C10-C11-C12-C13
10	F	603	CLA	C10-C11-C12-C13
10	I	603	CLA	C8-C10-C11-C12
10	B	611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	D	608	CHL	C16-C17-C18-C19
10	B	603	CLA	C16-C17-C18-C19
9	D	607	CHL	C16-C17-C18-C19
9	E	609	CHL	C3-C5-C6-C7
10	C	613	CLA	C3-C5-C6-C7
9	H	608	CHL	O1D-CGD-O2D-CED
10	G	603	CLA	C15-C16-C17-C18
9	H	608	CHL	C8-C10-C11-C12
10	J	614	CLA	O1D-CGD-O2D-CED
7	J	9630	LHG	C15-C16-C17-C18
7	A	630	LHG	C15-C16-C17-C18
8	H	6632	DGD	C5A-C6A-C7A-C8A
8	I	8632	DGD	CEA-CFA-CGA-CHA
8	I	8632	DGD	CDB-CEB-CFB-CGB
7	F	5630	LHG	C9-C10-C11-C12
8	D	5632	DGD	C7A-C8A-C9A-CAA
8	D	5632	DGD	C6B-C7B-C8B-C9B
8	E	4632	DGD	C7A-C8A-C9A-CAA
8	G	9632	DGD	CCB-CDB-CEB-CFB
7	J	9630	LHG	C34-C35-C36-C37
2	I	8633	BNG	C3'-C4'-C5'-C6'
2	C	2633	BNG	C3'-C4'-C5'-C6'
8	B	2632	DGD	C7A-C8A-C9A-CAA
8	B	1632	DGD	C5A-C6A-C7A-C8A
2	D	3633	BNG	C5'-C6'-C7'-C8'
7	I	8630	LHG	C15-C16-C17-C18
2	H	7633	BNG	C5'-C6'-C7'-C8'
10	C	604	CLA	O1D-CGD-O2D-CED
10	B	603	CLA	C16-C17-C18-C20
9	C	607	CHL	C16-C17-C18-C19
10	H	603	CLA	C16-C17-C18-C20
2	J	9633	BNG	C3'-C4'-C5'-C6'
8	I	8632	DGD	CAA-CBA-CCA-CDA
8	I	8632	DGD	CCB-CDB-CEB-CFB
7	F	5630	LHG	C14-C15-C16-C17
7	H	7630	LHG	C9-C10-C11-C12
2	B	1633	BNG	C3'-C4'-C5'-C6'
8	G	9632	DGD	C7A-C8A-C9A-CAA
8	G	9632	DGD	CDB-CEB-CFB-CGB
8	H	7632	DGD	CDB-CEB-CFB-CGB
7	I	8630	LHG	C34-C35-C36-C37
8	D	3632	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
9	F	606	CHL	O1D-CGD-O2D-CED
9	D	608	CHL	C8-C10-C11-C12
10	J	602	CLA	C5-C6-C7-C8
10	A	603	CLA	CBD-CGD-O2D-CED
7	E	4630	LHG	C29-C30-C31-C32
7	H	7630	LHG	C30-C31-C32-C33
8	D	5632	DGD	C5A-C6A-C7A-C8A
8	E	4632	DGD	C6B-C7B-C8B-C9B
7	J	9630	LHG	C25-C26-C27-C28
7	B	1630	LHG	C14-C15-C16-C17
7	B	1630	LHG	C15-C16-C17-C18
8	H	7632	DGD	C5A-C6A-C7A-C8A
2	E	4633	BNG	C3'-C4'-C5'-C6'
10	H	602	CLA	O1D-CGD-O2D-CED
2	I	8633	BNG	C5'-C6'-C7'-C8'
2	C	2633	BNG	C5'-C6'-C7'-C8'
2	F	5633	BNG	C3'-C4'-C5'-C6'
8	H	7632	DGD	C7A-C8A-C9A-CAA
8	B	2632	DGD	CEA-CFA-CGA-CHA
8	H	6632	DGD	C7A-C8A-C9A-CAA
9	B	607	CHL	C15-C16-C17-C18
7	E	4630	LHG	O2-C2-C3-O3
7	H	7630	LHG	C14-C15-C16-C17
8	A	632	DGD	C7A-C8A-C9A-CAA
8	A	632	DGD	CDB-CEB-CFB-CGB
2	E	4633	BNG	C5'-C6'-C7'-C8'
8	B	1632	DGD	C7A-C8A-C9A-CAA
7	D	3630	LHG	C14-C15-C16-C17
9	B	601	CHL	C3-C5-C6-C7
7	B	1630	LHG	C23-C24-C25-C26
7	G	6630	LHG	C23-C24-C25-C26
10	D	602	CLA	O1D-CGD-O2D-CED
8	A	632	DGD	C2A-C3A-C4A-C5A
2	A	633	BNG	C3'-C4'-C5'-C6'
7	C	2630	LHG	C30-C31-C32-C33
2	G	6633	BNG	C3'-C4'-C5'-C6'
7	I	8630	LHG	C9-C10-C11-C12
8	H	6632	DGD	CAA-CBA-CCA-CDA
8	D	3632	DGD	C6B-C7B-C8B-C9B
7	D	3630	LHG	C30-C31-C32-C33
9	H	607	CHL	C16-C17-C18-C19
9	F	607	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
8	I	8632	DGD	C7A-C8A-C9A-CAA
7	E	4630	LHG	C14-C15-C16-C17
8	D	5632	DGD	C2A-C3A-C4A-C5A
2	A	633	BNG	C5'-C6'-C7'-C8'
8	G	9632	DGD	CEA-CFA-CGA-CHA
7	J	9630	LHG	C14-C15-C16-C17
7	J	9630	LHG	C32-C33-C34-C35
7	C	2630	LHG	C14-C15-C16-C17
8	B	2632	DGD	CDB-CEB-CFB-CGB
7	I	8630	LHG	C32-C33-C34-C35
8	H	6632	DGD	CDB-CEB-CFB-CGB
8	D	3632	DGD	C2A-C3A-C4A-C5A
7	D	3630	LHG	C15-C16-C17-C18
9	G	601	CHL	C6-C7-C8-C9
10	G	613	CLA	C11-C12-C13-C14
9	B	608	CHL	C14-C13-C15-C16
10	D	611	CLA	C14-C13-C15-C16
10	I	613	CLA	C11-C12-C13-C14
10	J	610	CLA	C14-C13-C15-C16
10	G	604	CLA	C6-C7-C8-C9
10	D	613	CLA	C11-C12-C13-C14
10	J	613	CLA	C11-C12-C13-C14
9	D	601	CHL	C6-C7-C8-C9
10	D	602	CLA	C14-C13-C15-C16
10	H	603	CLA	C11-C10-C8-C9
10	E	613	CLA	C14-C13-C15-C16
7	H	7630	LHG	C23-C24-C25-C26
7	C	2630	LHG	C23-C24-C25-C26
7	D	3630	LHG	C23-C24-C25-C26
2	J	9633	BNG	C5'-C6'-C7'-C8'
8	A	632	DGD	CCB-CDB-CEB-CFB
8	G	9632	DGD	C5A-C6A-C7A-C8A
7	J	9630	LHG	C28-C29-C30-C31
2	G	6633	BNG	C5'-C6'-C7'-C8'
7	A	630	LHG	C14-C15-C16-C17
7	G	6630	LHG	C14-C15-C16-C17
7	G	6630	LHG	C15-C16-C17-C18
8	H	6632	DGD	CCB-CDB-CEB-CFB
10	C	611	CLA	C15-C16-C17-C18
10	C	613	CLA	C13-C15-C16-C17
9	D	607	CHL	C5-C6-C7-C8
10	I	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	F	614	CLA	O1A-CGA-O2A-C1
8	D	3632	DGD	C7A-C8A-C9A-CAA
10	J	612	CLA	C3-C5-C6-C7
10	E	612	CLA	C3-C5-C6-C7
10	B	603	CLA	C5-C6-C7-C8
8	I	8632	DGD	C6B-C7B-C8B-C9B
7	E	4630	LHG	C15-C16-C17-C18
8	B	1632	DGD	C2A-C3A-C4A-C5A
7	G	6630	LHG	C28-C29-C30-C31
7	F	5630	LHG	C23-C24-C25-C26
8	I	8632	DGD	C5A-C6A-C7A-C8A
7	H	7630	LHG	C15-C16-C17-C18
8	D	5632	DGD	CAA-CBA-CCA-CDA
8	E	4632	DGD	CDB-CEB-CFB-CGB
2	B	1633	BNG	C5'-C6'-C7'-C8'
7	J	9630	LHG	C18-C19-C20-C21
2	F	5633	BNG	C5'-C6'-C7'-C8'
7	I	8630	LHG	C29-C30-C31-C32
7	G	6630	LHG	C9-C10-C11-C12
8	H	6632	DGD	C2A-C3A-C4A-C5A
7	D	3630	LHG	C28-C29-C30-C31
9	B	608	CHL	C16-C17-C18-C19
10	B	613	CLA	C16-C17-C18-C19
9	E	608	CHL	C16-C17-C18-C19
8	H	6632	DGD	O6D-C1D-O3G-C3G
10	D	603	CLA	C5-C6-C7-C8
9	J	609	CHL	C13-C15-C16-C17
8	E	4632	DGD	CAB-CBB-CCB-CDB
7	J	9630	LHG	C26-C27-C28-C29
7	C	2630	LHG	C34-C35-C36-C37
8	H	7632	DGD	CAA-CBA-CCA-CDA
2	H	7633	BNG	C3'-C4'-C5'-C6'
10	G	614	CLA	CBD-CGD-O2D-CED
10	G	602	CLA	O1D-CGD-O2D-CED
9	C	601	CHL	O1D-CGD-O2D-CED
10	E	614	CLA	O1D-CGD-O2D-CED
7	H	7630	LHG	C34-C35-C36-C37
8	D	5632	DGD	CAB-CBB-CCB-CDB
8	G	9632	DGD	CAA-CBA-CCA-CDA
8	B	1632	DGD	CCB-CDB-CEB-CFB
7	G	6630	LHG	C34-C35-C36-C37
8	B	1632	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
10	H	610	CLA	C10-C11-C12-C13
10	G	611	CLA	C10-C11-C12-C13
7	E	4630	LHG	C34-C35-C36-C37
7	C	2630	LHG	C28-C29-C30-C31
7	B	1630	LHG	C32-C33-C34-C35
8	H	7632	DGD	CAB-CBB-CCB-CDB
8	D	3632	DGD	CAA-CBA-CCA-CDA
7	H	7630	LHG	C11-C10-C9-C8
10	B	611	CLA	C3A-C2A-CAA-CBA
10	F	611	CLA	C3A-C2A-CAA-CBA
9	D	606	CHL	C3A-C2A-CAA-CBA
10	I	604	CLA	C3A-C2A-CAA-CBA
10	D	611	CLA	C3A-C2A-CAA-CBA
10	F	603	CLA	C3A-C2A-CAA-CBA
9	A	605	CHL	C3A-C2A-CAA-CBA
9	C	606	CHL	C3A-C2A-CAA-CBA
10	A	611	CLA	C3A-C2A-CAA-CBA
9	F	606	CHL	C3A-C2A-CAA-CBA
10	I	611	CLA	C3A-C2A-CAA-CBA
9	H	605	CHL	C3A-C2A-CAA-CBA
9	E	605	CHL	C3A-C2A-CAA-CBA
9	G	606	CHL	C3A-C2A-CAA-CBA
9	I	606	CHL	C3A-C2A-CAA-CBA
9	A	606	CHL	C3A-C2A-CAA-CBA
9	B	605	CHL	C3A-C2A-CAA-CBA
9	D	605	CHL	C3A-C2A-CAA-CBA
10	E	611	CLA	C3A-C2A-CAA-CBA
9	I	605	CHL	C3A-C2A-CAA-CBA
9	J	605	CHL	C3A-C2A-CAA-CBA
10	G	611	CLA	C3A-C2A-CAA-CBA
10	B	611	CLA	C10-C11-C12-C13
10	I	603	CLA	C5-C6-C7-C8
9	J	608	CHL	C8-C10-C11-C12
9	D	607	CHL	C13-C15-C16-C17
9	B	609	CHL	C13-C15-C16-C17
2	I	8633	BNG	O5-C5-C6-O6
8	D	5632	DGD	CDB-CEB-CFB-CGB
7	I	8630	LHG	C14-C15-C16-C17
7	G	6630	LHG	C11-C10-C9-C8
9	H	607	CHL	C16-C17-C18-C20
10	B	613	CLA	C16-C17-C18-C20
9	C	607	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
9	I	607	CHL	C16-C17-C18-C19
9	I	607	CHL	C16-C17-C18-C20
9	H	608	CHL	C16-C17-C18-C19
10	H	603	CLA	C16-C17-C18-C19
9	D	607	CHL	C16-C17-C18-C20
7	F	5630	LHG	C33-C34-C35-C36
8	E	4632	DGD	CAA-CBA-CCA-CDA
8	G	9632	DGD	C2A-C3A-C4A-C5A
2	D	3633	BNG	C3'-C4'-C5'-C6'
7	G	6630	LHG	C32-C33-C34-C35
8	H	6632	DGD	C6B-C7B-C8B-C9B
7	E	4630	LHG	C4-C5-C6-O8
2	D	3633	BNG	C1'-C2'-C3'-C4'
9	C	605	CHL	CBD-CGD-O2D-CED
7	F	5630	LHG	C29-C30-C31-C32
8	E	4632	DGD	C5A-C6A-C7A-C8A
8	B	2632	DGD	CCB-CDB-CEB-CFB
9	F	608	CHL	O2A-C1-C2-C3
8	D	3632	DGD	C1A-C2A-C3A-C4A
7	H	7630	LHG	C28-C29-C30-C31
7	B	1630	LHG	C13-C14-C15-C16
8	B	2632	DGD	C2A-C3A-C4A-C5A
8	B	1632	DGD	C6B-C7B-C8B-C9B
7	E	4630	LHG	O1-C1-C2-O2
7	H	7630	LHG	O1-C1-C2-O2
7	C	2630	LHG	O1-C1-C2-O2
7	B	1630	LHG	O1-C1-C2-O2
7	D	3630	LHG	O1-C1-C2-O2
7	E	4630	LHG	C28-C29-C30-C31
7	F	5630	LHG	C15-C16-C17-C18
7	A	630	LHG	C29-C30-C31-C32
8	B	2632	DGD	CAA-CBA-CCA-CDA
7	D	3630	LHG	C16-C17-C18-C19
10	C	612	CLA	C10-C11-C12-C13
10	E	613	CLA	C8-C10-C11-C12
7	B	1630	LHG	C9-C10-C11-C12
7	A	630	LHG	C11-C10-C9-C8
7	A	630	LHG	C34-C35-C36-C37
10	A	604	CLA	C3-C5-C6-C7
10	J	603	CLA	C3-C5-C6-C7
9	H	609	CHL	CBA-CGA-O2A-C1
8	B	1632	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
7	G	6630	LHG	C18-C19-C20-C21
7	D	3630	LHG	C9-C10-C11-C12
10	B	613	CLA	C15-C16-C17-C18
10	J	603	CLA	C5-C6-C7-C8
9	H	609	CHL	O1A-CGA-O2A-C1
2	A	633	BNG	C1'-C2'-C3'-C4'
2	A	633	BNG	C4-C5-C6-O6
7	F	5630	LHG	C13-C14-C15-C16
8	H	7632	DGD	CCB-CDB-CEB-CFB
9	B	608	CHL	C16-C17-C18-C20
9	A	609	CHL	C3-C5-C6-C7
10	I	612	CLA	C3-C5-C6-C7
7	J	9630	LHG	C9-C10-C11-C12
8	B	1632	DGD	CDB-CEB-CFB-CGB
8	D	3632	DGD	CAB-CBB-CCB-CDB
8	D	3632	DGD	CCB-CDB-CEB-CFB
9	A	609	CHL	CBA-CGA-O2A-C1
10	E	603	CLA	C13-C15-C16-C17
10	J	611	CLA	C5-C6-C7-C8
10	H	604	CLA	C5-C6-C7-C8
9	J	607	CHL	C15-C16-C17-C18
9	B	609	CHL	C15-C16-C17-C18
7	G	6630	LHG	C8-C7-O7-C5
8	A	632	DGD	CAA-CBA-CCA-CDA
8	E	4632	DGD	CEA-CFA-CGA-CHA
7	A	630	LHG	C32-C33-C34-C35
8	B	1632	DGD	CAB-CBB-CCB-CDB
9	C	606	CHL	O1D-CGD-O2D-CED
7	F	5630	LHG	C25-C26-C27-C28
8	A	632	DGD	C5A-C6A-C7A-C8A
8	E	4632	DGD	C2A-C3A-C4A-C5A
7	C	2630	LHG	C25-C26-C27-C28
8	B	2632	DGD	C5A-C6A-C7A-C8A
10	D	604	CLA	C5-C6-C7-C8
10	C	602	CLA	C5-C6-C7-C8
7	E	4630	LHG	C32-C33-C34-C35
7	I	8630	LHG	C11-C10-C9-C8
8	H	6632	DGD	CEA-CFA-CGA-CHA
8	H	6632	DGD	CEB-CFB-CGB-CHB
9	B	608	CHL	C4-C3-C5-C6
10	J	603	CLA	C4-C3-C5-C6
9	B	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
10	F	611	CLA	C6-C7-C8-C10
9	H	607	CHL	C12-C13-C15-C16
10	G	613	CLA	C11-C12-C13-C15
10	G	613	CLA	C12-C13-C15-C16
9	B	608	CHL	C2-C3-C5-C6
9	F	609	CHL	C11-C12-C13-C15
10	B	603	CLA	C11-C12-C13-C15
9	I	608	CHL	C6-C7-C8-C10
9	I	608	CHL	C12-C13-C15-C16
10	D	611	CLA	C6-C7-C8-C10
10	H	611	CLA	C6-C7-C8-C10
10	G	602	CLA	C11-C10-C8-C7
9	I	601	CHL	C6-C7-C8-C10
9	A	607	CHL	C12-C13-C15-C16
9	C	609	CHL	C12-C13-C15-C16
10	D	604	CLA	C11-C10-C8-C7
10	J	602	CLA	C11-C10-C8-C7
10	I	613	CLA	C11-C12-C13-C15
10	I	613	CLA	C12-C13-C15-C16
9	A	608	CHL	C6-C7-C8-C10
10	F	613	CLA	C11-C12-C13-C15
10	E	602	CLA	C11-C12-C13-C15
9	G	609	CHL	C11-C12-C13-C15
10	D	610	CLA	C11-C12-C13-C15
10	B	604	CLA	C11-C10-C8-C7
10	B	613	CLA	C12-C13-C15-C16
10	D	613	CLA	C12-C13-C15-C16
9	G	607	CHL	C12-C13-C15-C16
9	F	607	CHL	C12-C13-C15-C16
10	J	611	CLA	C6-C7-C8-C10
10	J	613	CLA	C11-C12-C13-C15
10	J	613	CLA	C12-C13-C15-C16
9	I	609	CHL	C11-C12-C13-C15
9	E	607	CHL	C12-C13-C15-C16
10	H	602	CLA	C11-C10-C8-C7
10	A	613	CLA	C12-C13-C15-C16
10	C	603	CLA	C11-C10-C8-C7
10	J	603	CLA	C2-C3-C5-C6
10	H	604	CLA	C11-C10-C8-C7
10	F	604	CLA	C11-C10-C8-C7
10	B	612	CLA	C11-C12-C13-C15
10	H	613	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
10	C	613	CLA	C12-C13-C15-C16
10	E	613	CLA	C12-C13-C15-C16
9	D	607	CHL	C11-C12-C13-C15
9	F	601	CHL	C3-C5-C6-C7
9	A	609	CHL	O1A-CGA-O2A-C1
9	G	609	CHL	O1A-CGA-O2A-C1
10	B	611	CLA	C8-C10-C11-C12
10	H	611	CLA	C10-C11-C12-C13
10	A	612	CLA	C15-C16-C17-C18
9	G	607	CHL	C5-C6-C7-C8
10	A	611	CLA	C8-C10-C11-C12
9	F	601	CHL	C13-C15-C16-C17
10	F	611	CLA	C16-C17-C18-C19
10	G	613	CLA	C16-C17-C18-C19
9	G	607	CHL	C16-C17-C18-C19
10	J	613	CLA	C16-C17-C18-C19
10	G	611	CLA	C16-C17-C18-C19
10	E	613	CLA	C16-C17-C18-C19
9	G	609	CHL	CBA-CGA-O2A-C1
10	B	611	CLA	C15-C16-C17-C18
10	I	602	CLA	C5-C6-C7-C8
10	C	603	CLA	C13-C15-C16-C17
7	J	9630	LHG	C11-C10-C9-C8
7	I	8630	LHG	C33-C34-C35-C36
7	D	3630	LHG	C11-C10-C9-C8
8	G	9632	DGD	C2B-C3B-C4B-C5B
8	H	6632	DGD	CAB-CBB-CCB-CDB
10	B	604	CLA	C5-C6-C7-C8
10	J	613	CLA	C15-C16-C17-C18
10	H	602	CLA	C5-C6-C7-C8
7	C	2630	LHG	C11-C10-C9-C8
7	C	2630	LHG	C15-C16-C17-C18
7	A	630	LHG	C9-C10-C11-C12
7	A	630	LHG	C28-C29-C30-C31
8	B	2632	DGD	C6B-C7B-C8B-C9B
2	E	4633	BNG	C1'-C2'-C3'-C4'
7	E	4630	LHG	C16-C17-C18-C19
9	D	606	CHL	CBD-CGD-O2D-CED
10	D	603	CLA	C15-C16-C17-C18
9	C	608	CHL	C13-C15-C16-C17
8	B	1632	DGD	CEA-CFA-CGA-CHA
7	A	630	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
10	B	612	CLA	O1D-CGD-O2D-CED
8	E	4632	DGD	CCB-CDB-CEB-CFB
8	B	2632	DGD	C2B-C3B-C4B-C5B
10	F	613	CLA	C13-C15-C16-C17
7	G	6630	LHG	C30-C31-C32-C33
7	C	2630	LHG	C13-C14-C15-C16
7	B	1630	LHG	C29-C30-C31-C32
8	H	7632	DGD	CEB-CFB-CGB-CHB
10	D	610	CLA	C13-C15-C16-C17
8	I	8632	DGD	O1G-C1G-C2G-O2G
8	H	7632	DGD	O1G-C1G-C2G-O2G
8	B	1632	DGD	O1G-C1G-C2G-O2G
7	E	4630	LHG	C25-C26-C27-C28
7	H	7630	LHG	C16-C17-C18-C19
2	A	633	BNG	C4'-C5'-C6'-C7'
10	F	612	CLA	C10-C11-C12-C13
2	H	7633	BNG	C1'-C2'-C3'-C4'
9	D	609	CHL	C14-C13-C15-C16
10	G	613	CLA	C14-C13-C15-C16
9	I	608	CHL	C6-C7-C8-C9
9	I	601	CHL	C6-C7-C8-C9
9	I	601	CHL	C14-C13-C15-C16
10	B	602	CLA	C11-C10-C8-C9
10	J	602	CLA	C11-C10-C8-C9
10	I	613	CLA	C14-C13-C15-C16
10	F	613	CLA	C11-C12-C13-C14
10	E	602	CLA	C11-C10-C8-C9
10	B	604	CLA	C6-C7-C8-C9
10	D	613	CLA	C14-C13-C15-C16
9	F	607	CHL	C14-C13-C15-C16
10	J	613	CLA	C14-C13-C15-C16
10	H	612	CLA	C14-C13-C15-C16
10	D	603	CLA	C11-C10-C8-C9
9	C	607	CHL	C14-C13-C15-C16
9	B	601	CHL	C14-C13-C15-C16
10	H	602	CLA	C14-C13-C15-C16
10	A	613	CLA	C14-C13-C15-C16
10	H	604	CLA	C11-C10-C8-C9
9	I	607	CHL	C14-C13-C15-C16
10	D	602	CLA	C11-C10-C8-C9
10	F	604	CLA	C6-C7-C8-C9
10	H	603	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
10	C	613	CLA	C14-C13-C15-C16
9	D	607	CHL	C14-C13-C15-C16
7	F	5630	LHG	C11-C10-C9-C8
7	D	3630	LHG	C25-C26-C27-C28
9	A	601	CHL	C3-C5-C6-C7
8	A	632	DGD	CEA-CFA-CGA-CHA
8	H	7632	DGD	CEA-CFA-CGA-CHA
9	J	606	CHL	CBA-CGA-O2A-C1
7	H	7630	LHG	C7-C8-C9-C10
7	E	4630	LHG	C11-C10-C9-C8
8	A	632	DGD	C6B-C7B-C8B-C9B
10	B	611	CLA	C1A-C2A-CAA-CBA
10	F	611	CLA	C1A-C2A-CAA-CBA
9	D	609	CHL	C1A-C2A-CAA-CBA
9	C	605	CHL	C1A-C2A-CAA-CBA
9	D	606	CHL	C1A-C2A-CAA-CBA
9	F	609	CHL	C1A-C2A-CAA-CBA
10	H	611	CLA	C1A-C2A-CAA-CBA
9	C	609	CHL	C1A-C2A-CAA-CBA
9	A	609	CHL	C1A-C2A-CAA-CBA
9	F	605	CHL	C1A-C2A-CAA-CBA
9	G	609	CHL	C1A-C2A-CAA-CBA
9	A	605	CHL	C1A-C2A-CAA-CBA
9	C	606	CHL	C1A-C2A-CAA-CBA
9	E	606	CHL	C1A-C2A-CAA-CBA
9	F	606	CHL	C1A-C2A-CAA-CBA
9	H	605	CHL	C1A-C2A-CAA-CBA
9	H	609	CHL	C1A-C2A-CAA-CBA
9	A	606	CHL	C1A-C2A-CAA-CBA
9	J	609	CHL	C1A-C2A-CAA-CBA
10	H	604	CLA	C1A-C2A-CAA-CBA
9	B	605	CHL	C1A-C2A-CAA-CBA
9	D	605	CHL	C1A-C2A-CAA-CBA
9	I	605	CHL	C1A-C2A-CAA-CBA
9	J	605	CHL	C1A-C2A-CAA-CBA
10	G	611	CLA	C1A-C2A-CAA-CBA
9	B	609	CHL	C1A-C2A-CAA-CBA
10	B	611	CLA	C16-C17-C18-C20
10	F	611	CLA	C16-C17-C18-C20
9	D	609	CHL	C16-C17-C18-C20
10	G	613	CLA	C16-C17-C18-C20
10	D	610	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
9	F	607	CHL	C16-C17-C18-C20
10	J	613	CLA	C16-C17-C18-C20
10	G	611	CLA	C16-C17-C18-C20
9	B	609	CHL	C16-C17-C18-C20
10	G	604	CLA	C13-C15-C16-C17
7	F	5630	LHG	C34-C35-C36-C37
8	G	9632	DGD	C3B-C4B-C5B-C6B
9	I	608	CHL	O1D-CGD-O2D-CED
9	G	609	CHL	C8-C10-C11-C12
10	F	612	CLA	C5-C6-C7-C8
2	B	1633	BNG	C1'-C2'-C3'-C4'
7	C	2630	LHG	C4-O6-P-O3
7	D	3630	LHG	C3-O3-P-O6
8	I	8632	DGD	C2B-C3B-C4B-C5B
9	B	609	CHL	C3-C5-C6-C7
8	A	632	DGD	C8B-C9B-CAB-CBB
9	J	606	CHL	O1A-CGA-O2A-C1
10	B	612	CLA	C10-C11-C12-C13
9	I	609	CHL	CBA-CGA-O2A-C1
7	F	5630	LHG	O6-C4-C5-C6
7	I	8630	LHG	O6-C4-C5-C6
8	B	2632	DGD	CAB-CBB-CCB-CDB
8	I	8632	DGD	C2A-C3A-C4A-C5A
7	F	5630	LHG	C32-C33-C34-C35
10	H	610	CLA	C16-C17-C18-C19
10	D	610	CLA	C16-C17-C18-C19
10	D	610	CLA	O1D-CGD-O2D-CED
8	H	7632	DGD	C3A-C4A-C5A-C6A
8	I	8632	DGD	C8B-C9B-CAB-CBB
7	E	4630	LHG	C10-C11-C12-C13
2	B	1633	BNG	C4'-C5'-C6'-C7'
8	E	4632	DGD	C7B-C8B-C9B-CAB
7	B	1630	LHG	C28-C29-C30-C31
2	H	7633	BNG	C4'-C5'-C6'-C7'
7	A	630	LHG	C13-C14-C15-C16
10	B	611	CLA	C16-C17-C18-C19
9	C	608	CHL	C16-C17-C18-C19
10	I	613	CLA	C3-C5-C6-C7
10	D	602	CLA	C3-C5-C6-C7
10	B	612	CLA	C3-C5-C6-C7
7	C	2630	LHG	C4-C5-C6-O8
7	D	3630	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
8	H	7632	DGD	C7B-C8B-C9B-CAB
7	A	630	LHG	C30-C31-C32-C33
2	E	4633	BNG	C6'-C7'-C8'-C9'
2	F	5633	BNG	C6'-C7'-C8'-C9'
10	C	604	CLA	C13-C15-C16-C17
9	B	607	CHL	O1D-CGD-O2D-CED
9	G	609	CHL	C13-C15-C16-C17
9	B	601	CHL	C13-C15-C16-C17
9	H	608	CHL	C5-C6-C7-C8
7	B	1630	LHG	C7-C8-C9-C10
9	B	609	CHL	O1A-CGA-O2A-C1
8	A	632	DGD	CAB-CBB-CCB-CDB
7	C	2630	LHG	C9-C10-C11-C12
2	G	6633	BNG	C6'-C7'-C8'-C9'
9	G	607	CHL	C16-C17-C18-C20
8	B	1632	DGD	C8B-C9B-CAB-CBB
9	G	606	CHL	CBA-CGA-O2A-C1
7	D	3630	LHG	C35-C36-C37-C38
10	B	613	CLA	C13-C15-C16-C17
9	I	609	CHL	O1A-CGA-O2A-C1
2	C	2633	BNG	C6'-C7'-C8'-C9'
7	I	8630	LHG	C18-C19-C20-C21
10	I	603	CLA	O1D-CGD-O2D-CED
7	H	7630	LHG	C19-C20-C21-C22
8	D	5632	DGD	C8B-C9B-CAB-CBB
2	D	3633	BNG	C4'-C5'-C6'-C7'
9	D	609	CHL	C16-C17-C18-C19
9	J	609	CHL	CBA-CGA-O2A-C1
9	B	609	CHL	CBA-CGA-O2A-C1
9	I	608	CHL	CBD-CGD-O2D-CED
10	E	602	CLA	C5-C6-C7-C8
9	B	607	CHL	C13-C15-C16-C17
2	I	8633	BNG	C6'-C7'-C8'-C9'
10	C	611	CLA	C2A-CAA-CBA-CGA
9	D	605	CHL	C2A-CAA-CBA-CGA
10	G	611	CLA	C15-C16-C17-C18
7	F	5630	LHG	C27-C28-C29-C30
8	B	2632	DGD	C8A-C9A-CAA-CBA
7	B	1630	LHG	C25-C26-C27-C28
2	D	3633	BNG	C6'-C7'-C8'-C9'
7	G	6630	LHG	C29-C30-C31-C32
7	F	5630	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
10	H	611	CLA	C16-C17-C18-C20
10	C	611	CLA	C16-C17-C18-C19
10	E	613	CLA	C16-C17-C18-C20
7	A	630	LHG	C18-C19-C20-C21
8	H	6632	DGD	C8B-C9B-CAB-CBB
10	H	612	CLA	C10-C11-C12-C13
10	J	603	CLA	C10-C11-C12-C13
9	J	608	CHL	O1D-CGD-O2D-CED
9	G	606	CHL	O1A-CGA-O2A-C1
9	J	609	CHL	O1A-CGA-O2A-C1
10	F	611	CLA	C8-C10-C11-C12
9	E	601	CHL	C15-C16-C17-C18
10	G	612	CLA	C13-C15-C16-C17
10	H	613	CLA	C15-C16-C17-C18
6	E	4623	NEX	C11-C10-C9-C8
7	H	7630	LHG	C25-C26-C27-C28
8	D	5632	DGD	CCB-CDB-CEB-CFB
7	A	630	LHG	O9-C7-O7-C5
7	G	6630	LHG	O9-C7-O7-C5
10	A	613	CLA	C15-C16-C17-C18
8	D	5632	DGD	CEA-CFA-CGA-CHA
7	C	2630	LHG	C27-C28-C29-C30
7	I	8630	LHG	C27-C28-C29-C30
7	F	5630	LHG	C30-C31-C32-C33
10	C	611	CLA	C10-C11-C12-C13
10	B	611	CLA	C6-C7-C8-C10
9	G	601	CHL	C11-C10-C8-C7
9	G	601	CHL	C12-C13-C15-C16
9	D	609	CHL	C11-C12-C13-C15
9	D	609	CHL	C12-C13-C15-C16
10	F	610	CLA	C11-C10-C8-C7
10	A	602	CLA	C6-C7-C8-C10
10	G	610	CLA	C11-C12-C13-C15
9	B	608	CHL	C11-C12-C13-C15
9	B	608	CHL	C12-C13-C15-C16
9	D	608	CHL	C6-C7-C8-C10
9	D	608	CHL	C11-C12-C13-C15
9	I	608	CHL	C11-C12-C13-C15
10	C	610	CLA	C11-C12-C13-C15
10	F	602	CLA	C6-C7-C8-C10
10	F	602	CLA	C11-C10-C8-C7
10	J	612	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
10	J	612	CLA	C12-C13-C15-C16
10	J	604	CLA	C6-C7-C8-C10
10	I	602	CLA	C11-C10-C8-C7
10	I	602	CLA	C11-C12-C13-C15
10	B	602	CLA	C6-C7-C8-C10
10	B	602	CLA	C11-C12-C13-C15
10	A	612	CLA	C11-C12-C13-C15
10	J	602	CLA	C6-C7-C8-C10
10	H	610	CLA	C11-C10-C8-C7
9	A	609	CHL	C11-C12-C13-C15
9	C	601	CHL	C11-C12-C13-C15
10	F	613	CLA	C12-C13-C15-C16
10	E	602	CLA	C11-C10-C8-C7
10	J	610	CLA	C11-C12-C13-C15
10	I	603	CLA	C12-C13-C15-C16
10	C	602	CLA	C11-C10-C8-C7
10	C	602	CLA	C11-C12-C13-C15
9	I	609	CHL	C6-C7-C8-C10
9	I	609	CHL	C12-C13-C15-C16
9	F	608	CHL	C12-C13-C15-C16
10	H	612	CLA	C11-C12-C13-C15
10	D	603	CLA	C11-C10-C8-C7
10	D	612	CLA	C11-C12-C13-C15
9	A	601	CHL	C11-C10-C8-C7
9	B	601	CHL	C11-C12-C13-C15
9	H	609	CHL	C6-C7-C8-C10
9	J	609	CHL	C11-C12-C13-C15
9	J	607	CHL	C12-C13-C15-C16
10	E	612	CLA	C11-C12-C13-C15
9	J	608	CHL	C6-C7-C8-C10
9	J	608	CHL	C11-C12-C13-C15
9	J	608	CHL	C12-C13-C15-C16
10	D	602	CLA	C11-C10-C8-C7
10	D	602	CLA	C11-C12-C13-C15
9	H	608	CHL	C2-C3-C5-C6
9	H	608	CHL	C12-C13-C15-C16
9	C	608	CHL	C6-C7-C8-C10
9	C	608	CHL	C12-C13-C15-C16
10	G	611	CLA	C6-C7-C8-C10
10	H	613	CLA	C12-C13-C15-C16
10	C	613	CLA	C11-C12-C13-C15
9	J	601	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
9	E	608	CHL	C6-C7-C8-C10
9	E	608	CHL	C12-C13-C15-C16
9	G	608	CHL	C6-C7-C8-C10
9	G	608	CHL	C12-C13-C15-C16
2	J	9633	BNG	C1'-C2'-C3'-C4'
9	C	601	CHL	C3-C5-C6-C7
9	G	609	CHL	C3-C5-C6-C7
10	J	613	CLA	C3-C5-C6-C7
10	B	611	CLA	C6-C7-C8-C9
9	G	601	CHL	C14-C13-C15-C16
10	F	611	CLA	C6-C7-C8-C9
9	H	607	CHL	C14-C13-C15-C16
10	A	602	CLA	C11-C10-C8-C9
9	H	601	CHL	C14-C13-C15-C16
9	D	608	CHL	C11-C12-C13-C14
9	F	609	CHL	C11-C12-C13-C14
10	B	603	CLA	C11-C12-C13-C14
10	F	602	CLA	C11-C10-C8-C9
10	H	611	CLA	C6-C7-C8-C9
10	G	602	CLA	C11-C10-C8-C9
9	A	607	CHL	C14-C13-C15-C16
10	I	602	CLA	C11-C10-C8-C9
10	B	602	CLA	C14-C13-C15-C16
9	C	609	CHL	C11-C12-C13-C14
10	D	604	CLA	C6-C7-C8-C9
9	C	601	CHL	C14-C13-C15-C16
9	A	608	CHL	C6-C7-C8-C9
10	F	613	CLA	C14-C13-C15-C16
9	G	609	CHL	C11-C12-C13-C14
10	B	613	CLA	C14-C13-C15-C16
9	G	607	CHL	C14-C13-C15-C16
10	I	603	CLA	C14-C13-C15-C16
10	A	611	CLA	C11-C10-C8-C9
10	C	602	CLA	C11-C10-C8-C9
10	D	603	CLA	C14-C13-C15-C16
10	I	611	CLA	C6-C7-C8-C9
9	E	607	CHL	C14-C13-C15-C16
10	G	603	CLA	C11-C12-C13-C14
10	D	612	CLA	C11-C12-C13-C14
9	A	601	CHL	C11-C10-C8-C9
10	H	602	CLA	C11-C10-C8-C9
10	C	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
10	J	603	CLA	C11-C12-C13-C14
9	J	608	CHL	C6-C7-C8-C9
10	D	602	CLA	C11-C12-C13-C14
10	B	612	CLA	C11-C12-C13-C14
9	C	608	CHL	C6-C7-C8-C9
10	H	613	CLA	C11-C12-C13-C14
10	H	613	CLA	C14-C13-C15-C16
10	C	613	CLA	C11-C12-C13-C14
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	B	607	CHL	C14-C13-C15-C16
10	I	602	CLA	CBD-CGD-O2D-CED
8	B	2632	DGD	CEB-CFB-CGB-CHB
9	F	609	CHL	CBA-CGA-O2A-C1
10	I	611	CLA	C15-C16-C17-C18
10	D	604	CLA	C2A-CAA-CBA-CGA
10	F	604	CLA	C2A-CAA-CBA-CGA
8	H	7632	DGD	CFA-CGA-CHA-CIA
10	C	611	CLA	C16-C17-C18-C20
10	I	611	CLA	C16-C17-C18-C19
10	J	603	CLA	C16-C17-C18-C20
10	E	613	CLA	C3-C5-C6-C7
10	D	611	CLA	C15-C16-C17-C18
9	C	609	CHL	C8-C10-C11-C12
10	G	611	CLA	C8-C10-C11-C12
9	C	609	CHL	CBA-CGA-O2A-C1
8	E	4632	DGD	CFA-CGA-CHA-CIA
7	G	6630	LHG	C7-C8-C9-C10
10	I	610	CLA	C8-C10-C11-C12
2	G	6633	BNG	C1'-C2'-C3'-C4'
2	F	5633	BNG	C1'-C2'-C3'-C4'
10	D	610	CLA	CBD-CGD-O2D-CED
8	I	8632	DGD	CAB-CBB-CCB-CDB
7	E	4630	LHG	C9-C10-C11-C12
9	A	607	CHL	C16-C17-C18-C19
9	E	608	CHL	C16-C17-C18-C20
7	H	7630	LHG	O6-C4-C5-C6
7	J	9630	LHG	O6-C4-C5-C6
7	D	3630	LHG	O6-C4-C5-C6
10	H	613	CLA	O1D-CGD-O2D-CED
7	J	9630	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
7	J	9630	LHG	C30-C31-C32-C33
7	C	2630	LHG	C11-C12-C13-C14
10	F	602	CLA	C5-C6-C7-C8
10	J	612	CLA	C10-C11-C12-C13
10	G	602	CLA	C5-C6-C7-C8
10	E	603	CLA	C8-C10-C11-C12
7	D	3630	LHG	C13-C14-C15-C16
8	H	7632	DGD	C6B-C7B-C8B-C9B
7	I	8630	LHG	C28-C29-C30-C31
7	C	2630	LHG	C12-C13-C14-C15
8	H	6632	DGD	CBB-CCB-CDB-CEB
9	I	608	CHL	C16-C17-C18-C19
9	A	609	CHL	C16-C17-C18-C20
10	J	611	CLA	C16-C17-C18-C19
8	H	6632	DGD	CFB-CGB-CHB-CIB
8	D	3632	DGD	CEA-CFA-CGA-CHA
9	C	601	CHL	CBA-CGA-O2A-C1
7	C	2630	LHG	C7-C8-C9-C10
7	I	8630	LHG	C7-C8-C9-C10
7	B	1630	LHG	C34-C35-C36-C37
7	I	8630	LHG	C25-C26-C27-C28
8	D	3632	DGD	C5A-C6A-C7A-C8A
10	G	614	CLA	O1D-CGD-O2D-CED
10	H	611	CLA	C3A-C2A-CAA-CBA
10	H	604	CLA	C3A-C2A-CAA-CBA
9	J	606	CHL	C3A-C2A-CAA-CBA
9	J	601	CHL	C3A-C2A-CAA-CBA
2	C	2633	BNG	C1'-C2'-C3'-C4'
2	J	9633	BNG	C4'-C5'-C6'-C7'
8	I	8632	DGD	C4A-C5A-C6A-C7A
8	G	9632	DGD	C6B-C7B-C8B-C9B
7	B	1630	LHG	C19-C20-C21-C22
7	G	6630	LHG	C19-C20-C21-C22
2	A	633	BNG	C6'-C7'-C8'-C9'
9	H	608	CHL	C16-C17-C18-C20
10	F	610	CLA	O1D-CGD-O2D-CED
9	E	609	CHL	C15-C16-C17-C18
8	I	8632	DGD	O1G-C1G-C2G-C3G
7	H	7630	LHG	C4-C5-C6-O8
8	H	7632	DGD	O1G-C1G-C2G-C3G
8	B	1632	DGD	O1G-C1G-C2G-C3G
9	F	609	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	E	607	CHL	O1D-CGD-O2D-CED
7	H	7630	LHG	C13-C14-C15-C16
7	C	2630	LHG	C29-C30-C31-C32
8	H	7632	DGD	C4A-C5A-C6A-C7A
8	H	6632	DGD	C7B-C8B-C9B-CAB
9	B	608	CHL	O2A-C1-C2-C3
9	H	608	CHL	O2A-C1-C2-C3
8	H	6632	DGD	O6E-C5E-C6E-O5E
2	I	8633	BNG	C1'-C2'-C3'-C4'
10	B	612	CLA	C15-C16-C17-C18
8	B	2632	DGD	C4A-C5A-C6A-C7A
7	I	8630	LHG	C13-C14-C15-C16
9	H	608	CHL	C4-C3-C5-C6
9	C	608	CHL	C16-C17-C18-C20
8	B	1632	DGD	CFA-CGA-CHA-CIA
10	A	614	CLA	O1D-CGD-O2D-CED
10	H	613	CLA	C8-C10-C11-C12
7	E	4630	LHG	C3-O3-P-O6
7	G	6630	LHG	C4-O6-P-O3
9	C	609	CHL	O1A-CGA-O2A-C1
8	H	6632	DGD	CFA-CGA-CHA-CIA
2	D	3633	BNG	C4-C5-C6-O6
9	A	607	CHL	C13-C15-C16-C17
10	G	612	CLA	C10-C11-C12-C13
8	I	8632	DGD	CFB-CGB-CHB-CIB
7	F	5630	LHG	C16-C17-C18-C19
10	J	611	CLA	C16-C17-C18-C20
8	H	6632	DGD	C6A-C7A-C8A-C9A
7	D	3630	LHG	C19-C20-C21-C22
8	H	6632	DGD	C3B-C4B-C5B-C6B
9	C	601	CHL	O1A-CGA-O2A-C1
7	J	9630	LHG	C19-C20-C21-C22
9	C	609	CHL	C3-C5-C6-C7
2	B	1633	BNG	C4-C5-C6-O6
7	F	5630	LHG	O7-C5-C6-O8
7	H	7630	LHG	O7-C5-C6-O8
8	G	9632	DGD	O1G-C1G-C2G-O2G
7	B	1630	LHG	O7-C5-C6-O8
7	A	630	LHG	O7-C5-C6-O8
8	H	6632	DGD	O1G-C1G-C2G-O2G
8	D	3632	DGD	O1G-C1G-C2G-O2G
7	D	3630	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
7	F	5630	LHG	C28-C29-C30-C31
7	H	7630	LHG	C29-C30-C31-C32
8	D	5632	DGD	CFA-CGA-CHA-CIA
10	A	602	CLA	C16-C17-C18-C20
9	B	609	CHL	C16-C17-C18-C19
8	G	9632	DGD	C3A-C4A-C5A-C6A
7	G	6630	LHG	C1-C2-C3-O3
8	I	8632	DGD	CFA-CGA-CHA-CIA
10	E	611	CLA	C4-C3-C5-C6
9	H	606	CHL	C2-C1-O2A-CGA
9	A	609	CHL	C2-C1-O2A-CGA
9	G	609	CHL	C2-C1-O2A-CGA
9	I	606	CHL	C2-C1-O2A-CGA
9	D	601	CHL	C2-C1-O2A-CGA
9	F	601	CHL	C2-C1-O2A-CGA
9	J	601	CHL	C2-C1-O2A-CGA
7	C	2630	LHG	C16-C17-C18-C19
8	B	2632	DGD	CBB-CCB-CDB-CEB
9	D	601	CHL	C13-C15-C16-C17
10	E	613	CLA	C15-C16-C17-C18
10	B	603	CLA	C14-C13-C15-C16
9	I	608	CHL	C11-C12-C13-C14
10	C	611	CLA	C6-C7-C8-C9
10	J	612	CLA	C11-C12-C13-C14
10	G	602	CLA	C11-C12-C13-C14
9	I	601	CHL	C11-C12-C13-C14
10	B	602	CLA	C11-C12-C13-C14
10	H	610	CLA	C11-C10-C8-C9
9	C	601	CHL	C11-C10-C8-C9
10	E	602	CLA	C11-C12-C13-C14
10	H	612	CLA	C11-C12-C13-C14
9	A	601	CHL	C14-C13-C15-C16
9	J	607	CHL	C14-C13-C15-C16
10	F	612	CLA	C11-C12-C13-C14
10	G	611	CLA	C6-C7-C8-C9
10	E	613	CLA	C11-C12-C13-C14
2	I	8633	BNG	C4'-C5'-C6'-C7'
10	F	610	CLA	CBD-CGD-O2D-CED
10	G	603	CLA	C10-C11-C12-C13
7	E	4630	LHG	C27-C28-C29-C30
7	A	630	LHG	C35-C36-C37-C38
10	F	603	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
10	H	610	CLA	C16-C17-C18-C20
10	I	611	CLA	C16-C17-C18-C20
4	C	2621	LUT	C1-C6-C7-C8
4	D	3621	LUT	C1-C6-C7-C8
4	B	1621	LUT	C5-C6-C7-C8
8	H	7632	DGD	C2A-C3A-C4A-C5A
10	J	613	CLA	C5-C6-C7-C8
10	I	611	CLA	C8-C10-C11-C12
9	D	608	CHL	C16-C17-C18-C20
10	A	602	CLA	C10-C11-C12-C13
10	E	602	CLA	C15-C16-C17-C18
9	C	605	CHL	O1D-CGD-O2D-CED
2	B	1633	BNG	O1-C1'-C2'-C3'
7	B	1630	LHG	C26-C27-C28-C29
10	C	602	CLA	C10-C11-C12-C13
7	C	2630	LHG	O6-C4-C5-C6
10	D	604	CLA	CAA-CBA-CGA-O2A
10	G	612	CLA	C4-C3-C5-C6
7	B	1630	LHG	C16-C17-C18-C19
7	I	8630	LHG	C16-C17-C18-C19
8	D	3632	DGD	CEB-CFB-CGB-CHB
10	A	602	CLA	C11-C12-C13-C15
9	D	608	CHL	C12-C13-C15-C16
9	F	609	CHL	C12-C13-C15-C16
10	F	602	CLA	C11-C12-C13-C15
10	G	602	CLA	C11-C12-C13-C15
9	I	601	CHL	C12-C13-C15-C16
10	F	603	CLA	C6-C7-C8-C10
10	A	612	CLA	C12-C13-C15-C16
10	C	604	CLA	C11-C12-C13-C15
10	D	604	CLA	C6-C7-C8-C10
10	J	602	CLA	C11-C12-C13-C15
9	A	609	CHL	C12-C13-C15-C16
9	C	601	CHL	C11-C10-C8-C7
9	E	601	CHL	C12-C13-C15-C16
9	A	608	CHL	C11-C12-C13-C15
9	A	608	CHL	C12-C13-C15-C16
9	G	609	CHL	C12-C13-C15-C16
10	E	603	CLA	C6-C7-C8-C10
10	D	610	CLA	C11-C10-C8-C7
10	G	604	CLA	C11-C10-C8-C7
10	G	604	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
10	A	604	CLA	C11-C12-C13-C15
10	D	613	CLA	C11-C12-C13-C15
10	I	610	CLA	C11-C10-C8-C7
9	G	607	CHL	C6-C7-C8-C10
10	I	603	CLA	C11-C12-C13-C15
10	C	602	CLA	C6-C7-C8-C10
10	G	612	CLA	C2-C3-C5-C6
10	G	612	CLA	C11-C12-C13-C15
9	F	608	CHL	C11-C12-C13-C15
10	D	603	CLA	C12-C13-C15-C16
10	G	603	CLA	C11-C10-C8-C7
10	G	603	CLA	C11-C12-C13-C15
10	B	610	CLA	C11-C10-C8-C7
9	E	609	CHL	C11-C12-C13-C15
9	A	601	CHL	C11-C12-C13-C15
9	A	601	CHL	C12-C13-C15-C16
10	H	602	CLA	C11-C12-C13-C15
10	E	610	CLA	C11-C10-C8-C7
9	H	609	CHL	C11-C12-C13-C15
9	H	609	CHL	C12-C13-C15-C16
9	D	601	CHL	C11-C10-C8-C7
10	J	603	CLA	C11-C12-C13-C15
9	J	609	CHL	C12-C13-C15-C16
10	I	612	CLA	C11-C12-C13-C15
10	F	612	CLA	C11-C12-C13-C15
10	E	612	CLA	C12-C13-C15-C16
9	H	608	CHL	C11-C12-C13-C15
10	F	604	CLA	C11-C12-C13-C15
10	B	612	CLA	C12-C13-C15-C16
10	H	603	CLA	C12-C13-C15-C16
10	E	613	CLA	C11-C12-C13-C15
9	J	601	CHL	C6-C7-C8-C10
9	J	601	CHL	C11-C10-C8-C7
9	J	601	CHL	C11-C12-C13-C15
9	E	608	CHL	C11-C12-C13-C15
9	G	608	CHL	C11-C12-C13-C15
10	A	603	CLA	C6-C7-C8-C10
10	A	603	CLA	C12-C13-C15-C16
9	B	609	CHL	C11-C12-C13-C15
9	B	609	CHL	C12-C13-C15-C16
10	F	602	CLA	C3-C5-C6-C7
7	G	6630	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
10	B	602	CLA	C5-C6-C7-C8
10	E	611	CLA	C8-C10-C11-C12
10	H	611	CLA	C16-C17-C18-C19
10	I	610	CLA	C16-C17-C18-C19
10	A	610	CLA	C15-C16-C17-C18
9	F	609	CHL	C8-C10-C11-C12
9	C	601	CHL	C2A-CAA-CBA-CGA
10	I	611	CLA	C2A-CAA-CBA-CGA
9	E	605	CHL	C2A-CAA-CBA-CGA
8	E	4632	DGD	CEB-CFB-CGB-CHB
7	D	3630	LHG	C29-C30-C31-C32
10	F	613	CLA	C3-C5-C6-C7
9	A	607	CHL	C16-C17-C18-C20
9	B	607	CHL	C16-C17-C18-C19
10	J	610	CLA	C13-C15-C16-C17
9	D	609	CHL	CBA-CGA-O2A-C1
8	D	5632	DGD	C7B-C8B-C9B-CAB
2	E	4633	BNG	C4'-C5'-C6'-C7'
10	E	602	CLA	O1D-CGD-O2D-CED
10	A	602	CLA	C5-C6-C7-C8
10	F	603	CLA	C8-C10-C11-C12
9	J	601	CHL	C15-C16-C17-C18
7	J	9630	LHG	C33-C34-C35-C36
10	B	603	CLA	CAD-CBD-CGD-O2D
10	E	603	CLA	CAD-CBD-CGD-O2D
10	I	603	CLA	CAD-CBD-CGD-O2D
10	D	603	CLA	CAD-CBD-CGD-O2D
10	C	603	CLA	CAD-CBD-CGD-O2D
10	J	603	CLA	CAD-CBD-CGD-O2D
10	H	603	CLA	CAD-CBD-CGD-O2D
10	A	603	CLA	CAD-CBD-CGD-O2D
10	I	613	CLA	C15-C16-C17-C18
10	D	603	CLA	C8-C10-C11-C12
10	D	612	CLA	C10-C11-C12-C13
10	C	613	CLA	C8-C10-C11-C12
10	C	613	CLA	C15-C16-C17-C18
2	B	1633	BNG	C6'-C7'-C8'-C9'
7	A	630	LHG	C25-C26-C27-C28
10	B	604	CLA	C4-C3-C5-C6
10	G	611	CLA	C4-C3-C5-C6
9	A	601	CHL	C16-C17-C18-C20
8	H	6632	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
2	B	1633	BNG	O5-C1-O1-C1'
8	H	7632	DGD	O6D-C1D-O3G-C3G
10	H	612	CLA	C2-C3-C5-C6
8	E	4632	DGD	C8B-C9B-CAB-CBB
7	B	1630	LHG	C30-C31-C32-C33
8	D	3632	DGD	CFA-CGA-CHA-CIA
7	F	5630	LHG	C4-C5-C6-O8
7	B	1630	LHG	C4-C5-C6-O8
7	I	8630	LHG	C4-C5-C6-O8
7	H	7630	LHG	O6-C4-C5-O7
7	A	630	LHG	O6-C4-C5-O7
10	E	612	CLA	C15-C16-C17-C18
10	I	614	CLA	O2A-C1-C2-C3
10	C	614	CLA	O2A-C1-C2-C3
2	J	9633	BNG	C6'-C7'-C8'-C9'
7	E	4630	LHG	C19-C20-C21-C22
10	A	614	CLA	CBD-CGD-O2D-CED
9	E	609	CHL	C16-C17-C18-C20
9	B	607	CHL	C16-C17-C18-C20
9	G	601	CHL	CHA-CBD-CGD-O1D
9	G	601	CHL	CHA-CBD-CGD-O2D
9	I	601	CHL	CHA-CBD-CGD-O2D
10	C	604	CLA	CHA-CBD-CGD-O1D
9	J	601	CHL	CHA-CBD-CGD-O2D
2	H	7633	BNG	C6'-C7'-C8'-C9'
10	G	610	CLA	O1A-CGA-O2A-C1
7	C	2630	LHG	C17-C18-C19-C20
7	D	3630	LHG	C33-C34-C35-C36
6	A	623	NEX	C11-C10-C9-C8
9	A	608	CHL	C15-C16-C17-C18
7	C	2630	LHG	C26-C27-C28-C29
7	E	4630	LHG	O7-C5-C6-O8
7	I	8630	LHG	O7-C5-C6-O8
8	I	8632	DGD	C9B-CAB-CBB-CCB
8	A	632	DGD	C4A-C5A-C6A-C7A
10	D	602	CLA	C5-C6-C7-C8
9	D	601	CHL	C16-C17-C18-C20
10	G	610	CLA	O1D-CGD-O2D-CED
7	E	4630	LHG	C33-C34-C35-C36
8	A	632	DGD	C6A-C7A-C8A-C9A
10	H	612	CLA	C4-C3-C5-C6
9	D	609	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
8	B	1632	DGD	CFB-CGB-CHB-CIB
9	D	608	CHL	C6-C7-C8-C9
10	F	602	CLA	C11-C12-C13-C14
10	I	602	CLA	C11-C12-C13-C14
10	A	612	CLA	C11-C12-C13-C14
10	I	603	CLA	C11-C10-C8-C9
10	I	603	CLA	C11-C12-C13-C14
10	J	611	CLA	C6-C7-C8-C9
9	I	609	CHL	C11-C12-C13-C14
10	G	603	CLA	C11-C10-C8-C9
9	B	601	CHL	C6-C7-C8-C9
9	J	609	CHL	C11-C12-C13-C14
10	I	612	CLA	C11-C12-C13-C14
10	E	612	CLA	C11-C12-C13-C14
9	J	601	CHL	C11-C10-C8-C9
7	B	1630	LHG	C35-C36-C37-C38
9	A	608	CHL	O1A-CGA-O2A-C1
8	A	632	DGD	C2B-C3B-C4B-C5B
8	B	2632	DGD	CFB-CGB-CHB-CIB
10	F	611	CLA	C2A-CAA-CBA-CGA
9	I	606	CHL	O1D-CGD-O2D-CED
8	H	7632	DGD	CBB-CCB-CDB-CEB
7	I	8630	LHG	O1-C1-C2-C3
10	G	613	CLA	C3-C5-C6-C7
10	D	612	CLA	C3-C5-C6-C7
8	D	3632	DGD	CBB-CCB-CDB-CEB
10	D	613	CLA	C1A-C2A-CAA-CBA
10	D	603	CLA	C1A-C2A-CAA-CBA
10	F	604	CLA	C1A-C2A-CAA-CBA
10	H	603	CLA	C1A-C2A-CAA-CBA
2	E	4633	BNG	C4-C5-C6-O6
7	D	3630	LHG	C26-C27-C28-C29
9	E	609	CHL	C13-C15-C16-C17
7	H	7630	LHG	C26-C27-C28-C29
10	C	603	CLA	O1D-CGD-O2D-CED
9	C	607	CHL	C4-C3-C5-C6
10	F	604	CLA	C4-C3-C5-C6
10	E	604	CLA	C3-C5-C6-C7
9	C	608	CHL	C3-C5-C6-C7
10	B	604	CLA	C2-C3-C5-C6
9	F	608	CHL	C2-C3-C5-C6
10	G	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	B	1630	LHG	C11-C10-C9-C8
7	G	6630	LHG	C35-C36-C37-C38
7	B	1630	LHG	C4-O6-P-O4
7	A	630	LHG	C4-O6-P-O4
7	G	6630	LHG	C4-O6-P-O4
7	D	3630	LHG	C3-O3-P-O4
9	E	609	CHL	C16-C17-C18-C19
10	J	603	CLA	C16-C17-C18-C19
10	E	611	CLA	C16-C17-C18-C19
2	C	2633	BNG	O5-C1-O1-C1'
2	E	4633	BNG	O5-C1-O1-C1'
2	D	3633	BNG	O5-C1-O1-C1'
2	H	7633	BNG	O5-C1-O1-C1'
10	H	602	CLA	CBA-CGA-O2A-C1
7	A	630	LHG	O6-C4-C5-C6
7	A	630	LHG	C27-C28-C29-C30
8	H	6632	DGD	C2B-C3B-C4B-C5B
10	D	613	CLA	C15-C16-C17-C18
8	H	7632	DGD	C6A-C7A-C8A-C9A
9	A	609	CHL	C16-C17-C18-C19
10	D	603	CLA	C16-C17-C18-C20
9	E	607	CHL	C16-C17-C18-C19
8	G	9632	DGD	CAB-CBB-CCB-CDB
10	J	604	CLA	CAD-CBD-CGD-O1D
10	I	614	CLA	CAD-CBD-CGD-O1D
10	C	604	CLA	CAD-CBD-CGD-O1D
10	H	602	CLA	C15-C16-C17-C18
8	D	3632	DGD	C8A-C9A-CAA-CBA
7	D	3630	LHG	C32-C33-C34-C35
10	H	604	CLA	C3-C5-C6-C7
7	H	7630	LHG	C27-C28-C29-C30
8	B	2632	DGD	C8B-C9B-CAB-CBB
7	I	8630	LHG	C30-C31-C32-C33
9	A	608	CHL	CBA-CGA-O2A-C1
10	G	603	CLA	O1D-CGD-O2D-CED
7	B	1630	LHG	C33-C34-C35-C36
7	D	3630	LHG	C27-C28-C29-C30
9	I	608	CHL	C16-C17-C18-C20
10	G	610	CLA	C11-C10-C8-C7
9	B	608	CHL	C6-C7-C8-C10
9	F	609	CHL	C11-C10-C8-C7
10	C	610	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
7	E	4630	LHG	O6-C4-C5-O7
7	F	5630	LHG	O6-C4-C5-O7
10	G	602	CLA	C6-C7-C8-C10
9	H	606	CHL	C3A-C2A-CAA-CBA
10	I	602	CLA	C6-C7-C8-C10
9	C	609	CHL	C11-C10-C8-C7
10	C	612	CLA	C11-C12-C13-C15
10	H	610	CLA	C11-C12-C13-C15
7	J	9630	LHG	O6-C4-C5-O7
10	E	602	CLA	C6-C7-C8-C10
10	J	610	CLA	C11-C10-C8-C7
7	C	2630	LHG	O6-C4-C5-O7
10	I	610	CLA	C11-C12-C13-C15
10	I	603	CLA	C11-C10-C8-C7
10	J	611	CLA	C3A-C2A-CAA-CBA
9	F	608	CHL	C11-C10-C8-C7
9	E	609	CHL	C12-C13-C15-C16
10	H	602	CLA	C6-C7-C8-C10
9	F	601	CHL	C11-C10-C8-C7
9	F	601	CHL	C12-C13-C15-C16
9	J	609	CHL	C6-C7-C8-C10
10	H	604	CLA	C11-C12-C13-C15
7	I	8630	LHG	O6-C4-C5-O7
10	F	604	CLA	C12-C13-C15-C16
9	C	608	CHL	C11-C12-C13-C15
7	D	3630	LHG	O6-C4-C5-O7
7	C	2630	LHG	C33-C34-C35-C36
9	D	601	CHL	O1D-CGD-O2D-CED
8	A	632	DGD	CFA-CGA-CHA-CIA
8	H	6632	DGD	C3A-C4A-C5A-C6A
7	A	630	LHG	C33-C34-C35-C36
7	I	8630	LHG	C8-C7-O7-C5
7	H	7630	LHG	C33-C34-C35-C36
8	G	9632	DGD	CFA-CGA-CHA-CIA
9	E	609	CHL	O1A-CGA-O2A-C1
7	G	6630	LHG	O2-C2-C3-O3
8	D	3632	DGD	C8B-C9B-CAB-CBB
10	H	614	CLA	CBD-CGD-O2D-CED
10	A	611	CLA	C2A-CAA-CBA-CGA
9	G	606	CHL	C2A-CAA-CBA-CGA
9	I	605	CHL	C2A-CAA-CBA-CGA
9	D	601	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
2	F	5633	BNG	C4-C5-C6-O6
8	H	6632	DGD	C9A-CAA-CBA-CCA
10	C	612	CLA	C3-C5-C6-C7
8	G	9632	DGD	O1G-C1G-C2G-C3G
7	J	9630	LHG	C4-C5-C6-O8
7	A	630	LHG	C4-C5-C6-O8
8	H	6632	DGD	C5B-C6B-C7B-C8B
7	C	2630	LHG	O7-C5-C6-O8
7	G	6630	LHG	O7-C5-C6-O8
9	B	601	CHL	C16-C17-C18-C20
10	F	602	CLA	C10-C11-C12-C13
7	B	1630	LHG	C27-C28-C29-C30
9	D	606	CHL	O1D-CGD-O2D-CED
8	B	1632	DGD	CEB-CFB-CGB-CHB
10	H	602	CLA	O1A-CGA-O2A-C1
9	F	607	CHL	C8-C10-C11-C12
10	G	604	CLA	C4-C3-C5-C6
10	J	611	CLA	C4-C3-C5-C6
9	F	608	CHL	C4-C3-C5-C6
8	G	9632	DGD	C5B-C6B-C7B-C8B
8	B	1632	DGD	C4A-C5A-C6A-C7A
10	G	610	CLA	C11-C10-C8-C9
10	D	611	CLA	C6-C7-C8-C9
10	F	602	CLA	C14-C13-C15-C16
10	B	602	CLA	C6-C7-C8-C9
10	C	612	CLA	C11-C12-C13-C14
10	J	602	CLA	C6-C7-C8-C9
10	J	602	CLA	C11-C12-C13-C14
9	A	608	CHL	C11-C12-C13-C14
10	E	602	CLA	C14-C13-C15-C16
10	G	604	CLA	C11-C12-C13-C14
10	I	610	CLA	C11-C10-C8-C9
10	A	611	CLA	C6-C7-C8-C9
10	C	602	CLA	C6-C7-C8-C9
10	C	602	CLA	C14-C13-C15-C16
9	F	608	CHL	C11-C10-C8-C9
10	H	602	CLA	C11-C12-C13-C14
10	C	603	CLA	C14-C13-C15-C16
10	E	611	CLA	C6-C7-C8-C9
9	J	608	CHL	C11-C12-C13-C14
10	F	604	CLA	C11-C12-C13-C14
10	A	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
10	A	603	CLA	C14-C13-C15-C16
9	B	609	CHL	C14-C13-C15-C16
7	F	5630	LHG	C7-C8-C9-C10
2	A	633	BNG	O5-C1-O1-C1'
9	E	608	CHL	O1A-CGA-O2A-C1
10	G	604	CLA	C2A-CAA-CBA-CGA
7	G	6630	LHG	C25-C26-C27-C28
9	C	608	CHL	O1D-CGD-O2D-CED
9	J	608	CHL	CBD-CGD-O2D-CED
8	B	2632	DGD	C4E-C5E-C6E-O5E
10	D	611	CLA	C4-C3-C5-C6
10	C	611	CLA	C4-C3-C5-C6
10	A	612	CLA	C4-C3-C5-C6
9	F	607	CHL	C4-C3-C5-C6
10	A	611	CLA	C4-C3-C5-C6
10	H	604	CLA	C4-C3-C5-C6
10	C	604	CLA	CAA-CBA-CGA-O2A
10	E	611	CLA	C2-C3-C5-C6
10	F	611	CLA	C15-C16-C17-C18
10	C	612	CLA	C5-C6-C7-C8
9	J	609	CHL	C16-C17-C18-C20
10	B	614	CLA	C1-C2-C3-C4
10	H	614	CLA	C1-C2-C3-C4
10	I	614	CLA	C1-C2-C3-C4
10	G	614	CLA	C1-C2-C3-C4
10	J	614	CLA	C1-C2-C3-C4
10	C	614	CLA	C1-C2-C3-C4
10	F	614	CLA	C1-C2-C3-C4
10	A	614	CLA	C1-C2-C3-C4
10	D	614	CLA	C1-C2-C3-C4
10	E	614	CLA	C1-C2-C3-C4
10	J	613	CLA	O1D-CGD-O2D-CED
7	E	4630	LHG	O6-C4-C5-C6
10	C	604	CLA	C2A-CAA-CBA-CGA
9	D	601	CHL	C2A-CAA-CBA-CGA
8	G	9632	DGD	CFB-CGB-CHB-CIB
8	H	6632	DGD	C8A-C9A-CAA-CBA
9	G	601	CHL	C2-C1-O2A-CGA
9	E	606	CHL	C2-C1-O2A-CGA
9	A	606	CHL	C2-C1-O2A-CGA
9	B	609	CHL	C2-C1-O2A-CGA
10	A	602	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
10	B	603	CLA	C15-C16-C17-C18
10	J	602	CLA	C3-C5-C6-C7
9	G	608	CHL	C3-C5-C6-C7
9	B	608	CHL	C5-C6-C7-C8
10	B	611	CLA	C4-C3-C5-C6
7	I	8630	LHG	C26-C27-C28-C29
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	J	9621	LUT	C1-C6-C7-C8
4	J	9621	LUT	C5-C6-C7-C8
4	C	2621	LUT	C5-C6-C7-C8
4	J	9620	LUT	C1-C6-C7-C8
4	D	3621	LUT	C5-C6-C7-C8
4	B	1621	LUT	C1-C6-C7-C8
4	I	8621	LUT	C1-C6-C7-C8
4	A	621	LUT	C1-C6-C7-C8
7	H	7630	LHG	C12-C13-C14-C15
8	B	1632	DGD	C3A-C4A-C5A-C6A
10	E	610	CLA	O1D-CGD-O2D-CED
10	E	611	CLA	C16-C17-C18-C20
2	G	6633	BNG	O5-C1-O1-C1'
8	D	5632	DGD	CEB-CFB-CGB-CHB
7	J	9630	LHG	C13-C14-C15-C16
10	E	612	CLA	C10-C11-C12-C13
10	A	603	CLA	C5-C6-C7-C8
6	B	1623	NEX	C11-C10-C9-C8
2	G	6633	BNG	C4-C5-C6-O6
7	J	9630	LHG	O7-C5-C6-O8
7	J	9630	LHG	C31-C32-C33-C34
9	B	608	CHL	CBD-CGD-O2D-CED
7	F	5630	LHG	C3-O3-P-O6
7	H	7630	LHG	C3-O3-P-O6
7	J	9630	LHG	C3-O3-P-O6
7	C	2630	LHG	C3-O3-P-O6
7	I	8630	LHG	C3-O3-P-O6
7	G	6630	LHG	C4-C5-C6-O8
8	H	6632	DGD	O1G-C1G-C2G-C3G
8	D	3632	DGD	O1G-C1G-C2G-C3G
10	I	612	CLA	C4-C3-C5-C6
10	A	610	CLA	C11-C12-C13-C15
10	F	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	C	609	CHL	C11-C12-C13-C15
9	G	609	CHL	C6-C7-C8-C10
10	G	604	CLA	C12-C13-C15-C16
10	I	611	CLA	C6-C7-C8-C10
9	C	607	CHL	C2-C3-C5-C6
9	B	601	CHL	C6-C7-C8-C10
9	H	608	CHL	C11-C10-C8-C7
10	H	603	CLA	C11-C10-C8-C7
9	B	607	CHL	C11-C12-C13-C15
10	A	602	CLA	C6-C7-C8-C9
10	A	602	CLA	C11-C12-C13-C14
9	B	608	CHL	C6-C7-C8-C9
9	F	609	CHL	C11-C10-C8-C9
10	F	603	CLA	C6-C7-C8-C9
9	C	609	CHL	C11-C10-C8-C9
10	C	604	CLA	C11-C12-C13-C14
10	E	602	CLA	C6-C7-C8-C9
10	E	603	CLA	C6-C7-C8-C9
10	J	610	CLA	C11-C10-C8-C9
10	A	611	CLA	C11-C12-C13-C14
10	G	612	CLA	C11-C12-C13-C14
10	D	603	CLA	C6-C7-C8-C9
10	H	602	CLA	C6-C7-C8-C9
9	H	609	CHL	C6-C7-C8-C9
10	A	613	CLA	C11-C12-C13-C14
9	J	609	CHL	C6-C7-C8-C9
10	I	610	CLA	C16-C17-C18-C20
8	D	5632	DGD	C2B-C3B-C4B-C5B
7	I	8630	LHG	O9-C7-O7-C5
8	E	4632	DGD	C8A-C9A-CAA-CBA
7	F	5630	LHG	C26-C27-C28-C29
8	D	3632	DGD	C7B-C8B-C9B-CAB
8	G	9632	DGD	C8A-C9A-CAA-CBA
2	C	2633	BNG	C4'-C5'-C6'-C7'
9	E	609	CHL	CBA-CGA-O2A-C1
10	G	613	CLA	C15-C16-C17-C18
8	G	9632	DGD	O6E-C5E-C6E-O5E
10	A	614	CLA	O2A-C1-C2-C3
10	D	614	CLA	O2A-C1-C2-C3
9	J	601	CHL	C13-C15-C16-C17
10	H	611	CLA	C4-C3-C5-C6
10	C	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	A	604	CLA	CAA-CBA-CGA-O2A
10	D	613	CLA	C16-C17-C18-C19
9	E	607	CHL	C16-C17-C18-C20
9	J	608	CHL	C16-C17-C18-C20
10	I	604	CLA	CBA-CGA-O2A-C1
9	I	609	CHL	C8-C10-C11-C12
9	I	601	CHL	O1A-CGA-O2A-C1
8	B	1632	DGD	O6E-C5E-C6E-O5E
10	F	602	CLA	C13-C15-C16-C17
9	E	608	CHL	CBA-CGA-O2A-C1
9	E	607	CHL	C2A-CAA-CBA-CGA
7	I	8630	LHG	C12-C13-C14-C15
8	I	8632	DGD	C3A-C4A-C5A-C6A
7	E	4630	LHG	C26-C27-C28-C29
9	B	608	CHL	O1A-CGA-O2A-C1
9	J	609	CHL	C16-C17-C18-C19
10	H	613	CLA	C16-C17-C18-C19
8	D	5632	DGD	C9A-CAA-CBA-CCA
7	C	2630	LHG	C32-C33-C34-C35
9	E	609	CHL	C4-C3-C5-C6
10	F	612	CLA	C4-C3-C5-C6
9	B	607	CHL	C4-C3-C5-C6
10	H	612	CLA	C5-C6-C7-C8
8	B	1632	DGD	C8A-C9A-CAA-CBA
10	C	613	CLA	C2-C3-C5-C6
7	H	7630	LHG	C32-C33-C34-C35
7	B	1630	LHG	C17-C18-C19-C20
9	F	609	CHL	C2-C1-O2A-CGA
9	E	601	CHL	C2-C1-O2A-CGA
9	F	606	CHL	C2-C1-O2A-CGA
9	I	609	CHL	C2-C1-O2A-CGA
9	E	609	CHL	C2-C1-O2A-CGA
9	H	609	CHL	C2-C1-O2A-CGA
10	G	604	CLA	C5-C6-C7-C8
10	B	602	CLA	C16-C17-C18-C20
8	D	5632	DGD	CFB-CGB-CHB-CIB
7	J	9630	LHG	C35-C36-C37-C38
8	A	632	DGD	O1G-C1G-C2G-O2G
8	E	4632	DGD	O1G-C1G-C2G-O2G
9	B	606	CHL	C2A-CAA-CBA-CGA
9	I	607	CHL	C2A-CAA-CBA-CGA
9	D	607	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
10	A	611	CLA	C15-C16-C17-C18
9	D	608	CHL	C3-C5-C6-C7
10	F	612	CLA	C3-C5-C6-C7
10	G	604	CLA	C3A-C2A-CAA-CBA
9	F	608	CHL	C3A-C2A-CAA-CBA
9	D	601	CHL	C3A-C2A-CAA-CBA
10	F	604	CLA	C3A-C2A-CAA-CBA
8	H	7632	DGD	O6E-C5E-C6E-O5E
10	A	603	CLA	C4-C3-C5-C6
10	A	612	CLA	C2-C3-C5-C6
10	B	611	CLA	C11-C10-C8-C9
10	I	602	CLA	C6-C7-C8-C9
10	I	602	CLA	C14-C13-C15-C16
10	H	610	CLA	C14-C13-C15-C16
9	C	601	CHL	C11-C12-C13-C14
10	A	604	CLA	C11-C12-C13-C14
10	I	610	CLA	C14-C13-C15-C16
9	I	609	CHL	C6-C7-C8-C9
9	C	607	CHL	C11-C10-C8-C9
9	J	601	CHL	C6-C7-C8-C9
9	J	601	CHL	C14-C13-C15-C16
7	A	630	LHG	C19-C20-C21-C22
8	G	9632	DGD	CBB-CCB-CDB-CEB
7	G	6630	LHG	C27-C28-C29-C30
6	D	3623	NEX	C39-C29-C30-C31
6	B	1623	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	C	2623	NEX	C39-C29-C30-C31
6	A	623	NEX	C39-C29-C30-C31
8	B	1632	DGD	C1G-C2G-C3G-O3G
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	A	630	LHG	C26-C27-C28-C29
8	B	1632	DGD	C7B-C8B-C9B-CAB
10	D	611	CLA	C16-C17-C18-C20
10	B	602	CLA	C16-C17-C18-C19
9	G	608	CHL	C16-C17-C18-C19
10	A	603	CLA	C16-C17-C18-C20
9	I	608	CHL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	G	9632	DGD	C8B-C9B-CAB-CBB
2	H	7633	BNG	C2'-C3'-C4'-C5'
9	E	605	CHL	O1D-CGD-O2D-CED
10	C	604	CLA	C1A-C2A-CAA-CBA
10	J	611	CLA	C1A-C2A-CAA-CBA
10	C	603	CLA	C1A-C2A-CAA-CBA
10	A	603	CLA	C1A-C2A-CAA-CBA
8	E	4632	DGD	CFB-CGB-CHB-CIB
7	I	8630	LHG	C19-C20-C21-C22
10	H	613	CLA	C16-C17-C18-C20
9	G	608	CHL	C16-C17-C18-C20
10	I	604	CLA	C12-C13-C15-C16
10	D	604	CLA	C11-C12-C13-C15
9	F	607	CHL	C6-C7-C8-C10
10	A	611	CLA	C6-C7-C8-C10
9	C	608	CHL	C11-C10-C8-C7
10	C	602	CLA	C13-C15-C16-C17
10	I	613	CLA	C5-C6-C7-C8
10	I	613	CLA	C16-C17-C18-C19
10	I	613	CLA	C16-C17-C18-C20
8	D	5632	DGD	O6E-C5E-C6E-O5E
10	A	610	CLA	O1D-CGD-O2D-CED
10	A	604	CLA	C2A-CAA-CBA-CGA
9	F	607	CHL	C2A-CAA-CBA-CGA
9	C	607	CHL	C2A-CAA-CBA-CGA
9	J	605	CHL	C2A-CAA-CBA-CGA
10	D	602	CLA	C15-C16-C17-C18
8	A	632	DGD	O6E-C5E-C6E-O5E
8	D	3632	DGD	CFB-CGB-CHB-CIB
10	D	611	CLA	C10-C11-C12-C13
10	H	611	CLA	C15-C16-C17-C18
7	B	1630	LHG	O6-C4-C5-C6
7	G	6630	LHG	O6-C4-C5-C6
8	A	632	DGD	CBB-CCB-CDB-CEB
9	B	608	CHL	C3-C5-C6-C7
9	A	607	CHL	C4-C3-C5-C6
10	I	611	CLA	C4-C3-C5-C6
10	D	612	CLA	C4-C3-C5-C6
9	I	607	CHL	C4-C3-C5-C6
10	E	612	CLA	C4-C3-C5-C6
2	A	633	BNG	O1-C1'-C2'-C3'
10	A	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	I	612	CLA	C2-C3-C5-C6
8	B	2632	DGD	C3B-C4B-C5B-C6B
10	C	603	CLA	C8-C10-C11-C12
7	A	630	LHG	C16-C17-C18-C19
8	B	2632	DGD	C7B-C8B-C9B-CAB
8	H	6632	DGD	CCA-CDA-CEA-CFA
6	D	3623	NEX	C28-C29-C30-C31
6	B	1623	NEX	C28-C29-C30-C31
6	E	4623	NEX	C28-C29-C30-C31
6	F	5623	NEX	C28-C29-C30-C31
6	G	6623	NEX	C28-C29-C30-C31
6	C	2623	NEX	C28-C29-C30-C31
6	A	623	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
9	A	609	CHL	C15-C16-C17-C18
9	J	605	CHL	O1D-CGD-O2D-CED
10	D	602	CLA	C10-C11-C12-C13
10	A	611	CLA	C16-C17-C18-C19
9	F	601	CHL	C15-C16-C17-C18
10	E	611	CLA	C15-C16-C17-C18
9	A	608	CHL	C3-C5-C6-C7
9	F	609	CHL	C4-C3-C5-C6
10	B	603	CLA	C4-C3-C5-C6
10	I	604	CLA	C4-C3-C5-C6
10	E	604	CLA	C4-C3-C5-C6
10	A	604	CLA	C4-C3-C5-C6
7	G	6630	LHG	C26-C27-C28-C29
9	D	606	CHL	C2-C1-O2A-CGA
9	I	601	CHL	C2-C1-O2A-CGA
9	C	606	CHL	C2-C1-O2A-CGA
9	A	601	CHL	C2-C1-O2A-CGA
9	J	609	CHL	C2-C1-O2A-CGA
10	B	611	CLA	C2-C3-C5-C6
10	D	611	CLA	C2-C3-C5-C6
10	C	611	CLA	C2-C3-C5-C6
9	A	607	CHL	C2-C3-C5-C6
10	C	604	CLA	C2-C3-C5-C6
10	G	604	CLA	C2-C3-C5-C6
10	J	611	CLA	C2-C3-C5-C6
10	D	612	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	H	604	CLA	C2-C3-C5-C6
10	I	604	CLA	O1A-CGA-O2A-C1
2	J	9633	BNG	C2'-C3'-C4'-C5'
8	D	5632	DGD	C3A-C4A-C5A-C6A
7	B	1630	LHG	C12-C13-C14-C15
10	H	604	CLA	O1A-CGA-O2A-C1
9	D	609	CHL	C13-C15-C16-C17
10	H	604	CLA	C2A-CAA-CBA-CGA
10	F	614	CLA	C2A-CAA-CBA-CGA
10	G	602	CLA	C16-C17-C18-C20
10	D	613	CLA	C16-C17-C18-C20
8	H	7632	DGD	C8A-C9A-CAA-CBA
8	H	7632	DGD	CFB-CGB-CHB-CIB
4	D	3620	LUT	C1-C6-C7-C8
4	F	5620	LUT	C1-C6-C7-C8
4	E	4621	LUT	C5-C6-C7-C8
4	H	7621	LUT	C5-C6-C7-C8
4	C	2620	LUT	C1-C6-C7-C8
4	E	4620	LUT	C1-C6-C7-C8
4	G	6620	LUT	C1-C6-C7-C8
4	A	620	LUT	C1-C6-C7-C8
4	G	6621	LUT	C1-C6-C7-C8
4	H	7620	LUT	C1-C6-C7-C8
4	I	8620	LUT	C1-C6-C7-C8
4	I	8621	LUT	C5-C6-C7-C8
4	B	1620	LUT	C1-C6-C7-C8
4	A	621	LUT	C5-C6-C7-C8
8	D	3632	DGD	CDA-CEA-CFA-CGA
10	H	604	CLA	CBA-CGA-O2A-C1
9	D	609	CHL	C4-C3-C5-C6
9	H	601	CHL	C4-C3-C5-C6
10	J	612	CLA	C4-C3-C5-C6
10	F	603	CLA	C4-C3-C5-C6
9	C	609	CHL	C4-C3-C5-C6
9	A	609	CHL	C4-C3-C5-C6
10	E	603	CLA	C4-C3-C5-C6
9	G	607	CHL	C4-C3-C5-C6
9	H	609	CHL	C4-C3-C5-C6
9	D	601	CHL	C4-C3-C5-C6
9	J	607	CHL	C4-C3-C5-C6
10	H	603	CLA	C4-C3-C5-C6
9	J	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	D	607	CHL	C4-C3-C5-C6
9	B	609	CHL	C4-C3-C5-C6
10	H	611	CLA	C2-C3-C5-C6
9	F	607	CHL	C2-C3-C5-C6
10	F	612	CLA	C2-C3-C5-C6
10	F	604	CLA	C2-C3-C5-C6
10	C	602	CLA	C3-C5-C6-C7
10	H	613	CLA	C3-C5-C6-C7
2	A	633	BNG	C2'-C3'-C4'-C5'
9	J	609	CHL	C15-C16-C17-C18
7	G	6630	LHG	O6-C4-C5-O7
10	D	614	CLA	C2A-CAA-CBA-CGA
9	H	607	CHL	C4-C3-C5-C6
10	J	604	CLA	C4-C3-C5-C6
9	J	609	CHL	C4-C3-C5-C6
9	H	607	CHL	C6-C7-C8-C10
10	A	604	CLA	C2-C3-C5-C6
9	I	609	CHL	C11-C10-C8-C7
10	D	612	CLA	C12-C13-C15-C16
9	E	609	CHL	C2-C3-C5-C6
9	I	607	CHL	C2-C3-C5-C6
9	I	607	CHL	C12-C13-C15-C16
10	A	603	CLA	C11-C12-C13-C15
9	D	607	CHL	C2-C3-C5-C6
9	B	607	CHL	C2-C3-C5-C6
10	G	610	CLA	CBA-CGA-O2A-C1
7	I	8630	LHG	O1-C1-C2-O2
10	D	612	CLA	C8-C10-C11-C12
9	H	609	CHL	C13-C15-C16-C17
10	D	611	CLA	C16-C17-C18-C19
10	H	602	CLA	C13-C15-C16-C17
9	B	608	CHL	CBA-CGA-O2A-C1
7	H	7630	LHG	O8-C23-C24-C25
7	B	1630	LHG	O8-C23-C24-C25
10	F	611	CLA	C4-C3-C5-C6
9	I	601	CHL	C4-C3-C5-C6
10	D	604	CLA	C4-C3-C5-C6
9	G	609	CHL	C4-C3-C5-C6
9	I	609	CHL	C4-C3-C5-C6
10	B	603	CLA	C2-C3-C5-C6
10	I	604	CLA	C2-C3-C5-C6
10	E	604	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	C	612	CLA	C2-C3-C5-C6
10	I	611	CLA	C2-C3-C5-C6
9	J	607	CHL	C2-C3-C5-C6
10	E	612	CLA	C2-C3-C5-C6
10	F	603	CLA	C16-C17-C18-C19
10	F	611	CLA	C11-C10-C8-C9
10	F	611	CLA	C11-C12-C13-C14
10	D	611	CLA	C11-C12-C13-C14
10	G	602	CLA	C6-C7-C8-C9
9	A	609	CHL	C6-C7-C8-C9
9	E	601	CHL	C14-C13-C15-C16
9	G	609	CHL	C6-C7-C8-C9
10	E	603	CLA	C14-C13-C15-C16
10	B	613	CLA	C11-C12-C13-C14
10	J	611	CLA	C11-C12-C13-C14
10	C	602	CLA	C11-C12-C13-C14
10	B	610	CLA	C11-C10-C8-C9
10	E	610	CLA	C14-C13-C15-C16
9	F	601	CHL	C14-C13-C15-C16
10	H	604	CLA	C11-C12-C13-C14
10	D	602	CLA	C6-C7-C8-C9
9	H	608	CHL	C11-C10-C8-C9
10	F	604	CLA	C14-C13-C15-C16
9	C	608	CHL	C11-C12-C13-C14
9	E	608	CHL	C11-C12-C13-C14
9	G	608	CHL	C11-C12-C13-C14
8	A	632	DGD	C8A-C9A-CAA-CBA
9	I	609	CHL	C3A-C2A-CAA-CBA
10	D	603	CLA	C3A-C2A-CAA-CBA
10	H	603	CLA	C3A-C2A-CAA-CBA
10	A	603	CLA	C3A-C2A-CAA-CBA
9	C	605	CHL	CAA-CBA-CGA-O2A
7	F	5630	LHG	O7-C7-C8-C9
9	I	605	CHL	CAA-CBA-CGA-O2A
10	A	602	CLA	CAD-CBD-CGD-O2D
10	B	614	CLA	CAD-CBD-CGD-O2D
10	E	604	CLA	CAD-CBD-CGD-O2D
10	C	612	CLA	CAD-CBD-CGD-O2D
10	D	604	CLA	CAD-CBD-CGD-O2D
10	G	604	CLA	CAD-CBD-CGD-O2D
10	A	604	CLA	CAD-CBD-CGD-O2D
10	J	614	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
10	G	603	CLA	CAD-CBD-CGD-O2D
10	H	604	CLA	CAD-CBD-CGD-O2D
10	D	602	CLA	CAD-CBD-CGD-O2D
10	A	614	CLA	CAD-CBD-CGD-O2D
9	J	608	CHL	C16-C17-C18-C19
10	I	611	CLA	C2-C1-O2A-CGA
7	J	9630	LHG	C16-C17-C18-C19
9	A	605	CHL	CAA-CBA-CGA-O2A
7	G	6630	LHG	O7-C7-C8-C9
2	G	6633	BNG	C4'-C5'-C6'-C7'
10	C	612	CLA	C4-C3-C5-C6
9	E	601	CHL	C4-C3-C5-C6
10	G	603	CLA	C4-C3-C5-C6
10	B	612	CLA	C4-C3-C5-C6
10	C	613	CLA	C4-C3-C5-C6
9	J	608	CHL	C3-C5-C6-C7
10	F	611	CLA	C2-C3-C5-C6
9	D	609	CHL	C2-C3-C5-C6
9	C	609	CHL	C2-C3-C5-C6
9	H	609	CHL	C2-C3-C5-C6
10	A	603	CLA	C2-C3-C5-C6
9	B	609	CHL	C2-C3-C5-C6
7	E	4630	LHG	O8-C23-C24-C25
9	H	605	CHL	CAA-CBA-CGA-O2A
8	H	7632	DGD	O1G-C1A-C2A-C3A
7	G	6630	LHG	O8-C23-C24-C25
9	J	605	CHL	CAA-CBA-CGA-O2A
8	D	3632	DGD	O1G-C1A-C2A-C3A
7	D	3630	LHG	O8-C23-C24-C25
8	B	1632	DGD	CBB-CCB-CDB-CEB
5	B	5622	XAT	O24-C26-C27-C28
5	E	2622	XAT	O24-C26-C27-C28
5	B	1622	XAT	O24-C26-C27-C28
5	F	6622	XAT	O24-C26-C27-C28
7	B	1630	LHG	O6-C4-C5-O7
7	C	2630	LHG	O7-C7-C8-C9
7	A	630	LHG	O8-C23-C24-C25
9	B	605	CHL	CAA-CBA-CGA-O2A
10	F	611	CLA	O2A-C1-C2-C3
9	D	608	CHL	O2A-C1-C2-C3
9	A	608	CHL	O2A-C1-C2-C3
10	J	611	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	E	611	CLA	O2A-C1-C2-C3
9	J	608	CHL	O2A-C1-C2-C3
9	C	608	CHL	O2A-C1-C2-C3
9	E	608	CHL	O2A-C1-C2-C3
9	G	608	CHL	O2A-C1-C2-C3
9	H	607	CHL	C2A-CAA-CBA-CGA
9	G	607	CHL	C2A-CAA-CBA-CGA
9	H	605	CHL	C2A-CAA-CBA-CGA
10	H	614	CLA	O1D-CGD-O2D-CED
7	H	7630	LHG	O7-C7-C8-C9
7	I	8630	LHG	O7-C7-C8-C9
10	C	602	CLA	CBD-CGD-O2D-CED
9	E	608	CHL	C3-C5-C6-C7
10	J	603	CLA	C13-C15-C16-C17
9	G	609	CHL	C16-C17-C18-C20
10	A	611	CLA	C16-C17-C18-C20
10	B	602	CLA	CBD-CGD-O2D-CED
10	I	604	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-O2D
10	J	604	CLA	CHA-CBD-CGD-O1D
10	F	603	CLA	CHA-CBD-CGD-O1D
10	F	603	CLA	CHA-CBD-CGD-O2D
10	I	602	CLA	CHA-CBD-CGD-O2D
10	B	602	CLA	CHA-CBD-CGD-O2D
10	C	604	CLA	CHA-CBD-CGD-O2D
10	J	602	CLA	CHA-CBD-CGD-O1D
10	J	602	CLA	CHA-CBD-CGD-O2D
9	C	601	CHL	CHA-CBD-CGD-O1D
9	C	601	CHL	CHA-CBD-CGD-O2D
10	E	602	CLA	CHA-CBD-CGD-O2D
10	G	604	CLA	CHA-CBD-CGD-O1D
10	J	614	CLA	CHA-CBD-CGD-O1D
9	B	601	CHL	CHA-CBD-CGD-O1D
10	H	602	CLA	CHA-CBD-CGD-O2D
9	D	601	CHL	CHA-CBD-CGD-O1D
9	D	601	CHL	CHA-CBD-CGD-O2D
9	F	601	CHL	CHA-CBD-CGD-O1D
9	F	601	CHL	CHA-CBD-CGD-O2D
8	D	5632	DGD	CBB-CCB-CDB-CEB
10	J	612	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	I	609	CHL	C2-C3-C5-C6
10	B	612	CLA	C2-C3-C5-C6
10	H	603	CLA	C2-C3-C5-C6
9	C	607	CHL	C13-C15-C16-C17
8	G	9632	DGD	C9B-CAB-CBB-CCB
10	C	603	CLA	C16-C17-C18-C20
8	D	5632	DGD	O1G-C1G-C2G-O2G
10	B	602	CLA	O1D-CGD-O2D-CED
8	I	8632	DGD	CBB-CCB-CDB-CEB
10	A	602	CLA	C15-C16-C17-C18
9	E	601	CHL	CAA-CBA-CGA-O2A
10	D	613	CLA	CAA-CBA-CGA-O2A
7	I	8630	LHG	O8-C23-C24-C25
10	F	612	CLA	CAA-CBA-CGA-O2A
10	B	604	CLA	C2A-CAA-CBA-CGA
9	A	601	CHL	C13-C15-C16-C17
9	I	601	CHL	CBA-CGA-O2A-C1
9	G	601	CHL	C4-C3-C5-C6
2	E	4633	BNG	O1-C1'-C2'-C3'
10	J	604	CLA	C2-C3-C5-C6
10	E	604	CLA	C12-C13-C15-C16
10	D	604	CLA	C2-C3-C5-C6
10	B	604	CLA	C12-C13-C15-C16
9	J	609	CHL	C11-C10-C8-C7
10	I	612	CLA	C12-C13-C15-C16
10	H	602	CLA	C16-C17-C18-C20
8	D	5632	DGD	C3B-C4B-C5B-C6B
2	I	8633	BNG	C2'-C3'-C4'-C5'
7	F	5630	LHG	O8-C23-C24-C25
7	A	630	LHG	O7-C7-C8-C9
9	J	606	CHL	CAA-CBA-CGA-O2A
10	B	611	CLA	C11-C12-C13-C14
9	D	609	CHL	C11-C12-C13-C14
10	F	610	CLA	C11-C10-C8-C9
9	B	608	CHL	C11-C10-C8-C9
10	C	610	CLA	C11-C10-C8-C9
10	F	602	CLA	C6-C7-C8-C9
9	A	609	CHL	C11-C12-C13-C14
9	E	601	CHL	C6-C7-C8-C9
10	D	610	CLA	C11-C10-C8-C9
10	I	611	CLA	C11-C12-C13-C14
9	G	608	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
10	A	603	CLA	C11-C12-C13-C14
2	B	1633	BNG	C2'-C3'-C4'-C5'
7	D	3630	LHG	O7-C7-C8-C9
9	H	609	CHL	C16-C17-C18-C20
10	D	602	CLA	C13-C15-C16-C17
10	D	611	CLA	C2A-CAA-CBA-CGA
7	A	630	LHG	C7-C8-C9-C10
7	C	2630	LHG	O8-C23-C24-C25
7	E	4630	LHG	O10-C23-C24-C25
9	H	605	CHL	CAA-CBA-CGA-O1A
8	H	7632	DGD	O1A-C1A-C2A-C3A
7	D	3630	LHG	O10-C23-C24-C25
10	I	603	CLA	C4-C3-C5-C6
9	G	605	CHL	CAA-CBA-CGA-O2A
7	C	2630	LHG	O9-C7-C8-C9
7	A	630	LHG	O10-C23-C24-C25
9	B	605	CHL	CAA-CBA-CGA-O1A
7	G	6630	LHG	O10-C23-C24-C25
10	H	610	CLA	C8-C10-C11-C12
9	I	608	CHL	C1A-C2A-CAA-CBA
10	G	603	CLA	C1A-C2A-CAA-CBA
9	E	609	CHL	C1A-C2A-CAA-CBA
9	D	601	CHL	C1A-C2A-CAA-CBA
9	J	608	CHL	C1A-C2A-CAA-CBA
9	H	608	CHL	C1A-C2A-CAA-CBA
10	H	613	CLA	C1A-C2A-CAA-CBA
9	J	601	CHL	C1A-C2A-CAA-CBA
7	H	7630	LHG	C11-C12-C13-C14
2	F	5633	BNG	C4'-C5'-C6'-C7'
9	J	605	CHL	CAA-CBA-CGA-O1A
9	G	609	CHL	O1D-CGD-O2D-CED
9	D	609	CHL	C2-C1-O2A-CGA
9	C	605	CHL	CAA-CBA-CGA-O1A
7	H	7630	LHG	O9-C7-C8-C9
7	H	7630	LHG	O10-C23-C24-C25
7	B	1630	LHG	O10-C23-C24-C25
7	I	8630	LHG	O9-C7-C8-C9
8	A	632	DGD	O1G-C1G-C2G-C3G
8	E	4632	DGD	O1G-C1G-C2G-C3G
10	C	611	CLA	CAA-CBA-CGA-O2A
9	B	605	CHL	C2A-CAA-CBA-CGA
10	A	613	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
9	A	605	CHL	CAA-CBA-CGA-O1A
10	C	614	CLA	O1D-CGD-O2D-CED
10	J	603	CLA	CAA-CBA-CGA-O2A
9	D	605	CHL	CAA-CBA-CGA-O2A
7	A	630	LHG	O9-C7-C8-C9
7	E	4630	LHG	C3-O3-P-O5
7	G	6630	LHG	O9-C7-C8-C9
9	I	605	CHL	CAA-CBA-CGA-O1A
8	D	3632	DGD	O1A-C1A-C2A-C3A
10	B	614	CLA	O2A-C1-C2-C3
10	J	612	CLA	C15-C16-C17-C18
4	F	5621	LUT	C5-C6-C7-C8
4	J	9620	LUT	C5-C6-C7-C8
4	G	6621	LUT	C5-C6-C7-C8
9	J	609	CHL	C8-C10-C11-C12
10	I	602	CLA	CAA-CBA-CGA-O2A
9	F	608	CHL	CAA-CBA-CGA-O2A
10	F	602	CLA	CBA-CGA-O2A-C1
7	F	5630	LHG	O9-C7-C8-C9
7	C	2630	LHG	O10-C23-C24-C25
10	F	612	CLA	CAA-CBA-CGA-O1A
10	J	611	CLA	C15-C16-C17-C18
10	D	604	CLA	CAA-CBA-CGA-O1A
9	J	606	CHL	CAA-CBA-CGA-O1A
7	D	3630	LHG	O9-C7-C8-C9
9	E	607	CHL	C4-C3-C5-C6
10	I	612	CLA	C10-C11-C12-C13
10	G	602	CLA	C16-C17-C18-C19
10	I	604	CLA	CAD-CBD-CGD-O1D
10	D	604	CLA	CAD-CBD-CGD-O1D
10	G	604	CLA	CAD-CBD-CGD-O1D
10	J	614	CLA	CAD-CBD-CGD-O1D
9	D	601	CHL	CAD-CBD-CGD-O1D
10	H	604	CLA	CAD-CBD-CGD-O1D
8	B	2632	DGD	C1G-C2G-O2G-C1B
8	B	2632	DGD	C3G-C2G-O2G-C1B
10	F	614	CLA	CAD-CBD-CGD-O1D
10	F	604	CLA	CAD-CBD-CGD-O1D
9	D	605	CHL	CAA-CBA-CGA-O1A
10	A	602	CLA	CAA-CBA-CGA-O2A
10	B	613	CLA	CAA-CBA-CGA-O2A
9	D	609	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
10	C	604	CLA	C6-C7-C8-C9
9	A	609	CHL	C11-C10-C8-C9
10	G	604	CLA	C14-C13-C15-C16
10	D	603	CLA	C11-C12-C13-C14
9	E	609	CHL	C11-C12-C13-C14
9	H	609	CHL	C11-C12-C13-C14
9	J	609	CHL	C11-C10-C8-C9
10	E	611	CLA	C11-C12-C13-C14
10	E	611	CLA	C14-C13-C15-C16
9	J	608	CHL	C11-C10-C8-C9
9	H	608	CHL	C6-C7-C8-C9
8	I	8632	DGD	O1G-C1A-C2A-C3A
10	F	613	CLA	CAA-CBA-CGA-O2A
7	J	9630	LHG	O8-C23-C24-C25
9	E	605	CHL	CAA-CBA-CGA-O2A
8	B	1632	DGD	O1G-C1A-C2A-C3A
10	F	604	CLA	C5-C6-C7-C8
7	E	4630	LHG	O7-C7-C8-C9
10	B	602	CLA	CAA-CBA-CGA-O2A
10	A	612	CLA	CAA-CBA-CGA-O2A
10	I	613	CLA	CAA-CBA-CGA-O2A
9	C	601	CHL	CAA-CBA-CGA-O2A
10	J	613	CLA	CAA-CBA-CGA-O2A
10	H	612	CLA	CAA-CBA-CGA-O2A
7	B	1630	LHG	O7-C7-C8-C9
10	D	602	CLA	CAA-CBA-CGA-O2A
8	A	632	DGD	C9B-CAB-CBB-CCB
8	H	7632	DGD	C9A-CAA-CBA-CCA
2	D	3633	BNG	C2'-C3'-C4'-C5'
9	B	601	CHL	C16-C17-C18-C19
10	A	610	CLA	C11-C10-C8-C7
10	F	610	CLA	C6-C7-C8-C10
10	C	611	CLA	C3A-C2A-CAA-CBA
10	J	604	CLA	C3A-C2A-CAA-CBA
9	A	607	CHL	C11-C12-C13-C15
10	C	604	CLA	C3A-C2A-CAA-CBA
10	D	604	CLA	C12-C13-C15-C16
9	A	609	CHL	C3A-C2A-CAA-CBA
9	A	609	CHL	C6-C7-C8-C10
9	C	601	CHL	C12-C13-C15-C16
9	E	601	CHL	C6-C7-C8-C10
9	A	608	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
9	G	609	CHL	C2-C3-C5-C6
10	A	604	CLA	C6-C7-C8-C10
10	D	603	CLA	C6-C7-C8-C10
9	C	607	CHL	C6-C7-C8-C10
10	C	603	CLA	C12-C13-C15-C16
10	H	604	CLA	C12-C13-C15-C16
9	B	606	CHL	C3A-C2A-CAA-CBA
9	J	608	CHL	C11-C10-C8-C7
9	H	608	CHL	C6-C7-C8-C10
9	E	608	CHL	C11-C10-C8-C7
9	G	608	CHL	C11-C10-C8-C7
7	E	4630	LHG	O9-C7-C8-C9
9	E	605	CHL	CAA-CBA-CGA-O1A
7	J	9630	LHG	O7-C7-C8-C9
10	E	603	CLA	CAA-CBA-CGA-O2A
10	A	613	CLA	CAA-CBA-CGA-O2A
9	J	608	CHL	CAA-CBA-CGA-O2A
8	B	2632	DGD	CFA-CGA-CHA-CIA
10	A	602	CLA	CAA-CBA-CGA-O1A
7	F	5630	LHG	O10-C23-C24-C25
9	J	607	CHL	C16-C17-C18-C20
9	G	601	CHL	CAA-CBA-CGA-O2A
9	I	608	CHL	CAA-CBA-CGA-O2A
9	H	608	CHL	CAA-CBA-CGA-O2A
10	I	612	CLA	C13-C15-C16-C17
7	C	2630	LHG	C19-C20-C21-C22
8	B	1632	DGD	O1A-C1A-C2A-C3A
7	G	6630	LHG	C33-C34-C35-C36
10	G	613	CLA	CAA-CBA-CGA-O2A
9	F	601	CHL	CAA-CBA-CGA-O2A
10	E	612	CLA	CAA-CBA-CGA-O2A
9	C	608	CHL	CAA-CBA-CGA-O2A
10	B	602	CLA	C13-C15-C16-C17
9	E	601	CHL	CAA-CBA-CGA-O1A
7	J	9630	LHG	O9-C7-C8-C9
7	I	8630	LHG	O10-C23-C24-C25
9	J	608	CHL	CAA-CBA-CGA-O1A
9	G	605	CHL	C2A-CAA-CBA-CGA
10	C	603	CLA	C15-C16-C17-C18
10	C	611	CLA	CAA-CBA-CGA-O1A
10	B	603	CLA	CAA-CBA-CGA-O2A
10	E	602	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
10	G	612	CLA	CAA-CBA-CGA-O2A
10	B	612	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

139 monomers are involved in 193 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	611	CLA	3	0
9	G	601	CHL	3	0
10	F	611	CLA	1	0
9	D	609	CHL	1	0
4	F	5620	LUT	1	0
10	A	610	CLA	2	0
10	F	610	CLA	1	0
10	A	602	CLA	3	0
10	G	610	CLA	1	0
9	H	601	CHL	1	0
9	B	608	CHL	1	0
9	F	609	CHL	1	0
10	B	603	CLA	4	0
10	I	604	CLA	1	0
10	C	610	CLA	1	0
8	I	8632	DGD	1	0
10	D	611	CLA	2	0
10	F	602	CLA	3	0
10	H	611	CLA	3	0
7	E	4630	LHG	1	0
7	F	5630	LHG	3	0
10	C	611	CLA	3	0
10	J	612	CLA	2	0
7	H	7630	LHG	2	0
10	G	602	CLA	2	0
9	I	601	CHL	2	0
4	E	4621	LUT	1	0
10	J	604	CLA	1	0
8	D	5632	DGD	1	0
10	E	604	CLA	1	0
10	G	604	CLA	1	0
10	F	603	CLA	3	0
10	I	602	CLA	2	0
4	F	5621	LUT	1	0
10	B	602	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	609	CHL	2	0
5	H	4622	XAT	1	0
10	C	612	CLA	2	0
10	A	612	CLA	2	0
4	H	7621	LUT	2	0
10	D	604	CLA	2	0
10	J	602	CLA	2	0
10	H	610	CLA	2	0
10	I	613	CLA	1	0
9	C	601	CHL	1	0
9	E	601	CHL	1	0
9	A	608	CHL	1	0
10	F	613	CLA	2	0
10	E	602	CLA	2	0
9	G	609	CHL	2	0
10	E	603	CLA	4	0
10	D	610	CLA	1	0
10	J	610	CLA	1	0
10	B	604	CLA	1	0
10	A	604	CLA	1	0
9	A	605	CHL	1	0
10	B	613	CLA	1	0
7	C	2630	LHG	1	0
4	E	4620	LUT	2	0
10	D	613	CLA	1	0
10	I	610	CLA	2	0
4	J	9621	LUT	1	0
10	J	614	CLA	1	0
10	J	611	CLA	3	0
10	A	611	CLA	3	0
10	J	613	CLA	1	0
10	I	603	CLA	3	0
10	E	611	CLA	1	0
10	C	602	CLA	3	0
5	J	3622	XAT	1	0
7	G	6630	LHG	2	0
10	G	612	CLA	2	0
4	D	3621	LUT	1	0
9	I	609	CHL	1	0
9	F	608	CHL	1	0
10	H	612	CLA	2	0
10	D	603	CLA	1	0

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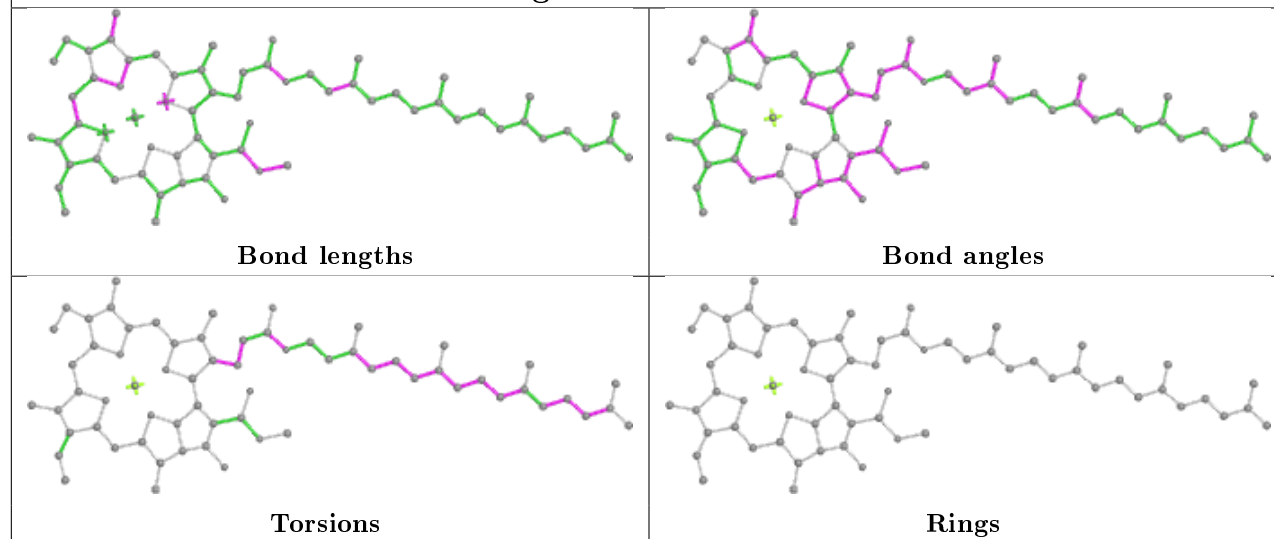
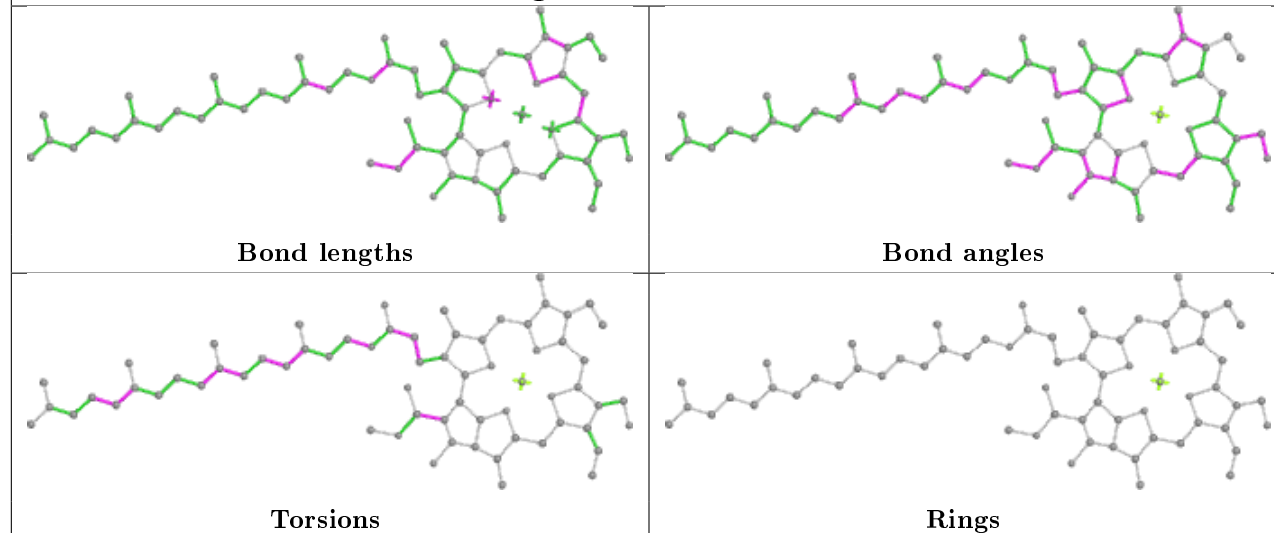
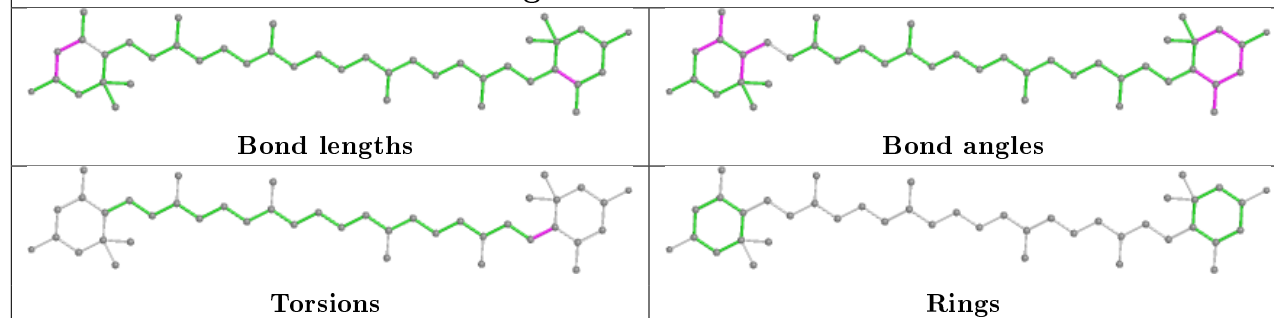
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	611	CLA	2	0
7	B	1630	LHG	3	0
4	A	620	LUT	2	0
10	G	613	CLA	1	0
9	H	605	CHL	1	0
10	G	603	CLA	3	0
9	G	607	CHL	1	0
9	E	605	CHL	1	0
10	B	610	CLA	2	0
10	C	614	CLA	1	0
9	E	609	CHL	1	0
9	G	606	CHL	1	0
9	A	601	CHL	2	0
9	B	601	CHL	3	0
10	H	602	CLA	3	0
10	E	610	CLA	1	0
9	I	606	CHL	1	0
9	H	609	CHL	2	0
7	A	630	LHG	2	0
10	C	603	CLA	4	0
9	D	601	CHL	1	0
9	F	601	CHL	3	0
10	J	603	CLA	3	0
5	E	2622	XAT	2	0
4	G	6621	LUT	1	0
4	B	1621	LUT	2	0
10	I	612	CLA	1	0
9	B	605	CHL	2	0
9	B	606	CHL	1	0
2	D	3633	BNG	1	0
7	I	8630	LHG	3	0
8	A	632	DGD	1	0
4	I	8620	LUT	2	0
9	I	605	CHL	1	0
10	D	612	CLA	2	0
4	I	8621	LUT	1	0
10	E	612	CLA	2	0
10	C	604	CLA	1	0
10	D	602	CLA	2	0
5	B	1622	XAT	1	0
9	H	608	CHL	1	0
6	G	6623	NEX	1	0

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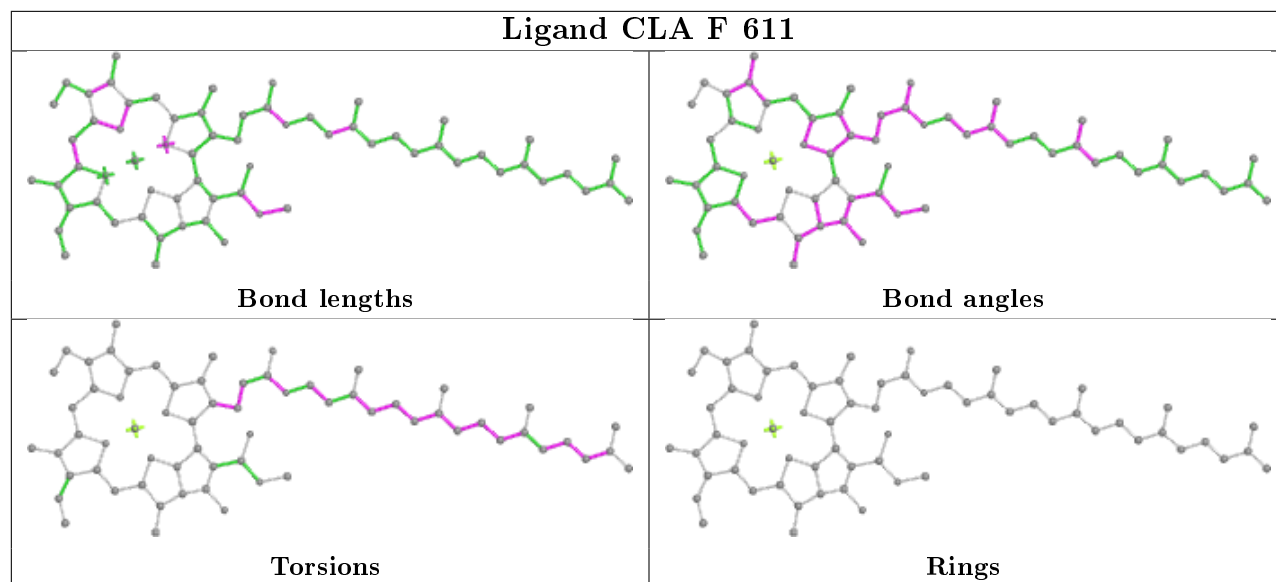
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	605	CHL	2	0
5	I	9622	XAT	1	0
10	F	604	CLA	1	0
10	B	612	CLA	2	0
4	C	2621	LUT	2	0
10	H	603	CLA	4	0
9	C	608	CHL	2	0
10	G	611	CLA	4	0
8	H	6632	DGD	1	0
10	H	613	CLA	1	0
4	B	1620	LUT	2	0
10	C	613	CLA	1	0
5	F	6622	XAT	1	0
10	E	613	CLA	1	0
9	G	608	CHL	2	0
10	A	603	CLA	3	0
10	E	614	CLA	1	0
9	B	609	CHL	1	0
4	A	621	LUT	1	0
7	D	3630	LHG	1	0

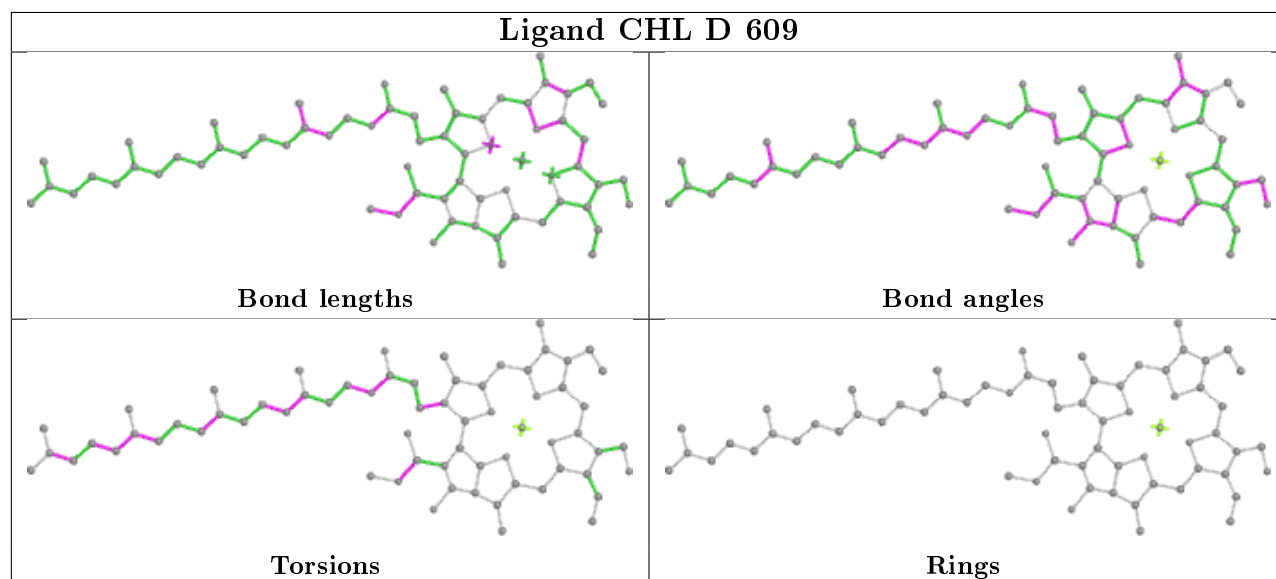
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA B 611**Ligand CHL G 601****Ligand LUT D 3620**

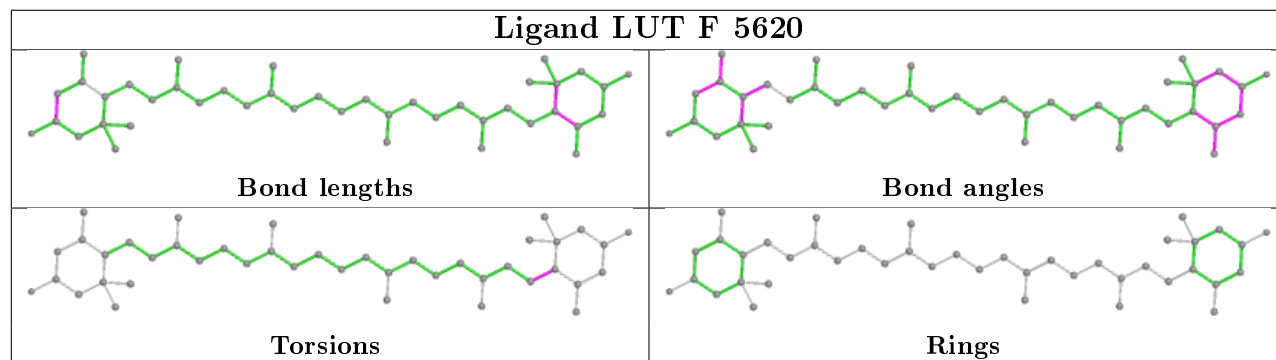
Ligand CLA F 611

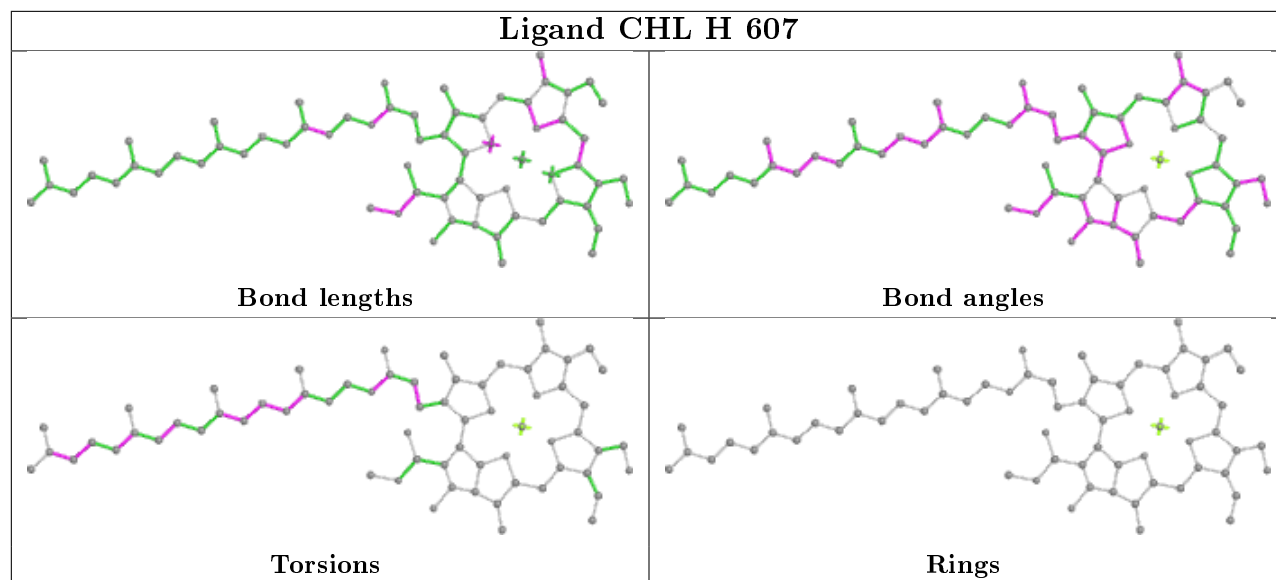
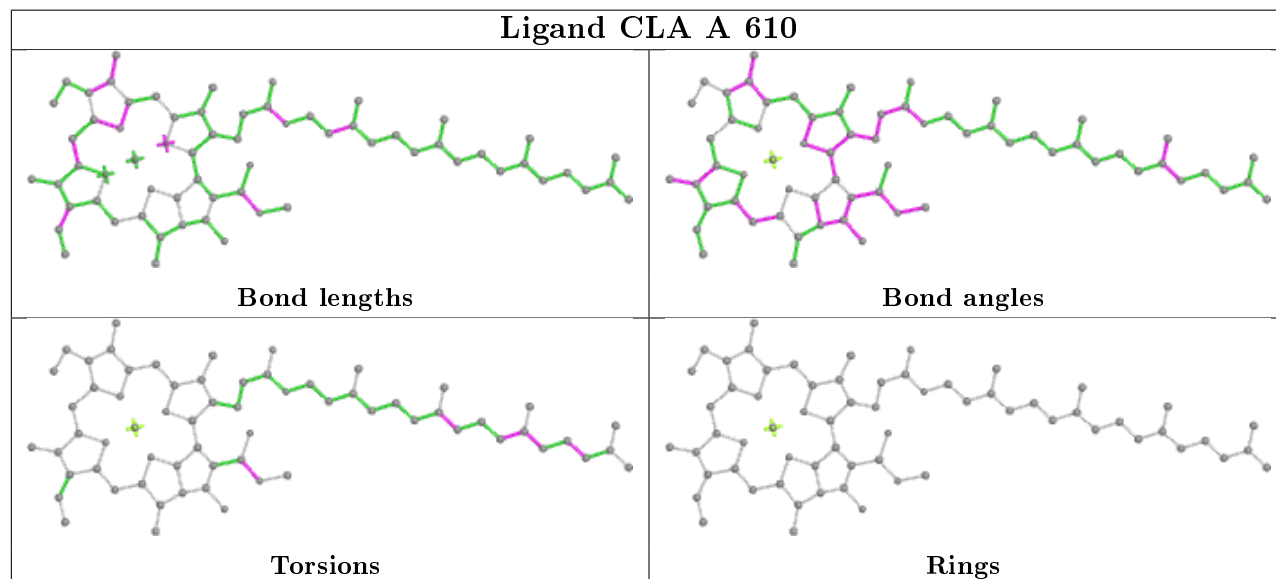
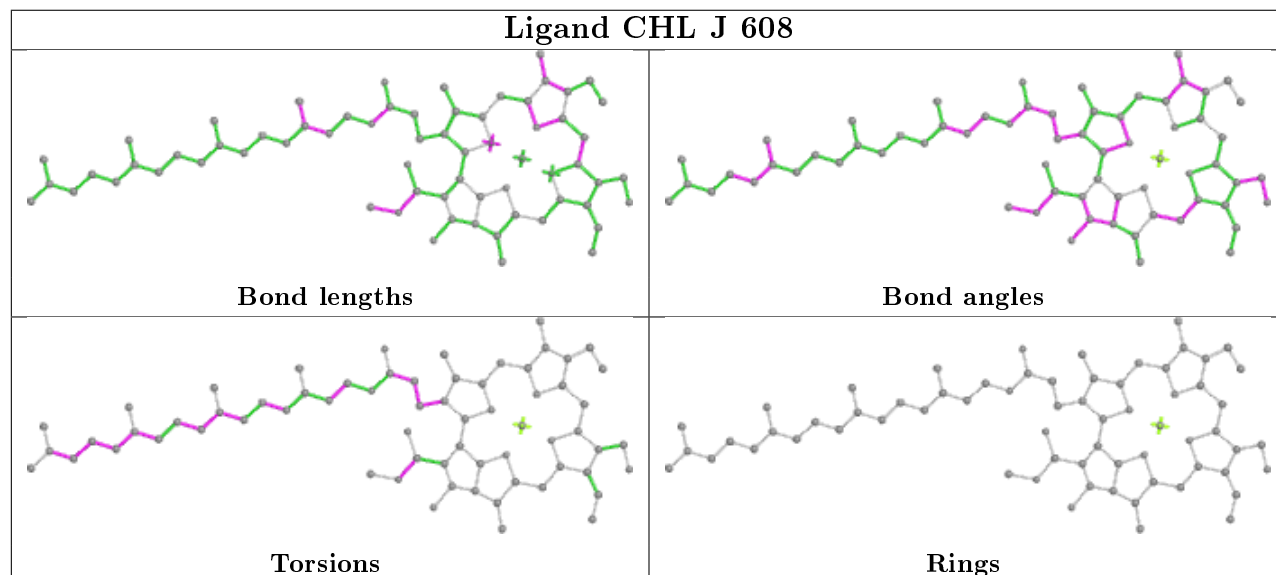


Ligand CHL D 609

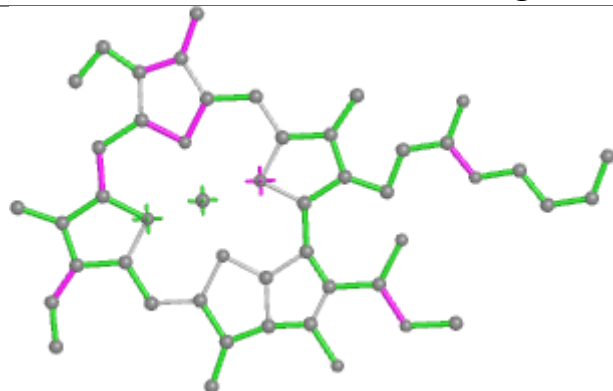


Ligand LUT F 5620

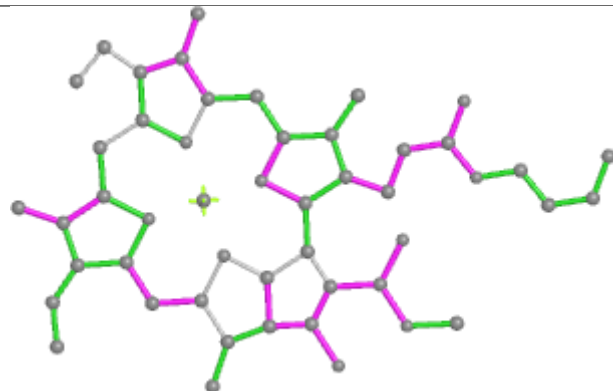


Ligand CHL H 607**Ligand CLA A 610****Ligand CHL J 608**

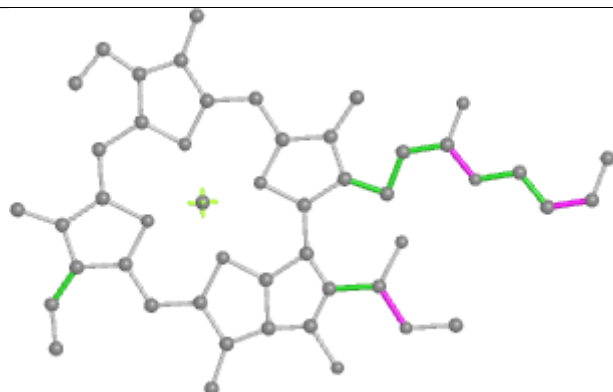
Ligand CLA G 614



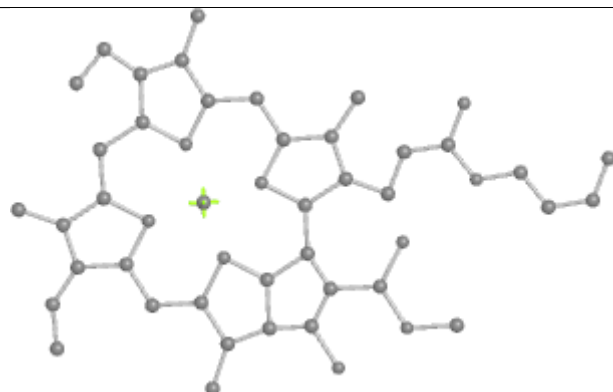
Bond lengths



Bond angles

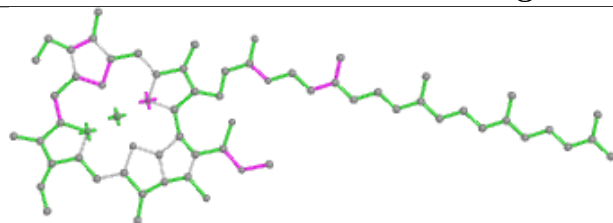


Torsions

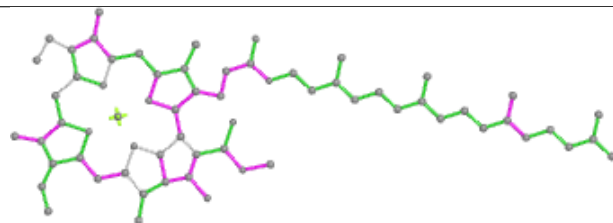


Rings

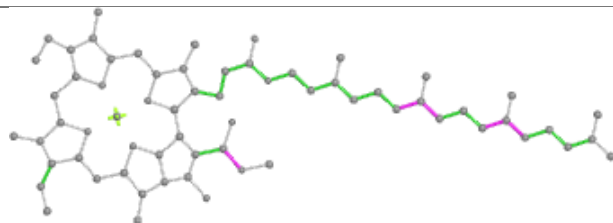
Ligand CLA F 610



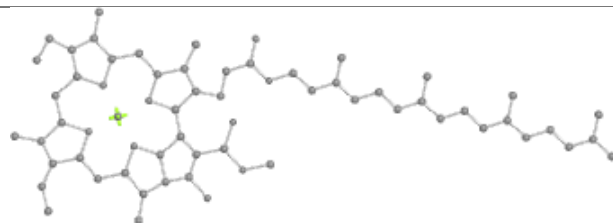
Bond lengths



Bond angles

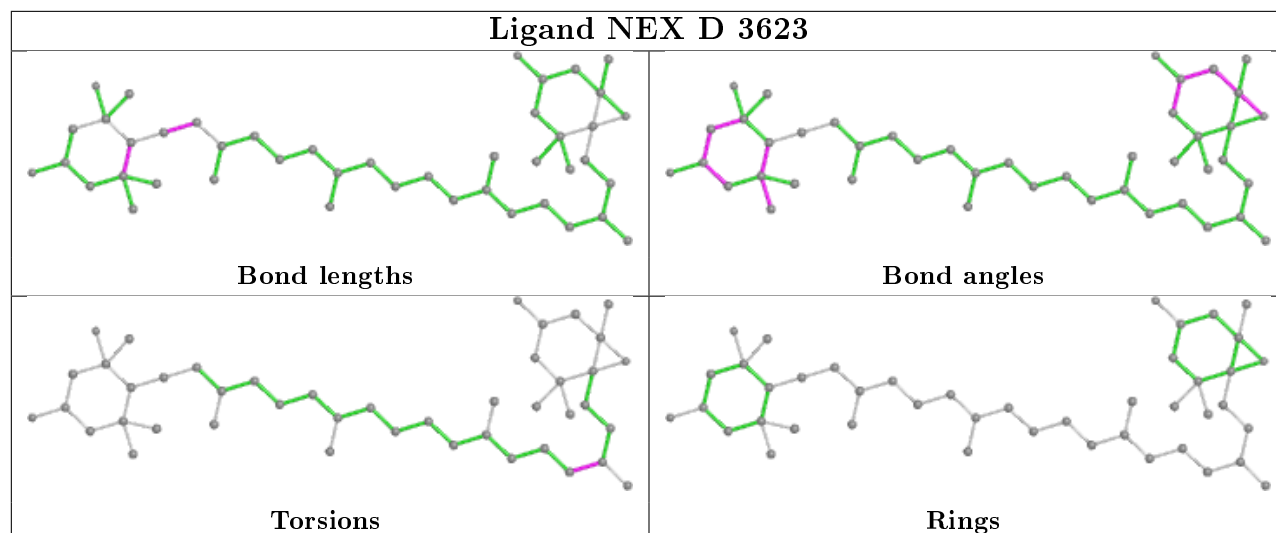


Torsions

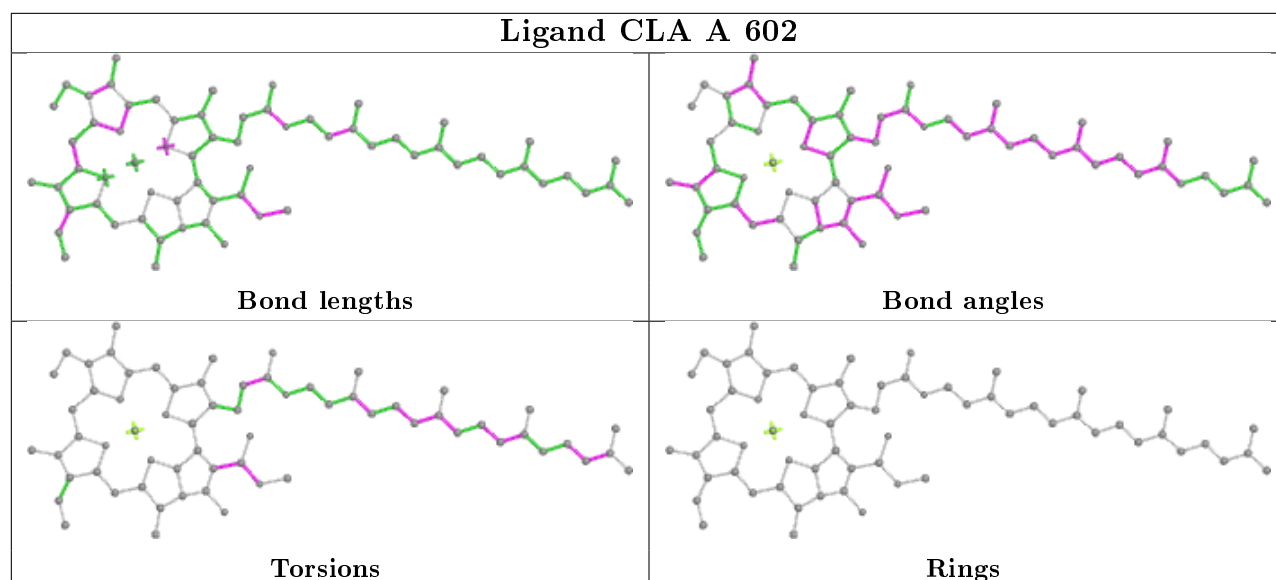


Rings

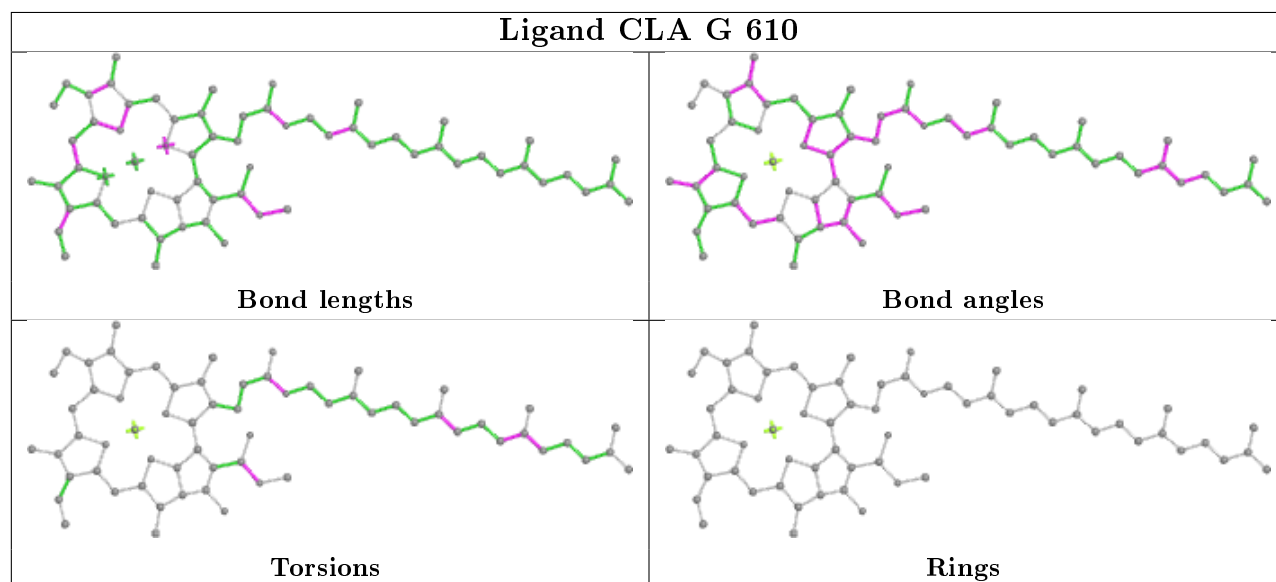
Ligand NEX D 3623

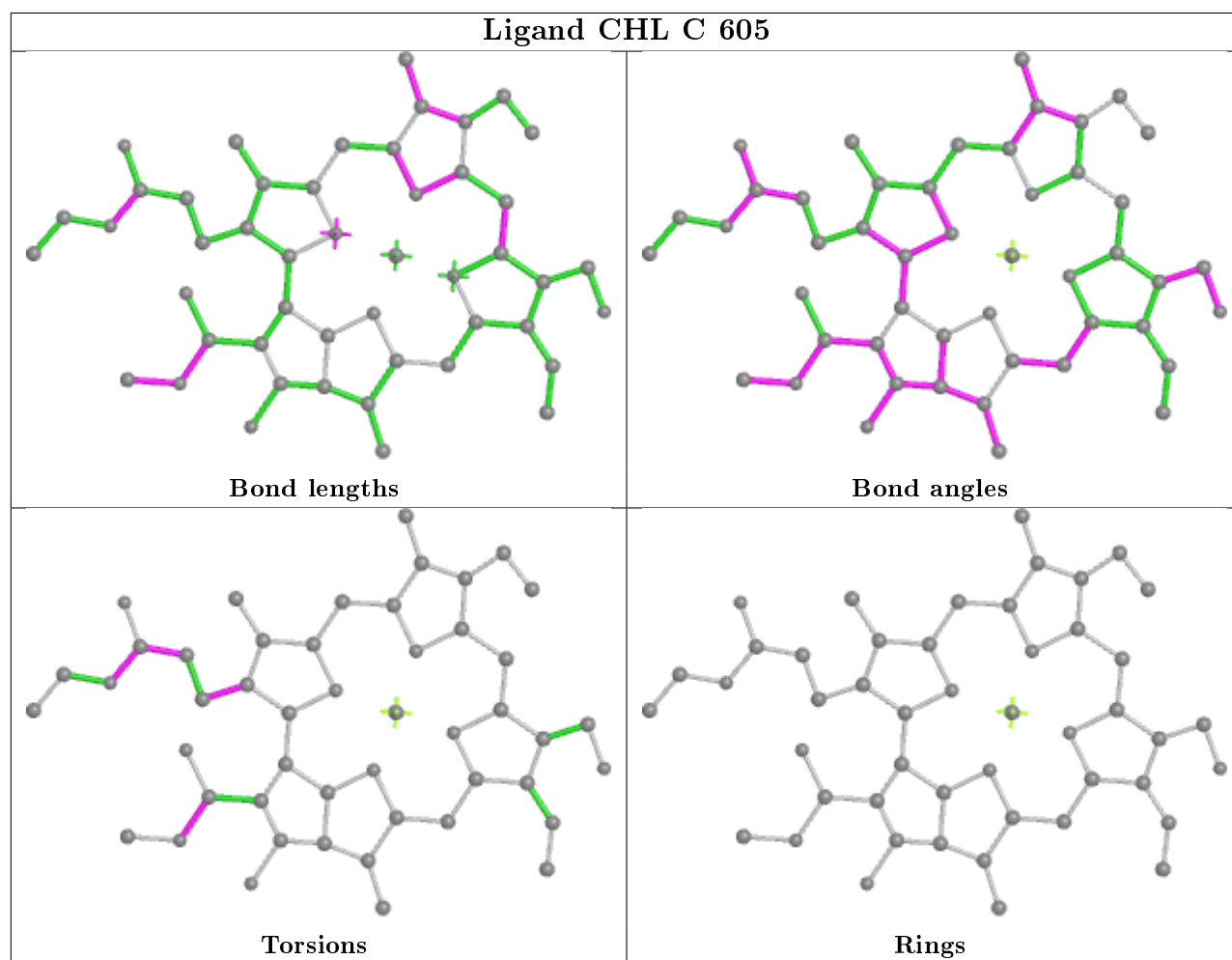
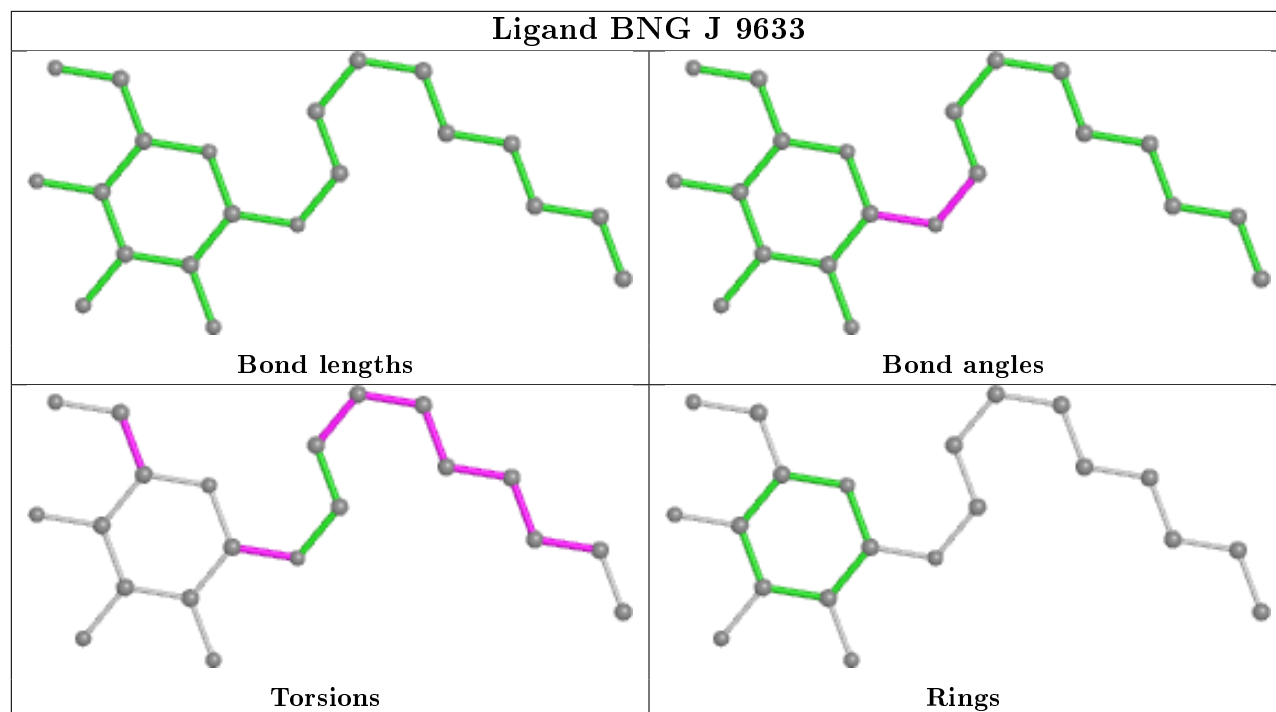


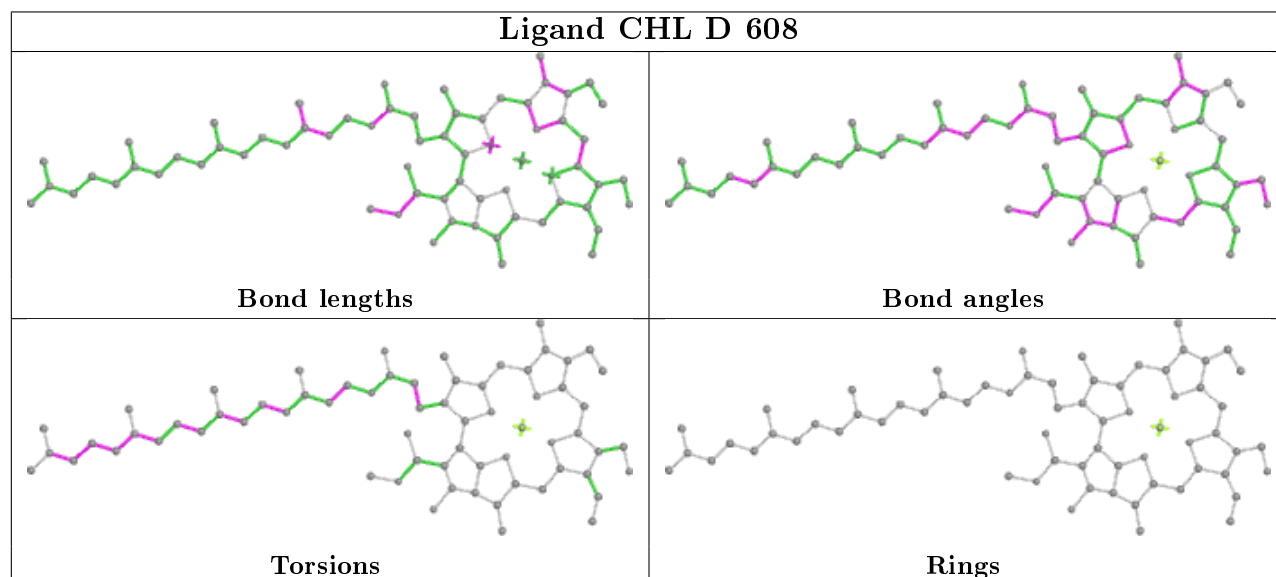
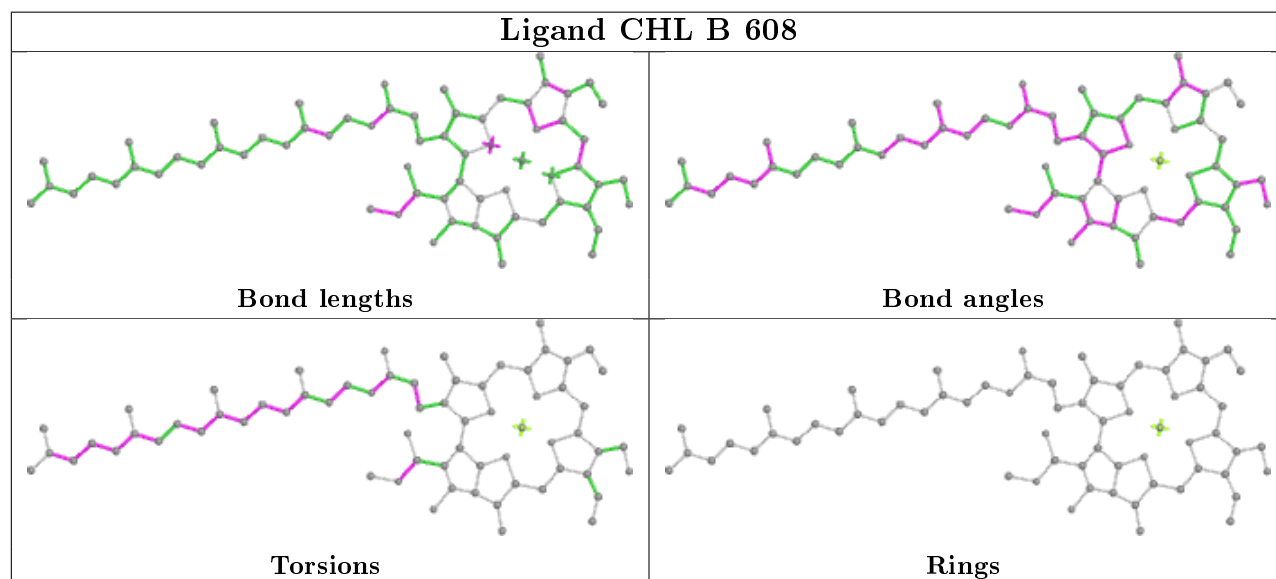
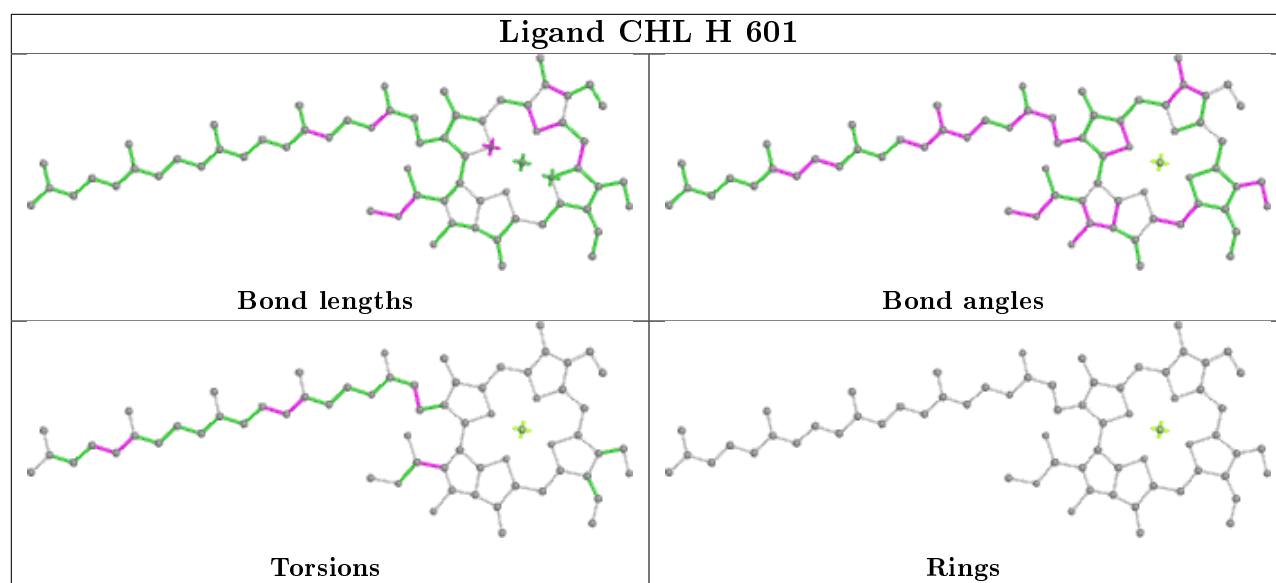
Ligand CLA A 602

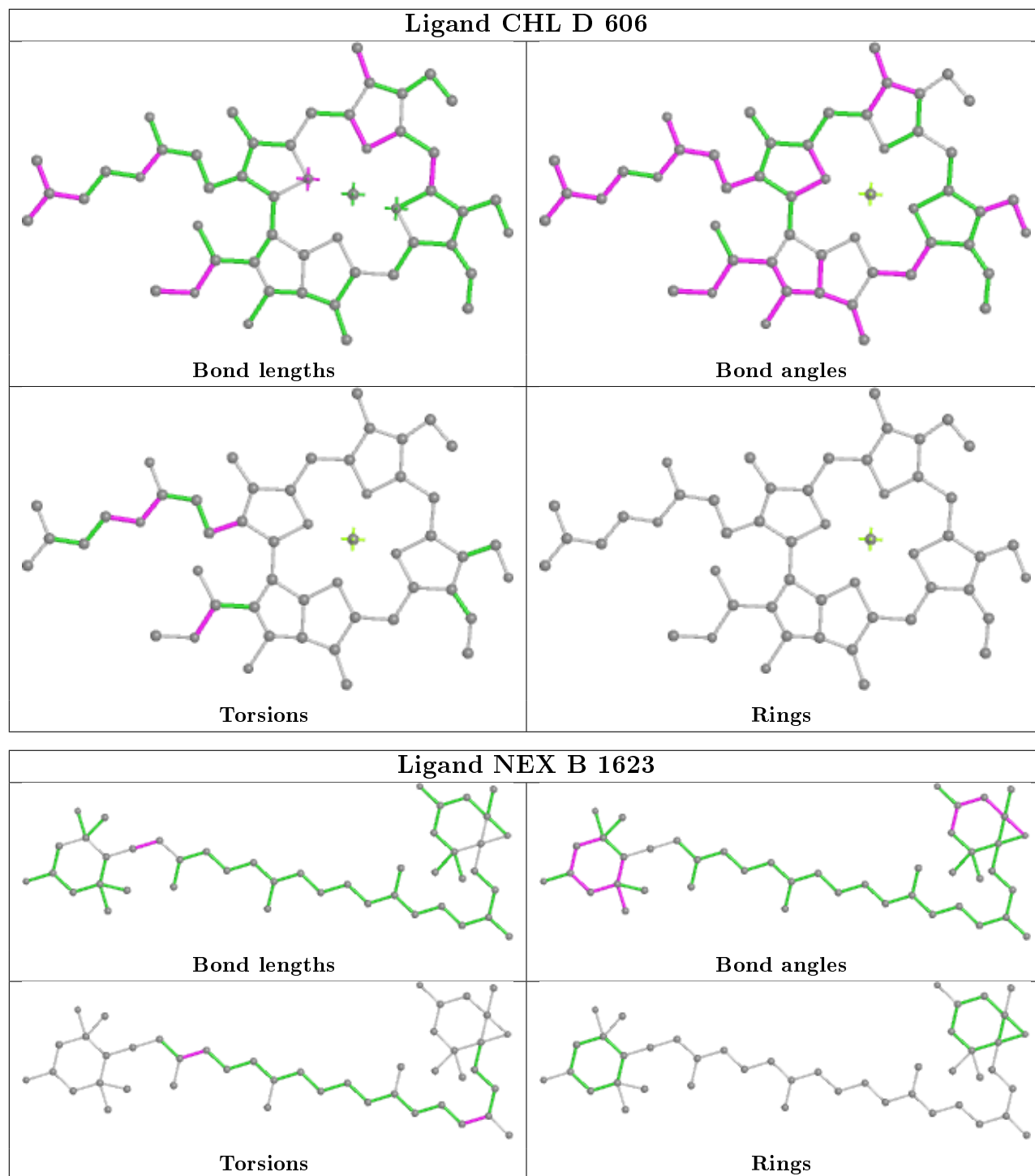


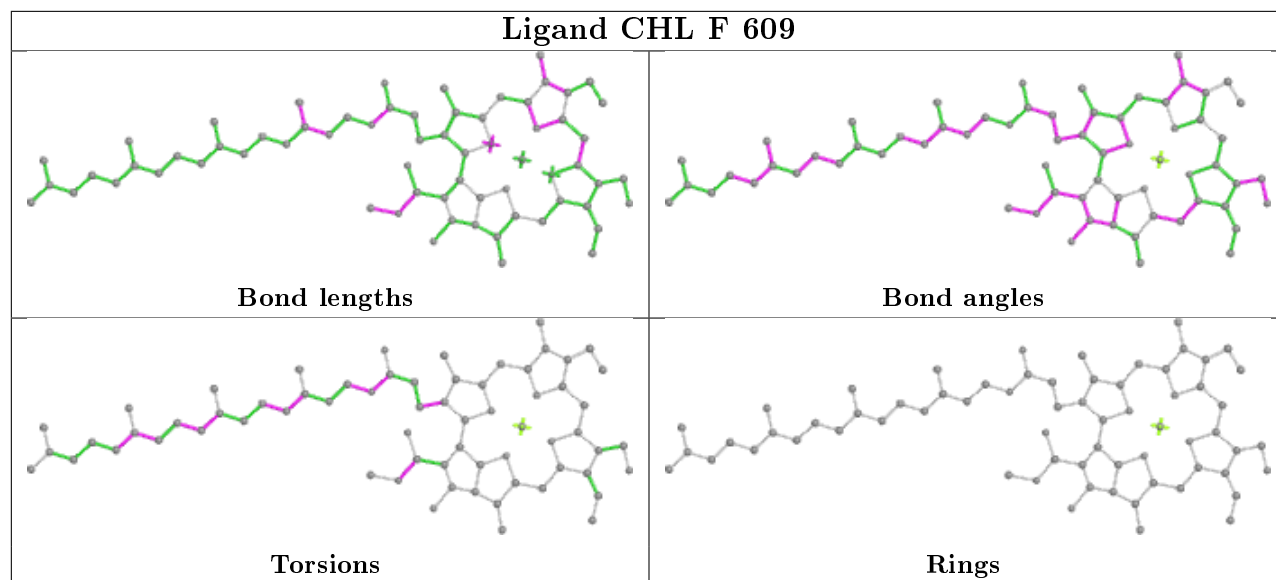
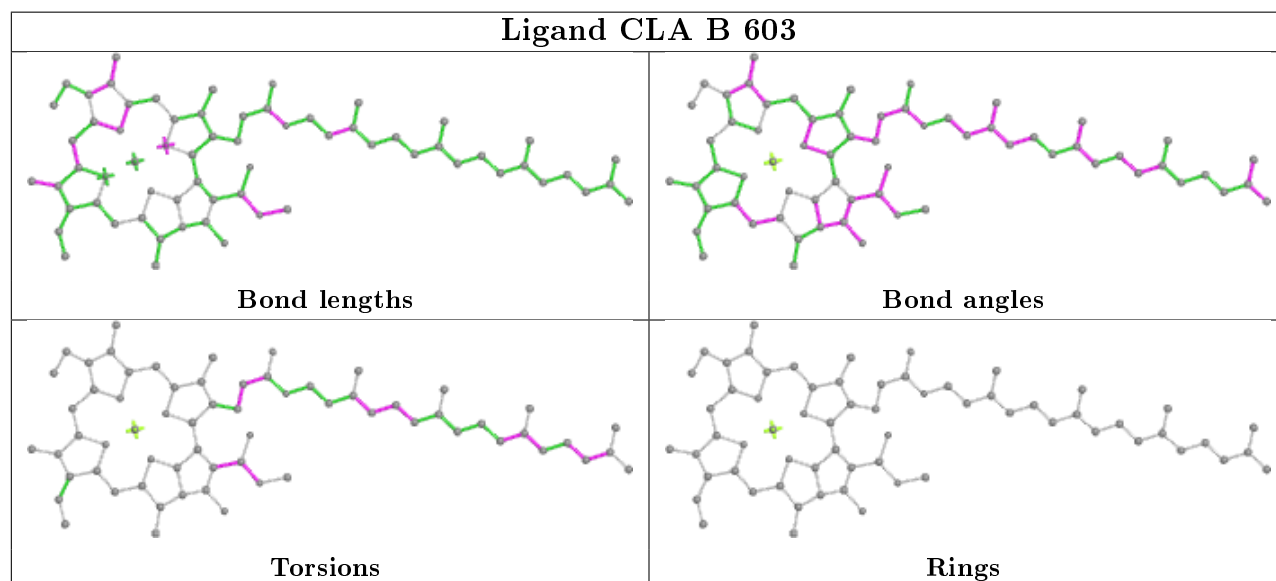
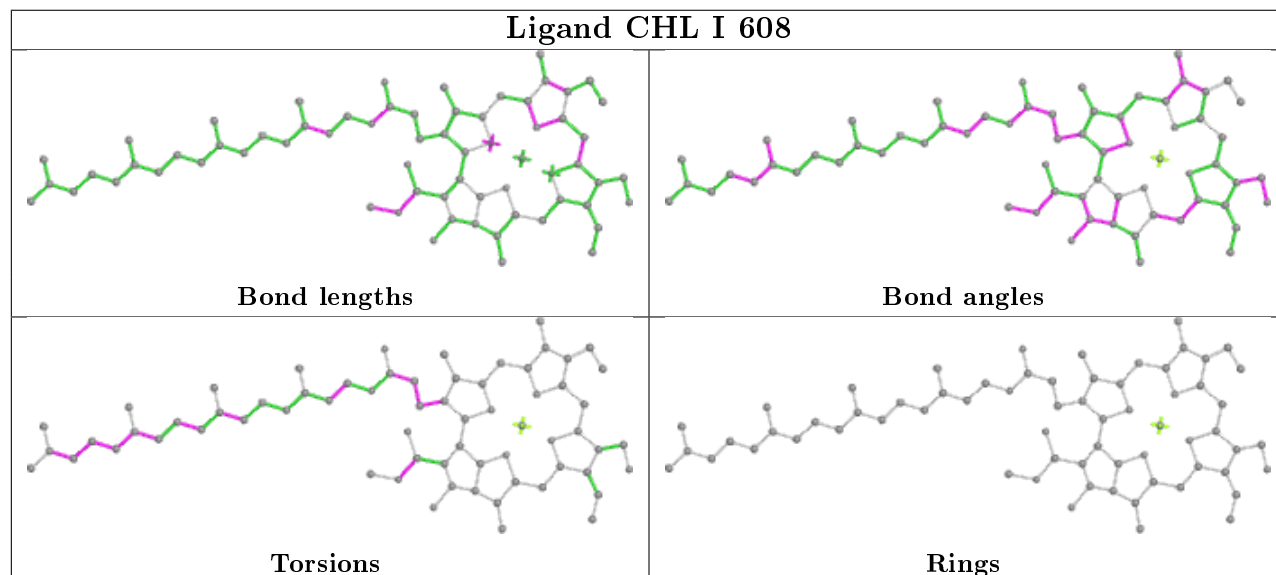
Ligand CLA G 610



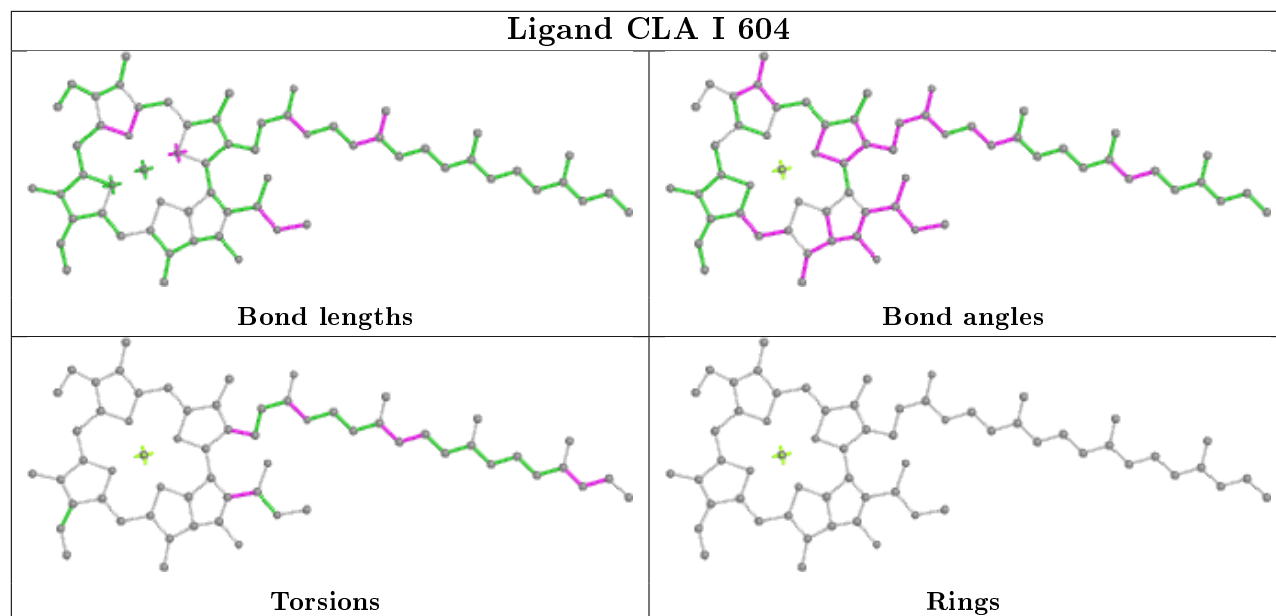




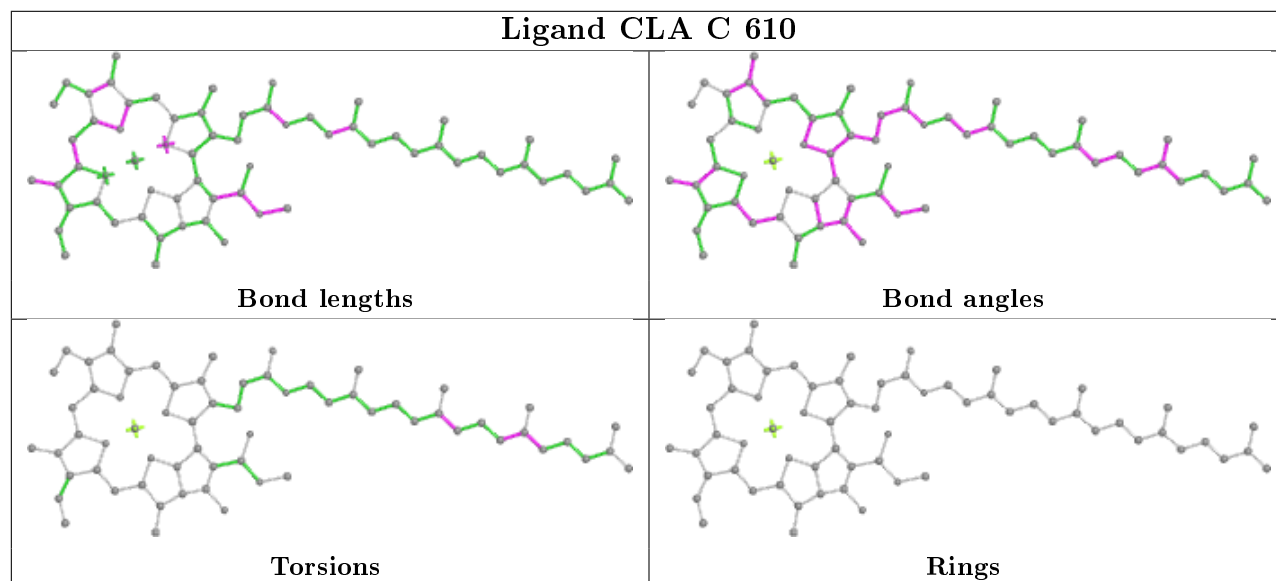


Ligand CHL F 609**Ligand CLA B 603****Ligand CHL I 608**

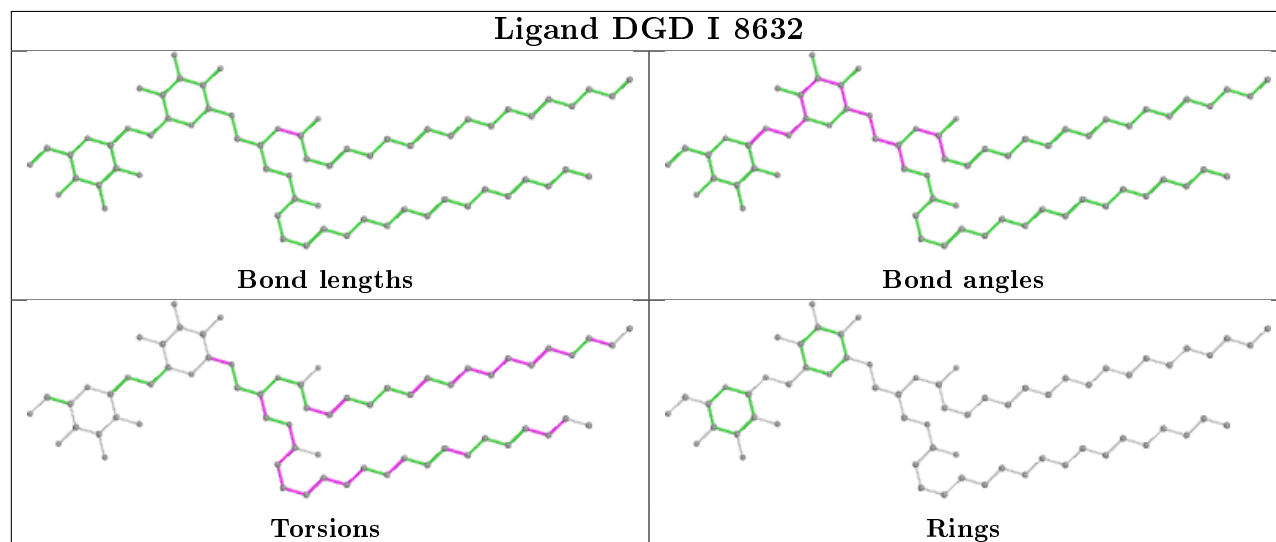
Ligand CLA I 604



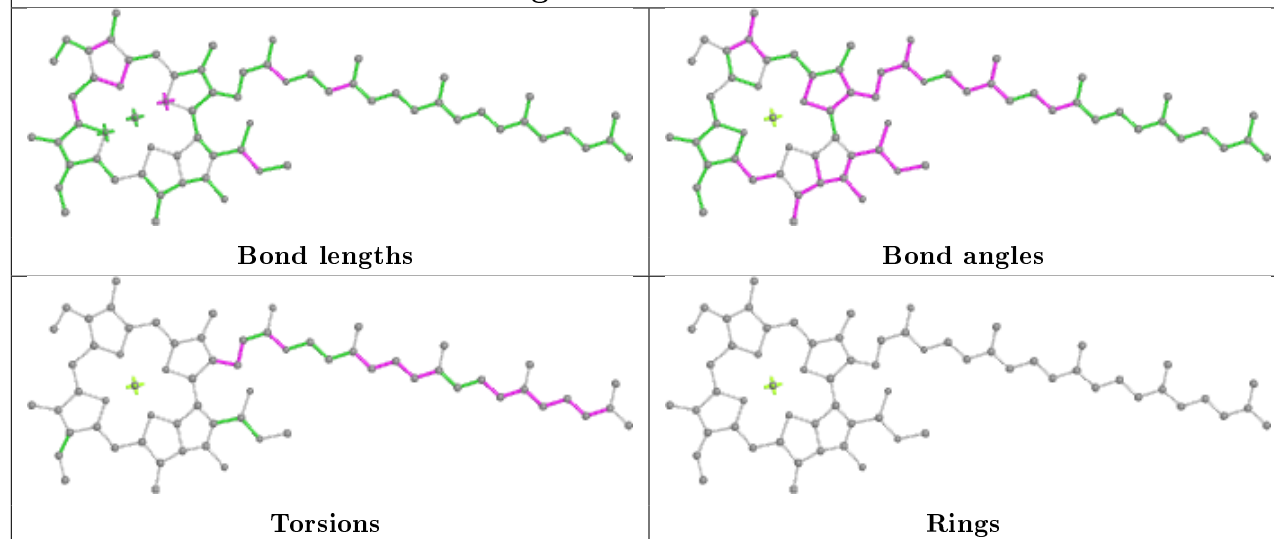
Ligand CLA C 610



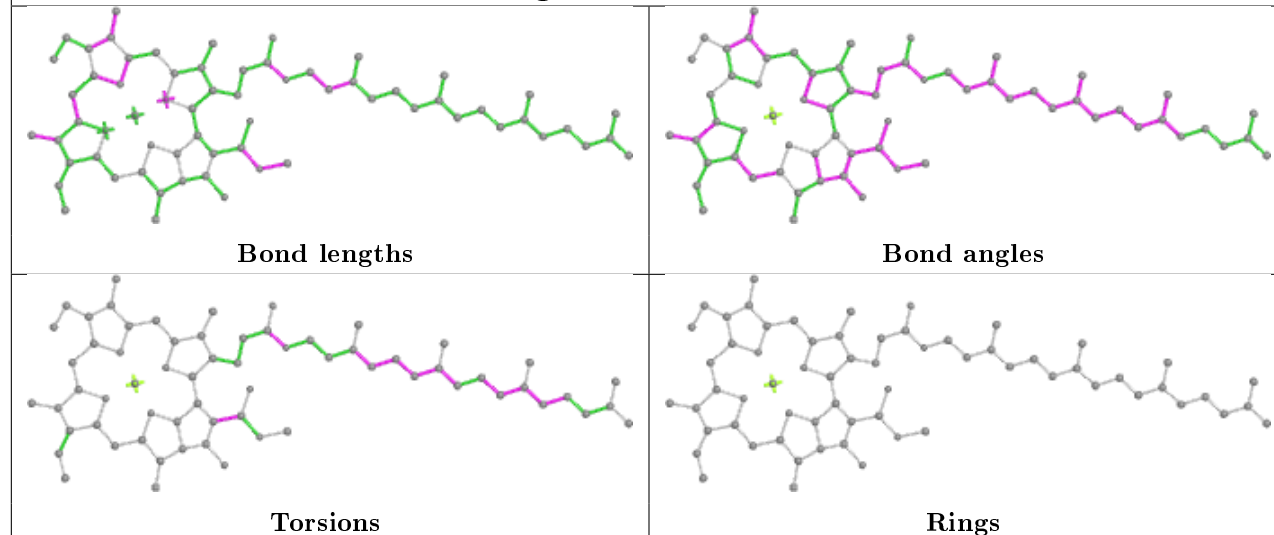
Ligand DGD I 8632



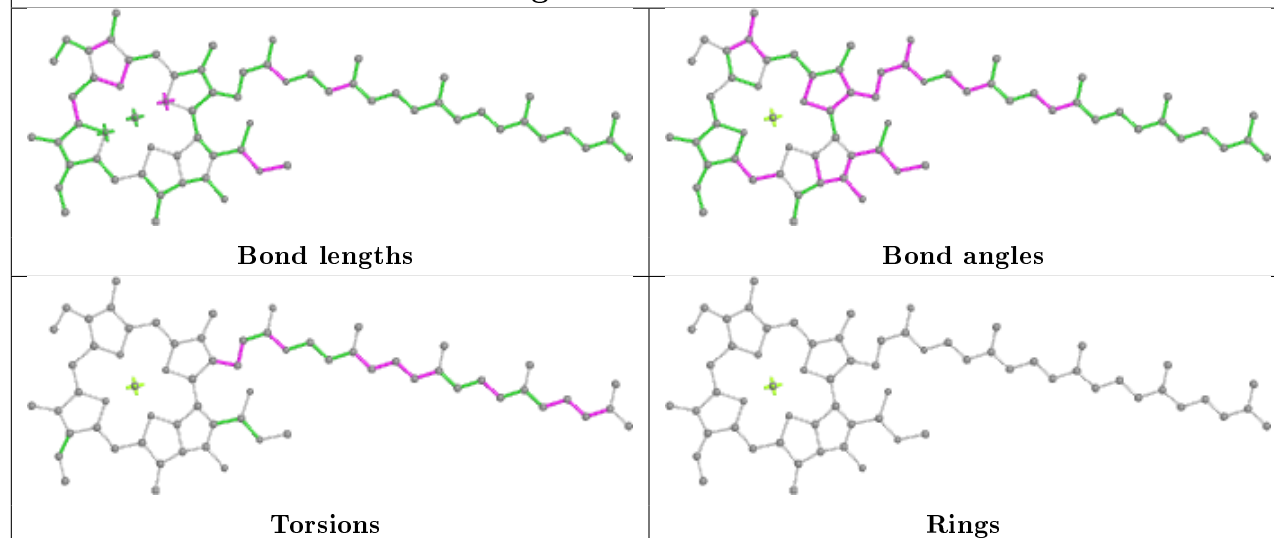
Ligand CLA D 611

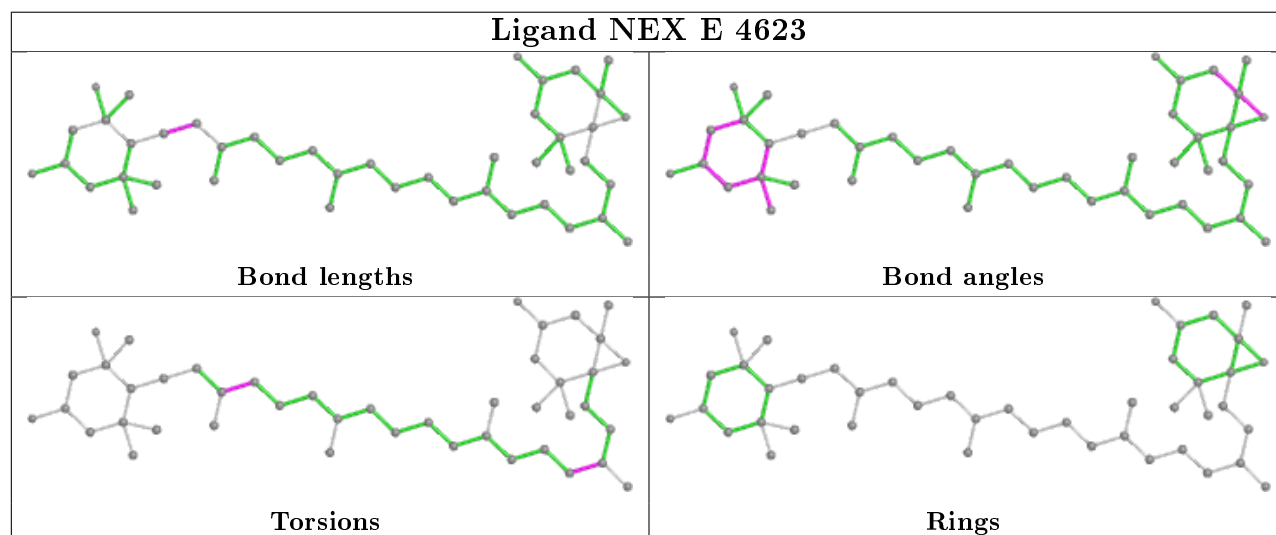
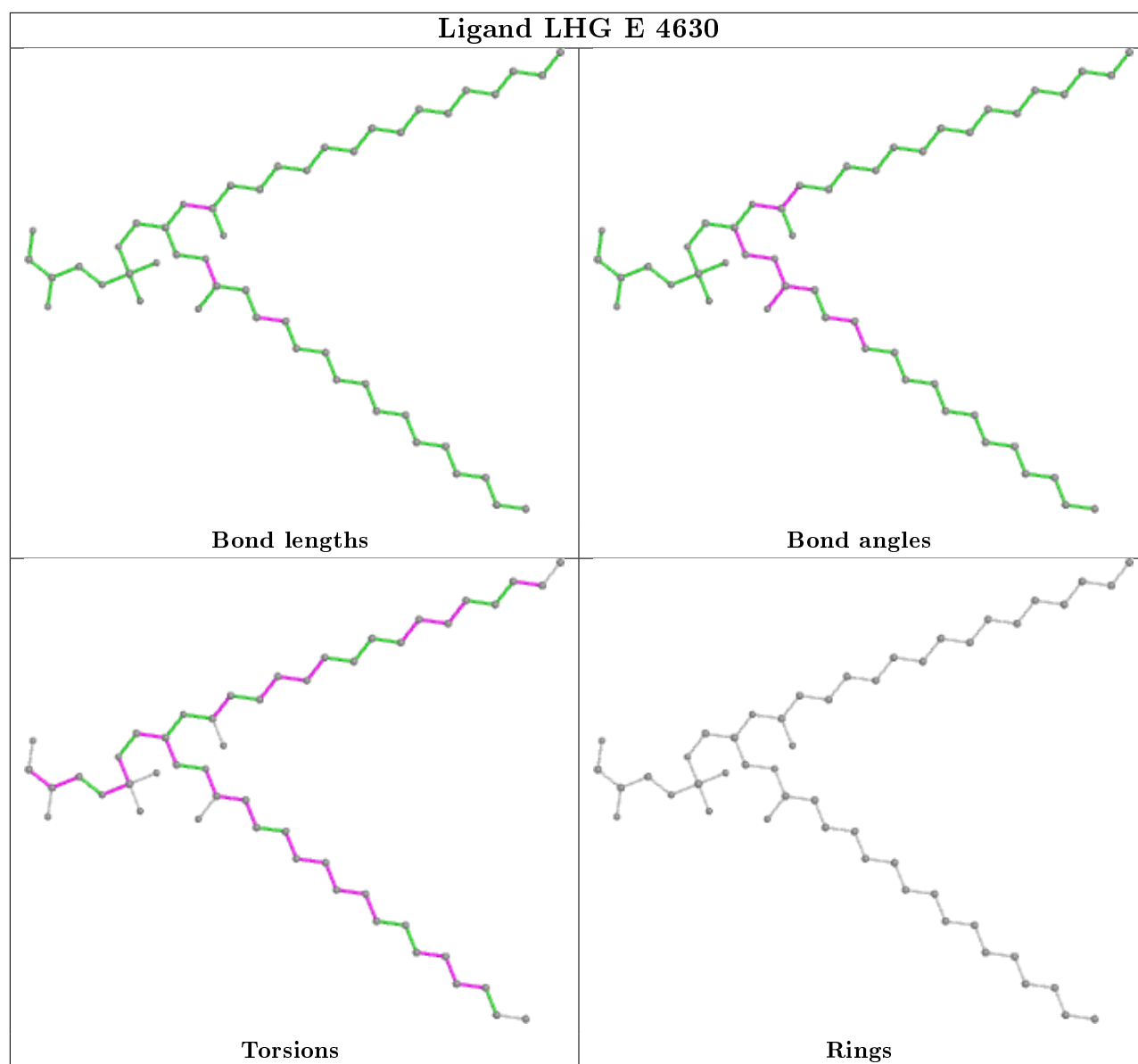


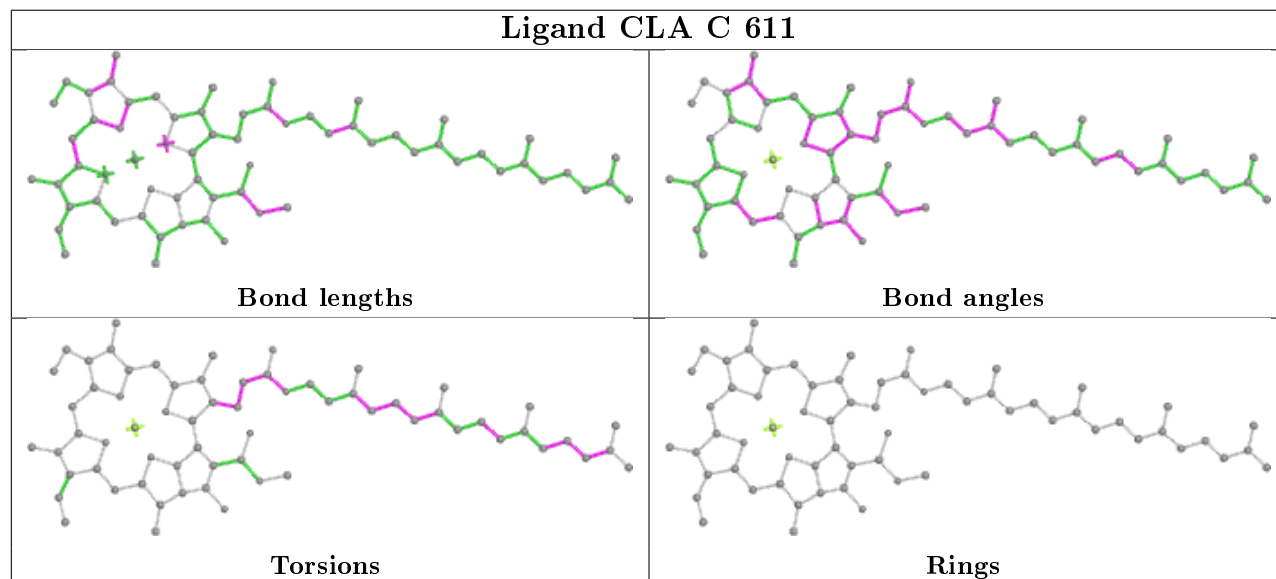
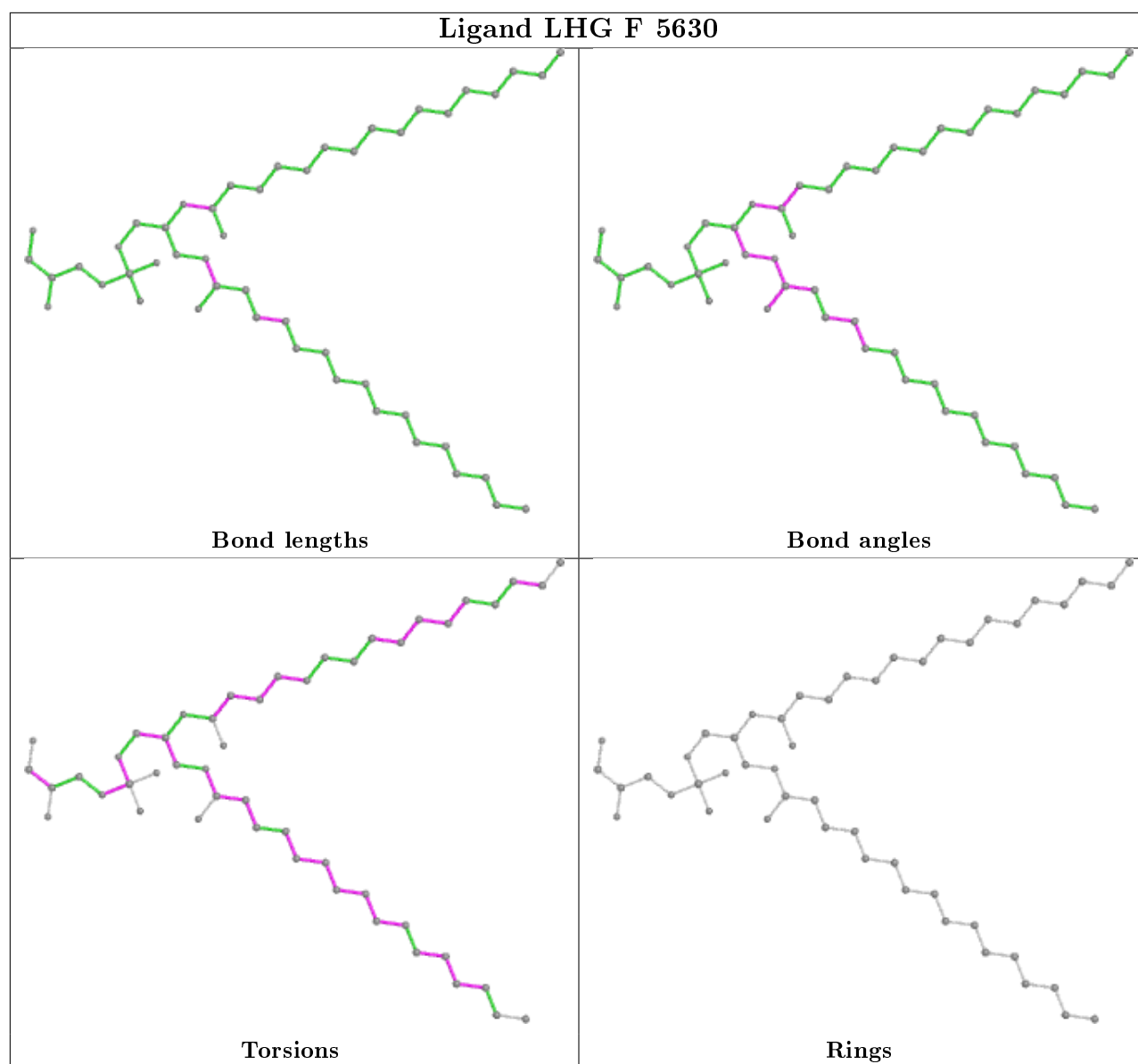
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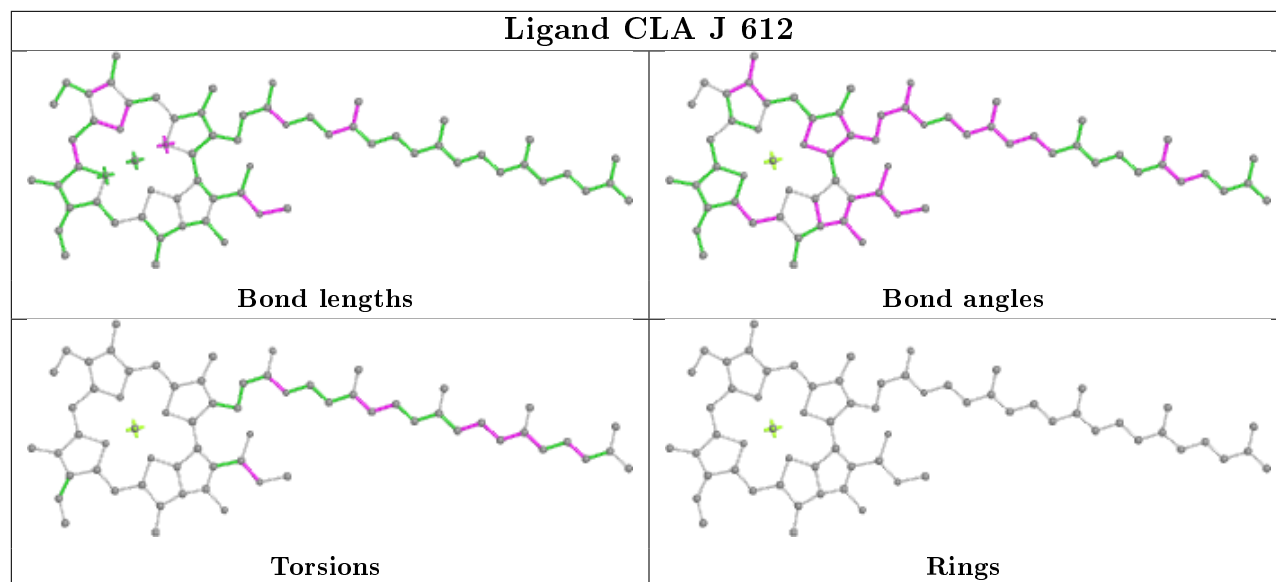
Ligand CLA H 611



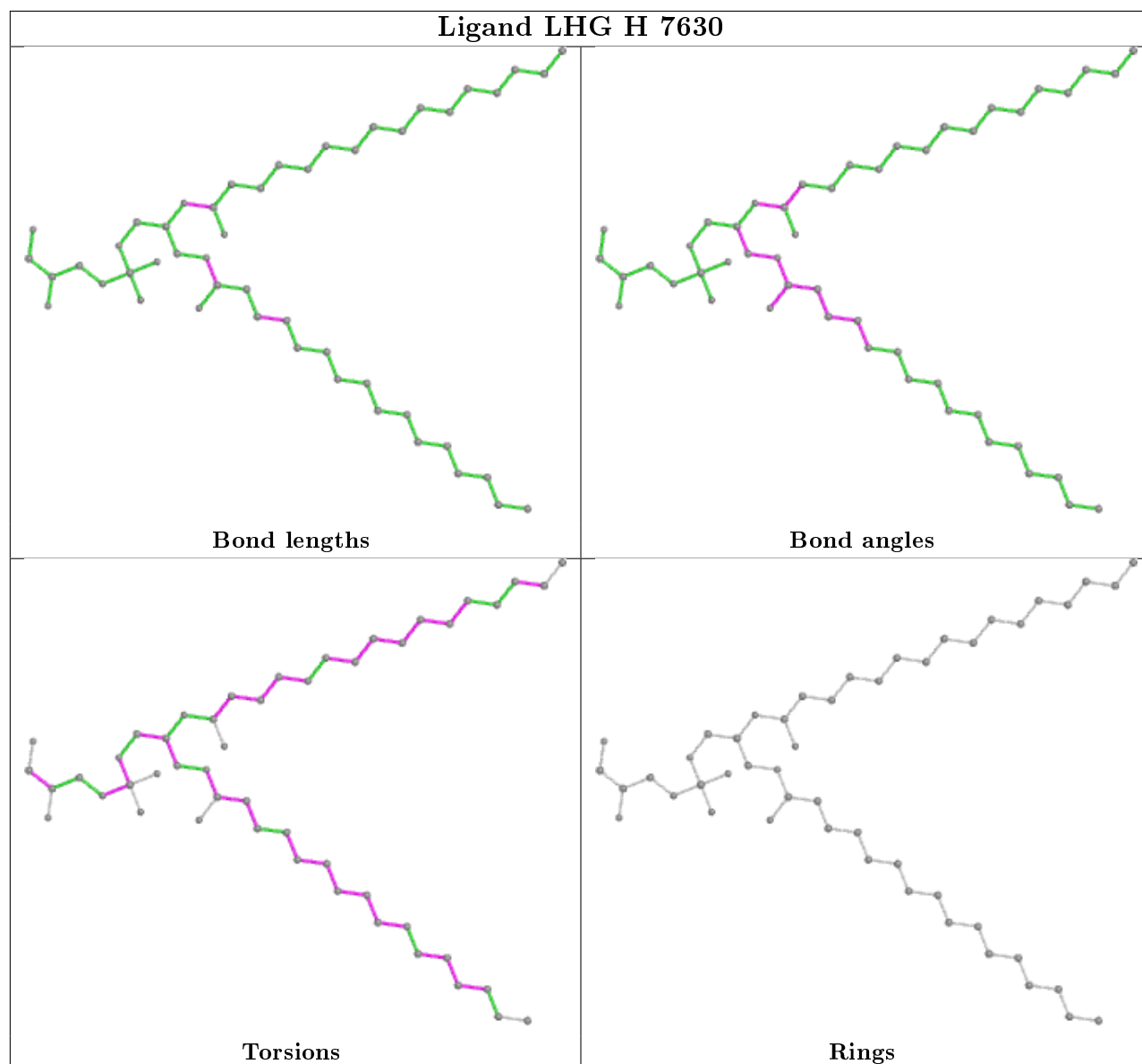




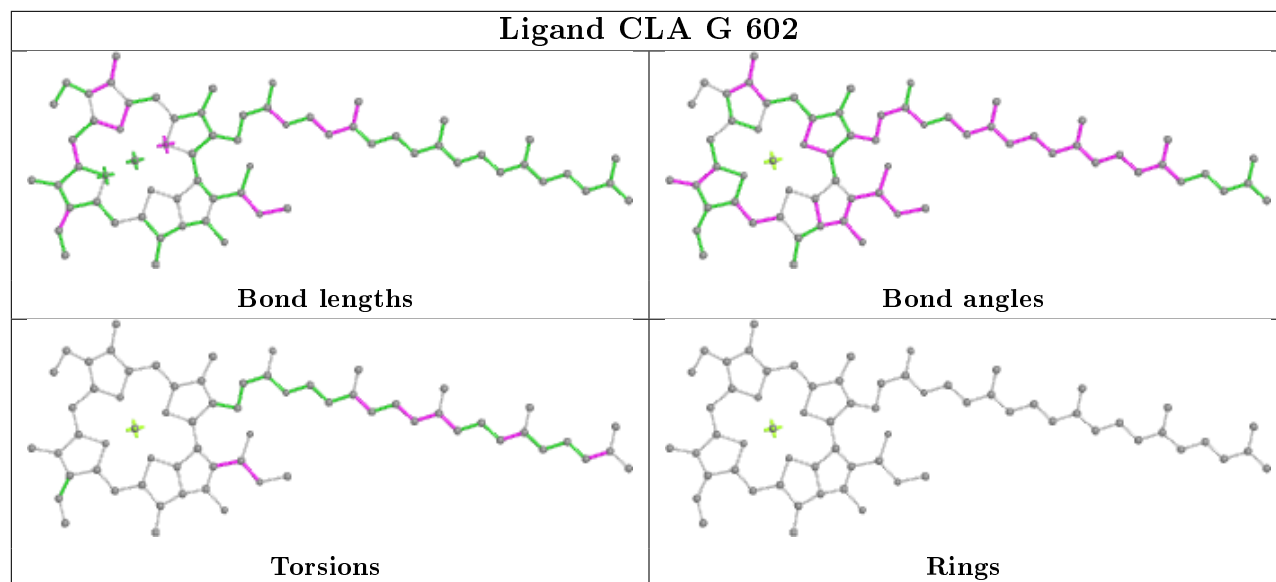
Ligand CLA J 612



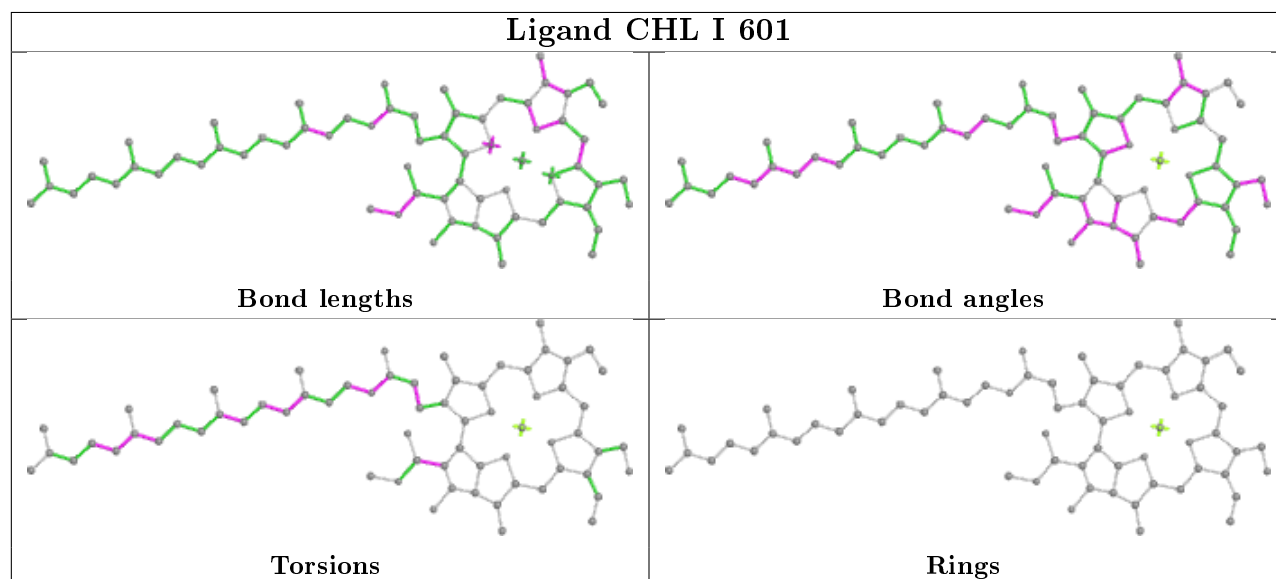
Ligand LHG H 7630



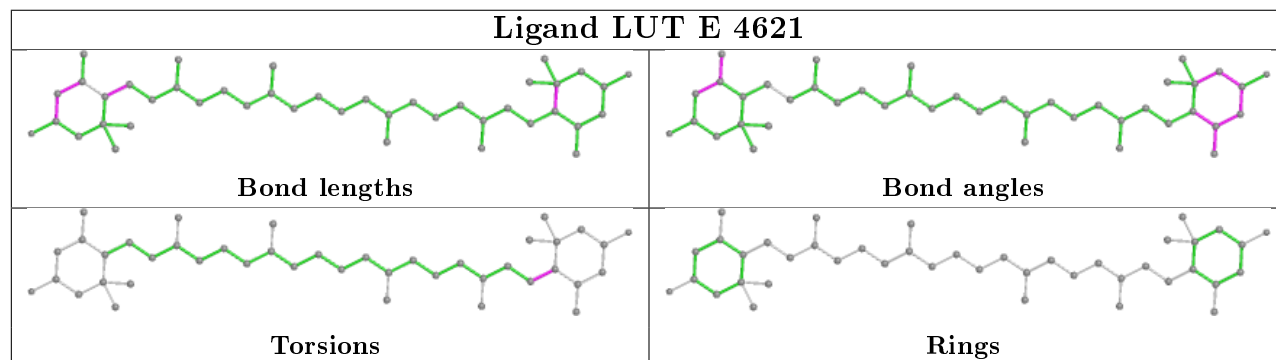
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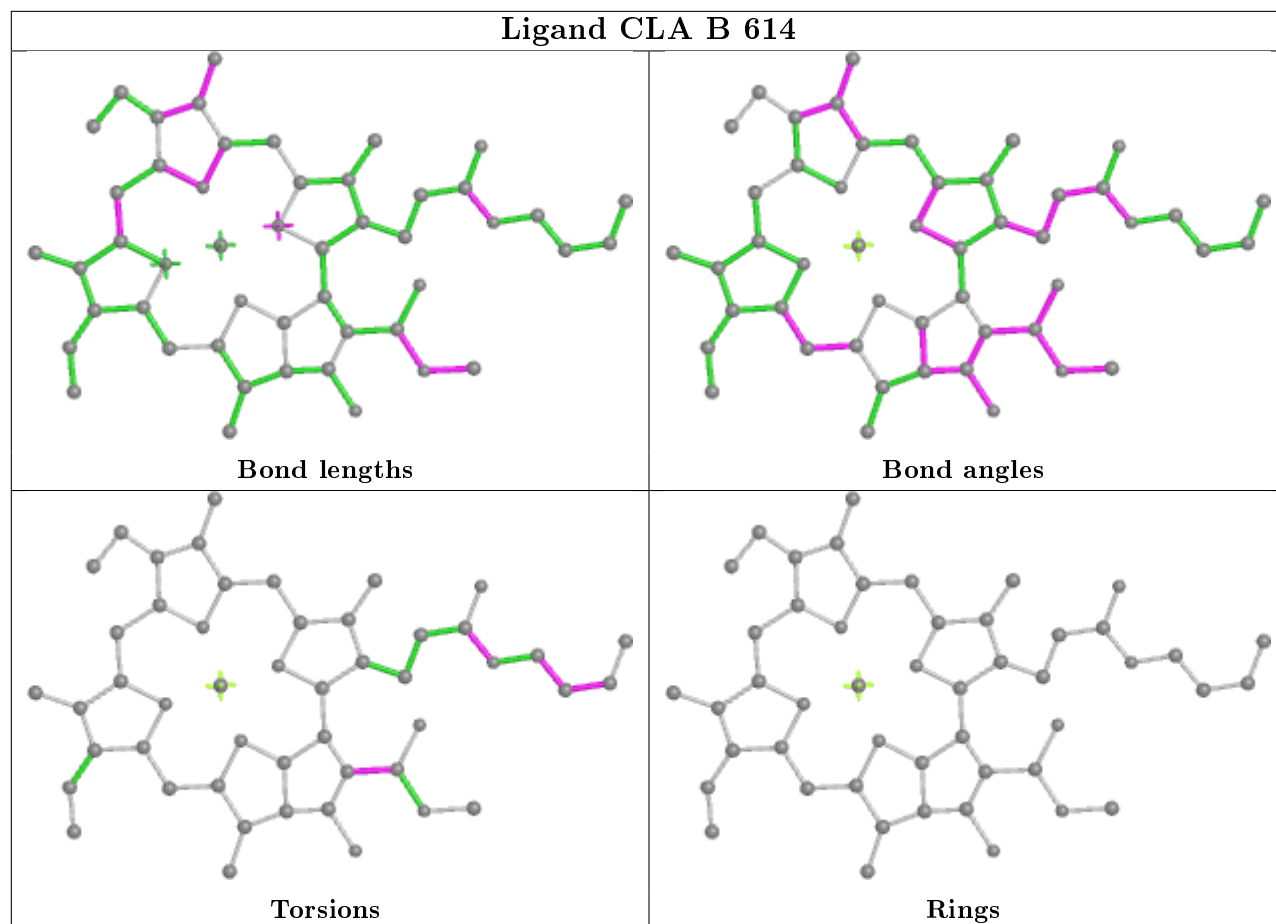
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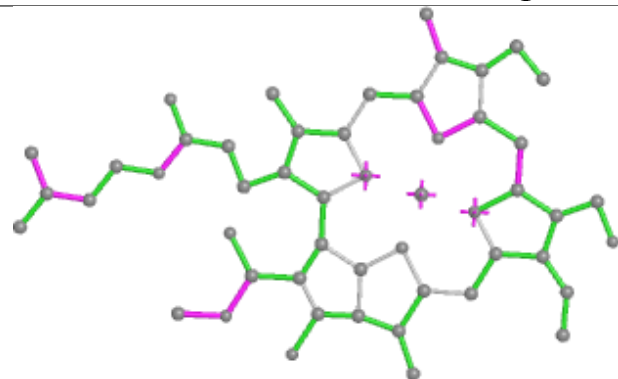
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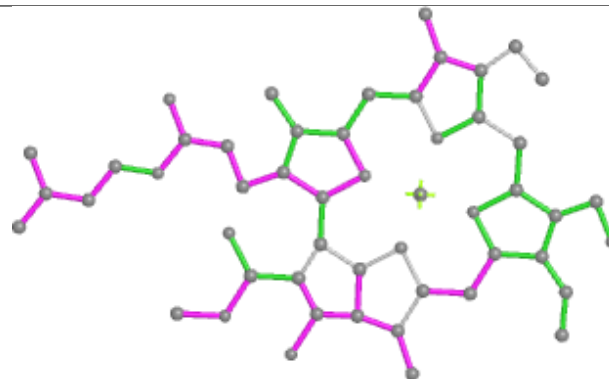
Ligand CLA B 614



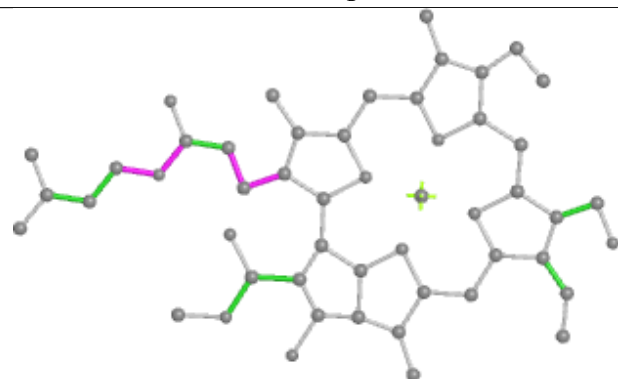
Ligand CHL H 606



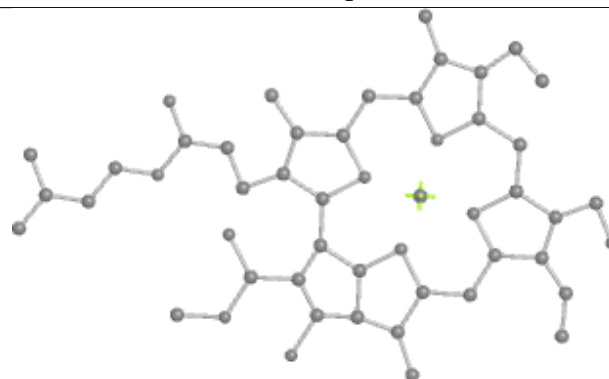
Bond lengths



Bond angles

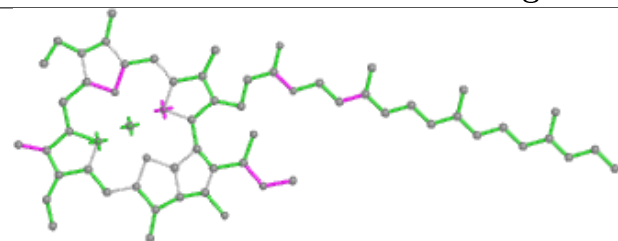


Torsions

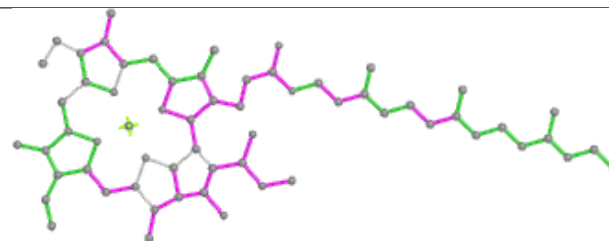


Rings

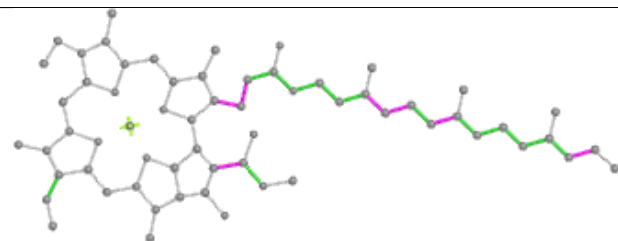
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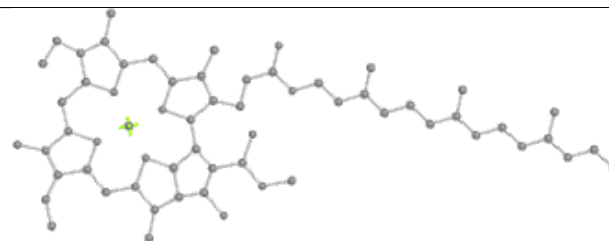
Bond lengths



Bond angles

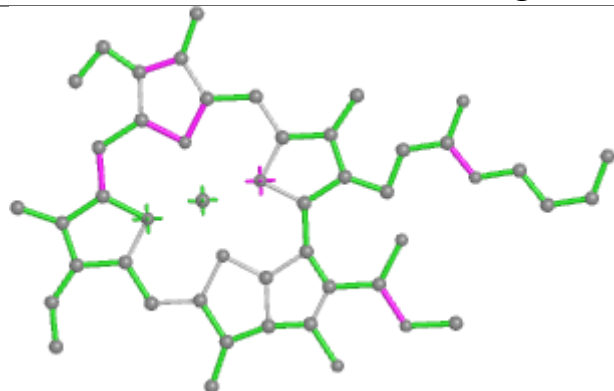


Torsions

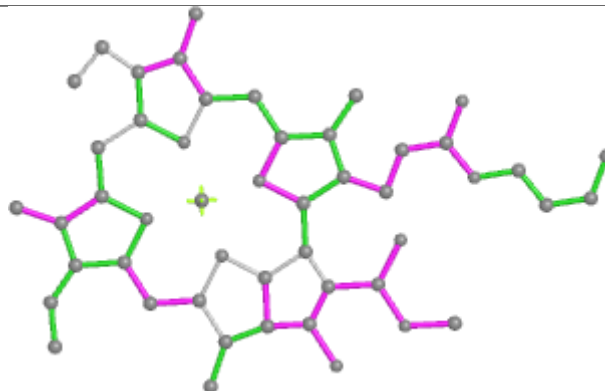


Rings

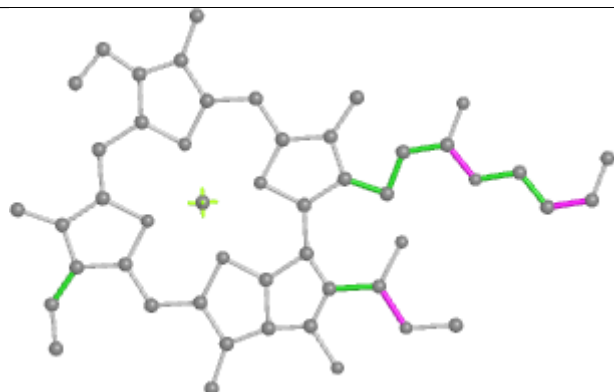
Ligand CLA H 614



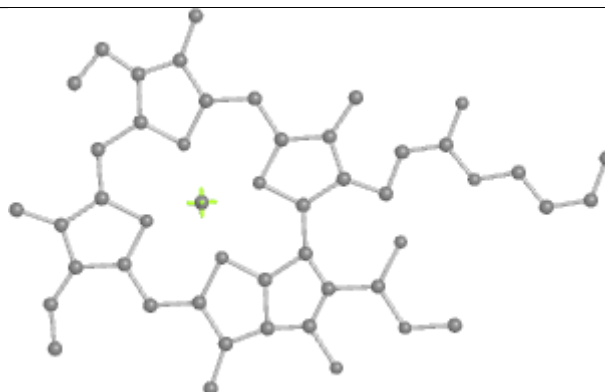
Bond lengths



Bond angles

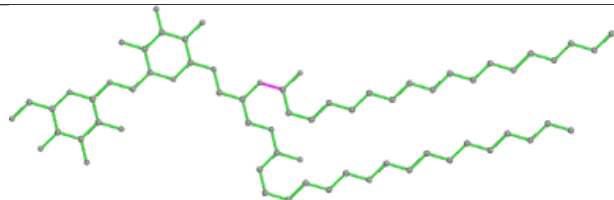


Torsions

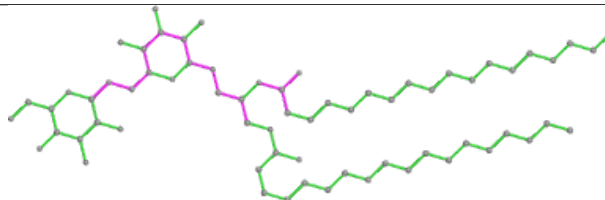


Rings

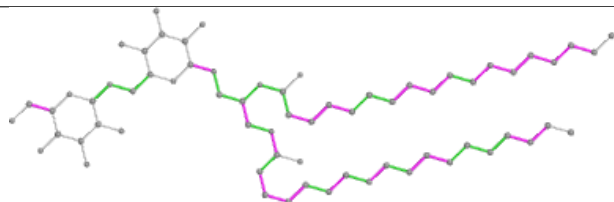
Ligand DGD D 5632



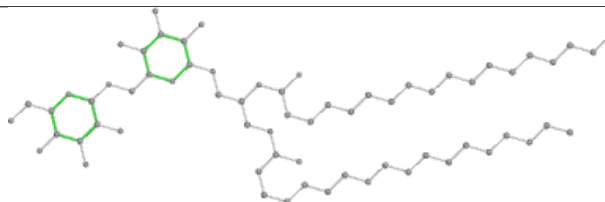
Bond lengths



Bond angles

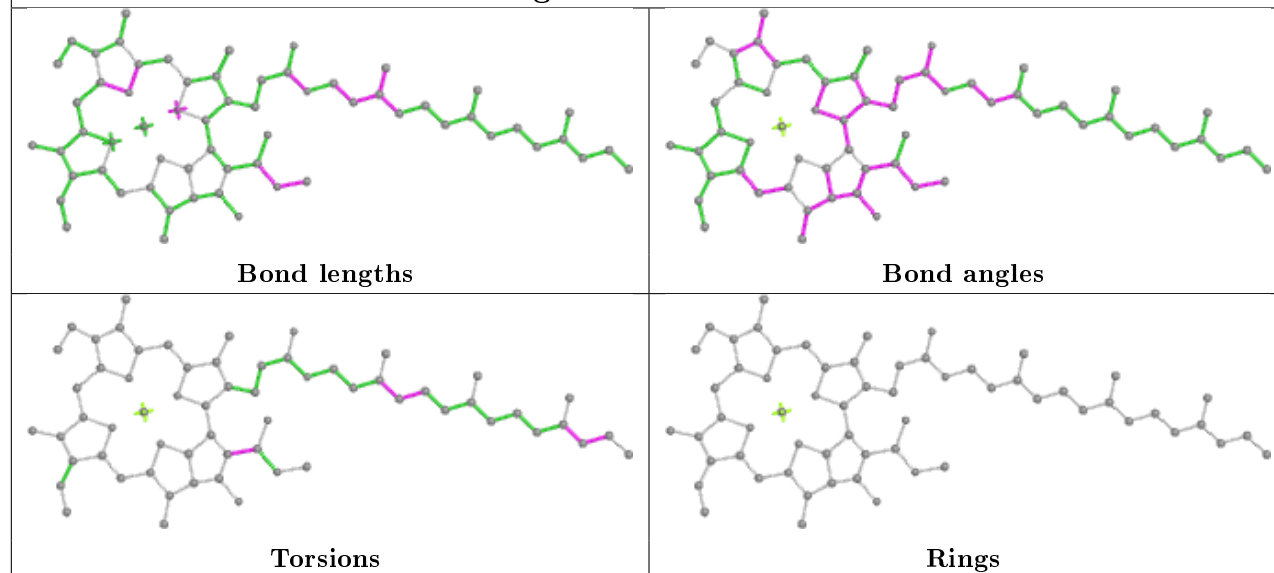


Torsions

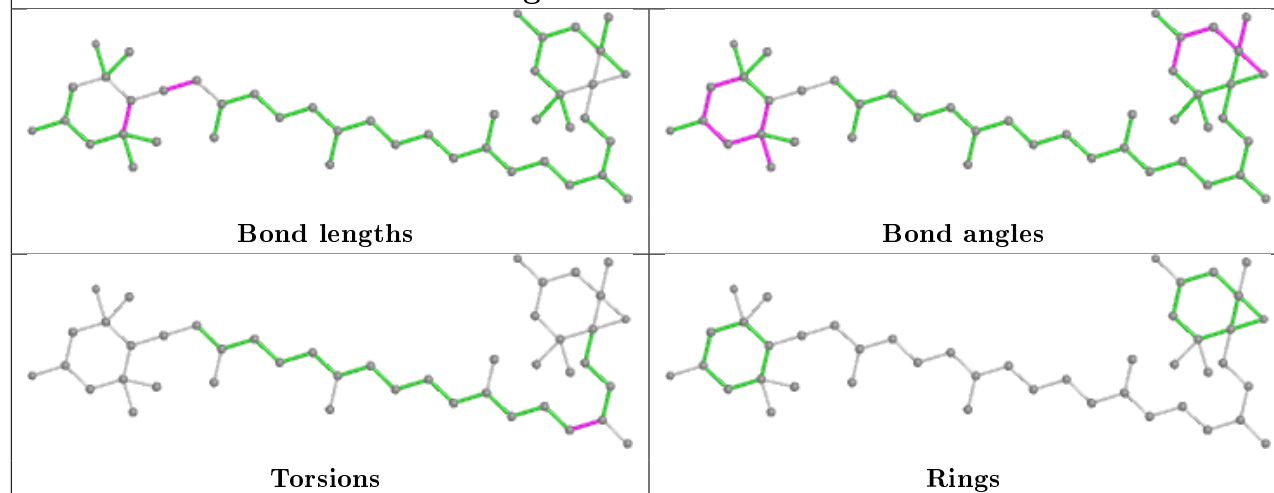


Rings

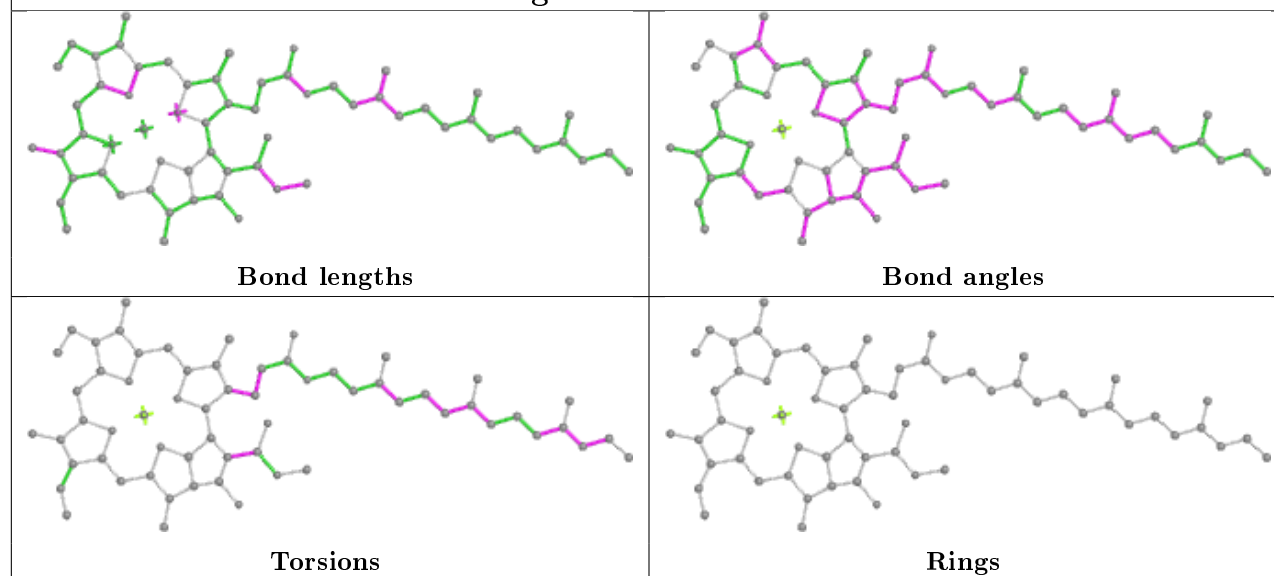
Ligand CLA E 604

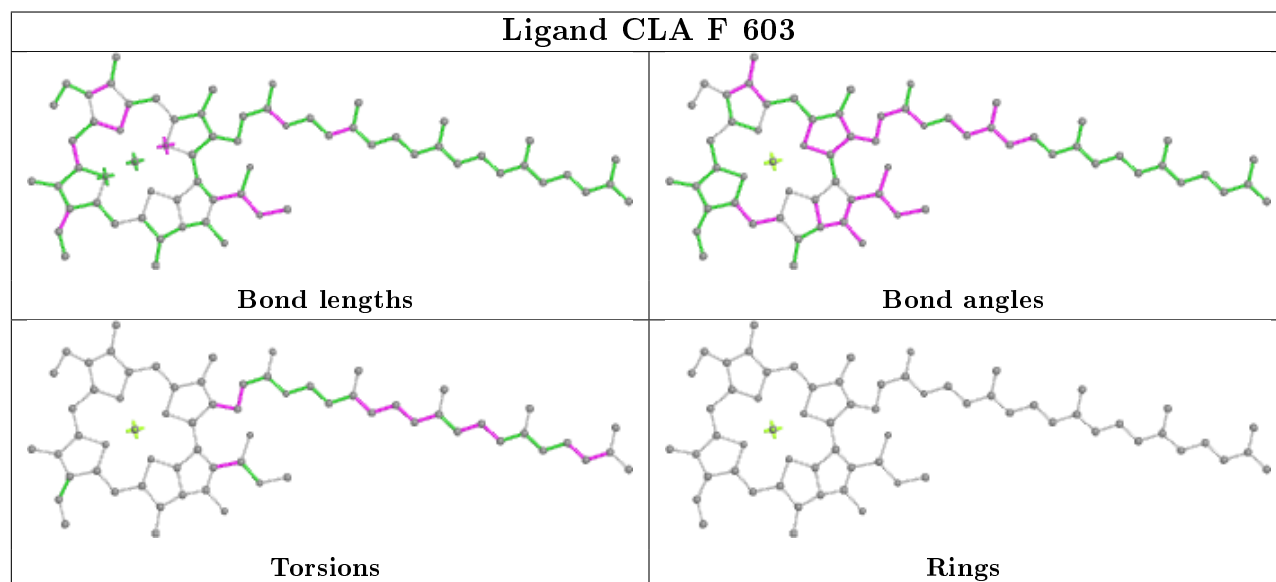
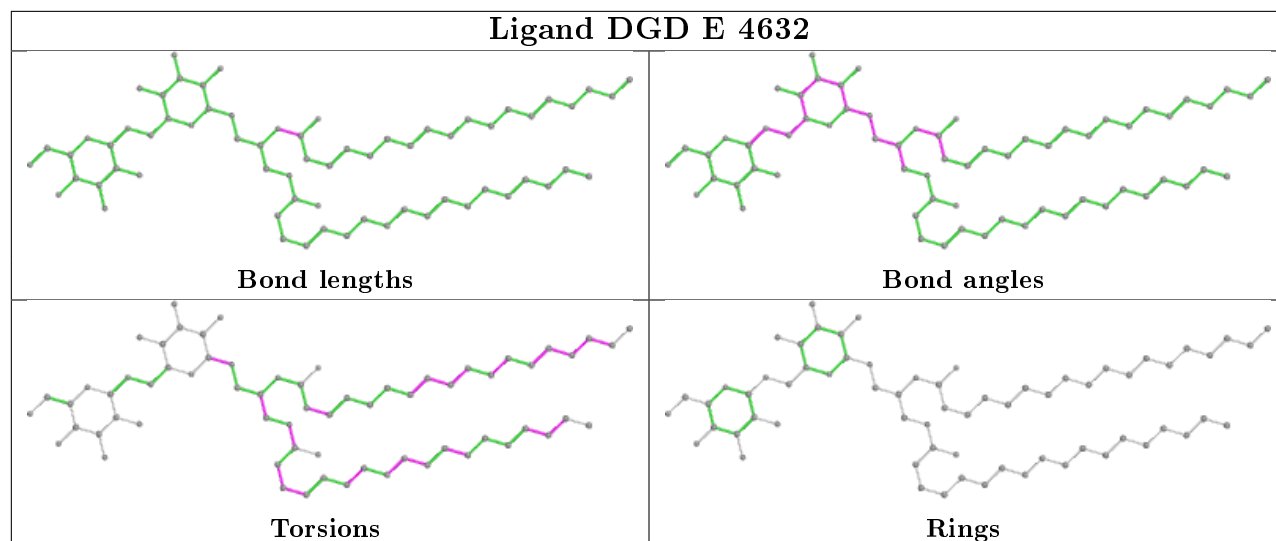


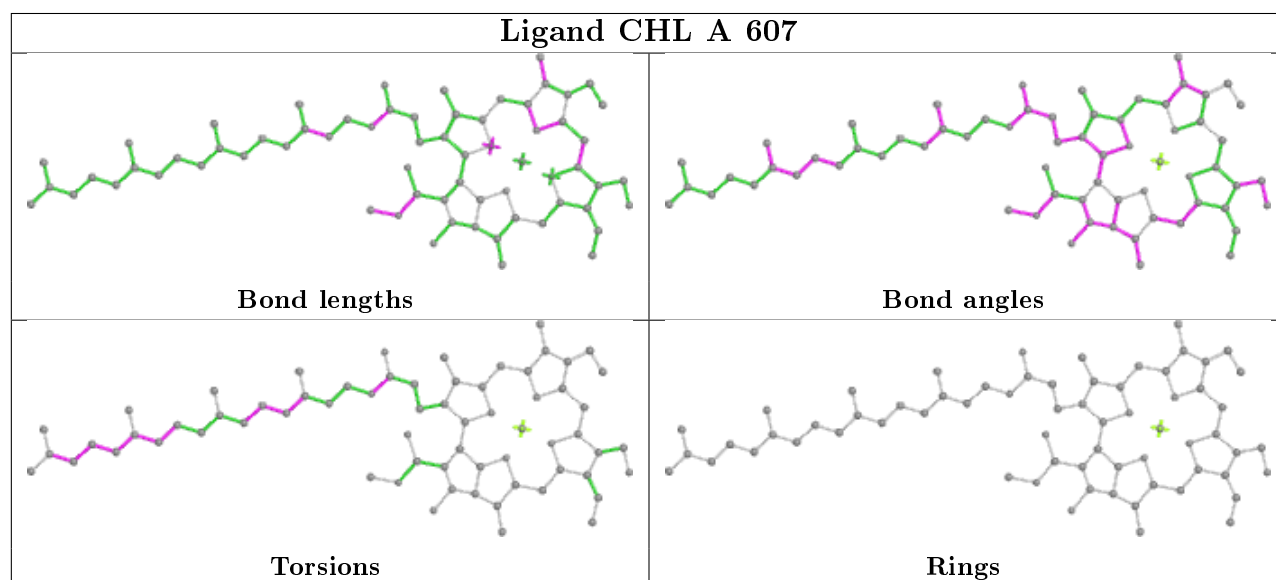
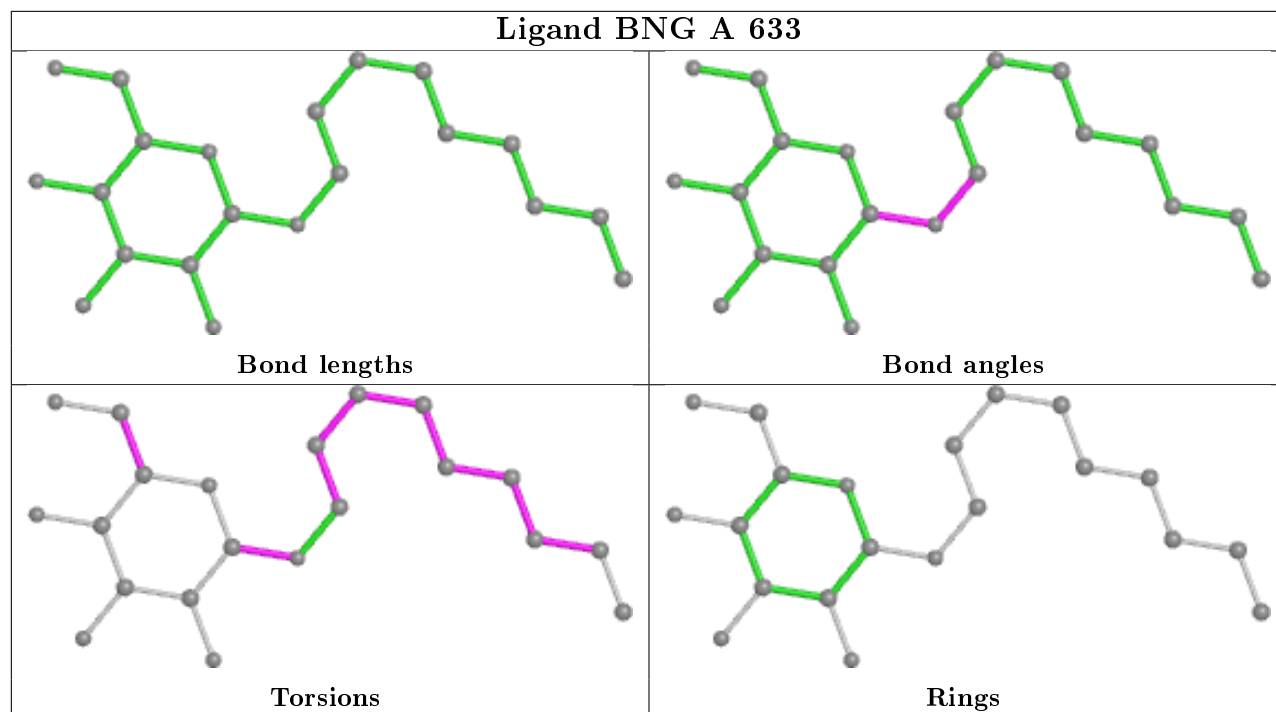
Ligand NEX F 5623

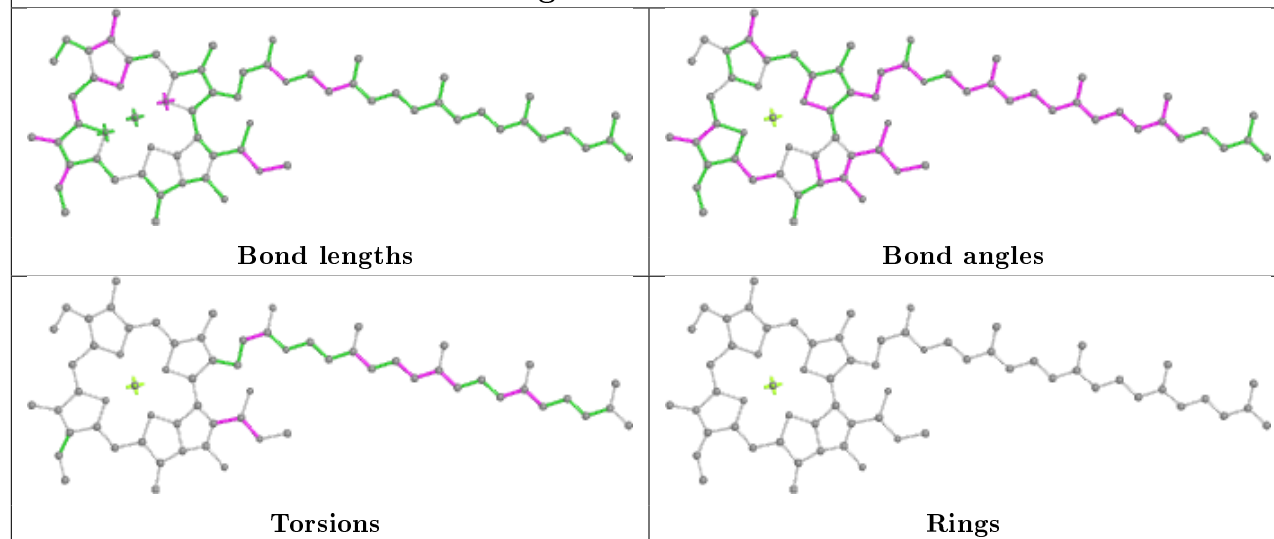
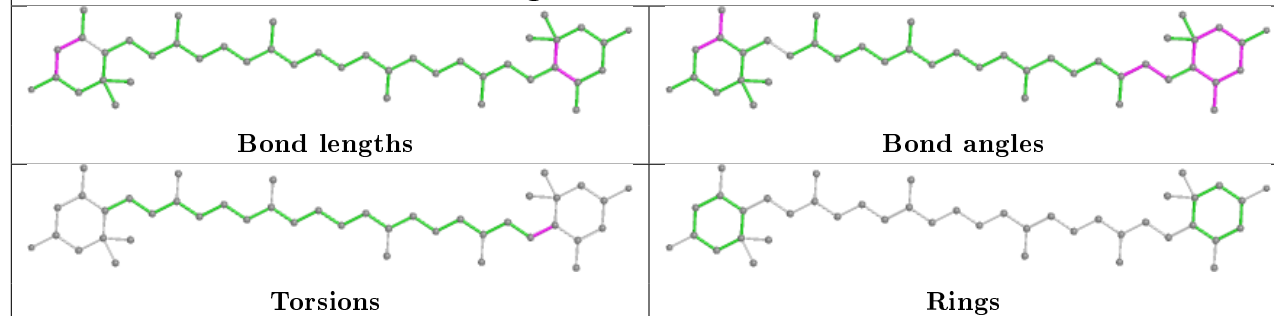
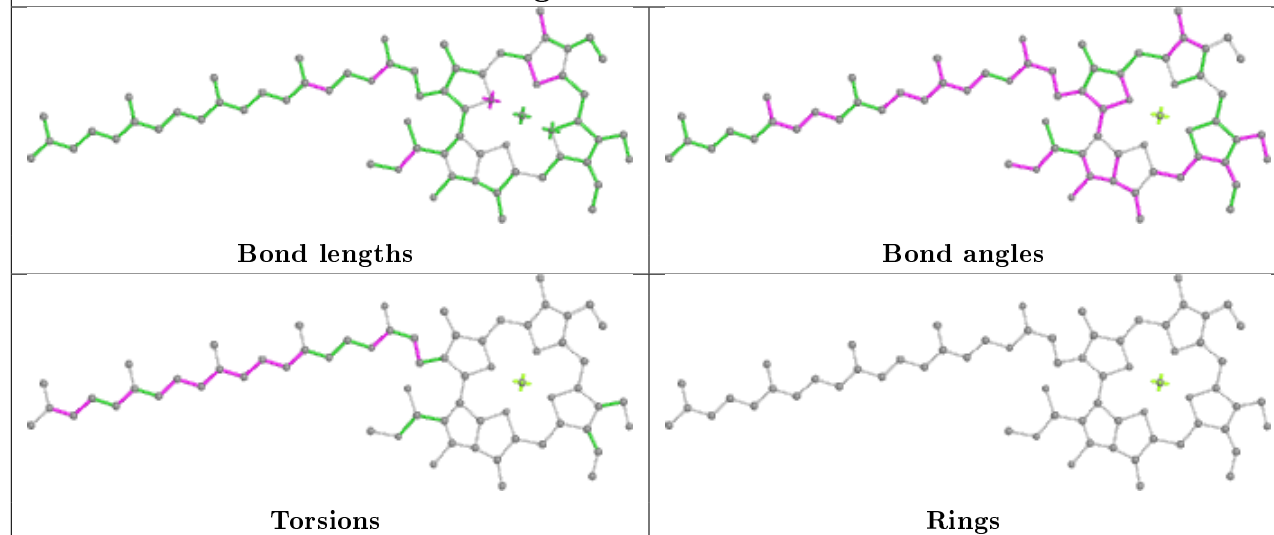


Ligand CLA G 604

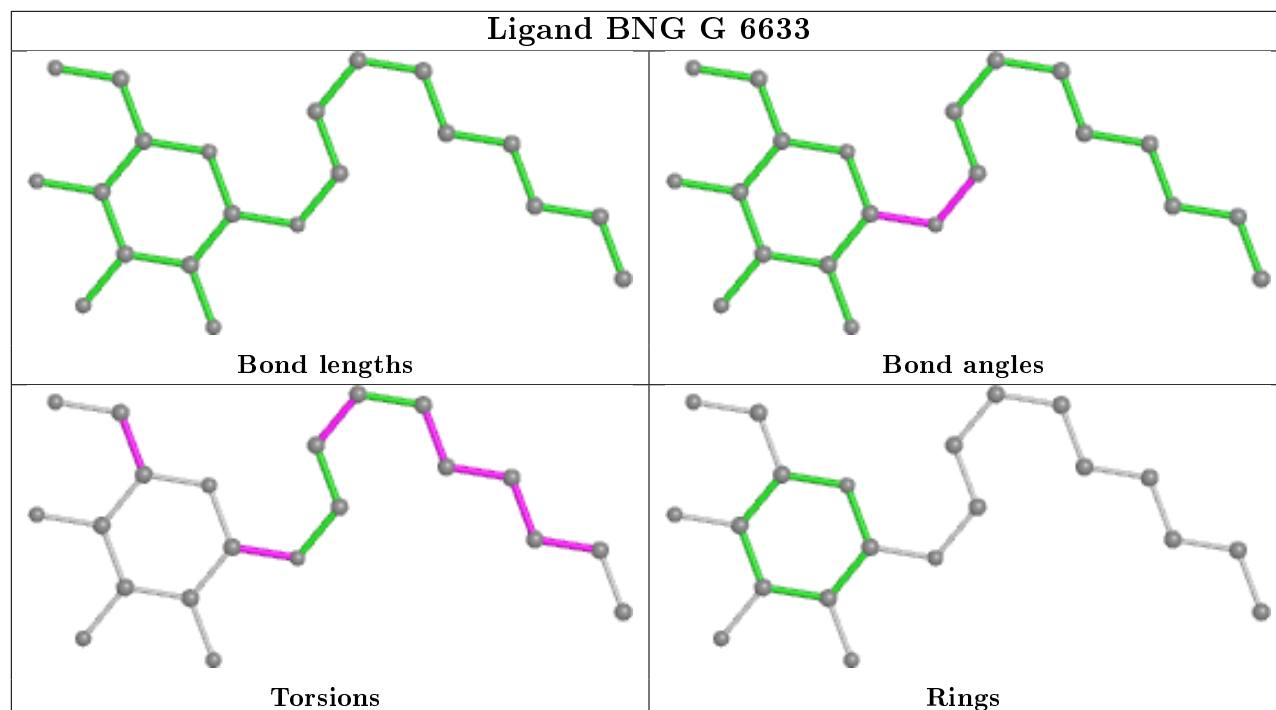




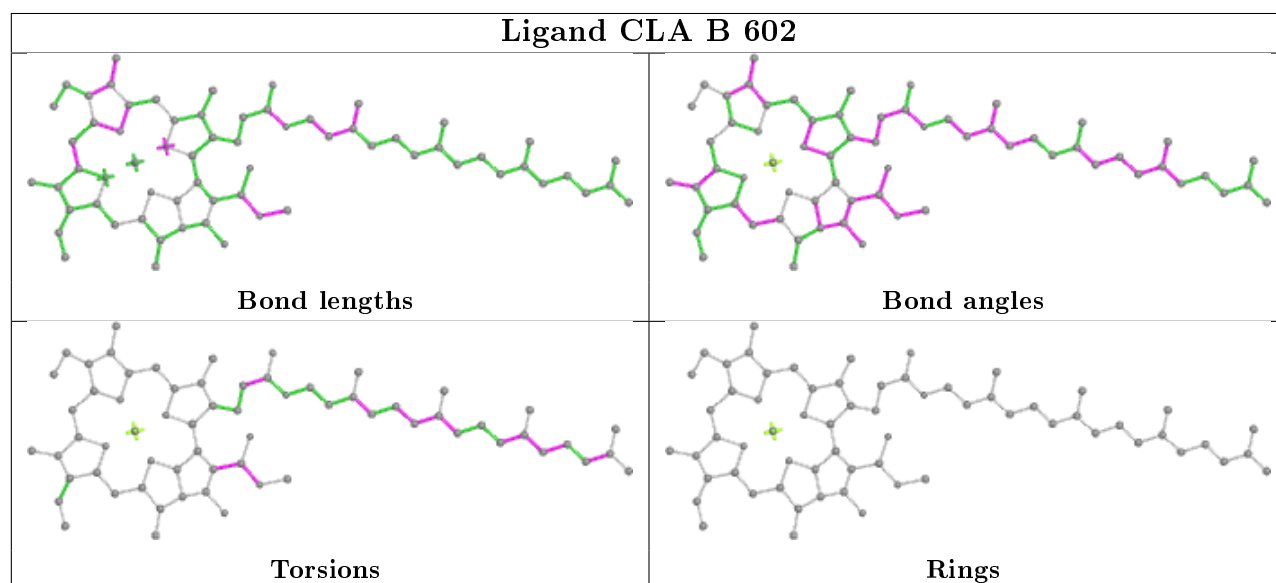


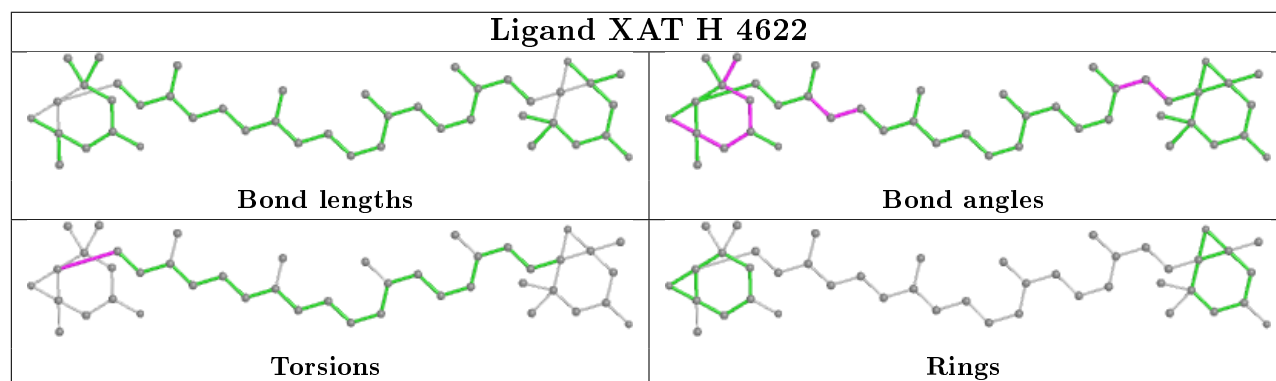
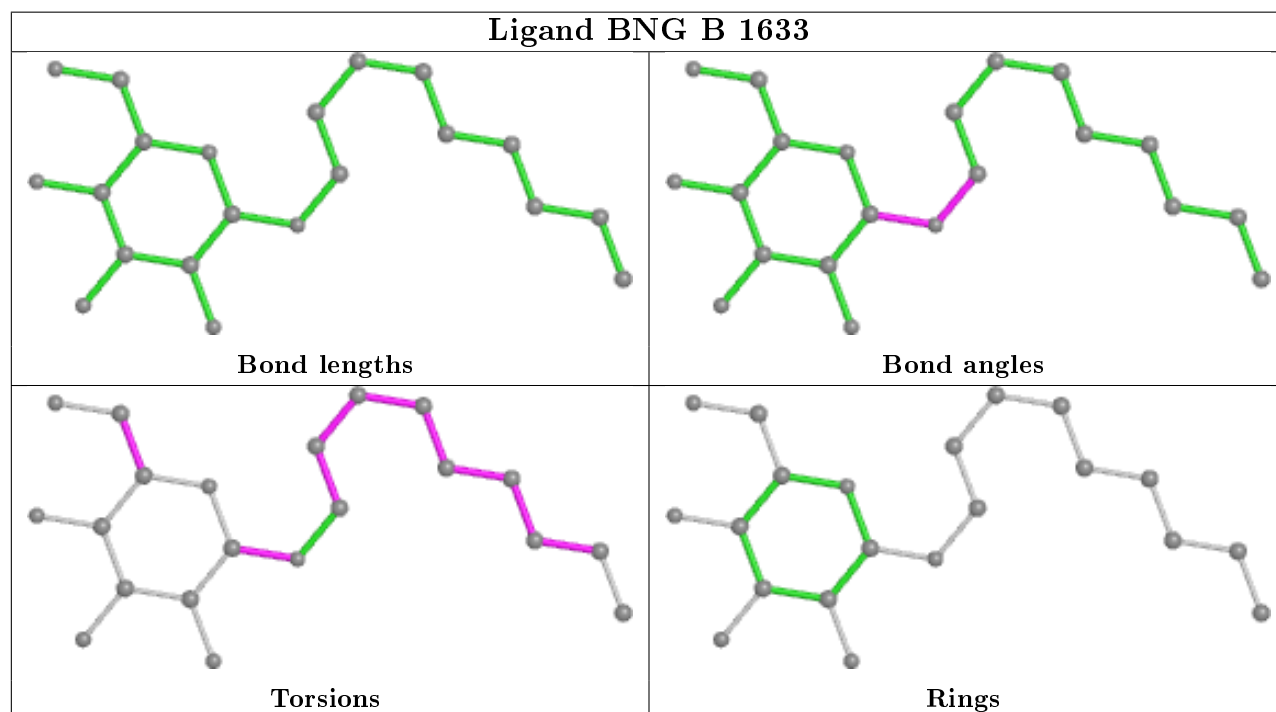
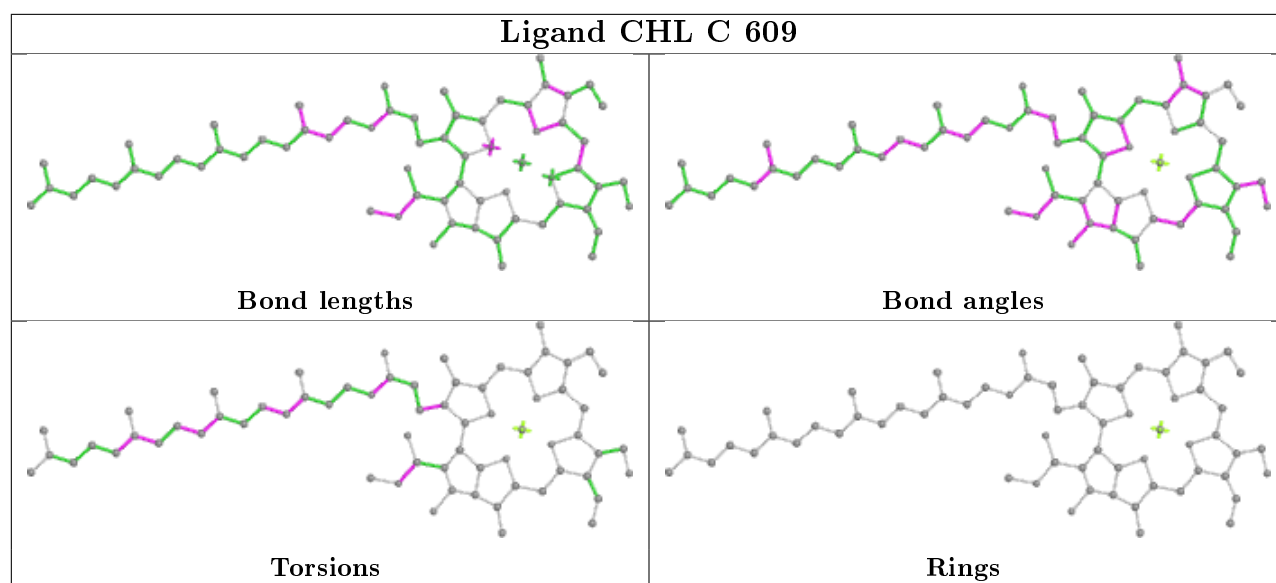
Ligand CLA I 602**Ligand LUT F 5621****Ligand CHL F 607**

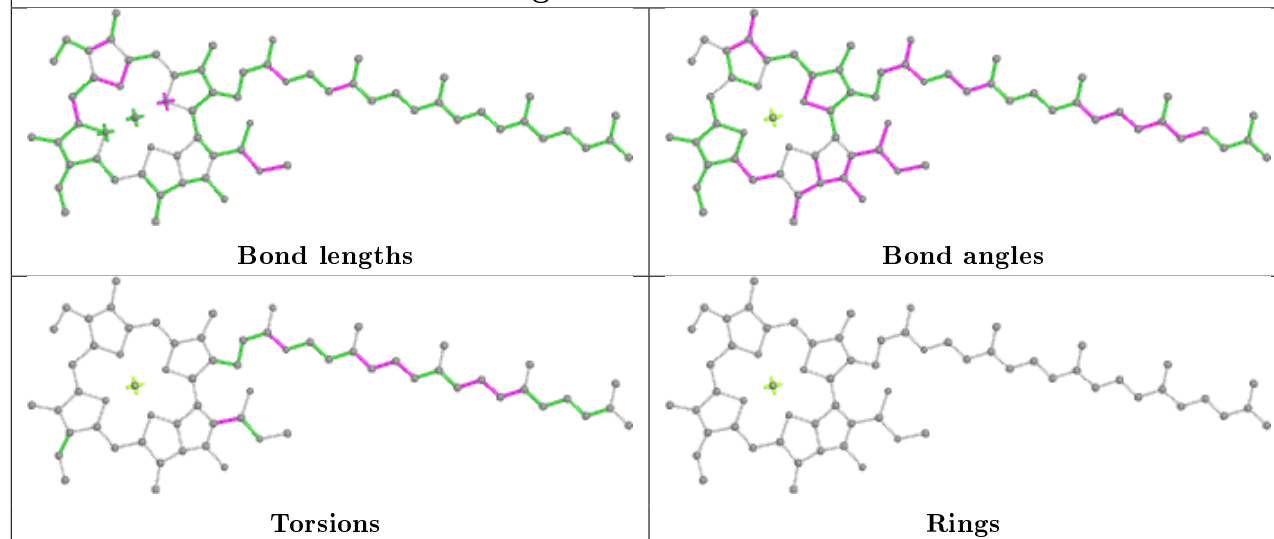
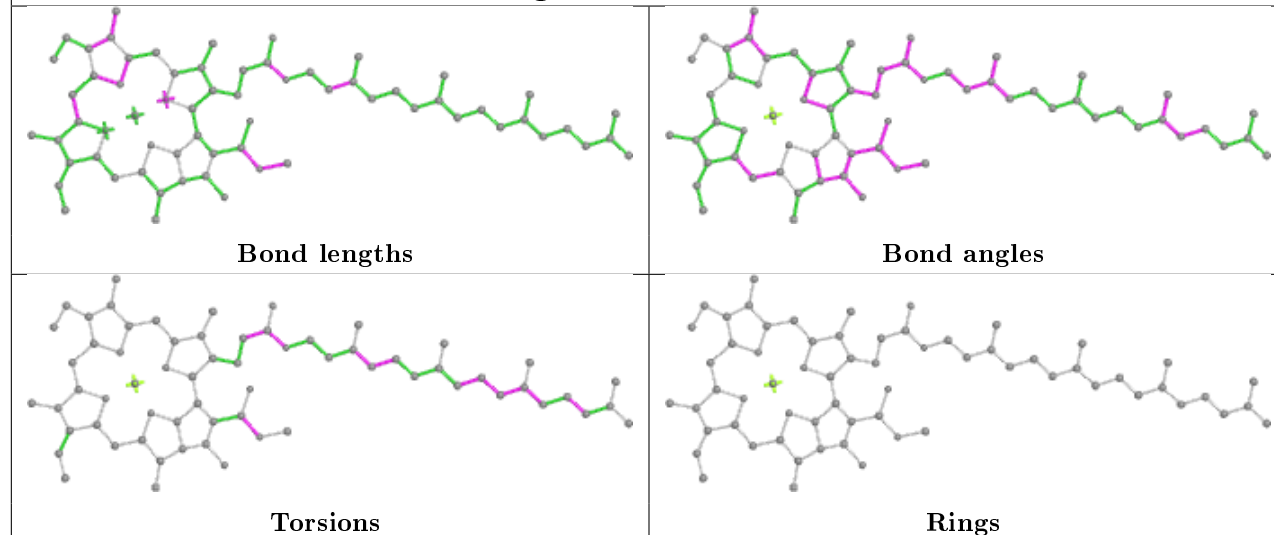
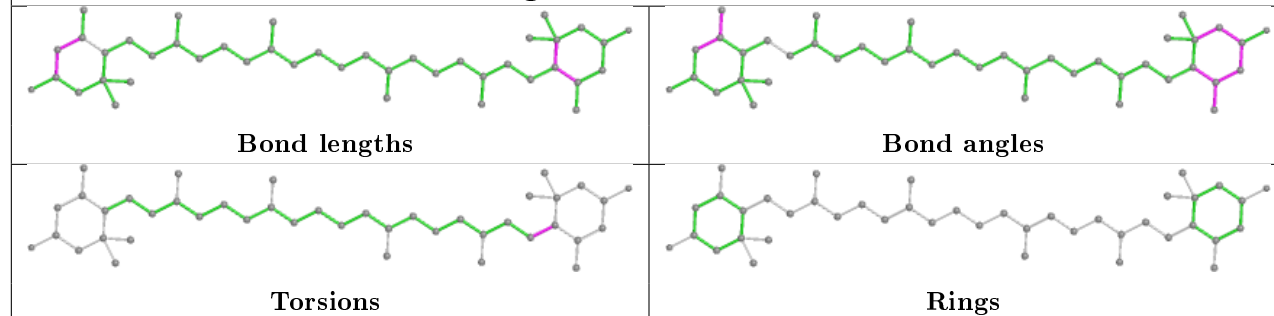
Ligand BNG G 6633



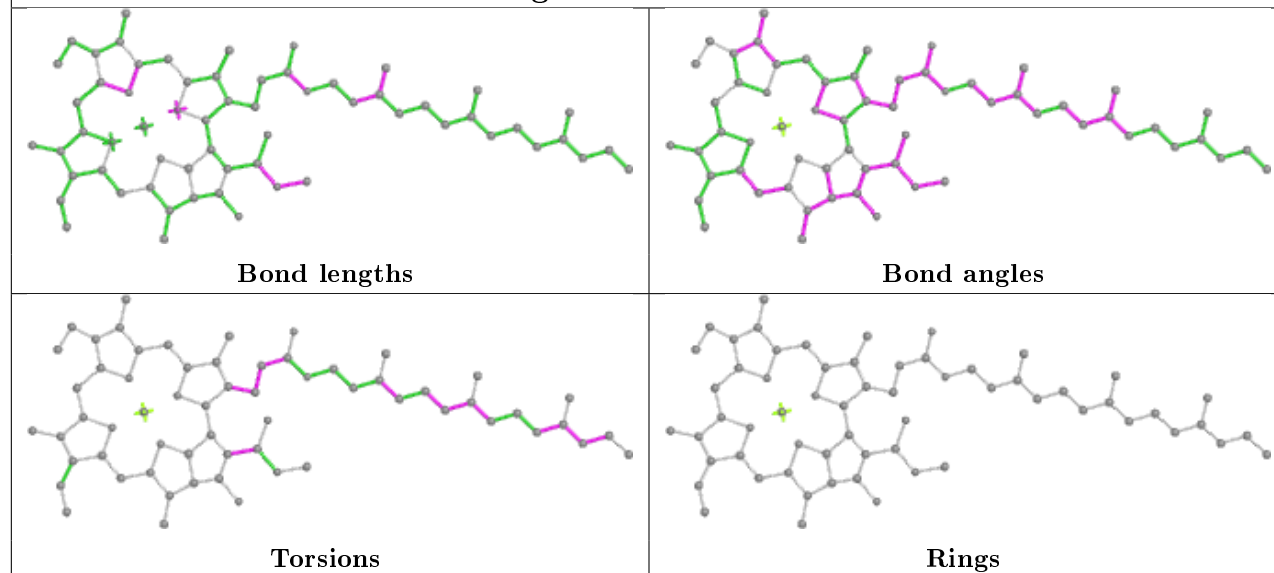
Ligand CLA B 602



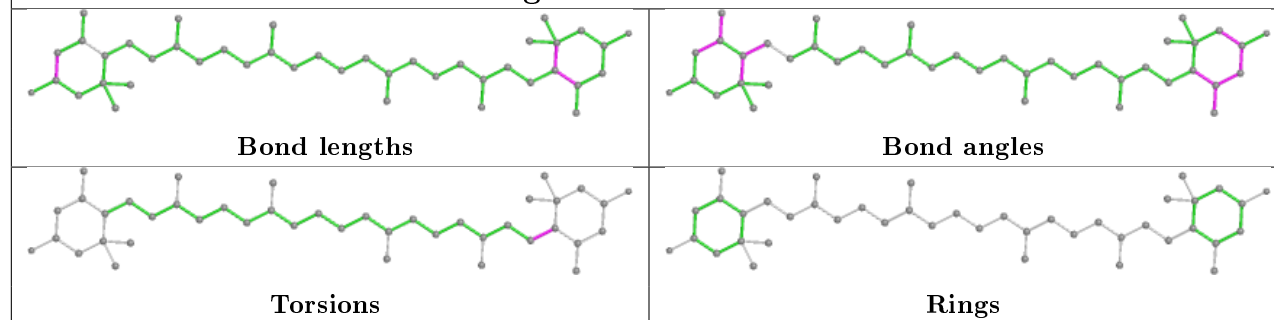


Ligand CLA C 612**Ligand CLA A 612****Ligand LUT H 7621**

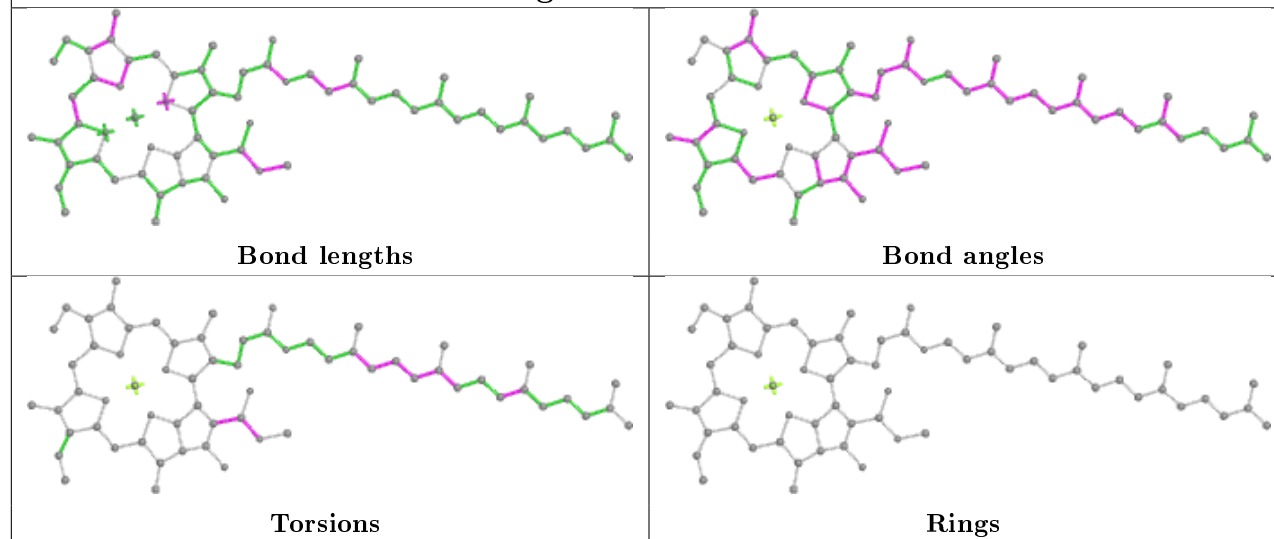
Ligand CLA D 604



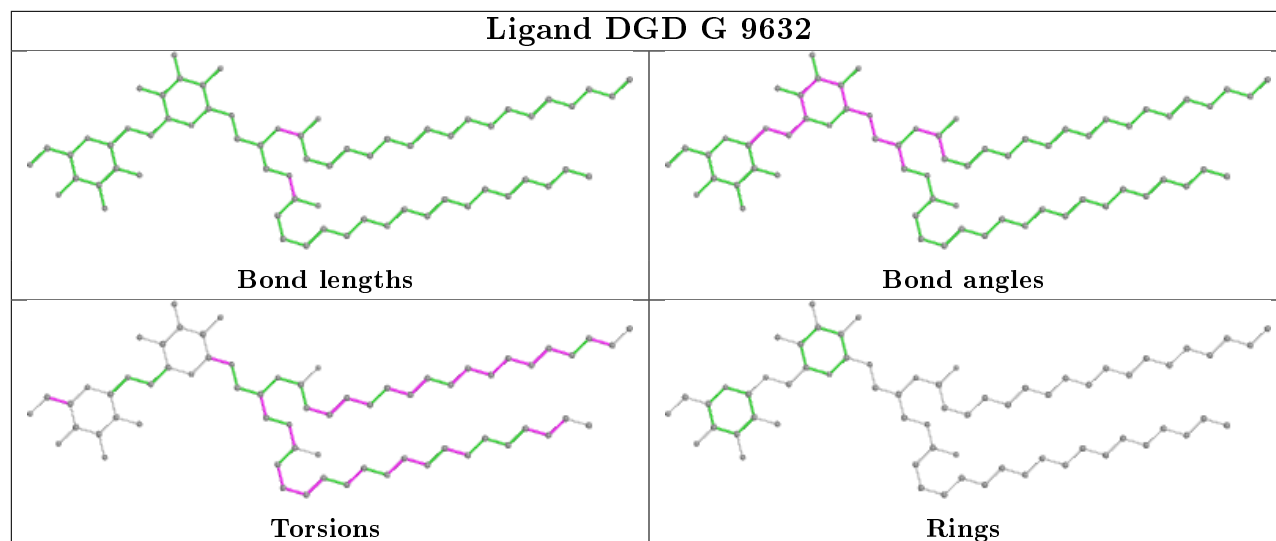
Ligand LUT C 2620



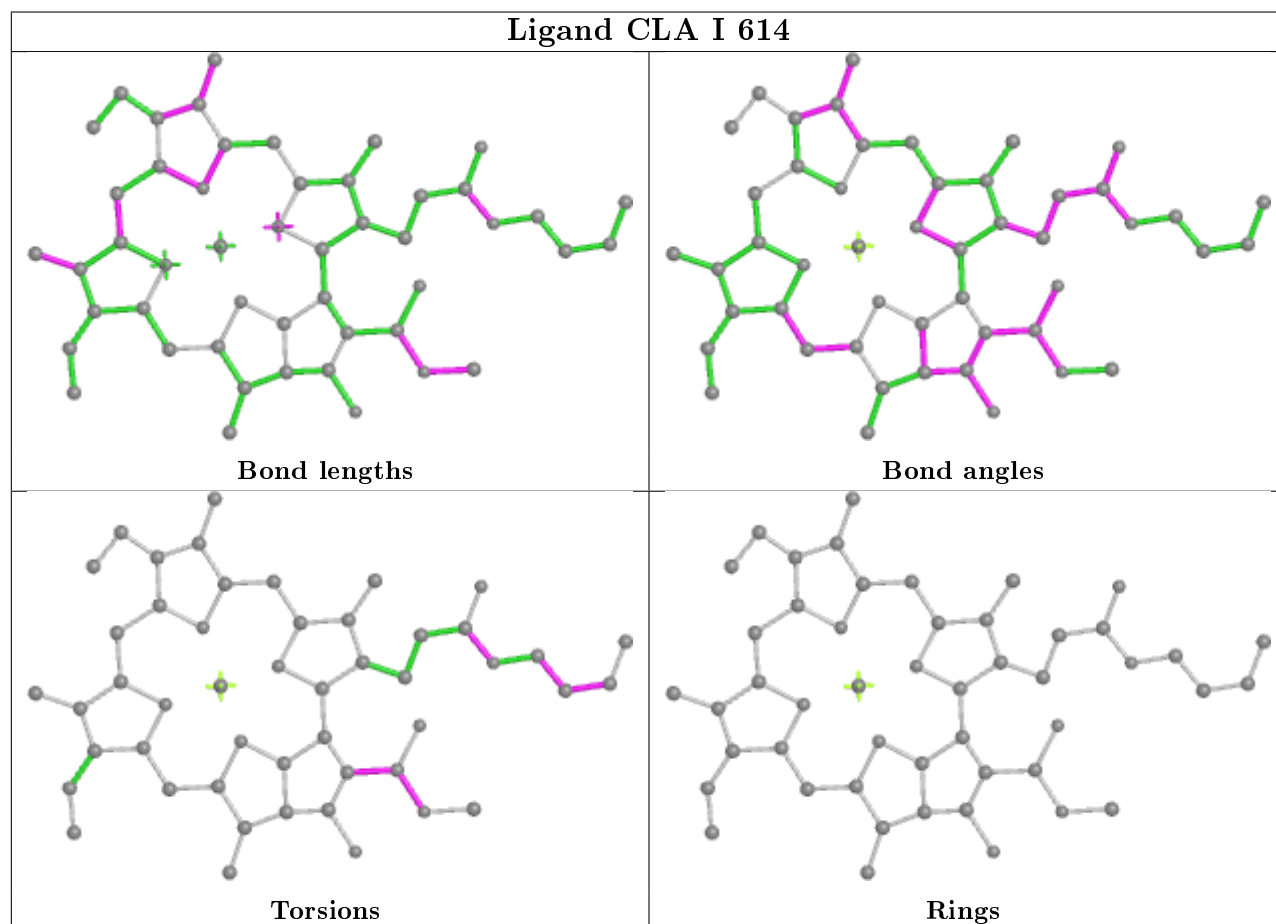
Ligand CLA J 602

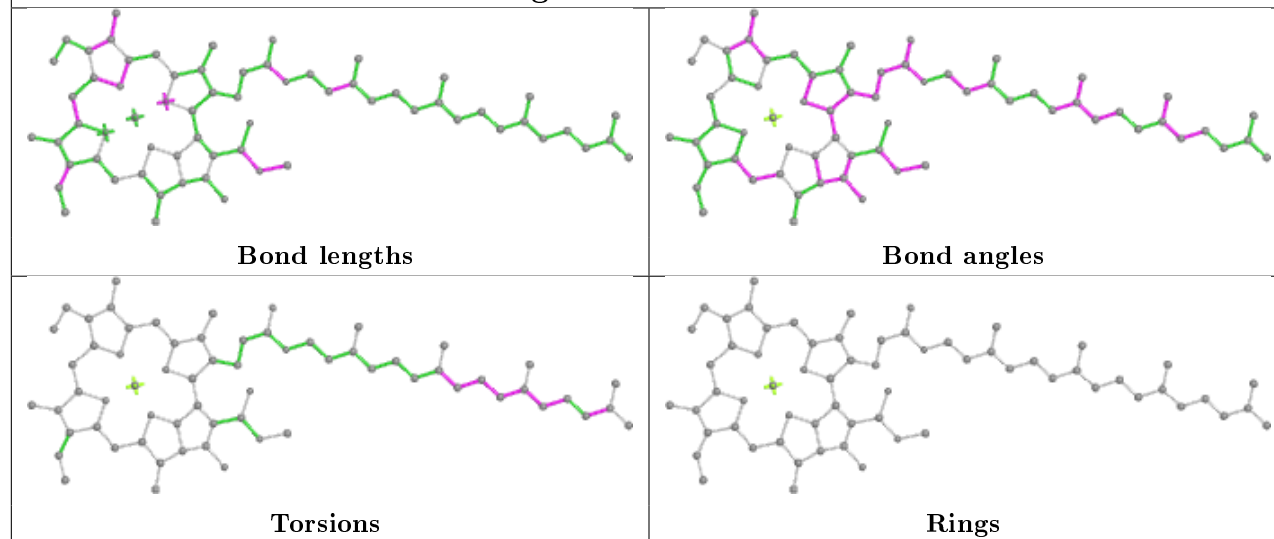
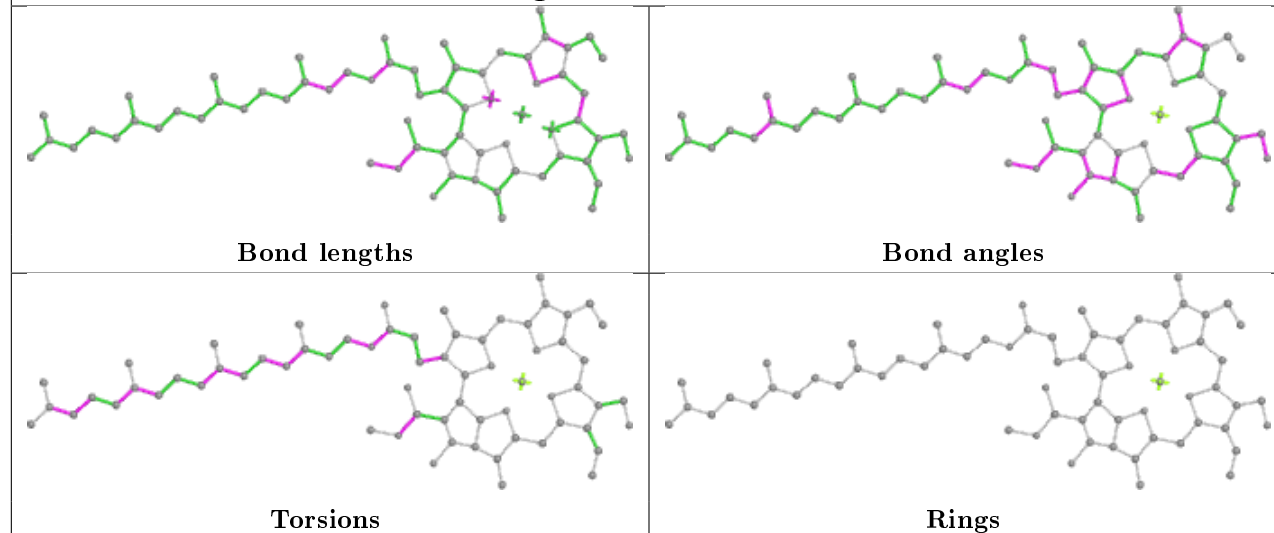
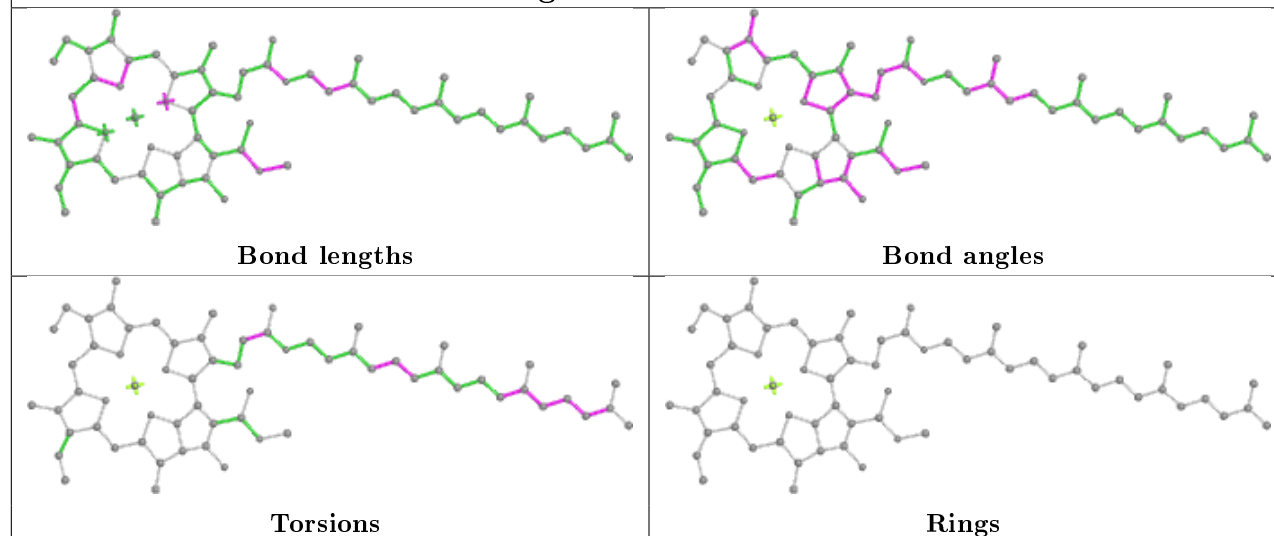


Ligand DGD G 9632

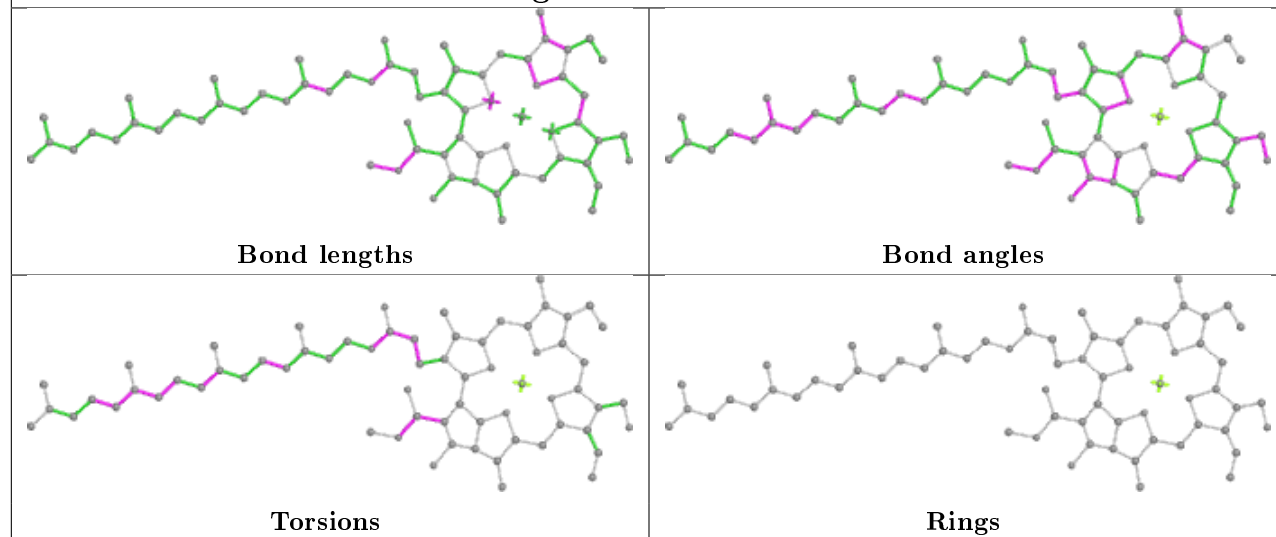


Ligand CLA I 614

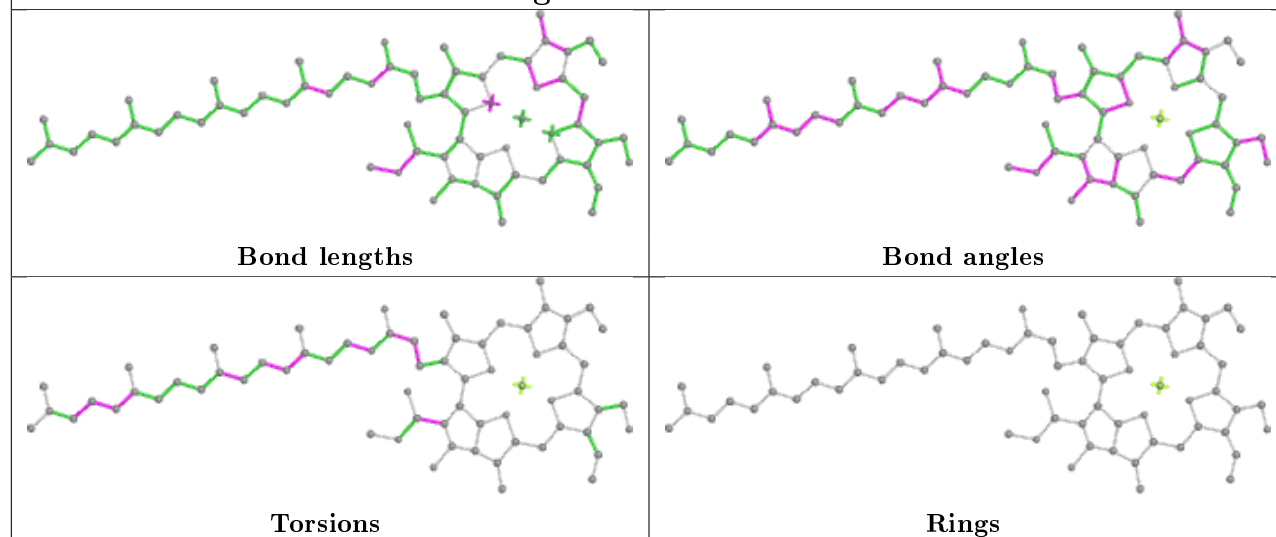


Ligand CLA H 610**Ligand CHL A 609****Ligand CLA I 613**

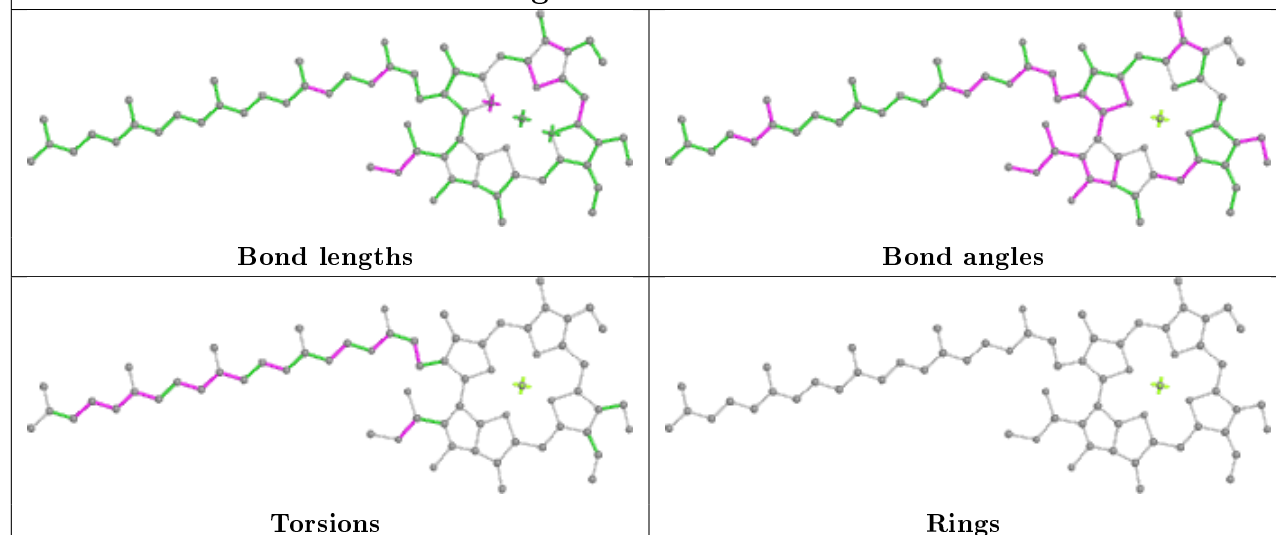
Ligand CHL C 601



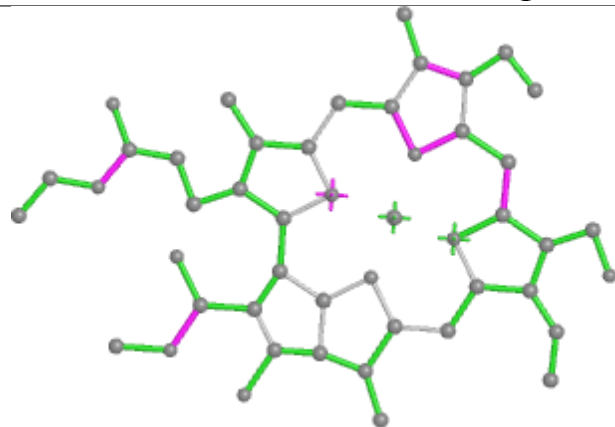
Ligand CHL E 601



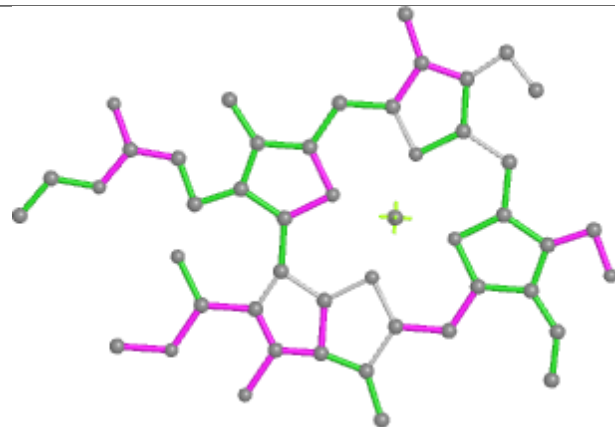
Ligand CHL A 608



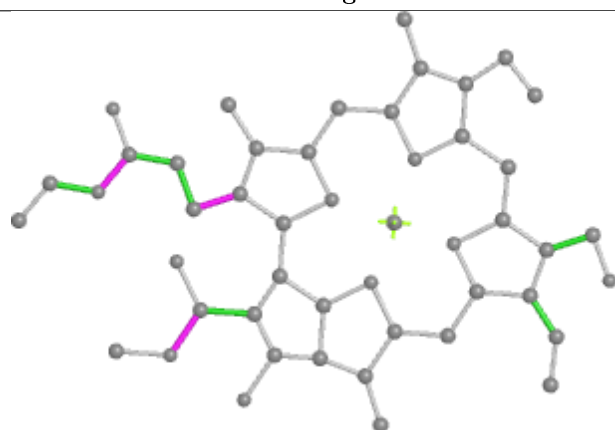
Ligand CHL F 605



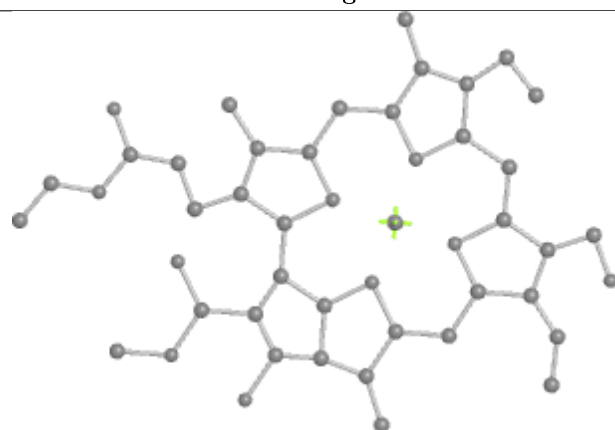
Bond lengths



Bond angles

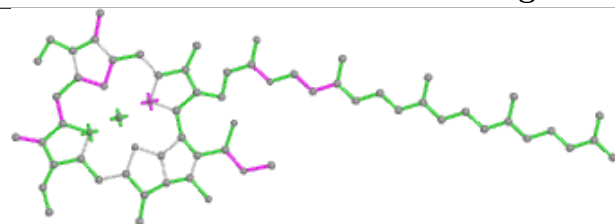


Torsions

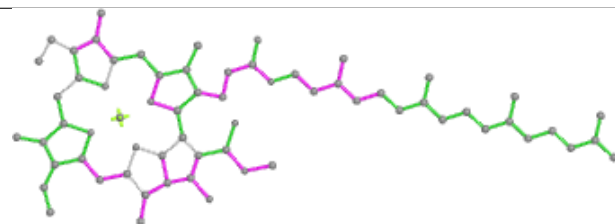


Rings

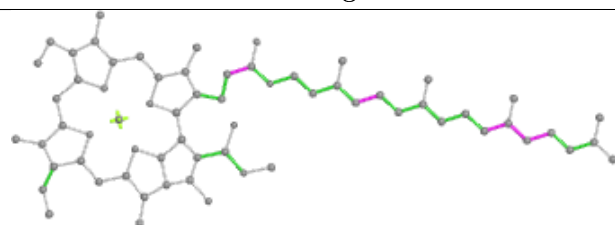
Ligand CLA F 613



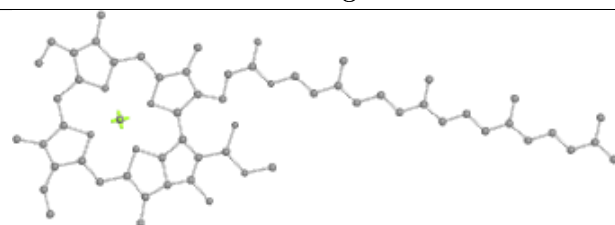
Bond lengths



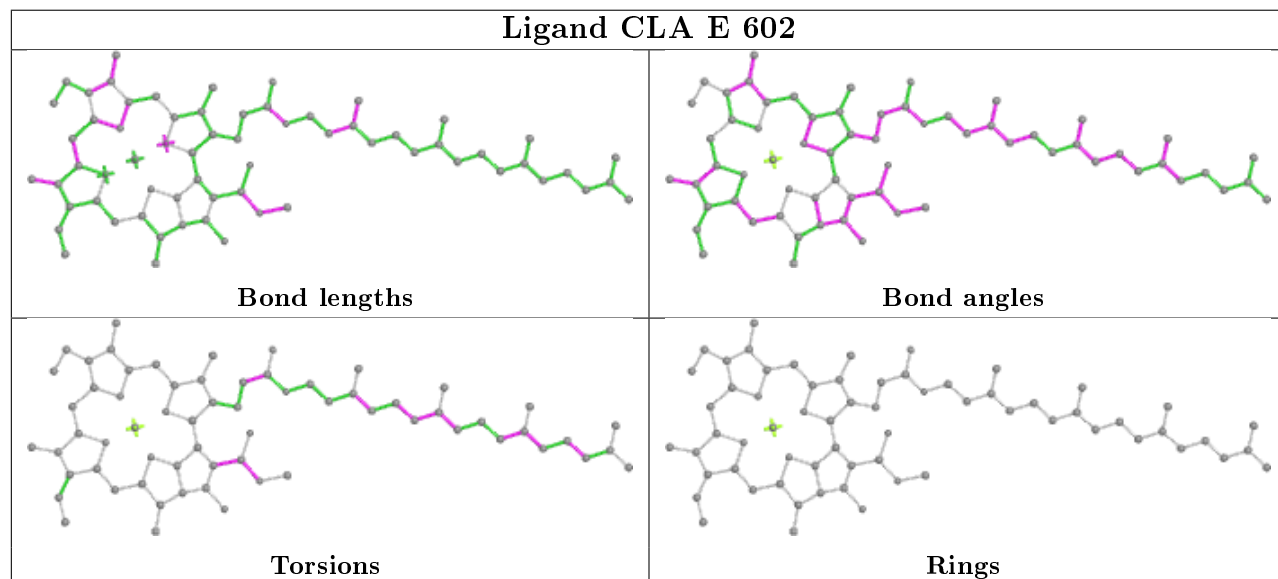
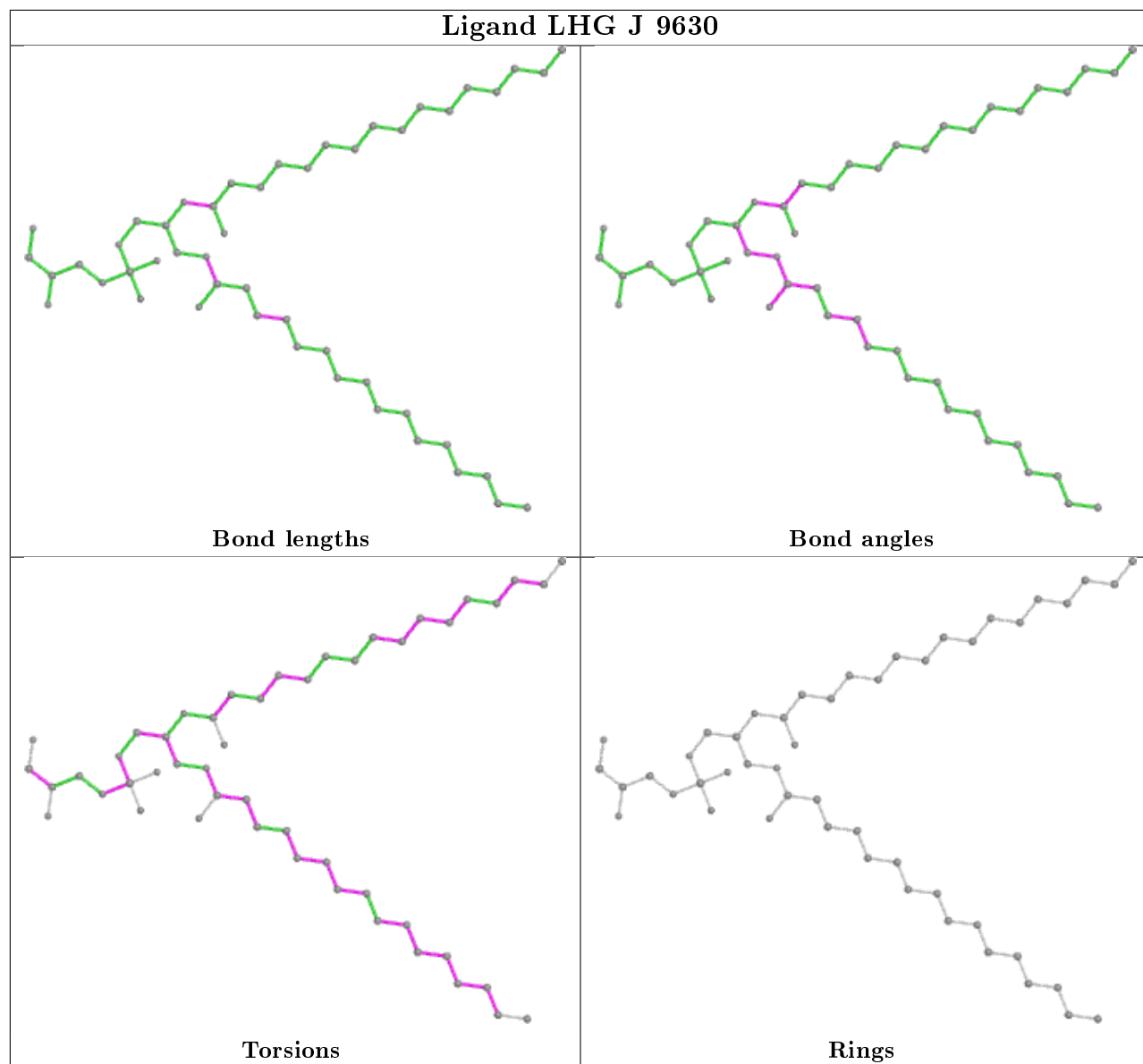
Bond angles

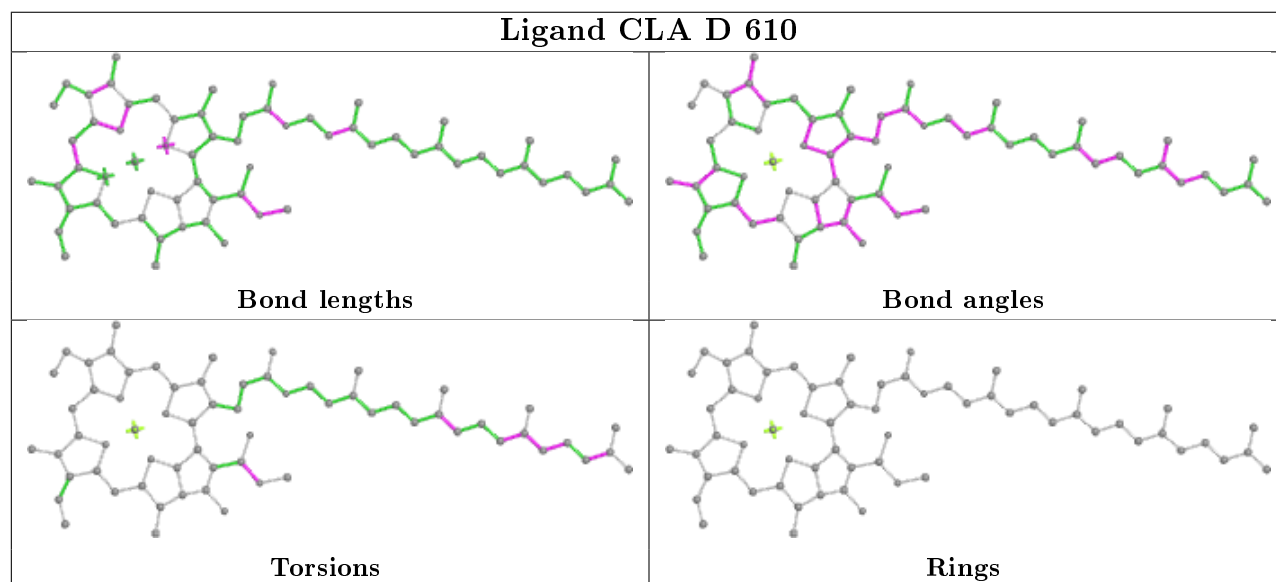
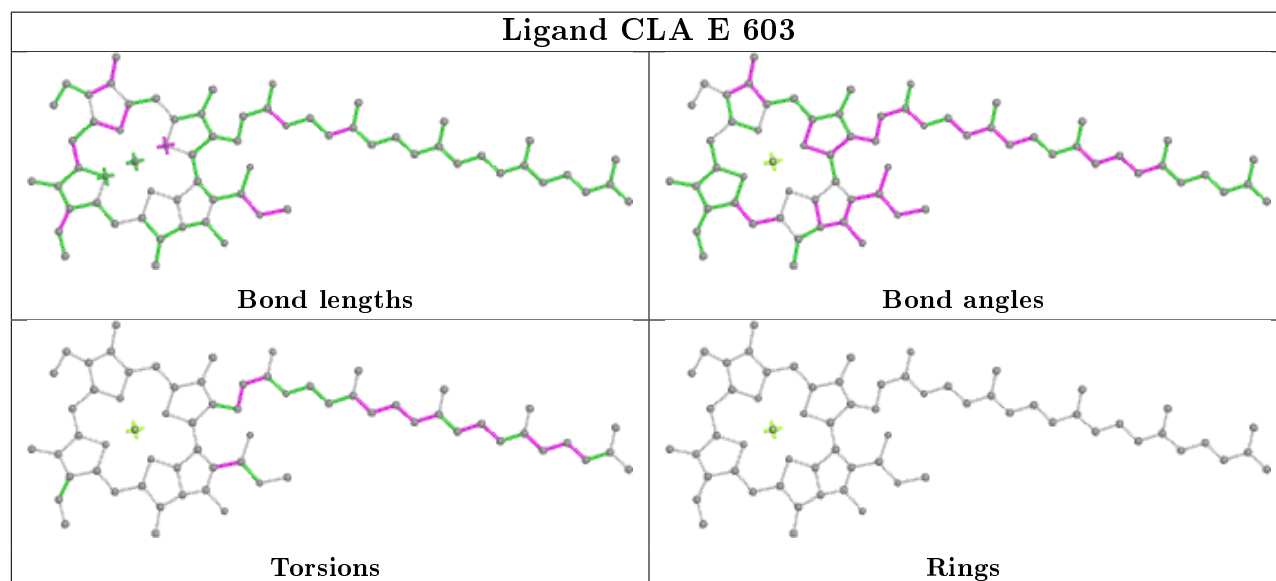
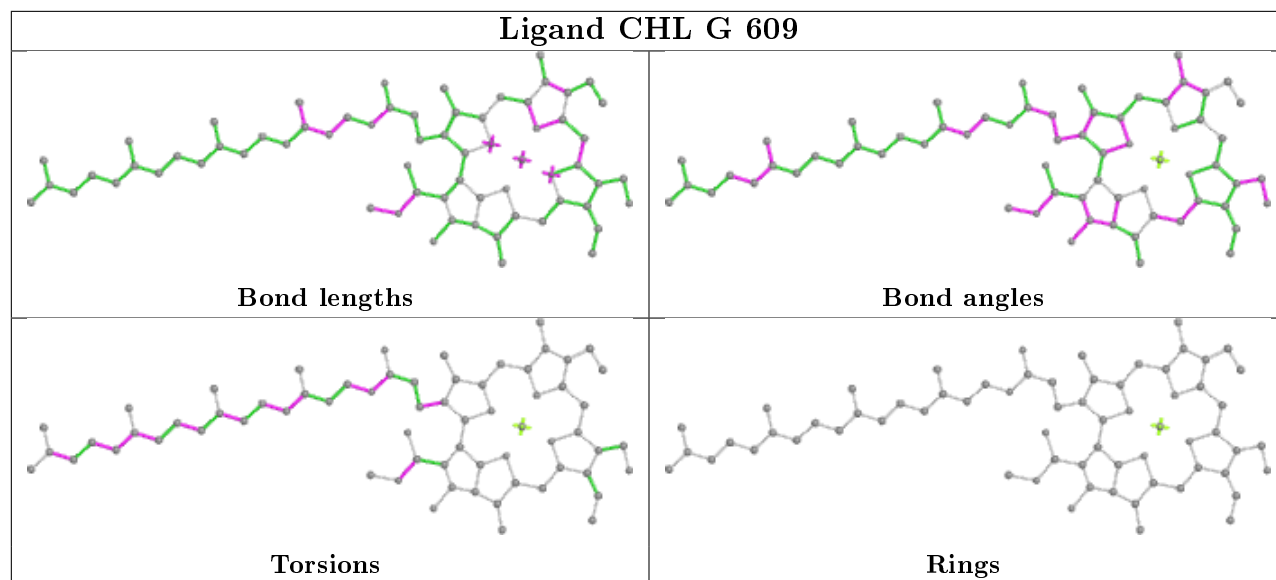


Torsions

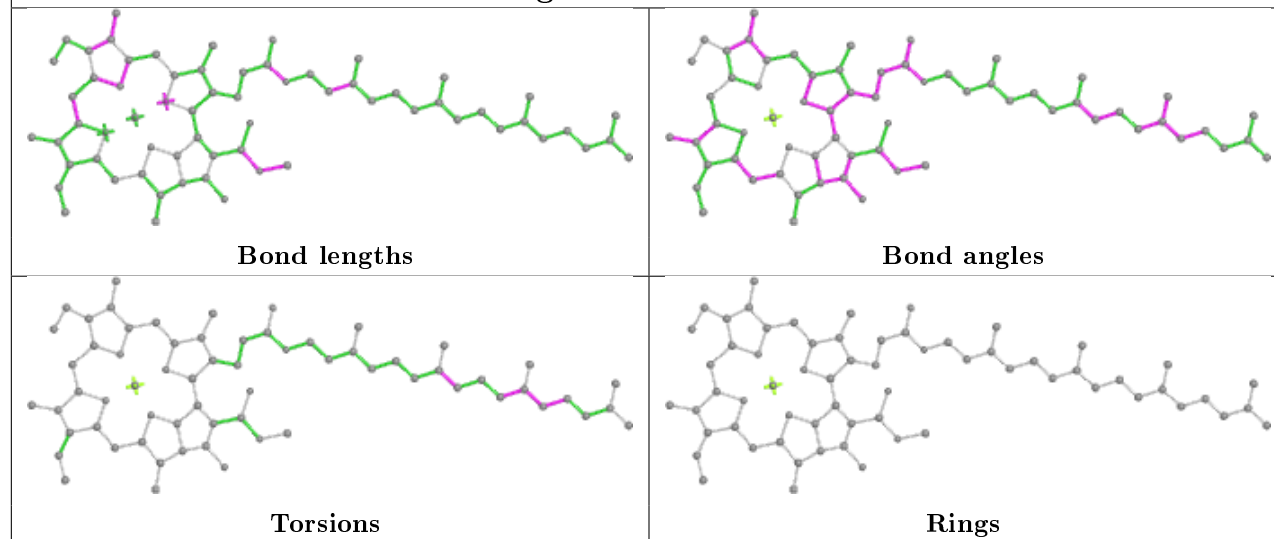


Rings

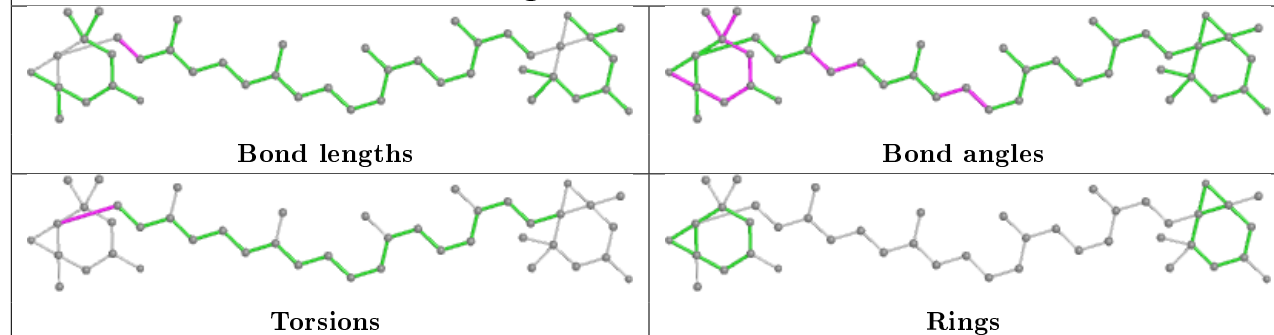




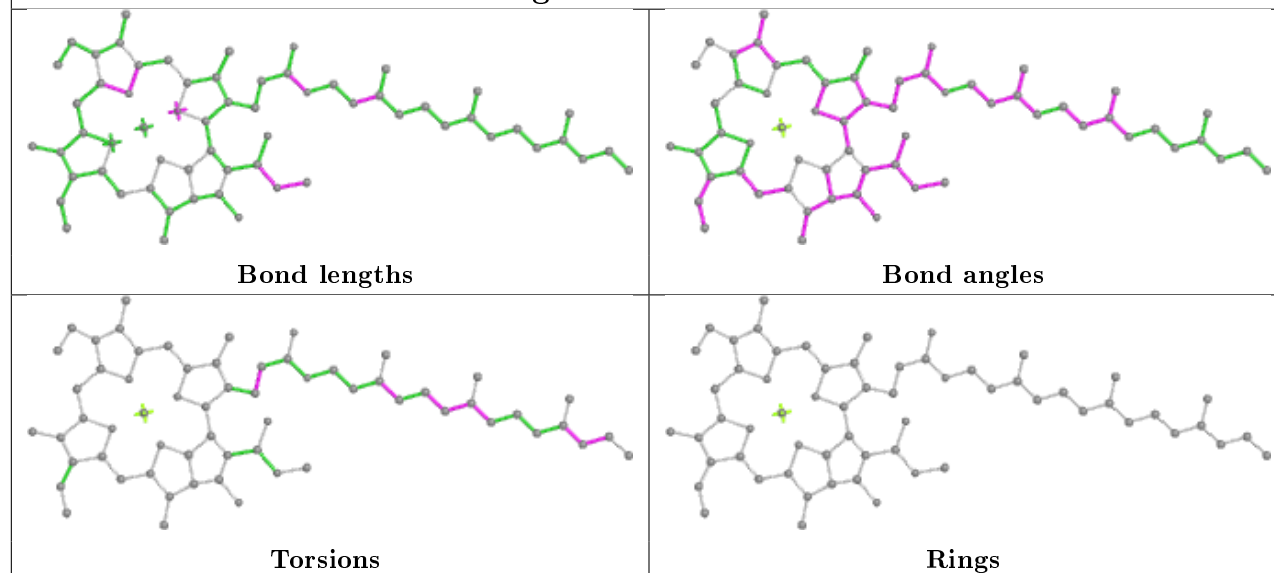
Ligand CLA J 610



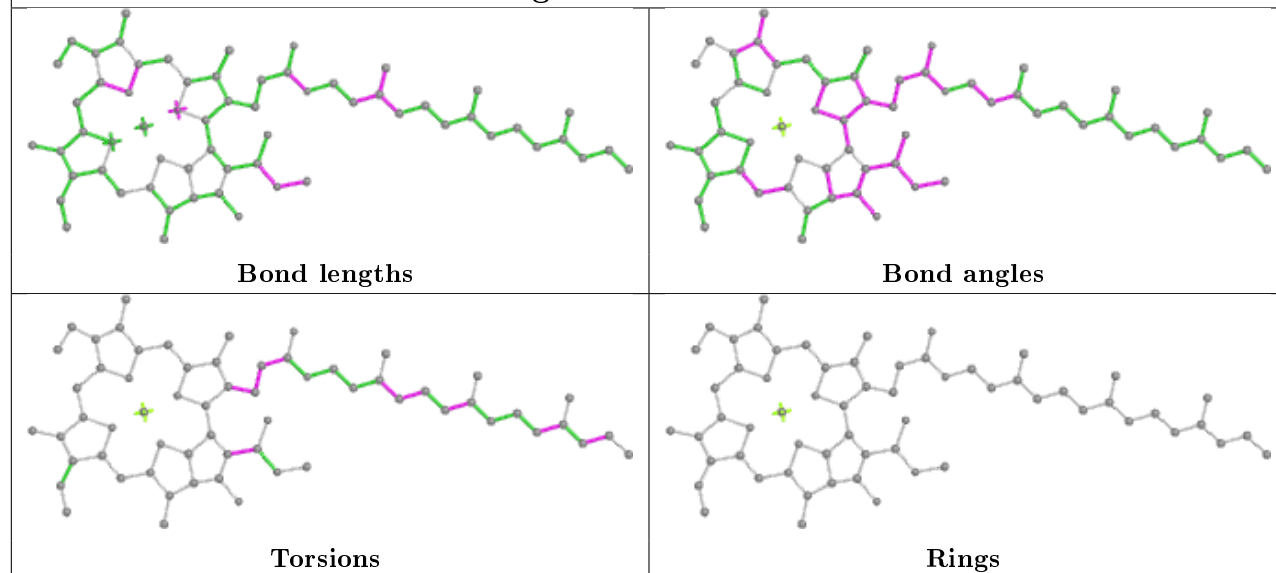
Ligand XAT D 8622



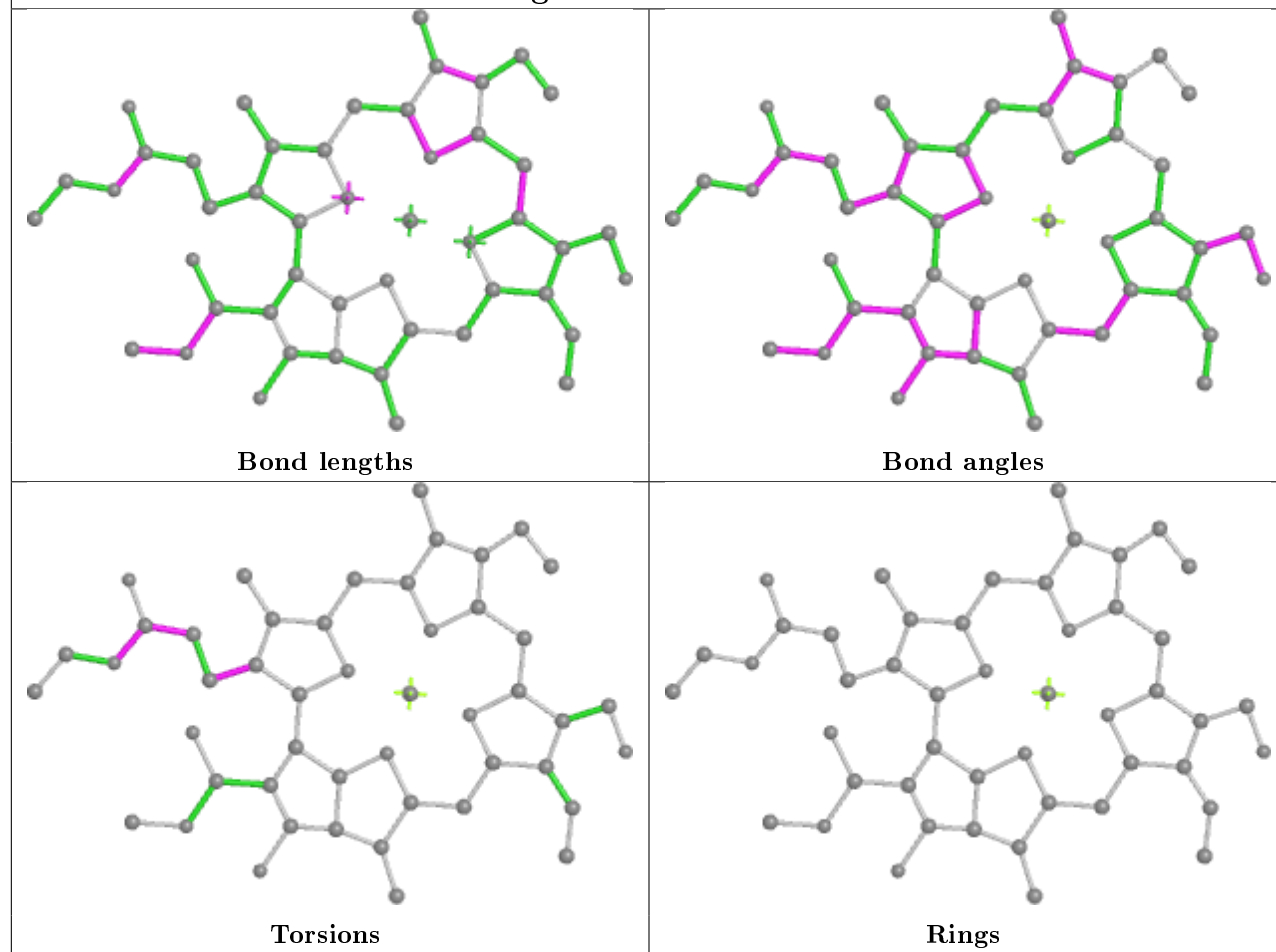
Ligand CLA B 604

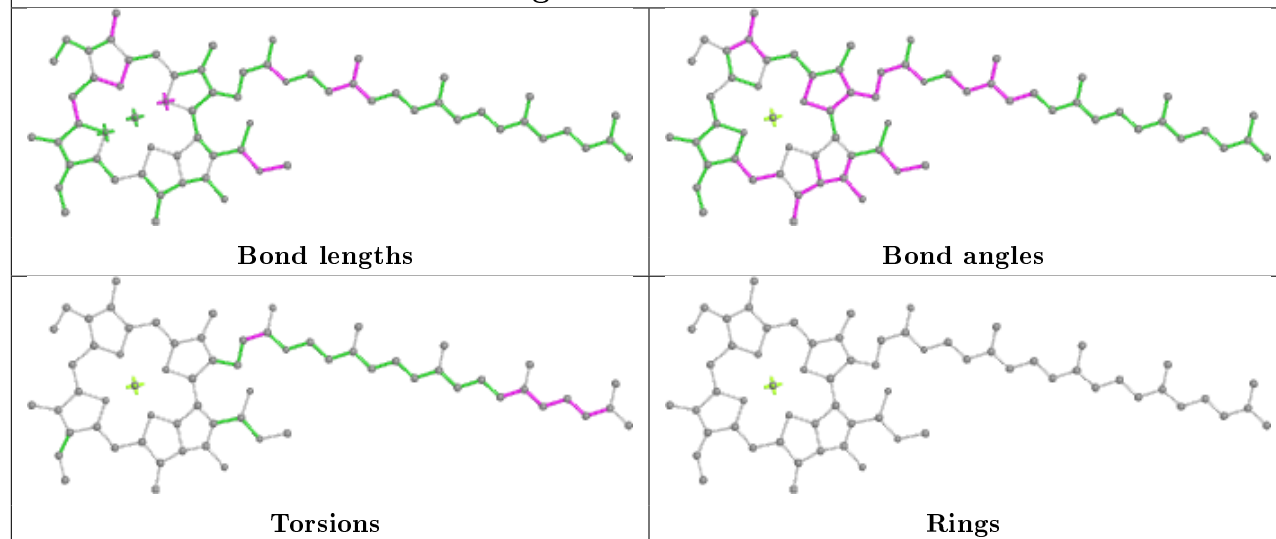
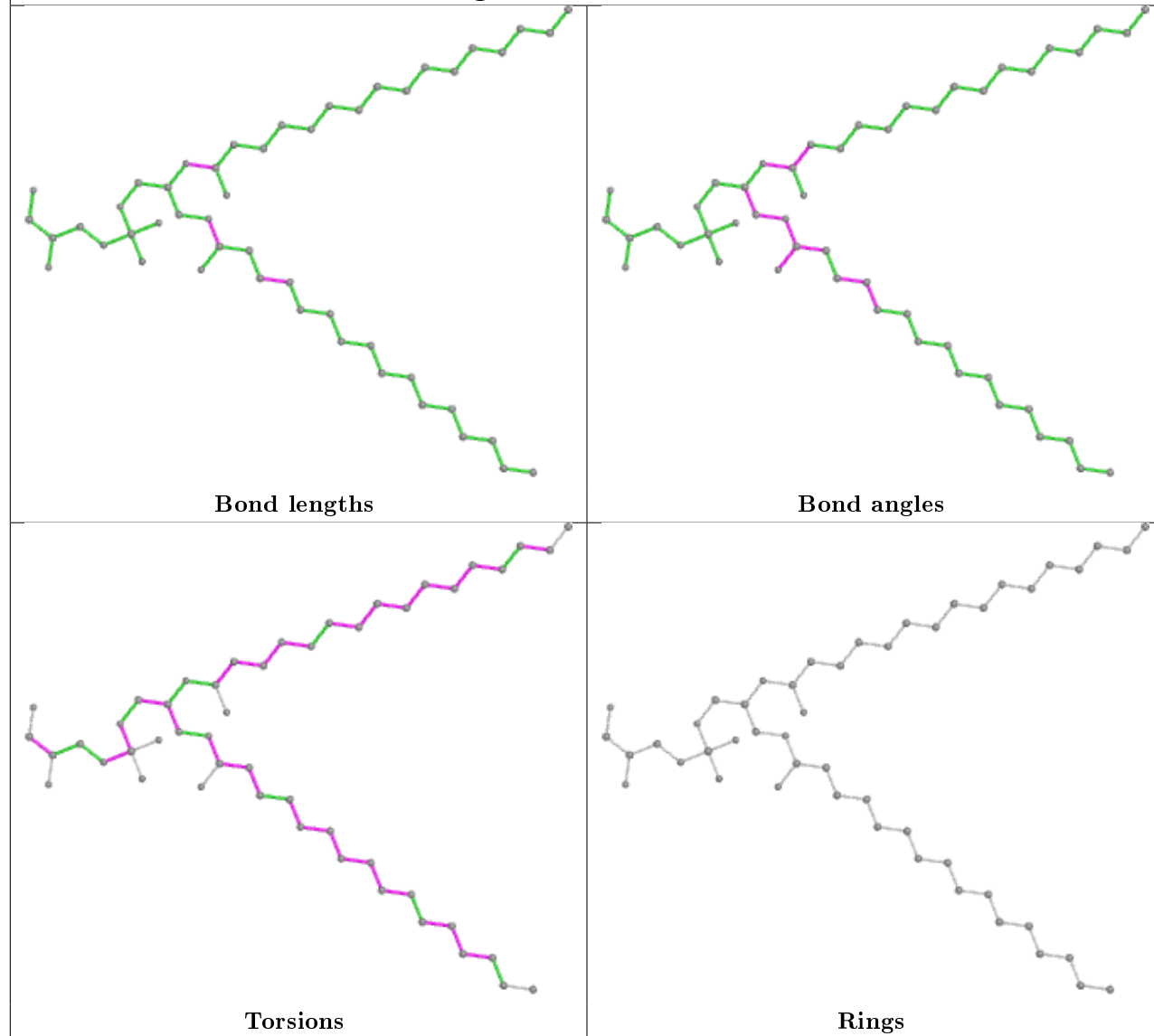


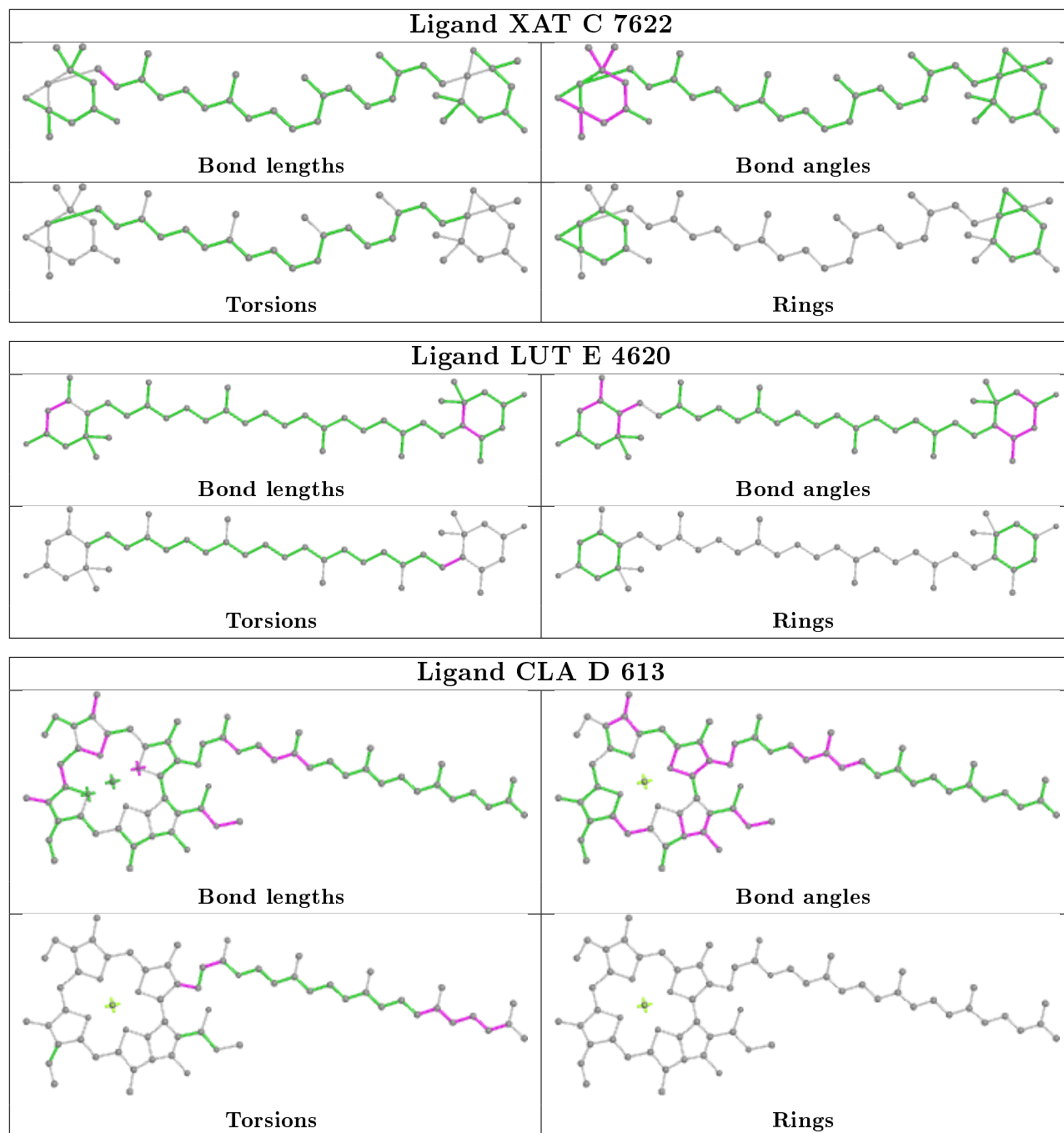
Ligand CLA A 604

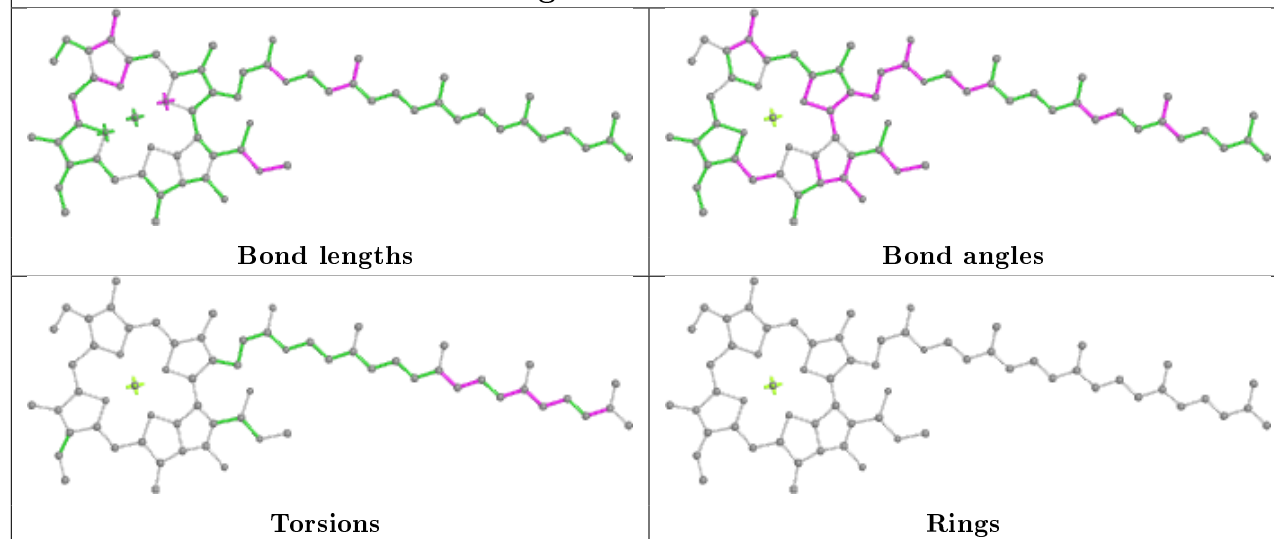
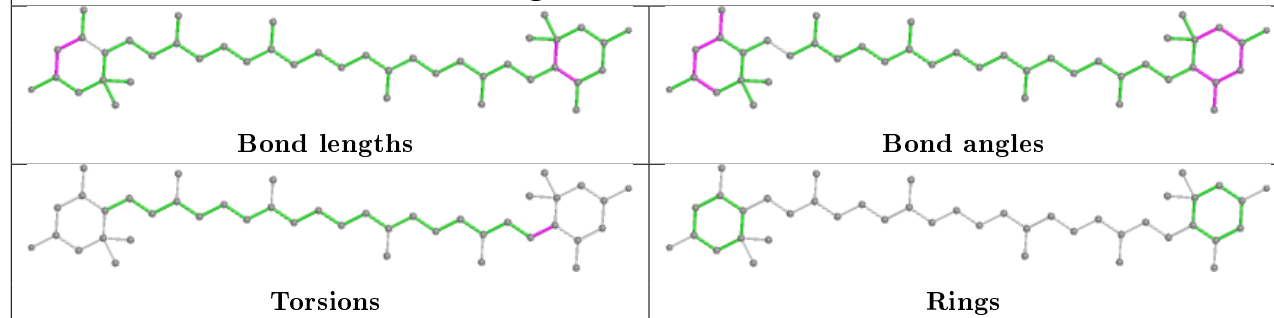


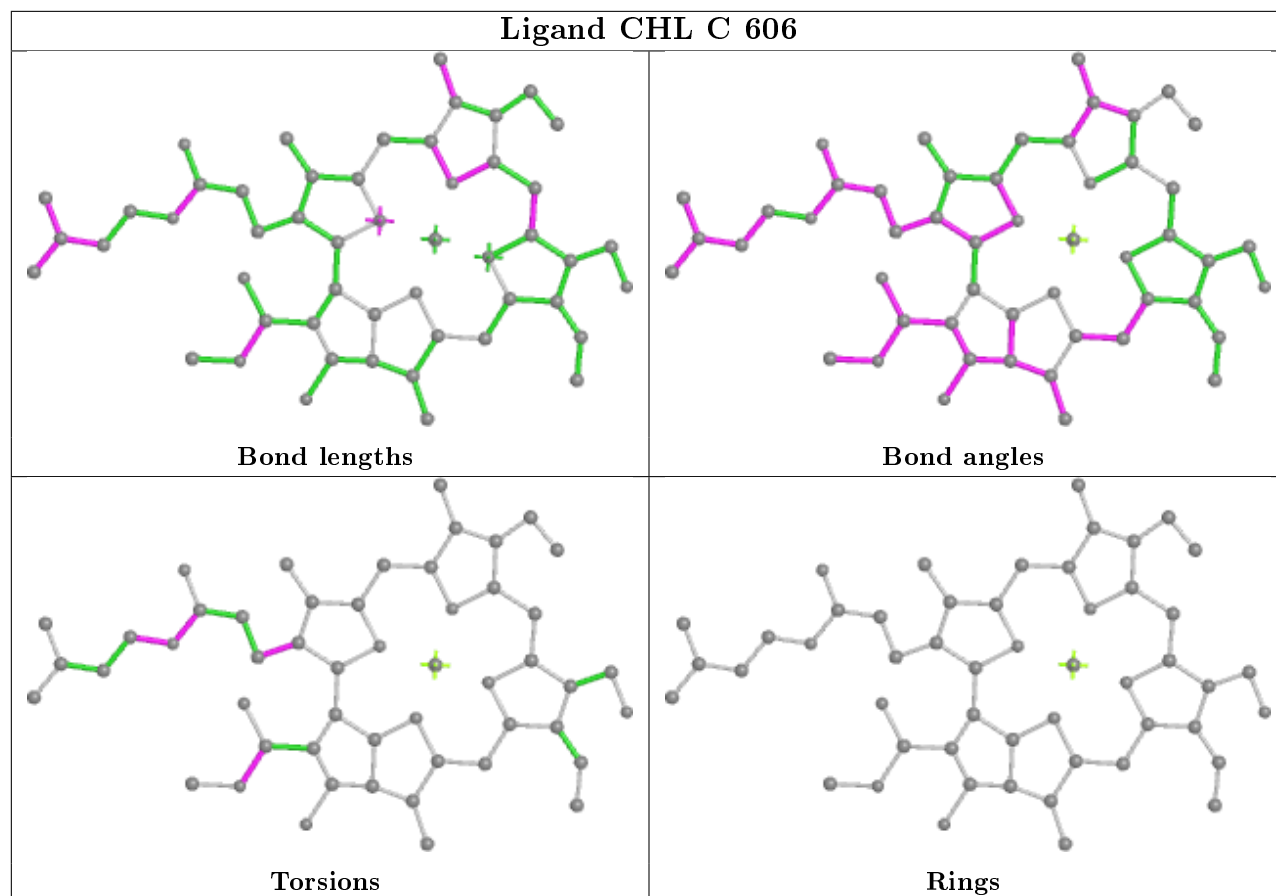
Ligand CHL A 605



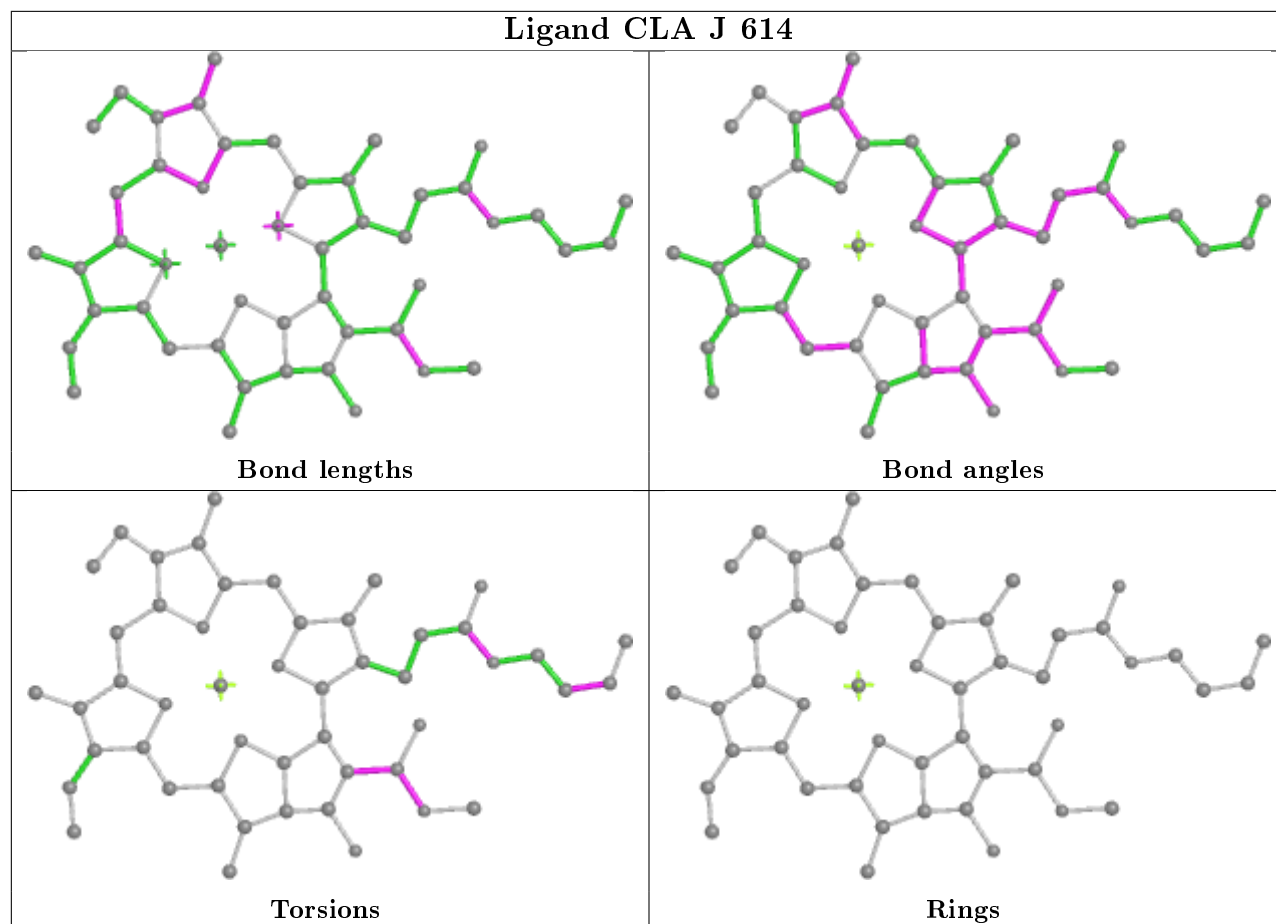
Ligand CLA B 613**Ligand LHG C 2630**



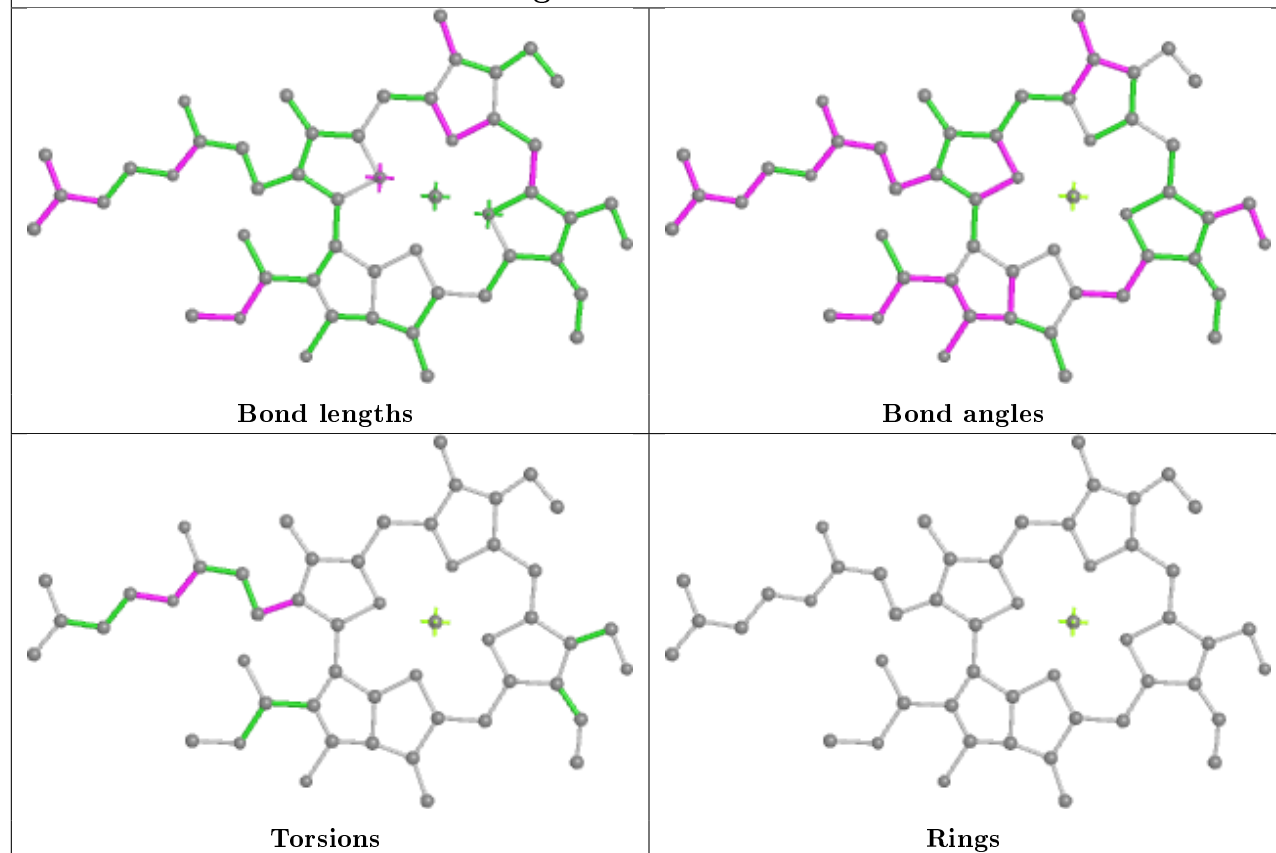
Ligand CLA I 610**Ligand LUT J 9621**



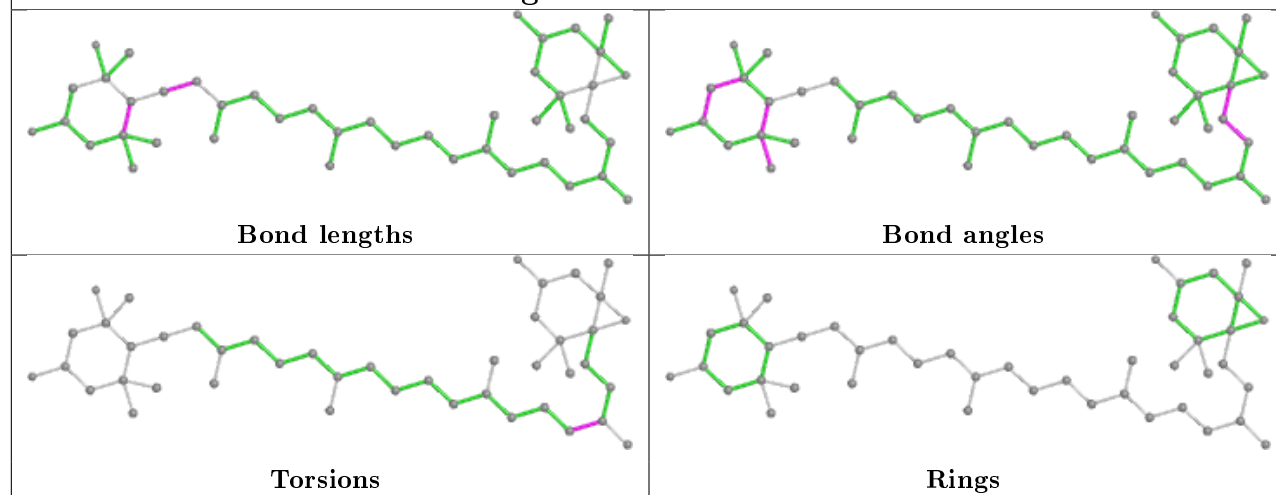
Ligand CLA J 614



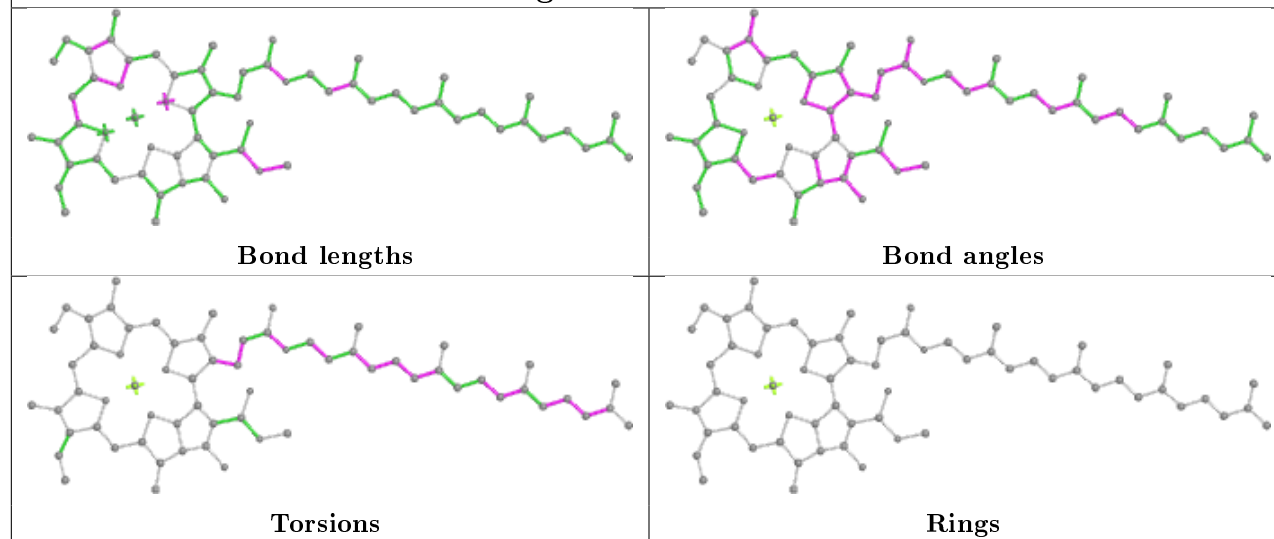
Ligand CHL E 606



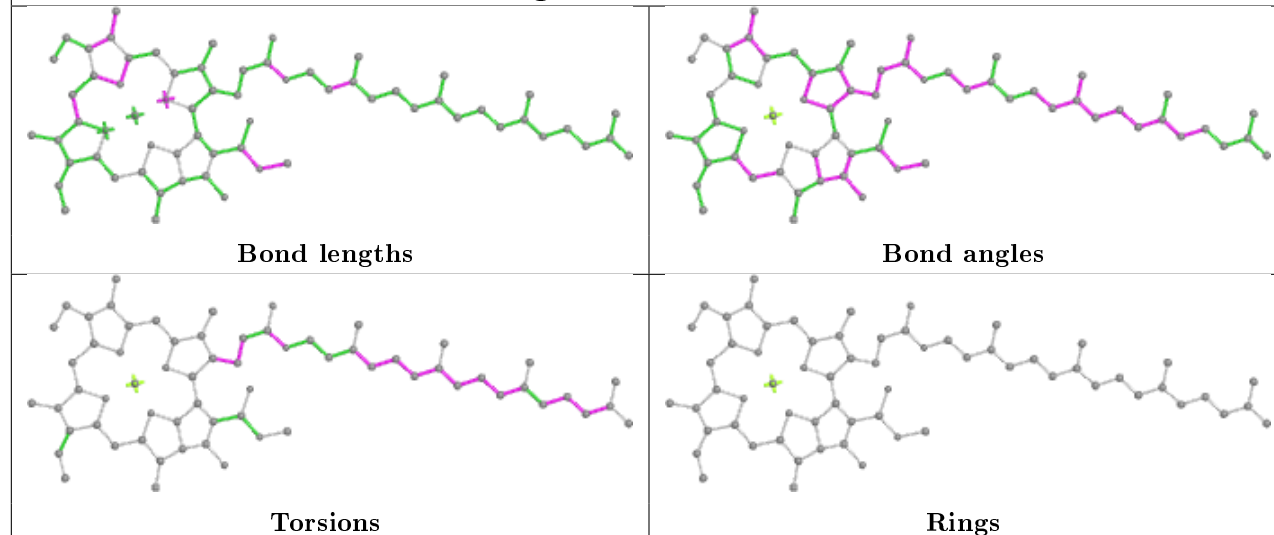
Ligand NEX C 2623



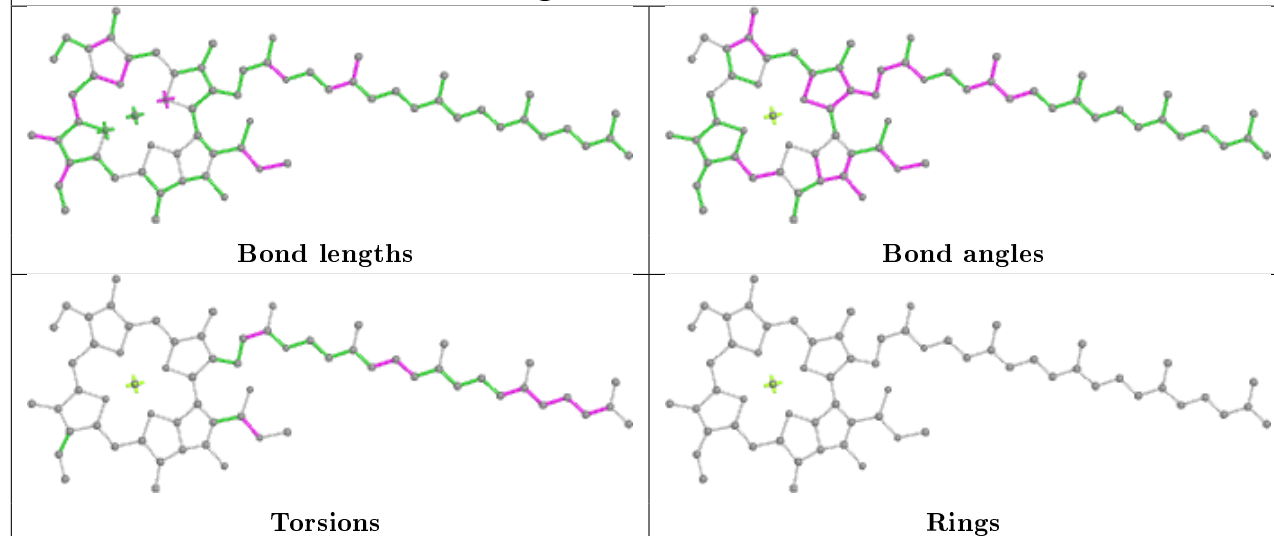
Ligand CLA J 611



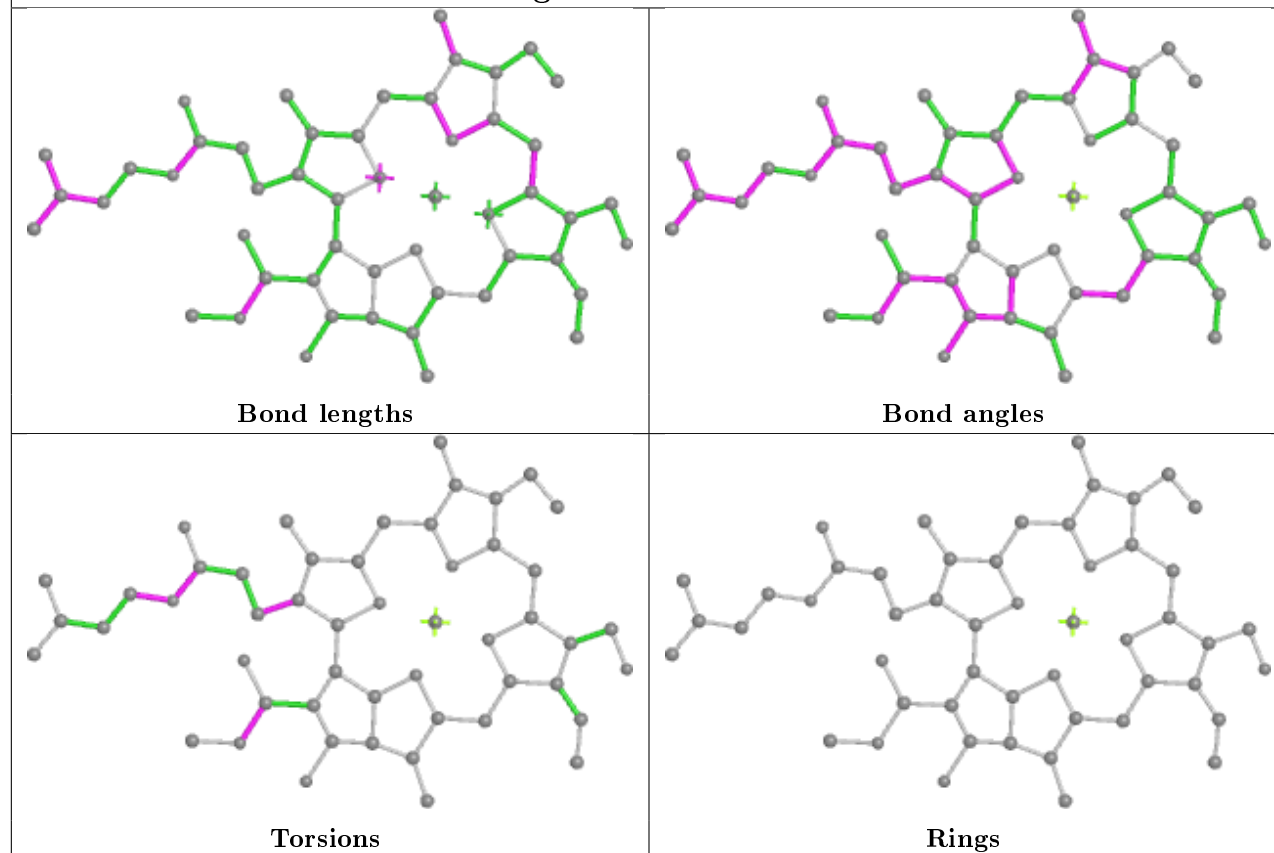
Ligand CLA A 611



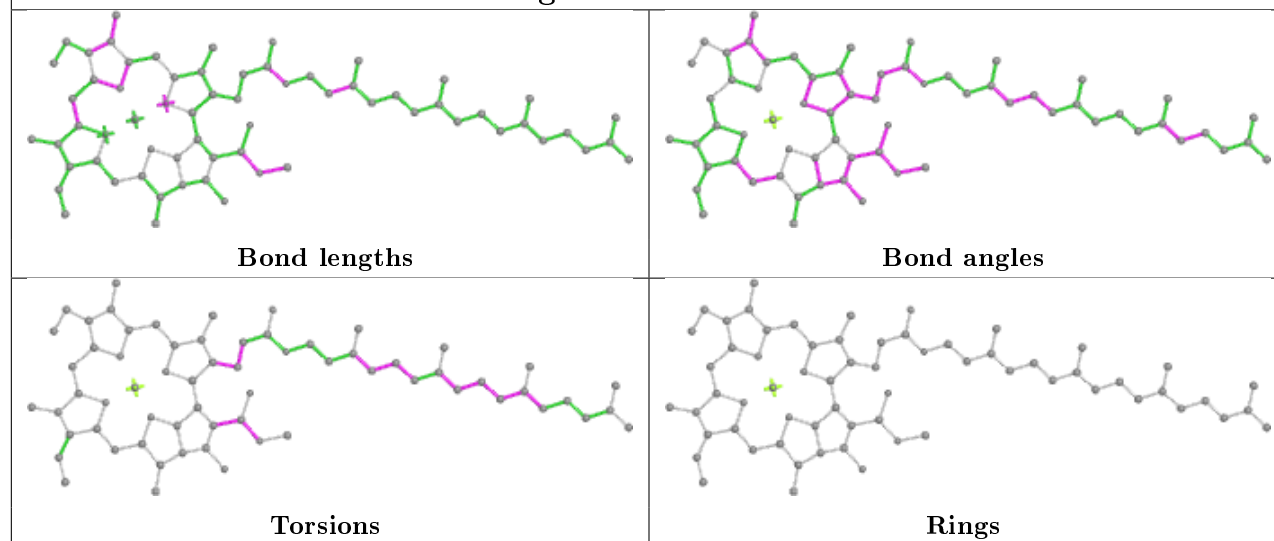
Ligand CLA J 613

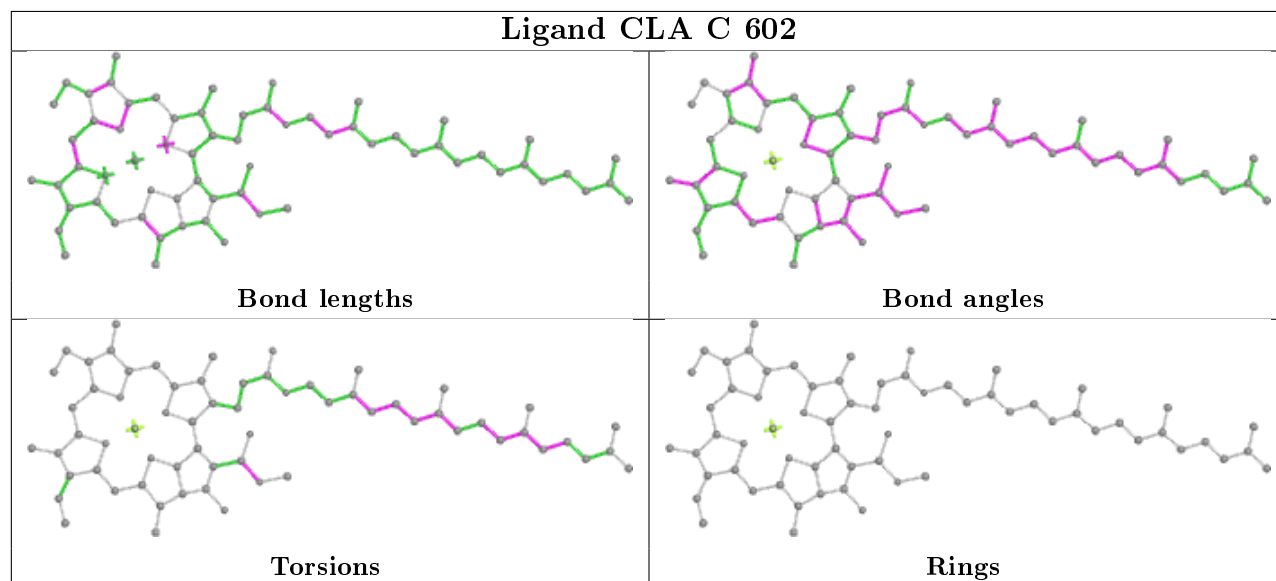
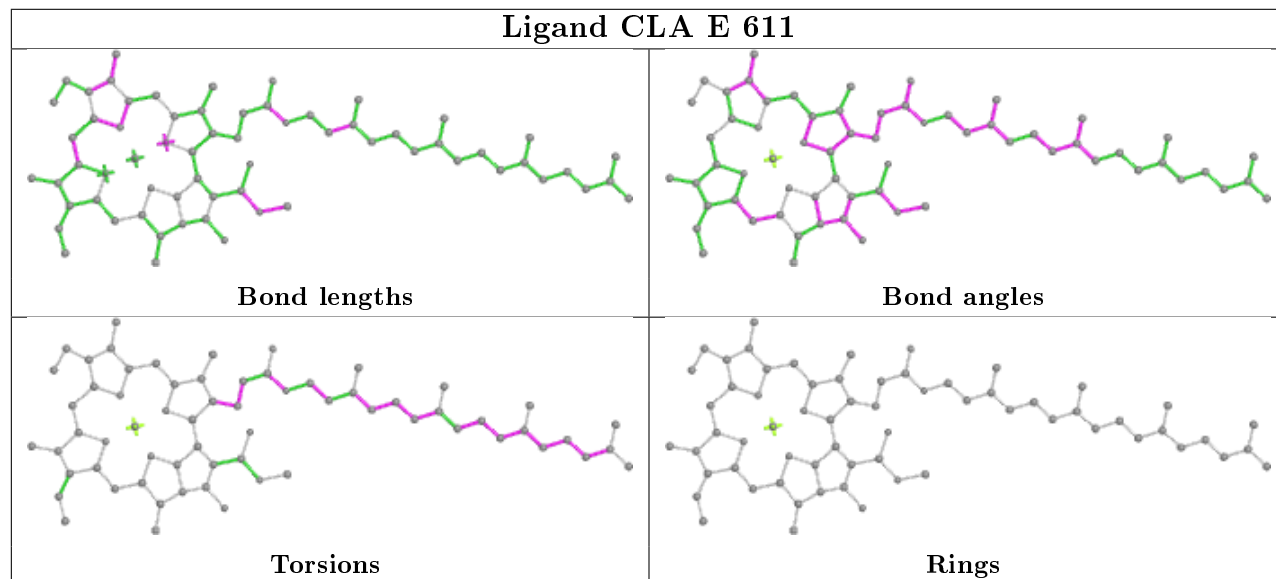
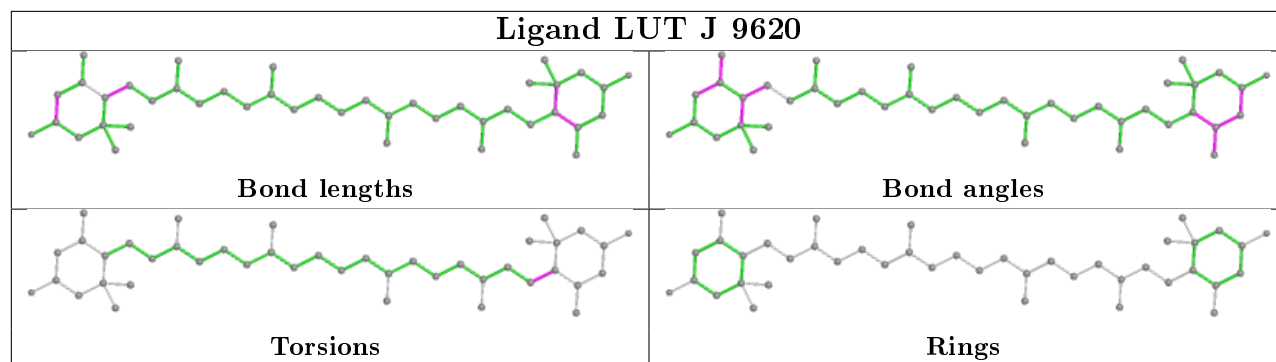


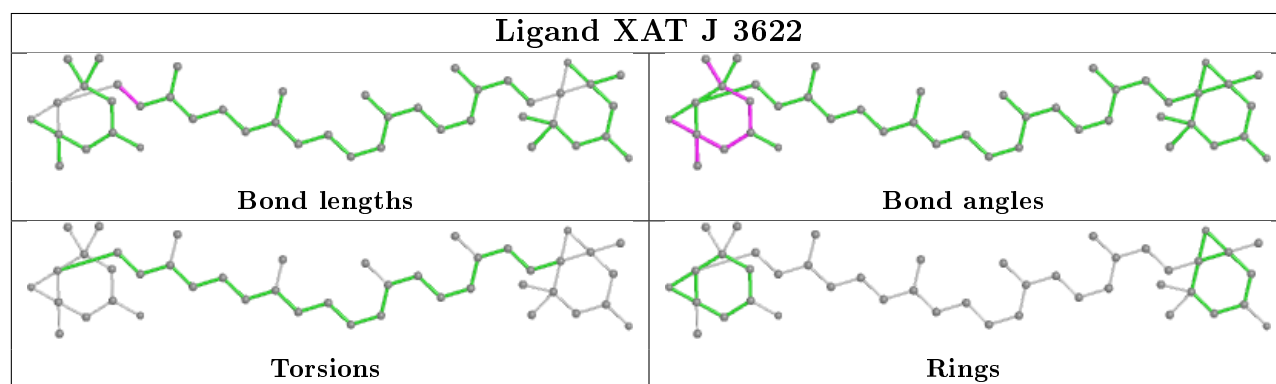
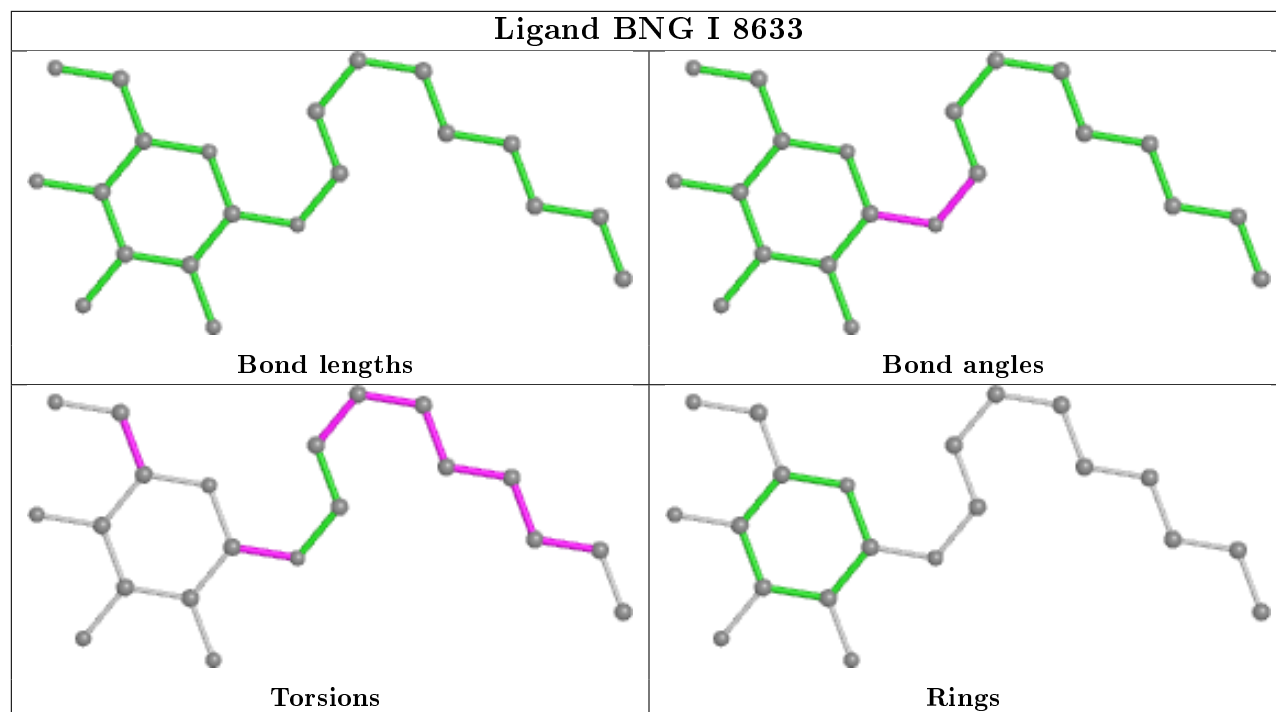
Ligand CHL F 606

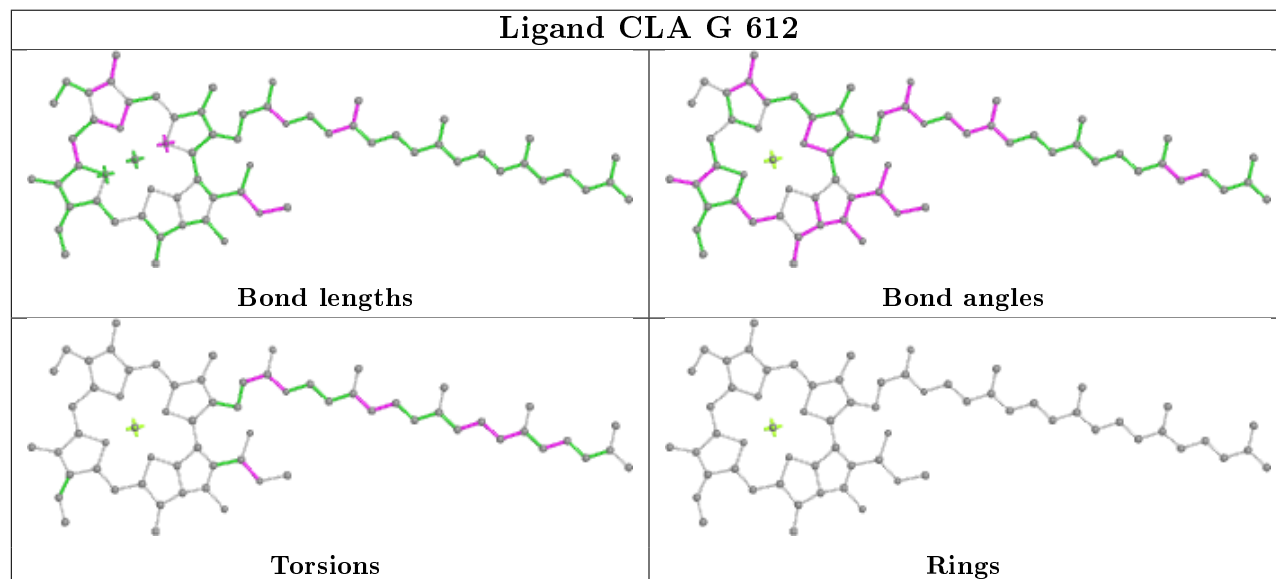
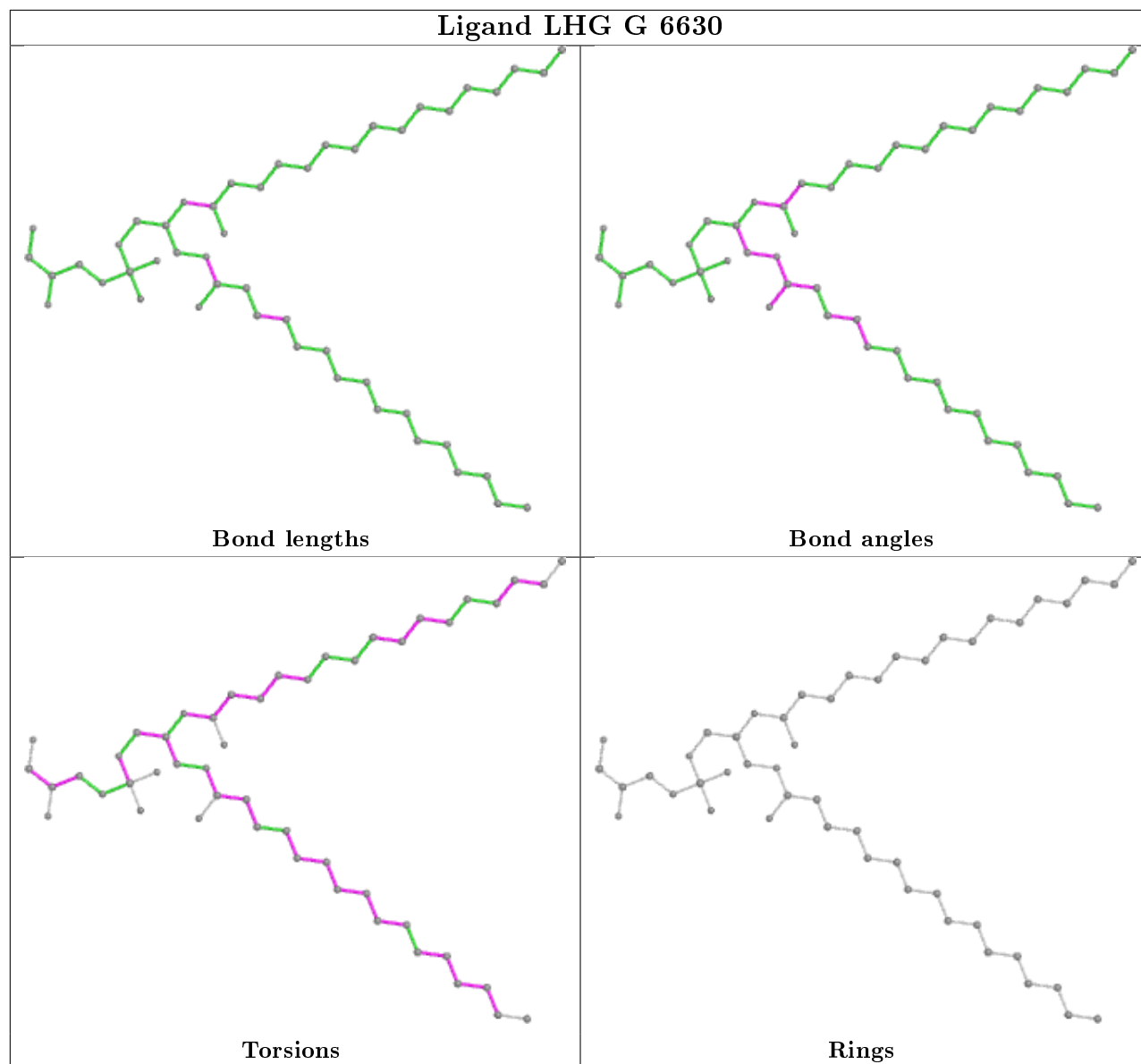


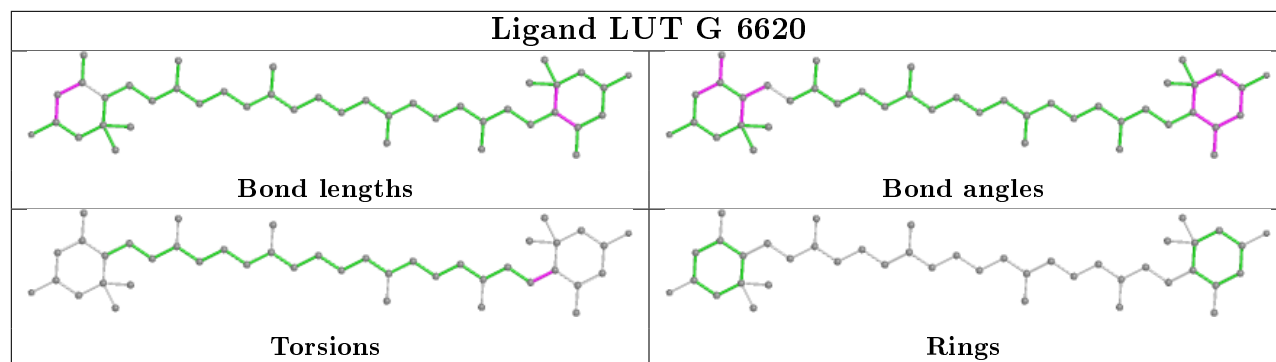
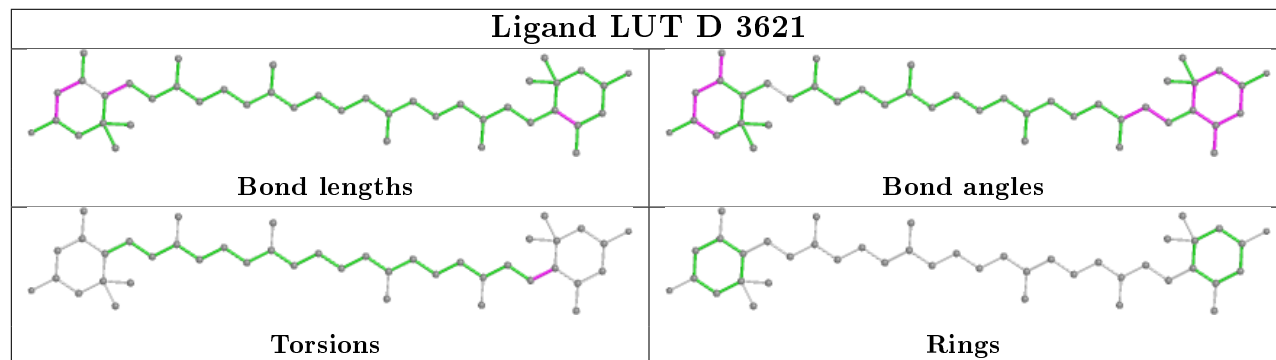
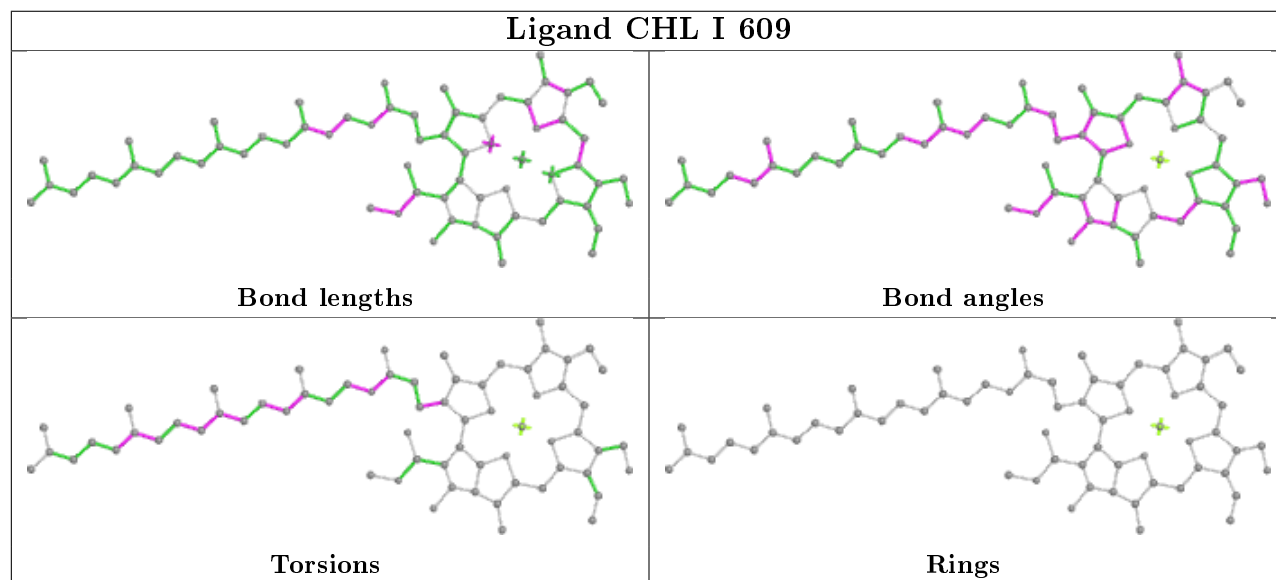
Ligand CLA I 603



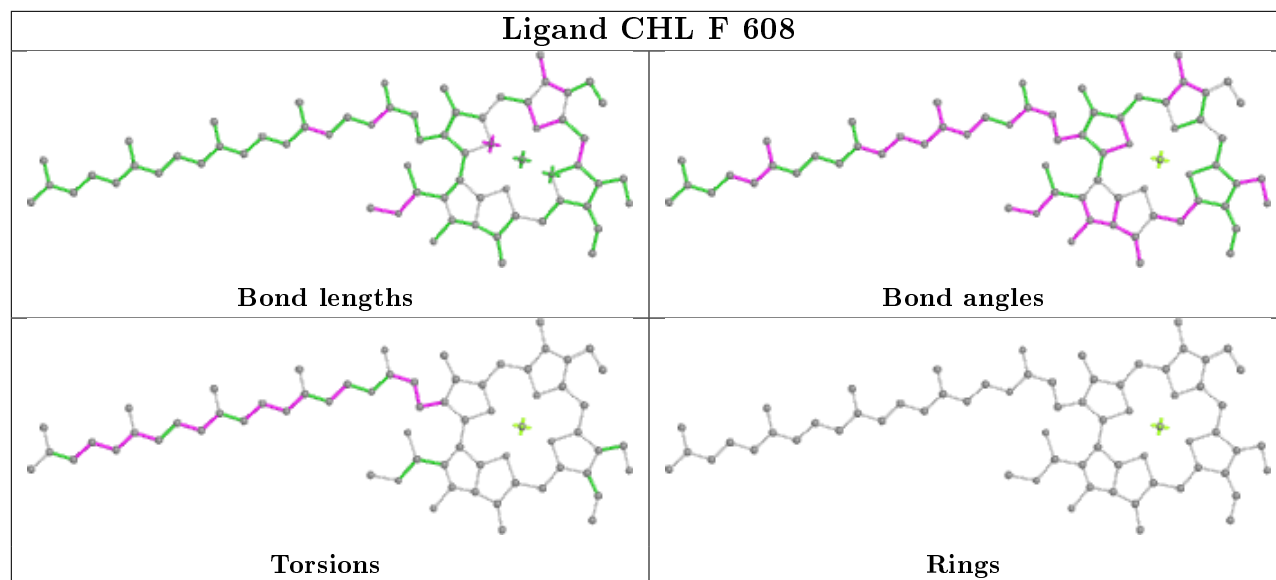




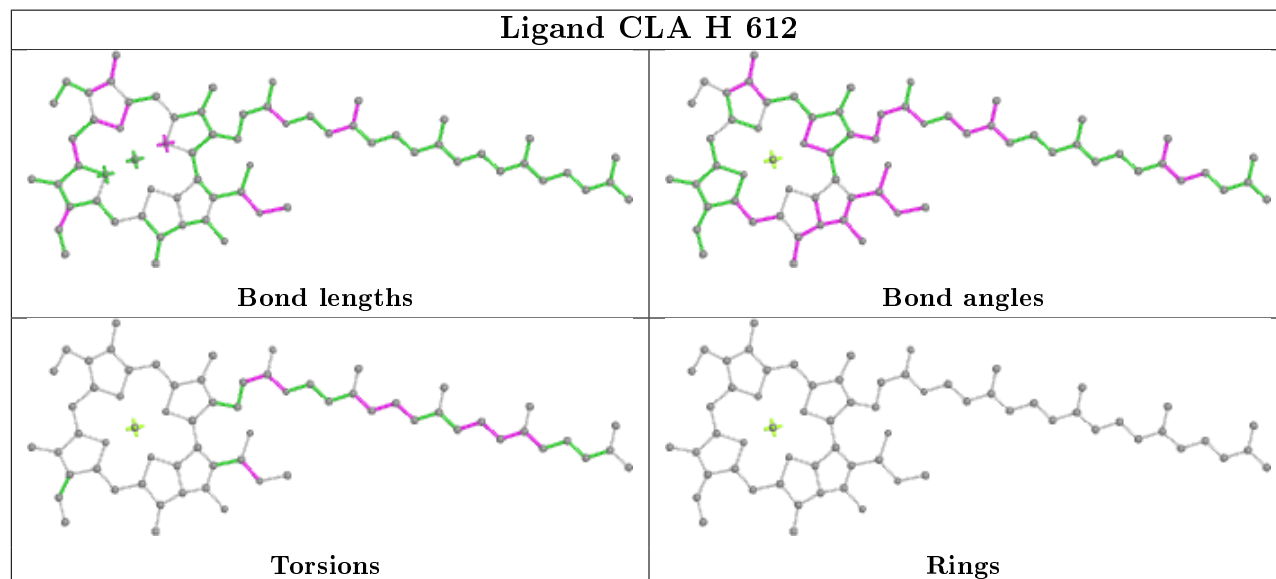


Ligand LUT G 6620**Ligand LUT D 3621****Ligand CHL I 609**

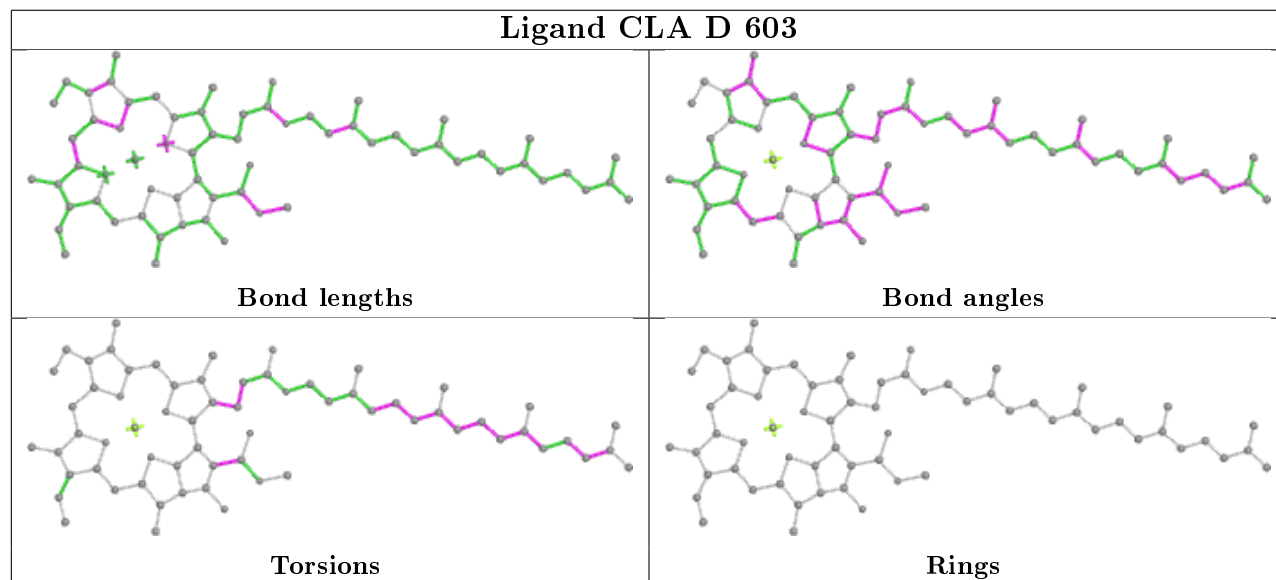
Ligand CHL F 608



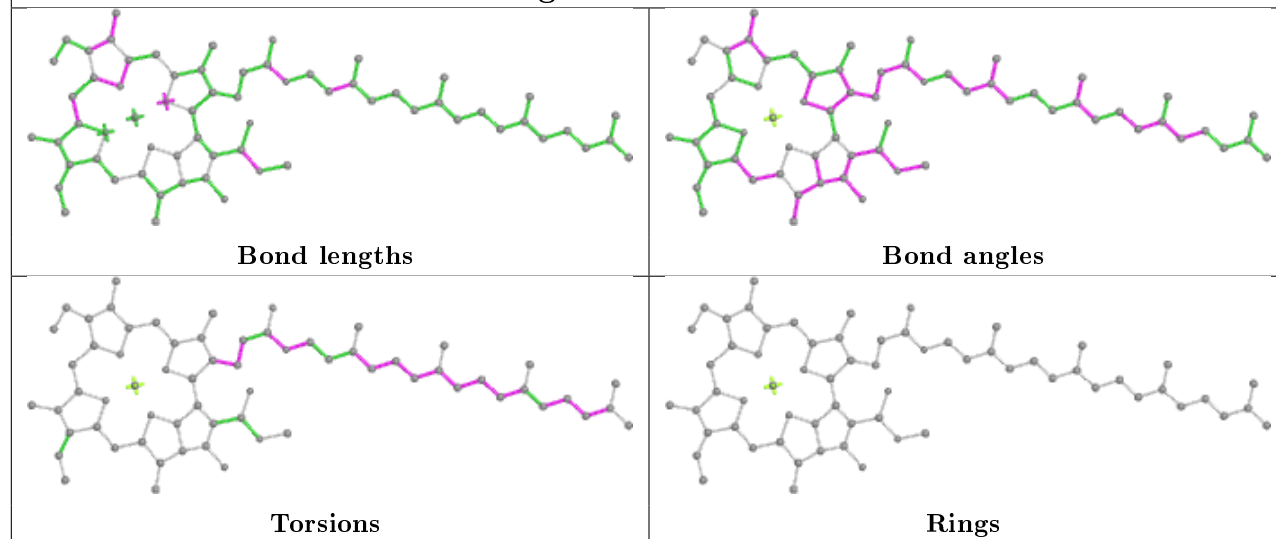
Ligand CLA H 612



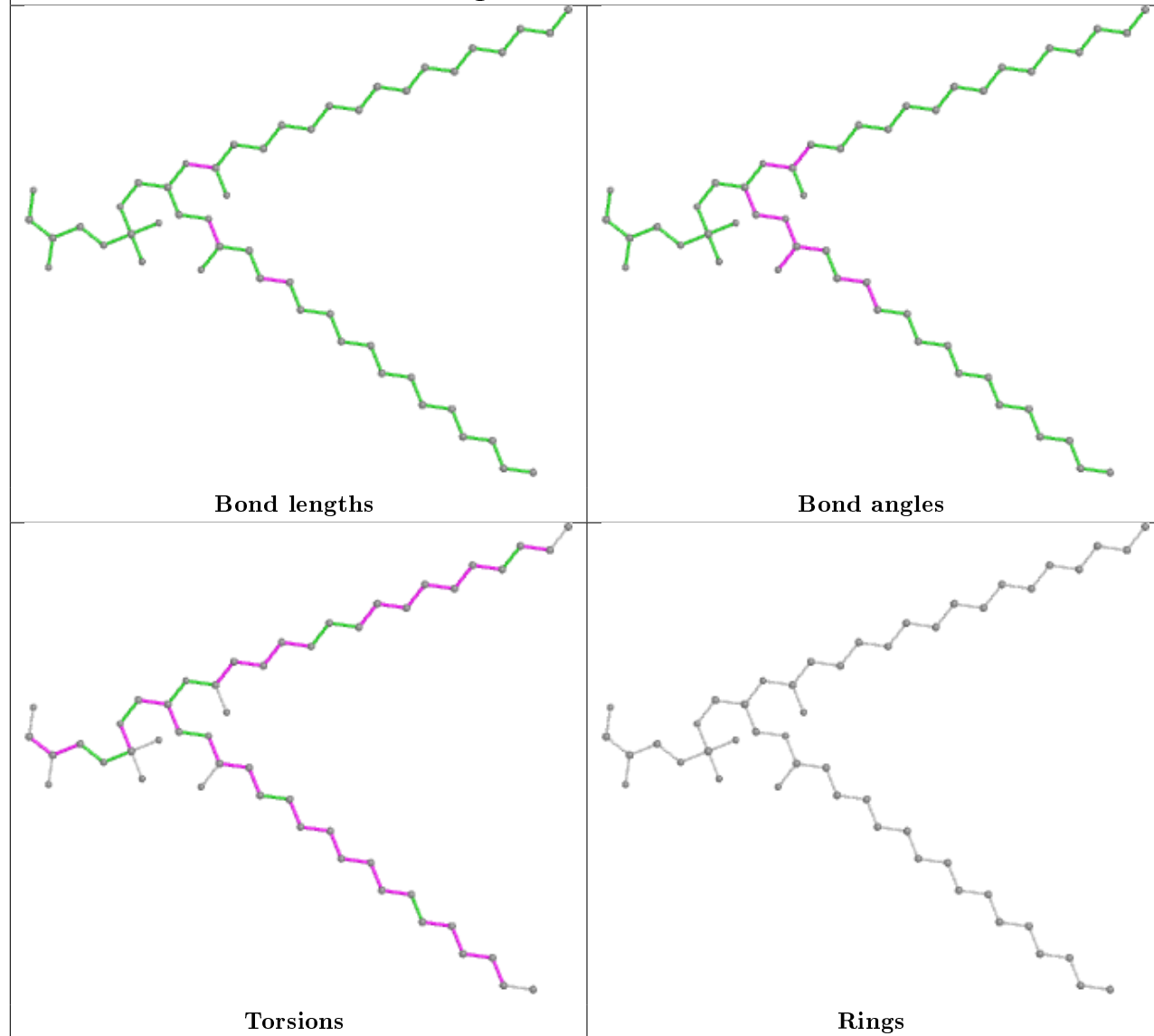
Ligand CLA D 603

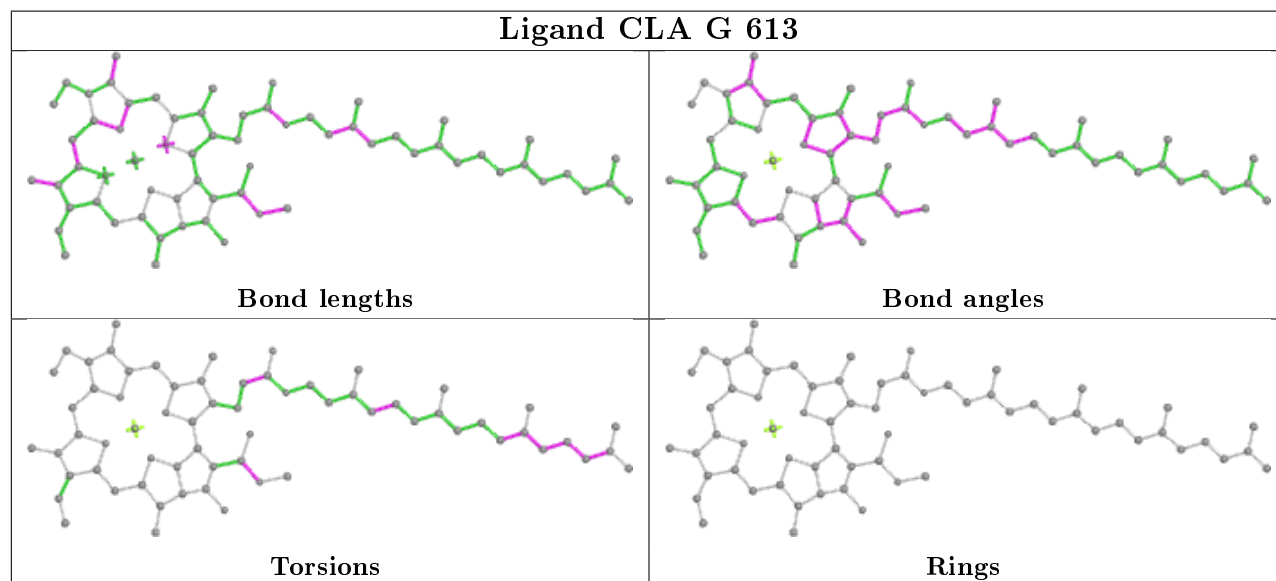
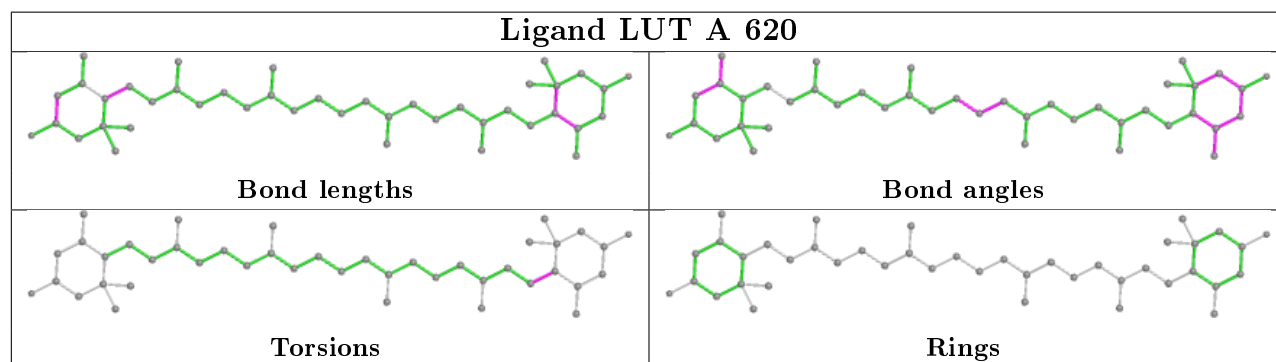
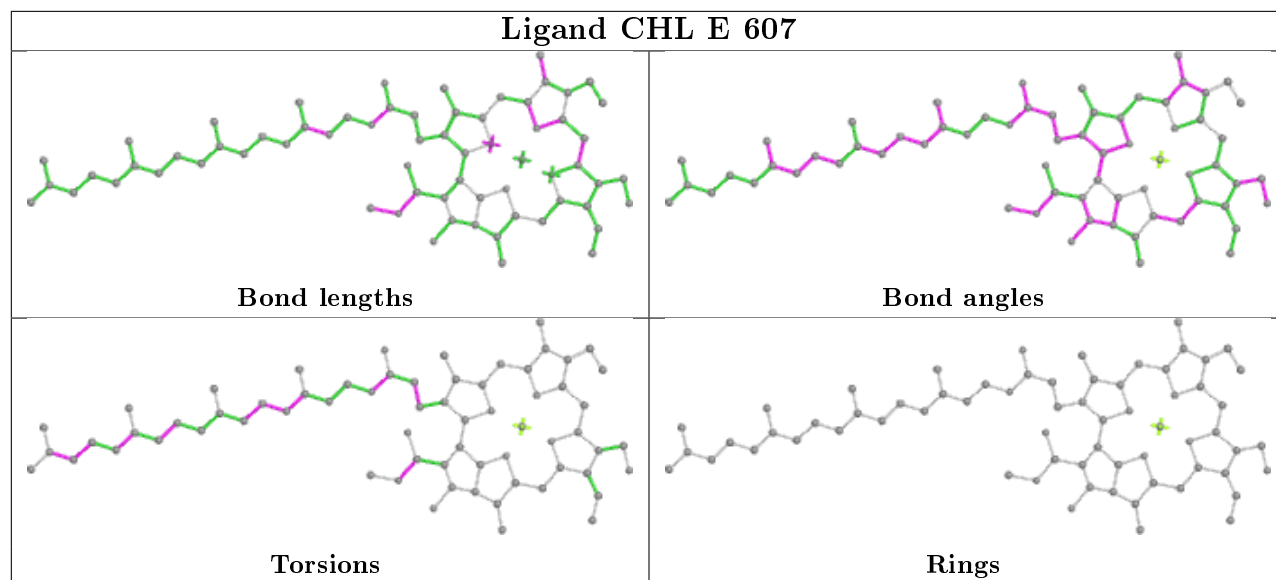


Ligand CLA I 611

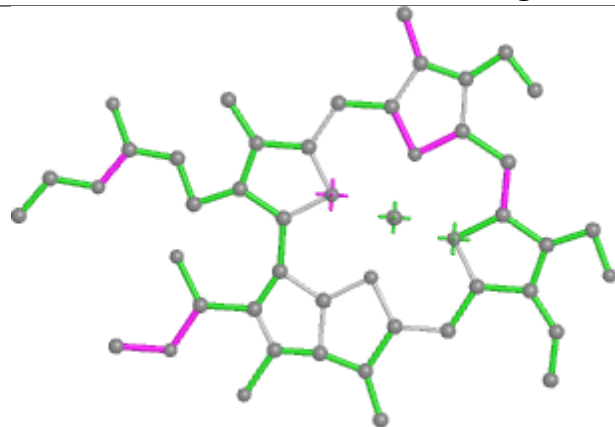


Ligand LHG B 1630

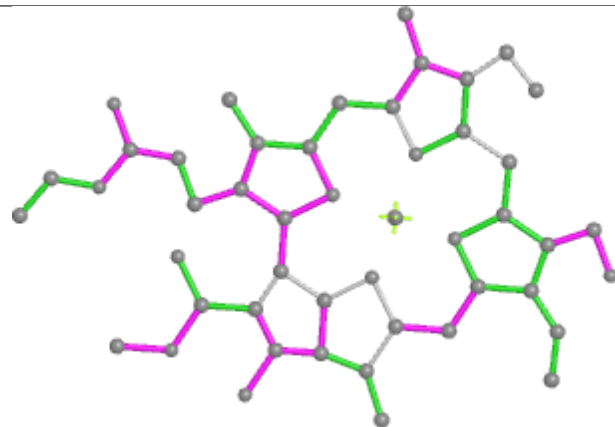




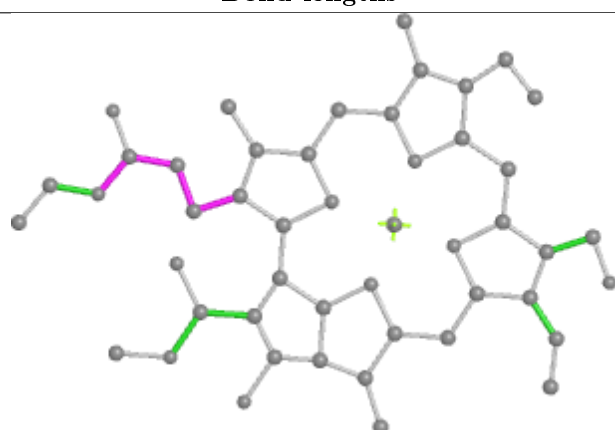
Ligand CHL H 605



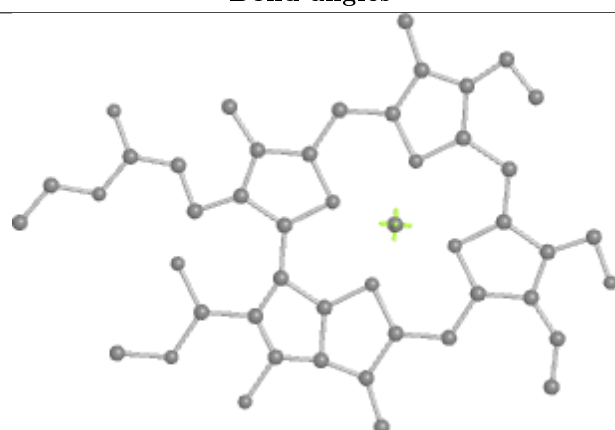
Bond lengths



Bond angles

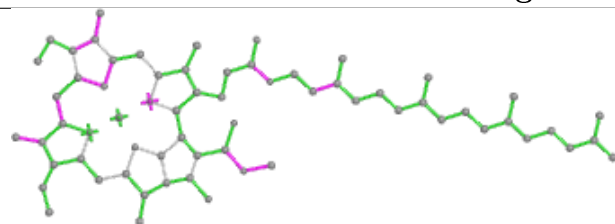


Torsions

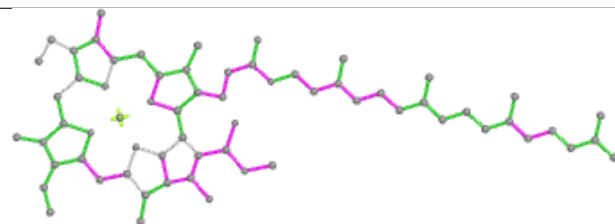


Rings

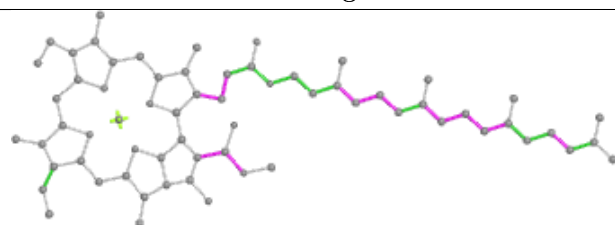
Ligand CLA G 603



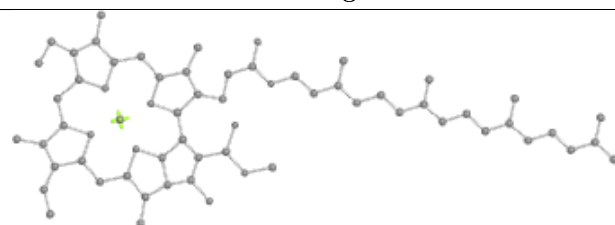
Bond lengths



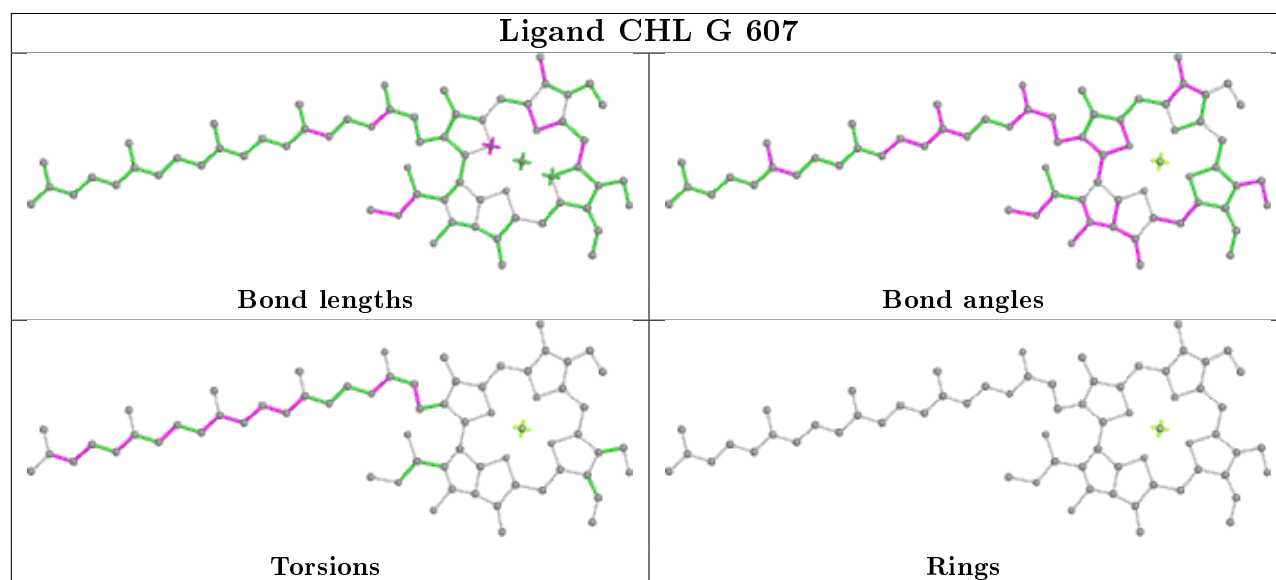
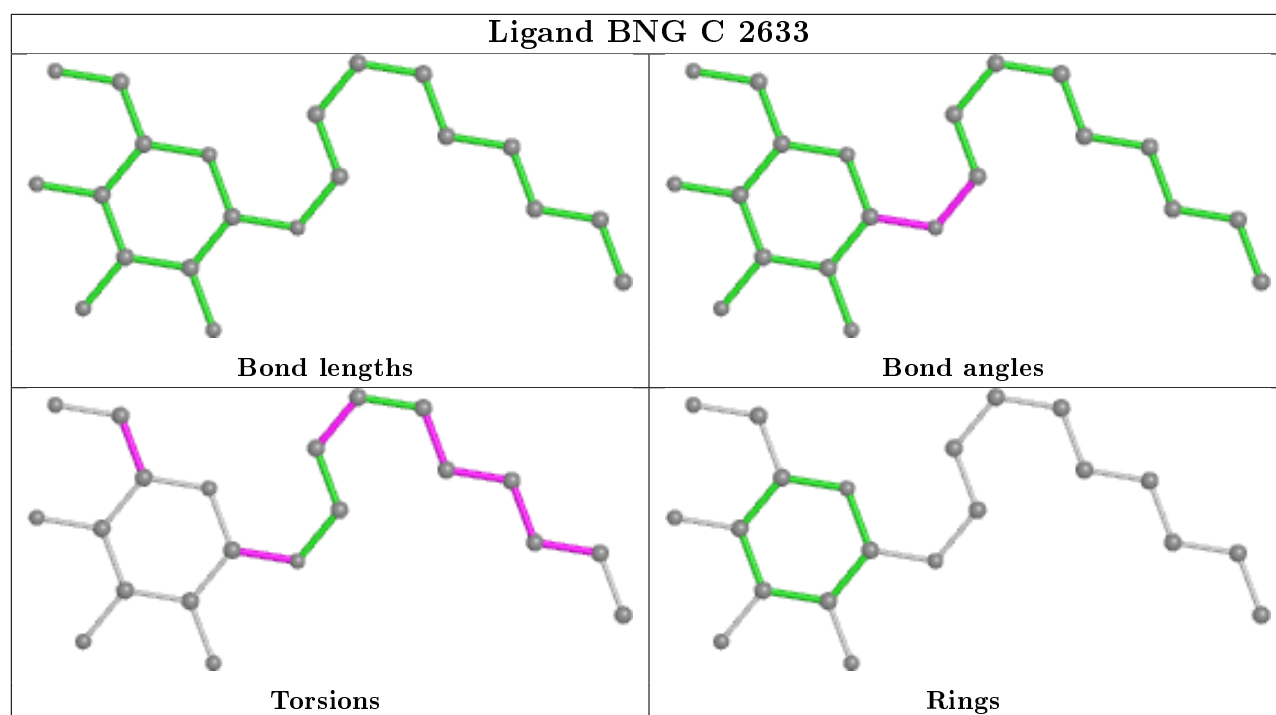
Bond angles



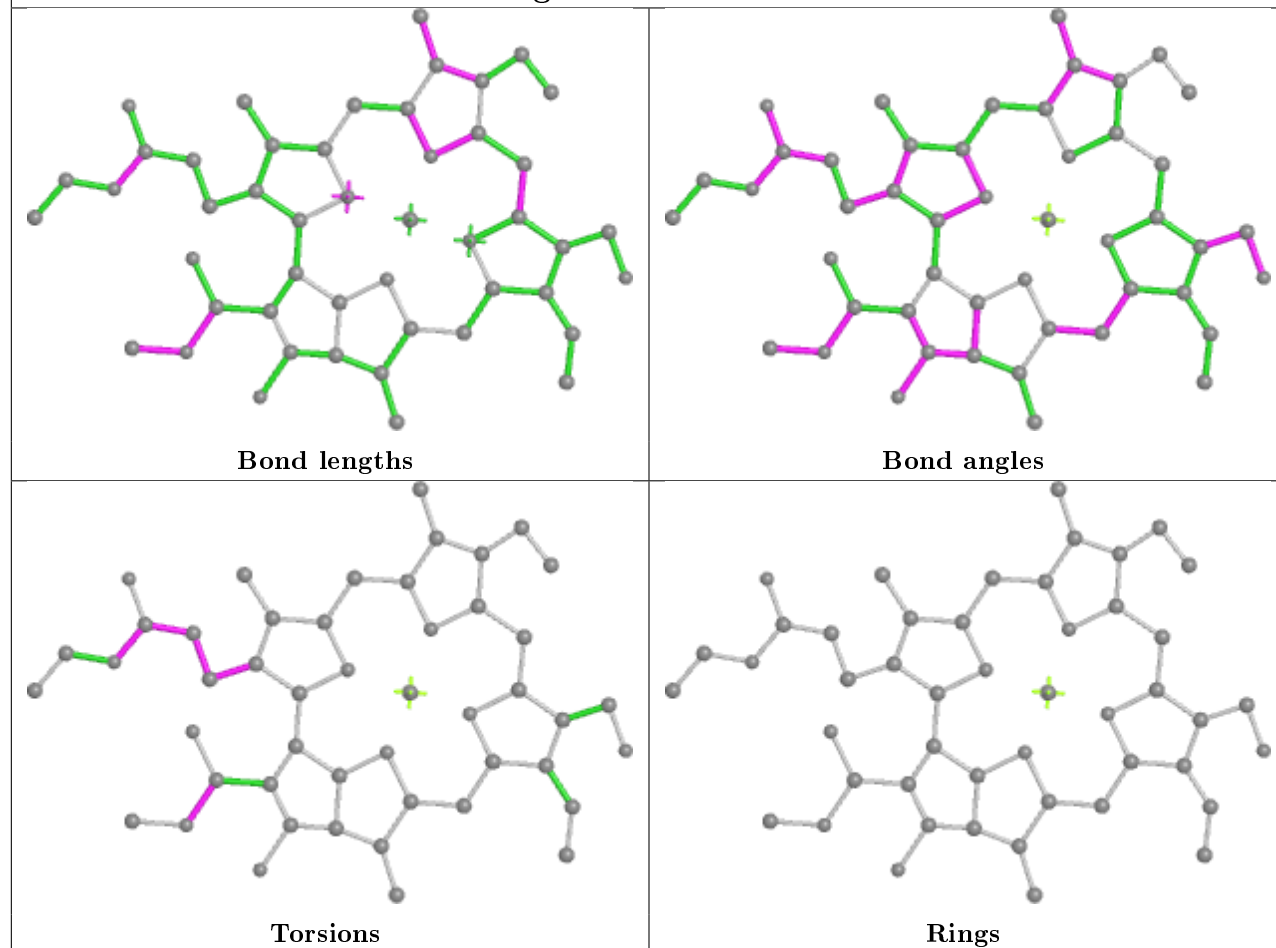
Torsions



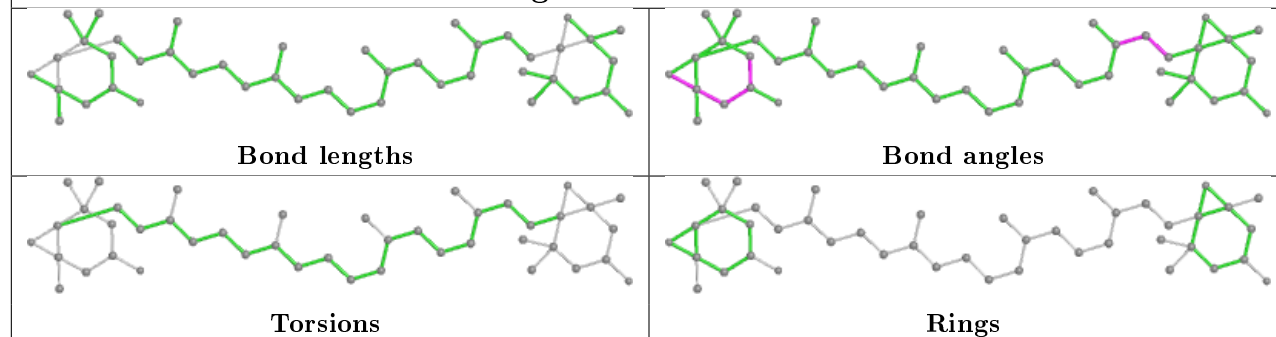
Rings



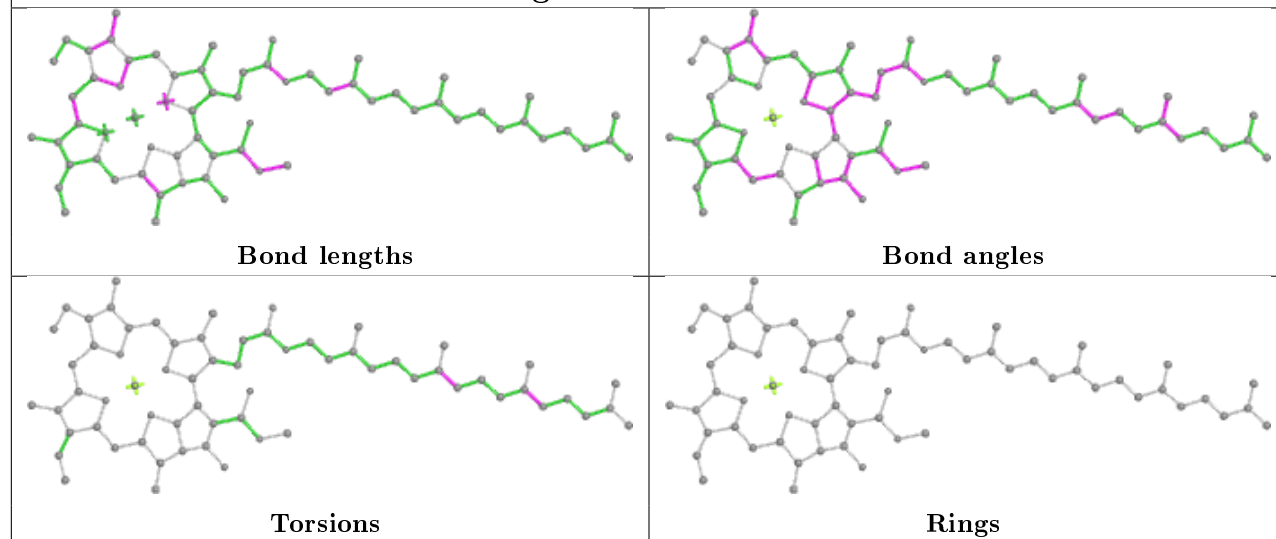
Ligand CHL E 605



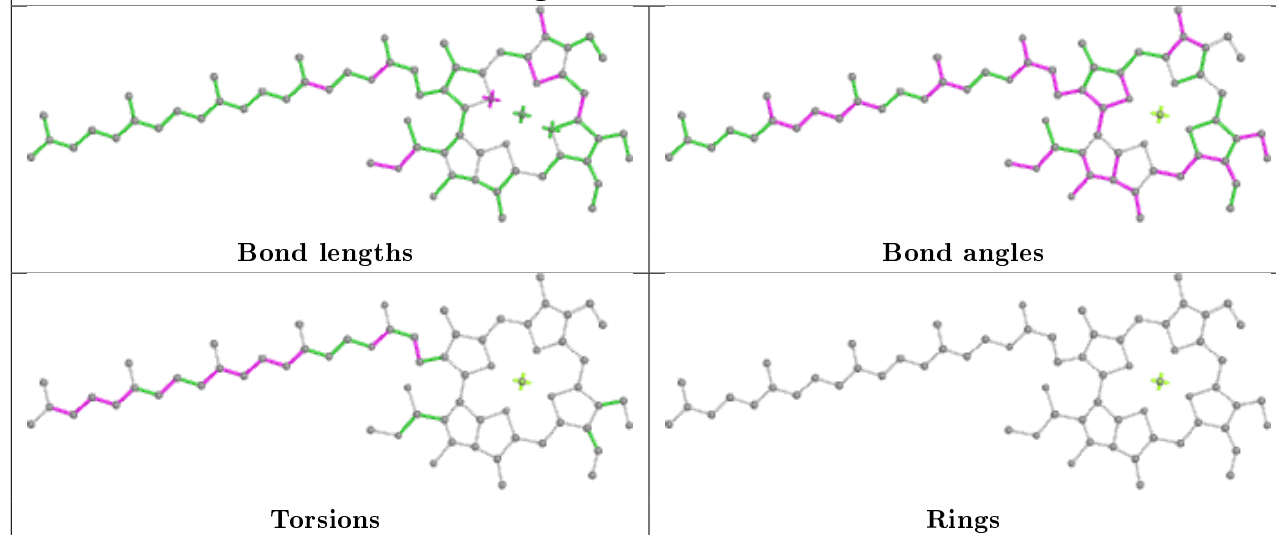
Ligand XAT A 622



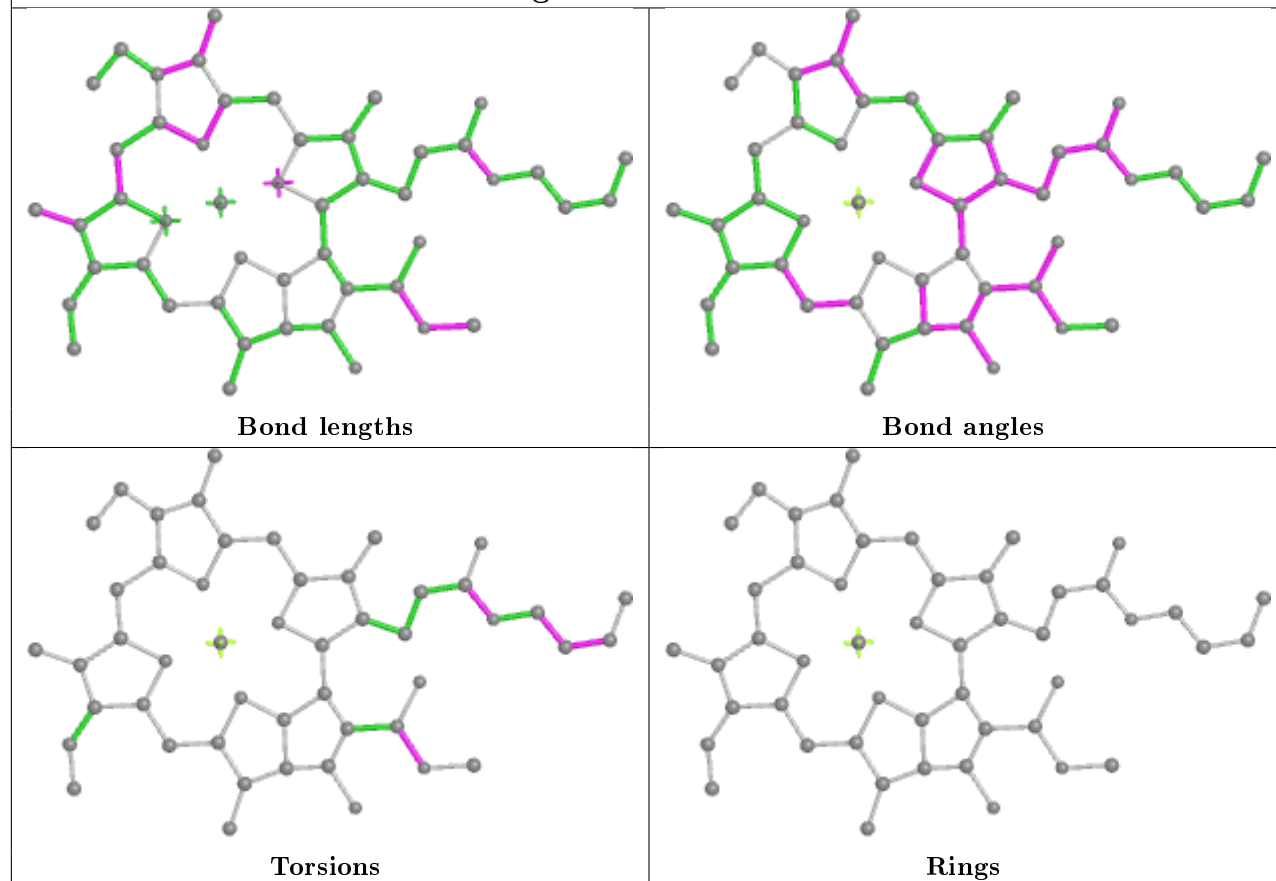
Ligand CLA B 610



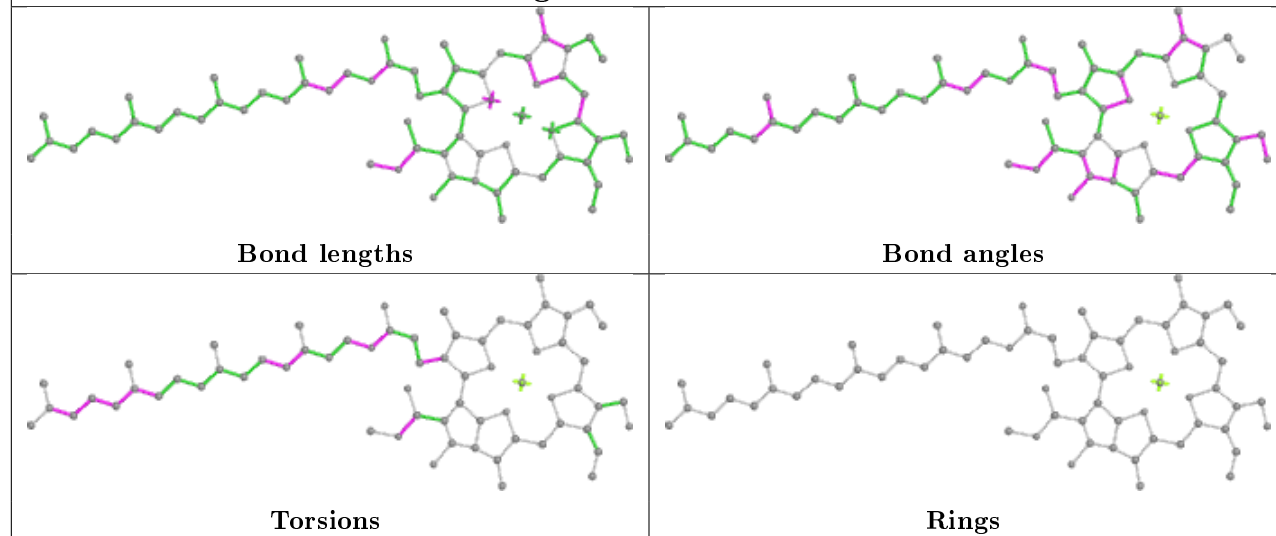
Ligand CHL C 607

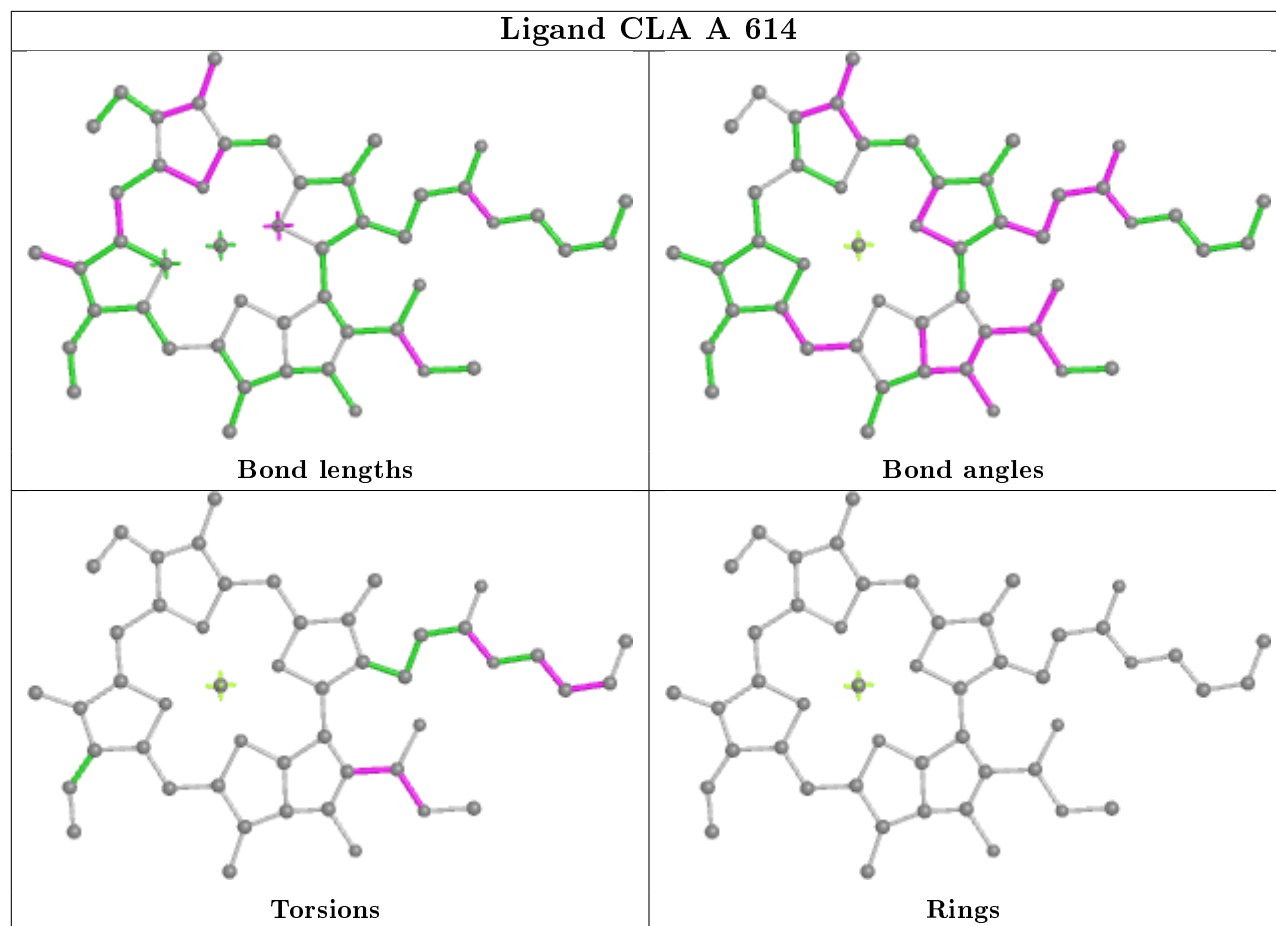


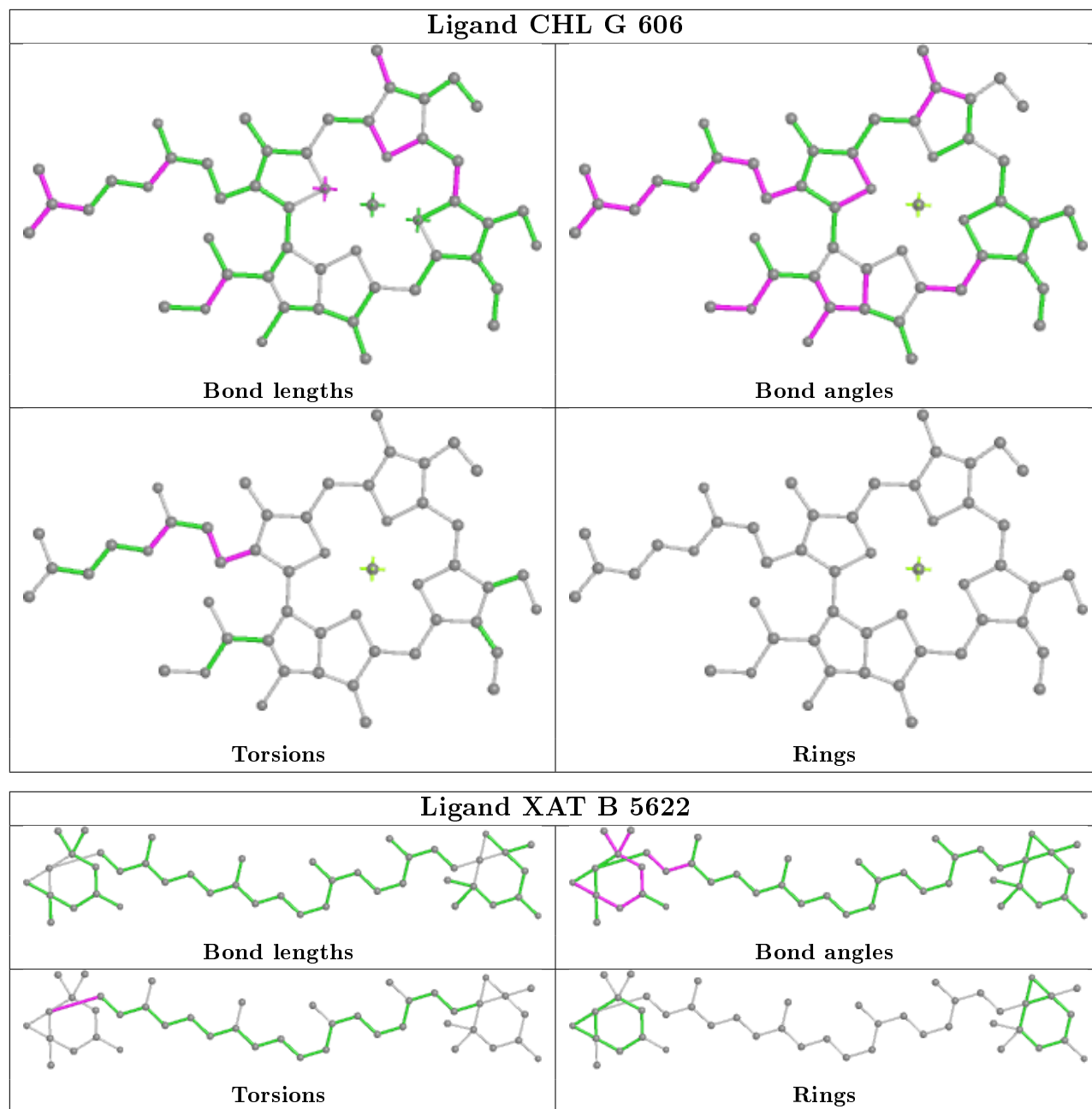
Ligand CLA C 614

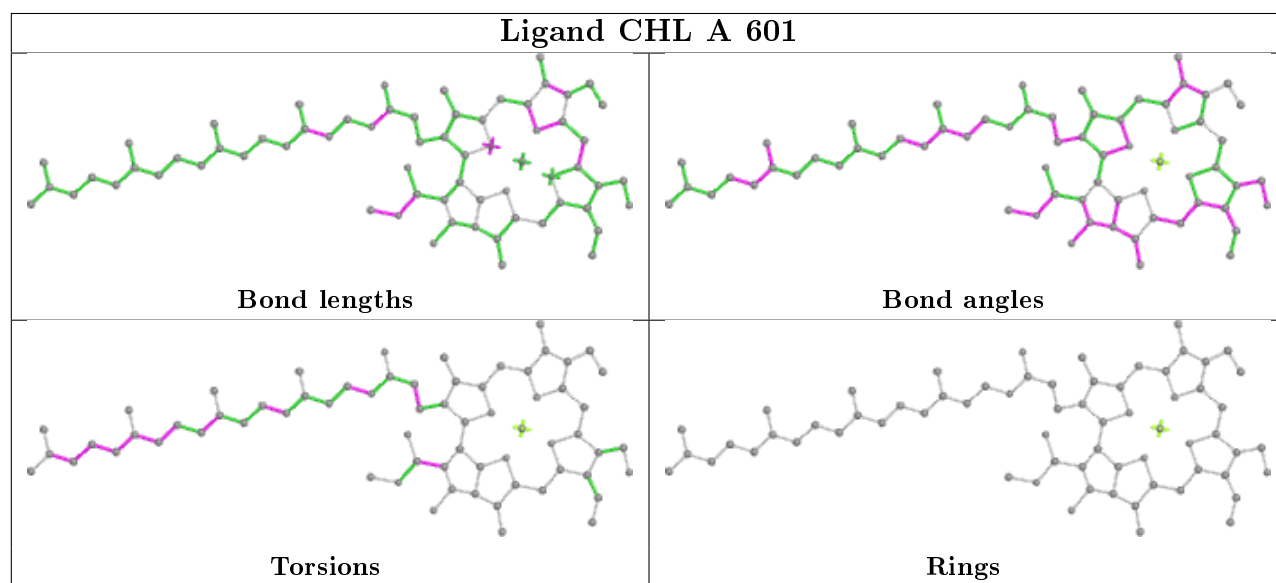
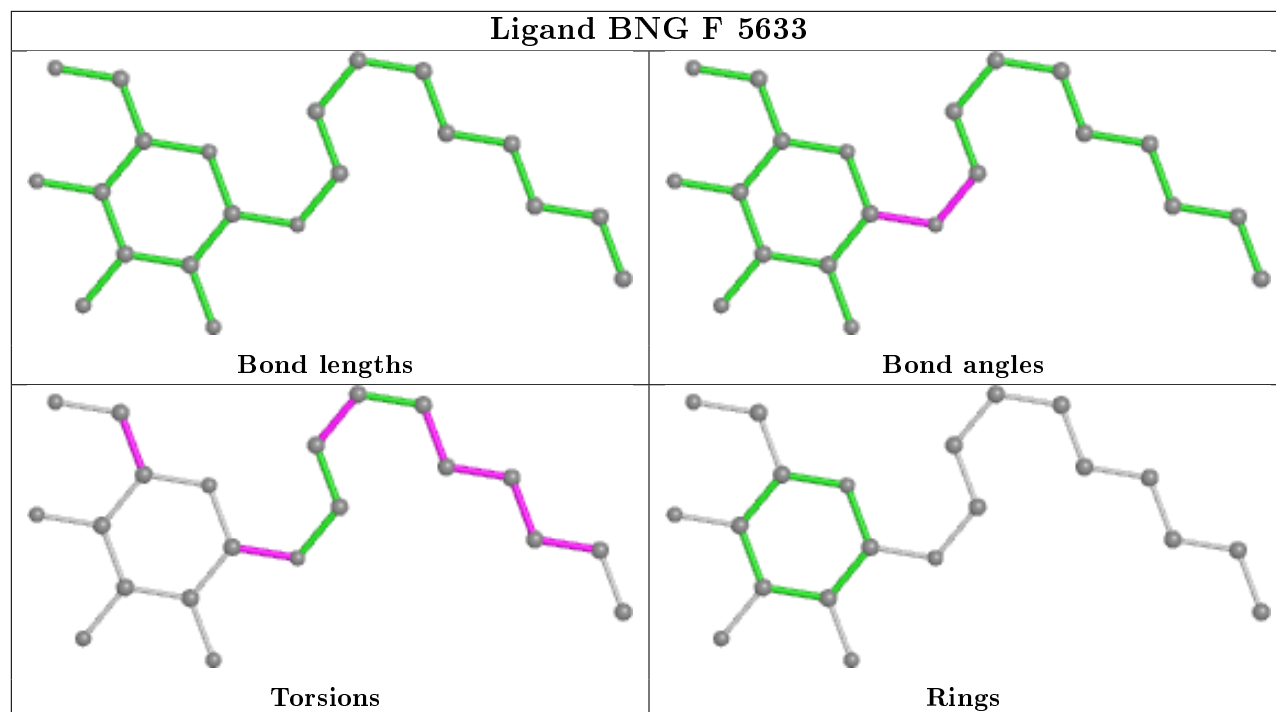


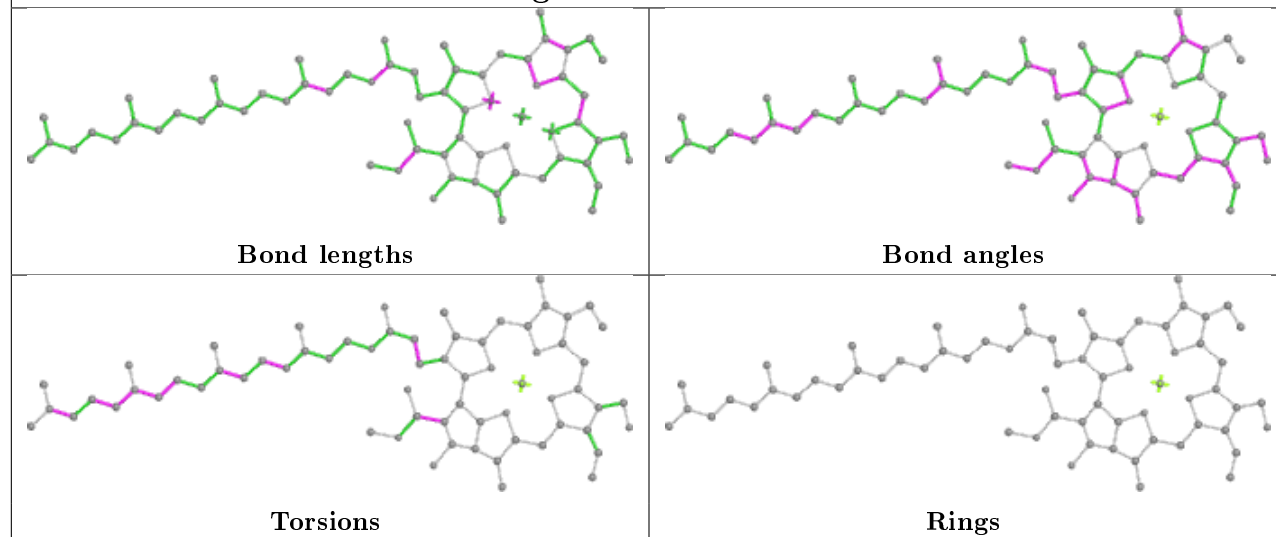
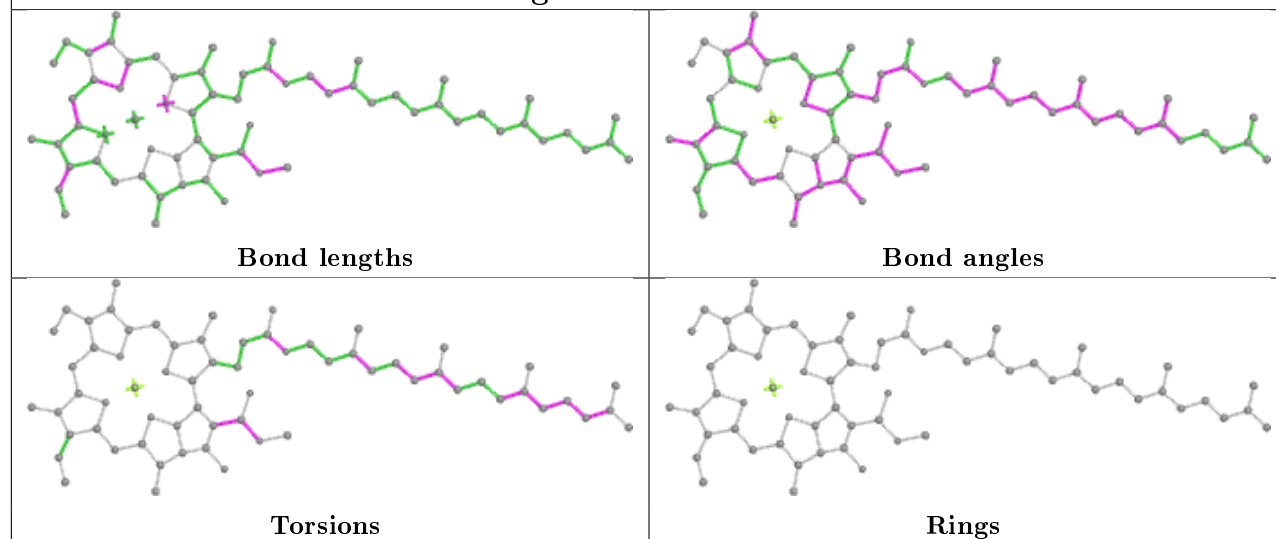
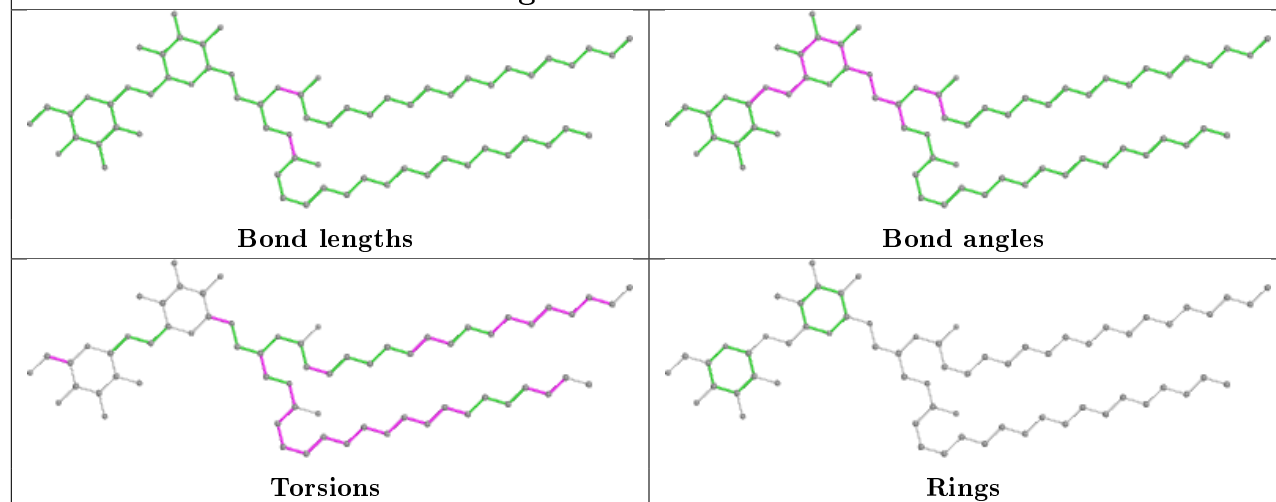
Ligand CHL E 609



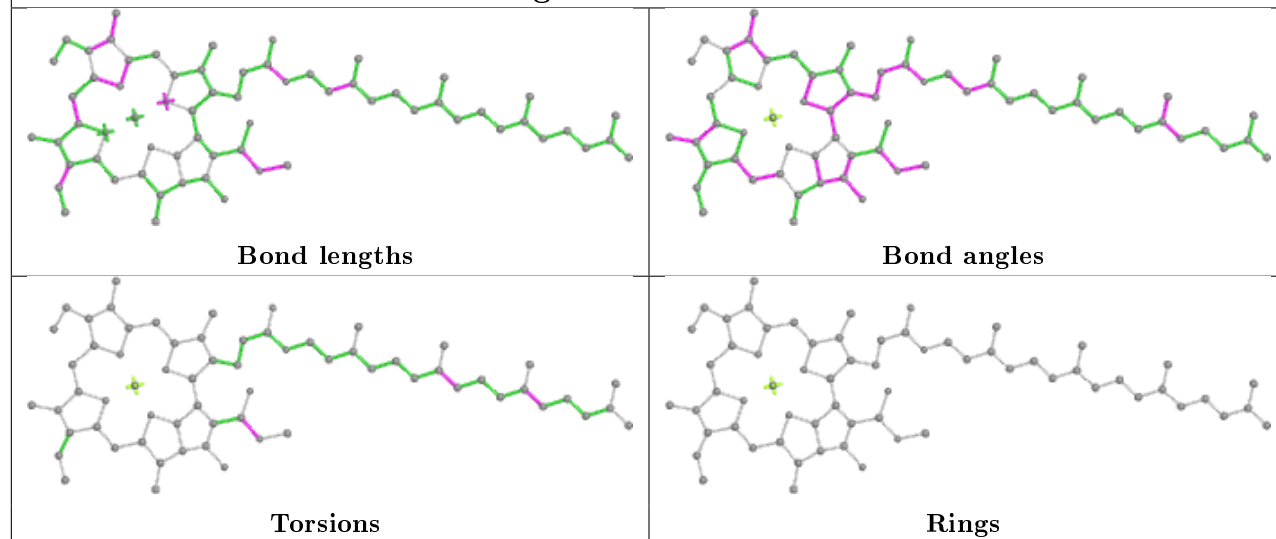




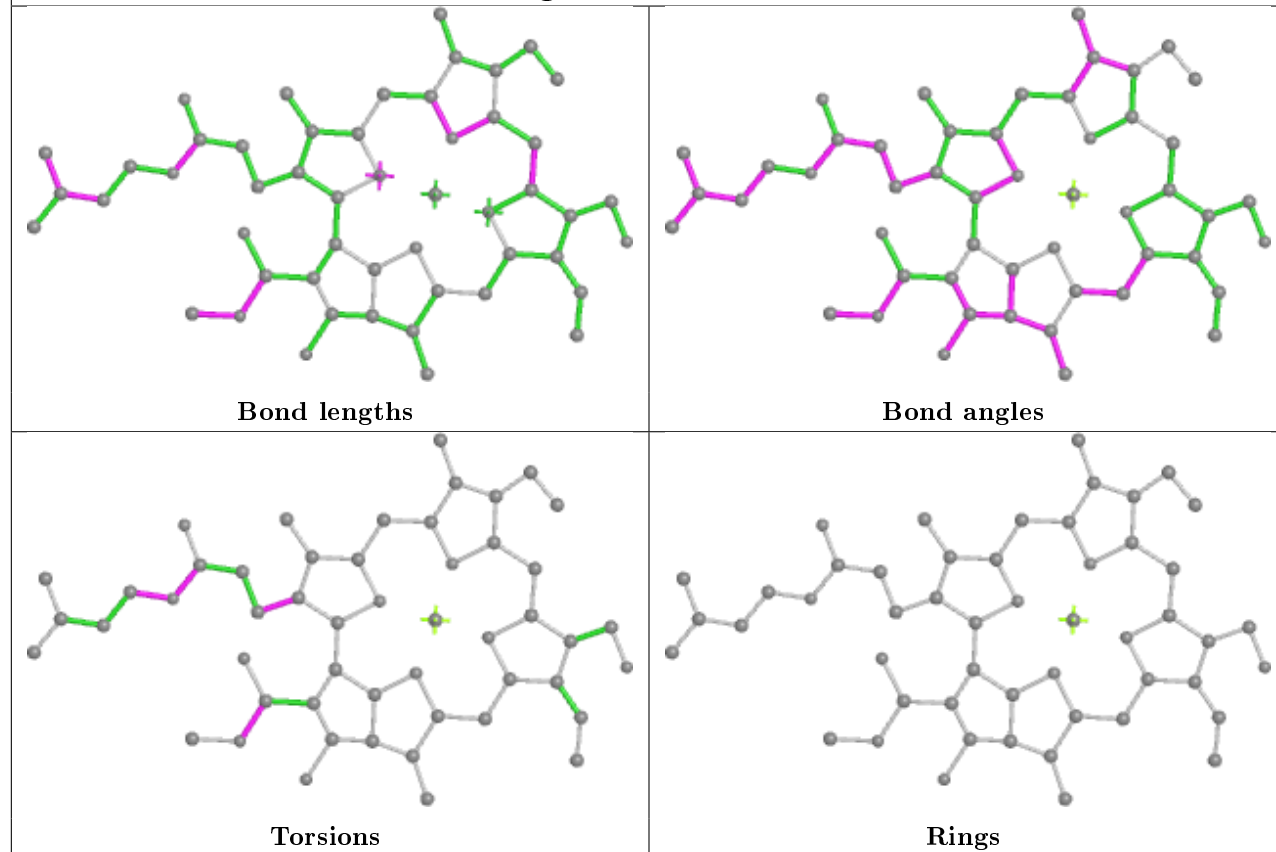


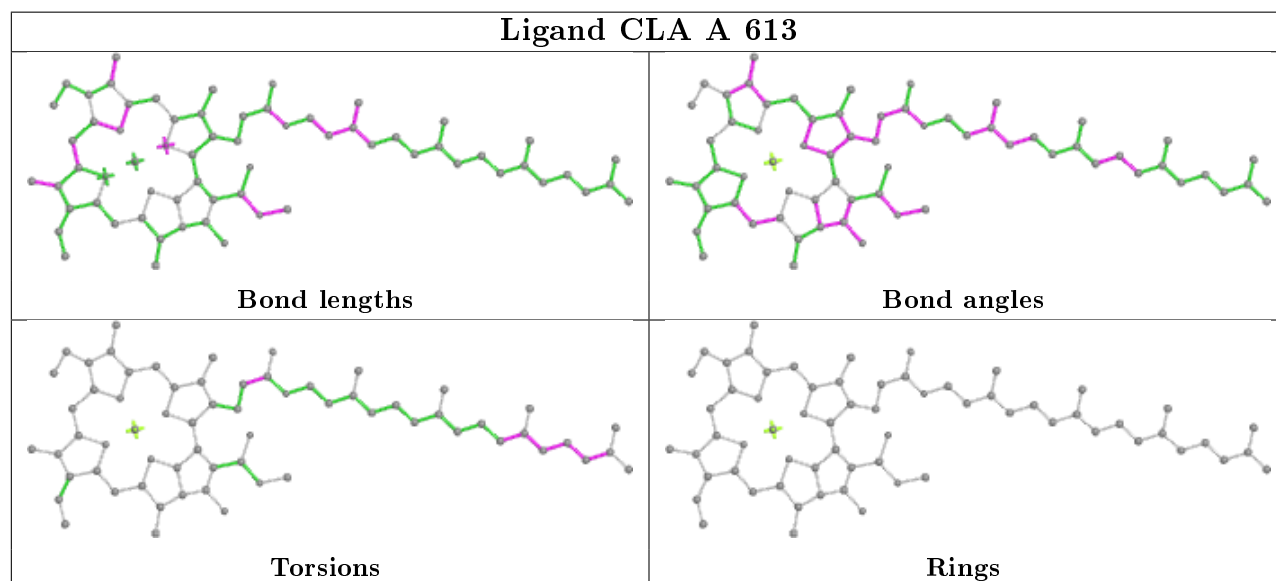
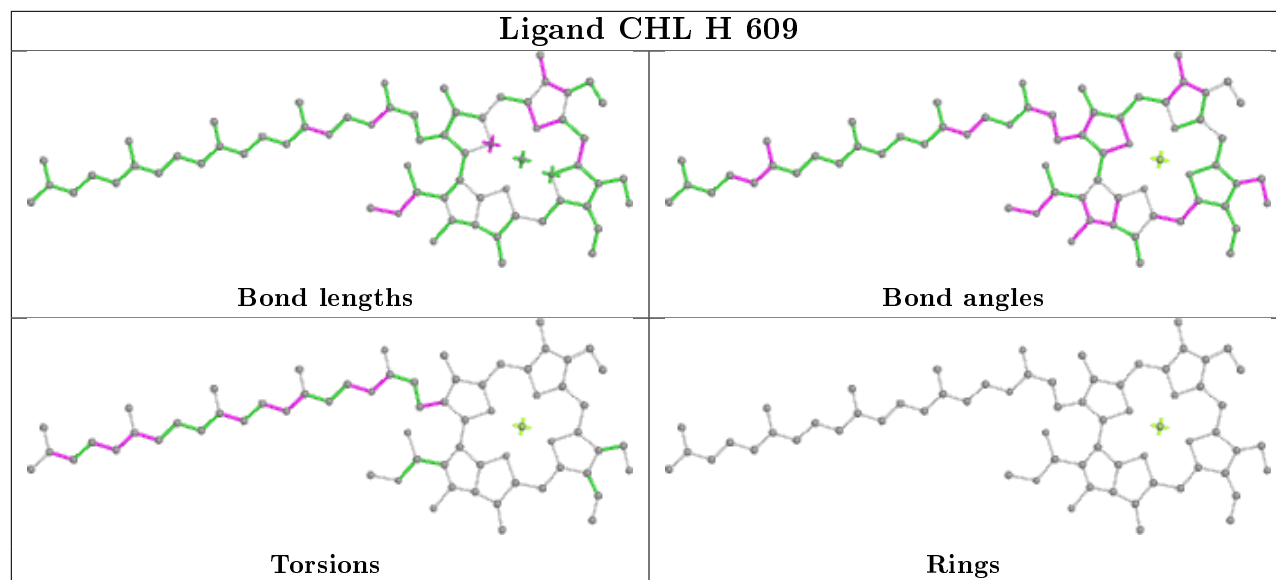
Ligand CHL B 601**Ligand CLA H 602****Ligand DGD H 7632**

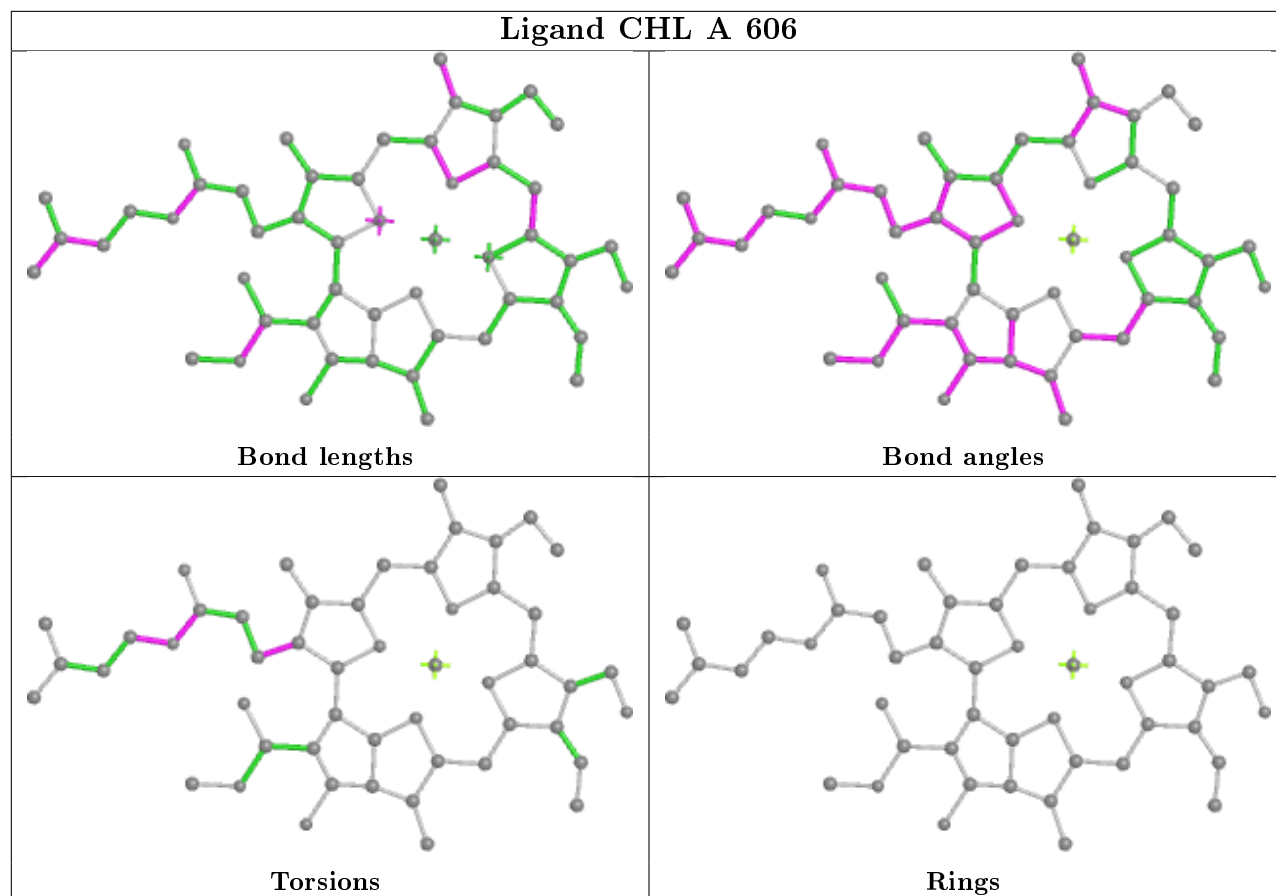
Ligand CLA E 610

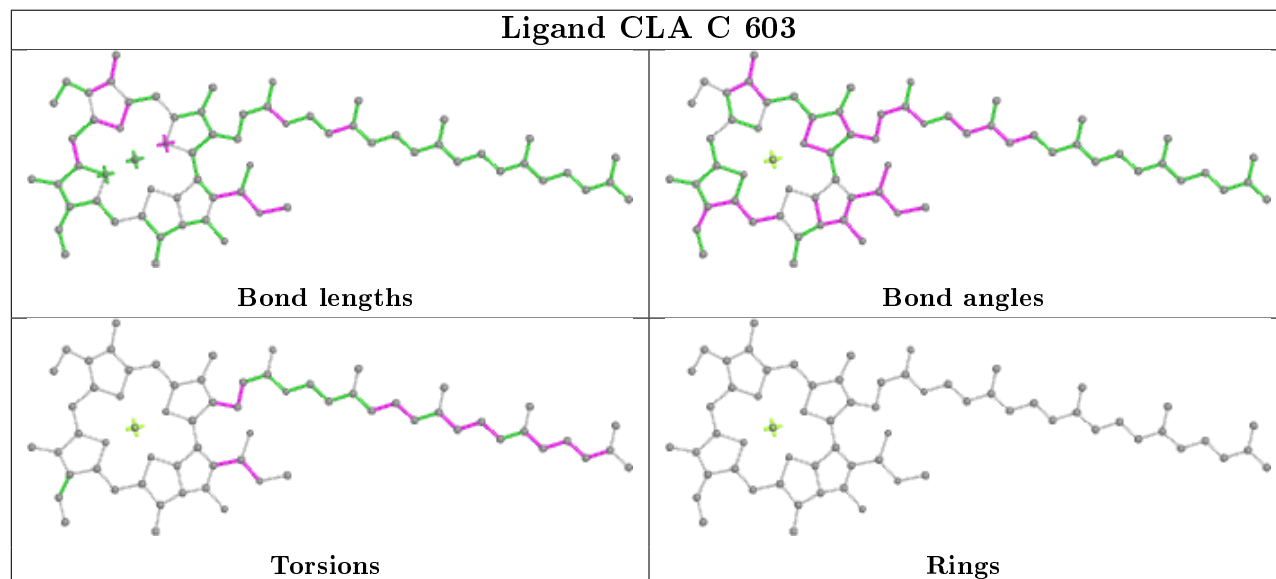
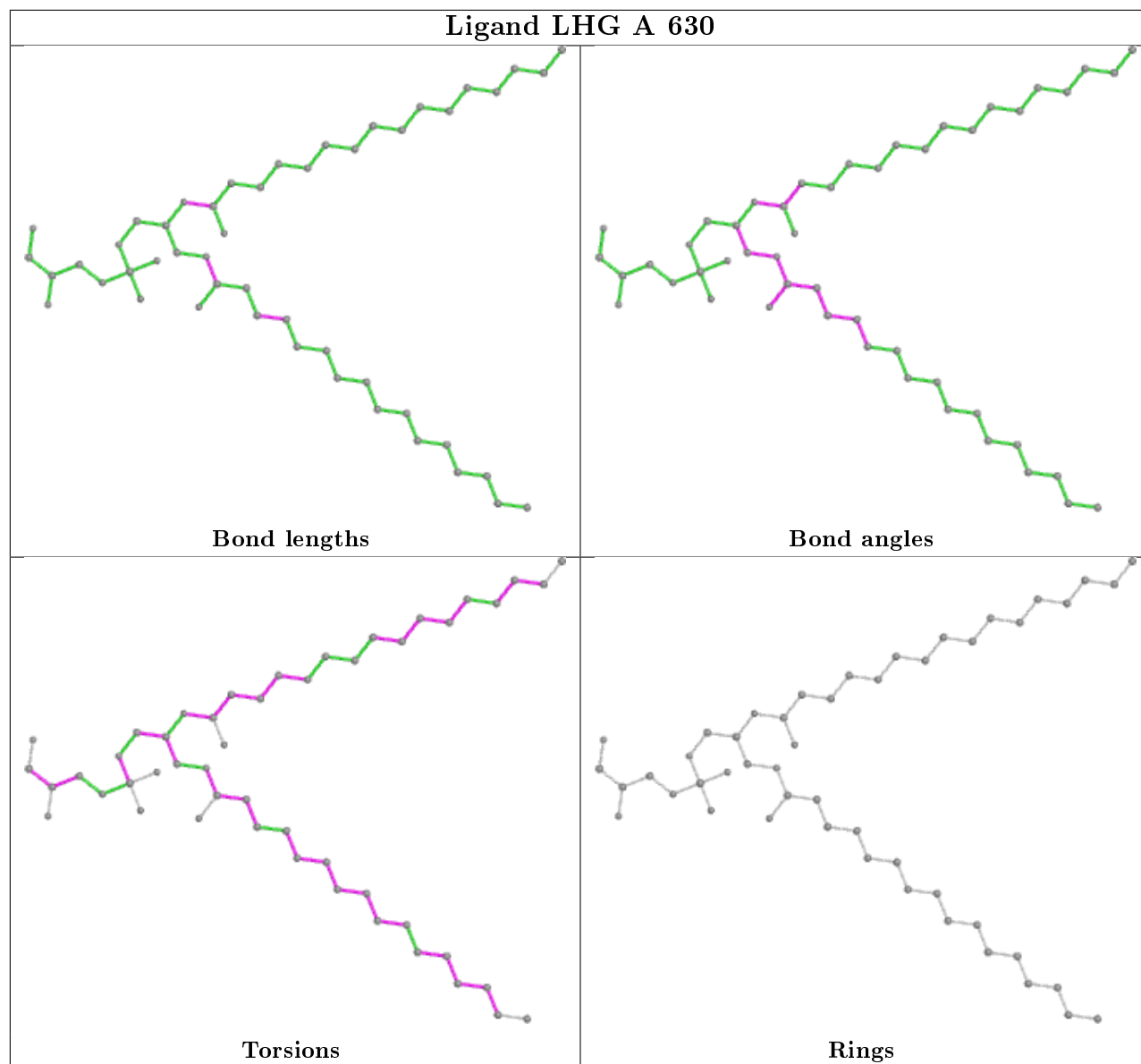


Ligand CHL I 606

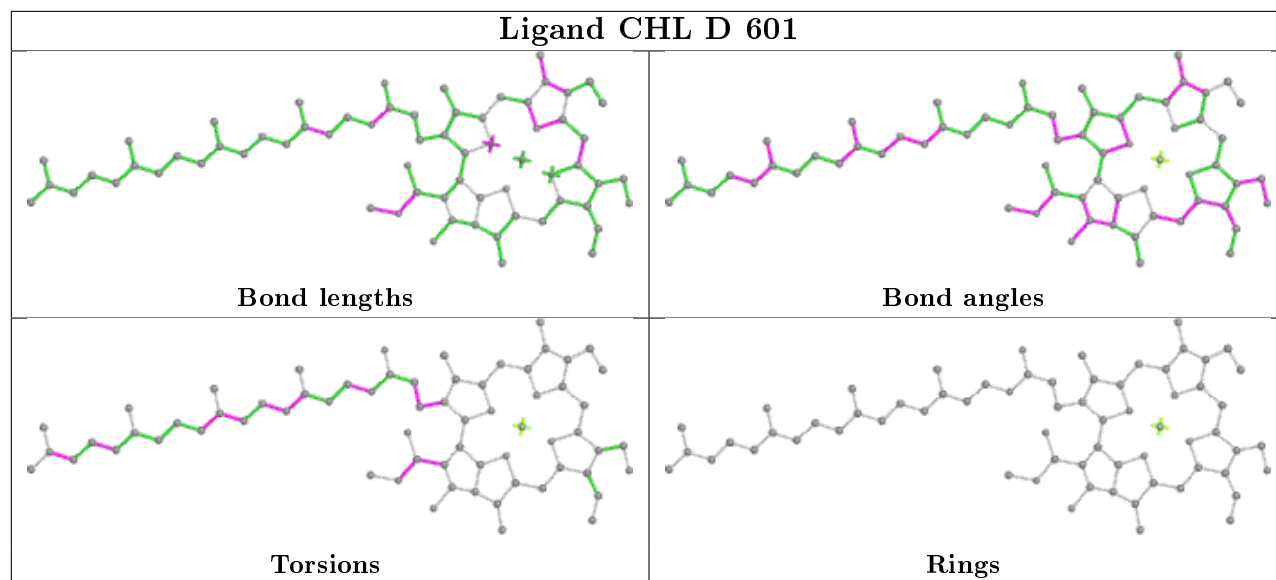




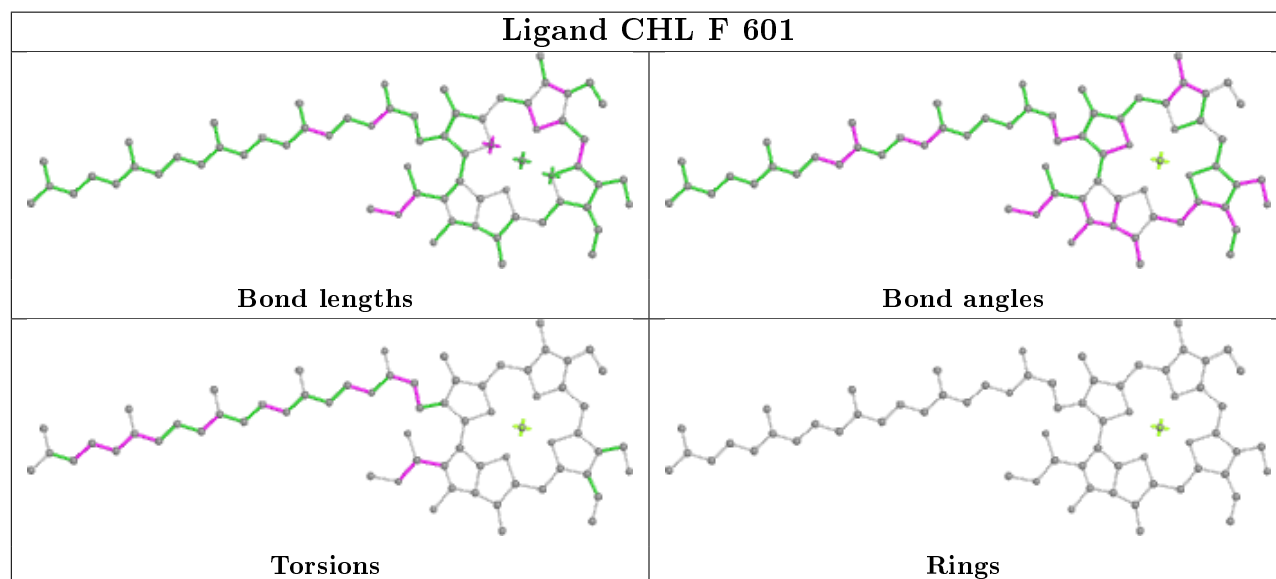




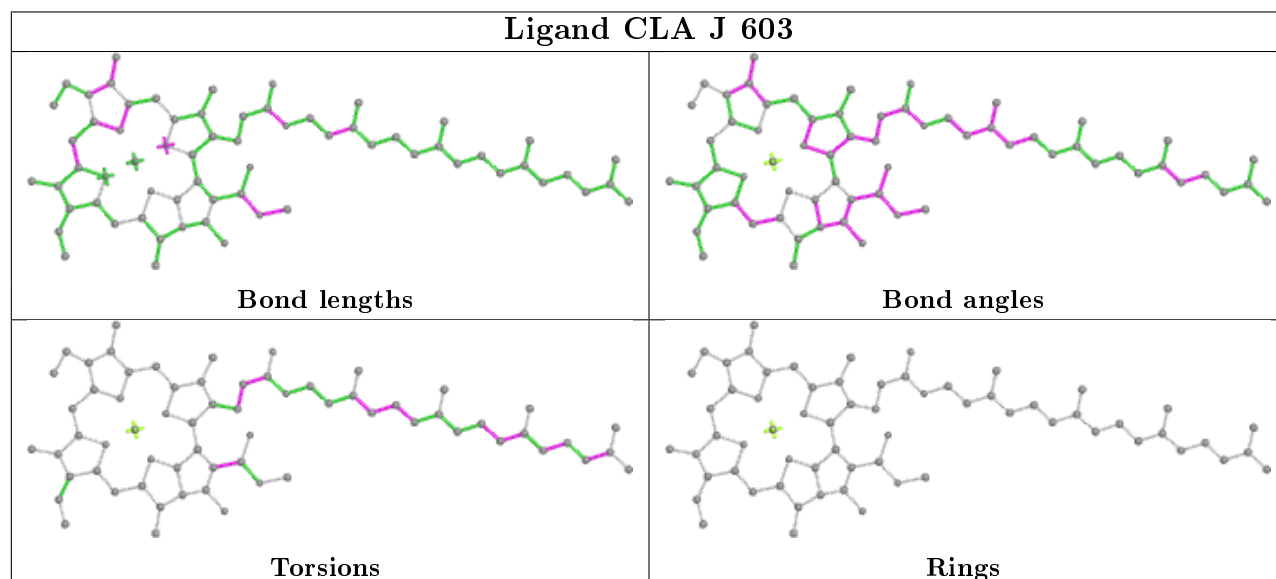
Ligand CHL D 601

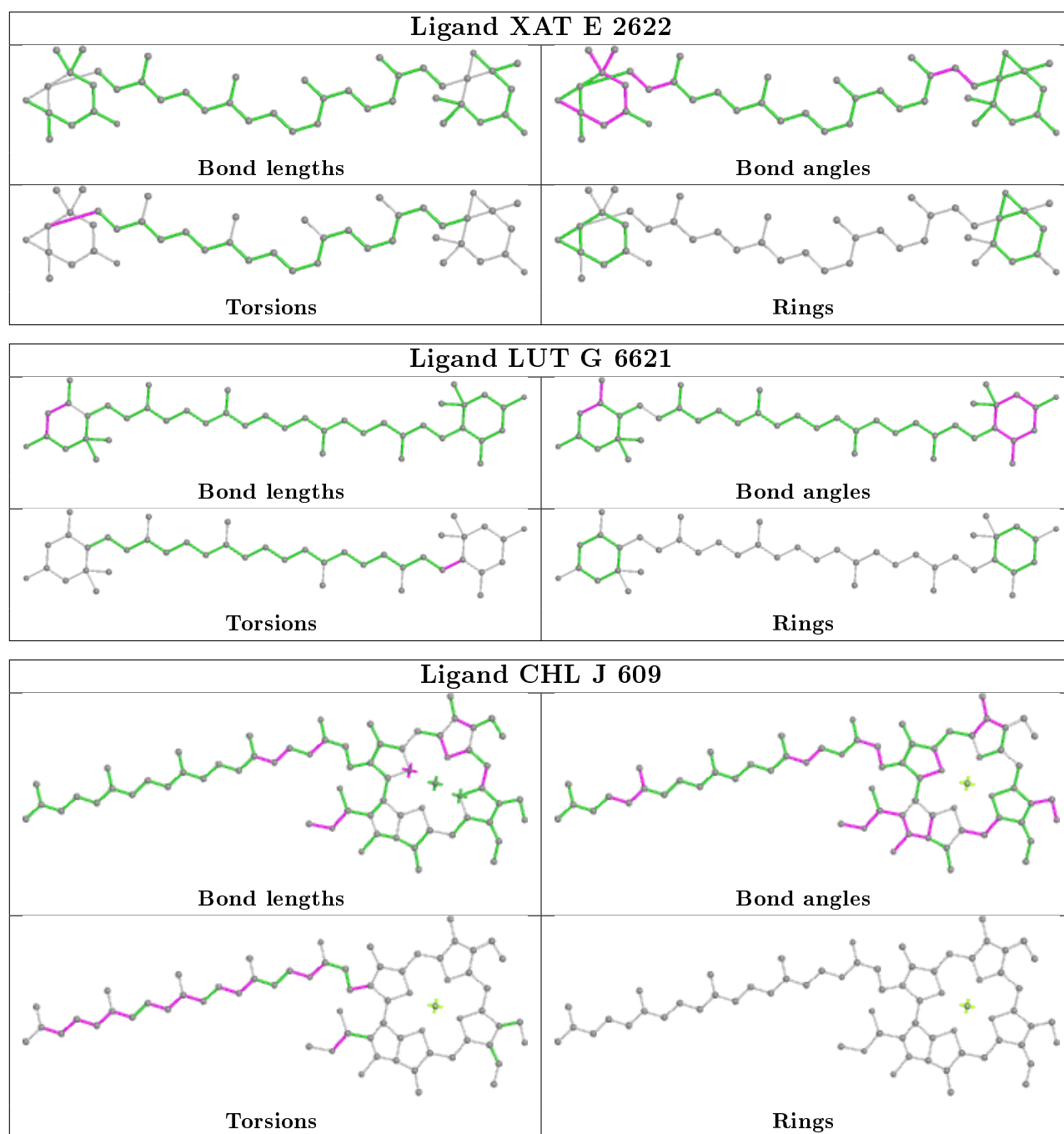


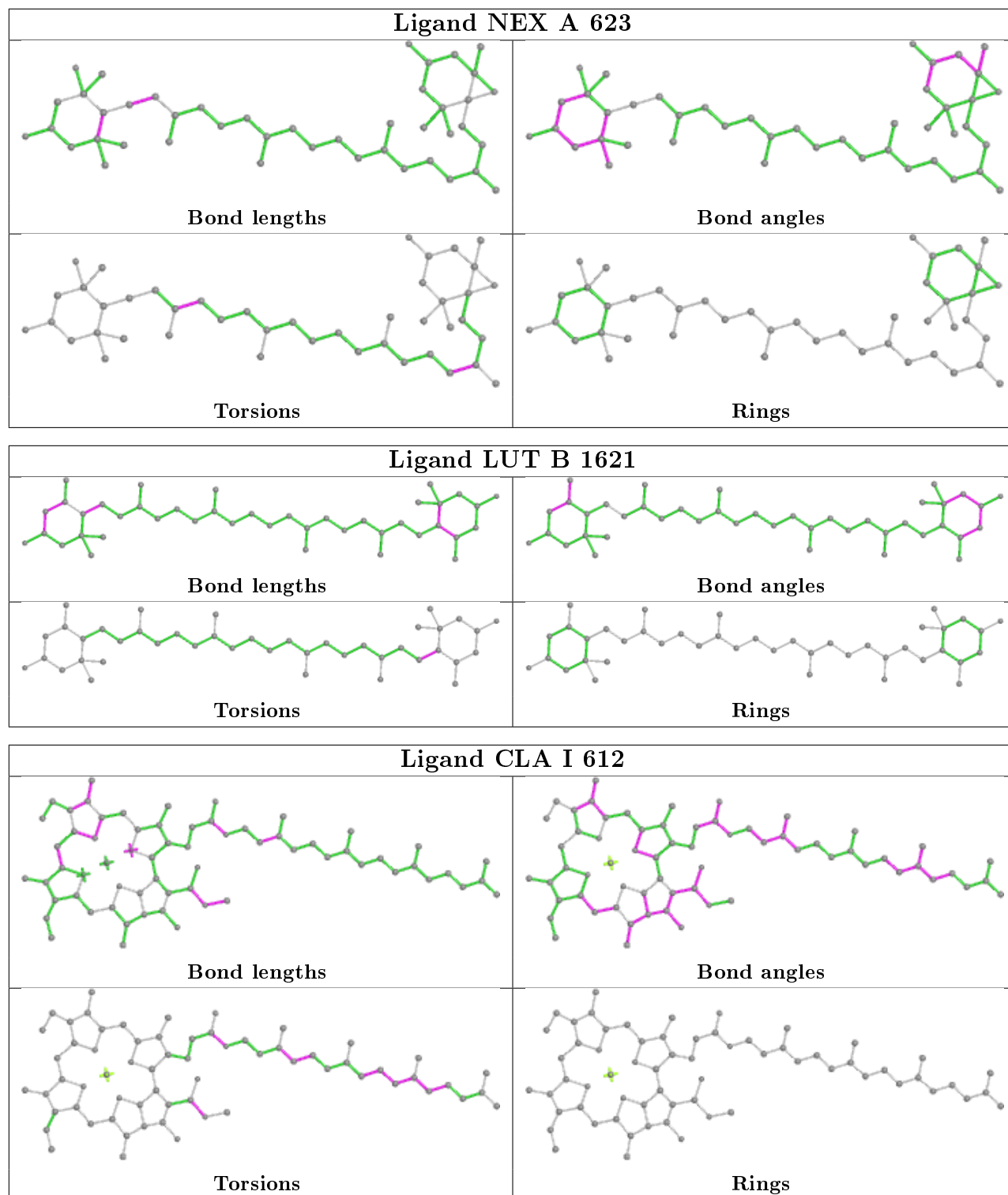
Ligand CHL F 601



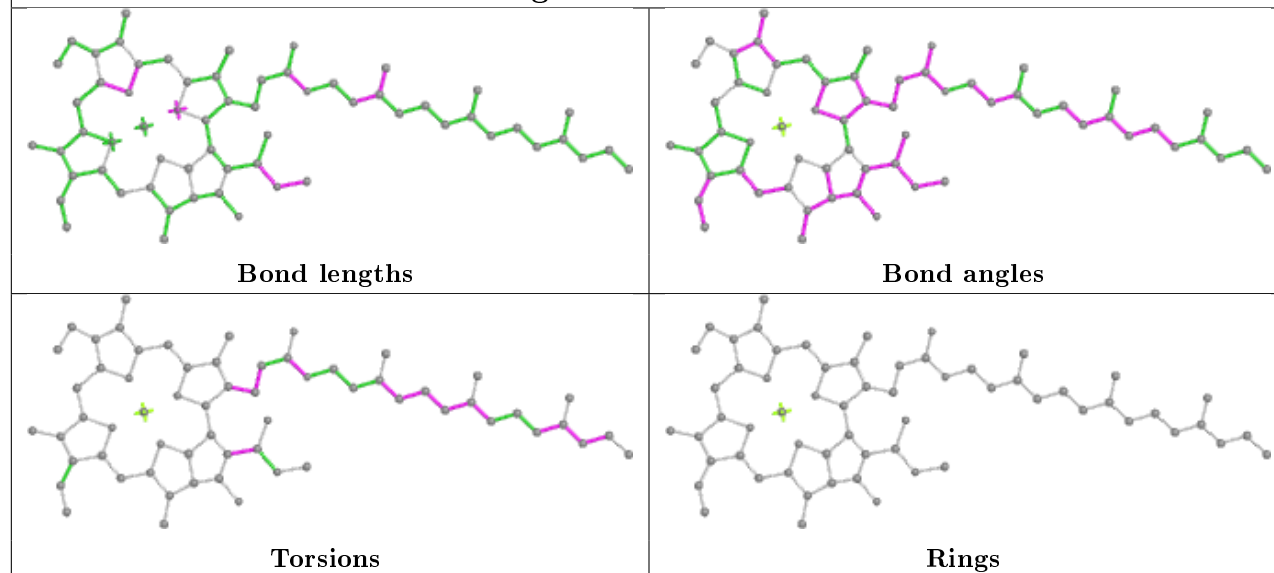
Ligand CLA J 603



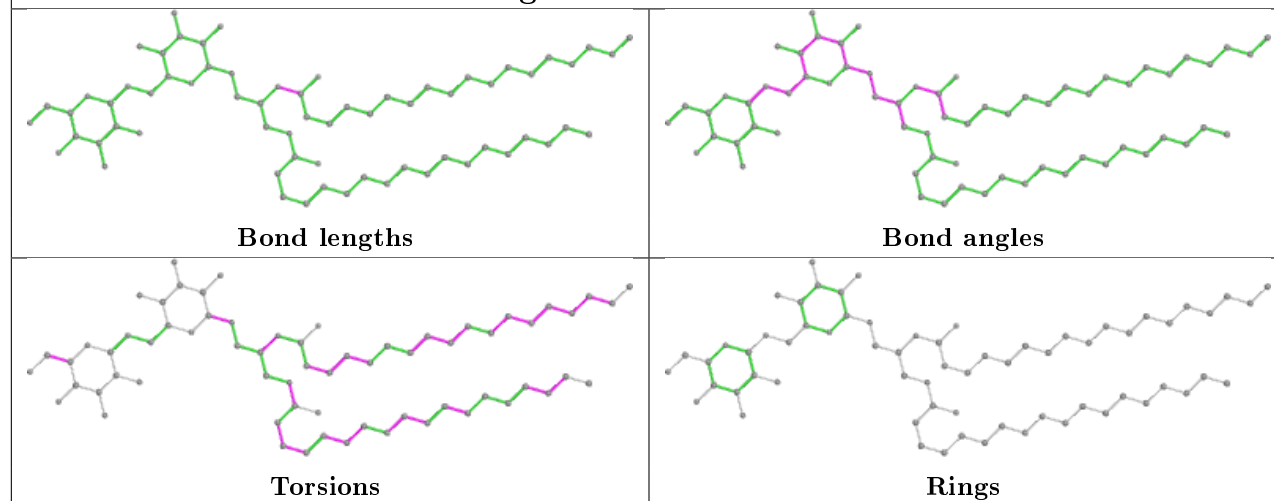




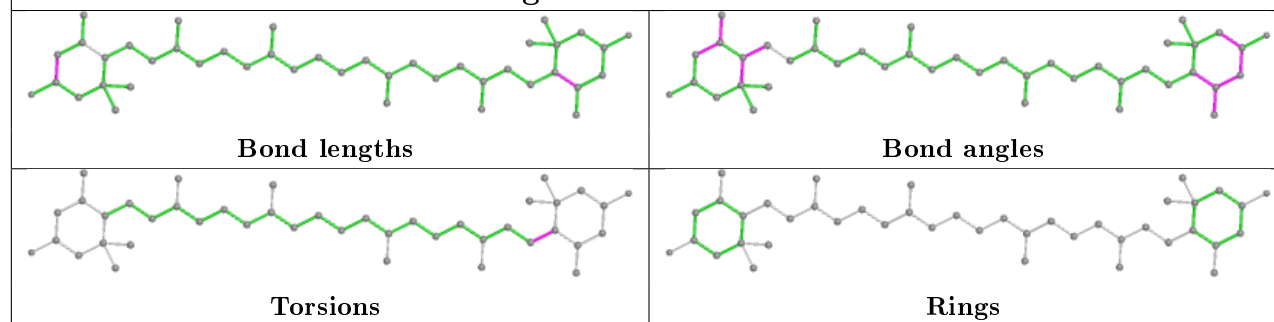
Ligand CLA H 604

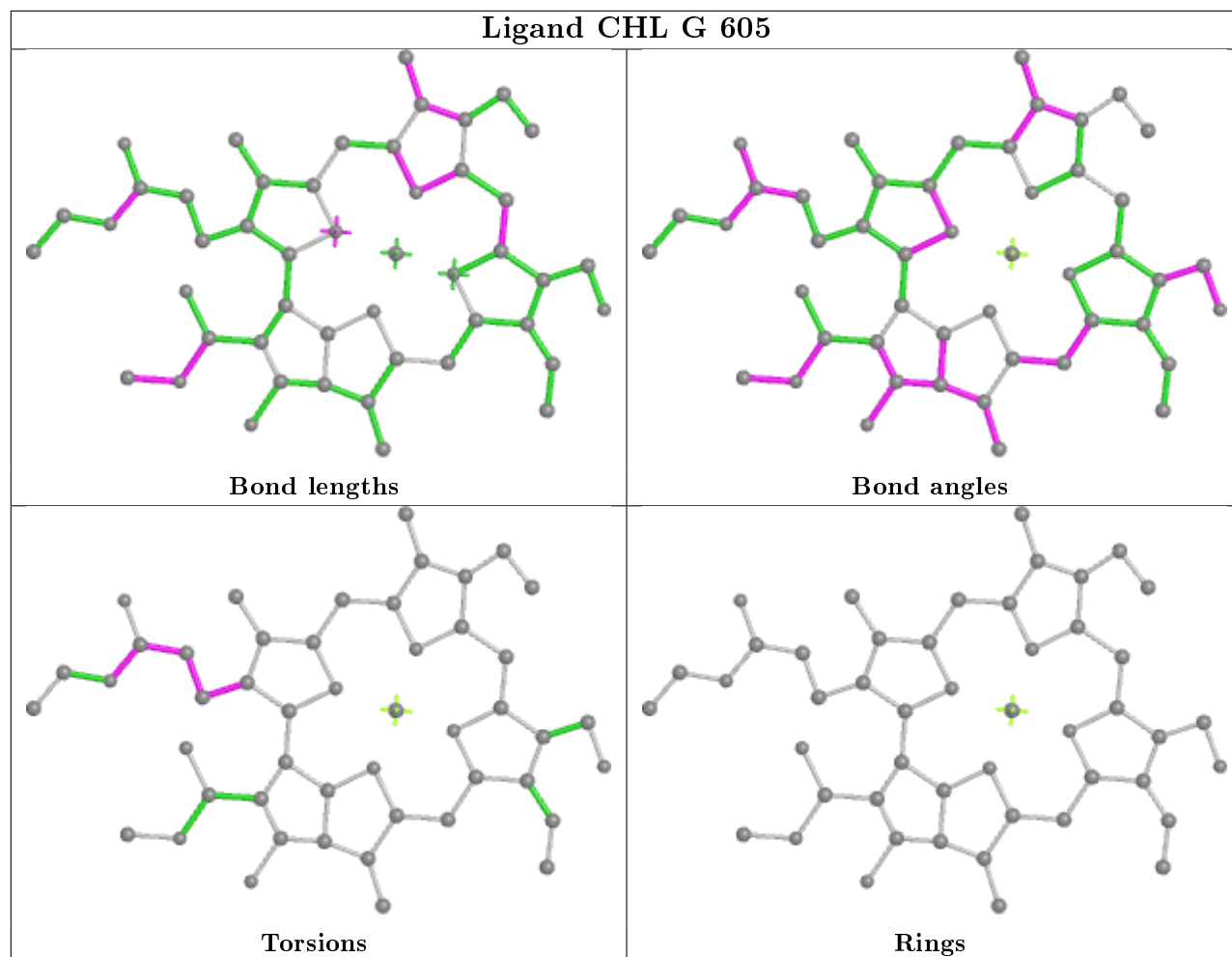


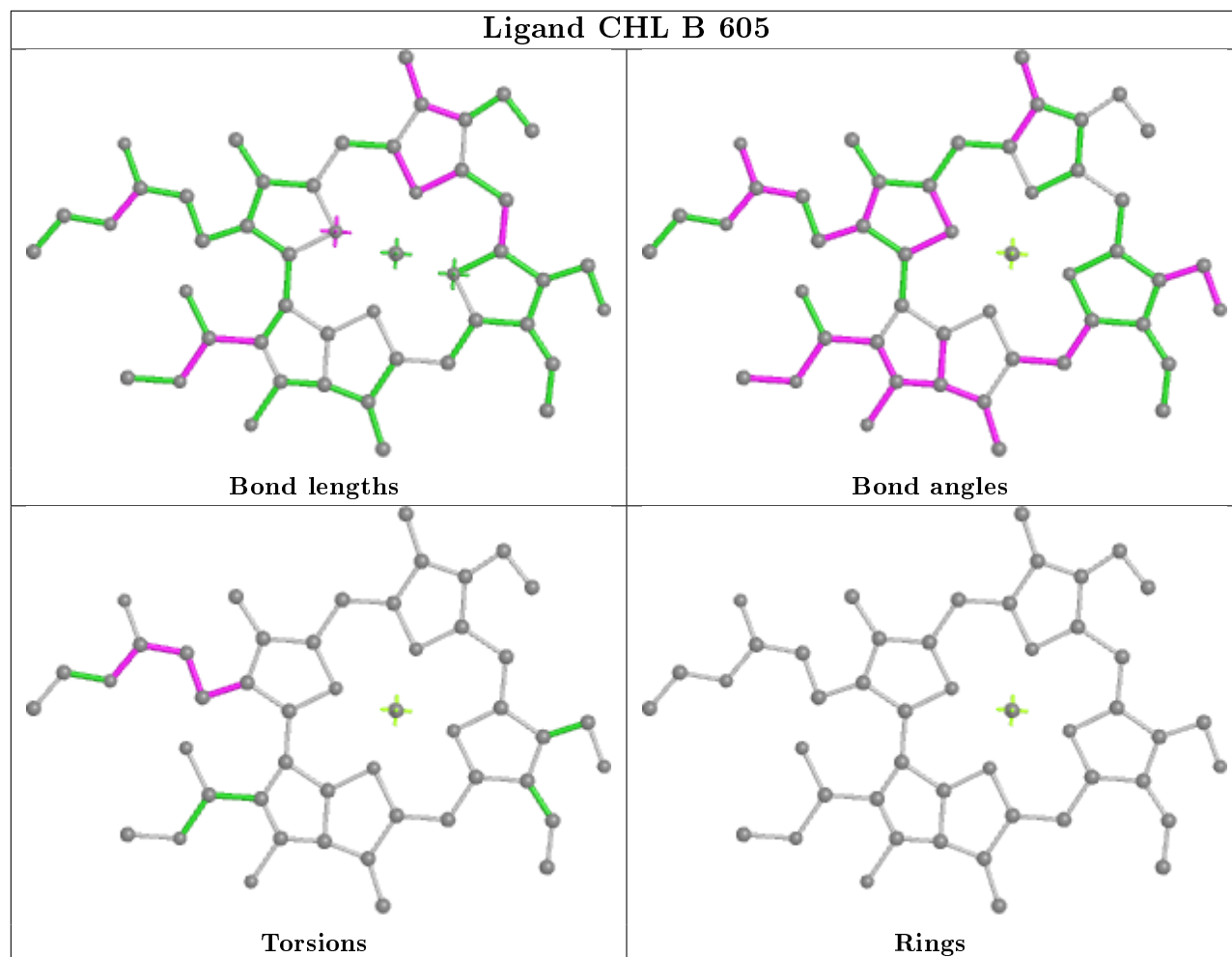
Ligand DGD B 2632

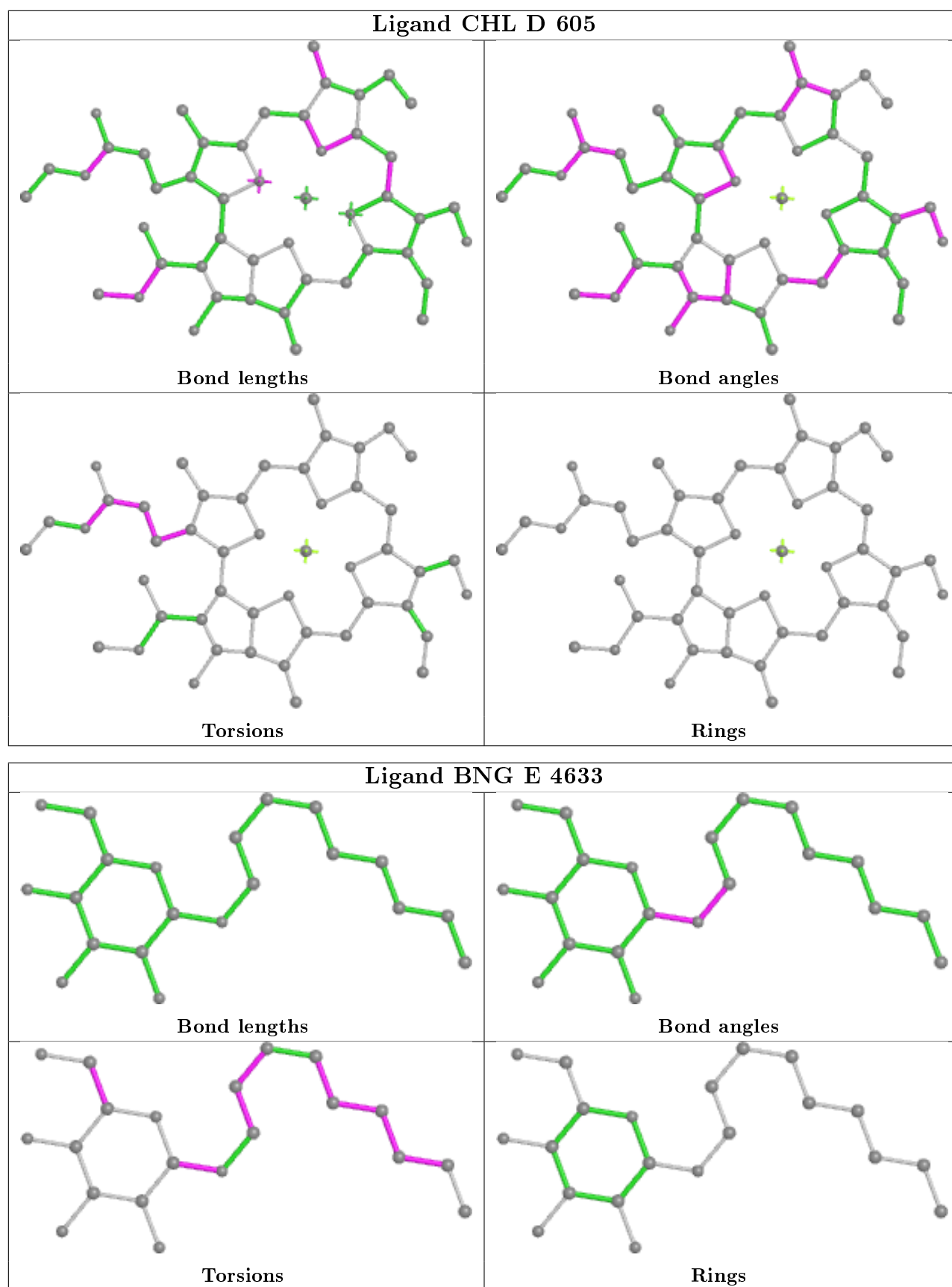


Ligand LUT H 7620

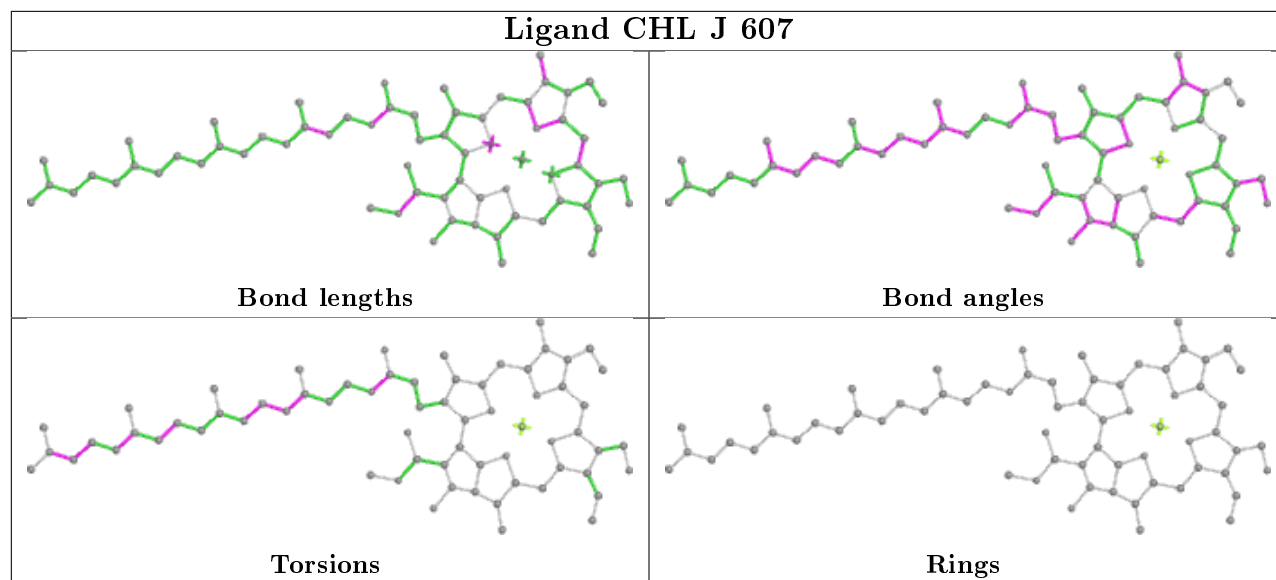




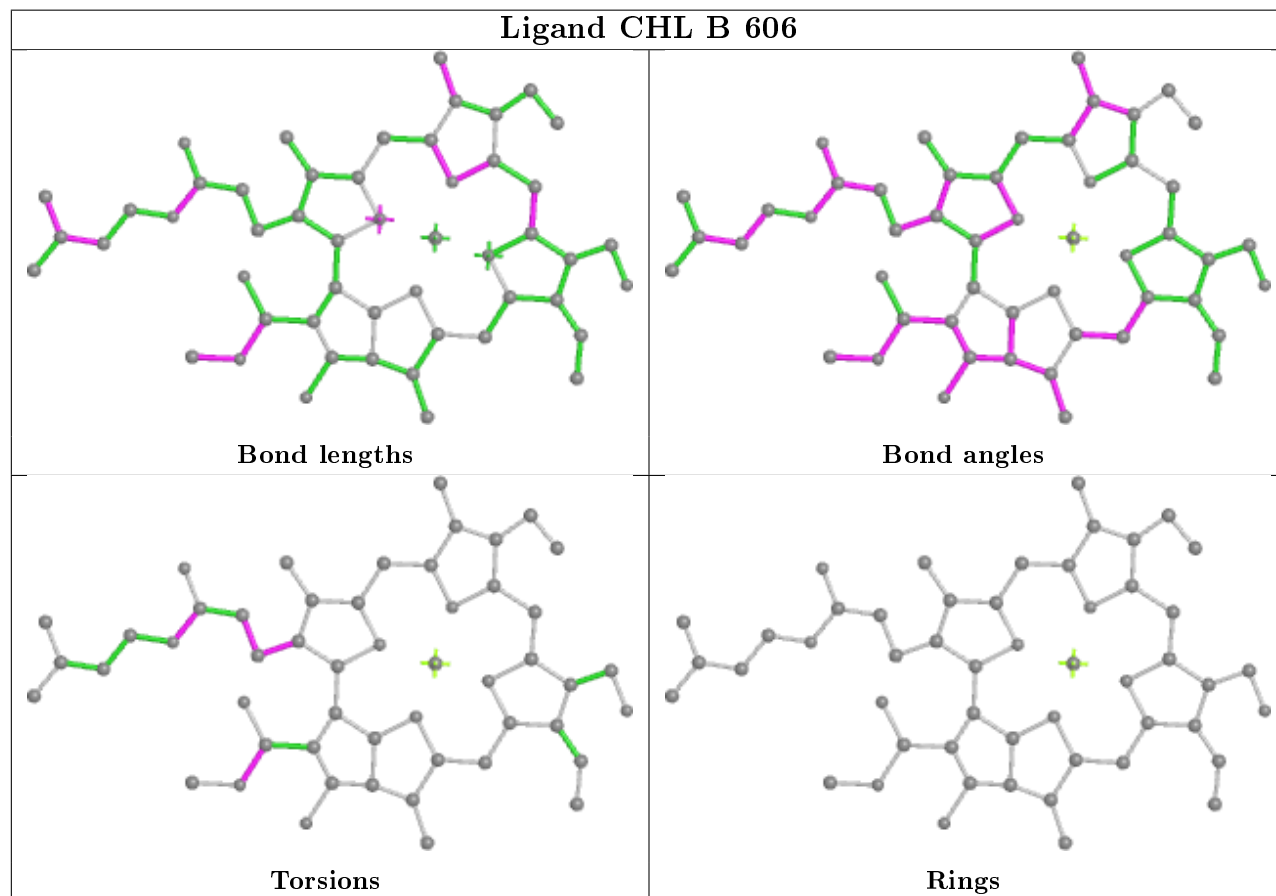




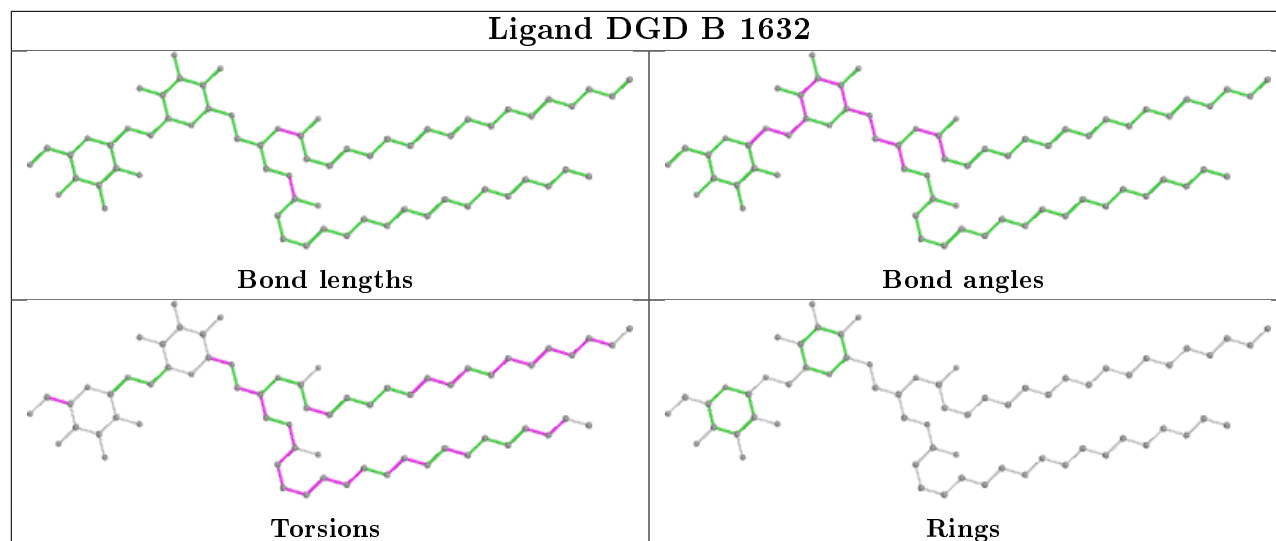
Ligand CHL J 607



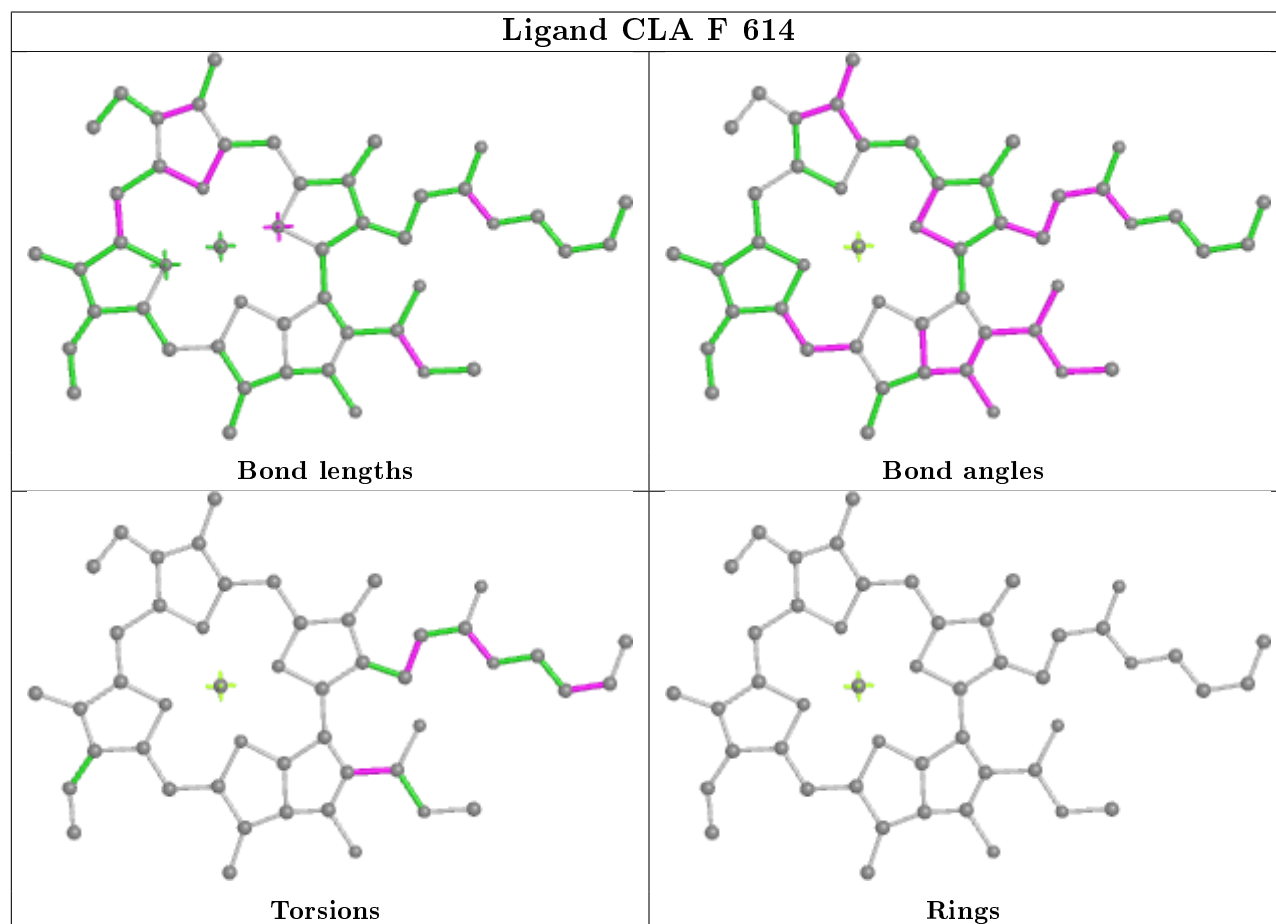
Ligand CHL B 606

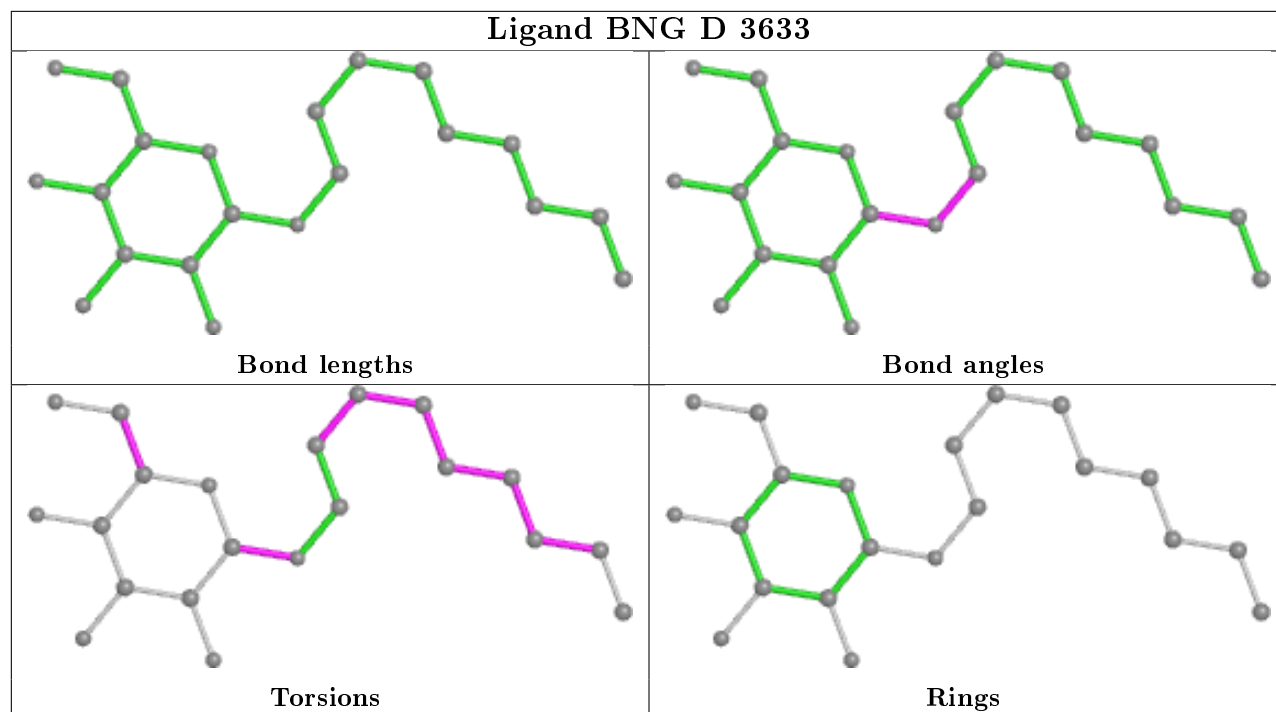


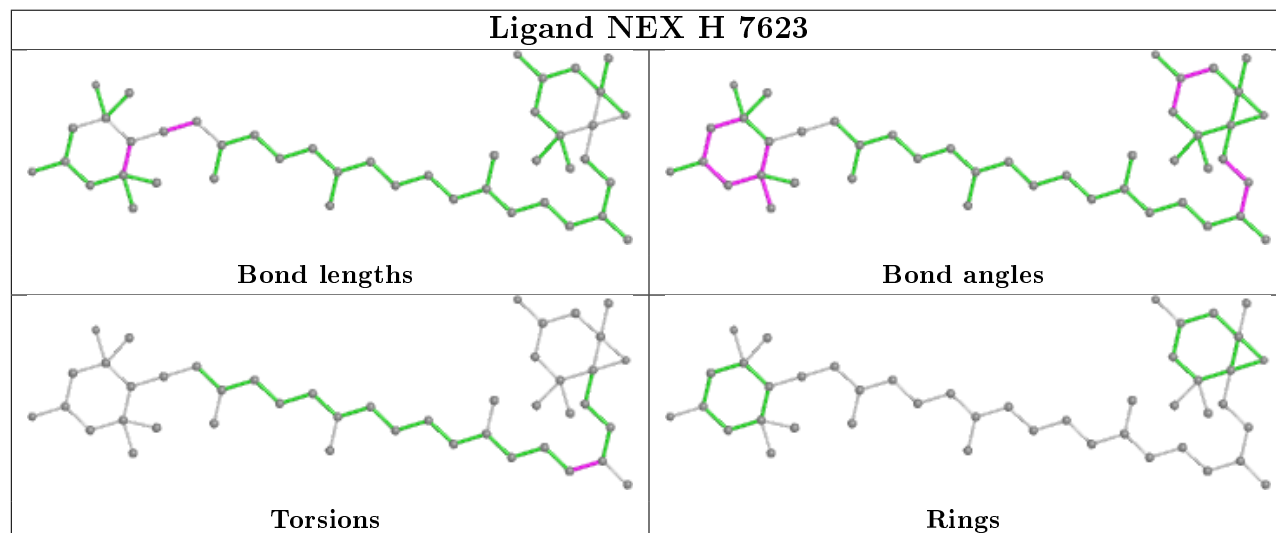
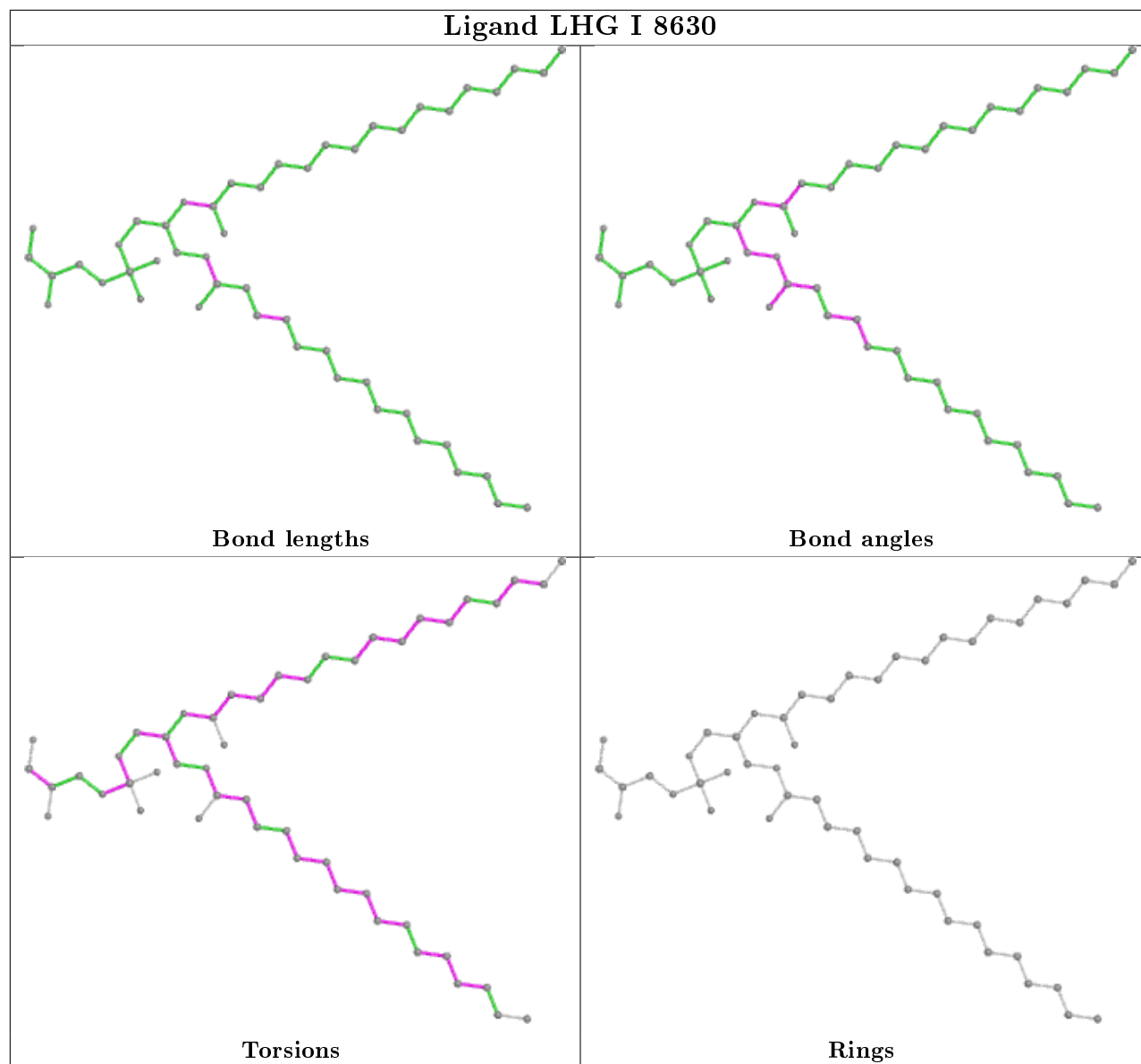
Ligand DGD B 1632



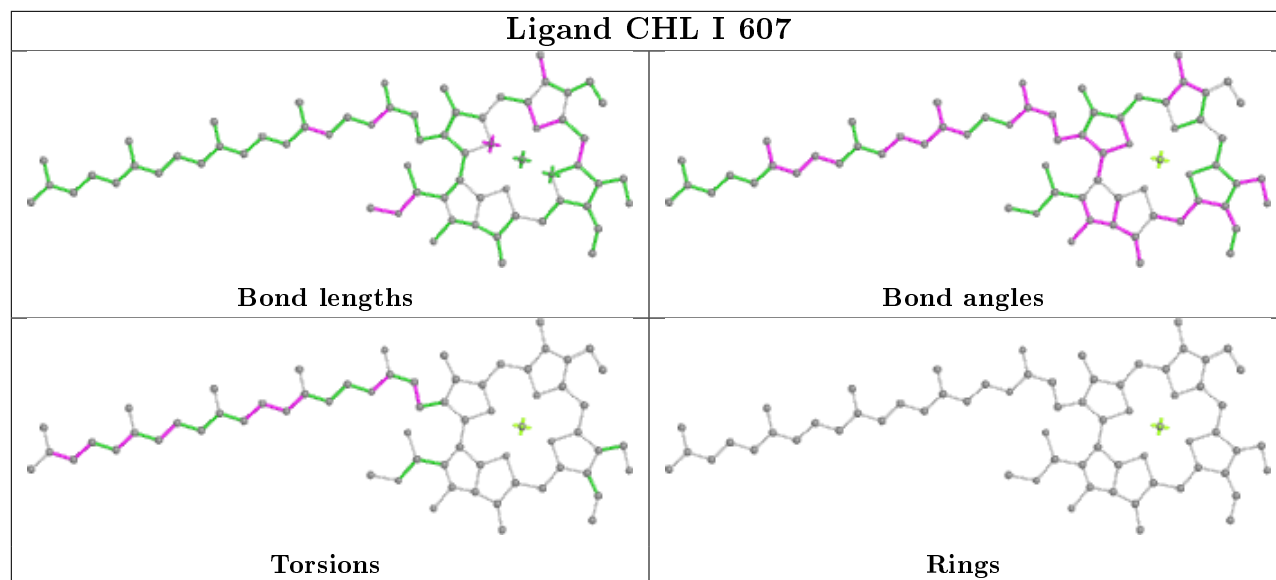
Ligand CLA F 614



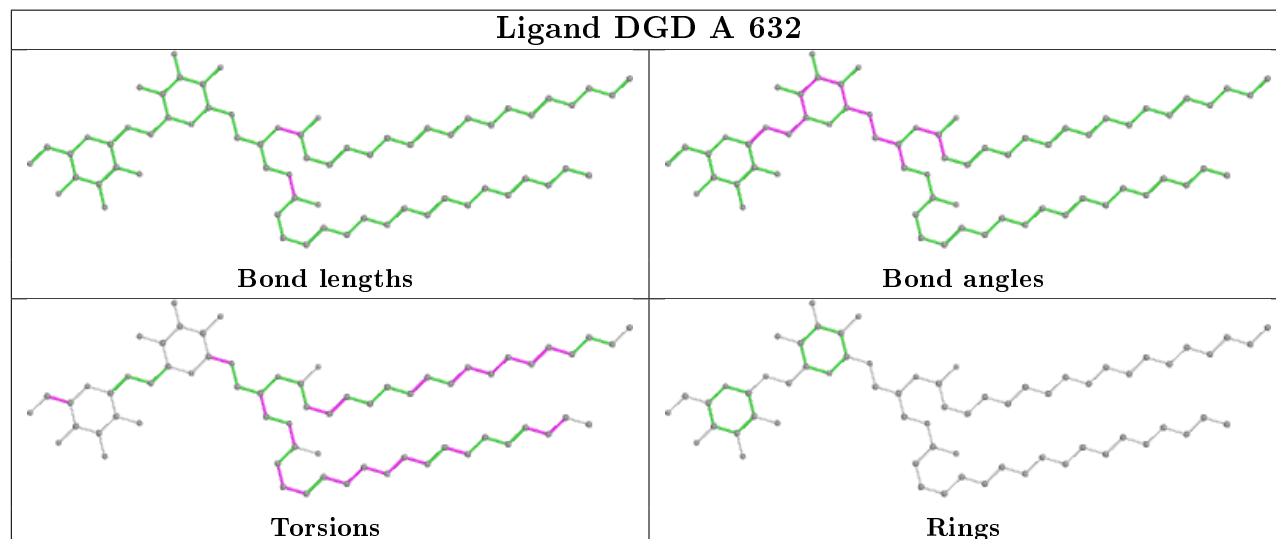




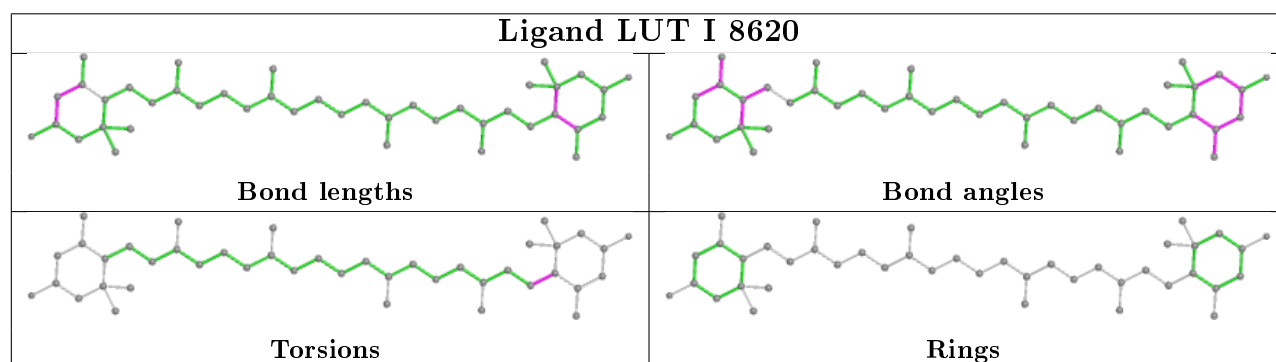
Ligand CHL I 607



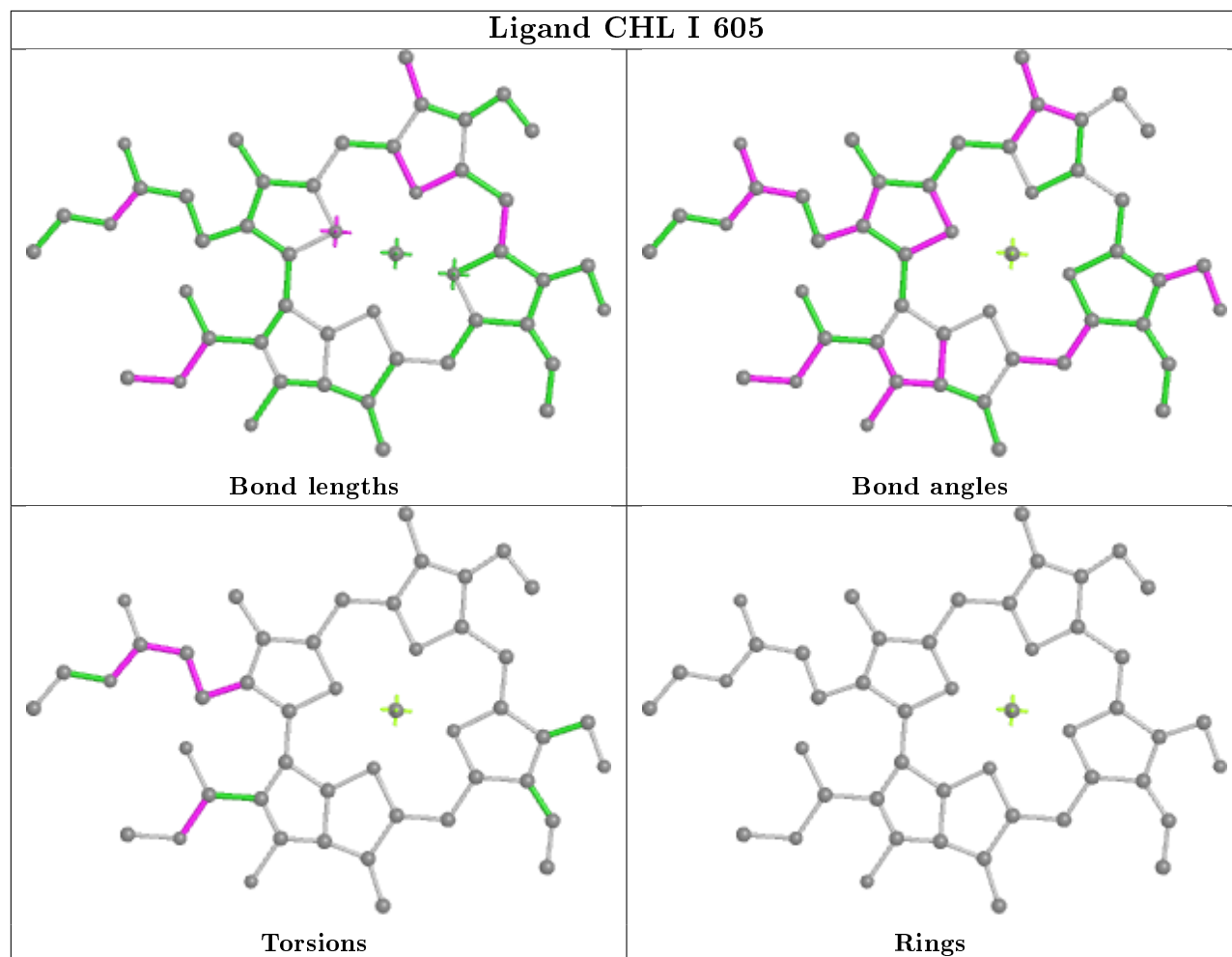
Ligand DGD A 632



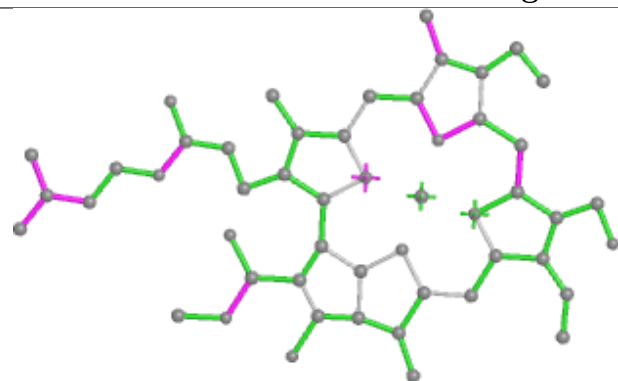
Ligand LUT I 8620



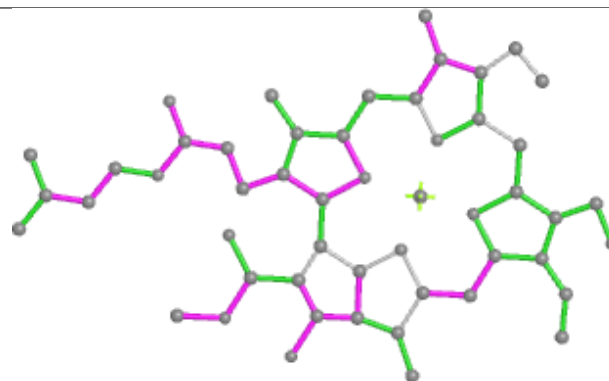
Ligand CHL I 605



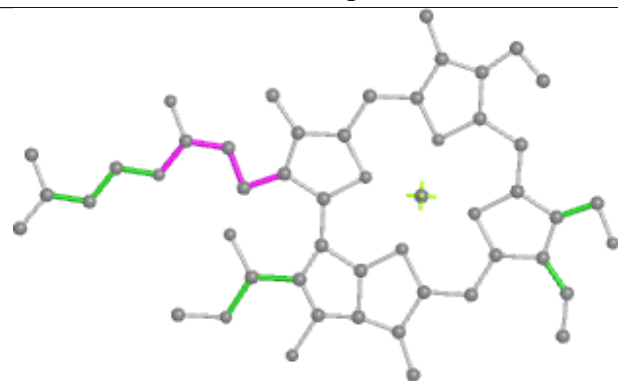
Ligand CHL J 606



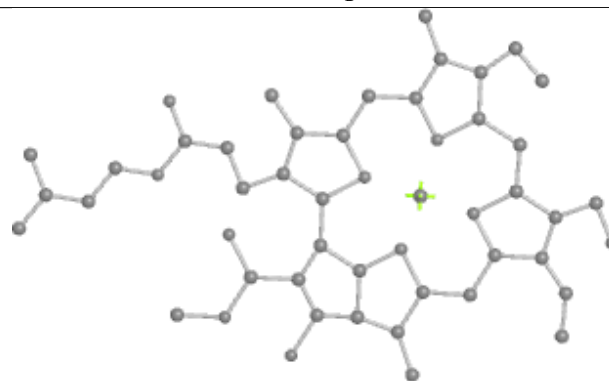
Bond lengths



Bond angles

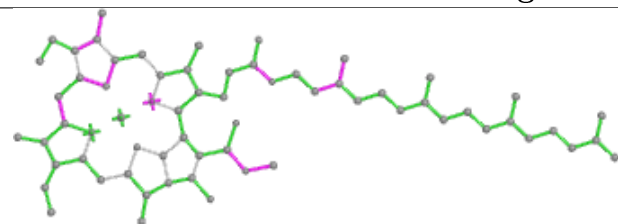


Torsions

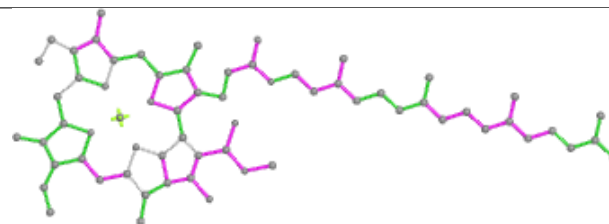


Rings

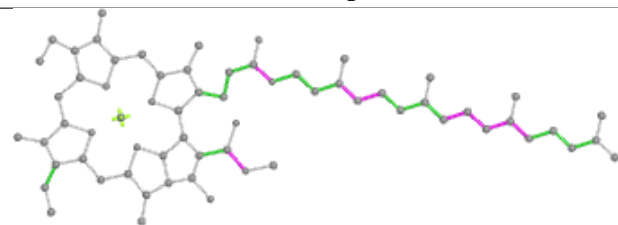
Ligand CLA D 612



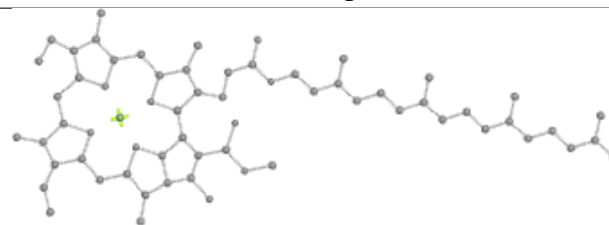
Bond lengths



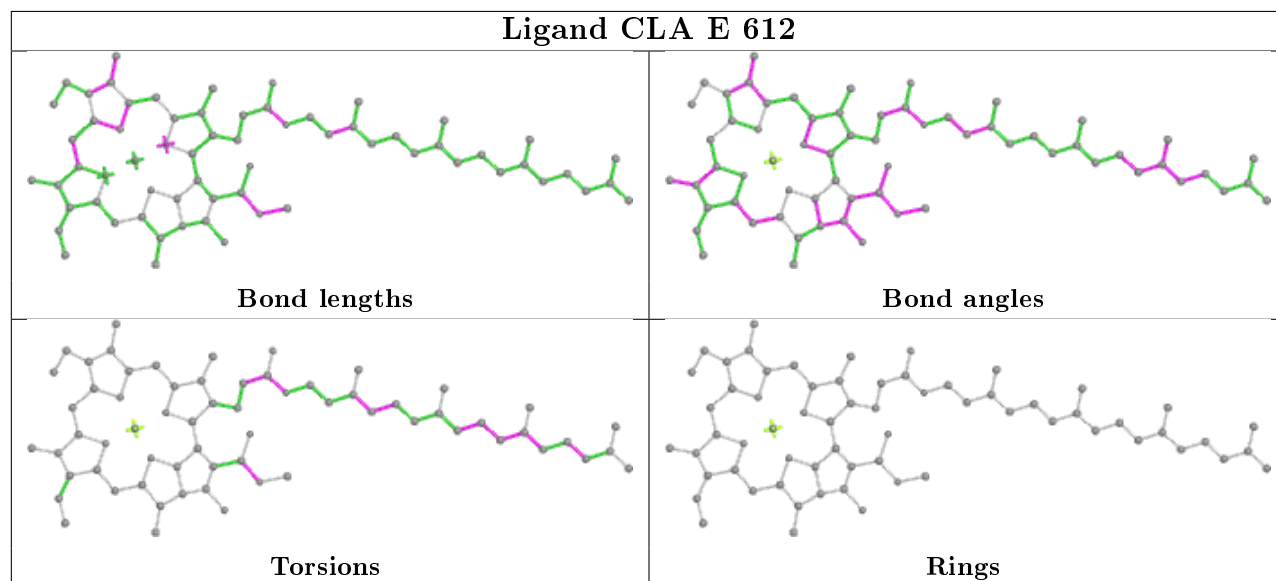
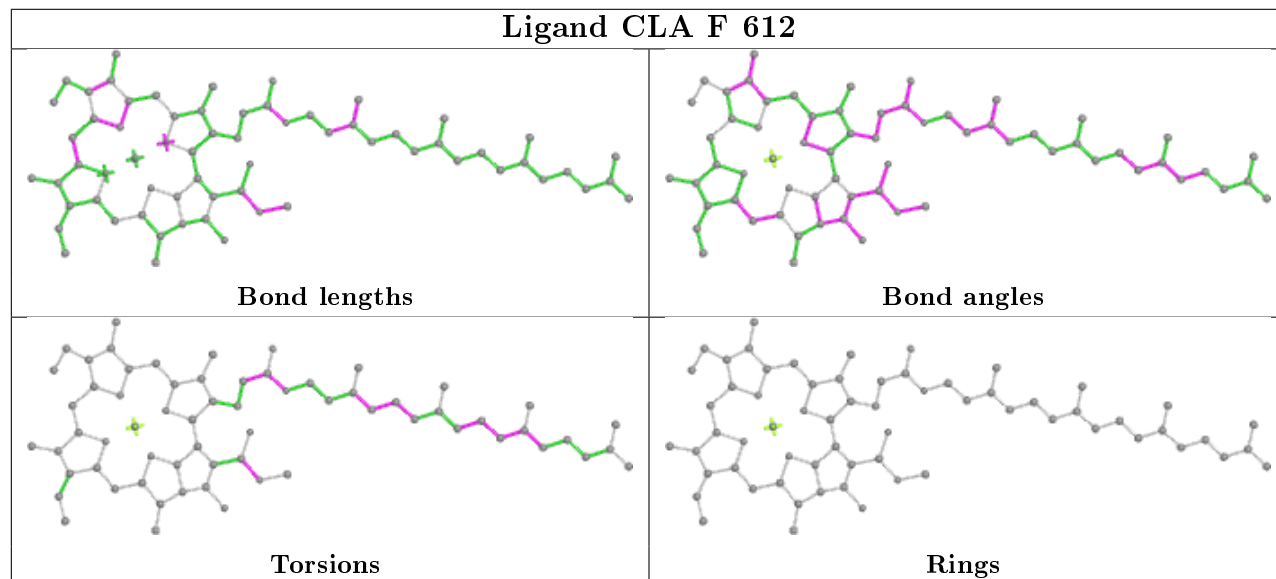
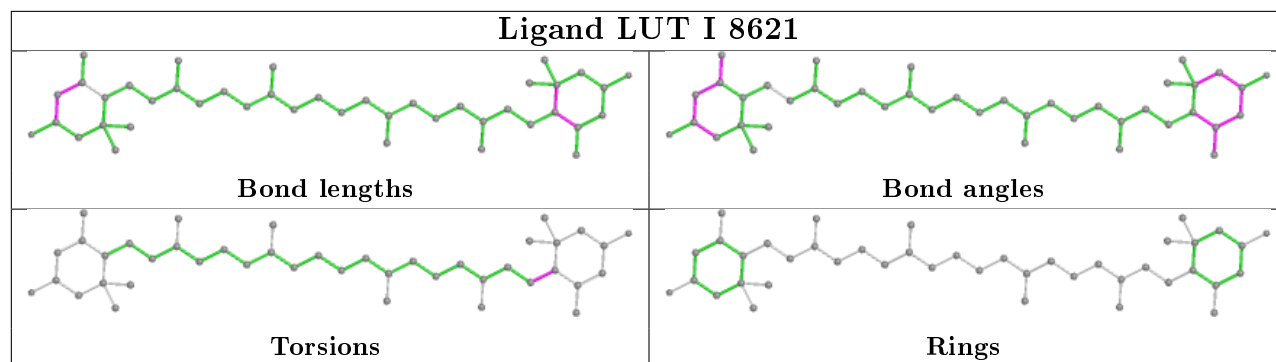
Bond angles



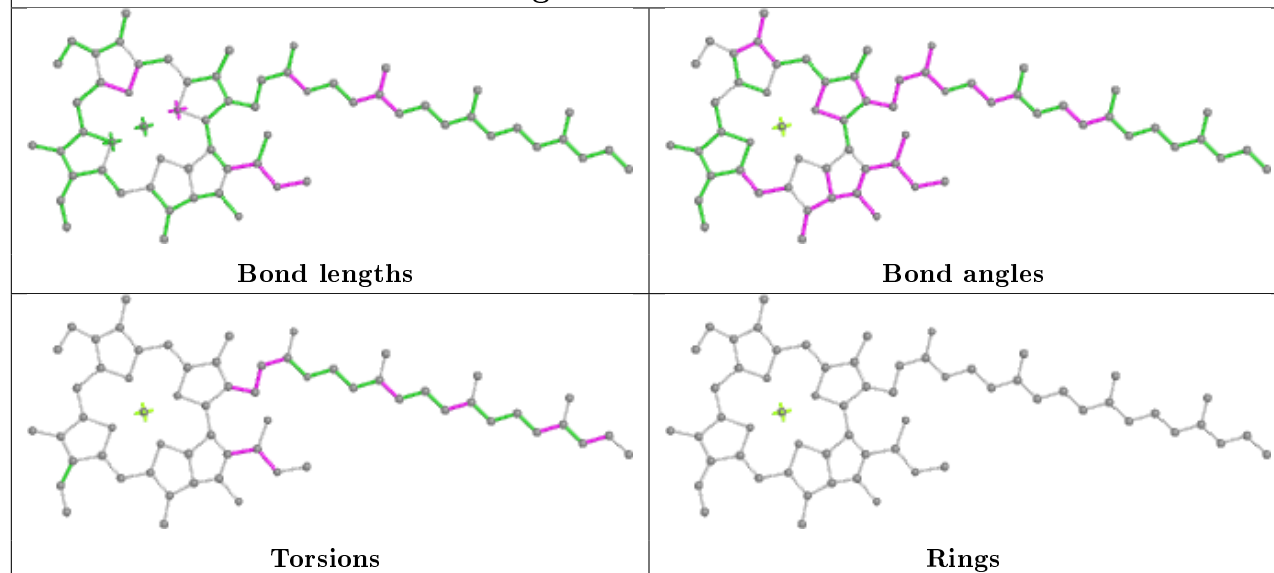
Torsions



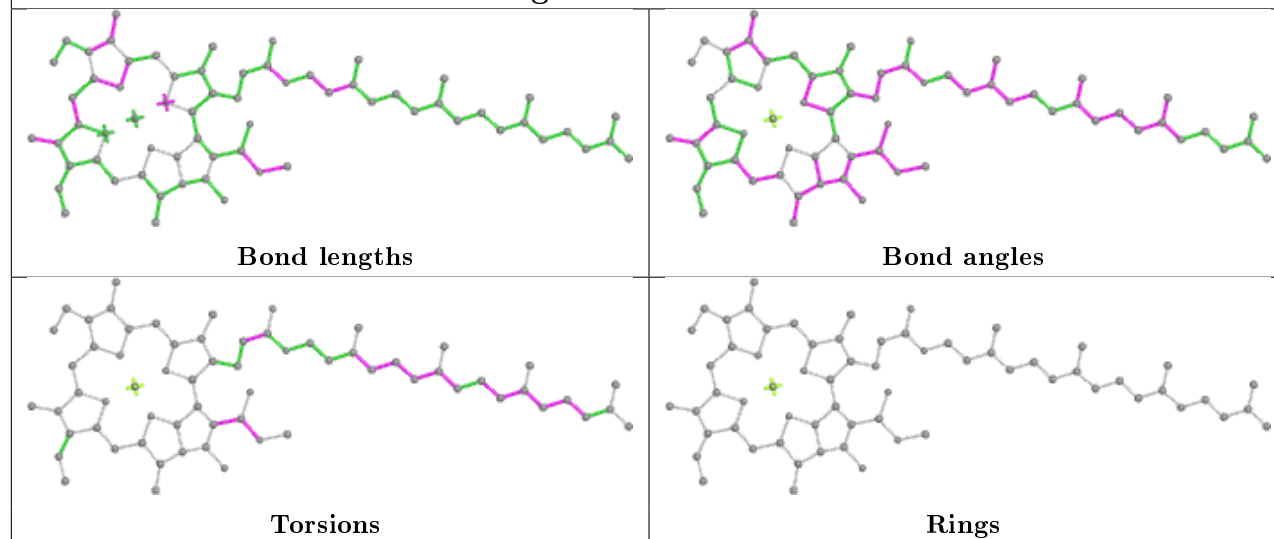
Rings



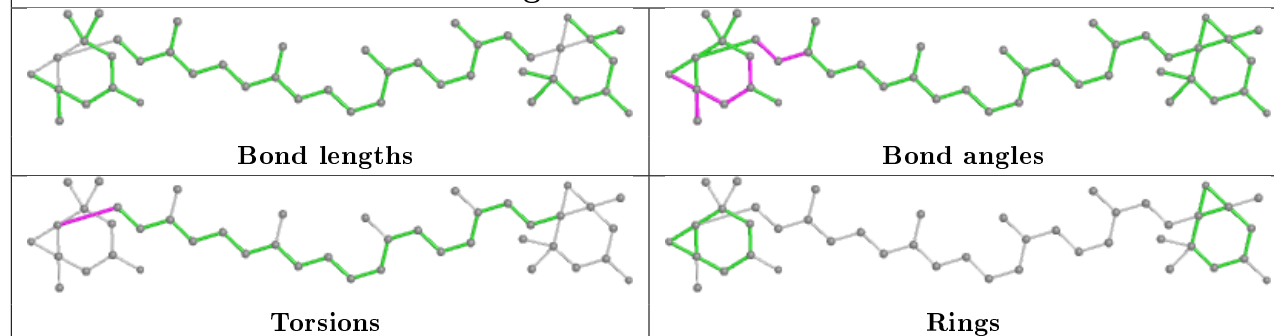
Ligand CLA C 604

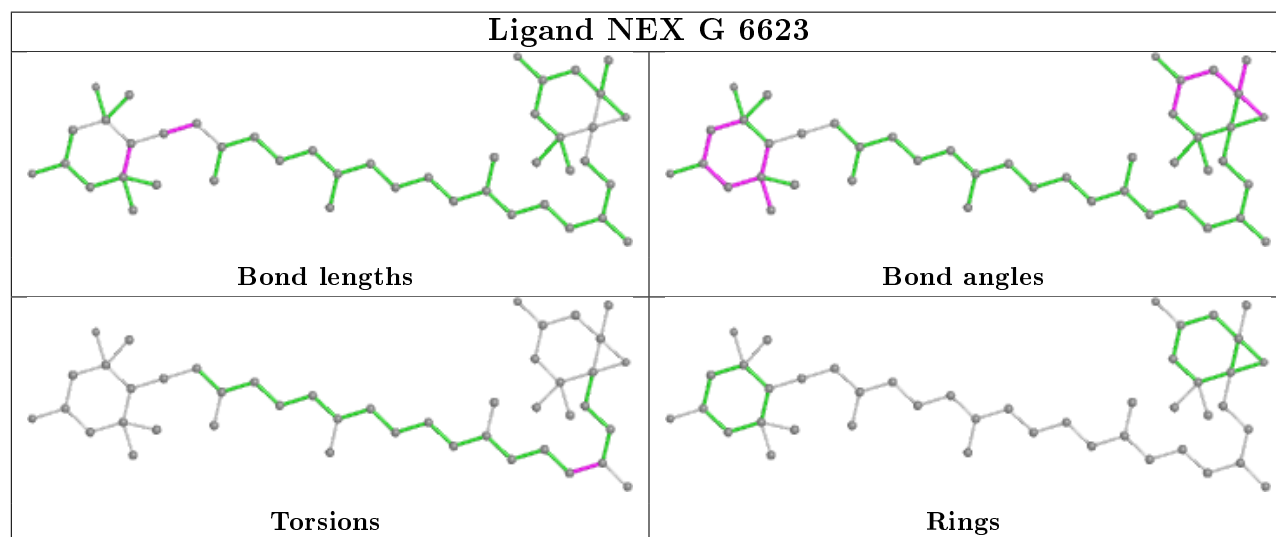
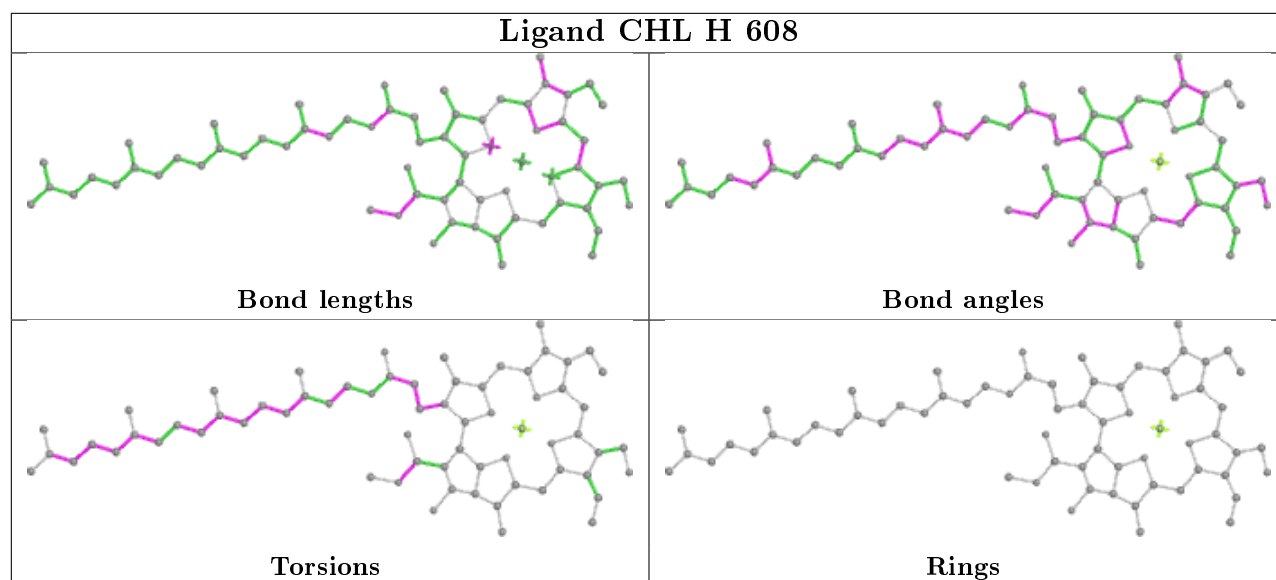
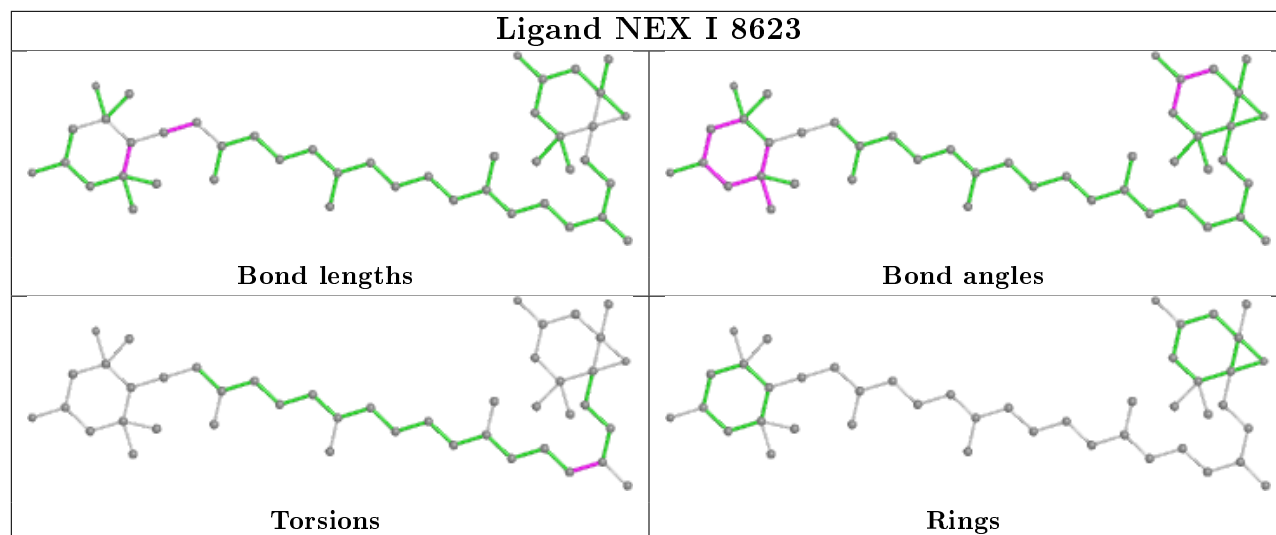


Ligand CLA D 602

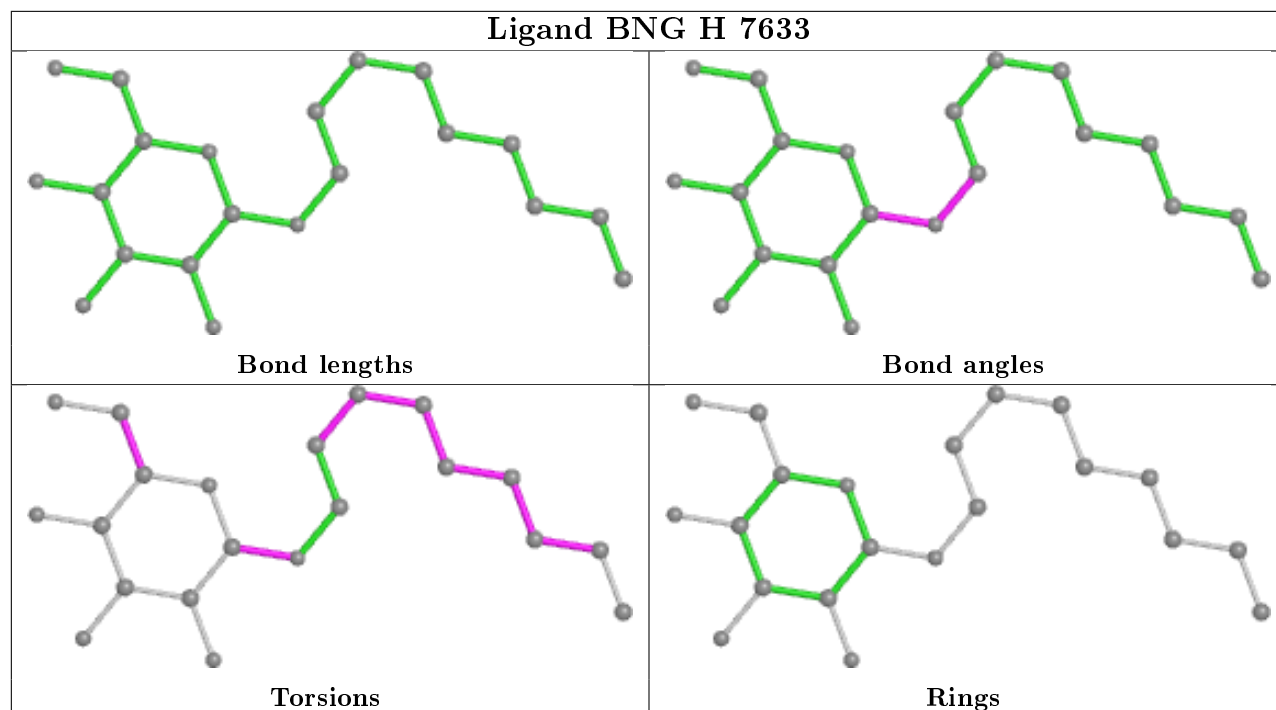


Ligand XAT B 1622

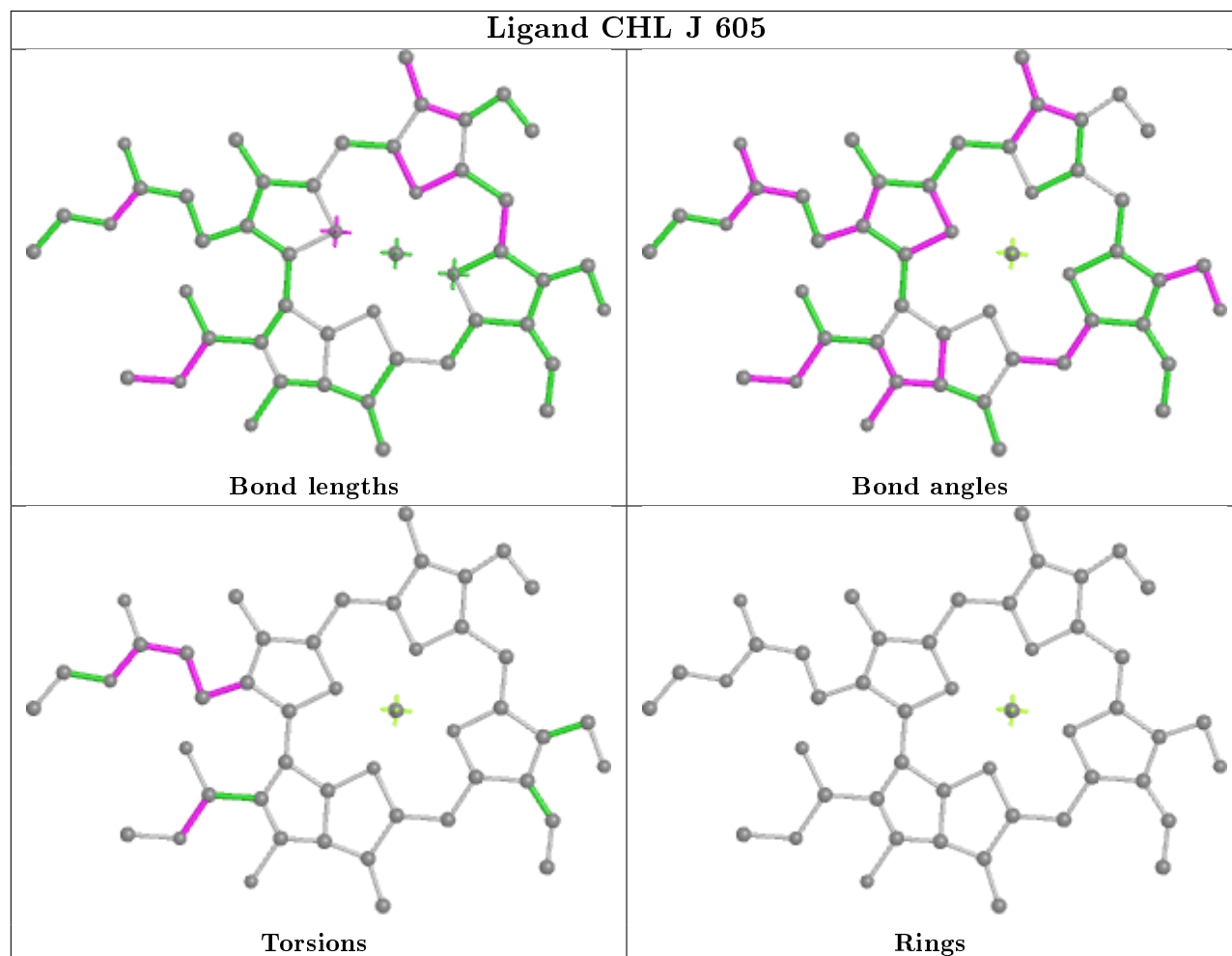


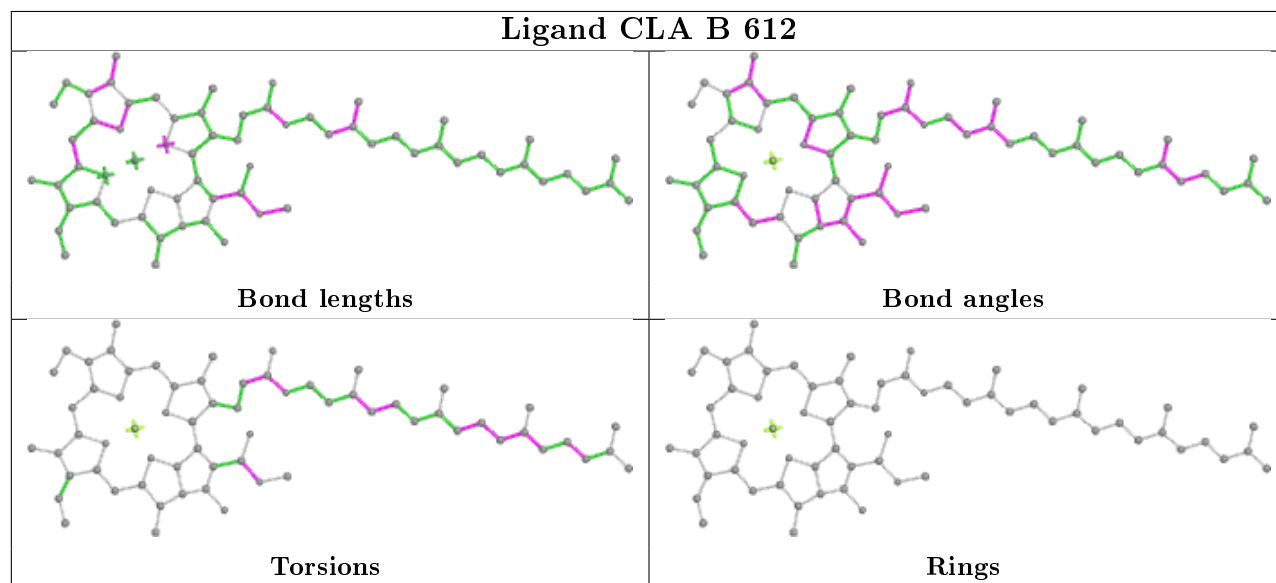
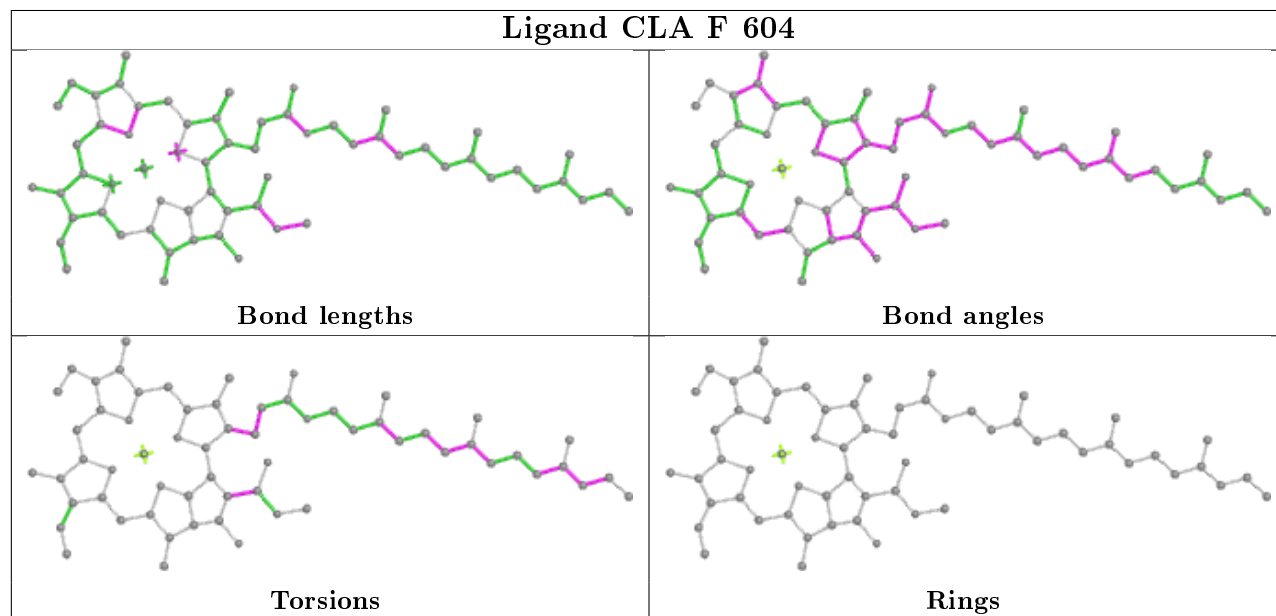
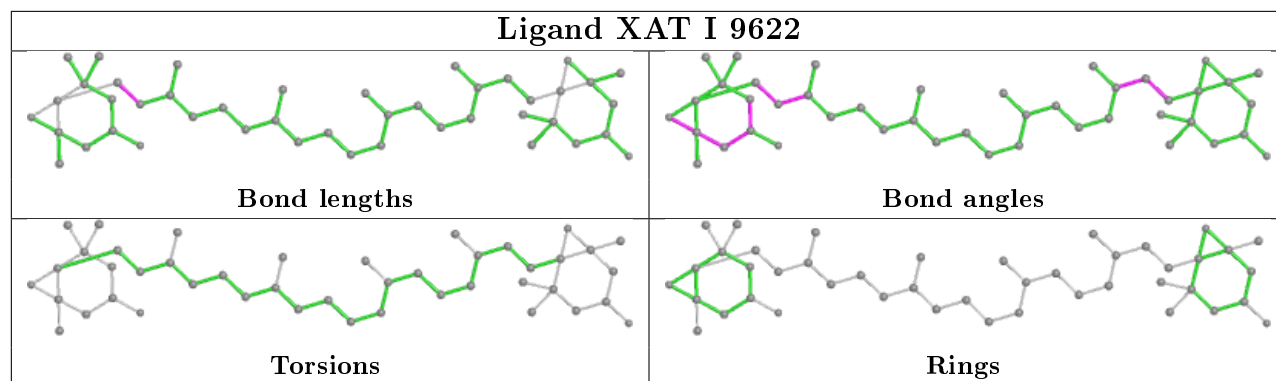


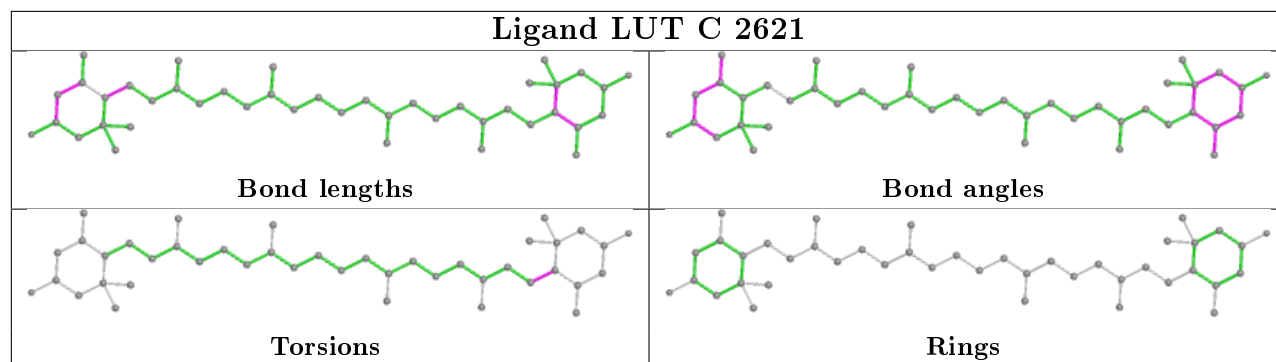
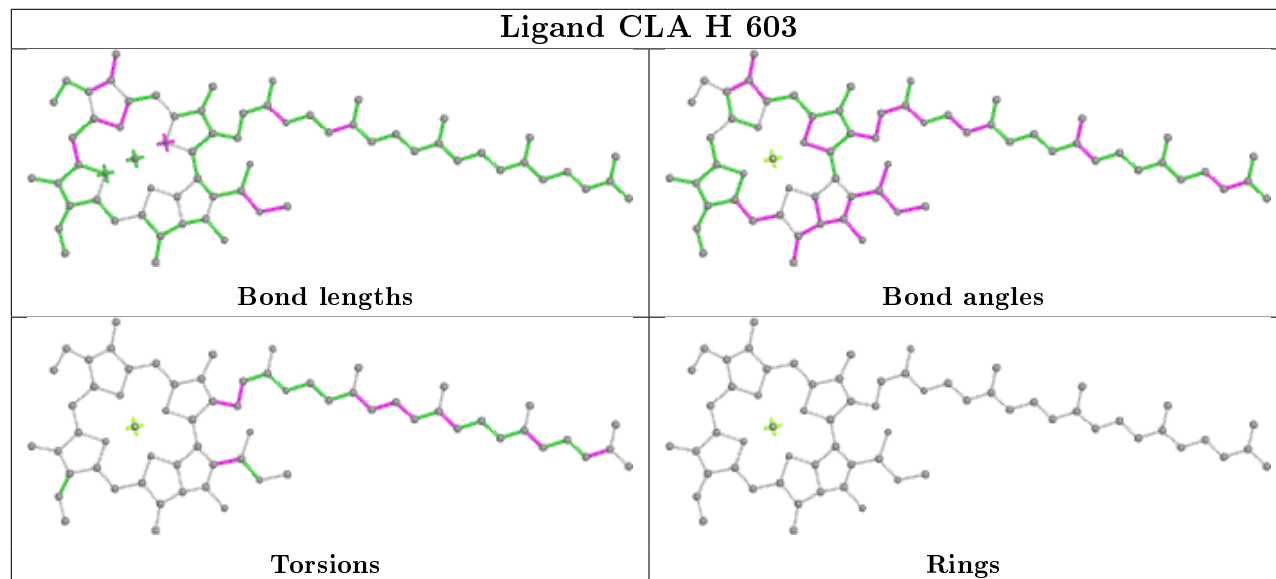
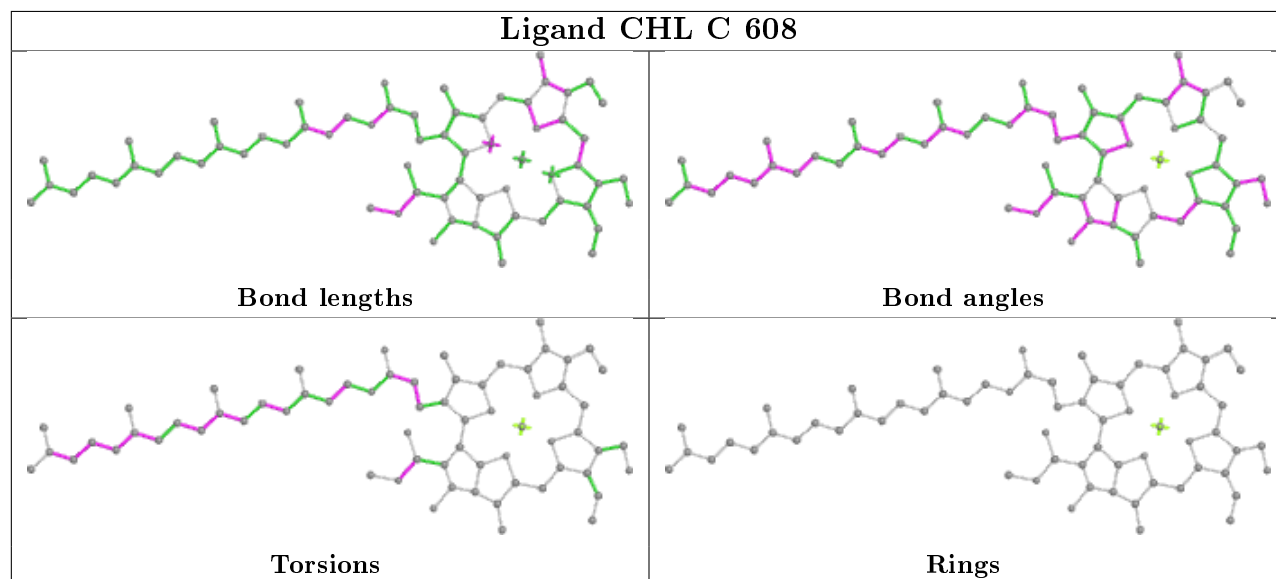
Ligand BNG H 7633

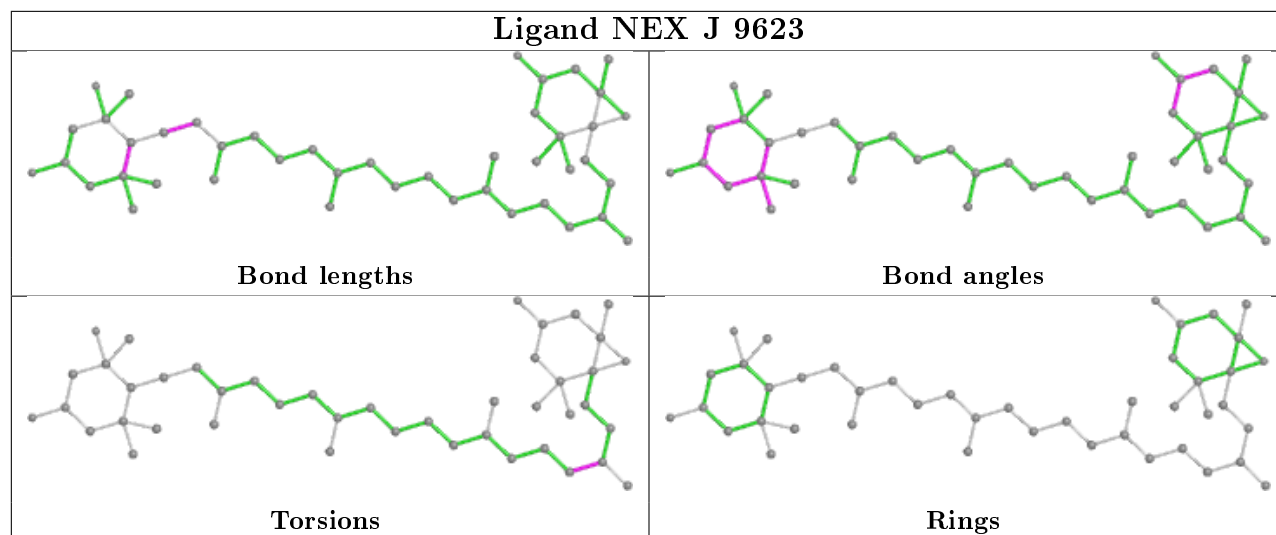
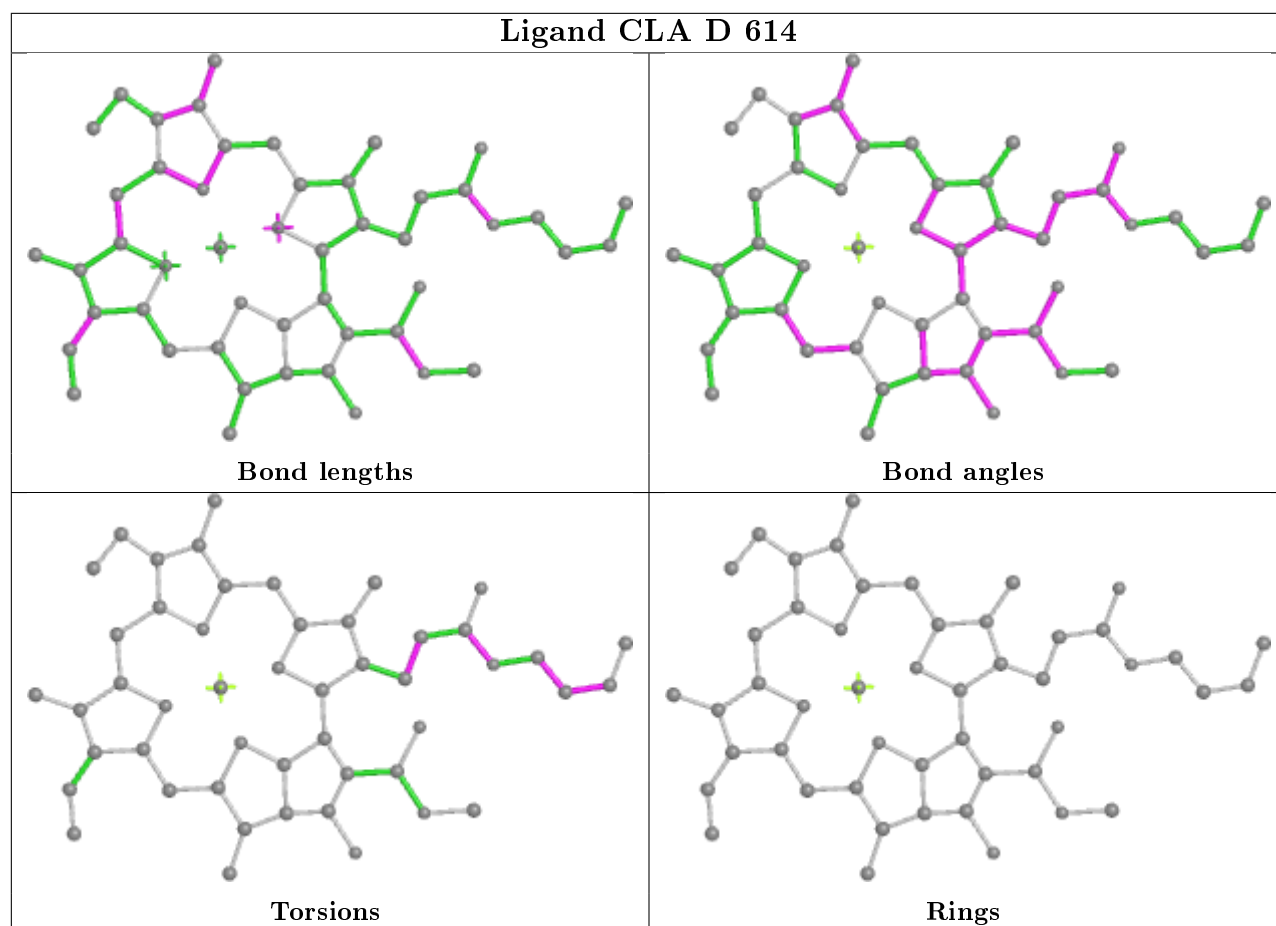


Ligand CHL J 605

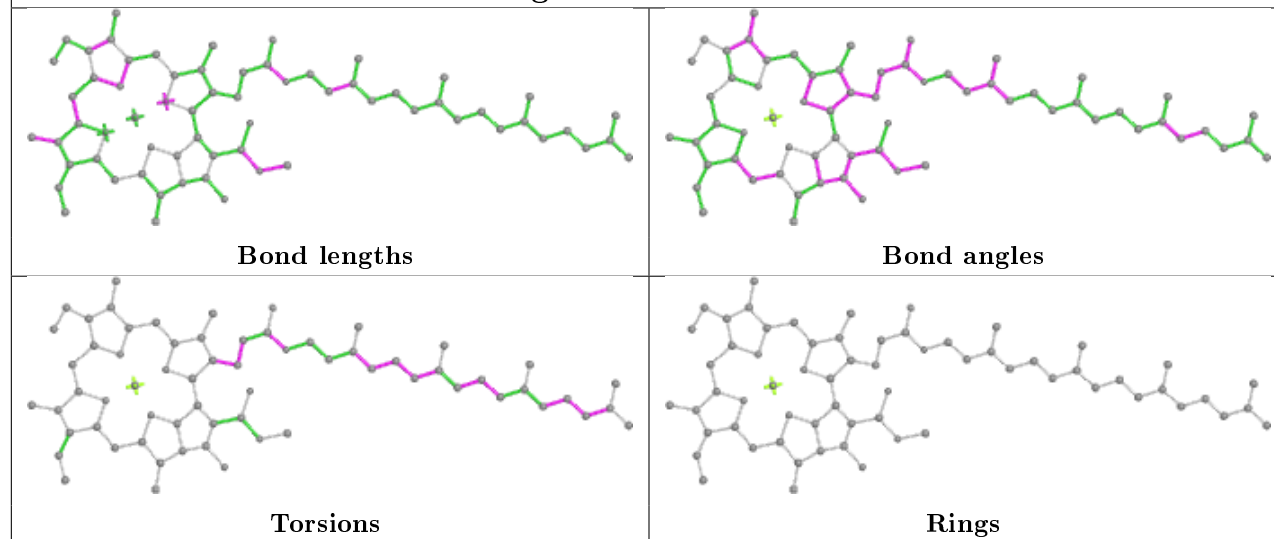




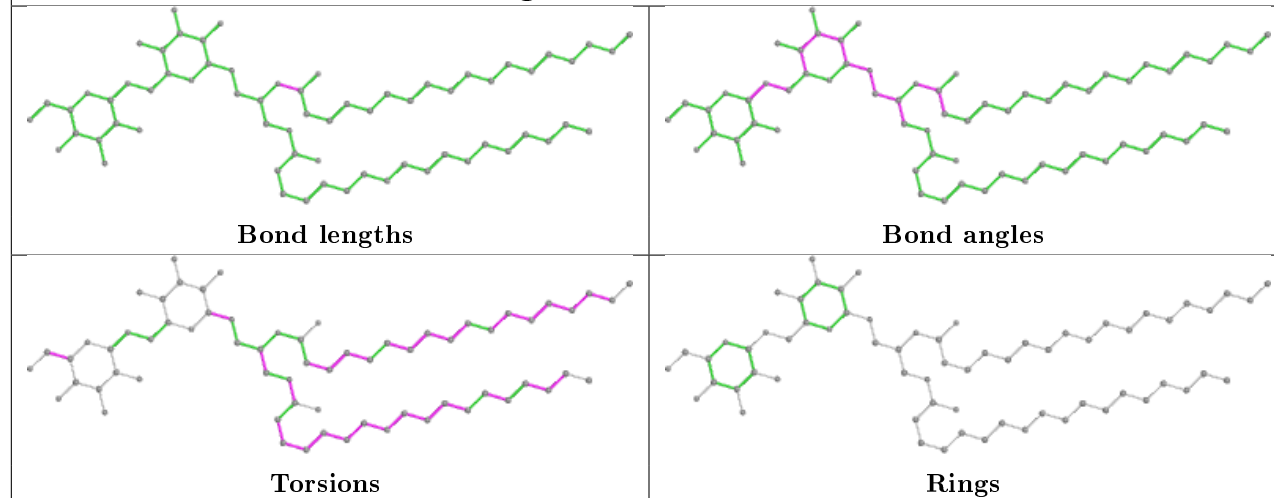
Ligand LUT C 2621**Ligand CLA H 603****Ligand CHL C 608**

Ligand NEX J 9623**Ligand CLA D 614**

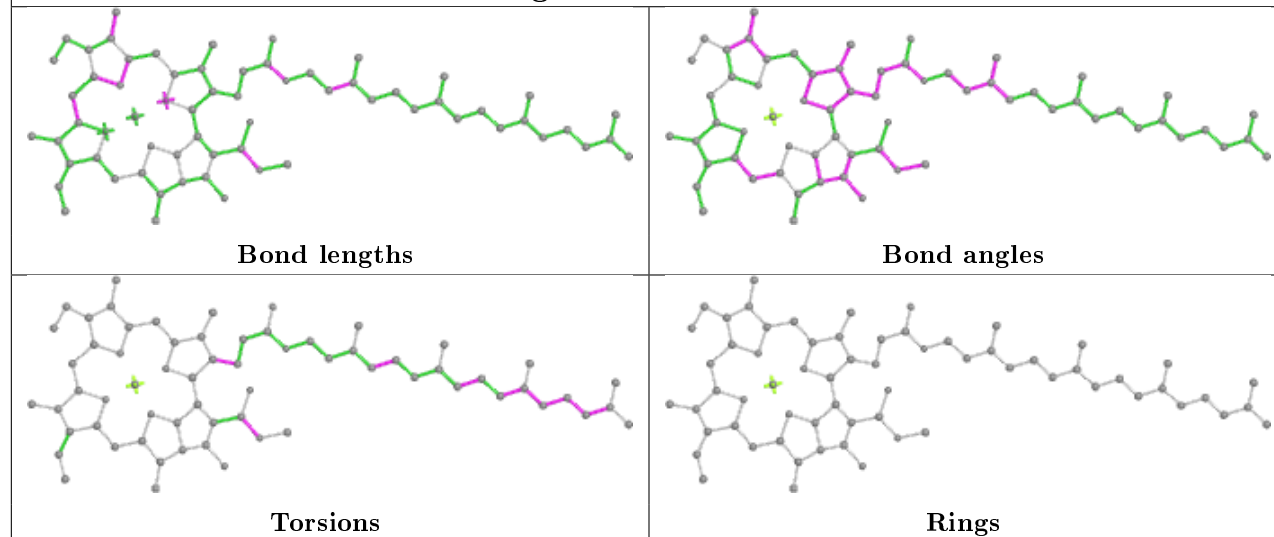
Ligand CLA G 611

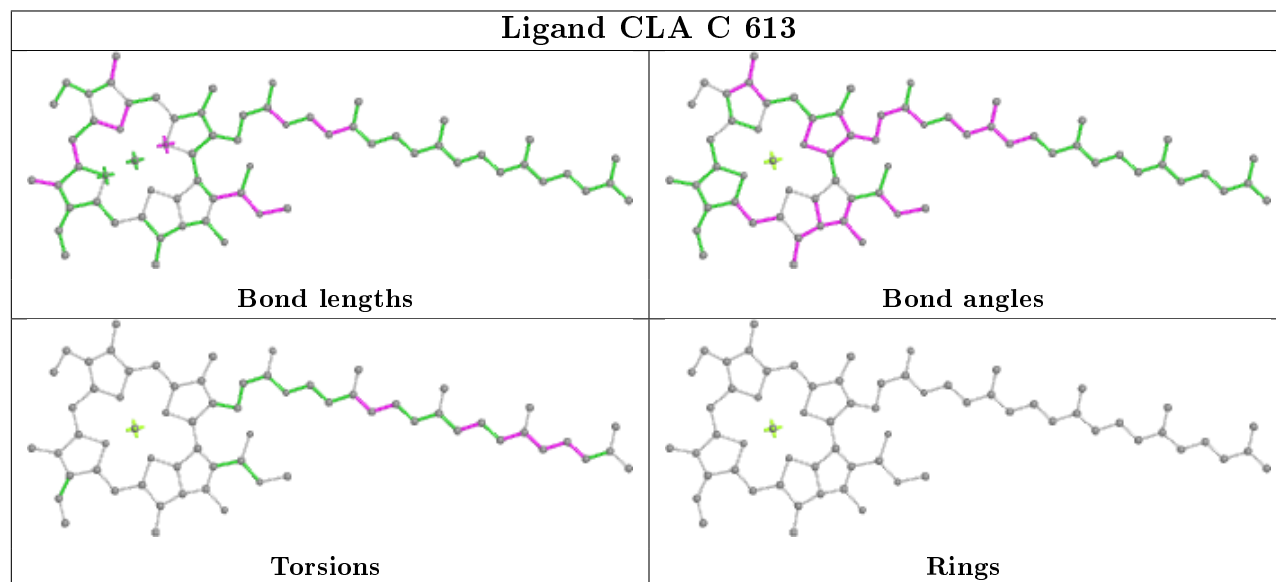
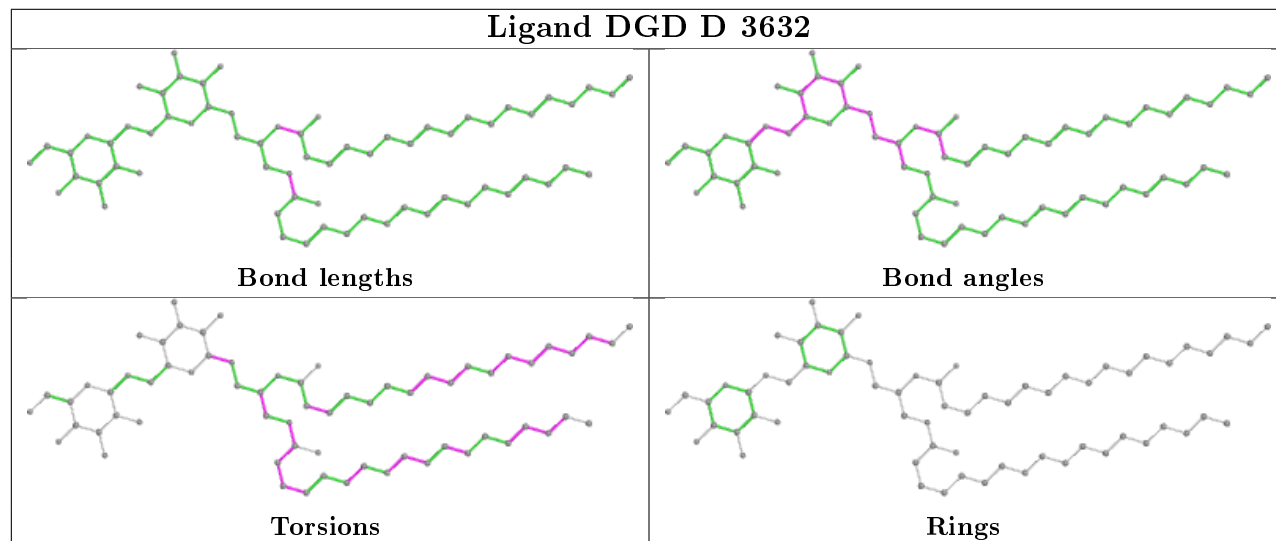
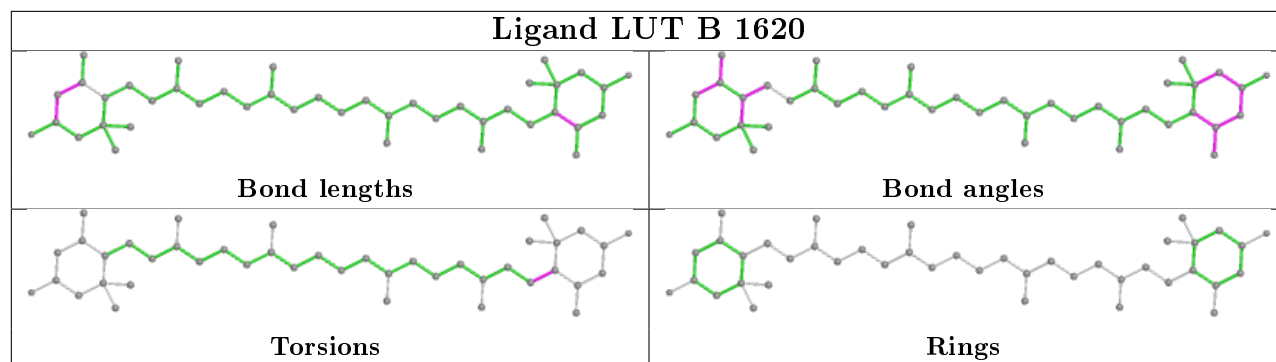


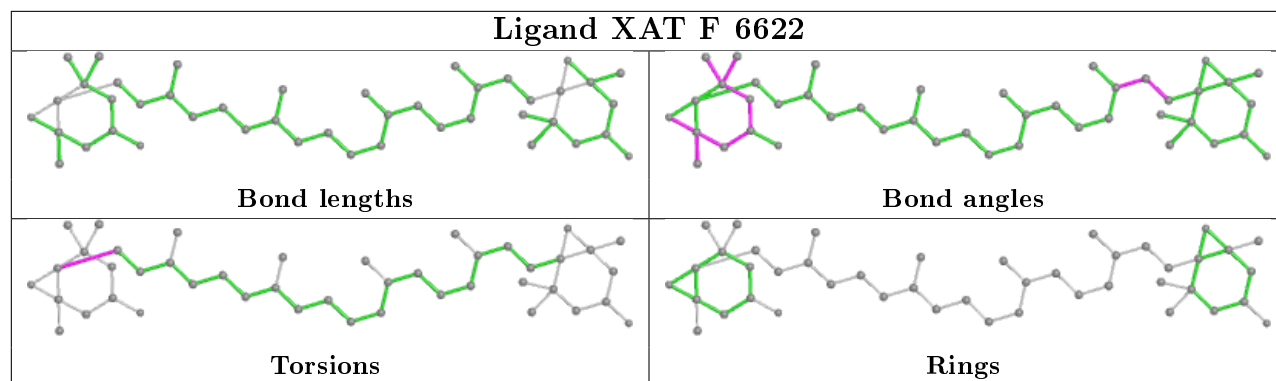
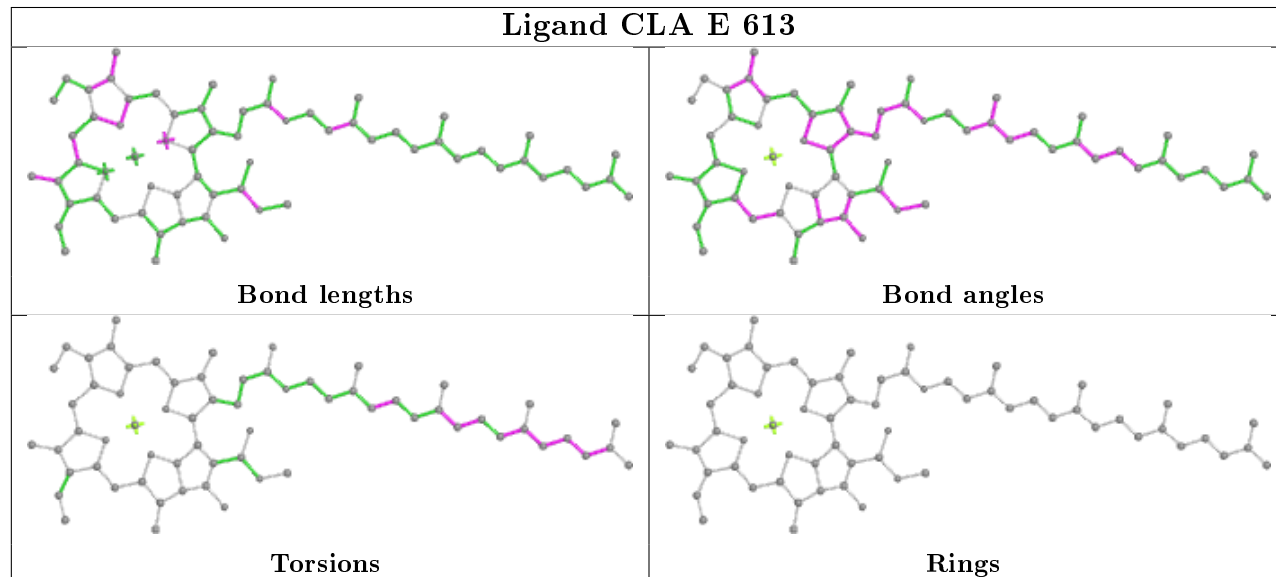
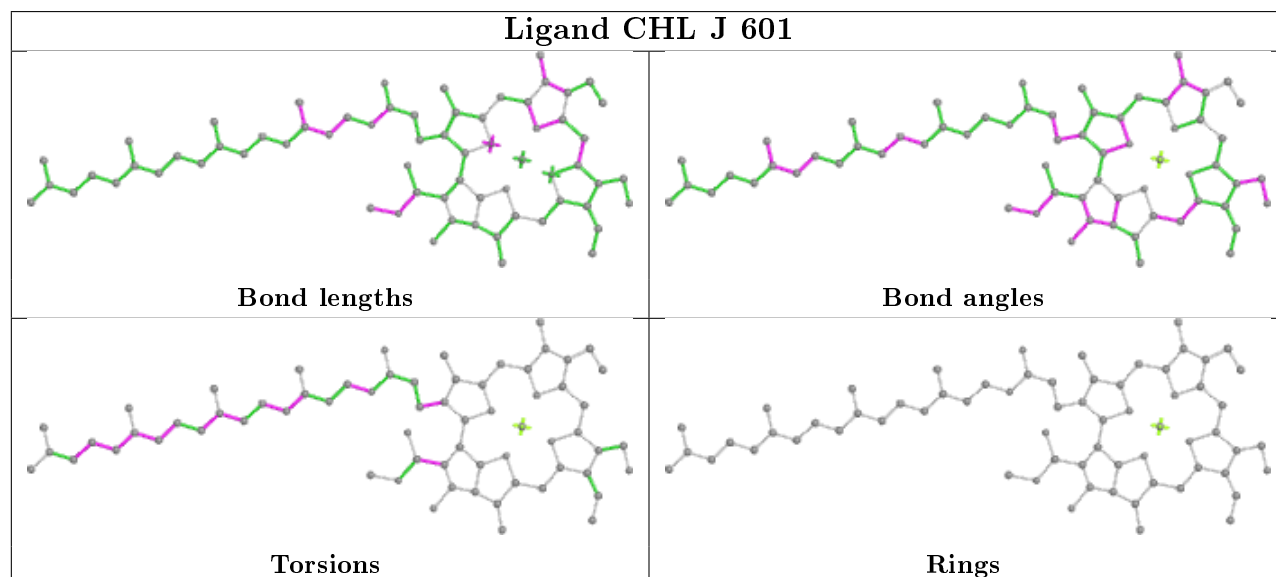
Ligand DGD H 6632



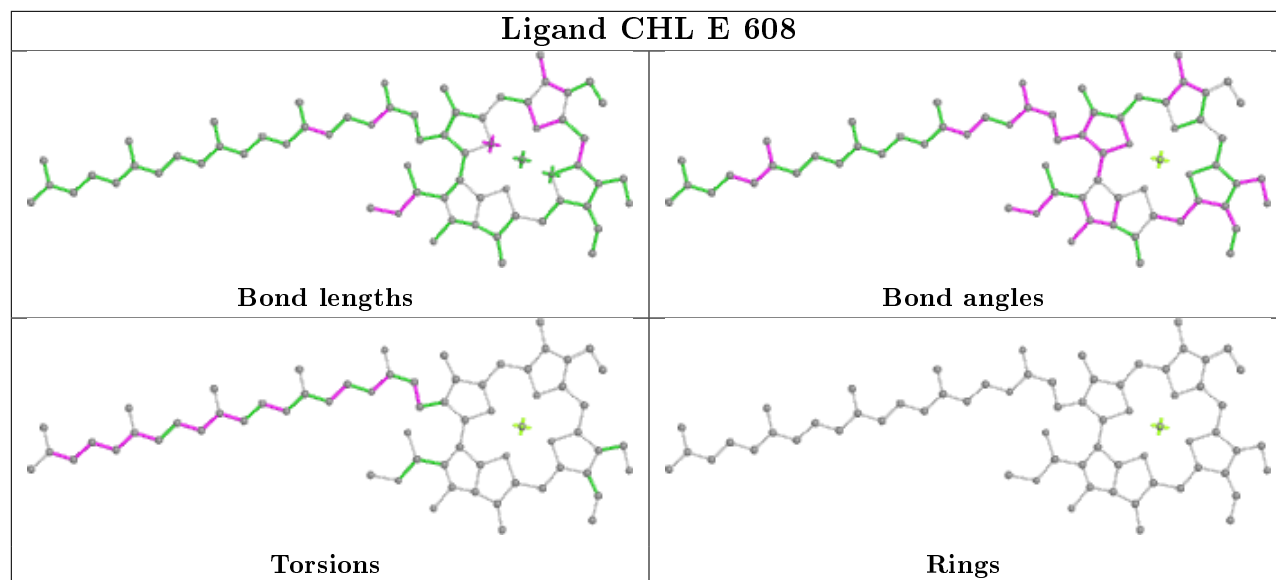
Ligand CLA H 613



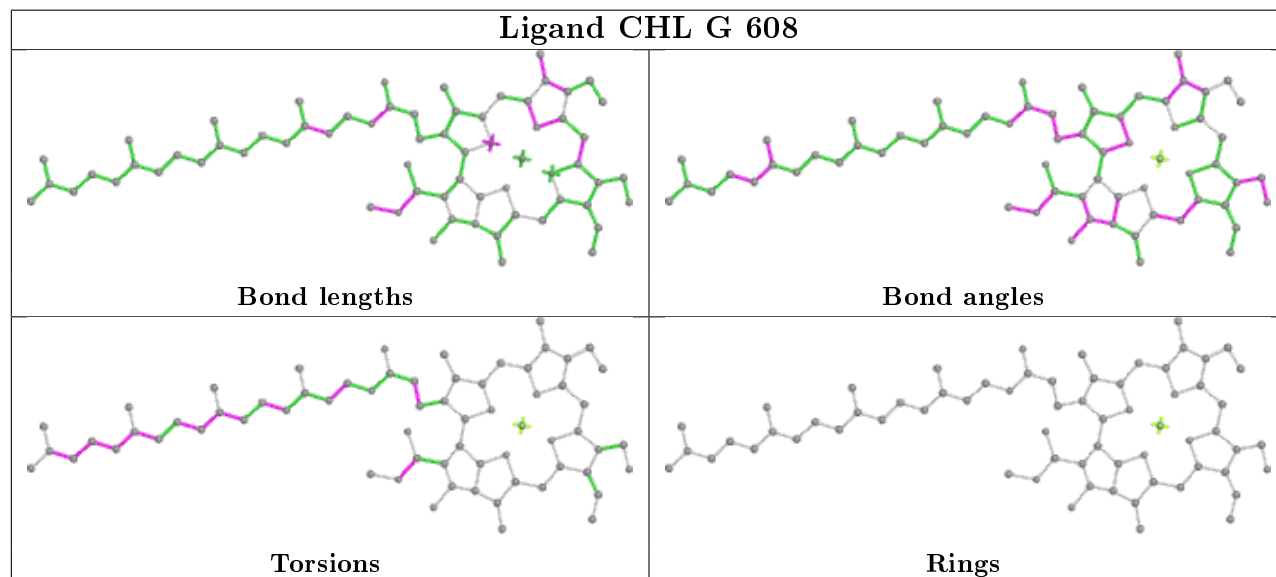


Ligand XAT F 6622**Ligand CLA E 613****Ligand CHL J 601**

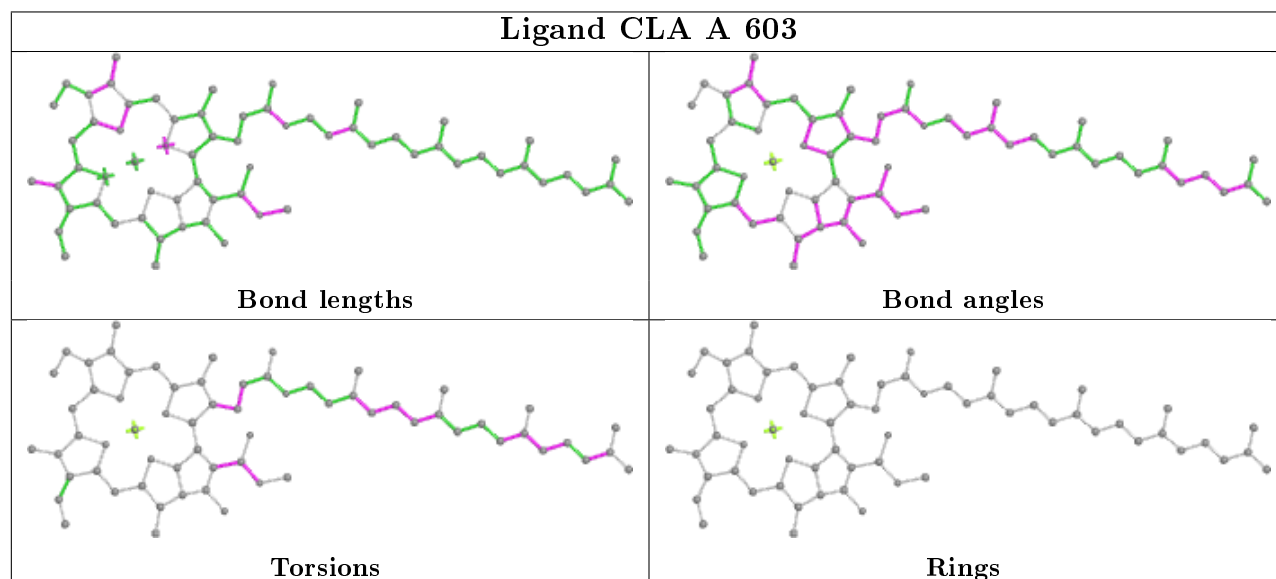
Ligand CHL E 608



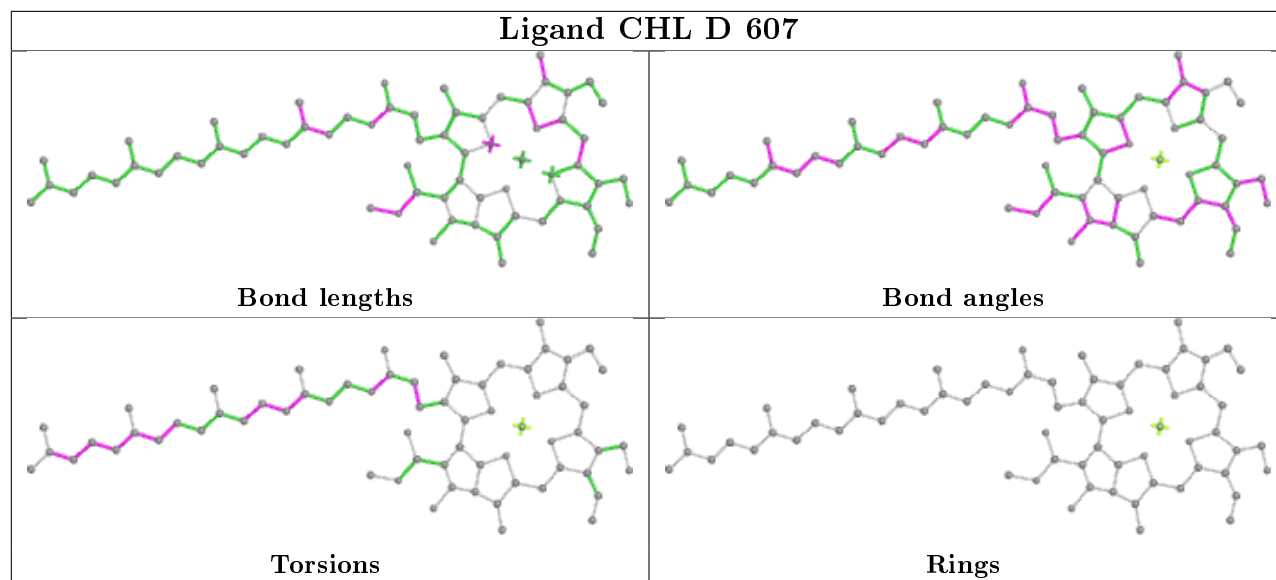
Ligand CHL G 608



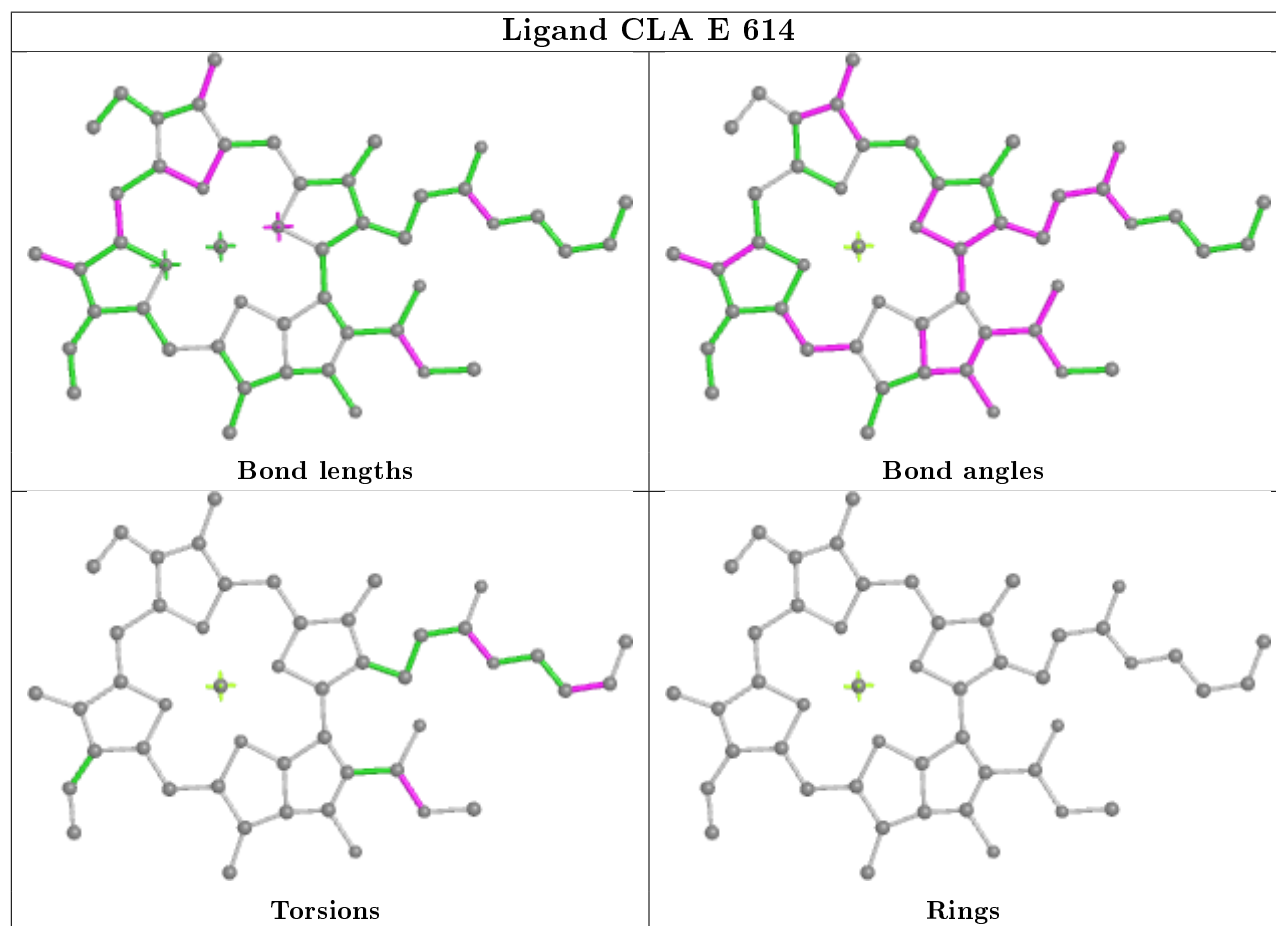
Ligand CLA A 603

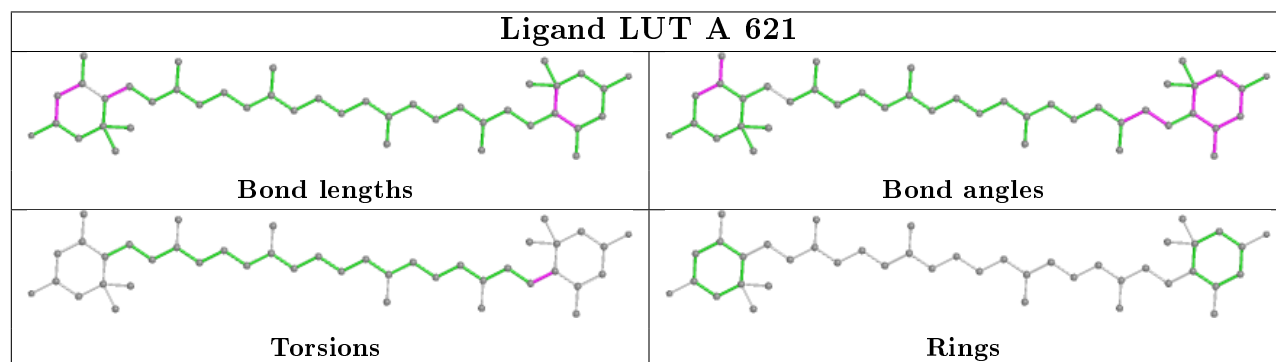
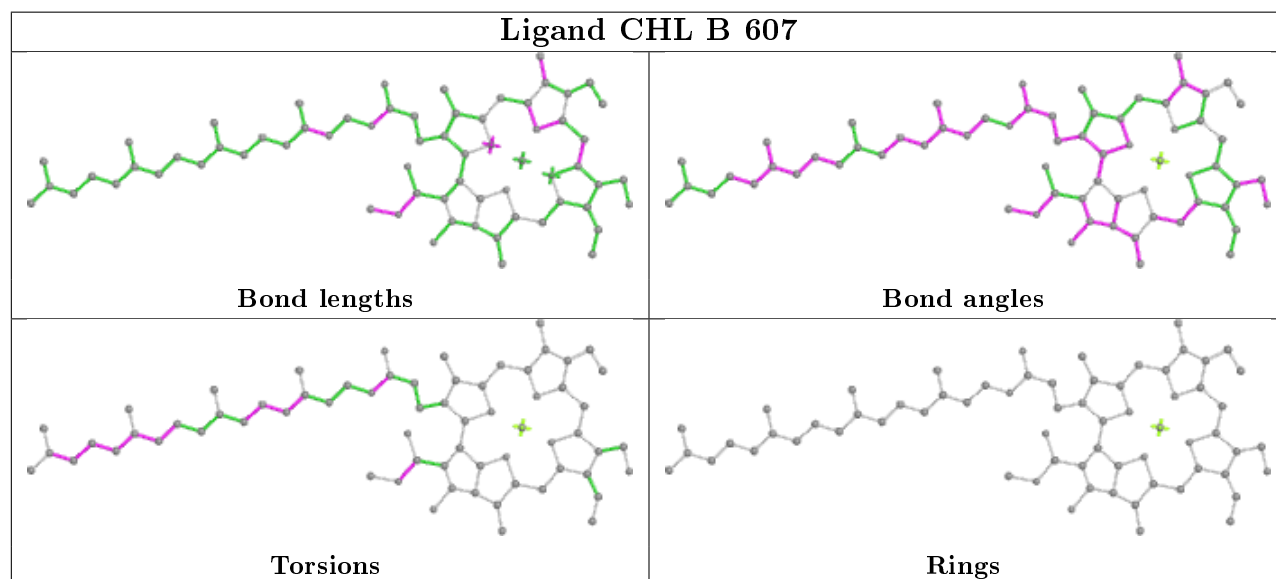
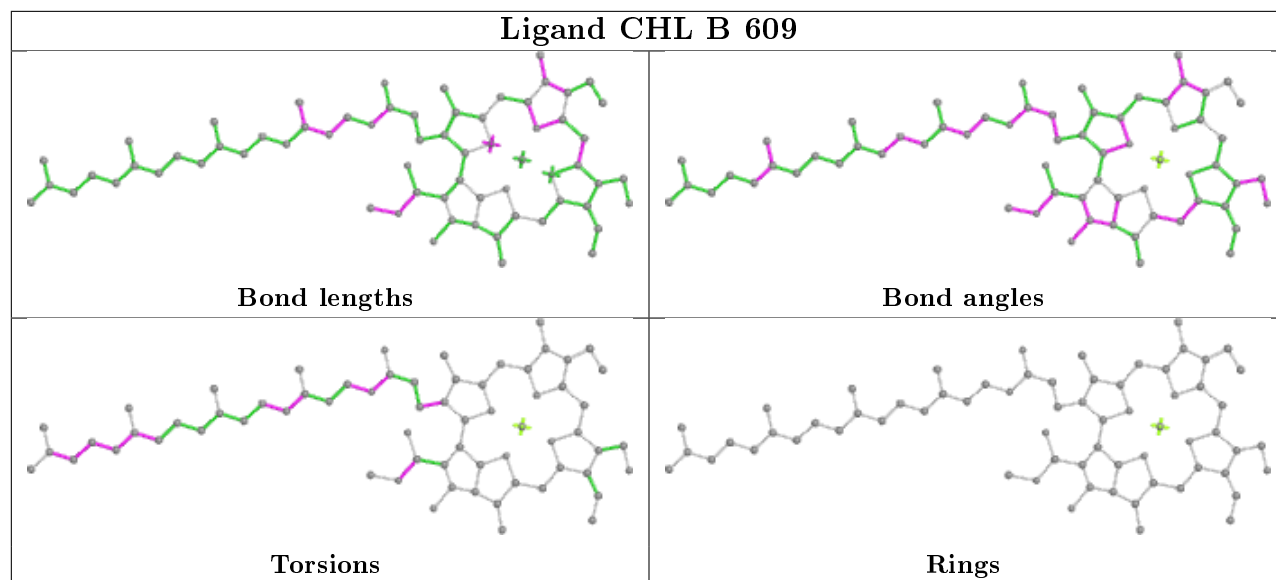


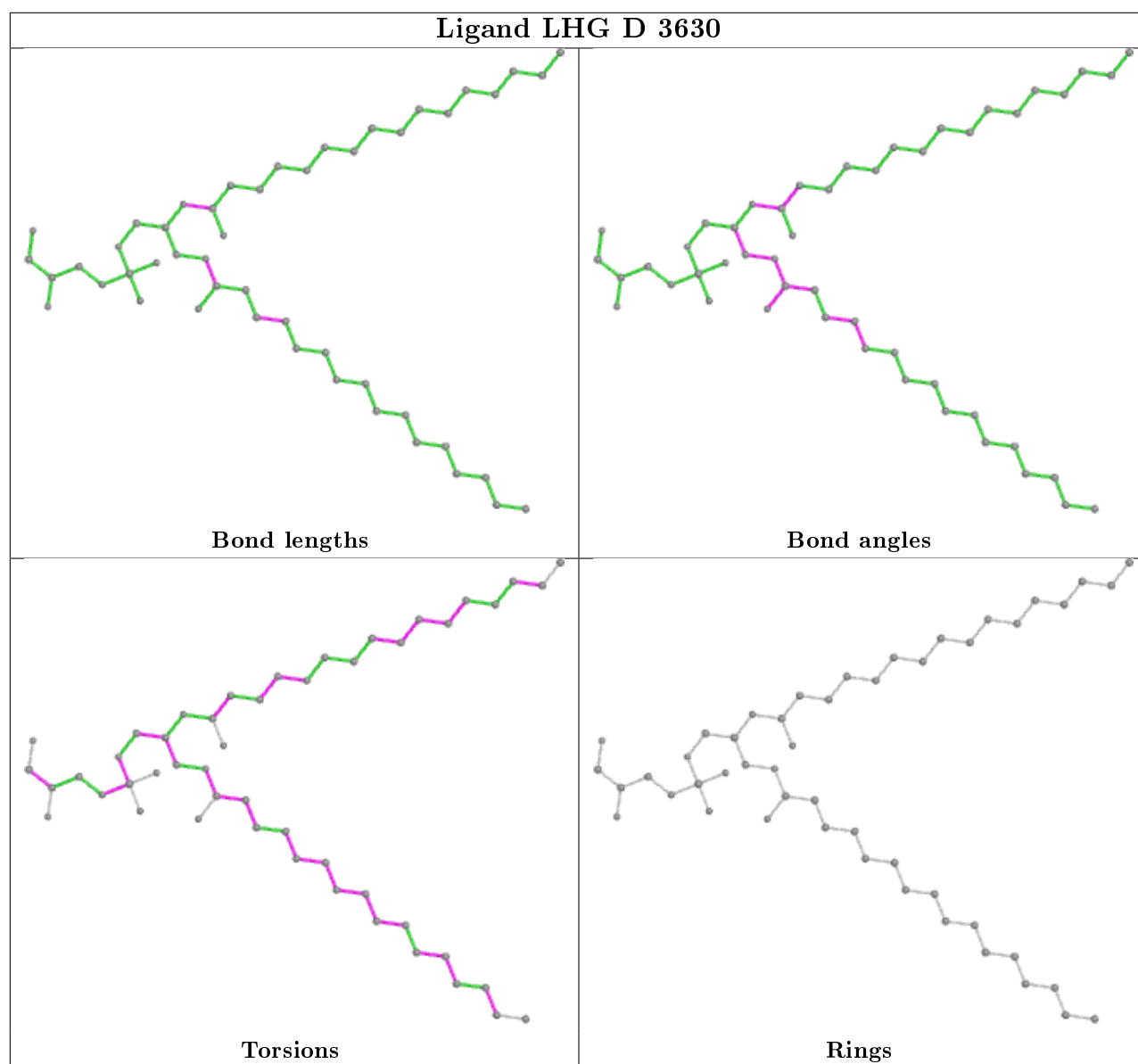
Ligand CHL D 607



Ligand CLA E 614







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/232 (93%)	-0.46	5 (2%) 60 62	18, 31, 53, 67	0
1	B	218/232 (93%)	-0.58	4 (1%) 68 70	15, 23, 42, 50	0
1	C	218/232 (93%)	-0.54	6 (2%) 53 54	14, 23, 40, 53	0
1	D	218/232 (93%)	-0.58	4 (1%) 68 70	16, 26, 44, 60	0
1	E	218/232 (93%)	-0.57	5 (2%) 60 62	14, 25, 41, 54	0
1	F	219/232 (94%)	-0.53	6 (2%) 54 55	14, 24, 42, 69	0
1	G	218/232 (93%)	-0.54	8 (3%) 41 41	16, 27, 47, 59	0
1	H	218/232 (93%)	-0.49	6 (2%) 53 54	18, 27, 49, 58	0
1	I	218/232 (93%)	-0.50	7 (3%) 47 48	17, 26, 45, 61	0
1	J	218/232 (93%)	-0.59	5 (2%) 60 62	15, 24, 42, 52	0
All	All	2181/2320 (94%)	-0.54	56 (2%) 56 57	14, 26, 46, 69	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	232	LYS	6.2
1	E	231	GLY	5.3
1	A	231	GLY	5.0
1	G	231	GLY	4.0
1	I	231	GLY	3.8
1	D	231	GLY	3.6
1	H	152	VAL	3.5
1	H	107	GLU	3.3
1	A	152	VAL	3.2
1	J	231	GLY	3.1
1	C	107	GLU	2.9
1	H	89	GLY	2.9
1	I	152	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	91	LYS	2.8
1	I	89	GLY	2.8
1	G	89	GLY	2.7
1	C	152	VAL	2.7
1	B	107	GLU	2.7
1	F	14	SER	2.7
1	C	89	GLY	2.6
1	J	168	ASP	2.6
1	D	89	GLY	2.6
1	A	168	ASP	2.6
1	H	231	GLY	2.6
1	D	107	GLU	2.5
1	A	107	GLU	2.5
1	G	88	ASN	2.5
1	E	89	GLY	2.5
1	E	168	ASP	2.5
1	H	91	LYS	2.5
1	J	152	VAL	2.4
1	F	88	ASN	2.4
1	B	20	ASP	2.4
1	E	88	ASN	2.4
1	J	88	ASN	2.4
1	E	107	GLU	2.3
1	G	31	GLU	2.3
1	F	168	ASP	2.2
1	G	107	GLU	2.2
1	H	31	GLU	2.2
1	B	88	ASN	2.2
1	A	20	ASP	2.2
1	C	168	ASP	2.2
1	J	107	GLU	2.2
1	I	20	ASP	2.2
1	G	19	PRO	2.2
1	F	107	GLU	2.2
1	I	31	GLU	2.2
1	I	165	GLY	2.2
1	F	89	GLY	2.1
1	G	170	PRO	2.1
1	I	91	LYS	2.1
1	B	89	GLY	2.1
1	C	91	LYS	2.1
1	C	231	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	171	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BNG	G	6633	21/21	0.61	0.43	75,96,102,104	0
2	BNG	D	3633	21/21	0.61	0.41	61,86,92,92	0
2	BNG	C	2633	21/21	0.62	0.36	59,85,92,93	0
2	BNG	A	633	21/21	0.63	0.34	72,92,95,96	0
2	BNG	E	4633	21/21	0.64	0.33	65,89,96,97	0
2	BNG	J	9633	21/21	0.64	0.36	63,83,92,93	0
2	BNG	H	7633	21/21	0.64	0.38	71,90,97,99	0
2	BNG	B	1633	21/21	0.66	0.36	63,86,92,93	0
2	BNG	F	5633	21/21	0.68	0.35	55,83,91,91	0
2	BNG	I	8633	21/21	0.70	0.35	67,86,93,93	0
6	NEX	H	7623	44/44	0.75	0.29	28,46,82,84	0
6	NEX	G	6623	44/44	0.76	0.28	30,42,80,82	0
6	NEX	J	9623	44/44	0.77	0.29	22,40,85,86	0
6	NEX	I	8623	44/44	0.78	0.27	27,36,77,80	0
6	NEX	D	3623	44/44	0.79	0.25	22,34,76,79	0
6	NEX	E	4623	44/44	0.80	0.25	16,30,74,76	0
6	NEX	A	623	44/44	0.80	0.25	27,53,90,91	0
6	NEX	B	1623	44/44	0.81	0.24	19,36,75,78	0
6	NEX	C	2623	44/44	0.83	0.25	17,35,85,87	0
6	NEX	F	5623	44/44	0.85	0.23	21,33,78,81	0
8	DGD	A	632	66/66	0.88	0.22	26,46,79,80	0
8	DGD	H	7632	66/66	0.88	0.22	30,50,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	DGD	G	9632	66/66	0.88	0.22	23,48,83,86	0
8	DGD	I	8632	66/66	0.89	0.24	24,49,85,86	0
8	DGD	D	5632	66/66	0.89	0.23	23,43,89,91	0
8	DGD	B	2632	66/66	0.89	0.22	21,44,77,79	0
8	DGD	E	4632	66/66	0.89	0.22	27,41,87,89	0
8	DGD	B	1632	66/66	0.89	0.22	20,45,80,82	0
8	DGD	H	6632	66/66	0.89	0.22	24,49,83,84	0
5	XAT	A	622	44/44	0.90	0.17	16,26,34,38	0
5	XAT	E	2622	44/44	0.90	0.16	16,22,27,30	0
10	CLA	A	611	65/65	0.90	0.19	40,48,78,78	0
8	DGD	D	3632	66/66	0.90	0.21	20,47,77,79	0
10	CLA	I	611	65/65	0.91	0.16	27,33,71,72	0
7	LHG	A	630	49/49	0.91	0.22	39,47,61,63	0
7	LHG	B	1630	49/49	0.91	0.21	32,40,55,60	0
10	CLA	D	611	65/65	0.91	0.18	25,34,65,66	0
10	CLA	H	611	65/65	0.91	0.17	33,39,71,72	0
10	CLA	G	611	65/65	0.91	0.18	33,39,75,77	0
5	XAT	B	5622	44/44	0.91	0.17	12,22,27,31	0
10	CLA	B	611	65/65	0.91	0.17	24,31,69,69	0
7	LHG	I	8630	49/49	0.92	0.19	29,34,55,57	0
3	NA	A	634	1/1	0.92	0.34	1,1,1,1	1
7	LHG	G	6630	49/49	0.92	0.20	31,38,57,61	0
5	XAT	D	8622	44/44	0.92	0.15	18,23,30,33	0
5	XAT	I	9622	44/44	0.92	0.15	15,22,29,32	0
5	XAT	C	7622	44/44	0.92	0.15	17,23,31,34	0
7	LHG	E	4630	49/49	0.92	0.21	28,37,52,55	0
10	CLA	E	611	65/65	0.92	0.17	26,32,70,72	0
5	XAT	H	4622	44/44	0.92	0.15	20,24,30,34	0
10	CLA	C	611	65/65	0.92	0.19	28,33,76,77	0
5	XAT	F	6622	44/44	0.92	0.15	15,22,29,32	0
7	LHG	D	3630	49/49	0.92	0.18	30,36,55,60	0
10	CLA	A	610	65/65	0.93	0.14	27,36,73,78	0
7	LHG	F	5630	49/49	0.93	0.19	25,33,48,52	0
10	CLA	J	611	65/65	0.93	0.15	20,26,68,69	0
9	CHL	A	601	66/66	0.93	0.16	31,36,39,43	0
10	CLA	F	611	65/65	0.93	0.15	20,26,73,75	0
9	CHL	J	606	51/66	0.93	0.16	16,22,60,62	0
5	XAT	B	1622	44/44	0.93	0.14	17,23,28,30	0
9	CHL	A	606	51/66	0.93	0.15	19,24,66,67	0
9	CHL	F	606	51/66	0.93	0.15	13,21,61,62	0
7	LHG	H	7630	49/49	0.93	0.20	30,37,57,62	0
7	LHG	J	9630	49/49	0.93	0.20	26,35,54,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	XAT	J	3622	44/44	0.93	0.14	17,24,29,31	0
10	CLA	J	604	62/65	0.93	0.16	15,22,72,76	0
9	CHL	G	605	48/66	0.93	0.15	24,27,59,75	0
10	CLA	B	604	62/65	0.93	0.17	19,22,75,78	0
7	LHG	C	2630	49/49	0.93	0.18	24,30,48,50	0
10	CLA	H	604	62/65	0.94	0.16	18,25,69,74	0
9	CHL	D	606	51/66	0.94	0.16	16,22,60,61	0
10	CLA	E	604	62/65	0.94	0.16	18,23,75,79	0
9	CHL	B	605	48/66	0.94	0.16	23,26,58,74	0
10	CLA	G	612	65/65	0.94	0.16	22,33,89,91	0
10	CLA	H	612	65/65	0.94	0.17	24,34,86,87	0
9	CHL	C	605	48/66	0.94	0.15	25,29,58,72	0
10	CLA	G	604	62/65	0.94	0.15	17,24,75,79	0
9	CHL	H	605	48/66	0.94	0.14	24,30,60,73	0
10	CLA	A	604	62/65	0.94	0.16	18,25,74,79	0
9	CHL	H	606	51/66	0.94	0.14	17,22,67,69	0
9	CHL	I	605	48/66	0.94	0.15	29,32,60,73	0
10	CLA	C	612	65/65	0.94	0.15	20,31,82,85	0
10	CLA	F	612	65/65	0.94	0.15	22,28,79,81	0
10	CLA	I	610	65/65	0.94	0.14	21,26,62,68	0
9	CHL	C	606	51/66	0.94	0.15	16,22,63,64	0
9	CHL	E	606	51/66	0.94	0.15	18,21,60,62	0
9	CHL	I	606	51/66	0.94	0.14	15,19,62,64	0
10	CLA	F	604	62/65	0.94	0.16	17,21,76,81	0
10	CLA	A	612	65/65	0.94	0.16	33,38,86,88	0
10	CLA	C	604	62/65	0.94	0.15	15,21,70,75	0
10	CLA	I	604	62/65	0.94	0.17	20,25,77,81	0
10	CLA	H	610	65/65	0.94	0.15	24,32,69,74	0
9	CHL	F	605	48/66	0.94	0.13	26,29,59,72	0
9	CHL	G	608	66/66	0.94	0.14	27,31,67,68	0
10	CLA	I	612	65/65	0.94	0.15	23,30,87,90	0
9	CHL	I	608	66/66	0.95	0.13	21,26,66,67	0
9	CHL	G	601	66/66	0.95	0.14	27,32,36,40	0
10	CLA	J	610	65/65	0.95	0.12	18,24,64,67	0
4	LUT	G	6620	42/42	0.95	0.14	16,25,36,37	0
9	CHL	F	608	66/66	0.95	0.13	22,28,63,65	0
9	CHL	D	605	48/66	0.95	0.15	23,29,57,71	0
10	CLA	C	610	65/65	0.95	0.13	15,21,65,70	0
9	CHL	A	607	66/66	0.95	0.13	17,20,48,49	0
9	CHL	B	606	51/66	0.95	0.14	11,20,60,62	0
9	CHL	I	601	66/66	0.95	0.14	22,26,34,35	0
10	CLA	I	614	49/65	0.95	0.14	20,23,58,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	CLA	G	603	65/65	0.95	0.12	17,22,69,71	0
9	CHL	A	605	48/66	0.95	0.15	19,25,57,71	0
9	CHL	E	605	48/66	0.95	0.15	20,25,58,71	0
10	CLA	B	614	49/65	0.95	0.11	10,22,59,69	0
10	CLA	D	612	65/65	0.95	0.14	22,30,83,85	0
9	CHL	G	606	51/66	0.95	0.14	15,23,59,60	0
10	CLA	E	612	65/65	0.95	0.12	19,25,80,82	0
9	CHL	J	608	66/66	0.95	0.14	19,26,67,68	0
9	CHL	H	601	66/66	0.95	0.14	28,31,32,36	0
9	CHL	B	608	66/66	0.95	0.12	16,22,63,63	0
9	CHL	H	608	66/66	0.95	0.15	28,31,69,72	0
10	CLA	H	614	49/65	0.95	0.12	16,26,60,68	0
9	CHL	B	601	66/66	0.95	0.14	22,26,37,38	0
9	CHL	J	605	48/66	0.95	0.13	20,26,59,71	0
10	CLA	J	614	49/65	0.95	0.13	14,22,57,67	0
10	CLA	B	612	65/65	0.95	0.13	18,27,88,89	0
10	CLA	A	614	49/65	0.95	0.13	20,27,59,66	0
9	CHL	C	608	66/66	0.95	0.13	23,28,60,61	0
10	CLA	E	610	65/65	0.95	0.13	17,25,59,66	0
9	CHL	D	608	66/66	0.95	0.14	24,29,65,67	0
10	CLA	D	604	62/65	0.95	0.16	20,25,66,70	0
10	CLA	G	610	65/65	0.95	0.14	24,31,73,79	0
10	CLA	F	610	65/65	0.95	0.12	15,20,63,68	0
9	CHL	E	601	66/66	0.95	0.14	23,28,31,33	0
10	CLA	A	603	65/65	0.95	0.11	20,26,77,78	0
9	CHL	A	608	66/66	0.95	0.12	30,35,67,68	0
10	CLA	I	603	65/65	0.96	0.11	16,20,64,65	0
9	CHL	J	607	66/66	0.96	0.12	12,17,45,47	0
10	CLA	B	610	65/65	0.96	0.12	19,25,62,68	0
10	CLA	G	613	65/65	0.96	0.13	14,17,55,56	0
10	CLA	F	614	49/65	0.96	0.11	12,20,57,68	0
10	CLA	C	614	49/65	0.96	0.11	14,18,54,65	0
10	CLA	E	602	65/65	0.96	0.15	13,20,48,49	0
10	CLA	E	603	65/65	0.96	0.11	11,20,73,74	0
10	CLA	D	610	65/65	0.96	0.12	21,26,64,69	0
4	LUT	I	8620	42/42	0.96	0.13	15,23,35,36	0
10	CLA	G	602	65/65	0.96	0.14	17,21,44,46	0
10	CLA	I	602	65/65	0.96	0.15	17,21,52,57	0
10	CLA	H	602	65/65	0.96	0.16	20,23,47,48	0
4	LUT	C	2620	42/42	0.96	0.14	18,23,28,29	0
10	CLA	J	602	65/65	0.96	0.16	12,17,47,48	0
10	CLA	G	614	49/65	0.96	0.12	12,22,58,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	LUT	D	3621	42/42	0.96	0.17	11,19,23,23	0
10	CLA	B	603	65/65	0.96	0.12	10,19,74,76	0
9	CHL	D	601	66/66	0.96	0.13	22,27,30,32	0
9	CHL	F	601	66/66	0.96	0.14	22,24,32,33	0
10	CLA	J	603	65/65	0.96	0.11	13,20,71,72	0
10	CLA	A	602	65/65	0.96	0.15	20,30,52,54	0
10	CLA	D	603	65/65	0.96	0.10	14,21,74,75	0
9	CHL	A	609	66/66	0.96	0.12	23,27,50,54	0
10	CLA	H	603	65/65	0.96	0.11	15,19,78,79	0
4	LUT	B	1621	42/42	0.96	0.14	8,14,23,25	0
9	CHL	C	601	66/66	0.96	0.13	17,22,32,33	0
10	CLA	D	614	49/65	0.96	0.12	10,21,54,64	0
9	CHL	E	607	66/66	0.96	0.13	16,20,51,51	0
4	LUT	A	620	42/42	0.96	0.12	19,26,38,39	0
4	LUT	H	7620	42/42	0.96	0.12	16,22,35,36	0
4	LUT	D	3620	42/42	0.96	0.13	18,24,35,36	0
9	CHL	J	601	66/66	0.96	0.14	19,23,29,33	0
9	CHL	E	608	66/66	0.96	0.12	14,19,67,69	0
10	CLA	J	612	65/65	0.96	0.14	18,25,79,82	0
9	CHL	F	607	66/66	0.96	0.12	13,19,41,43	0
10	CLA	E	614	49/65	0.96	0.12	15,23,57,68	0
10	CLA	F	603	65/65	0.96	0.11	14,22,74,77	0
10	CLA	F	602	65/65	0.97	0.14	9,17,42,48	0
9	CHL	G	609	66/66	0.97	0.12	18,25,42,46	0
10	CLA	C	603	65/65	0.97	0.11	12,18,76,78	0
9	CHL	I	607	66/66	0.97	0.11	11,17,53,56	0
4	LUT	I	8621	42/42	0.97	0.14	12,20,22,24	0
9	CHL	D	609	66/66	0.97	0.10	18,23,42,46	0
4	LUT	J	9621	42/42	0.97	0.14	14,19,21,24	0
9	CHL	F	609	66/66	0.97	0.11	14,22,43,47	0
10	CLA	D	602	65/65	0.97	0.14	13,20,45,46	0
4	LUT	F	5621	42/42	0.97	0.14	11,19,22,24	0
4	LUT	G	6621	42/42	0.97	0.15	16,21,23,25	0
10	CLA	I	613	65/65	0.97	0.12	15,19,49,51	0
9	CHL	J	609	66/66	0.97	0.11	13,19,39,43	0
4	LUT	H	7621	42/42	0.97	0.15	13,20,24,25	0
10	CLA	J	613	65/65	0.97	0.12	11,17,56,59	0
4	LUT	F	5620	42/42	0.97	0.12	15,22,26,26	0
4	LUT	C	2621	42/42	0.97	0.14	13,18,21,22	0
4	LUT	J	9620	42/42	0.97	0.10	11,18,34,35	0
9	CHL	C	607	66/66	0.97	0.12	15,18,46,49	0
9	CHL	H	607	66/66	0.97	0.12	12,18,49,50	0

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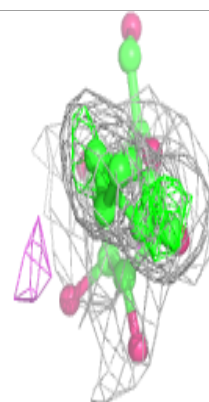
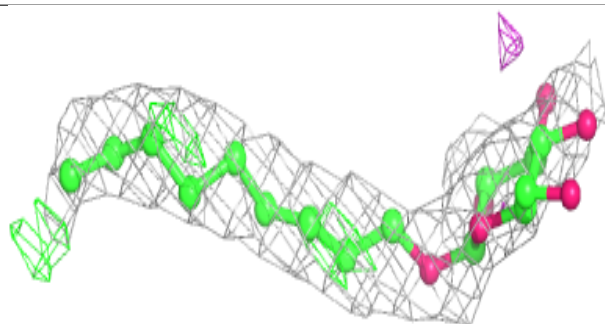
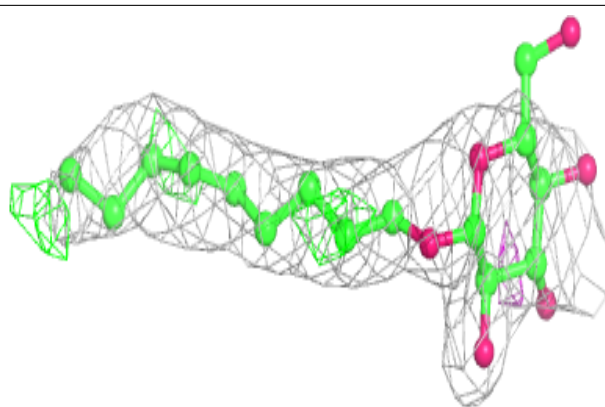
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	CHL	E	609	66/66	0.97	0.11	16,19,40,43	0
10	CLA	C	602	65/65	0.97	0.15	10,19,38,39	0
10	CLA	B	613	65/65	0.97	0.13	13,17,52,56	0
10	CLA	B	602	65/65	0.97	0.14	16,21,51,54	0
10	CLA	H	613	65/65	0.97	0.12	10,17,55,57	0
4	LUT	B	1620	42/42	0.97	0.11	13,19,30,30	0
10	CLA	F	613	65/65	0.97	0.12	14,17,45,48	0
10	CLA	C	613	65/65	0.97	0.11	13,15,43,47	0
4	LUT	E	4620	42/42	0.97	0.10	16,21,29,30	0
10	CLA	E	613	65/65	0.97	0.12	15,18,54,57	0
10	CLA	D	613	65/65	0.97	0.12	15,18,50,52	0
9	CHL	I	609	66/66	0.97	0.12	17,20,45,50	0
9	CHL	C	609	66/66	0.97	0.10	15,22,41,42	0
9	CHL	G	607	66/66	0.97	0.13	15,17,49,51	0
9	CHL	D	607	66/66	0.97	0.12	11,14,52,57	0
9	CHL	H	609	66/66	0.97	0.11	21,26,45,51	0
9	CHL	B	609	66/66	0.97	0.11	14,20,43,47	0
9	CHL	B	607	66/66	0.97	0.12	13,16,44,45	0
4	LUT	A	621	42/42	0.97	0.15	17,20,25,26	0
10	CLA	A	613	65/65	0.97	0.13	15,19,46,49	0
4	LUT	E	4621	42/42	0.98	0.14	11,16,22,24	0

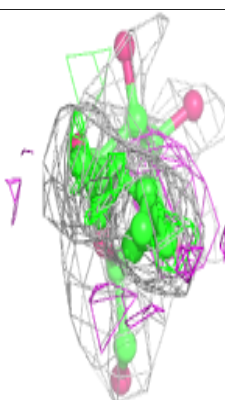
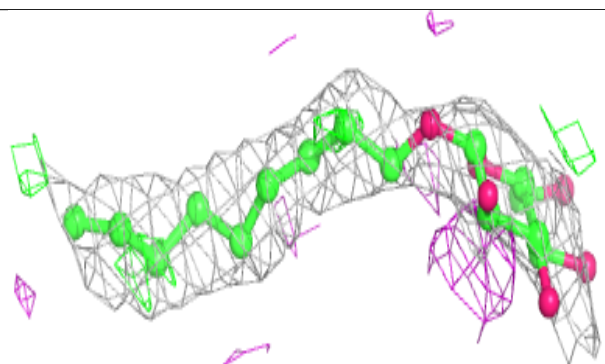
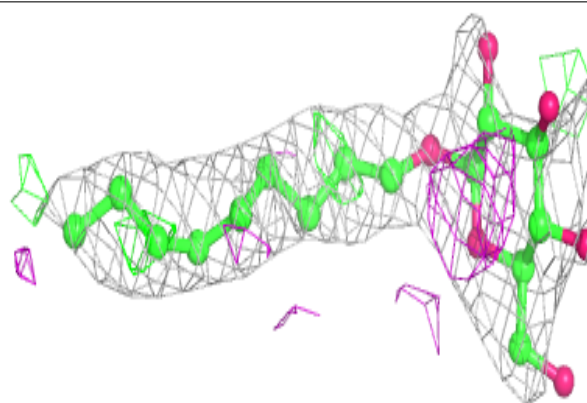
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BNG 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)

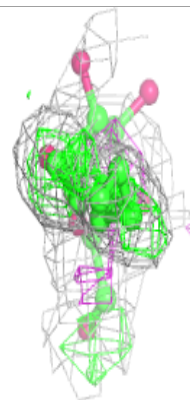
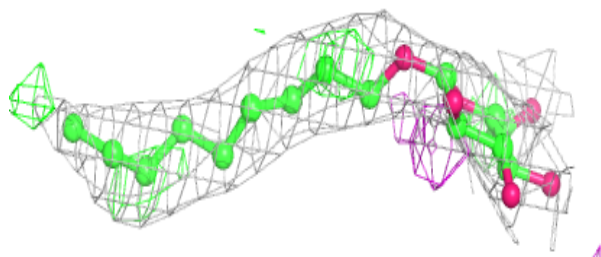
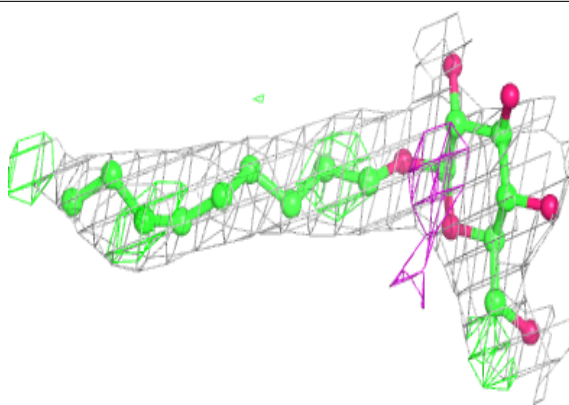
**Electron density around BNG D 3633:**

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

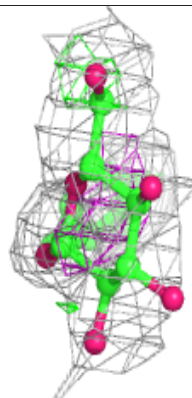
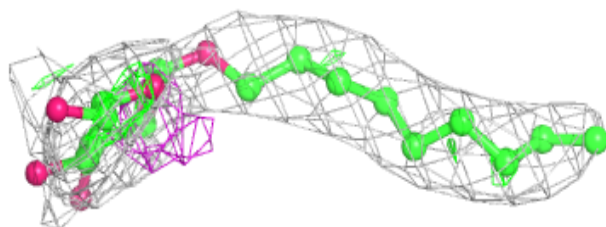
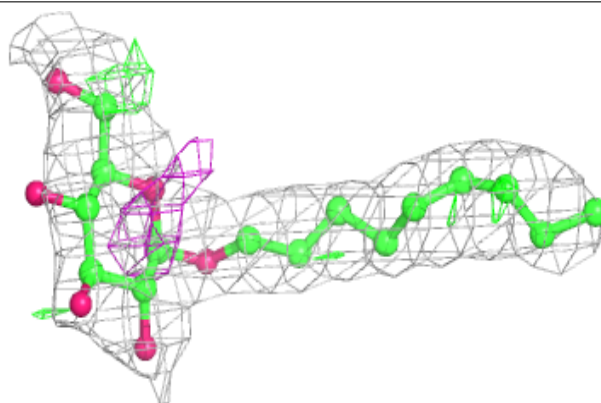


Electron density around BNG C 2633:

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

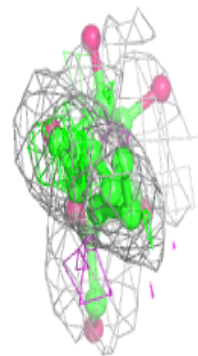
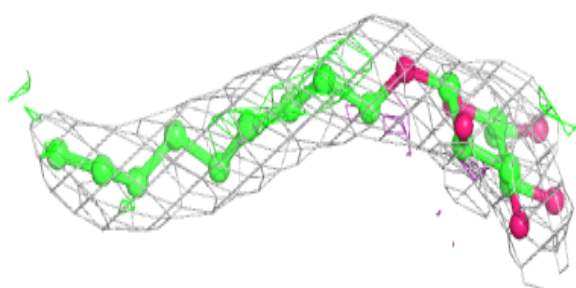
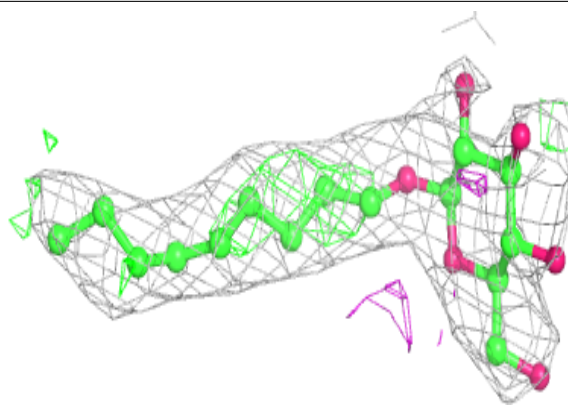
**Electron density around BNG A 633:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

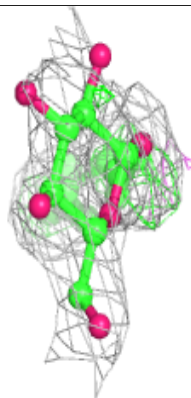
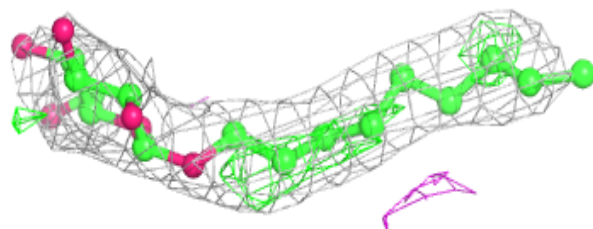
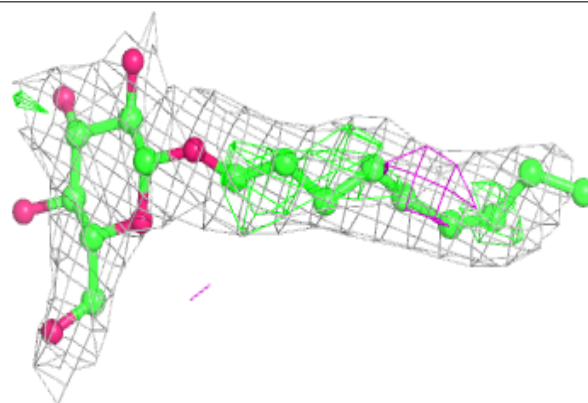


Electron density around BNG E 4633:

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

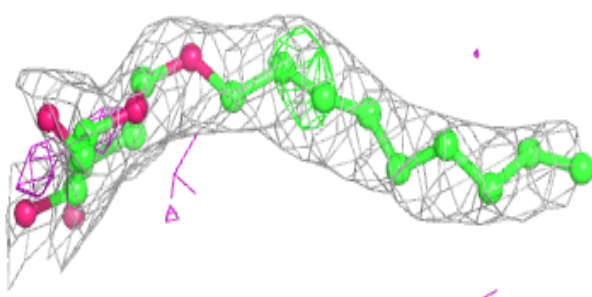
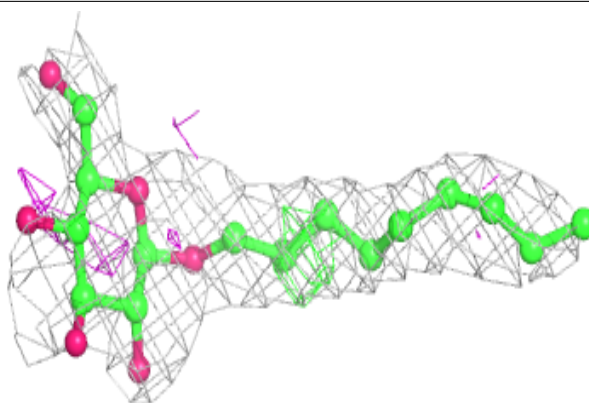
**Electron density around BNG J 9633:**

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

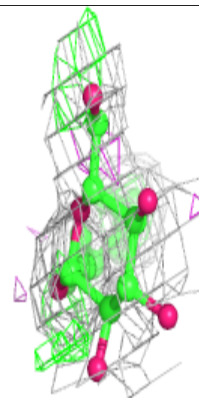
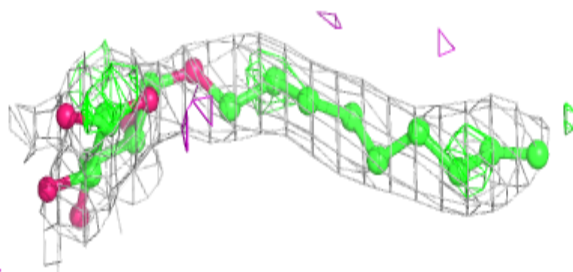
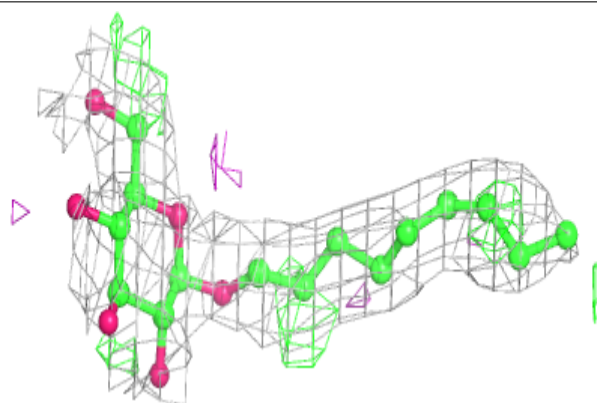


Electron density around BNG H 7633:

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

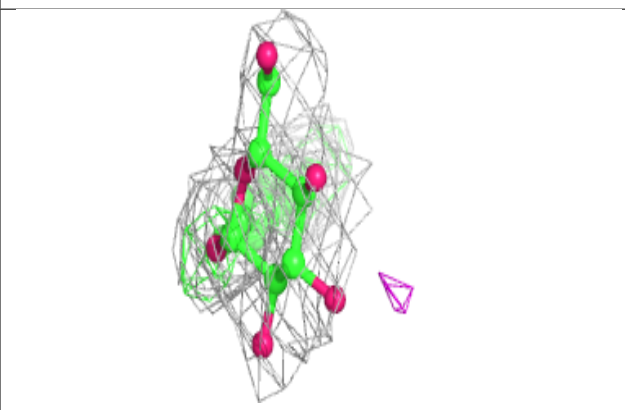
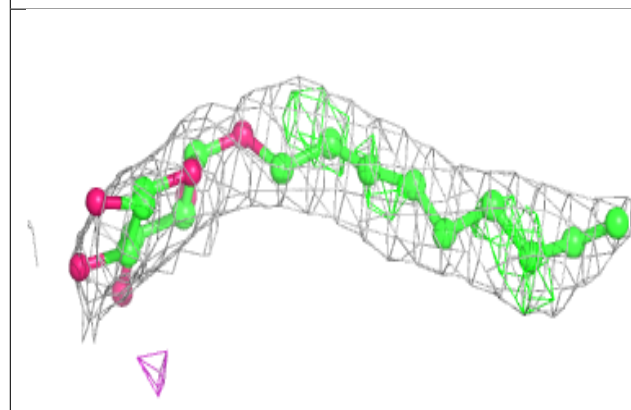
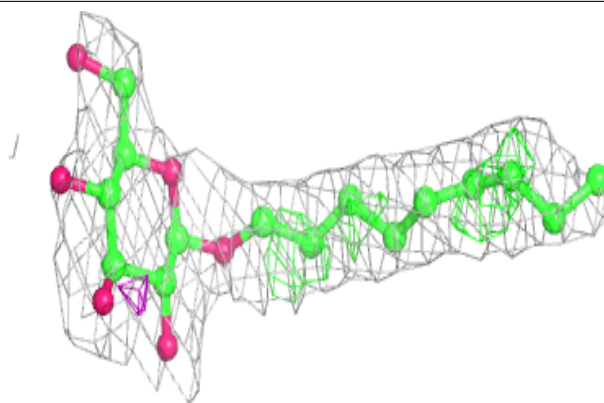
**Electron density around BNG B 1633:**

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

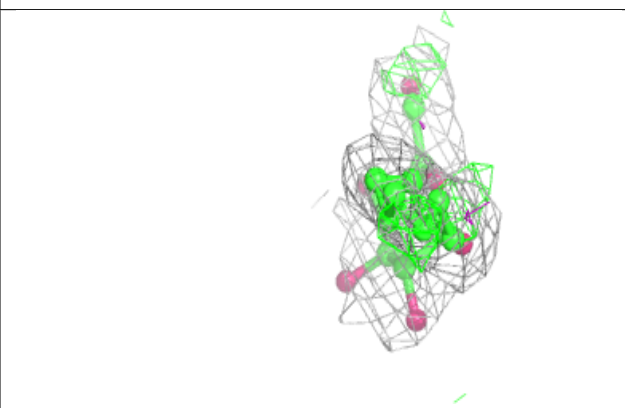
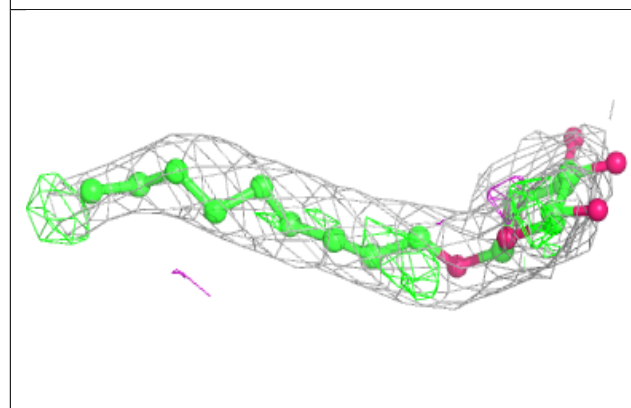
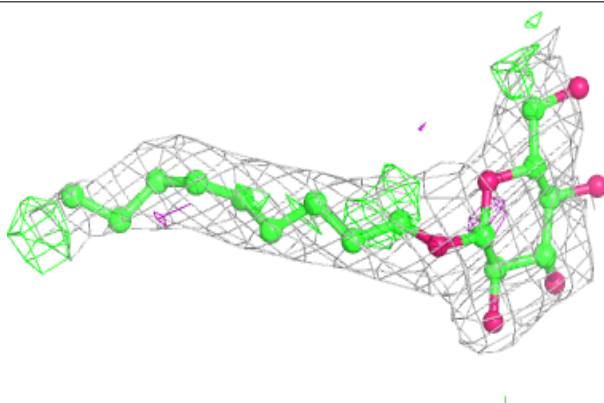


Electron density around BNG F 5633:

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

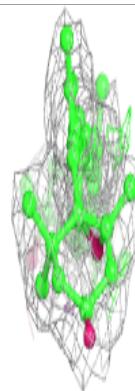
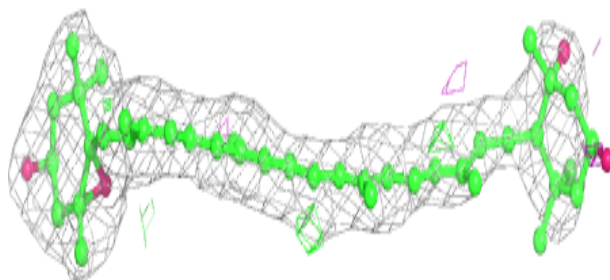
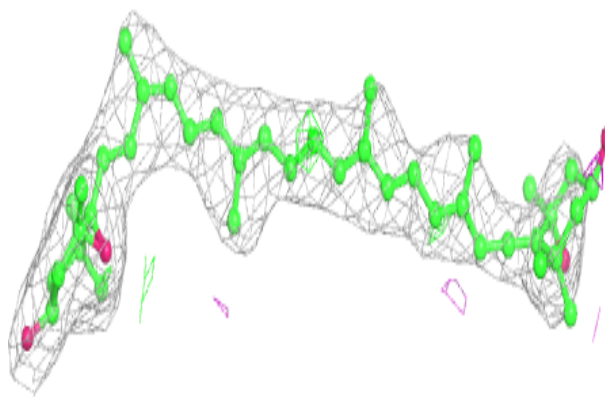
**Electron density around BNG I 8633:**

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

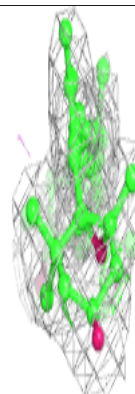
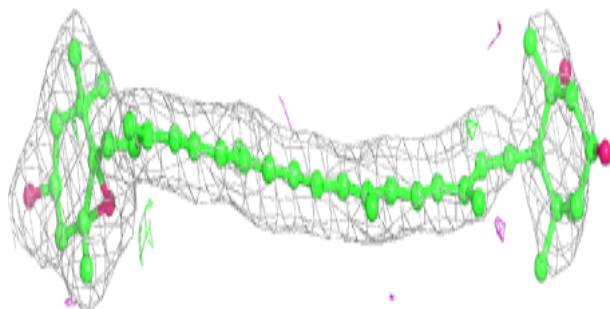
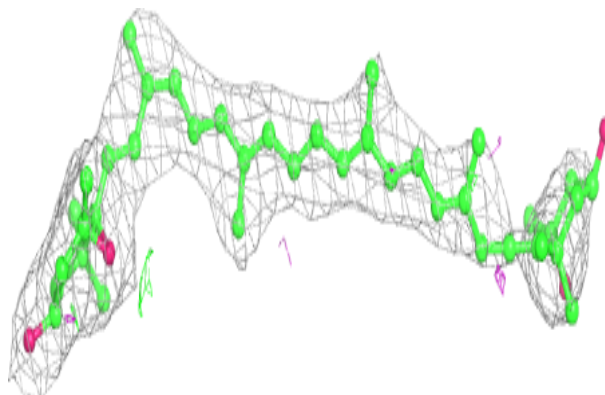


Electron density around NEX H 7623:

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

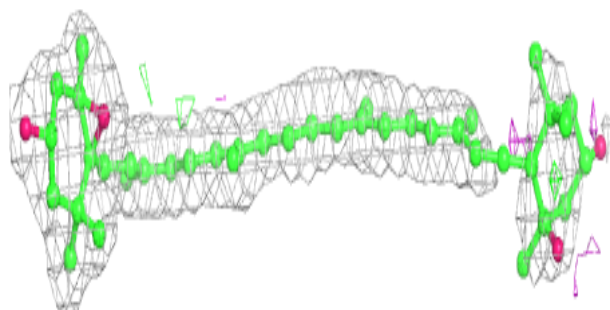
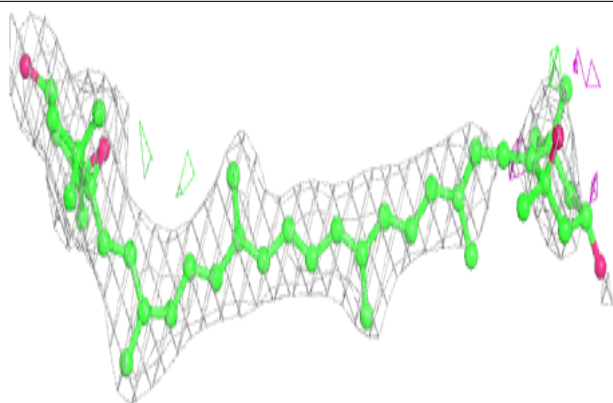
**Electron density around NEX G 6623:**

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

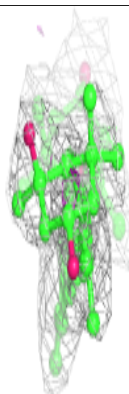
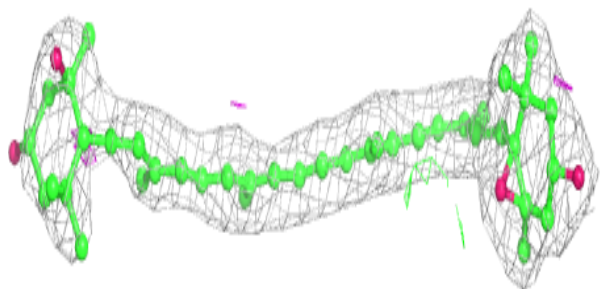
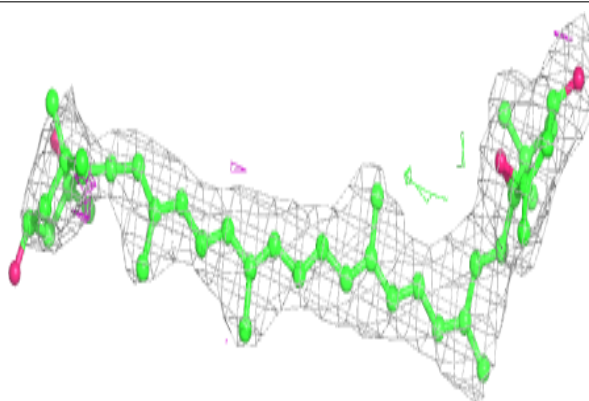


Electron density around NEX J 9623:

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

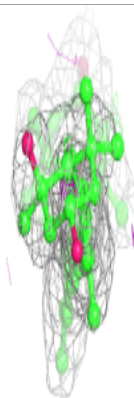
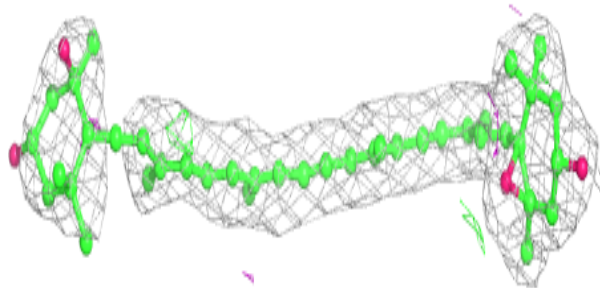
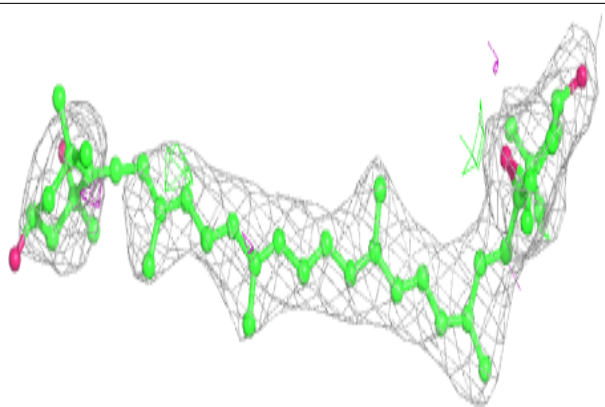
**Electron density around NEX I 8623:**

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

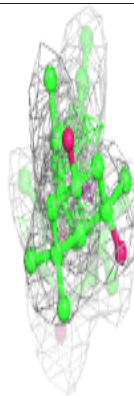
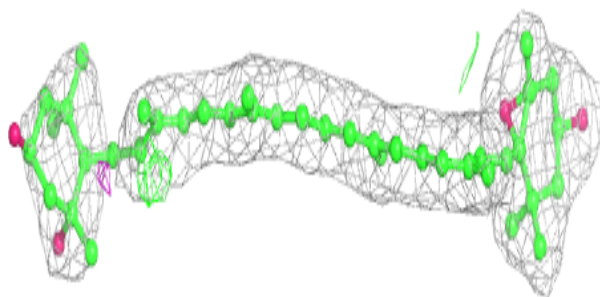
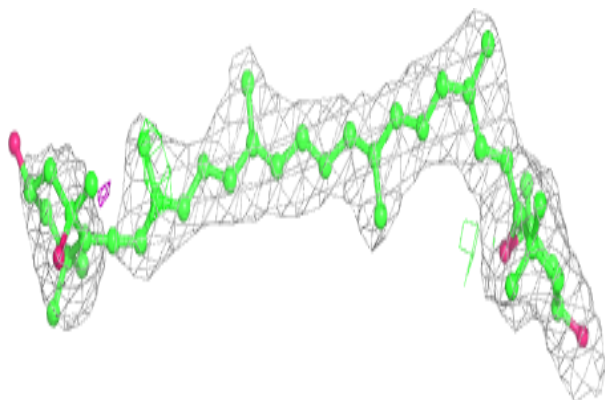


Electron density around NEX D 3623:

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

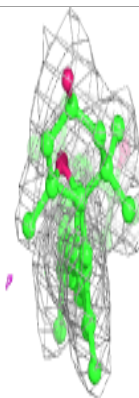
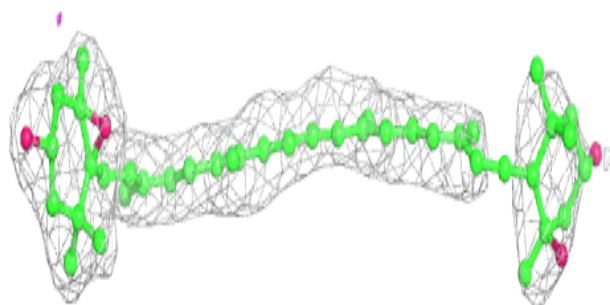
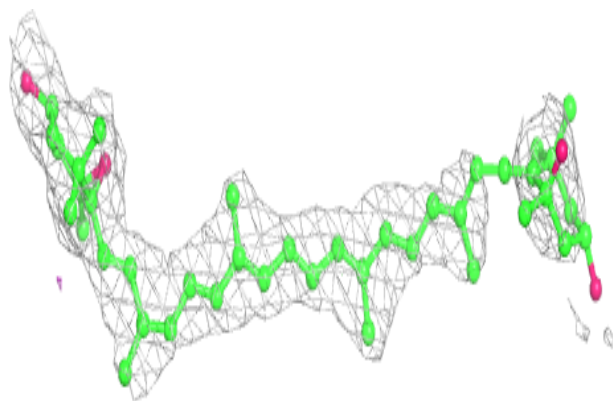
**Electron density around NEX E 4623:**

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

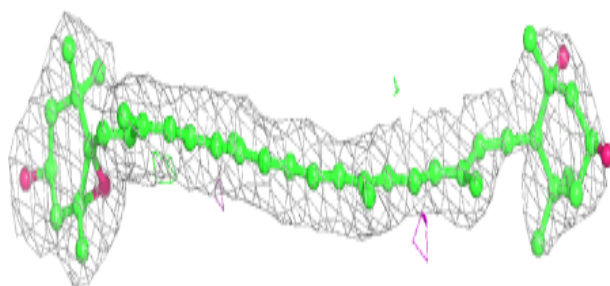
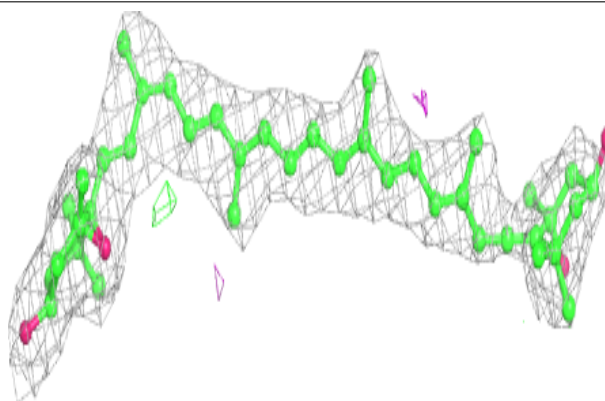


Electron density around NEX A 623:

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

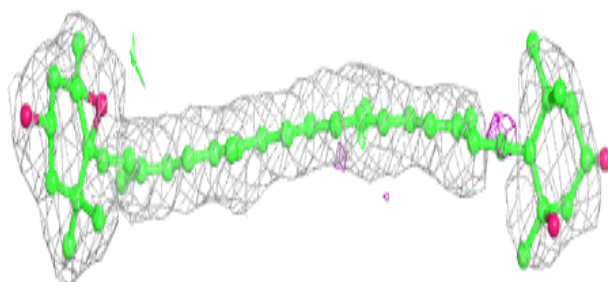
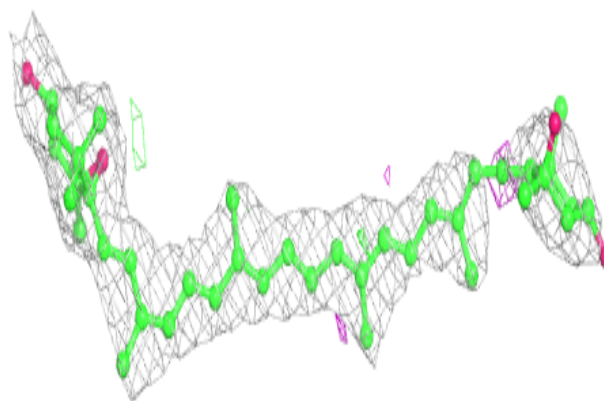
**Electron density around NEX B 1623:**

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

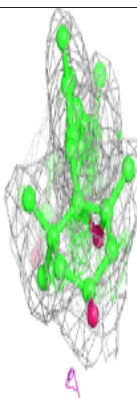
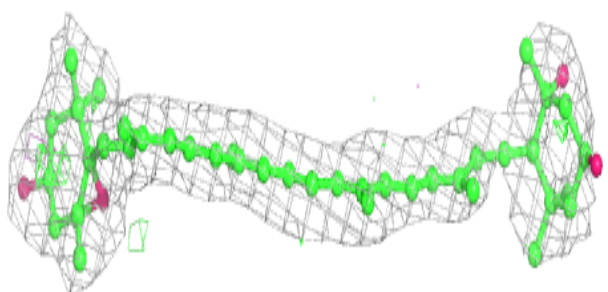
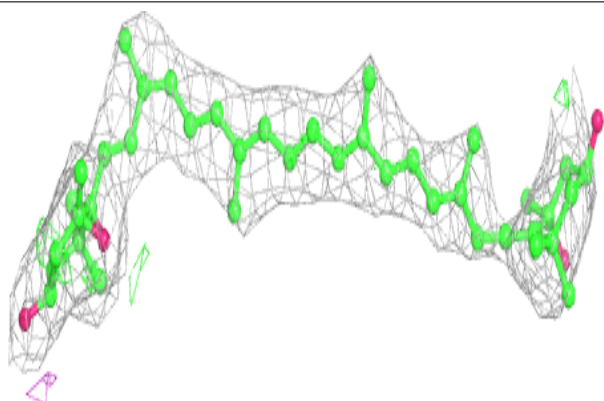


Electron density around NEX C 2623:

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

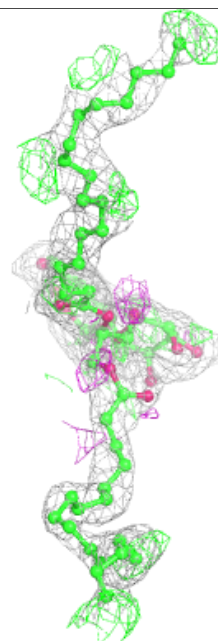
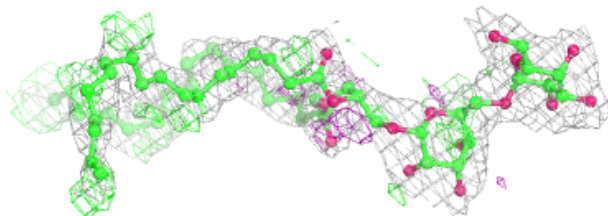
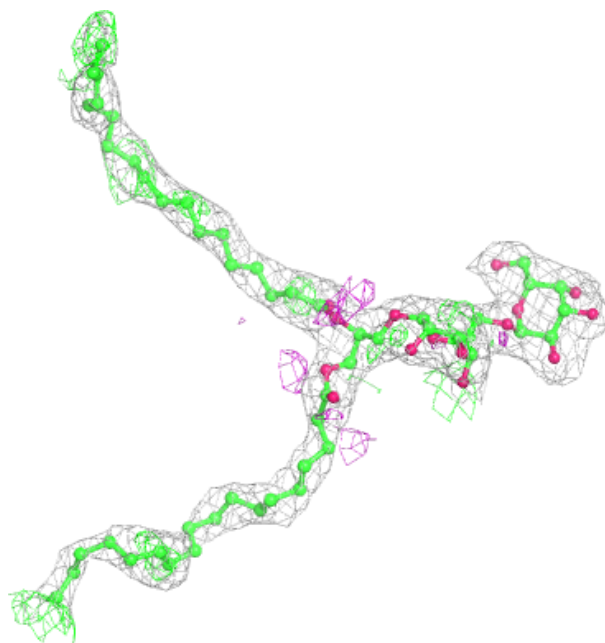
**Electron density around NEX F 5623:**

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



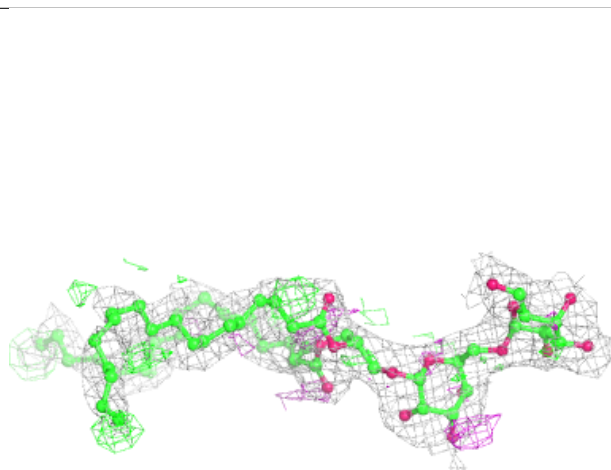
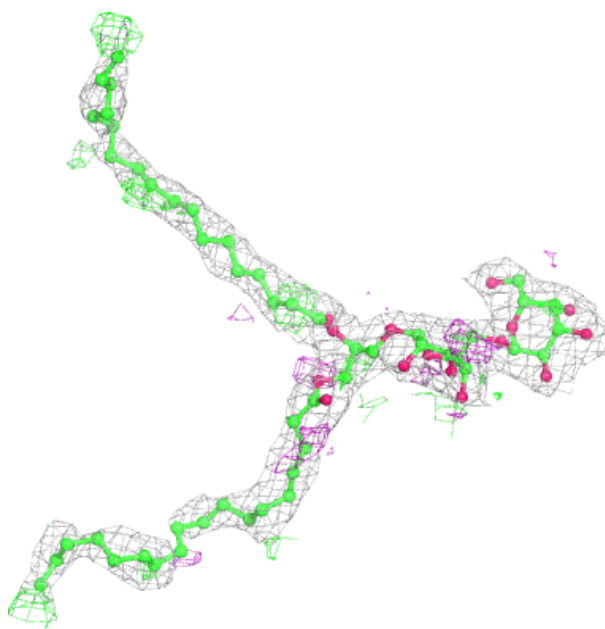
Electron density around DGD A 632:

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



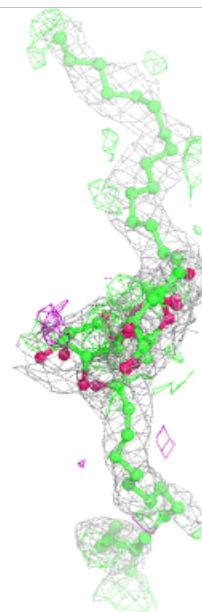
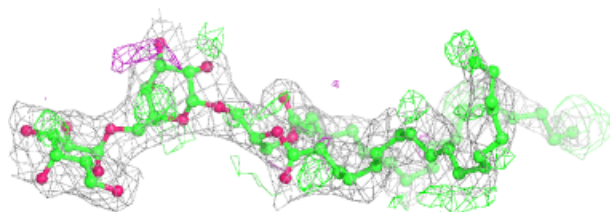
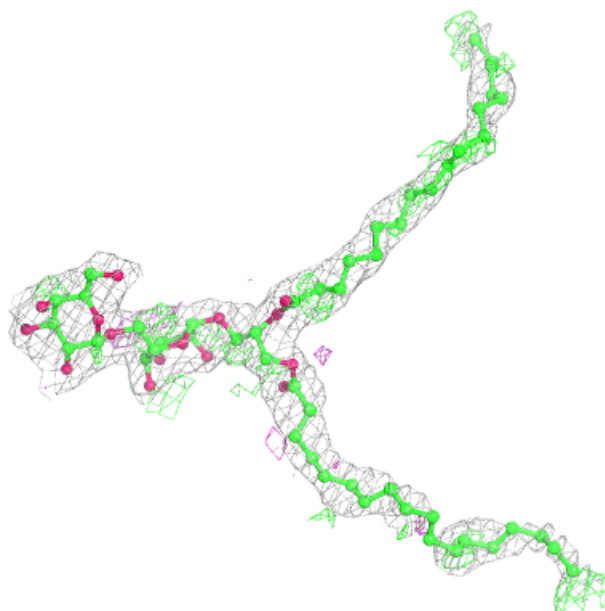
Electron density around DGD H 7632:

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



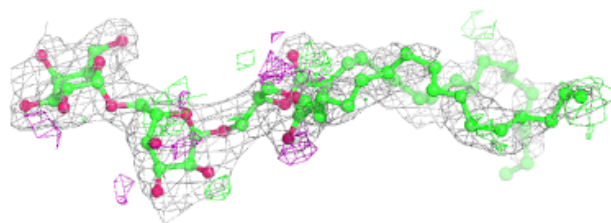
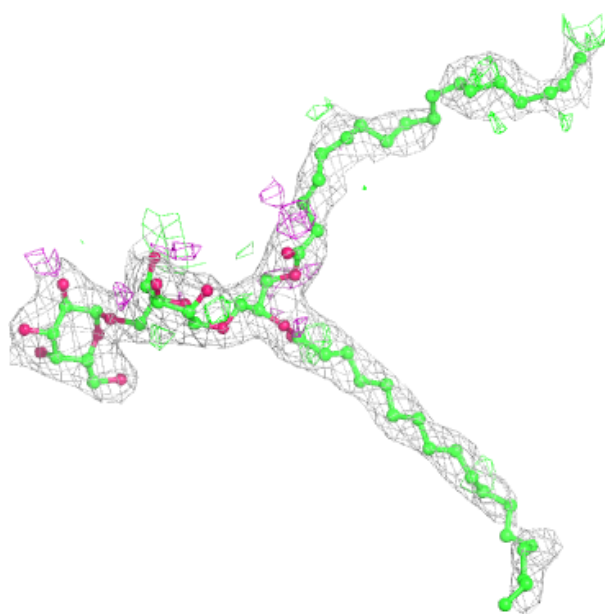
Electron density around DGD G 9632:

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



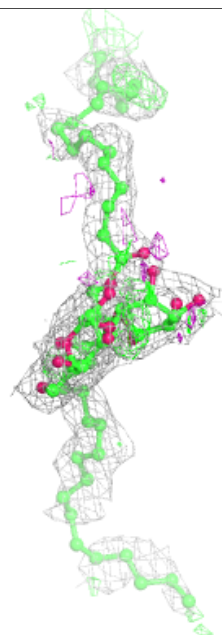
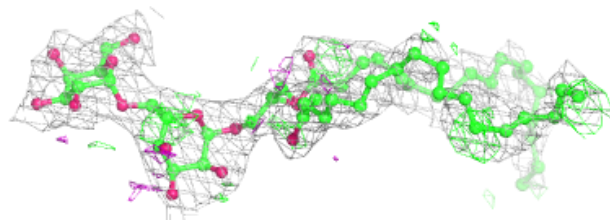
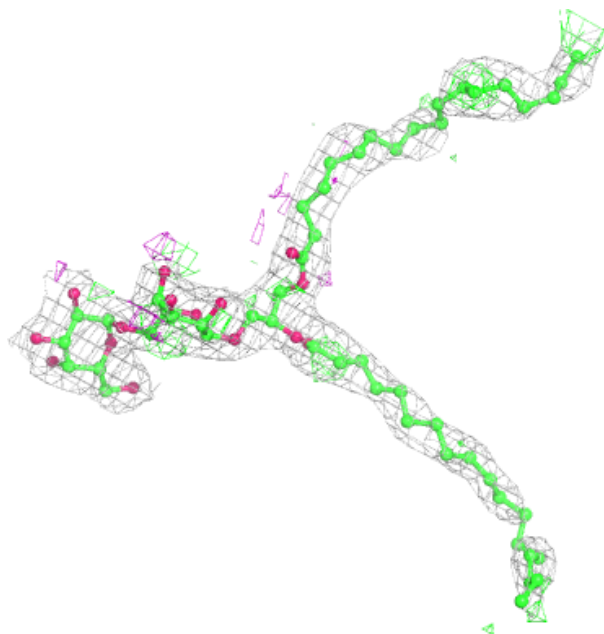
Electron density around DGD I 8632:

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



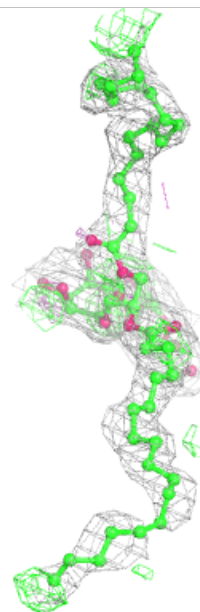
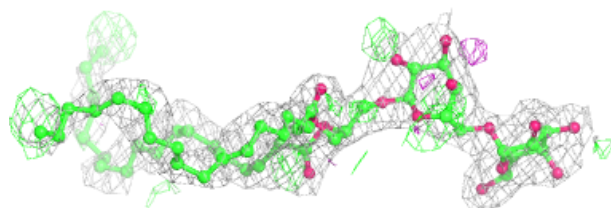
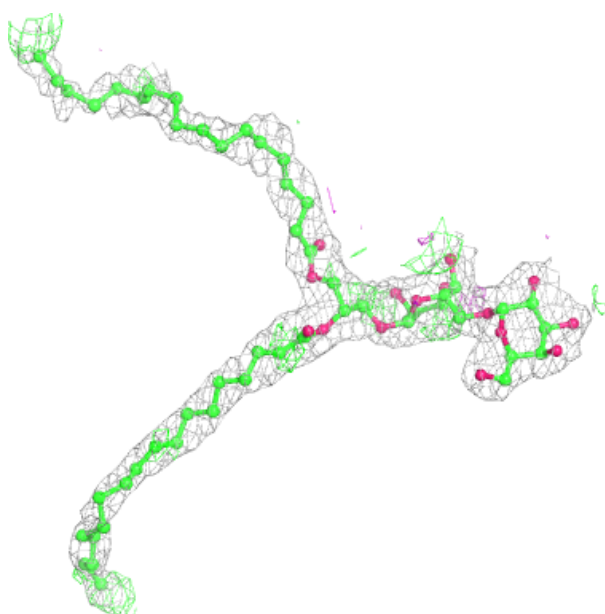
Electron density around DGD D 5632:

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



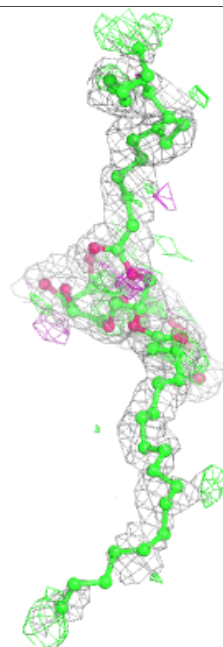
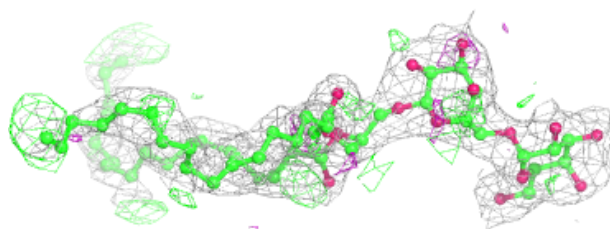
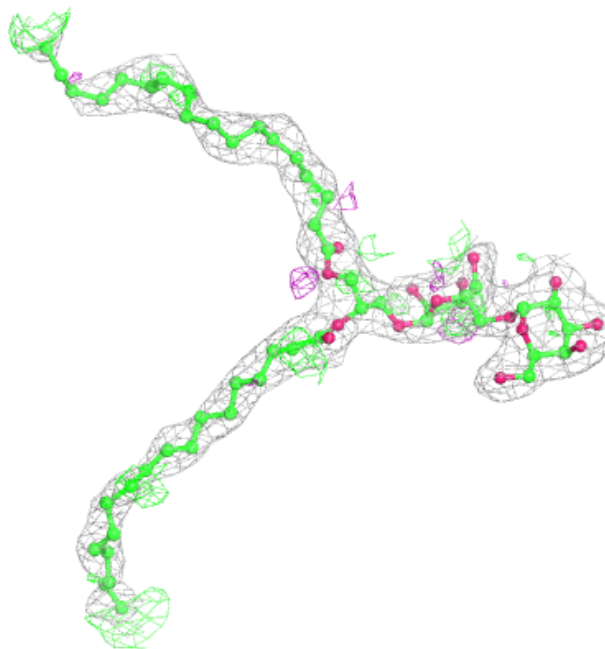
Electron density around DGD B 2632:

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



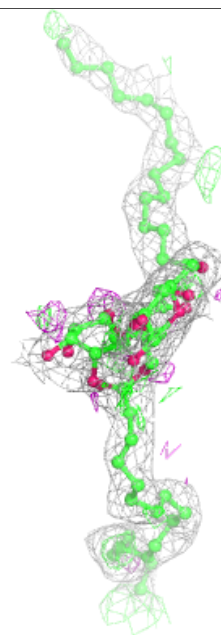
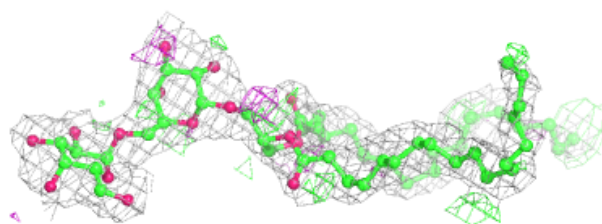
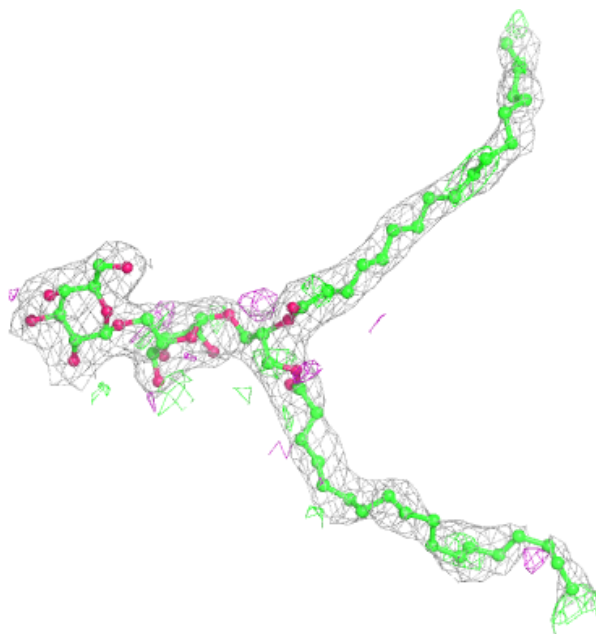
Electron density around DGD E 4632:

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



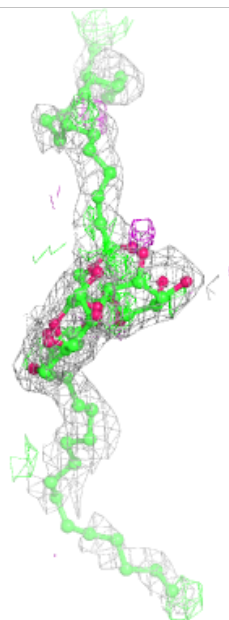
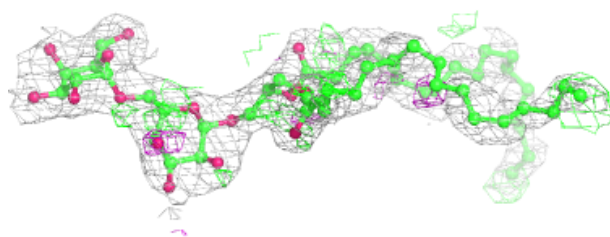
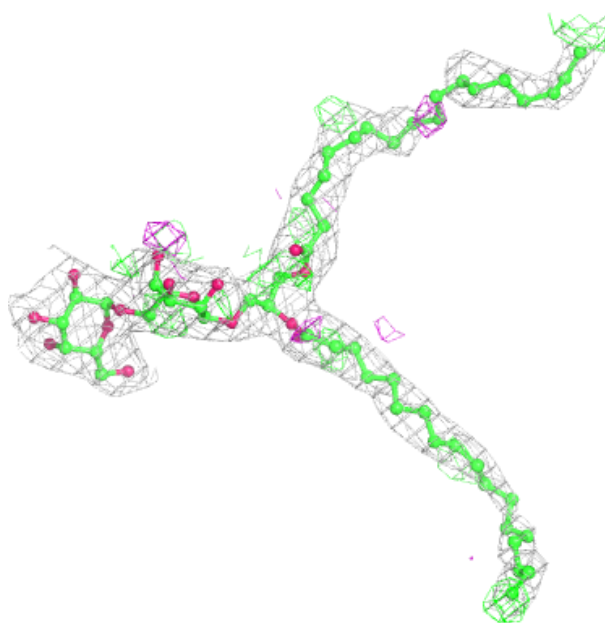
Electron density around DGD B 1632:

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



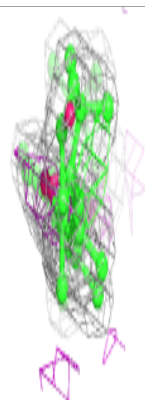
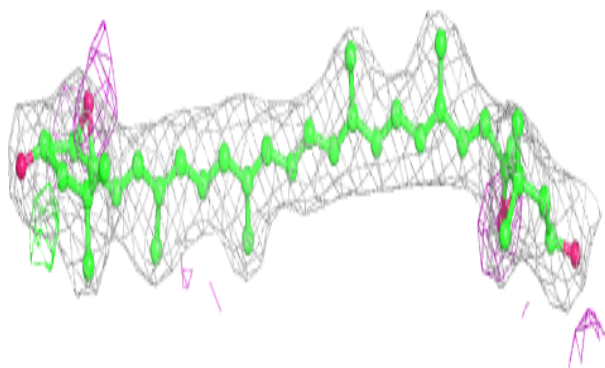
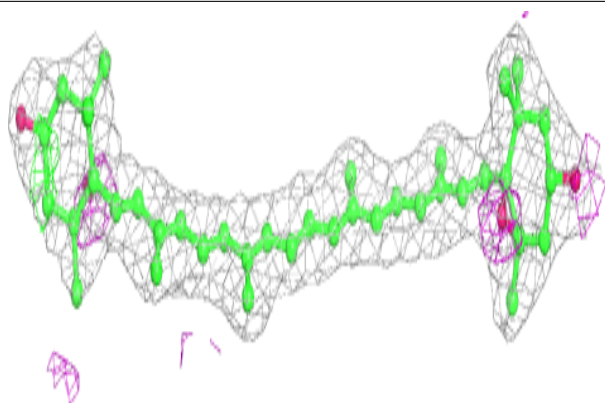
Electron density around DGD H 6632:

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

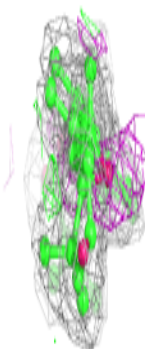
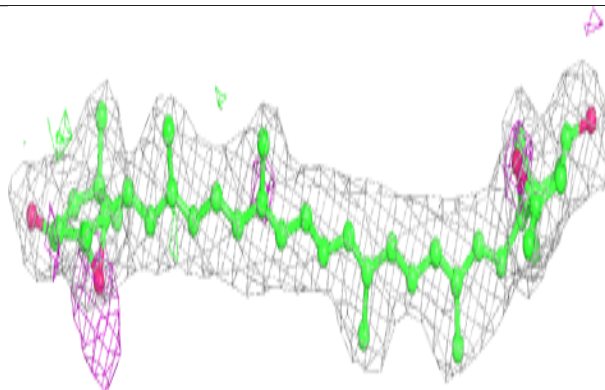
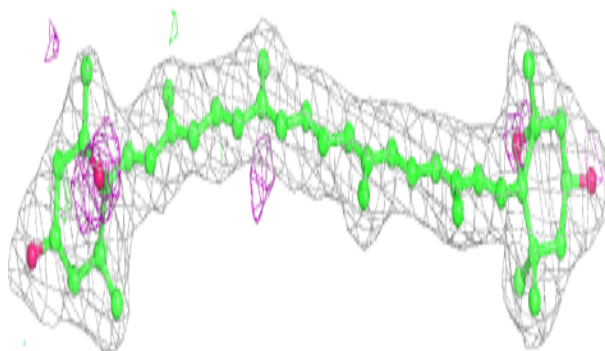


Electron density around XAT A 622:

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

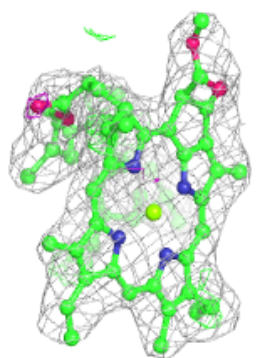
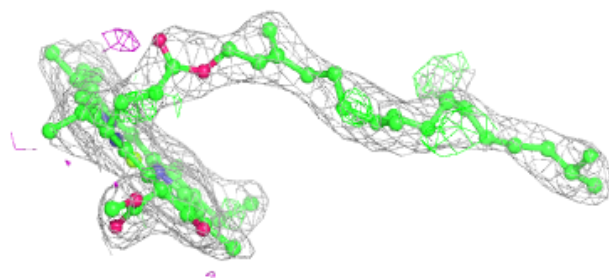
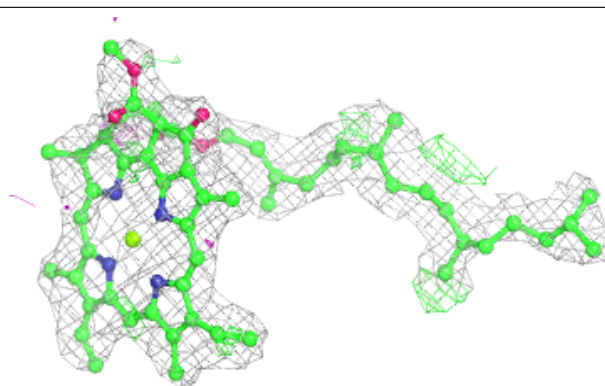
**Electron density around XAT E 2622:**

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



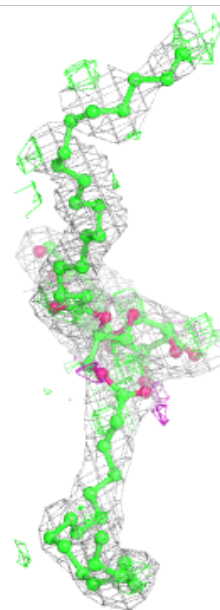
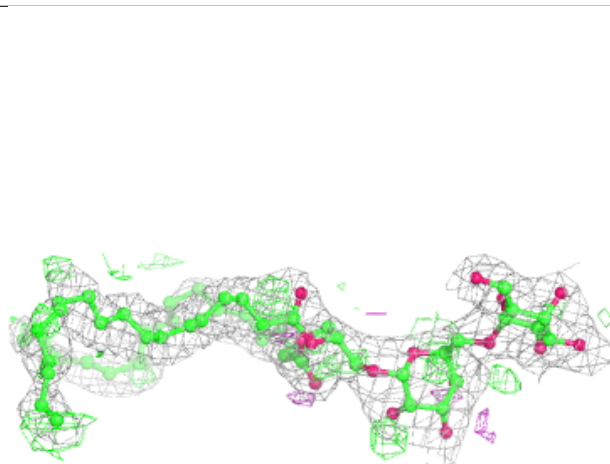
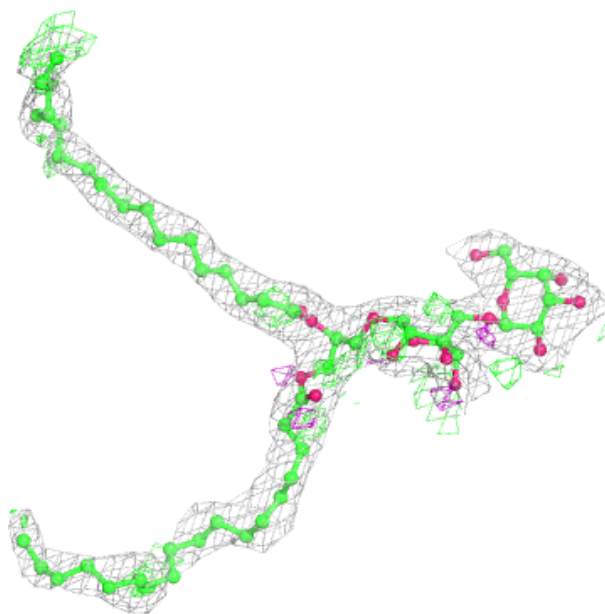
Electron density around CLA A 611:

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



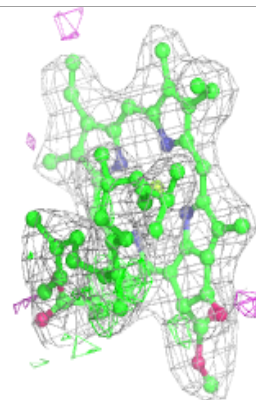
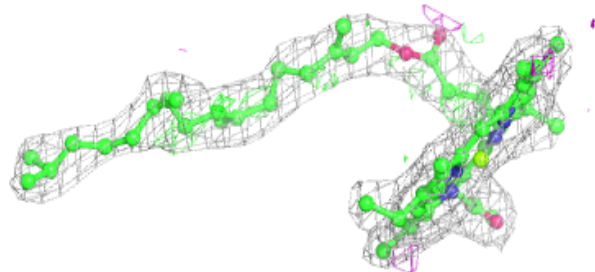
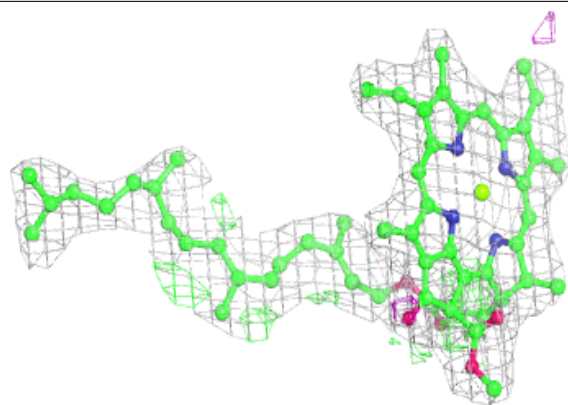
Electron density around DGD D 3632:

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

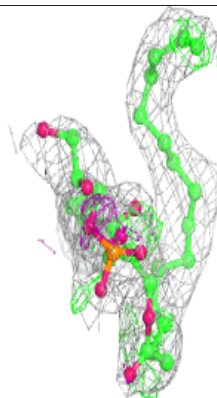
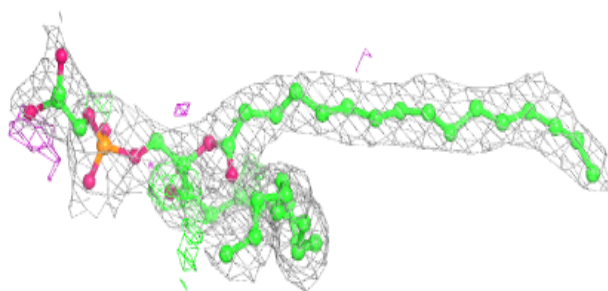
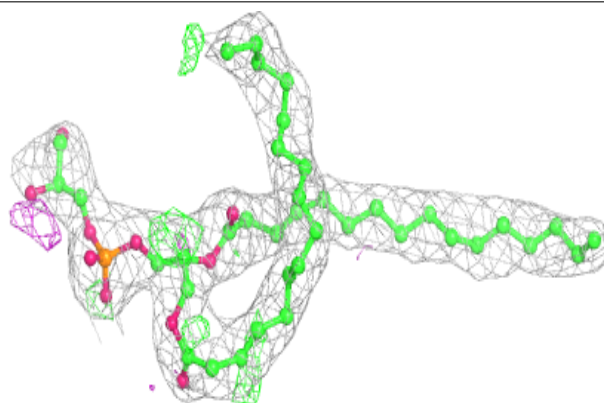


Electron density around CLA I 611:

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

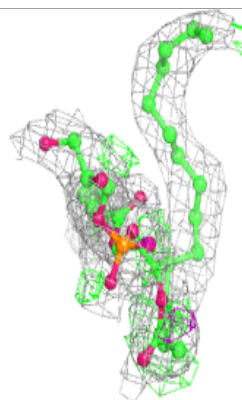
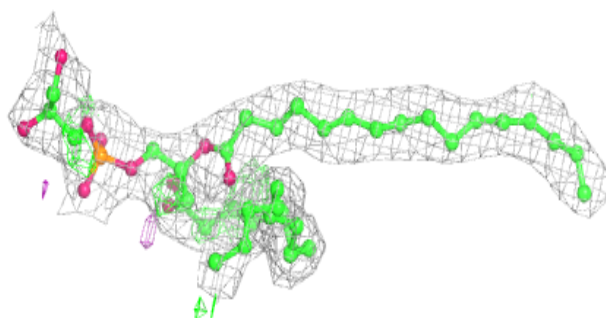
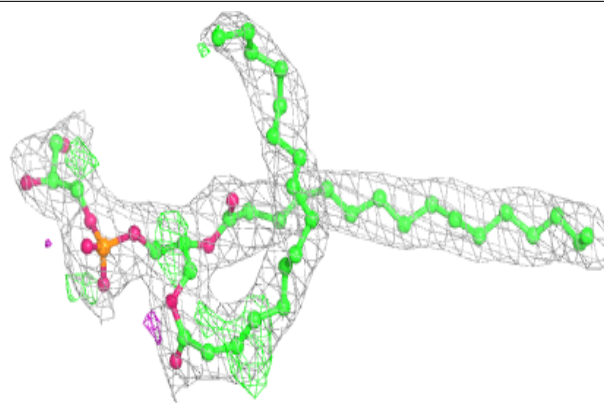
**Electron density around LHG A 630:**

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

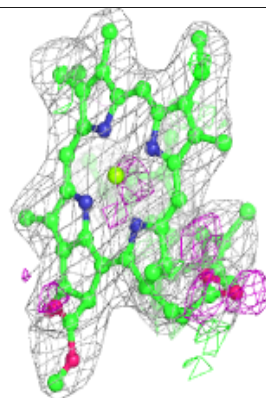
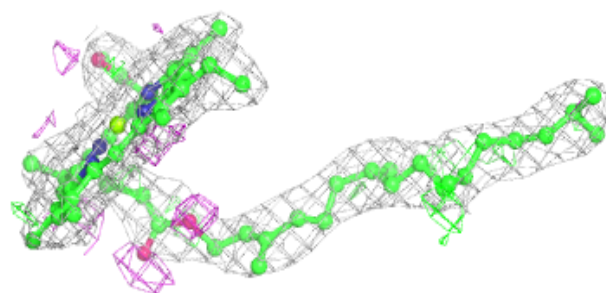
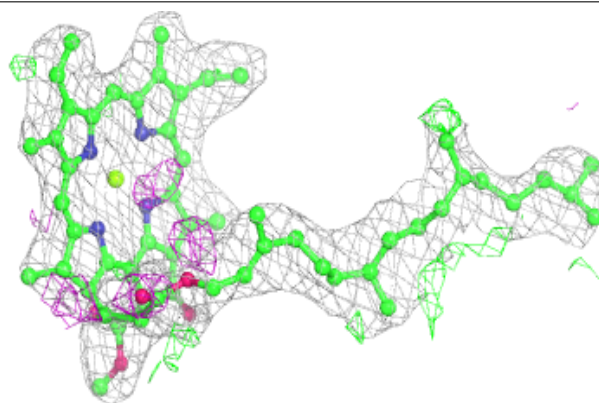


Electron density around LHG B 1630:

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

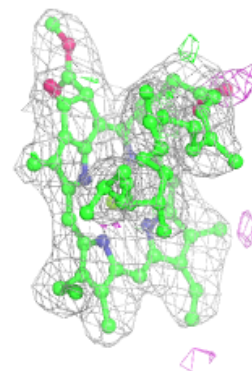
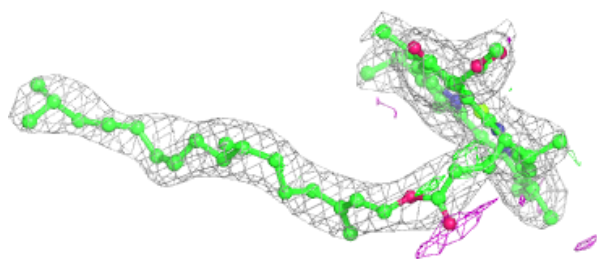
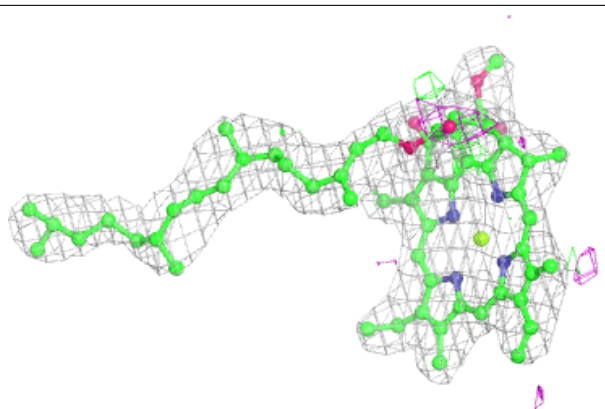
**Electron density around CLA D 611:**

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

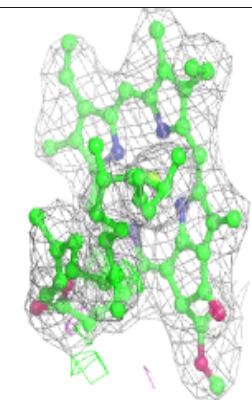
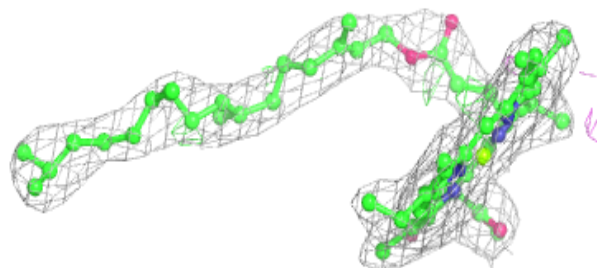
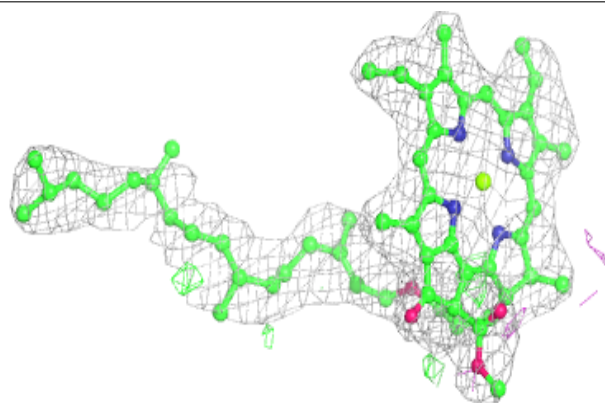


Electron density around CLA H 611:

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

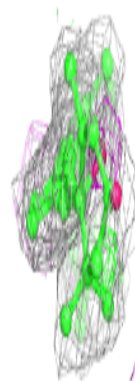
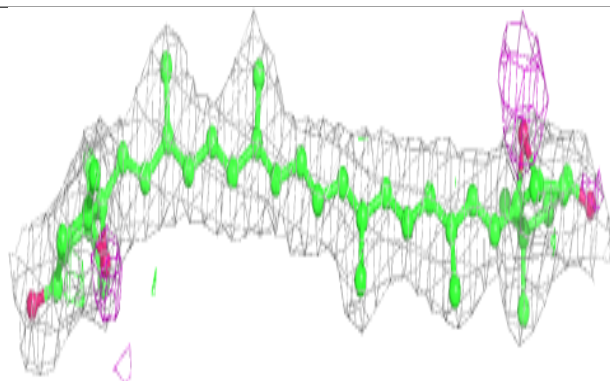
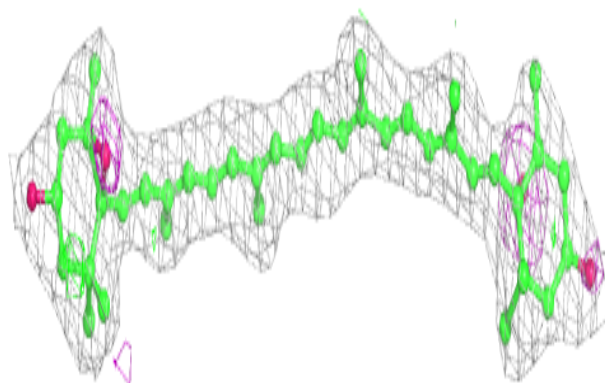
**Electron density around CLA G 611:**

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

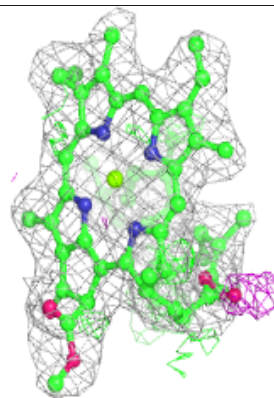
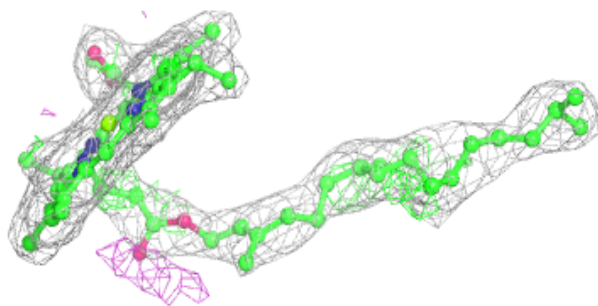
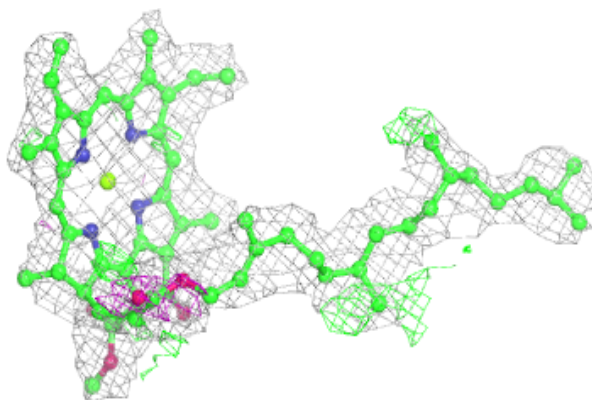


Electron density around XAT B 5622:

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

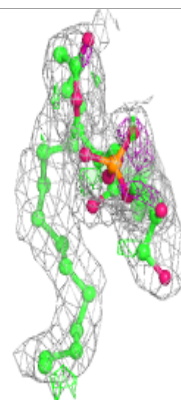
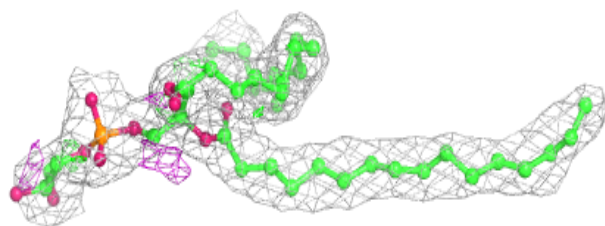
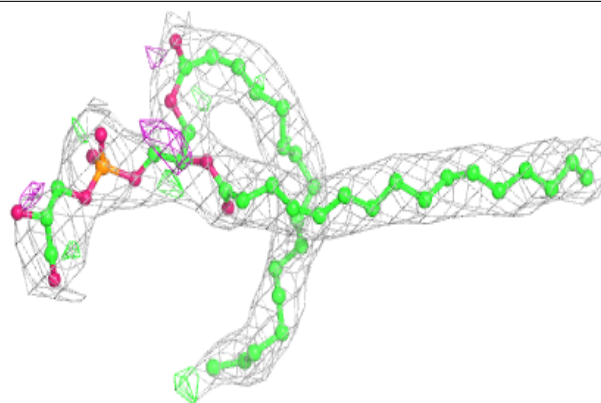
**Electron density around CLA B 611:**

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

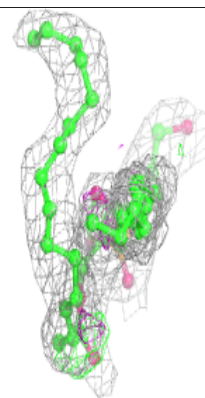
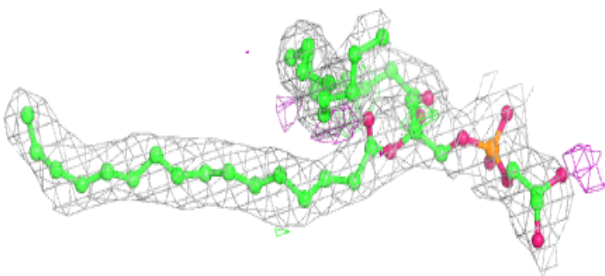
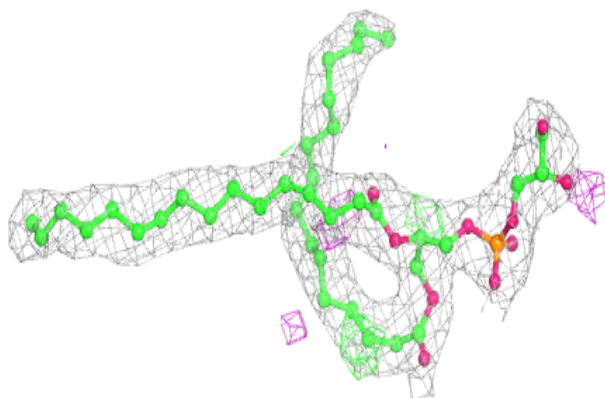


Electron density around LHG I 8630:

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

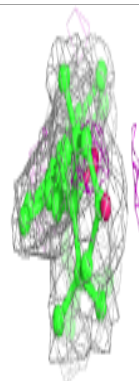
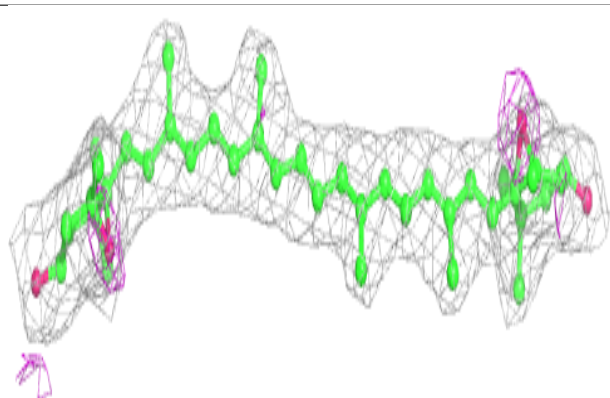
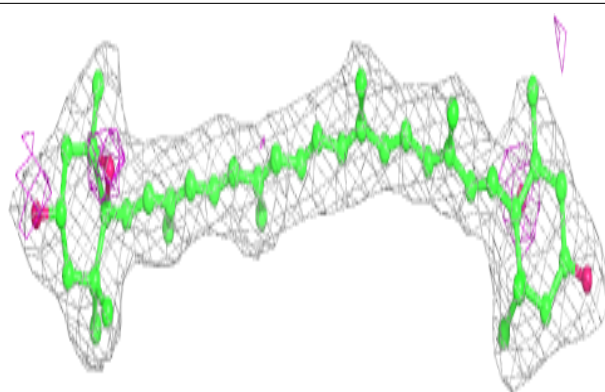
**Electron density around LHG G 6630:**

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

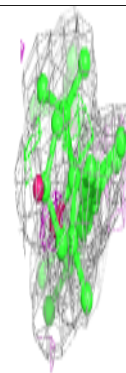
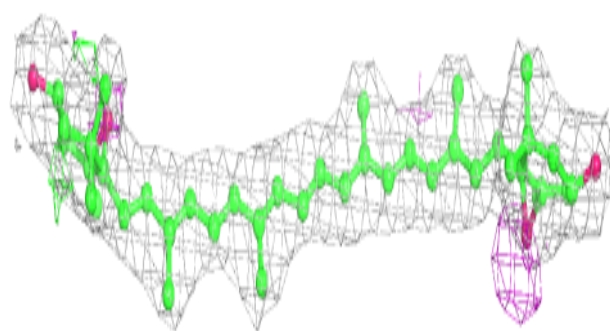
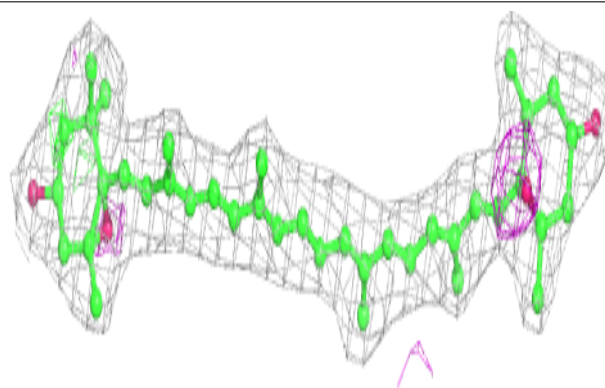


Electron density around XAT D 8622:

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

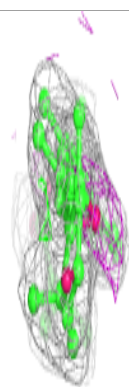
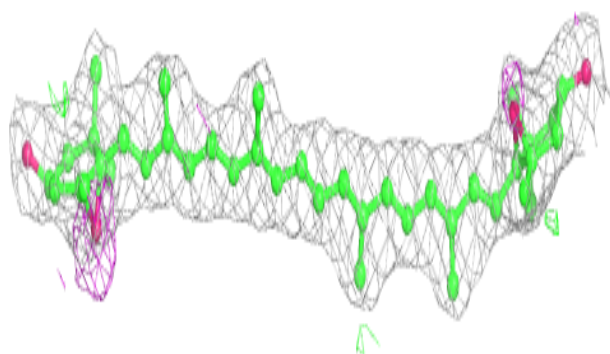
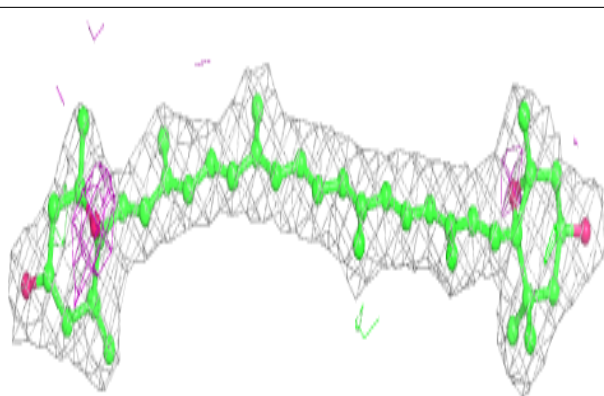
**Electron density around XAT I 9622:**

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

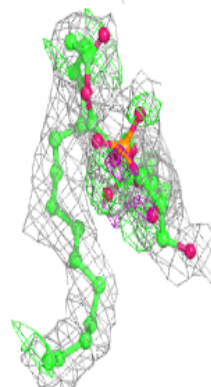
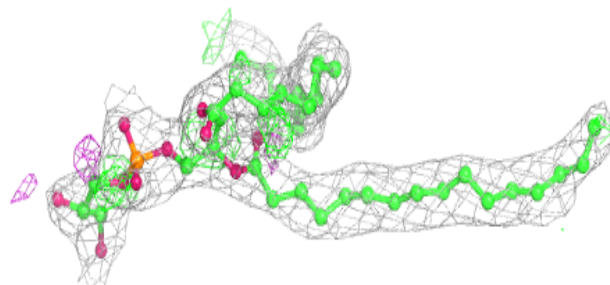
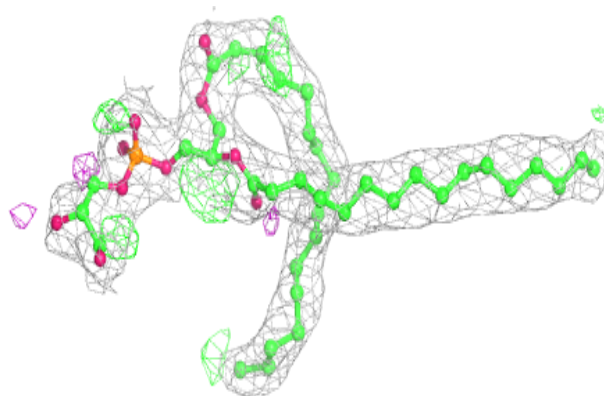


Electron density around XAT C 7622:

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

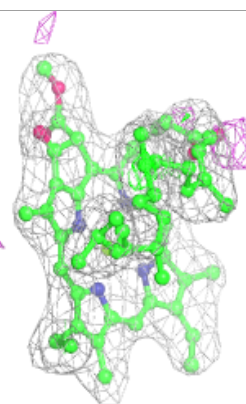
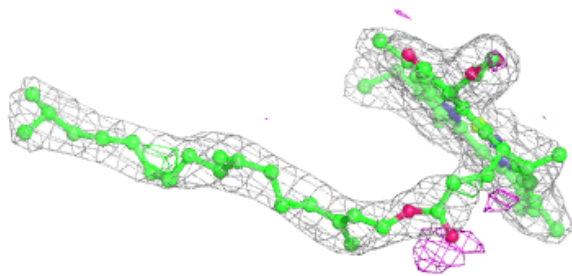
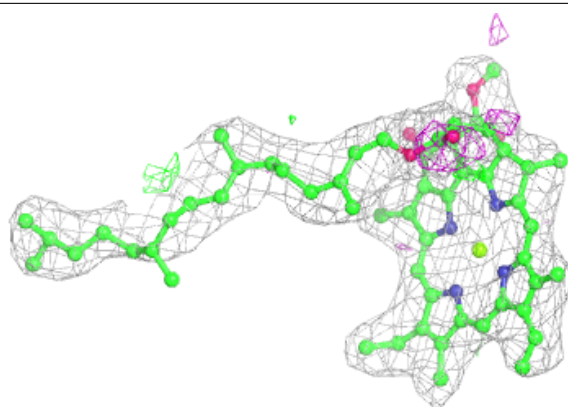
**Electron density around LHG E 4630:**

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

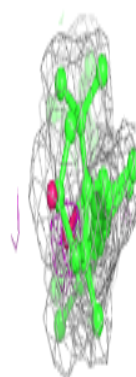
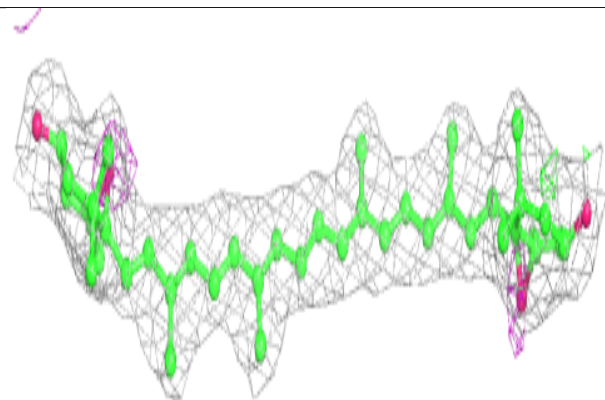
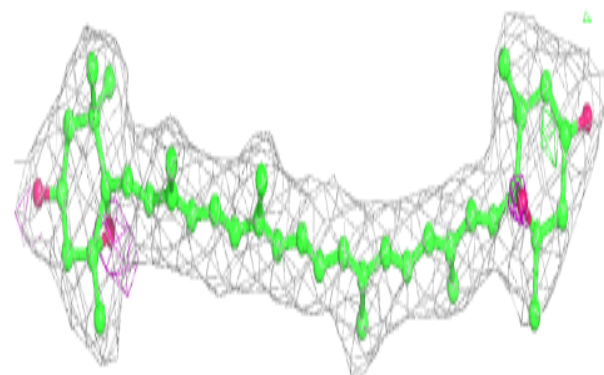


Electron density around CLA E 611:

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

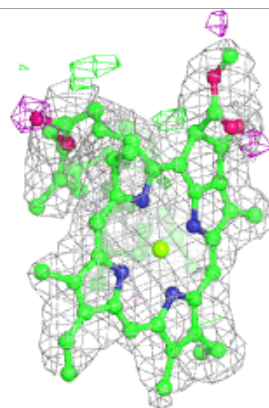
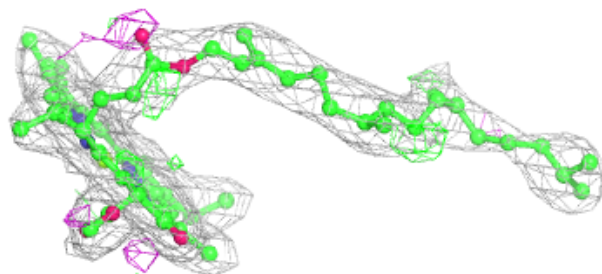
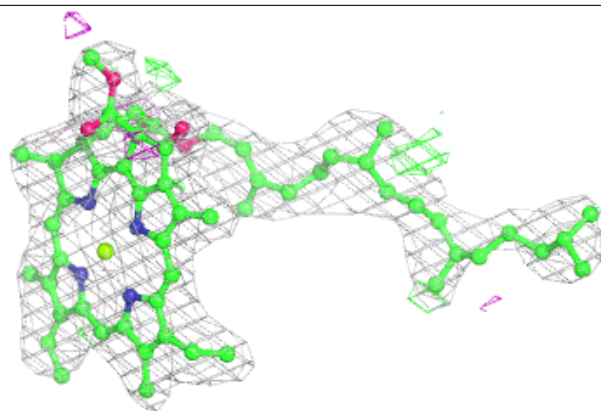
**Electron density around XAT H 4622:**

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

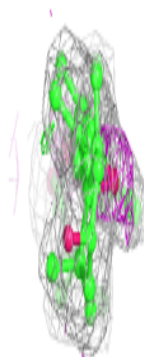
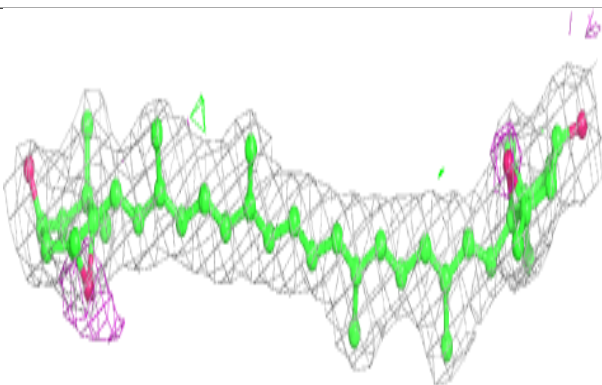
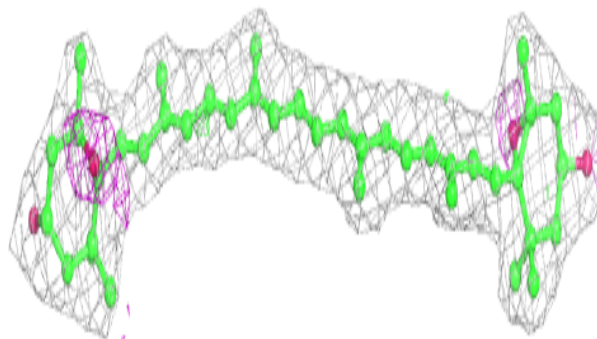


Electron density around CLA C 611:

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

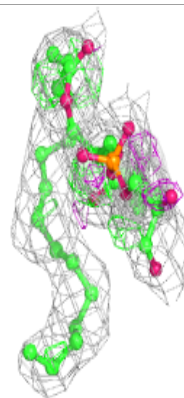
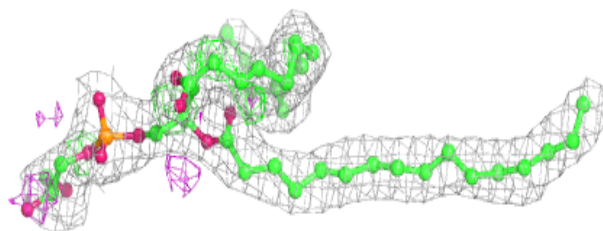
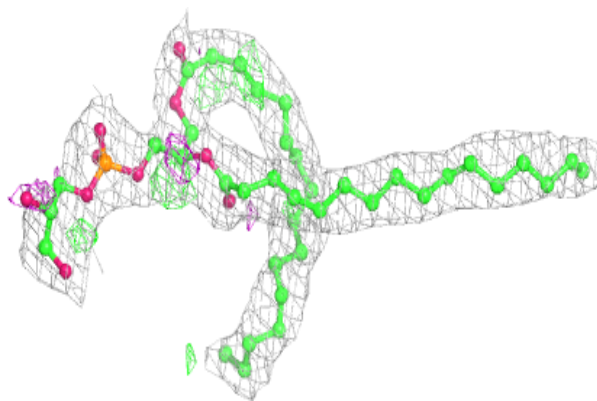
**Electron density around XAT F 6622:**

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

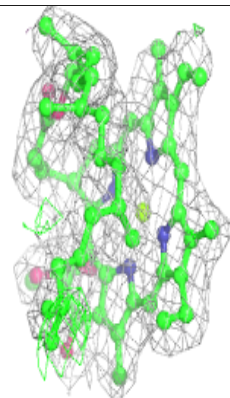
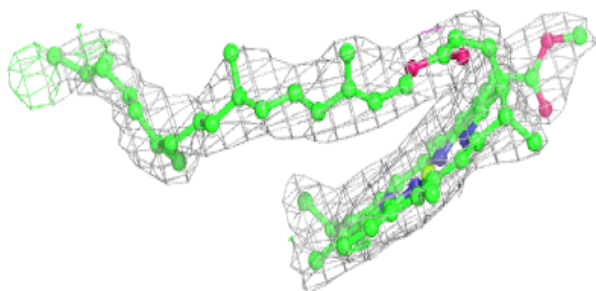
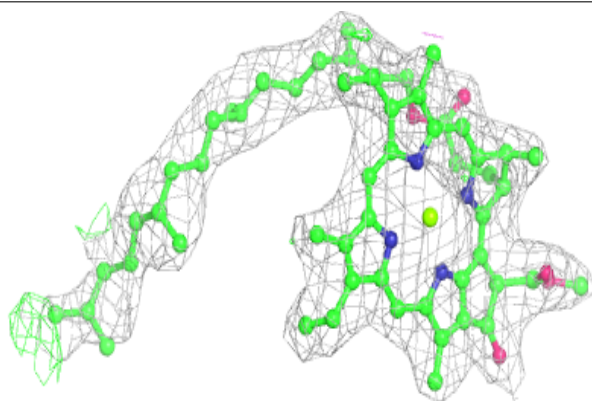


Electron density around LHG D 3630:

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

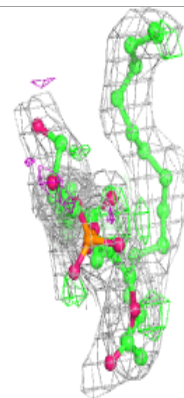
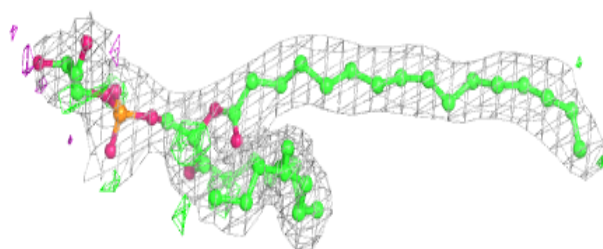
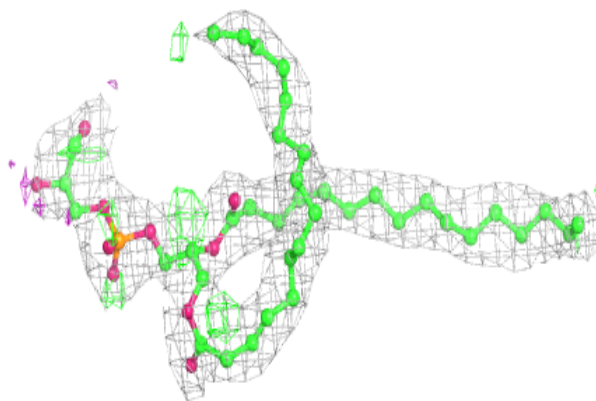
**Electron density around CLA A 610:**

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

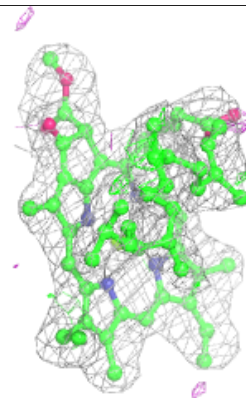
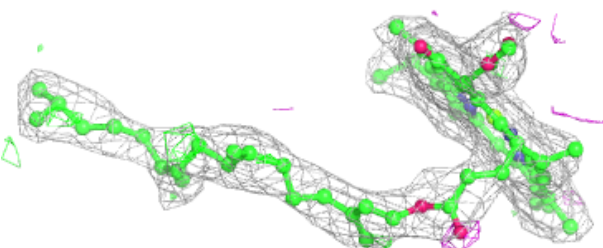
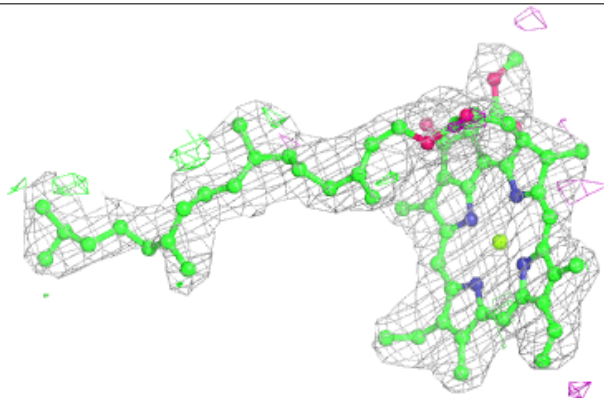


Electron density around LHG F 5630:

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

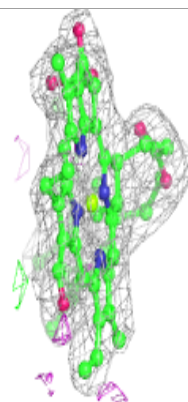
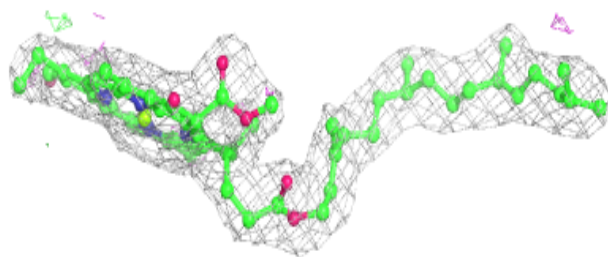
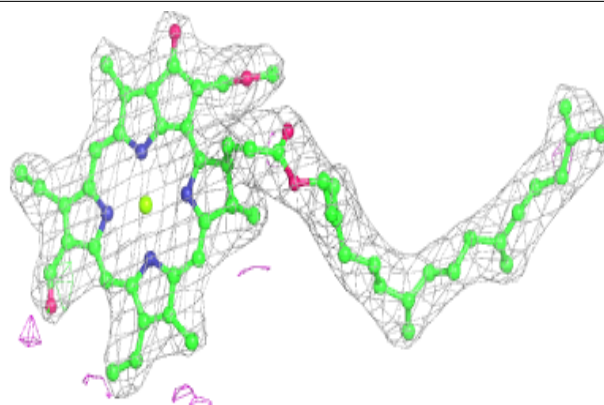
**Electron density around CLA J 611:**

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

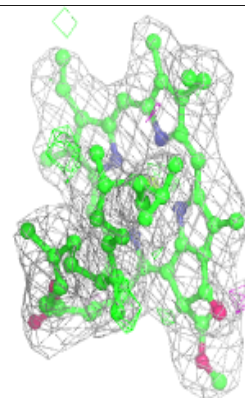
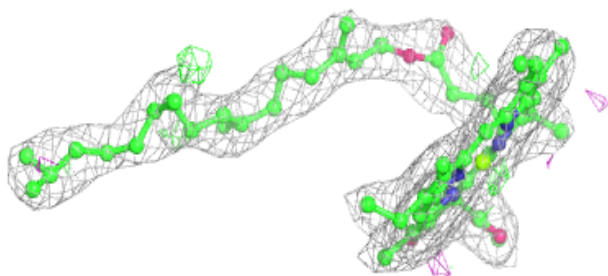
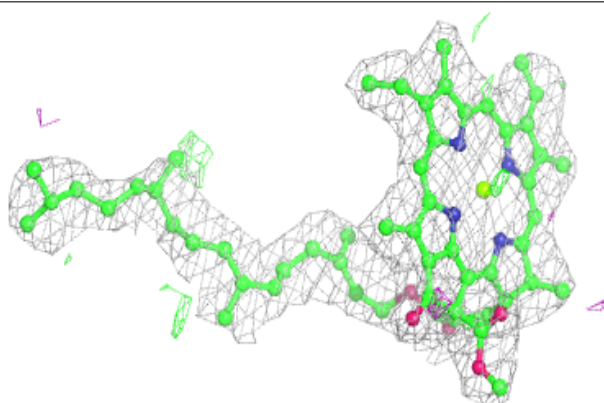


Electron density around CHL A 601:

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

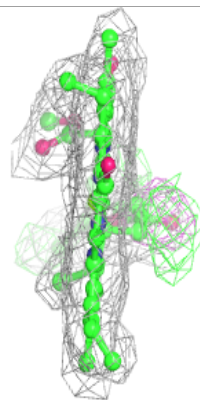
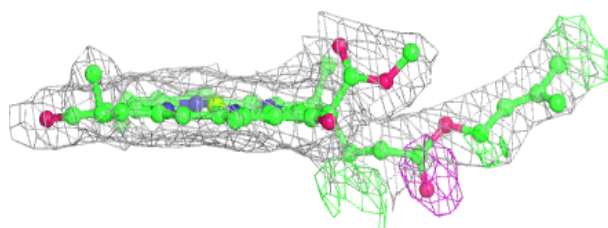
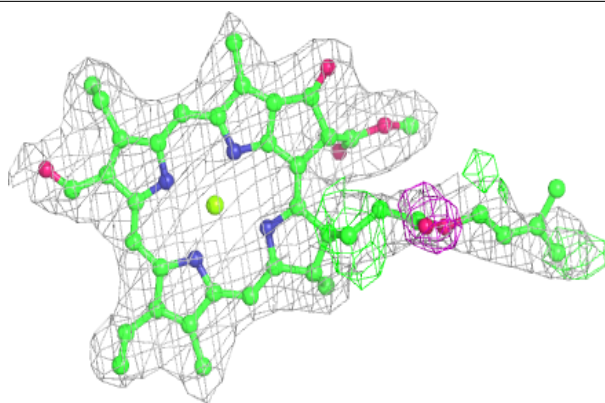
**Electron density around CLA F 611:**

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

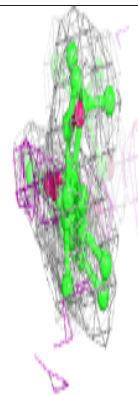
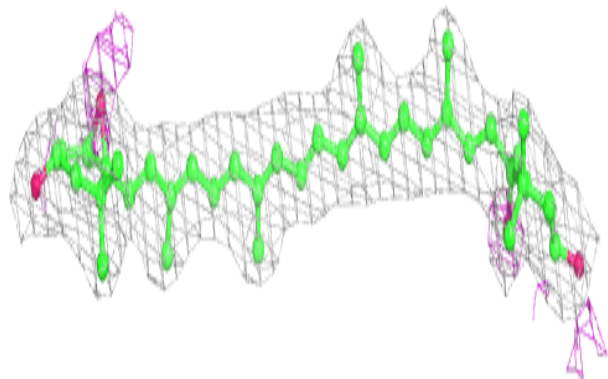
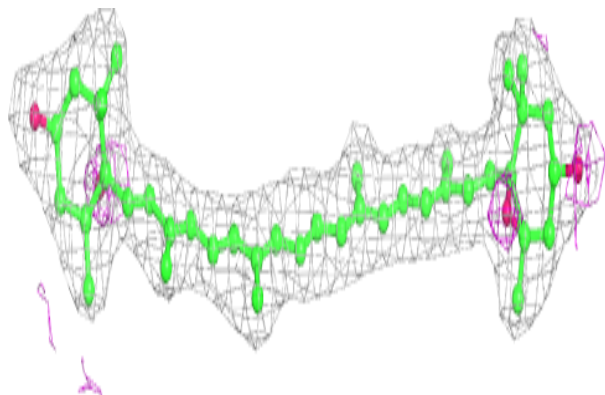


Electron density around CHL J 606:

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

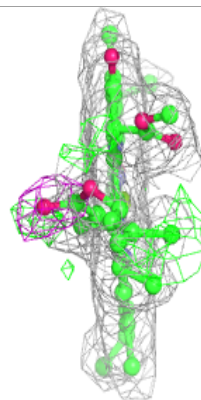
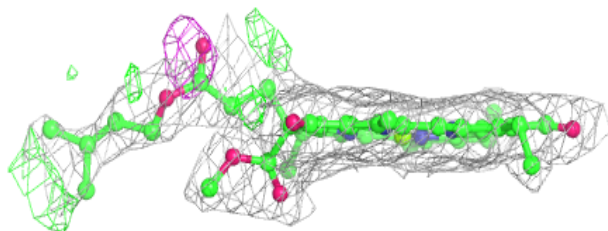
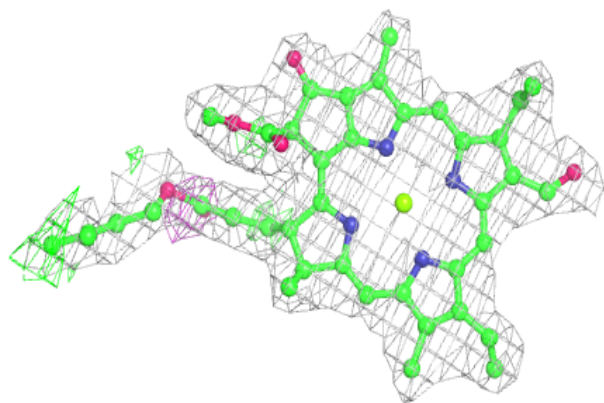
**Electron density around XAT B 1622:**

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

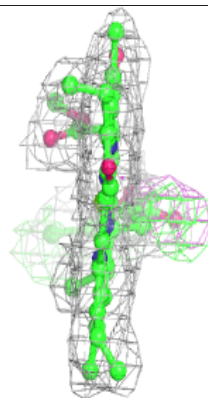
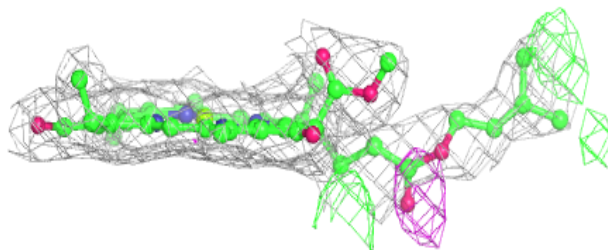
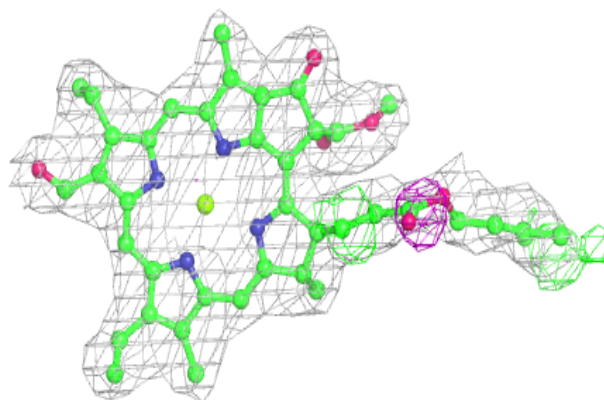


Electron density around CHL A 606:

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

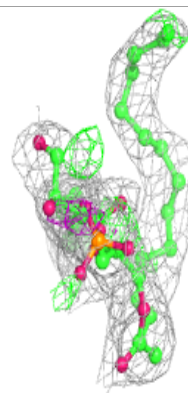
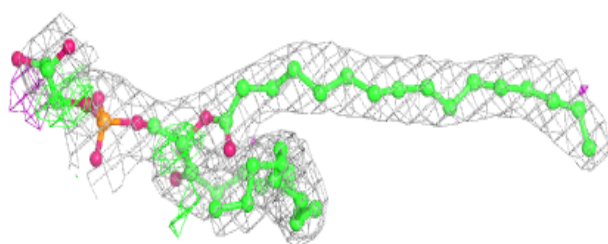
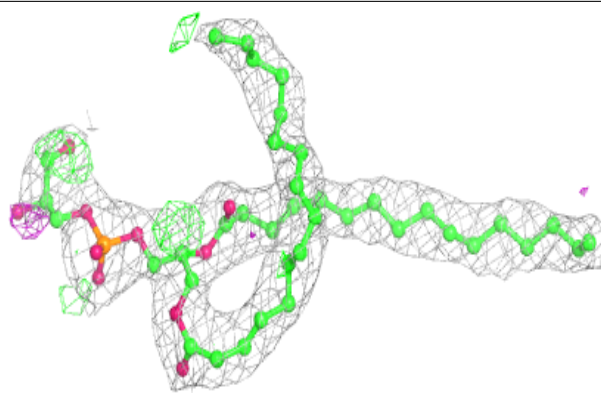
**Electron density around CHL F 606:**

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

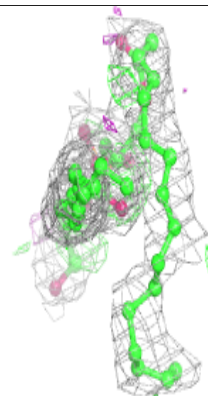
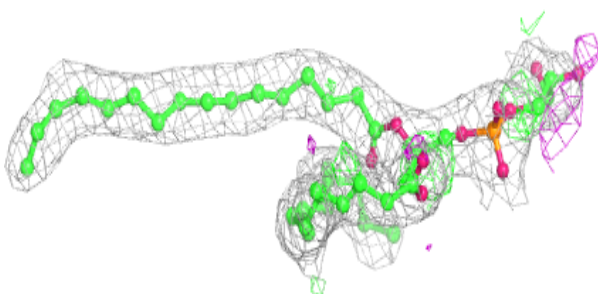
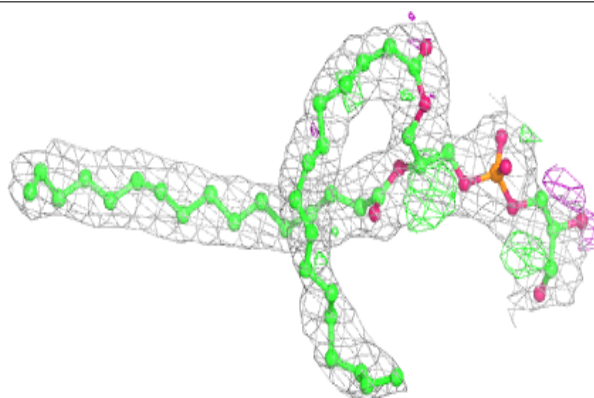


Electron density around LHG H 7630:

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

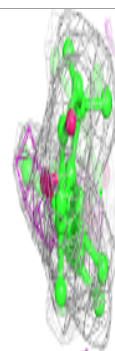
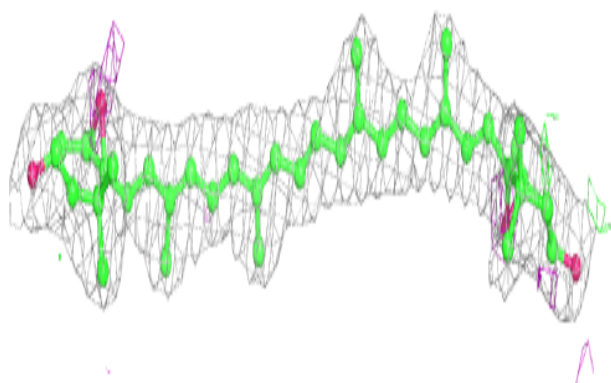
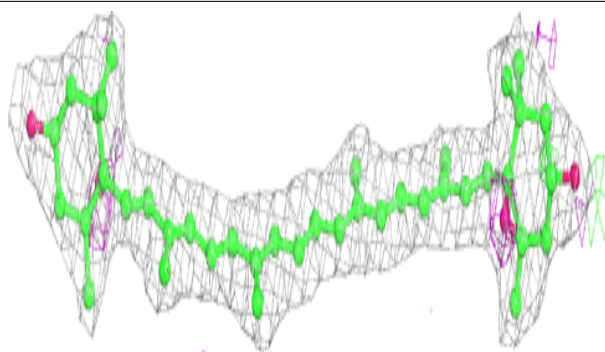
**Electron density around LHG J 9630:**

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

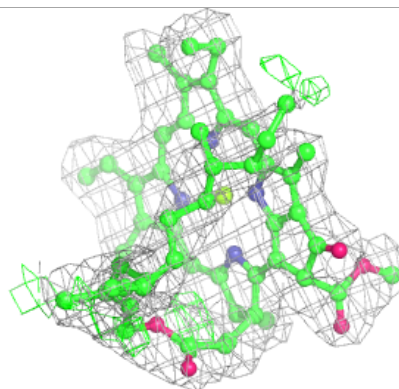
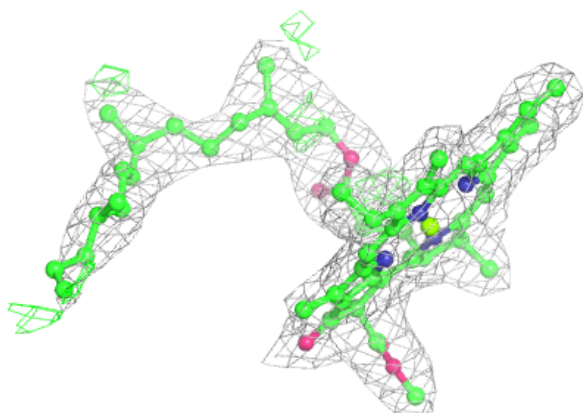
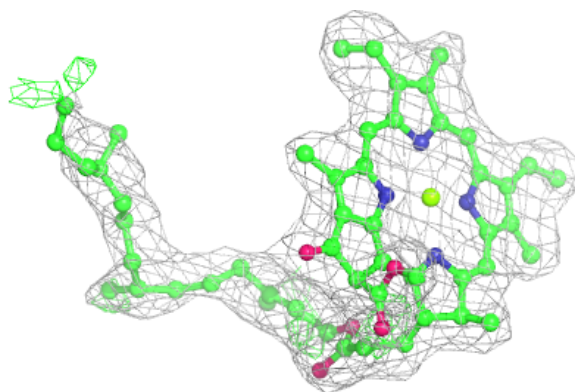


Electron density around XAT J 3622:

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

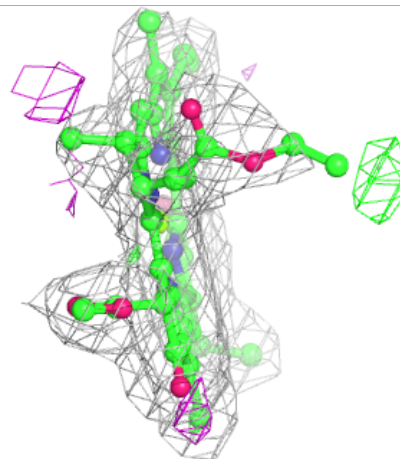
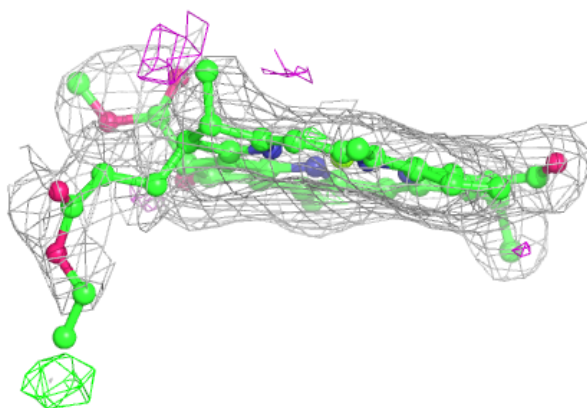
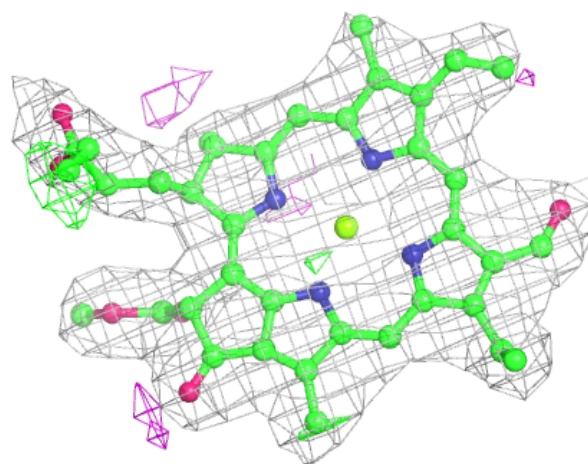
**Electron density around CLA J 604:**

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



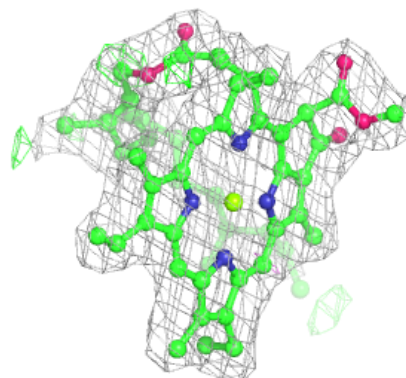
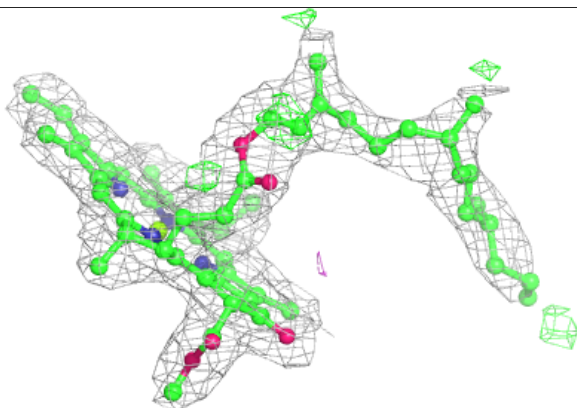
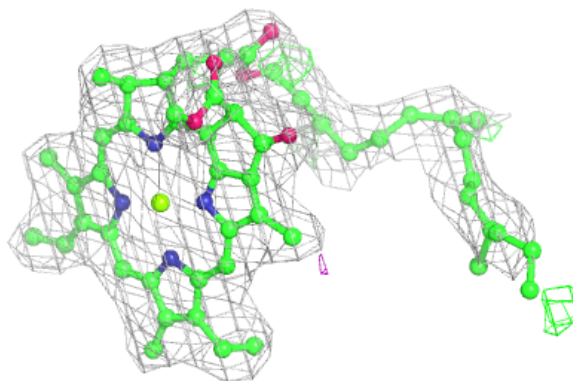
Electron density around CHL G 605:

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

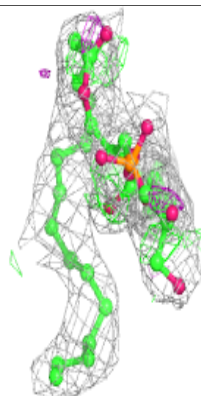
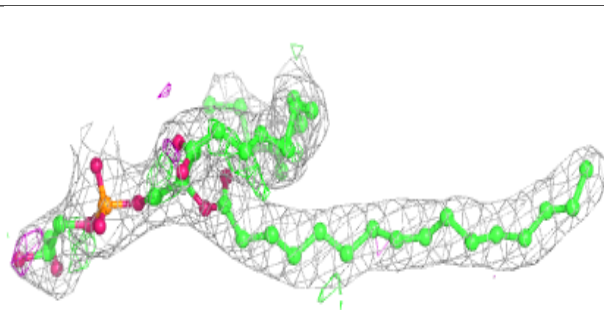
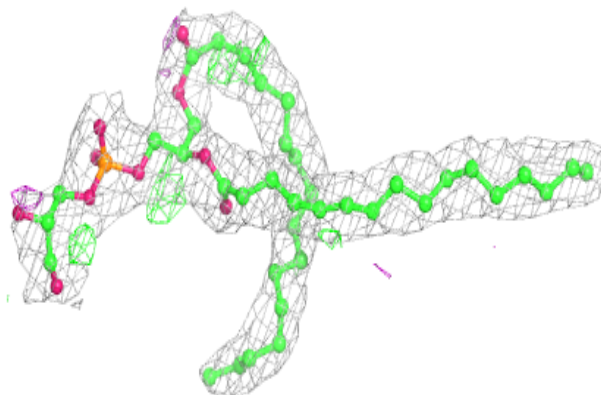


Electron density around CLA B 604:

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

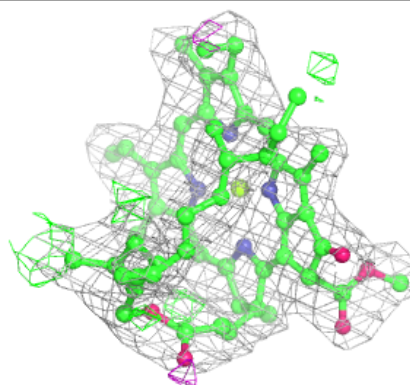
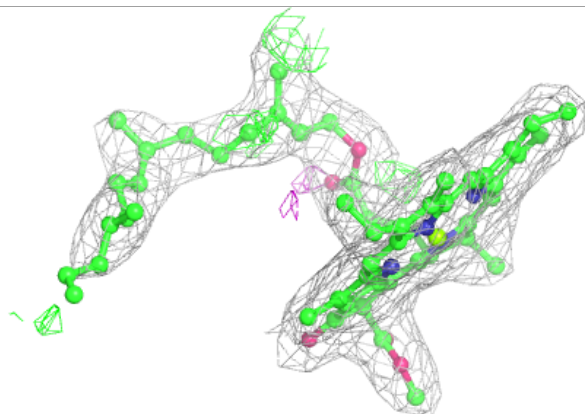
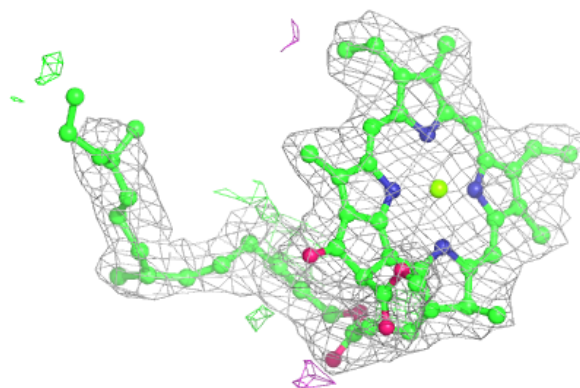
**Electron density around LHG C 2630:**

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

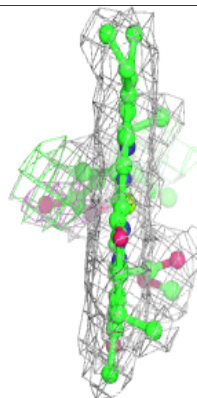
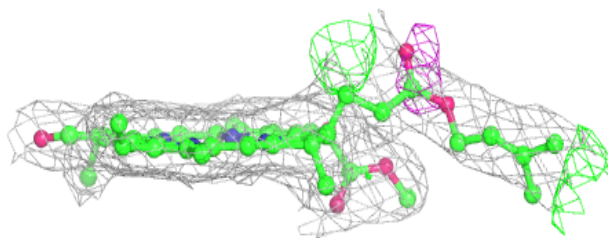
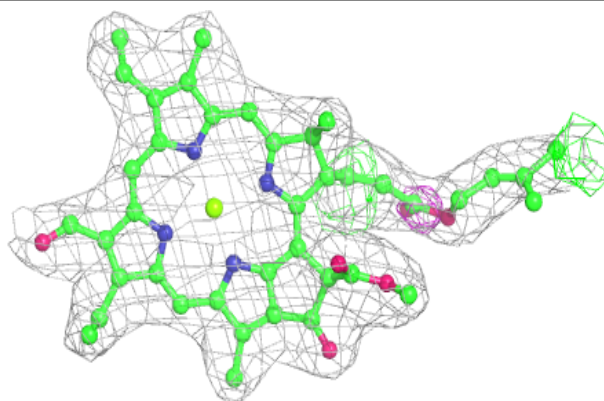


Electron density around CLA H 604:

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

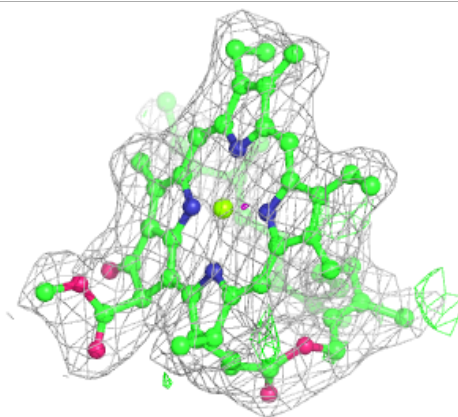
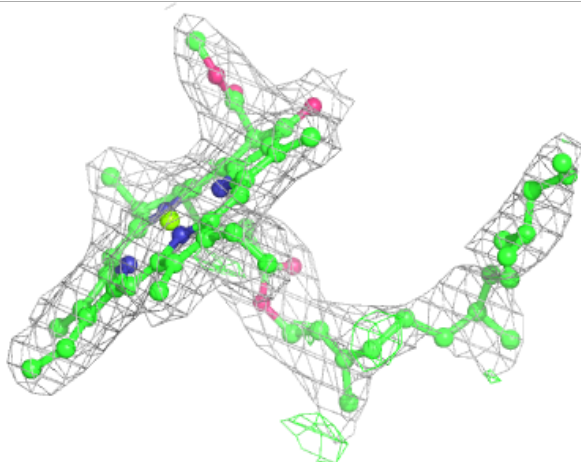
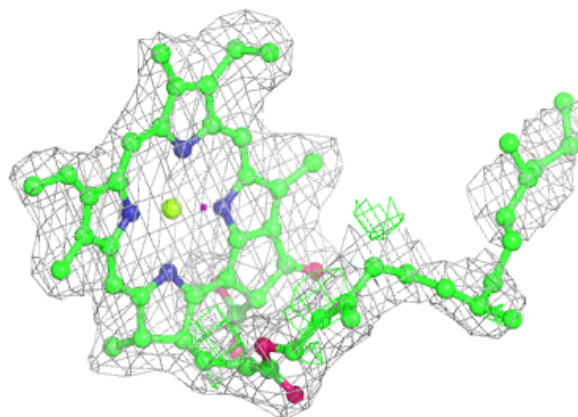
**Electron density around CHL D 606:**

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



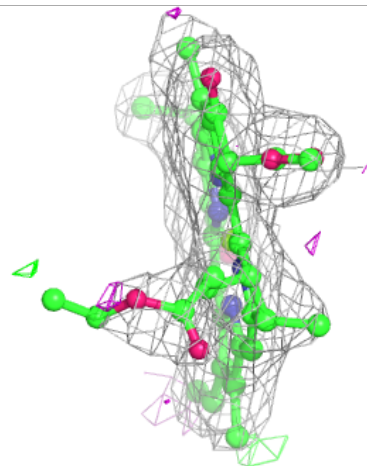
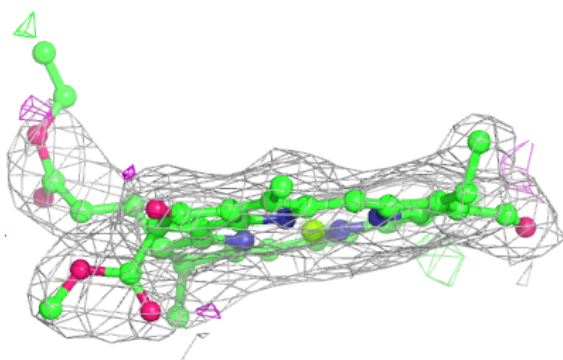
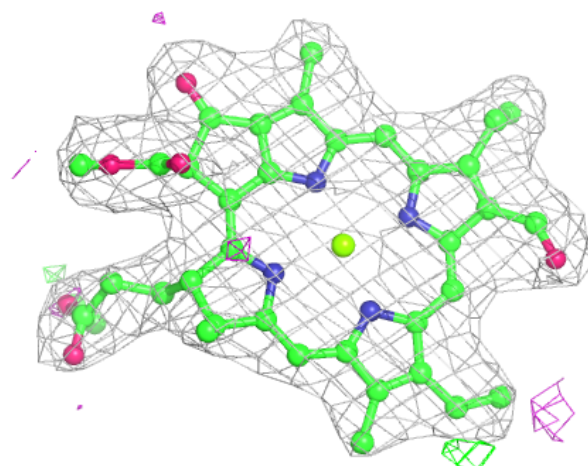
Electron density around CLA E 604:

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



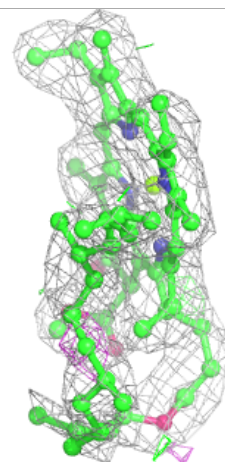
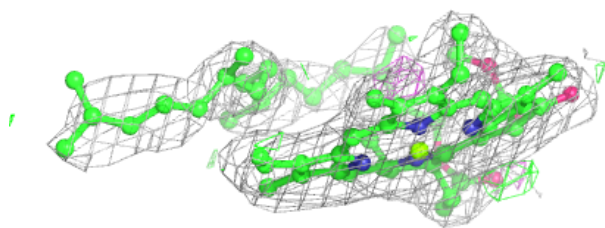
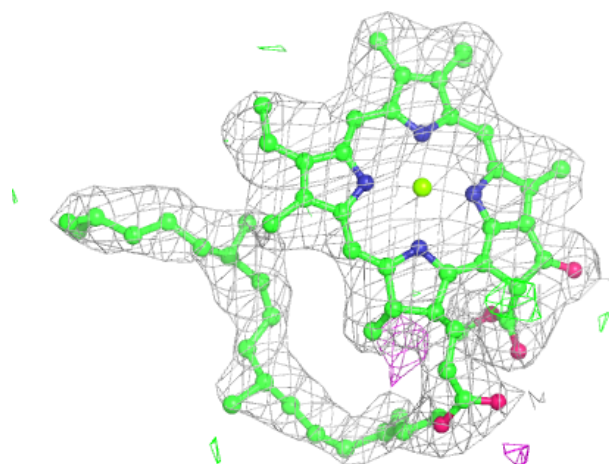
Electron density around CHL B 605:

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



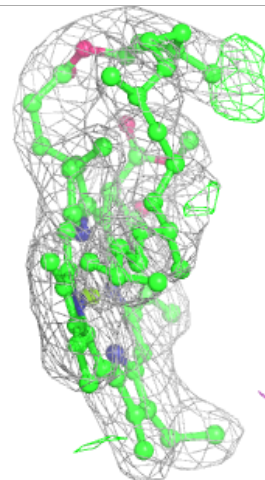
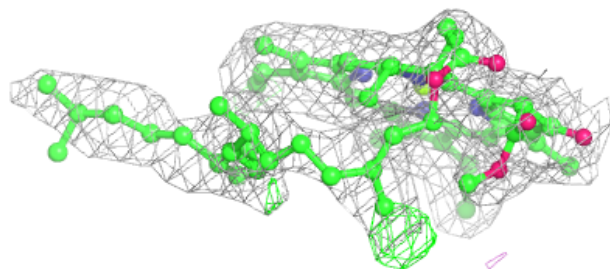
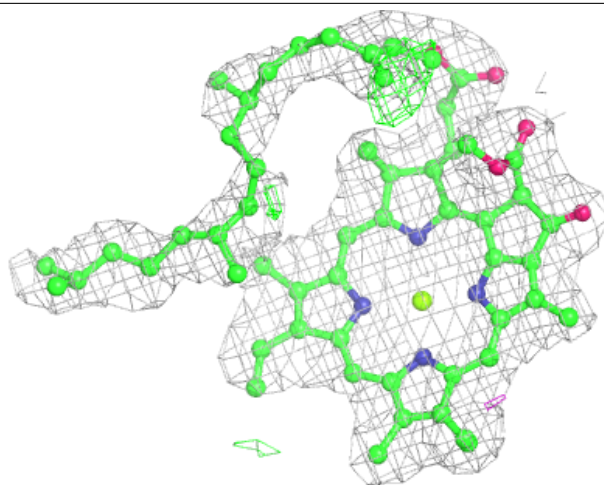
Electron density around CLA G 612:

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



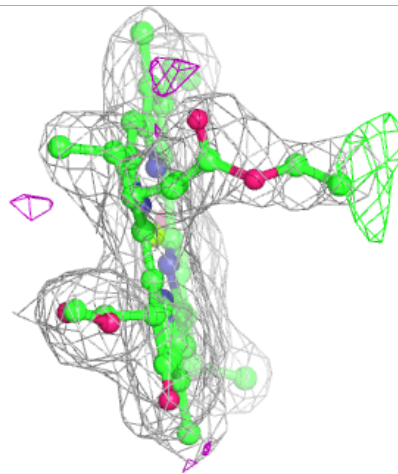
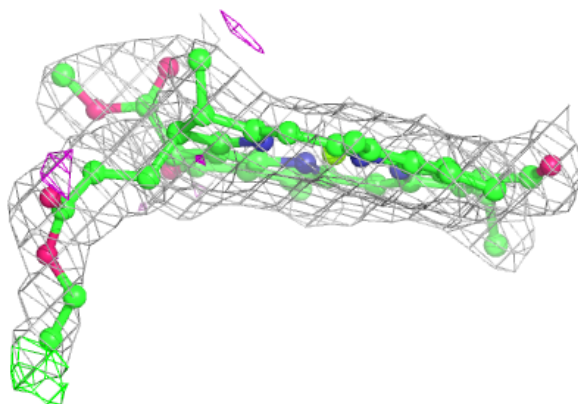
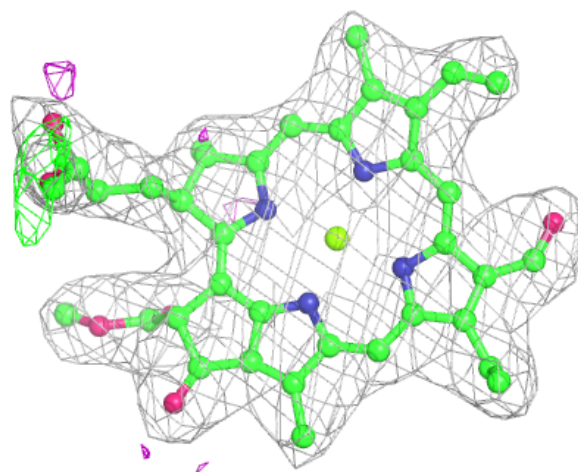
Electron density around CLA H 612:

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



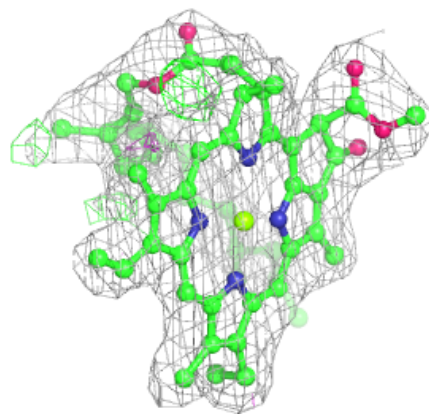
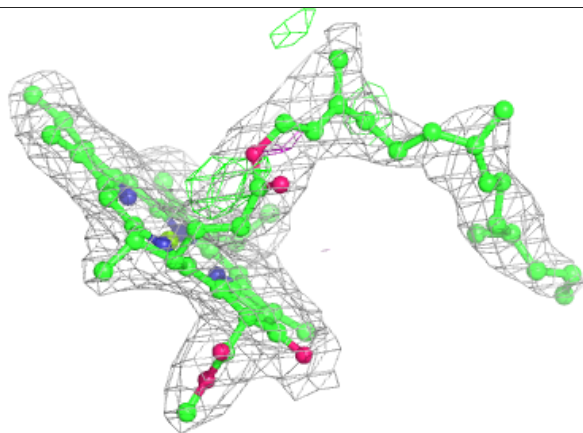
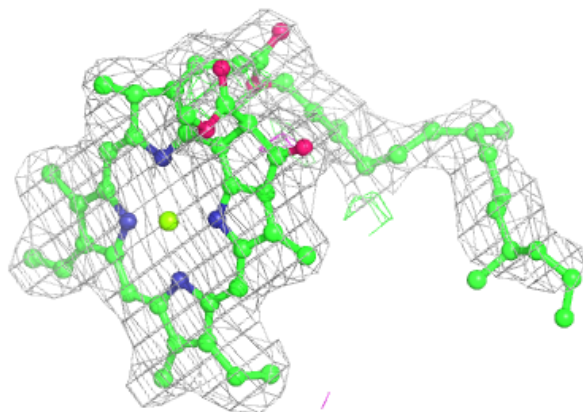
Electron density around CHL C 605:

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



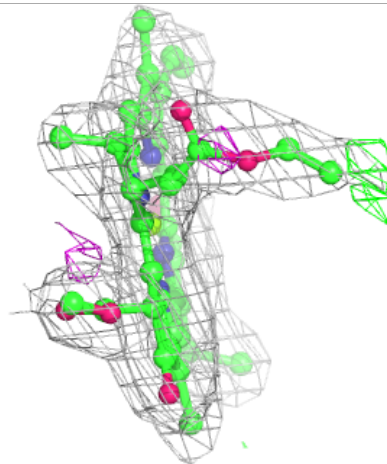
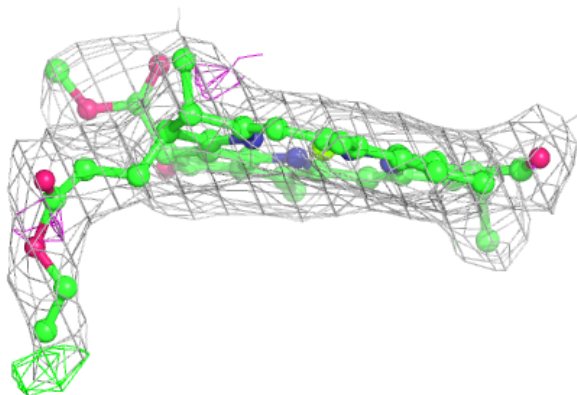
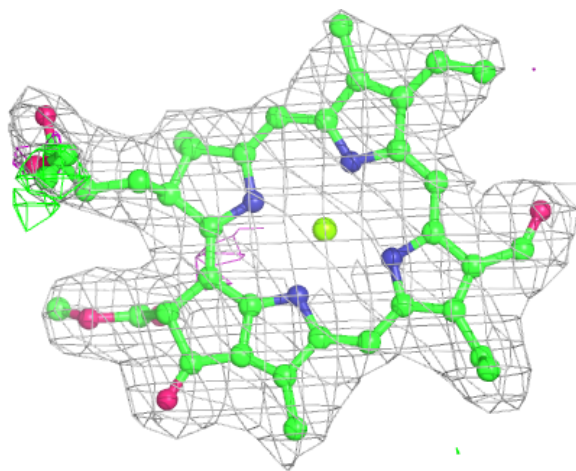
Electron density around CLA G 604:

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



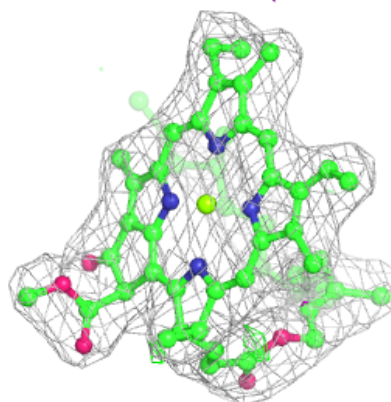
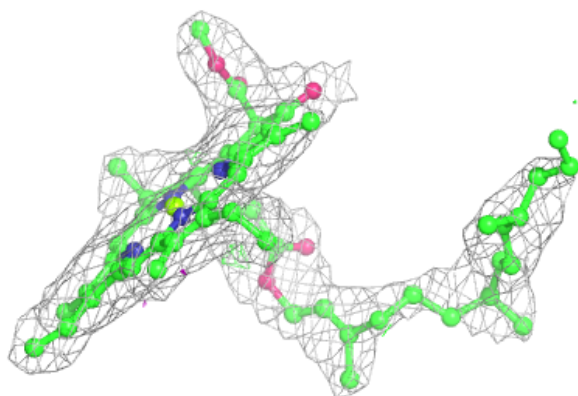
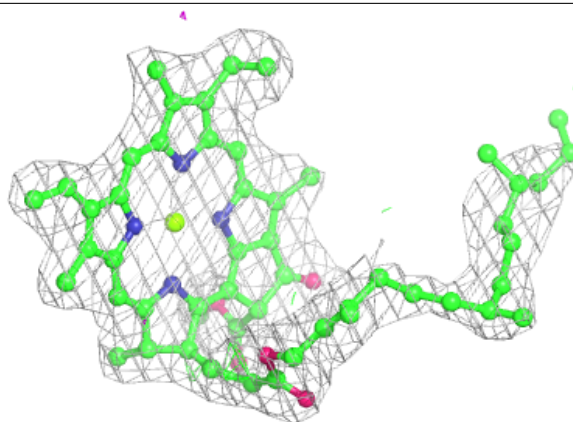
Electron density around CHL H 605:

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

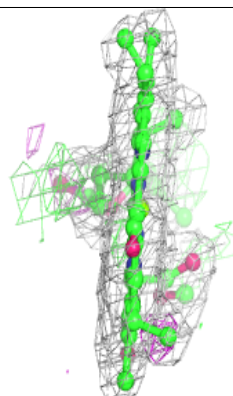
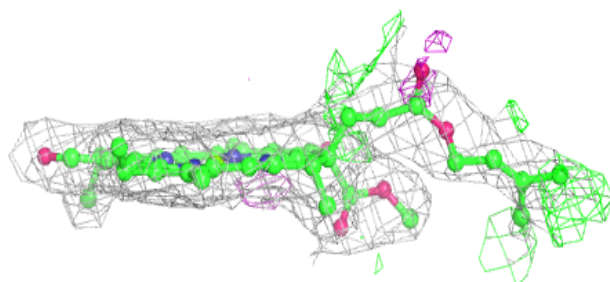
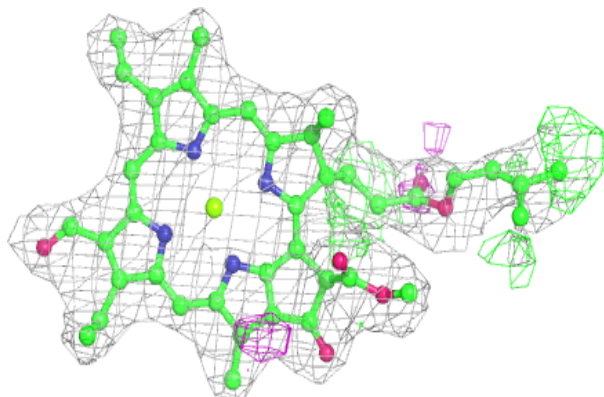


Electron density around CLA A 604:

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

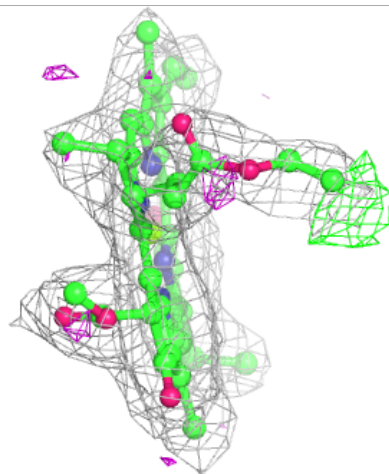
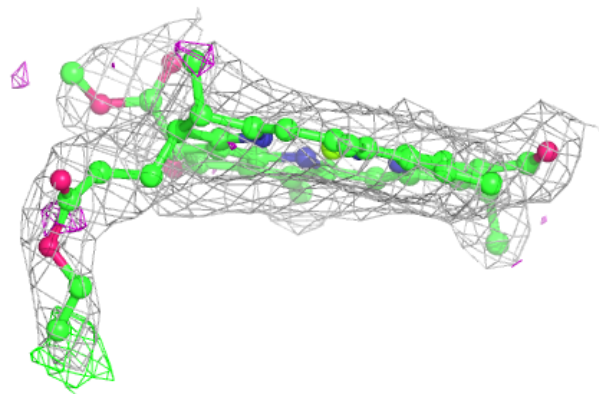
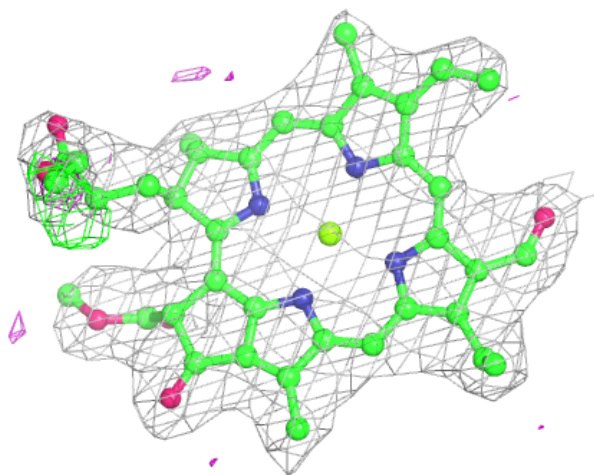
**Electron density around CHL H 606:**

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



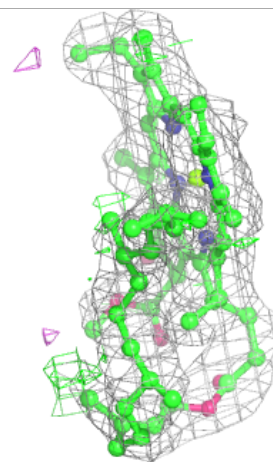
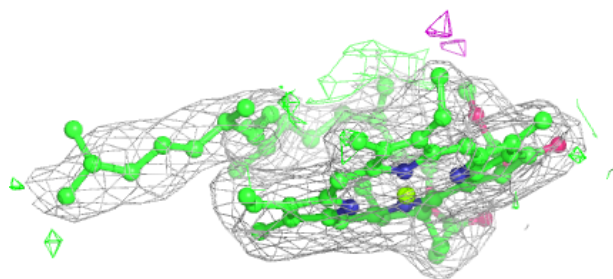
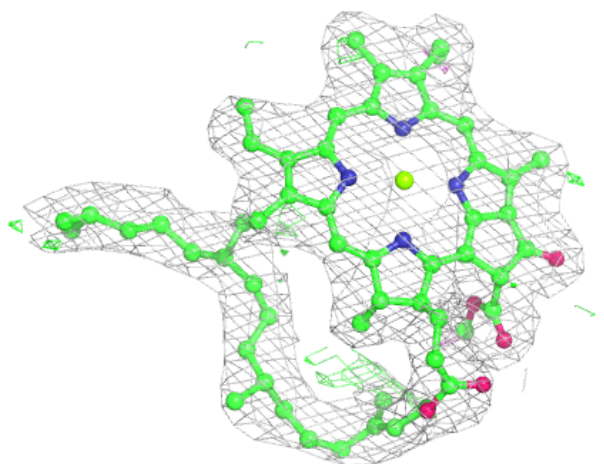
Electron density around CHL I 605:

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



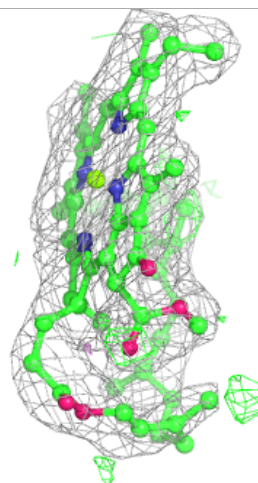
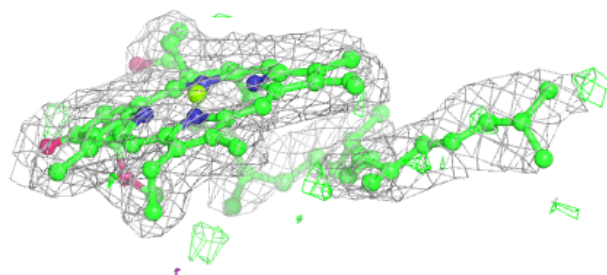
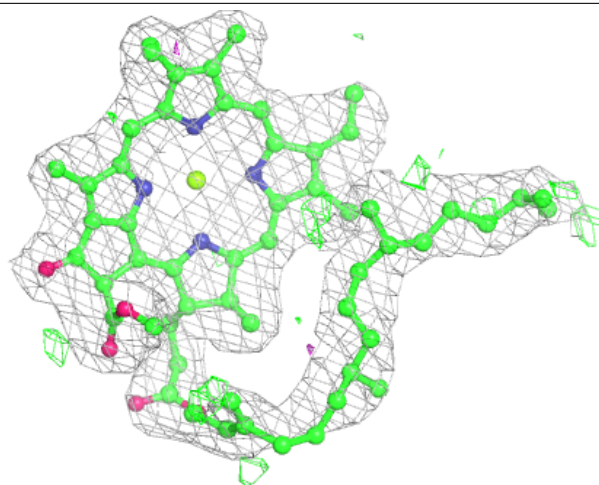
Electron density around CLA C 612:

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



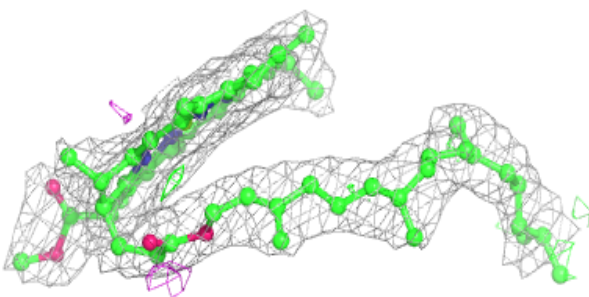
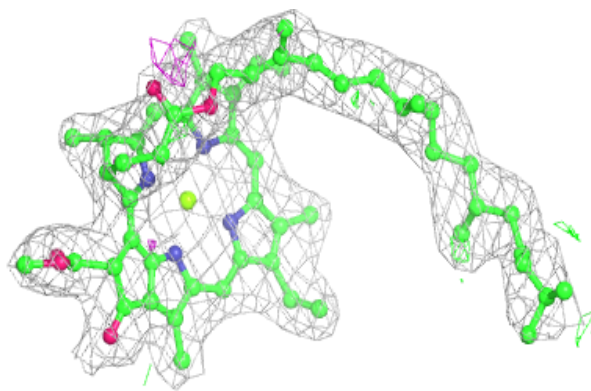
Electron density around CLA F 612:

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

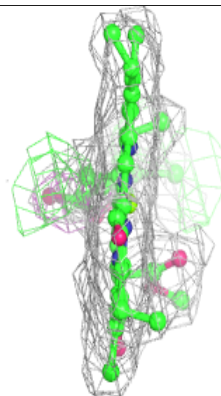
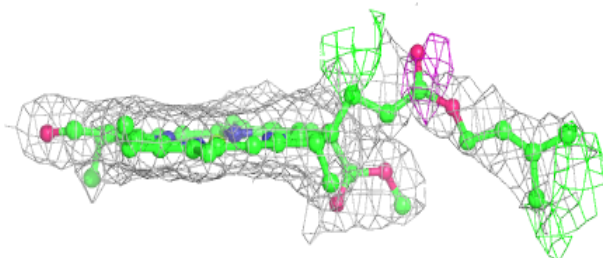
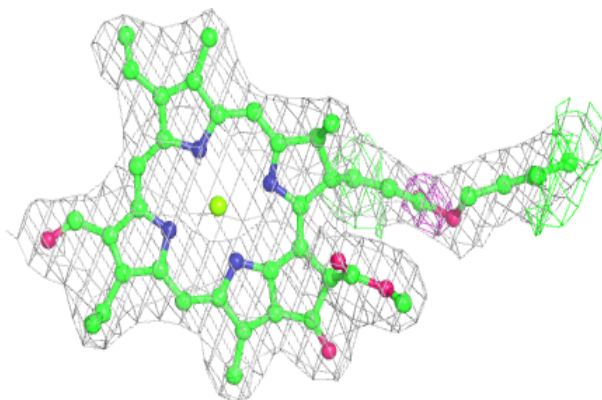


Electron density around CLA I 610:

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

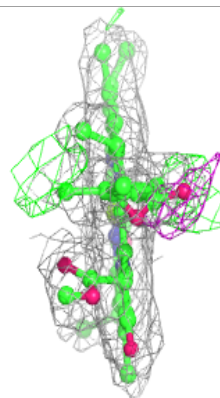
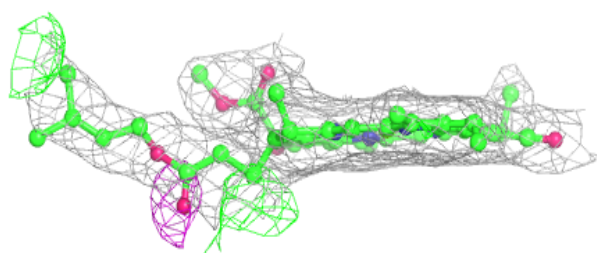
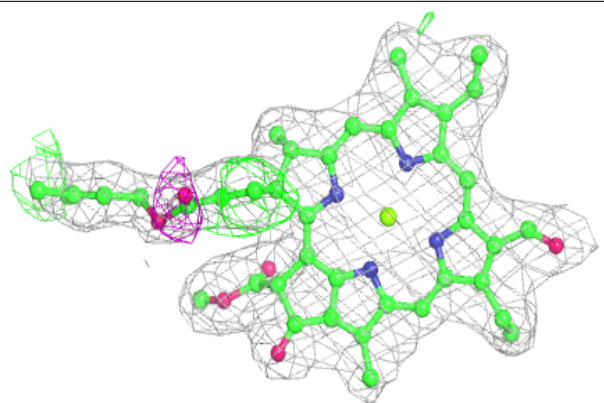
**Electron density around CHL C 606:**

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

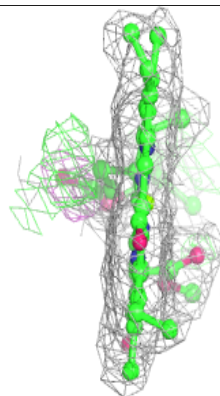
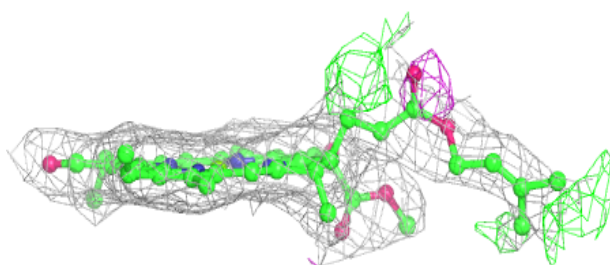
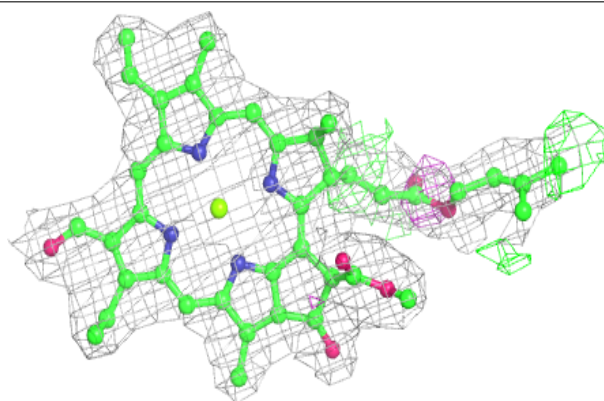


Electron density around CHL E 606:

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

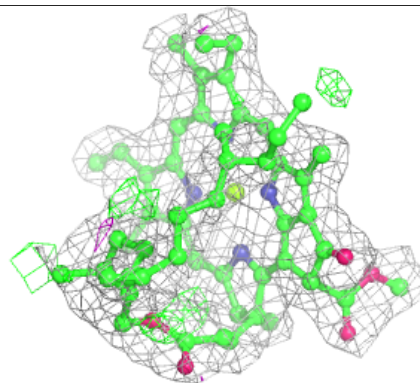
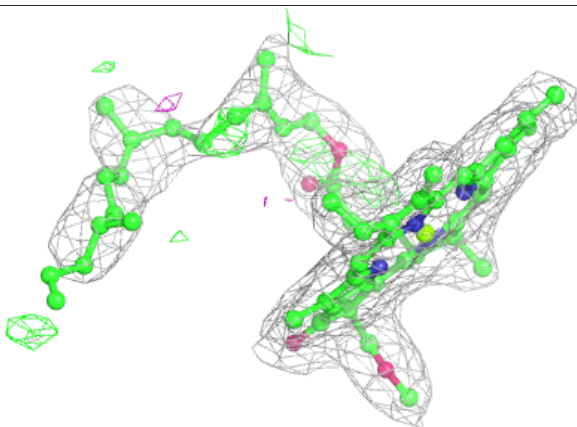
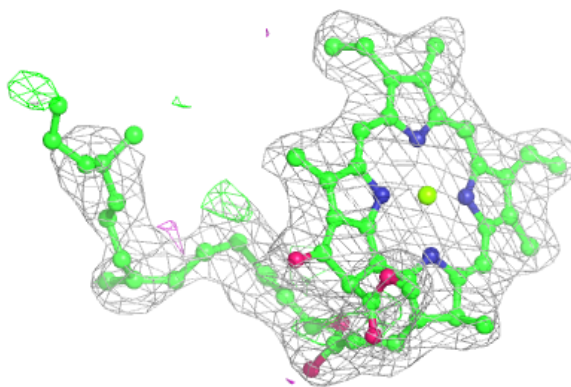
**Electron density around CHL I 606:**

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



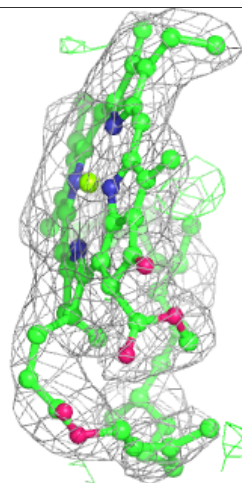
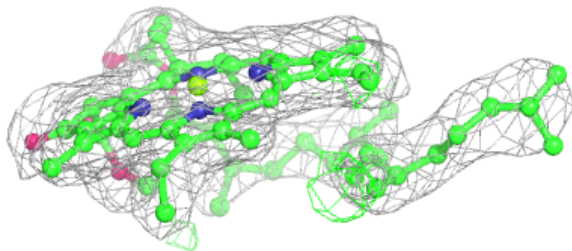
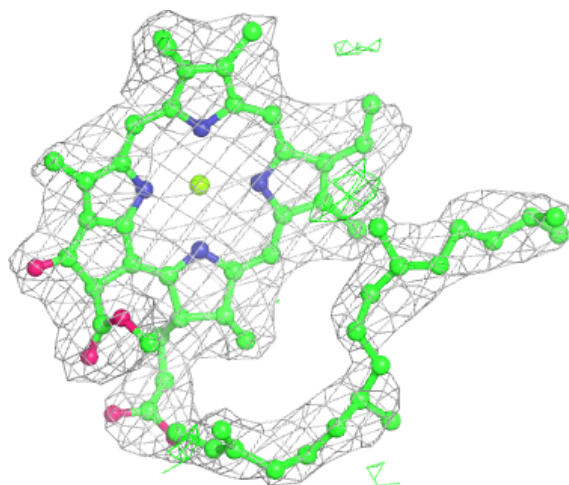
Electron density around CLA F 604:

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



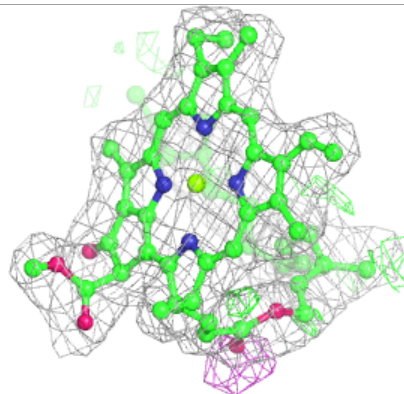
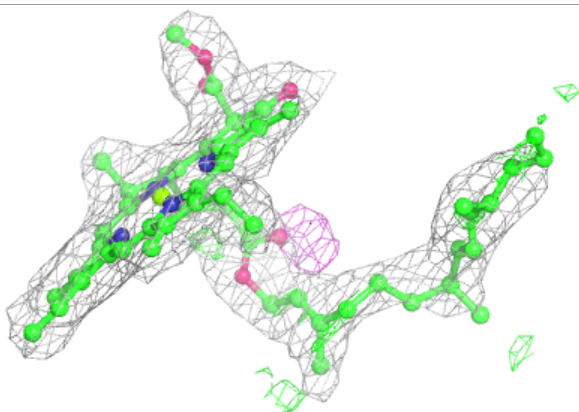
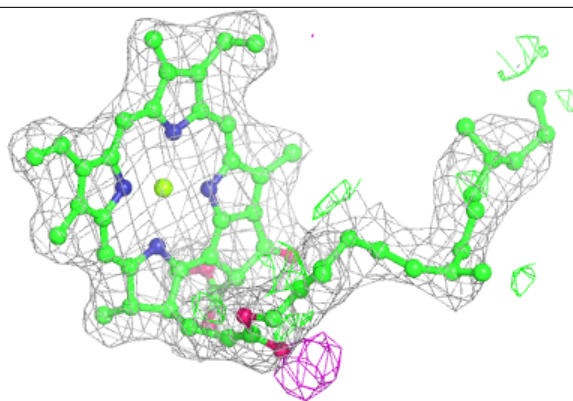
Electron density around CLA A 612:

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

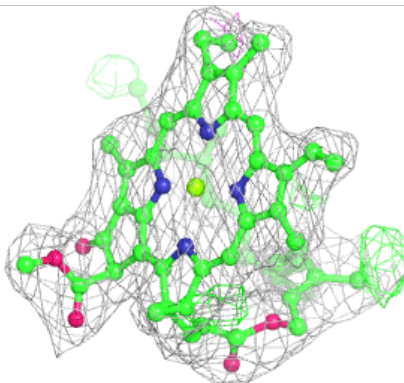
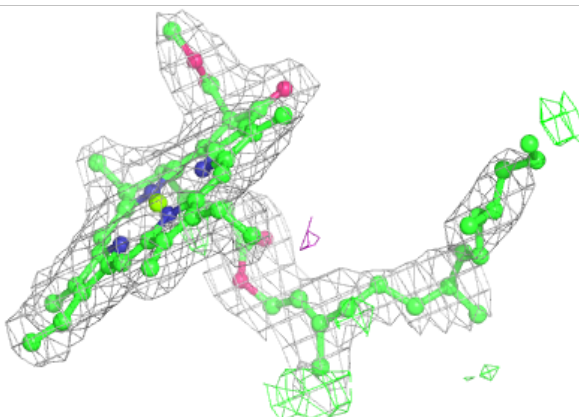
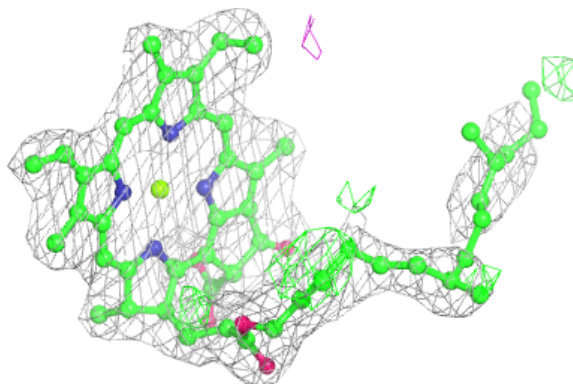


Electron density around CLA C 604:

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

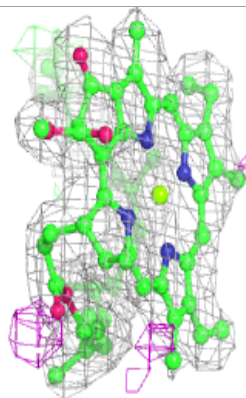
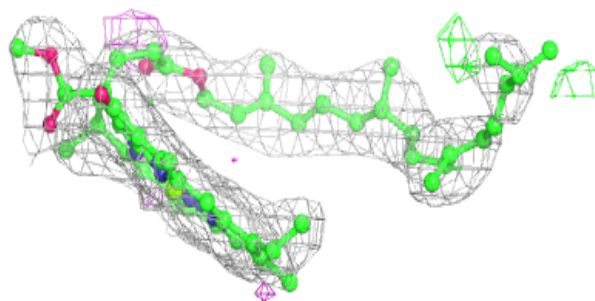
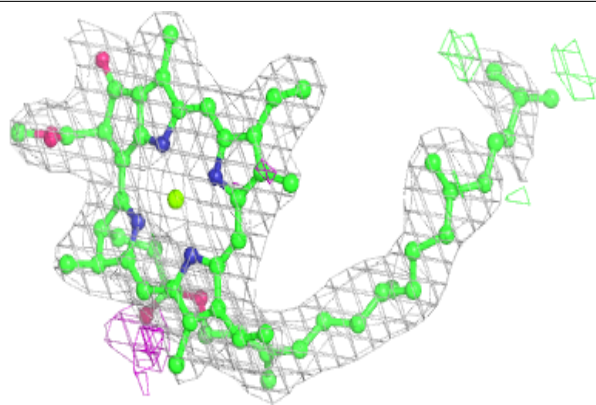
**Electron density around CLA I 604:**

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



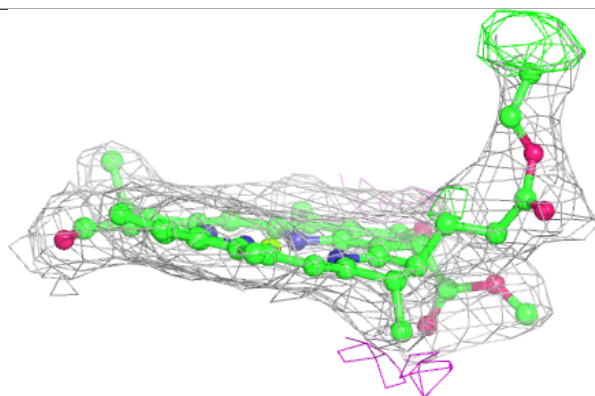
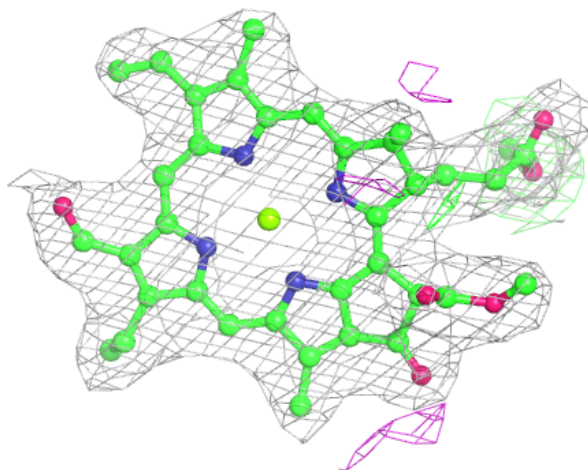
Electron density around CLA H 610:

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



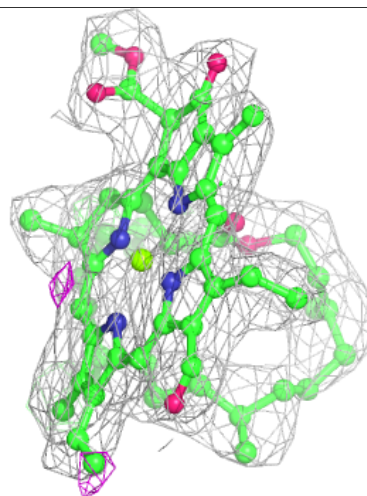
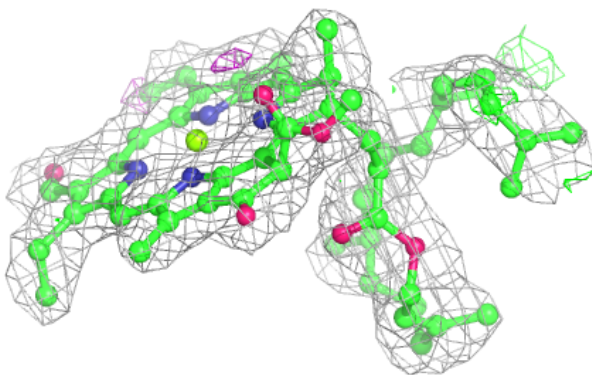
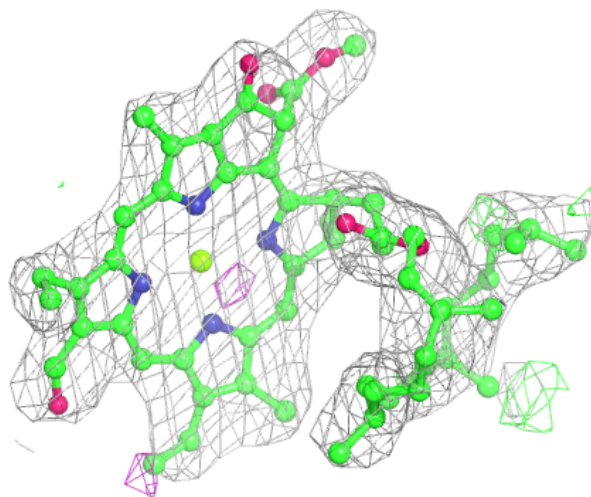
Electron density around CHL F 605:

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



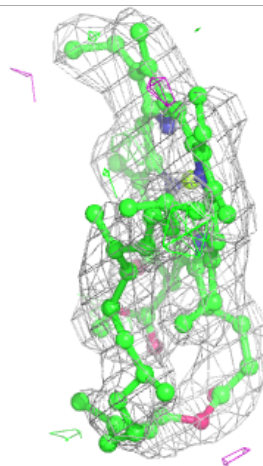
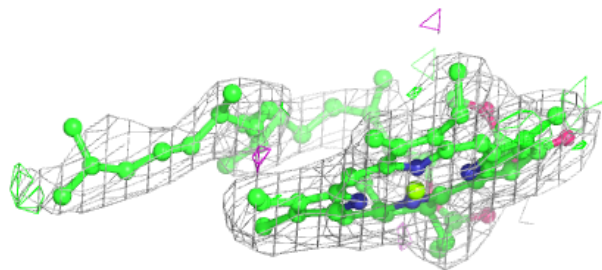
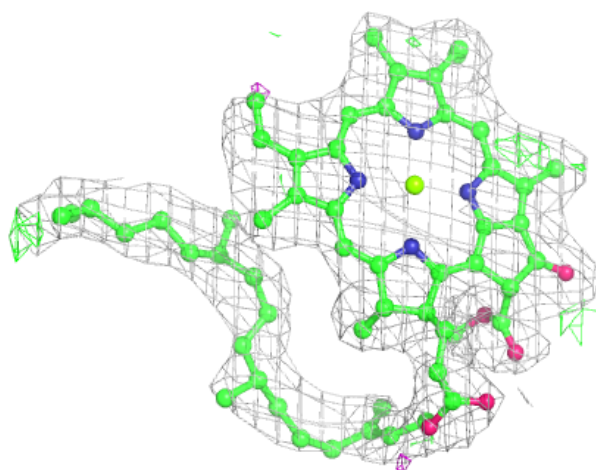
Electron density around CHL G 608:

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



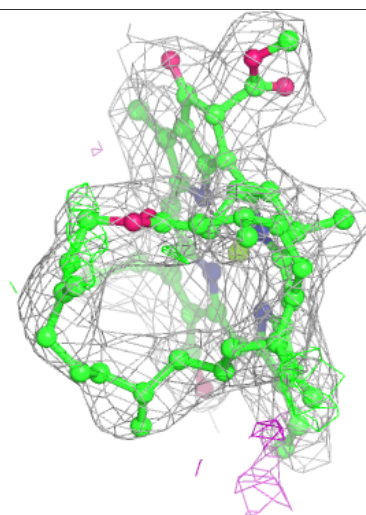
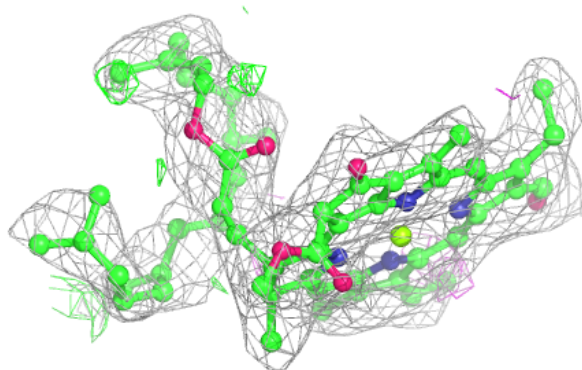
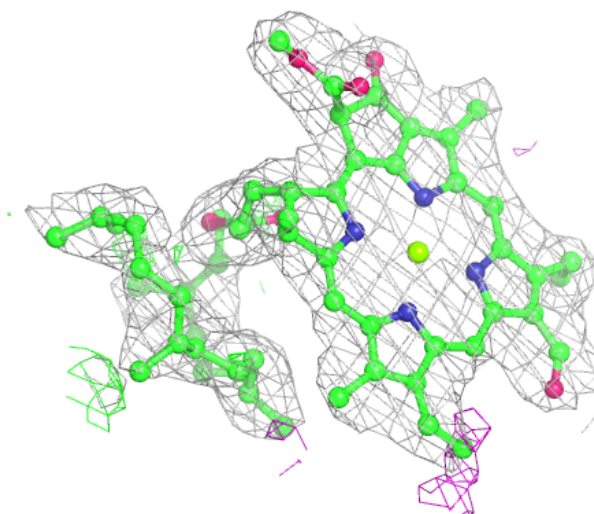
Electron density around CLA I 612:

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



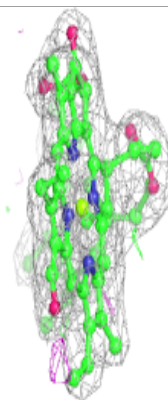
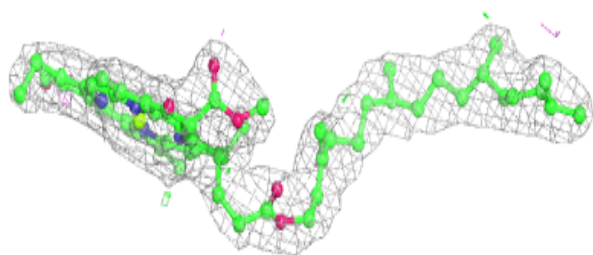
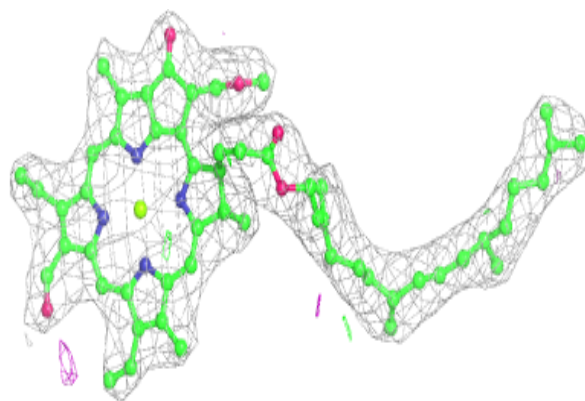
Electron density around CHL I 608:

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

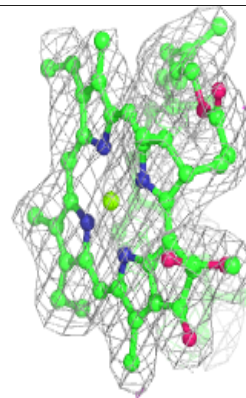
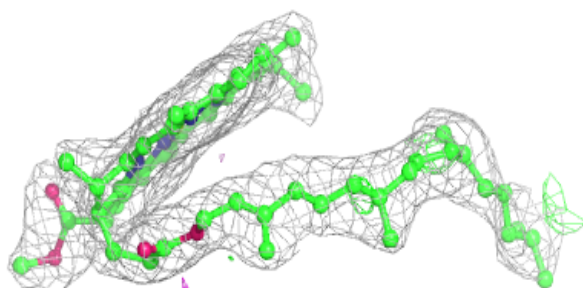
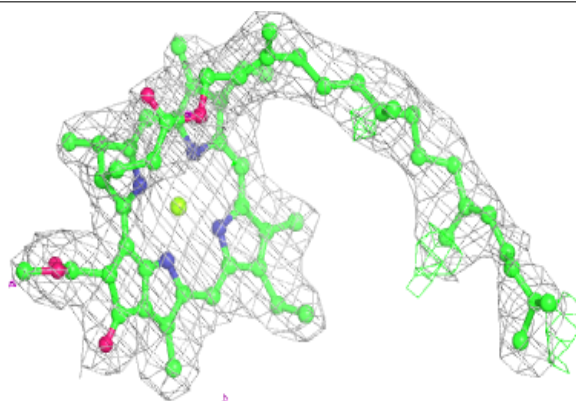


Electron density around CHL G 601:

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

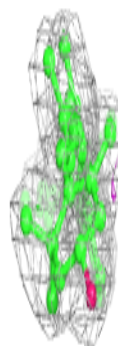
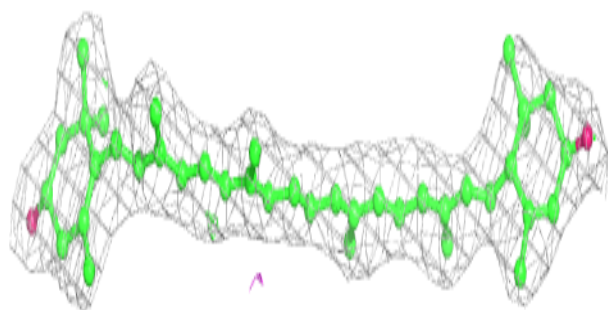
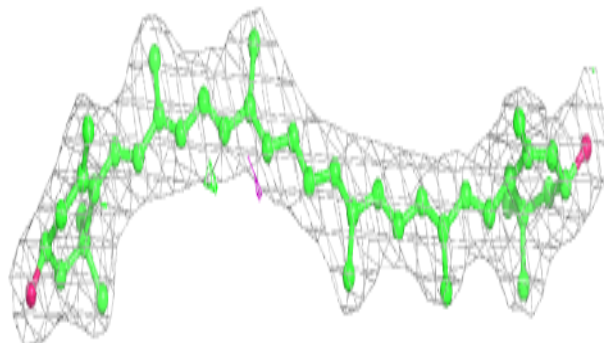
**Electron density around CLA J 610:**

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



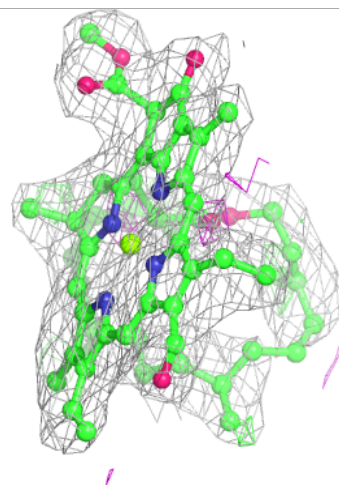
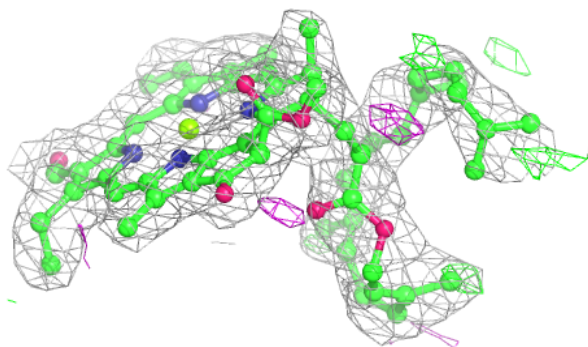
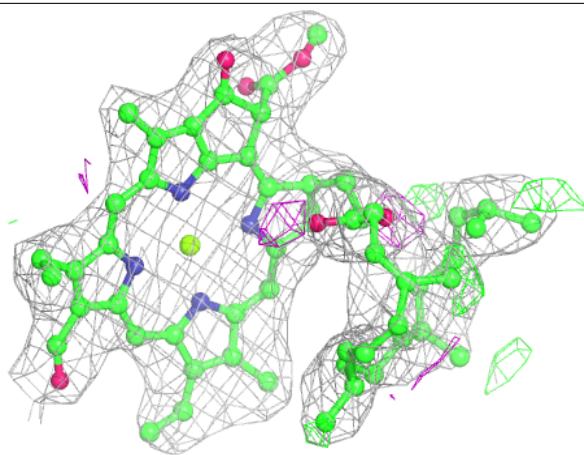
Electron density around LUT G 6620:

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



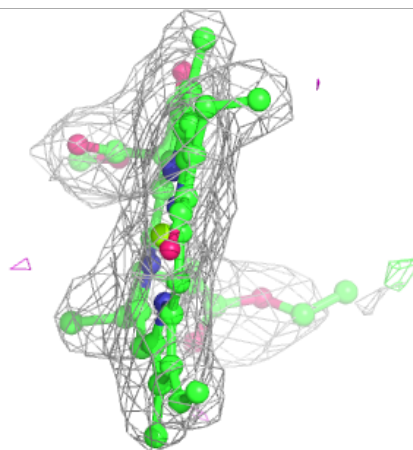
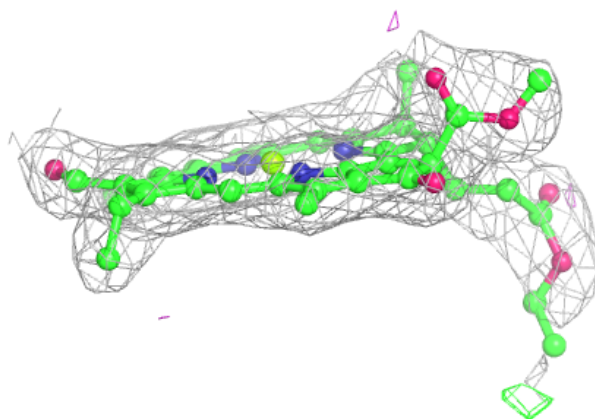
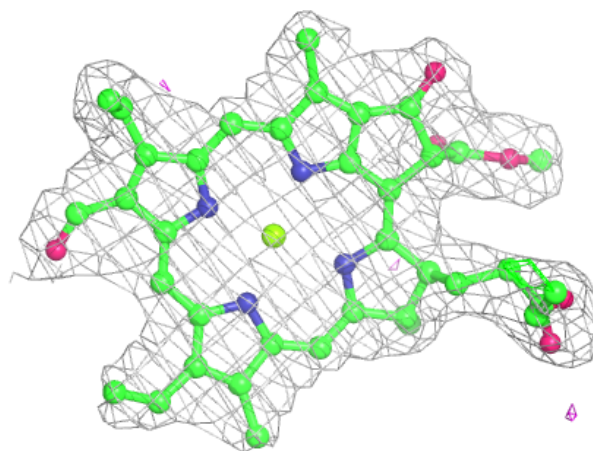
Electron density around CHL F 608:

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



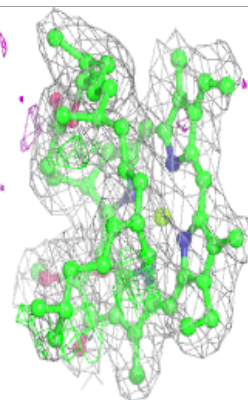
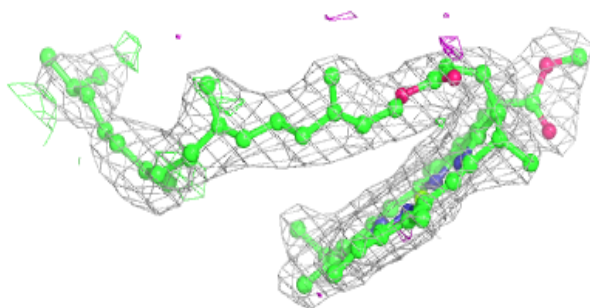
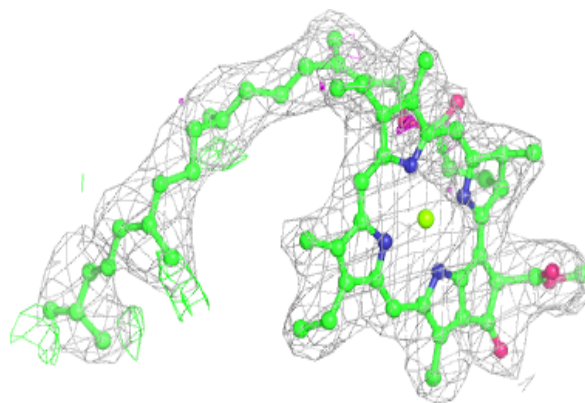
Electron density around CHL D 605:

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



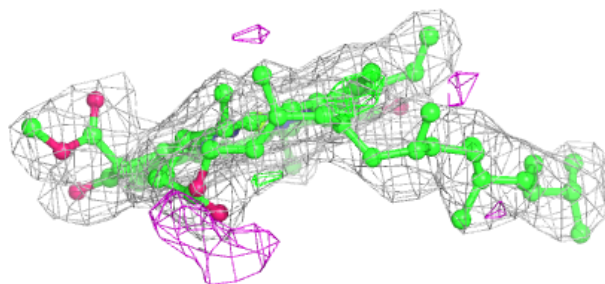
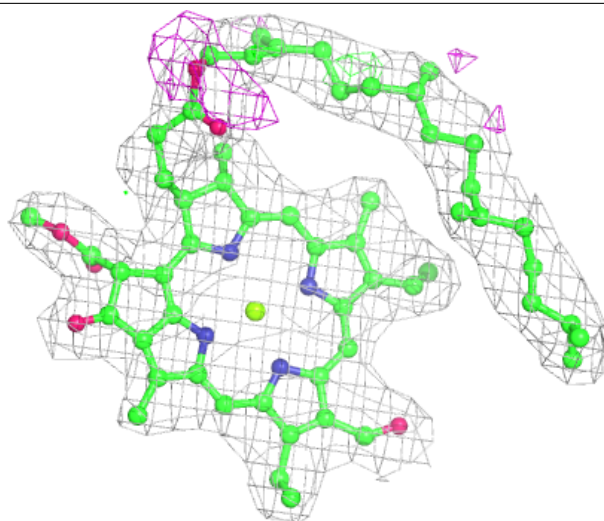
Electron density around CLA C 610:

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



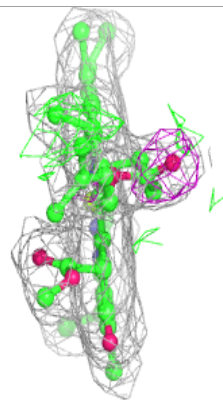
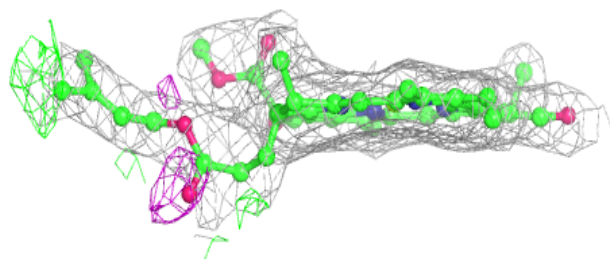
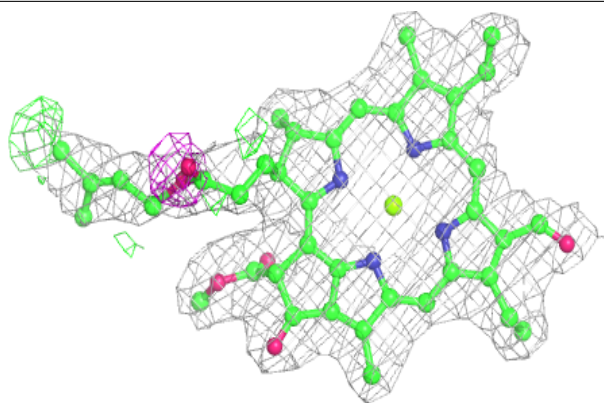
Electron density around CHL A 607:

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

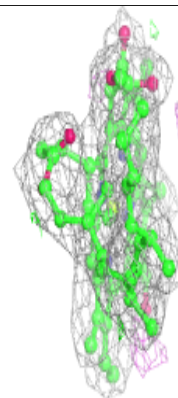
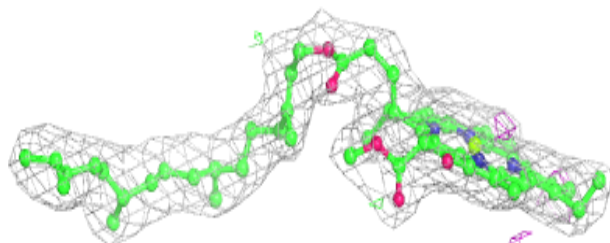
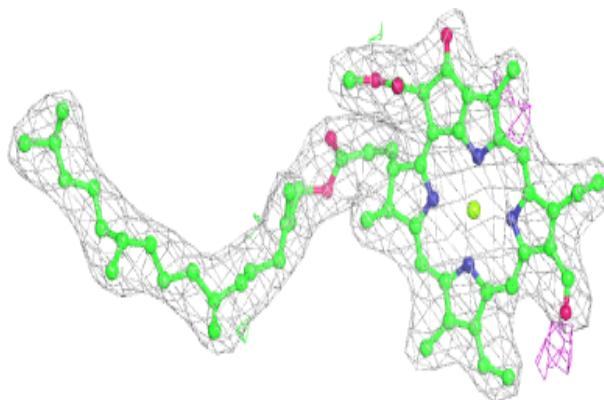


Electron density around CHL B 606:

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

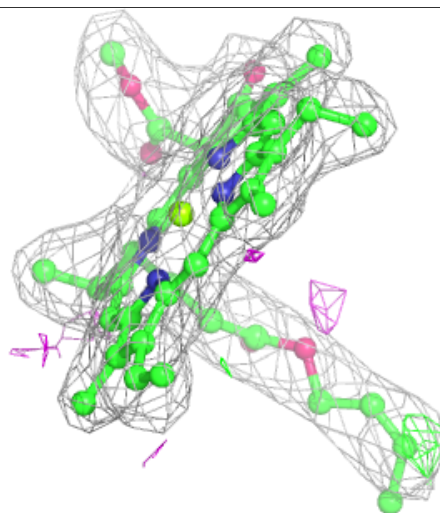
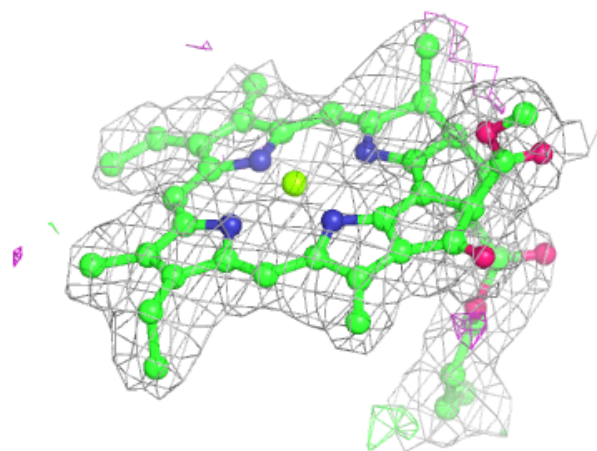
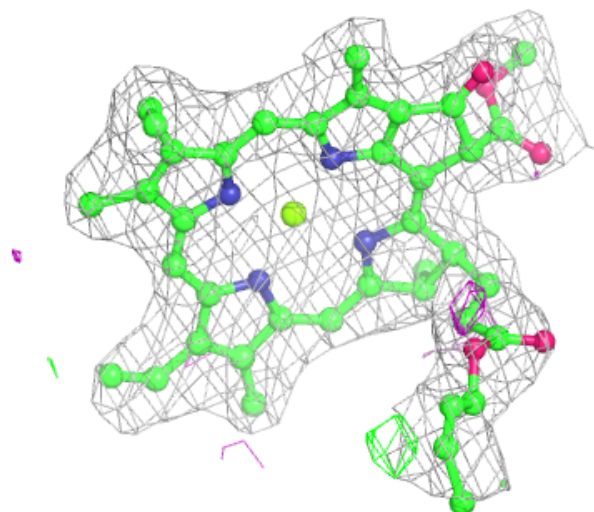
**Electron density around CHL I 601:**

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



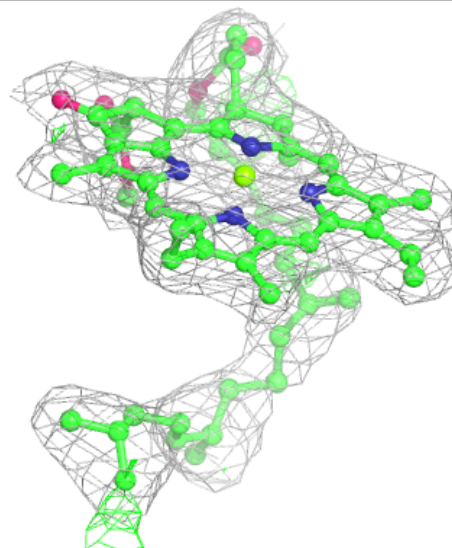
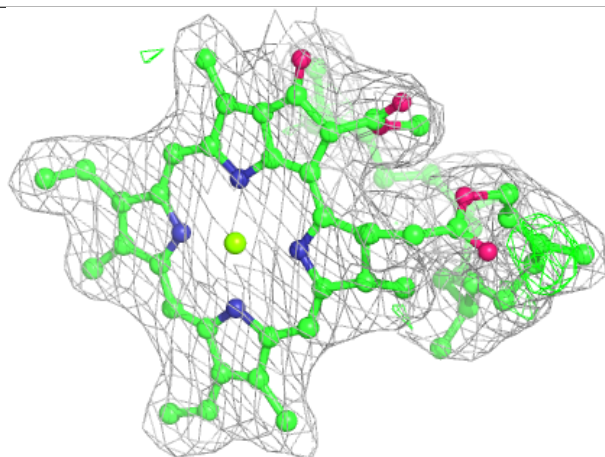
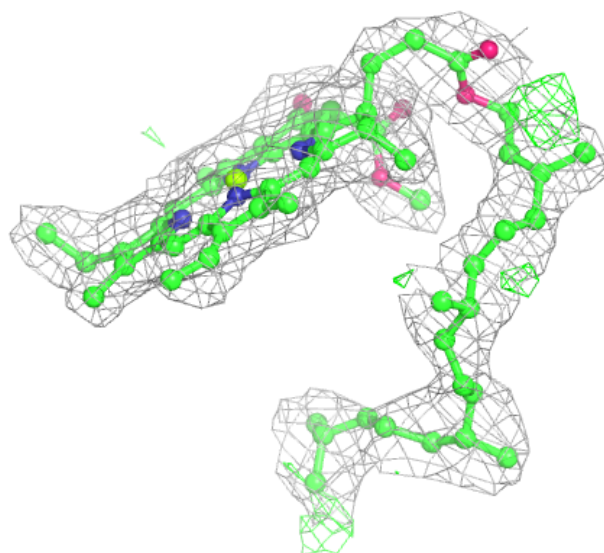
Electron density around CLA I 614:

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



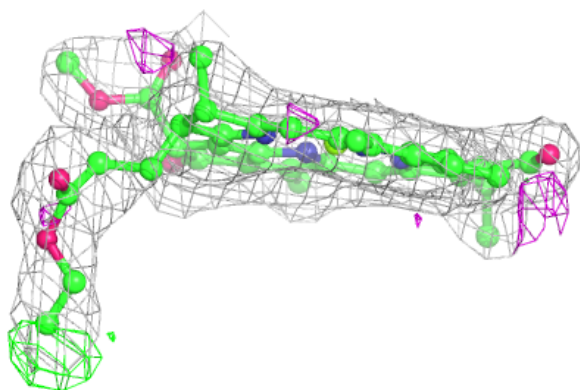
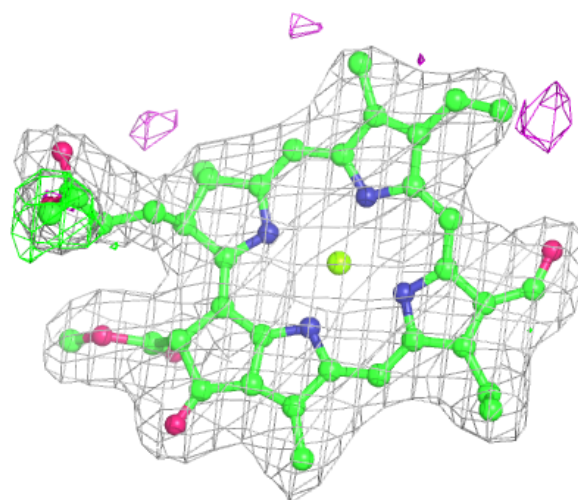
Electron density around CLA G 603:

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



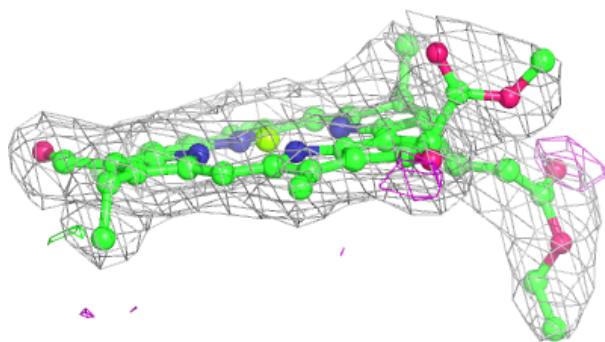
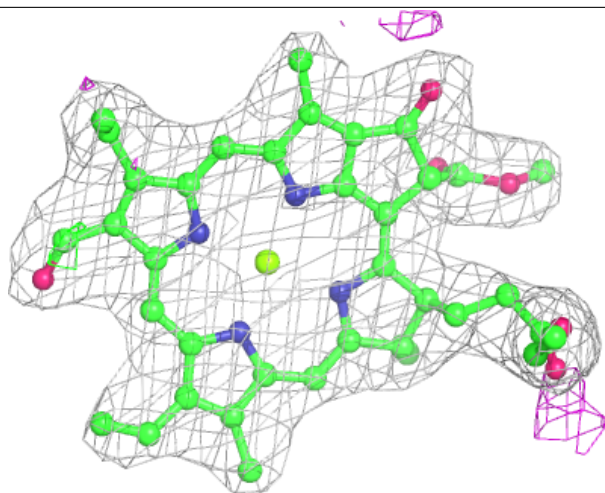
Electron density around CHL A 605:

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



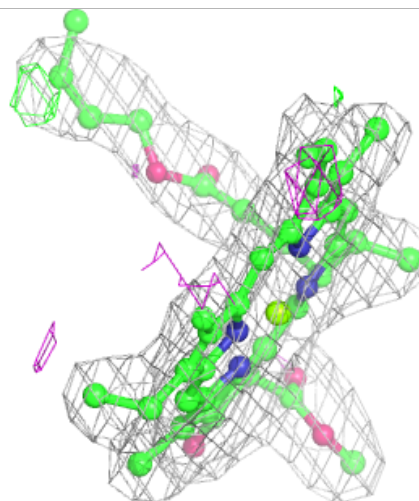
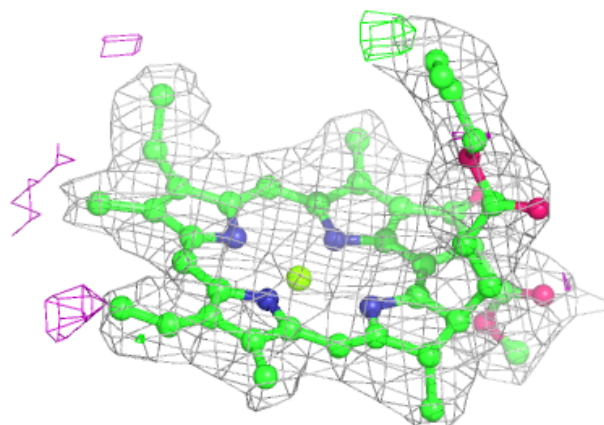
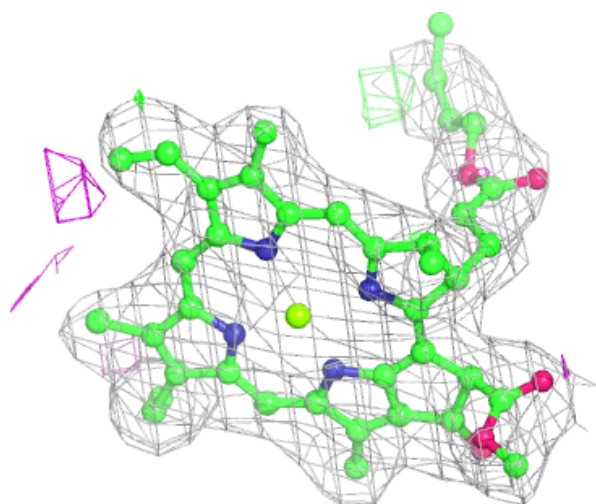
Electron density around CHL E 605:

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



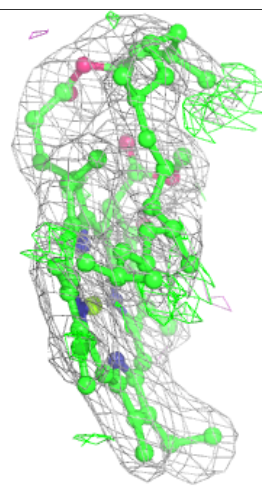
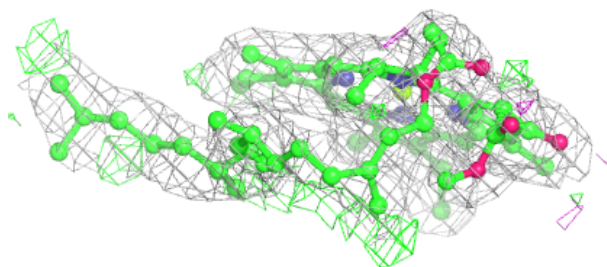
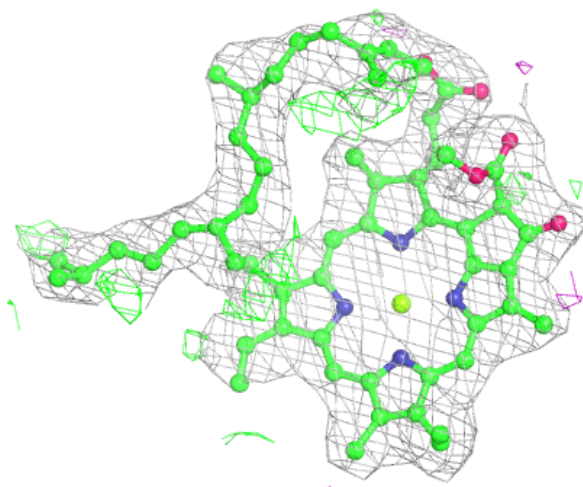
Electron density around CLA B 614:

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



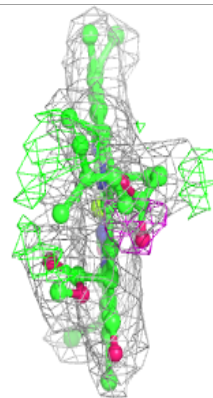
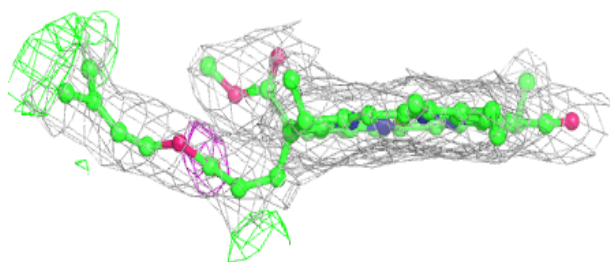
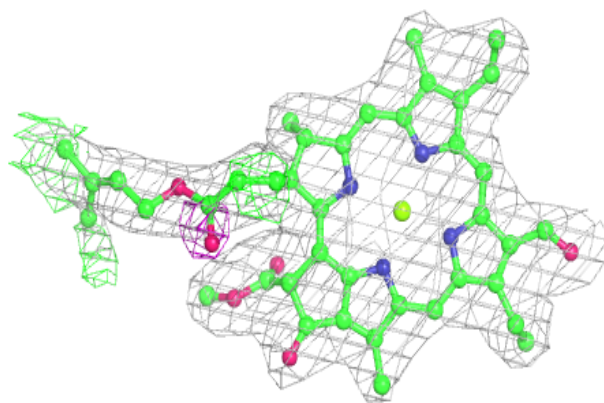
Electron density around CLA D 612:

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



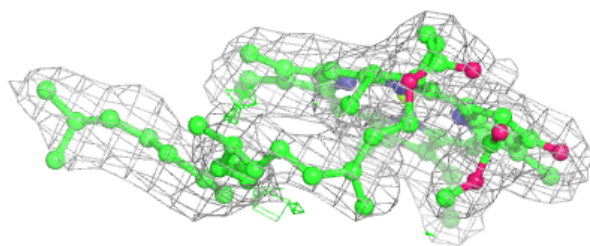
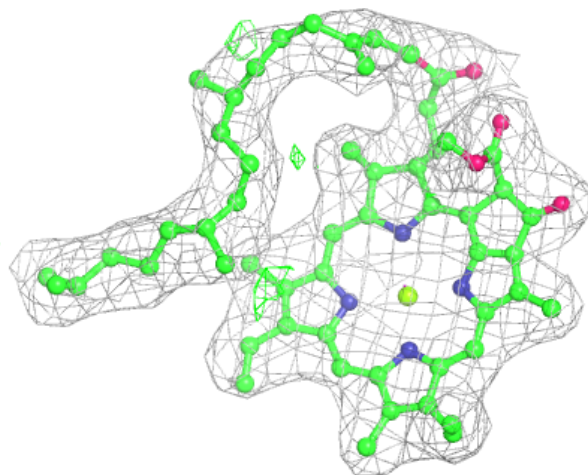
Electron density around CHL G 606:

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



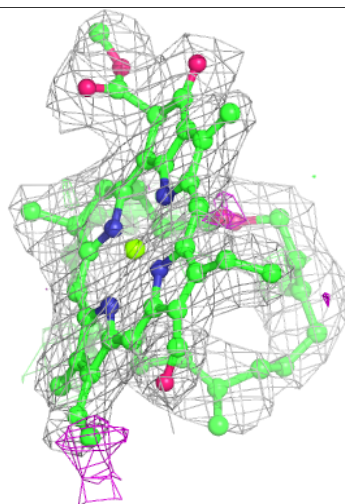
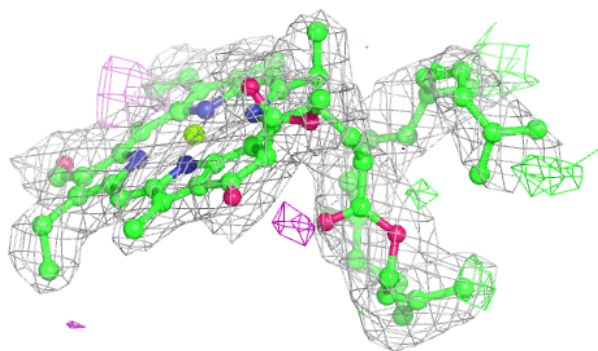
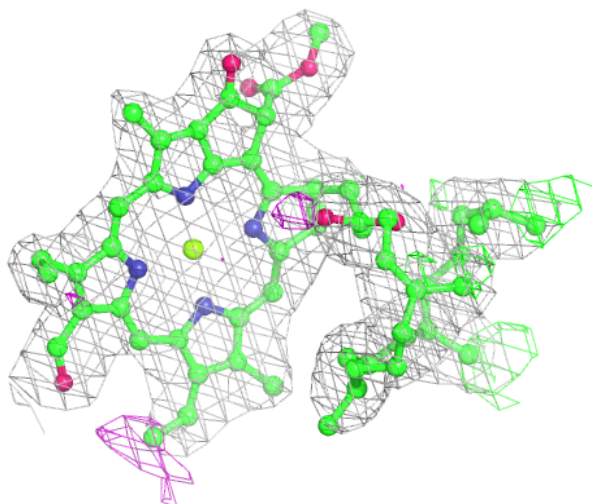
Electron density around CLA E 612:

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



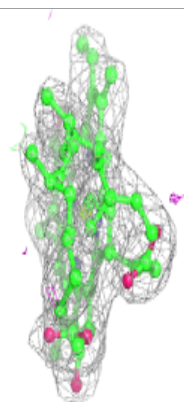
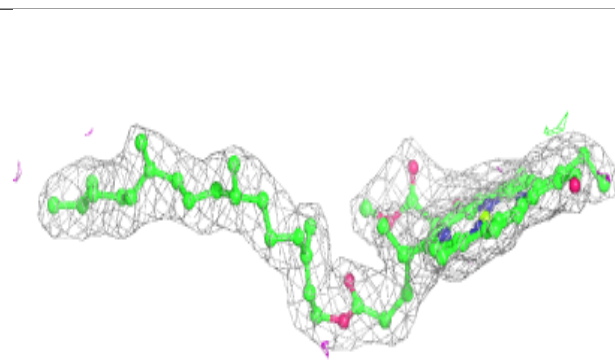
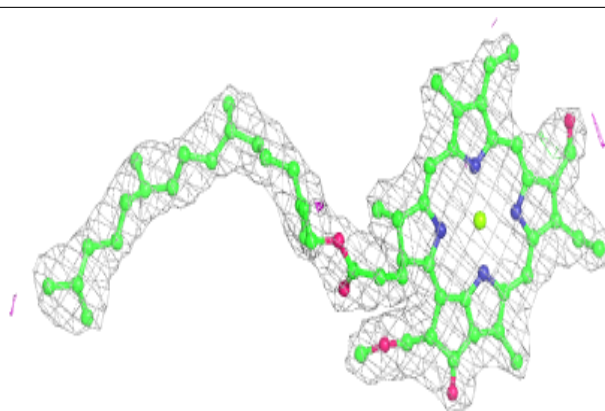
Electron density around CHL J 608:

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



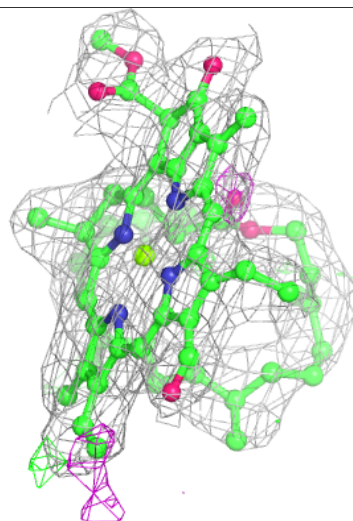
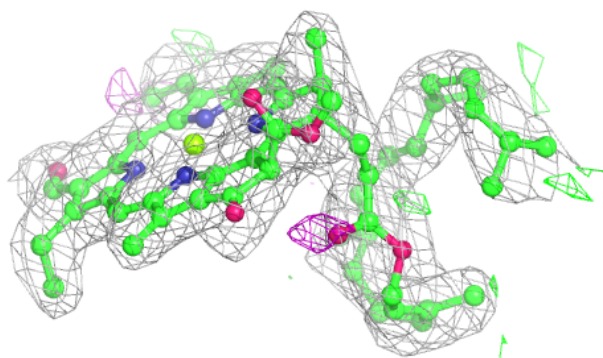
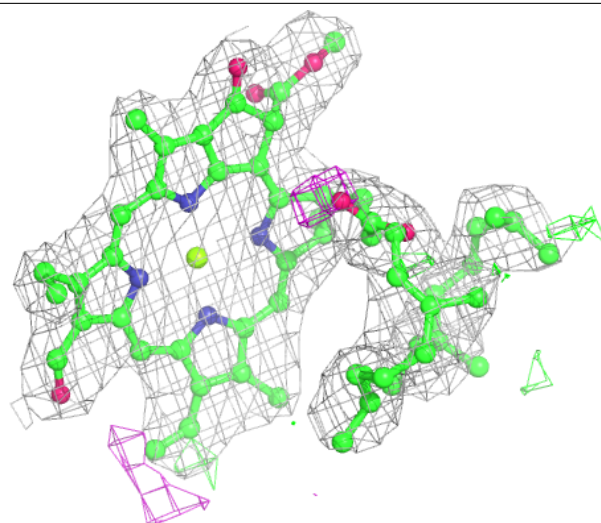
Electron density around CHL H 601:

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



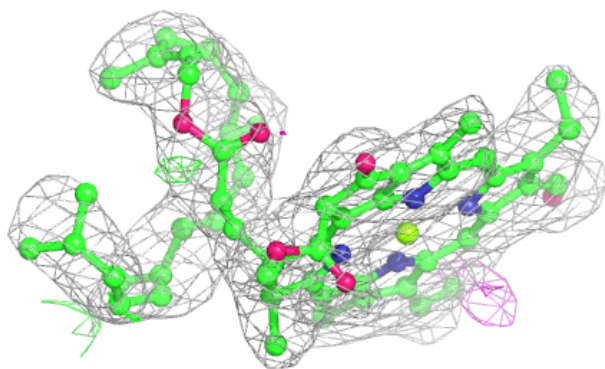
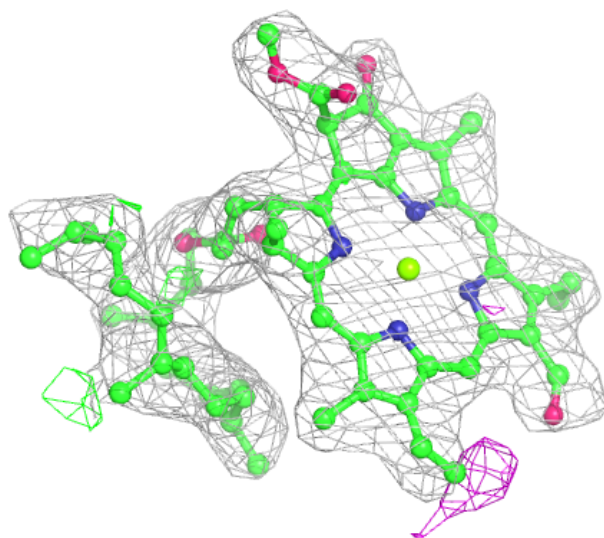
Electron density around CHL B 608:

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



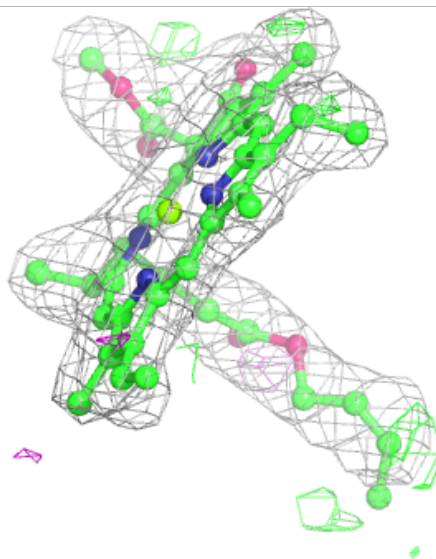
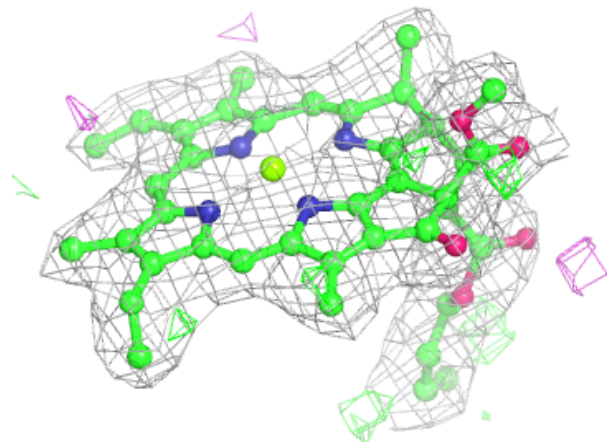
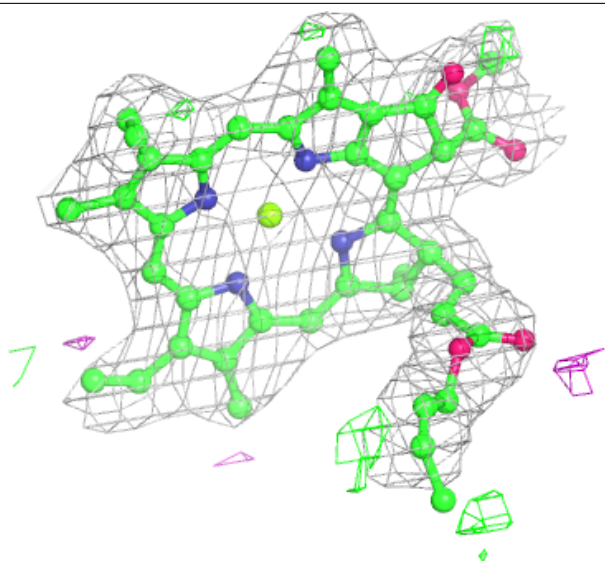
Electron density around CHL H 608:

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



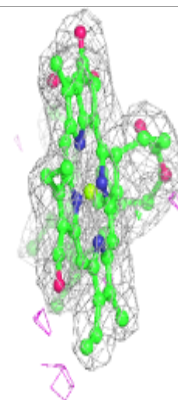
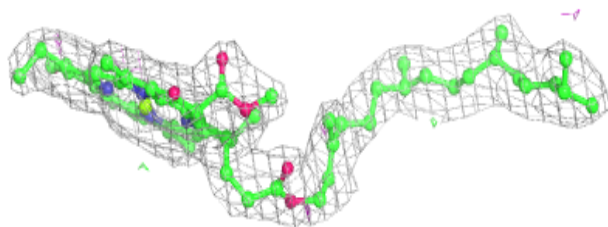
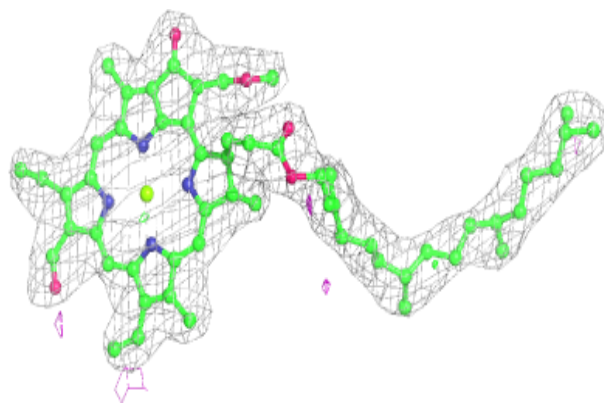
Electron density around CLA H 614:

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



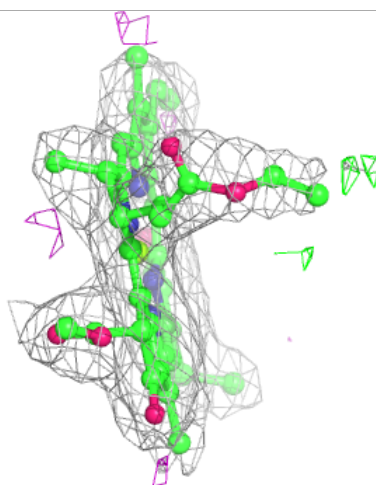
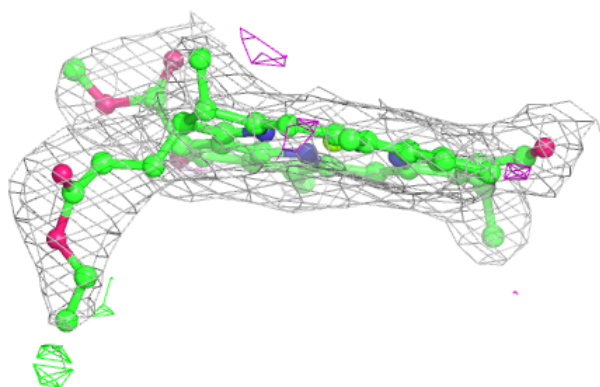
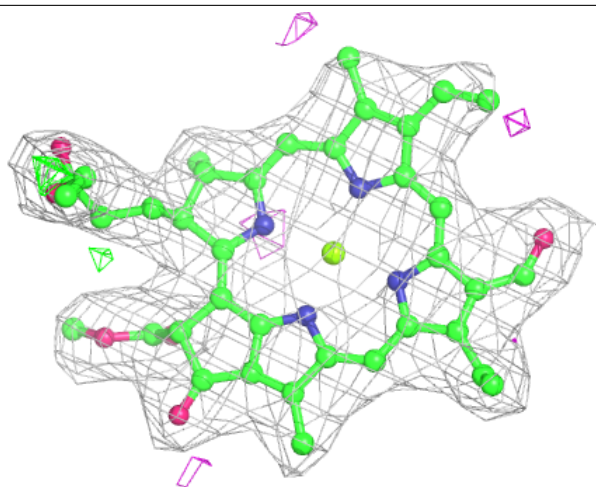
Electron density around CHL B 601:

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



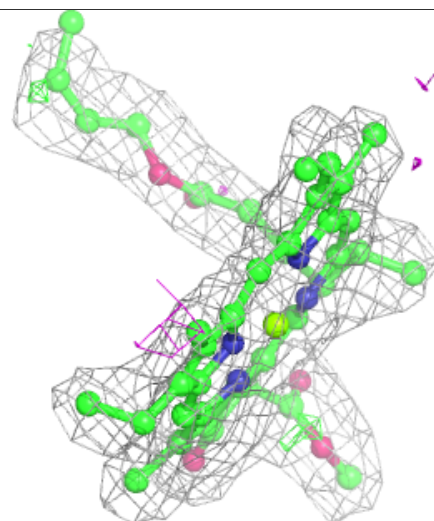
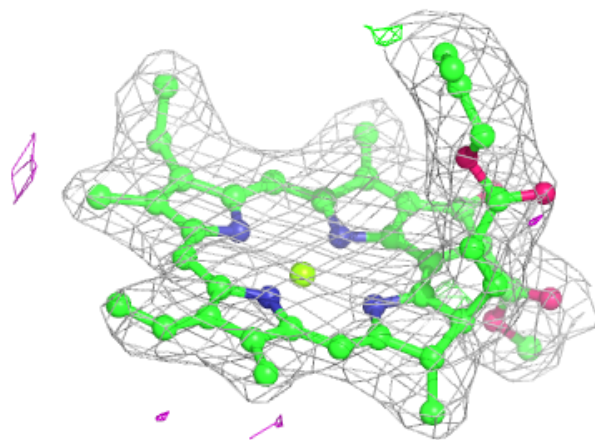
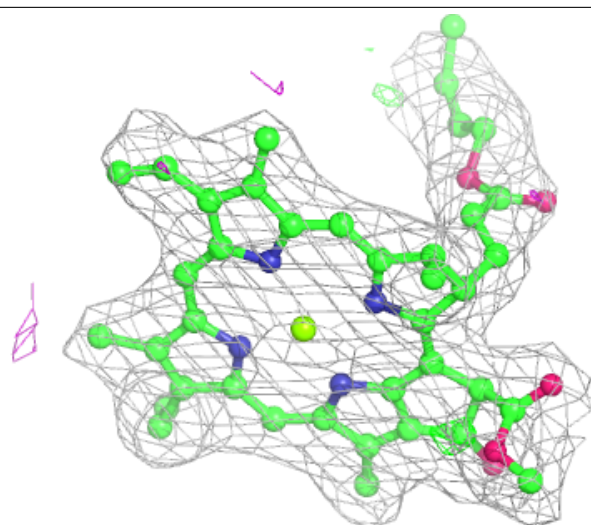
Electron density around CHL J 605:

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



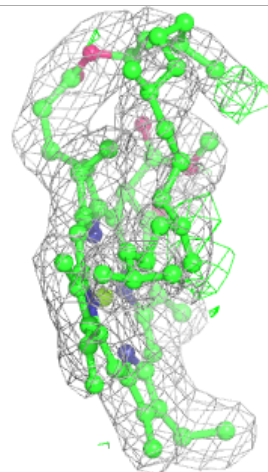
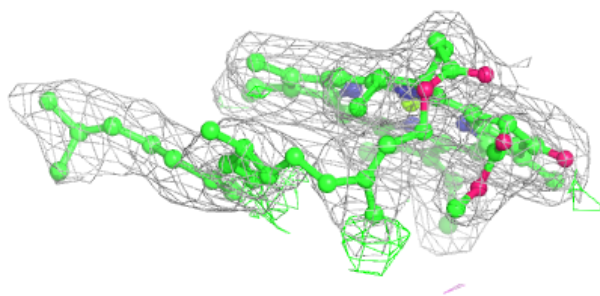
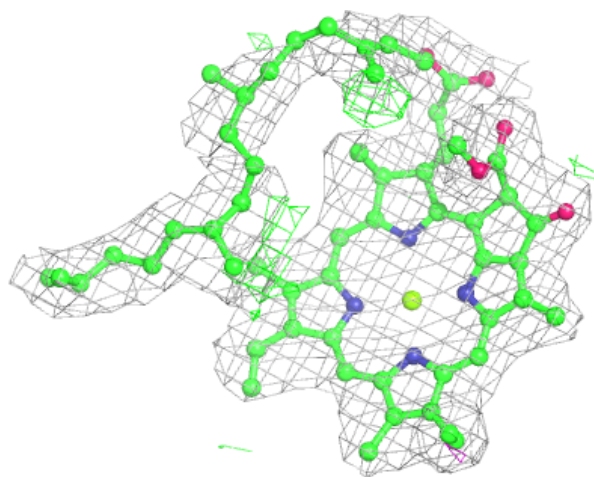
Electron density around CLA J 614:

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



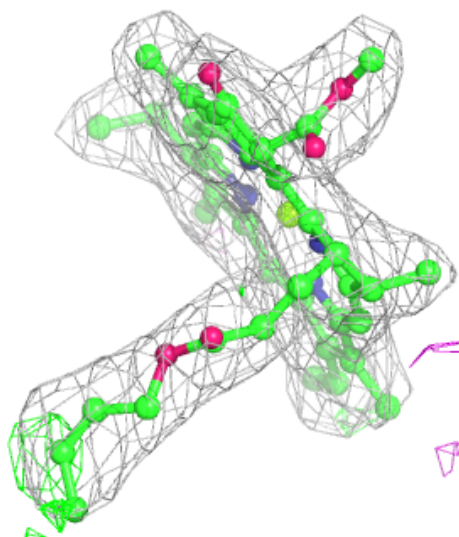
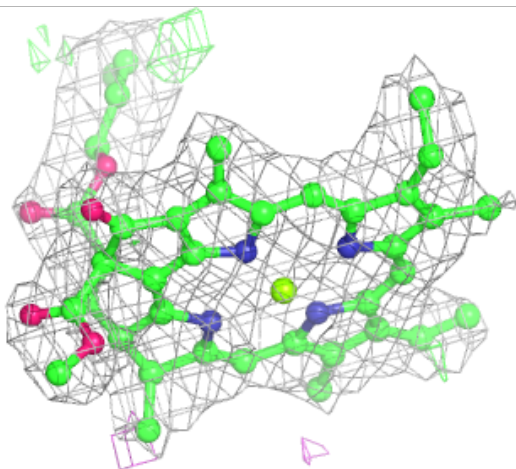
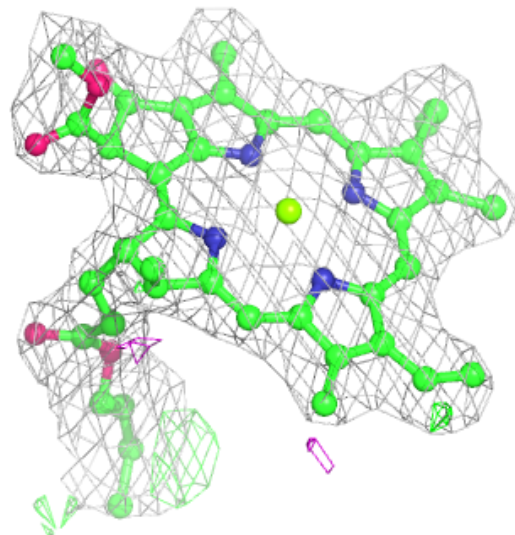
Electron density around CLA B 612:

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



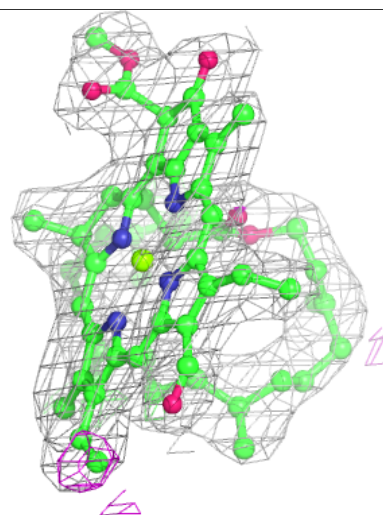
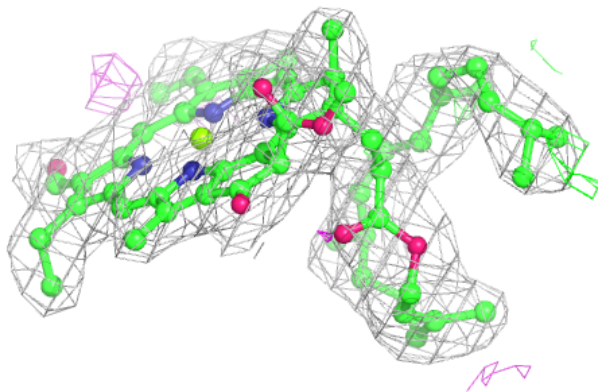
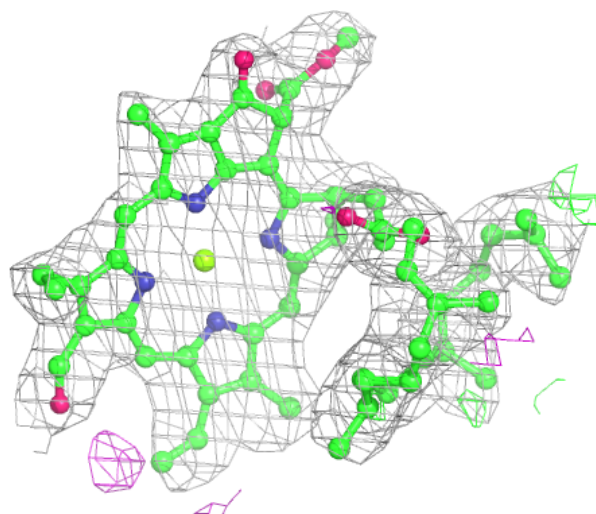
Electron density around CLA A 614:

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



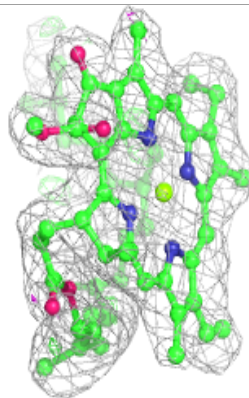
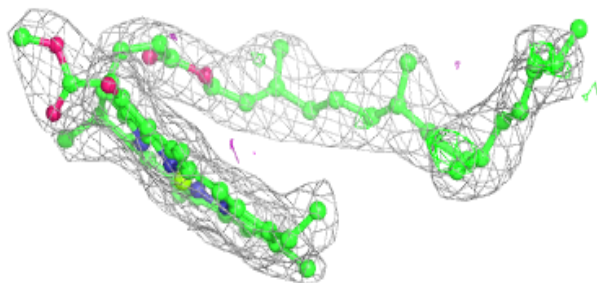
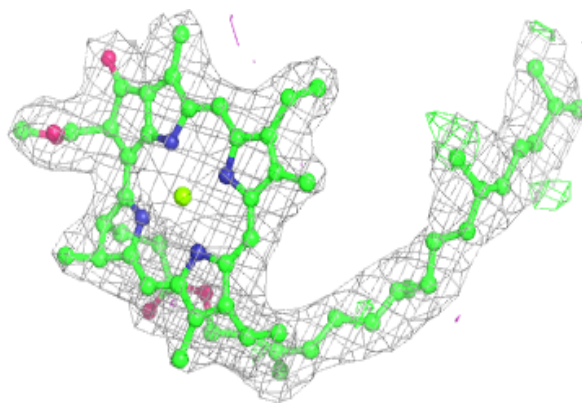
Electron density around CHL C 608:

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



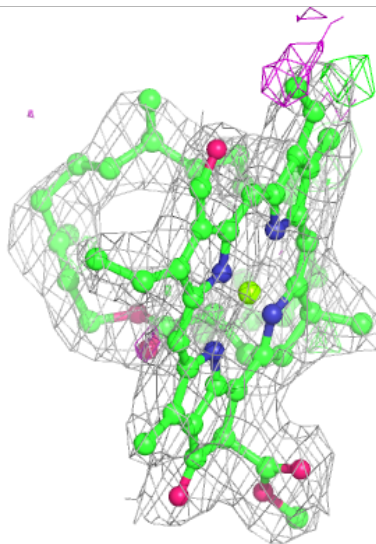
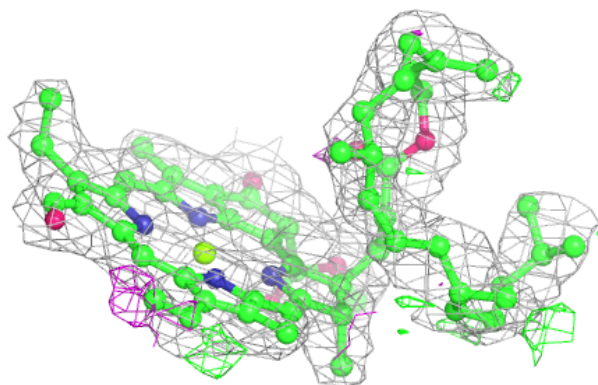
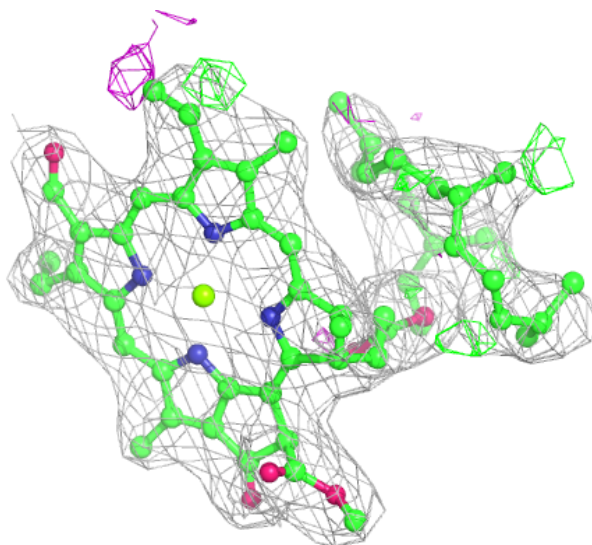
Electron density around CLA E 610:

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



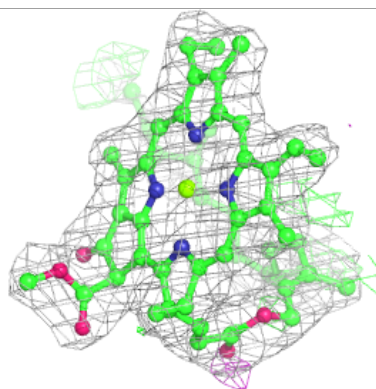
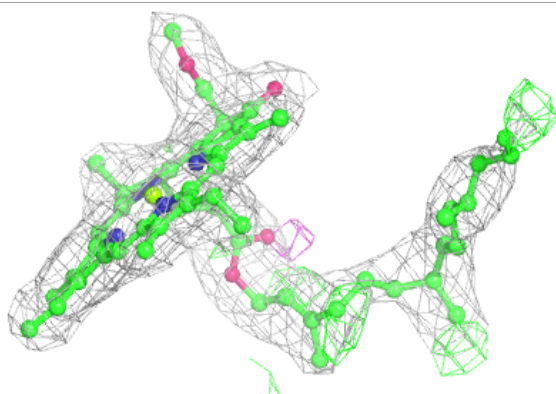
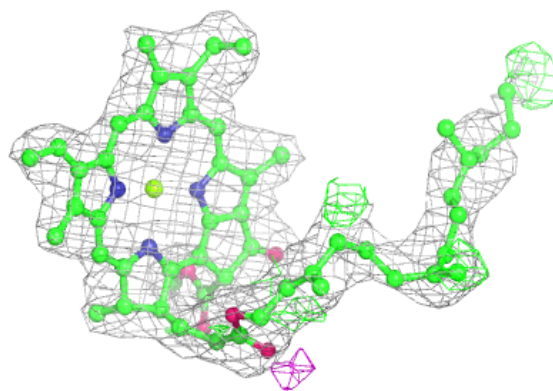
Electron density around CHL D 608:

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

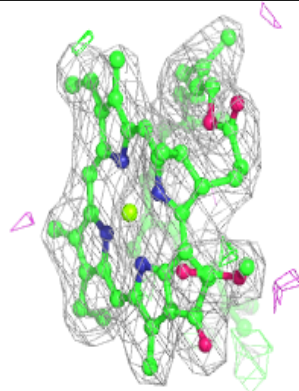
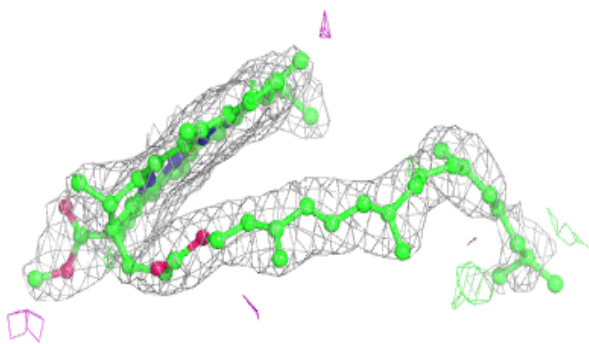
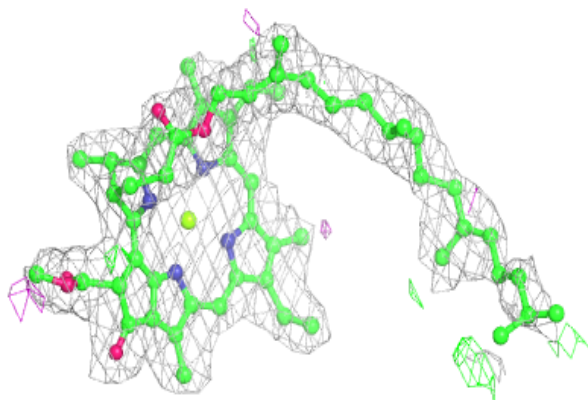


Electron density around CLA D 604:

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

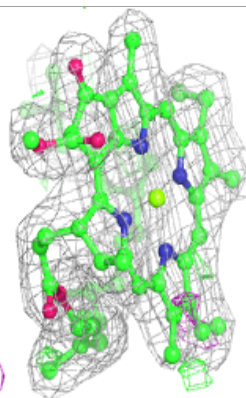
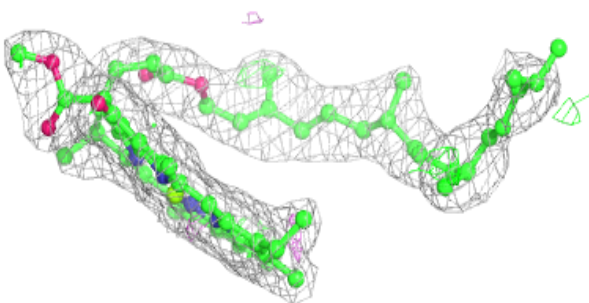
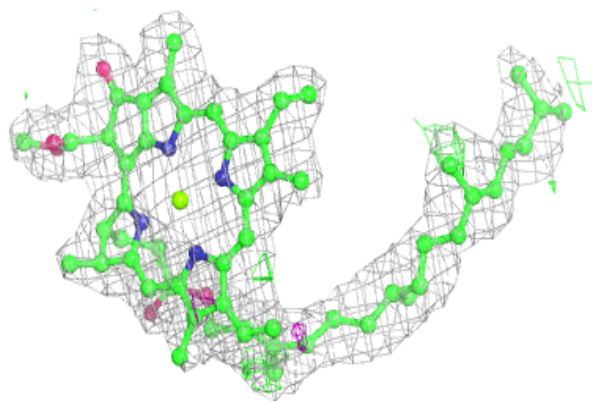
**Electron density around CLA G 610:**

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

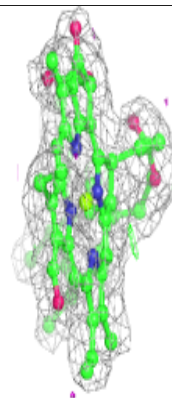
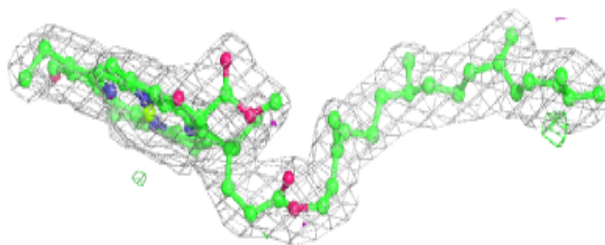
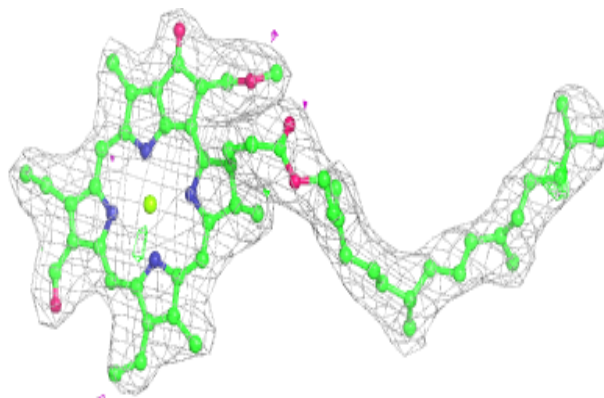


Electron density around CLA F 610:

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

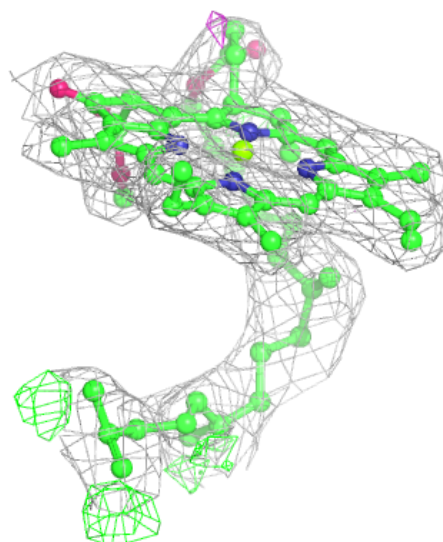
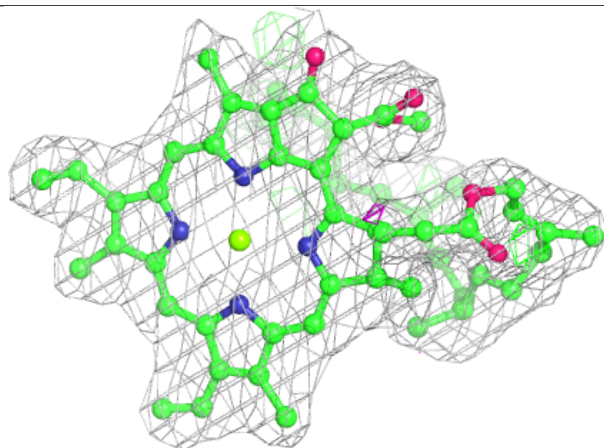
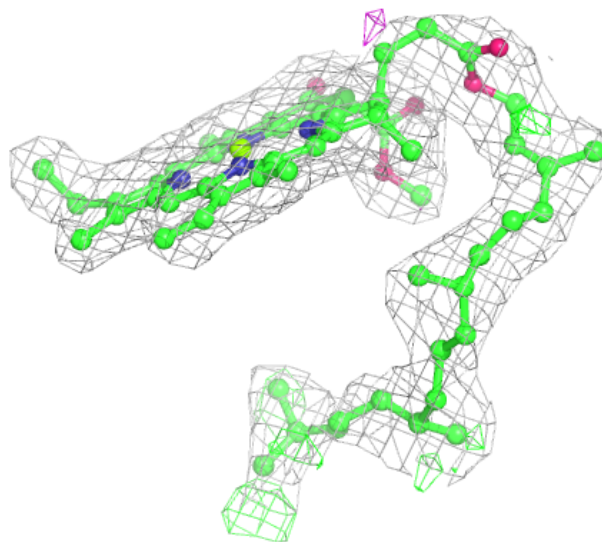
**Electron density around CHL E 601:**

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



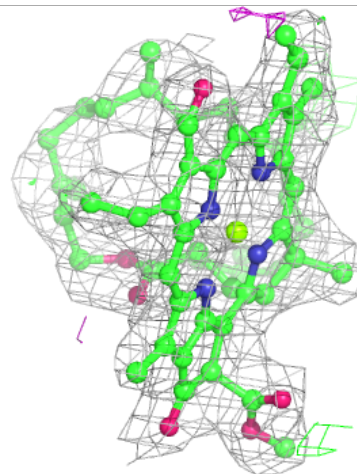
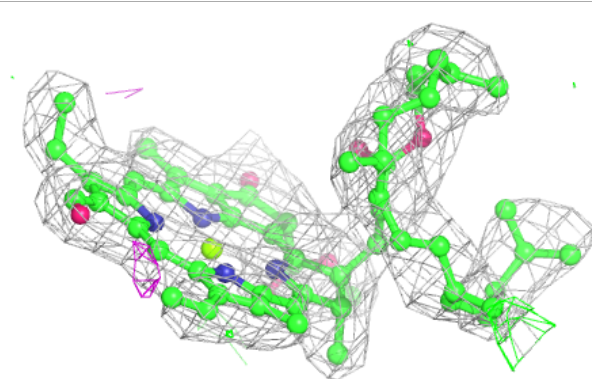
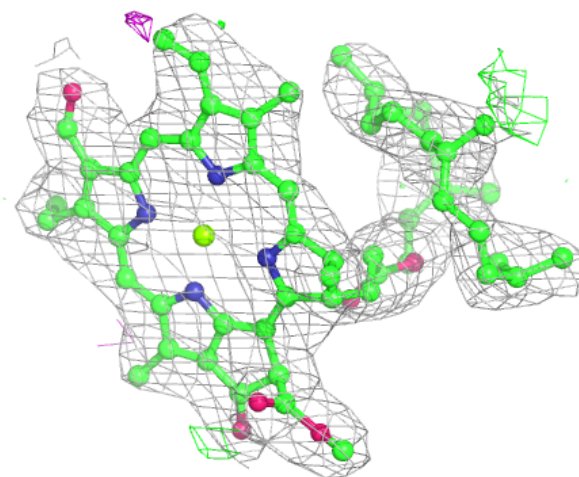
Electron density around CLA A 603:

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



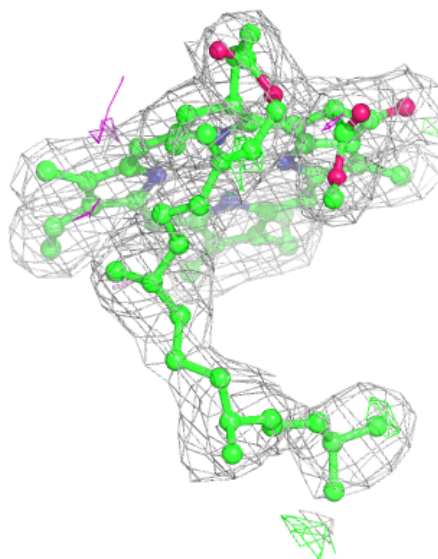
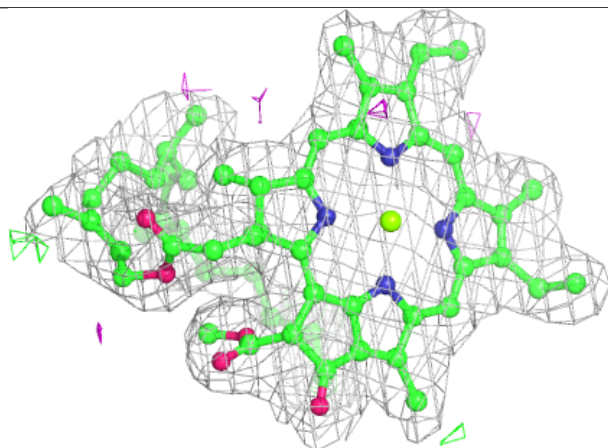
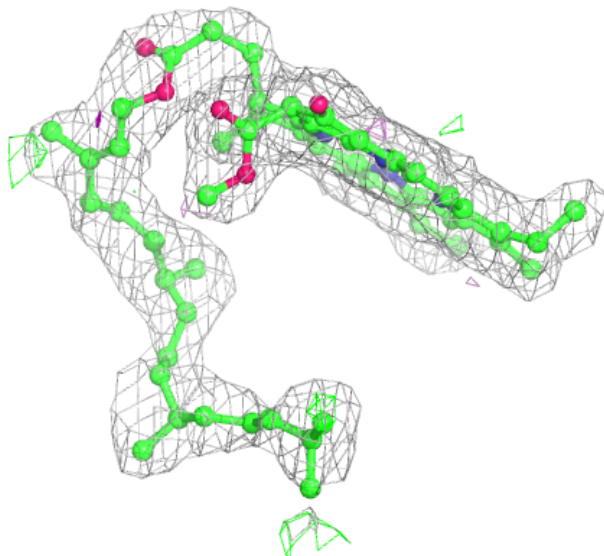
Electron density around CHL A 608:

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



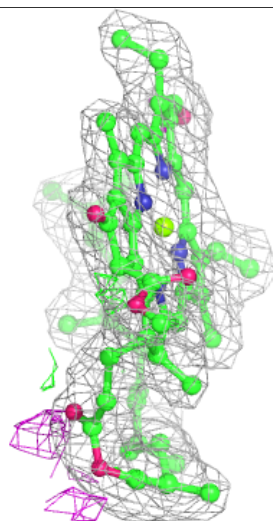
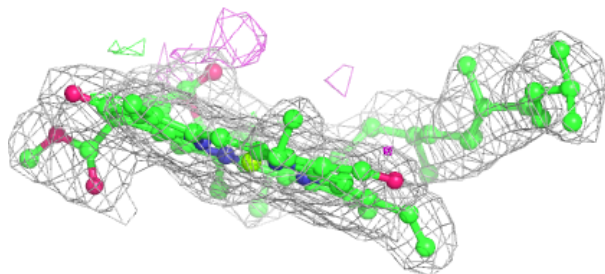
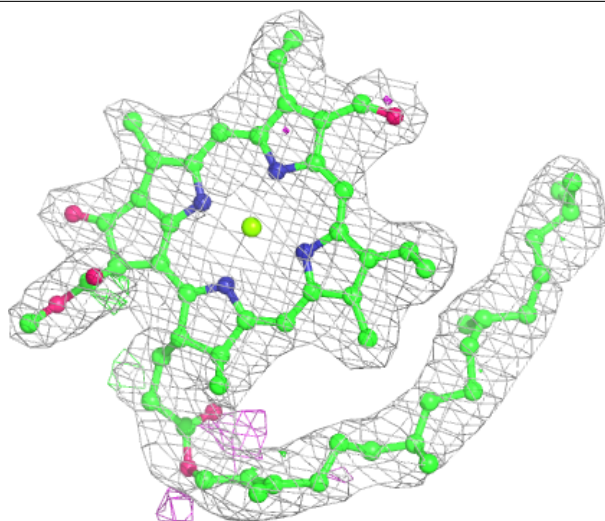
Electron density around CLA I 603:

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



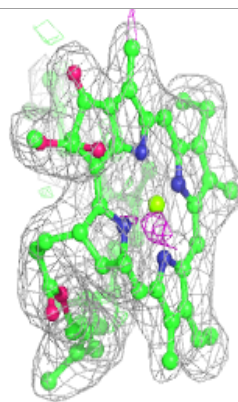
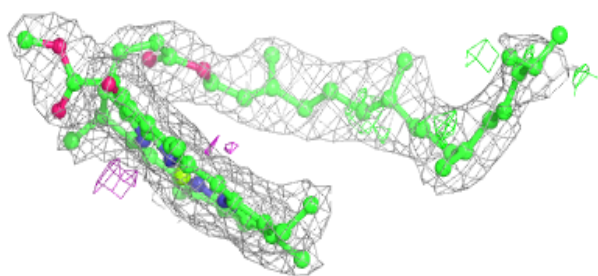
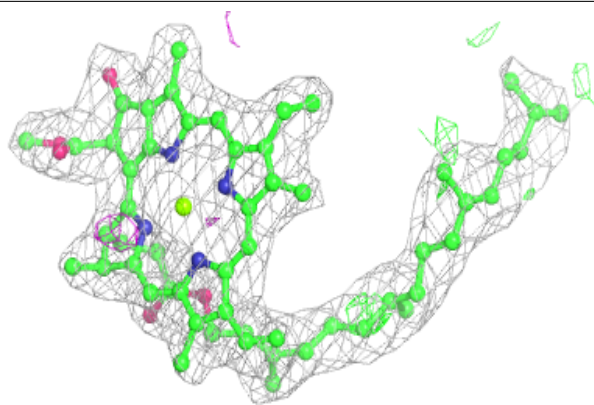
Electron density around CHL J 607:

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



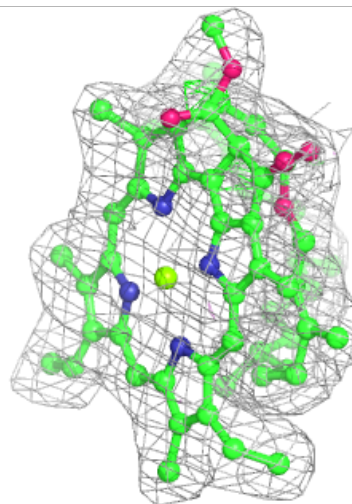
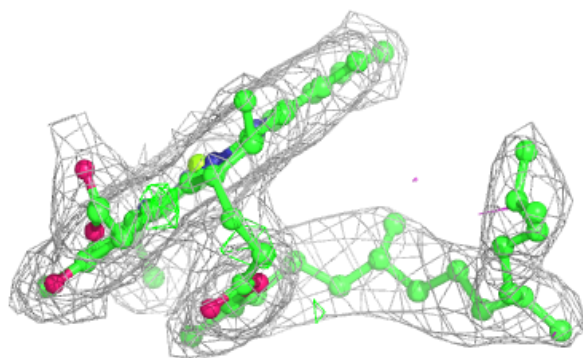
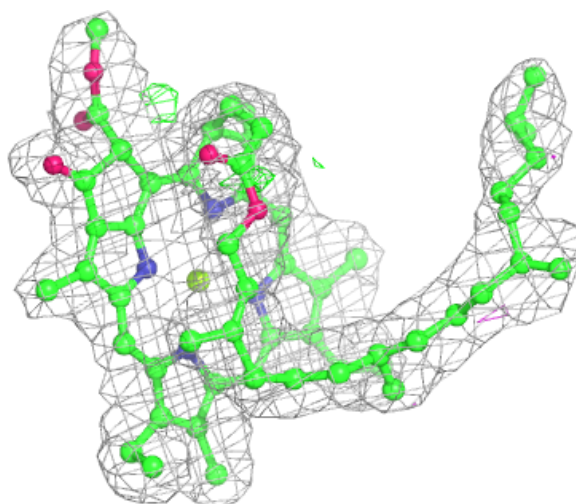
Electron density around CLA B 610:

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



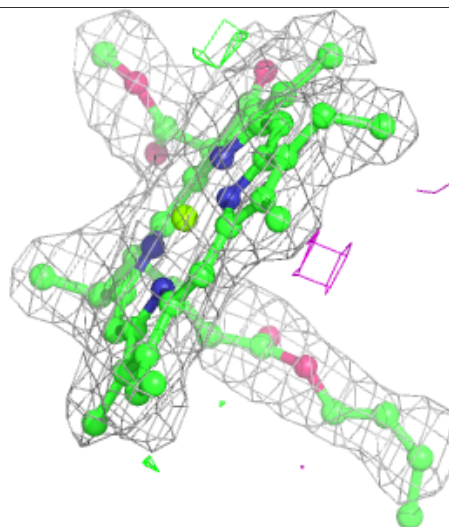
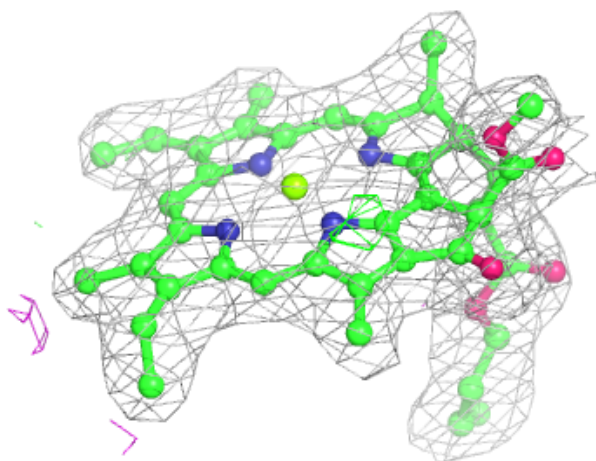
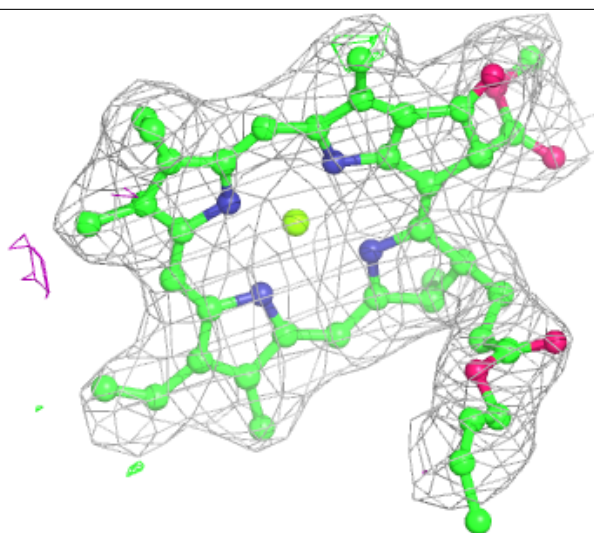
Electron density around CLA G 613:

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



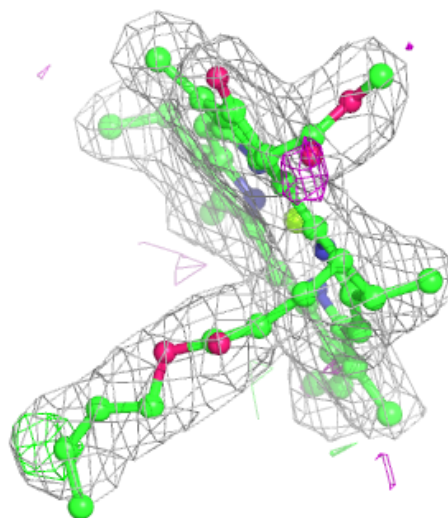
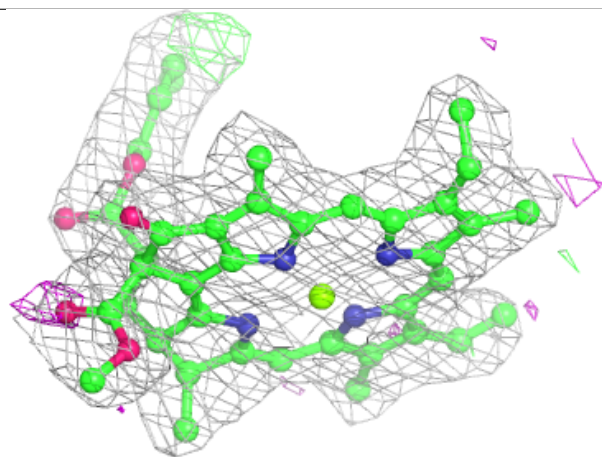
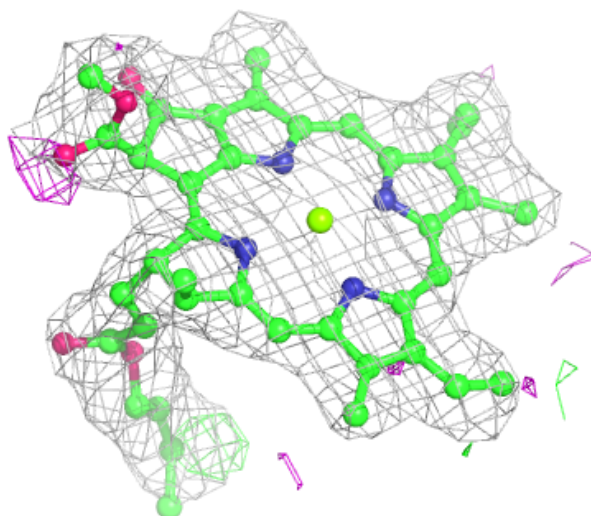
Electron density around CLA F 614:

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



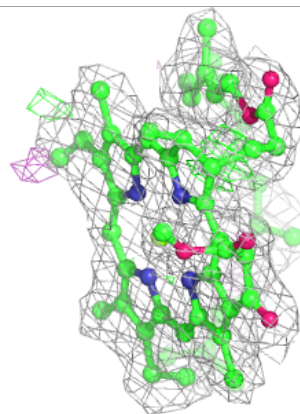
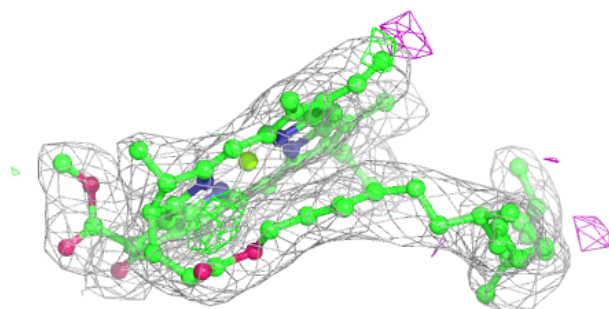
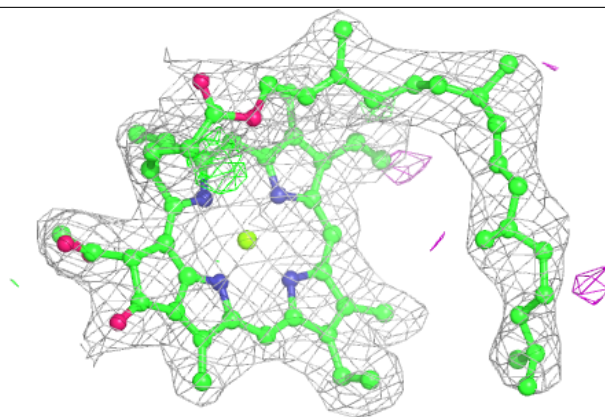
Electron density around CLA C 614:

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



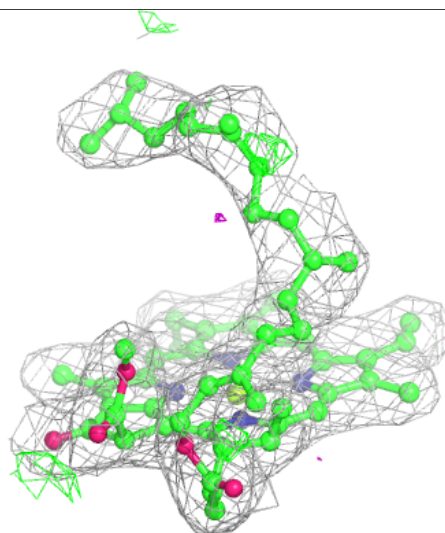
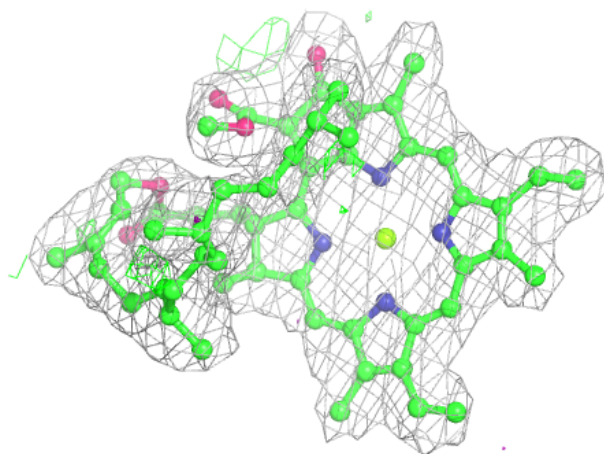
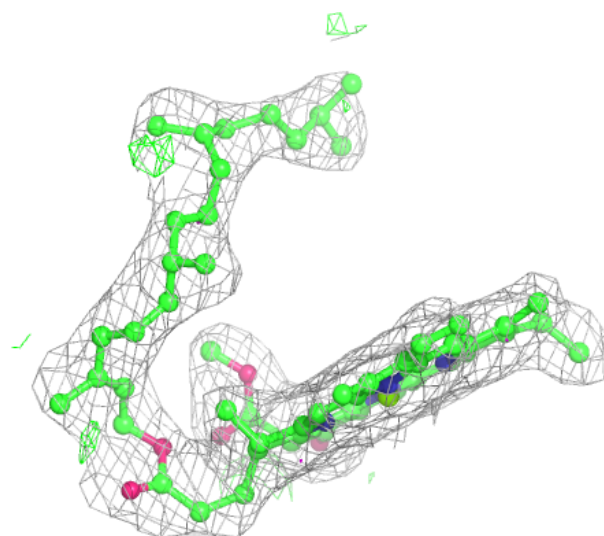
Electron density around CLA E 602:

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



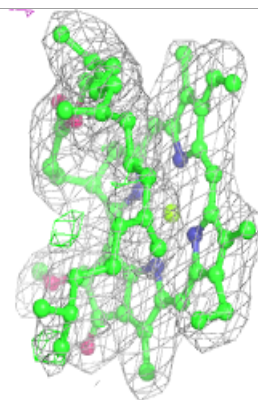
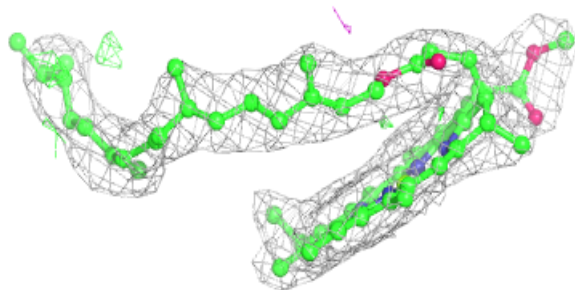
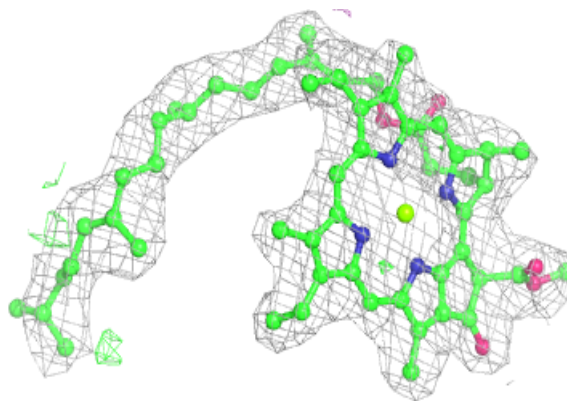
Electron density around CLA E 603:

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

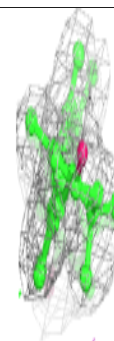
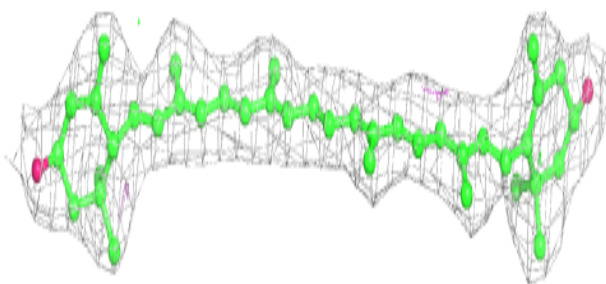
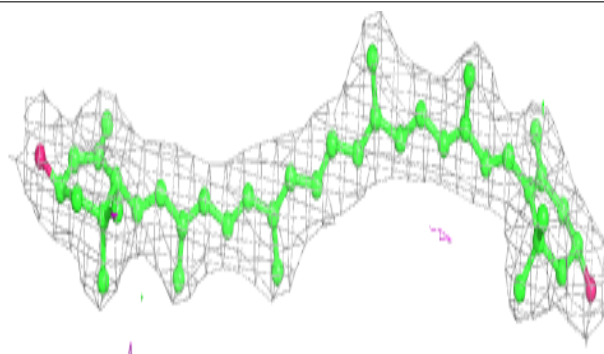


Electron density around CLA D 610:

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

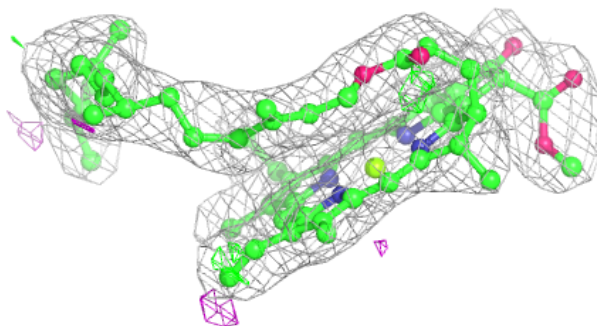
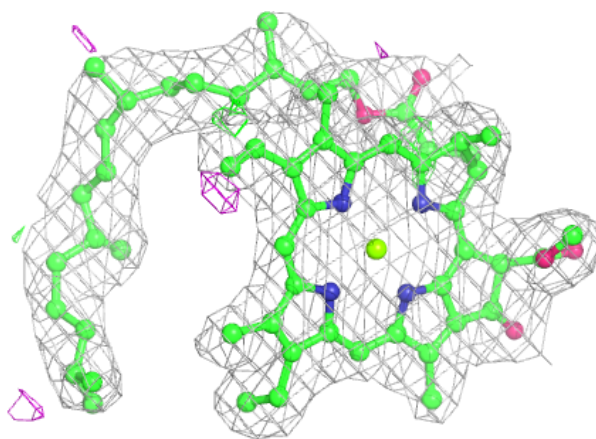
**Electron density around LUT I 8620:**

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



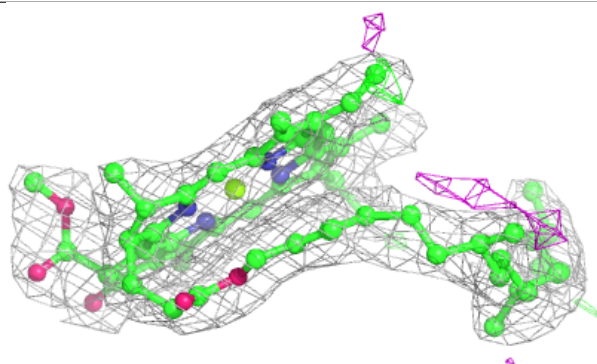
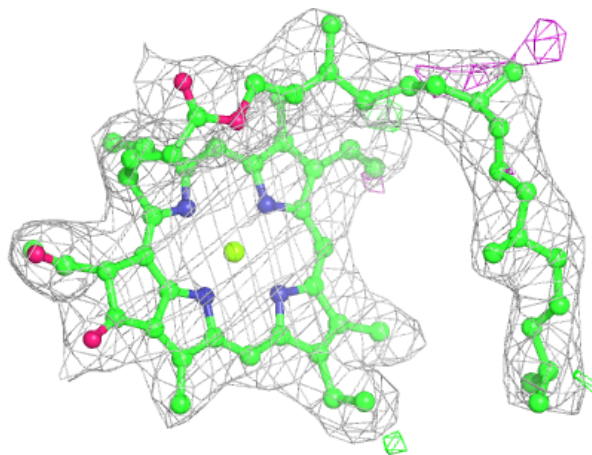
Electron density around CLA G 602:

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



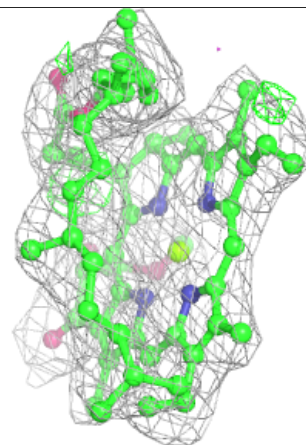
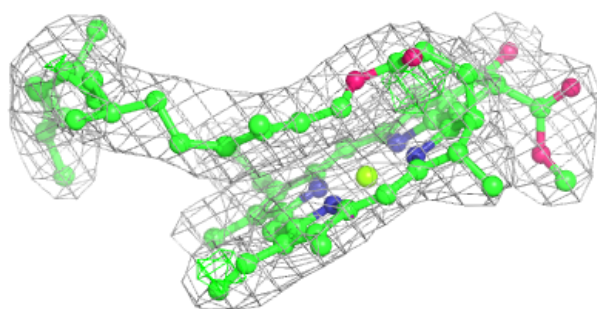
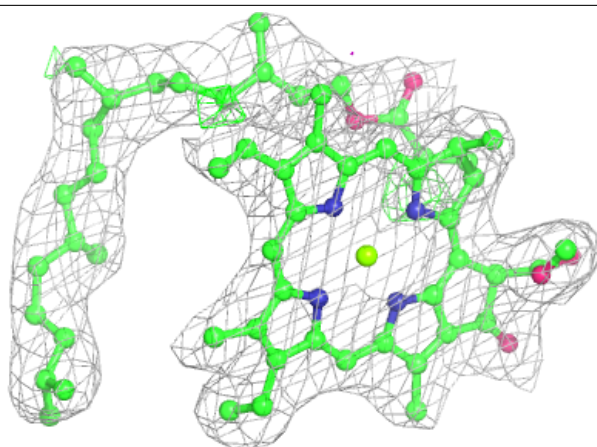
Electron density around CLA I 602:

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

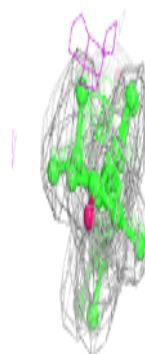
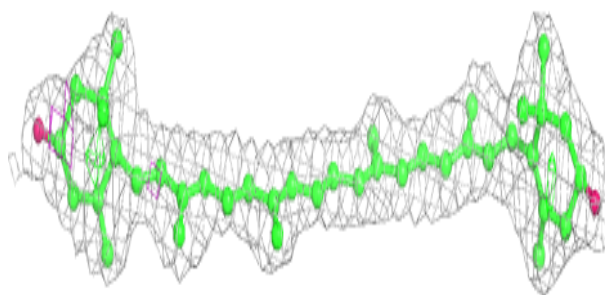
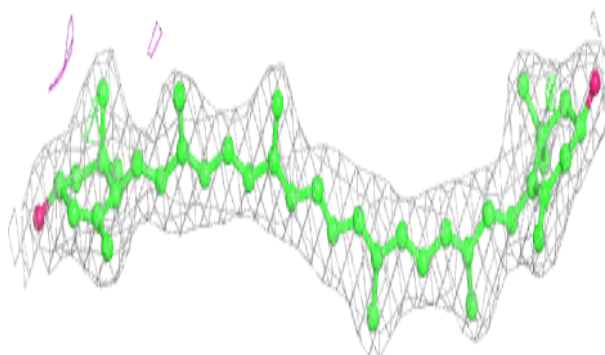


Electron density around CLA H 602:

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

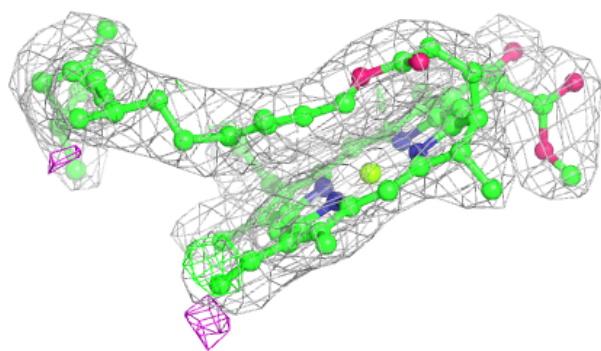
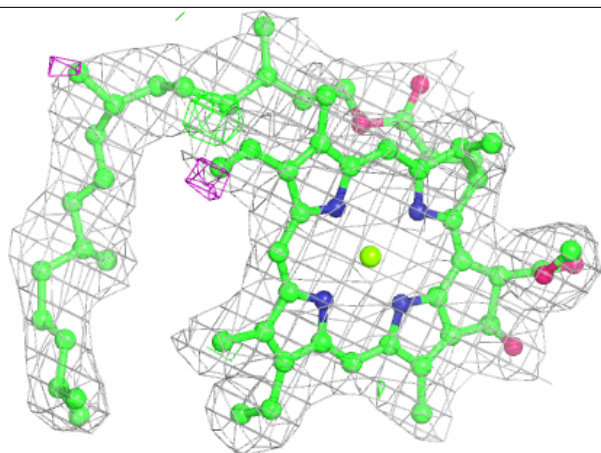
**Electron density around LUT C 2620:**

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



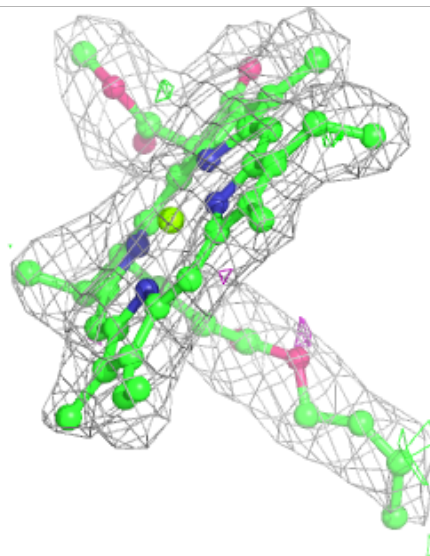
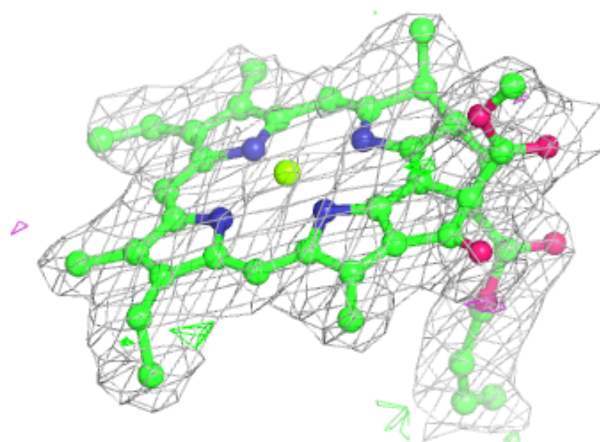
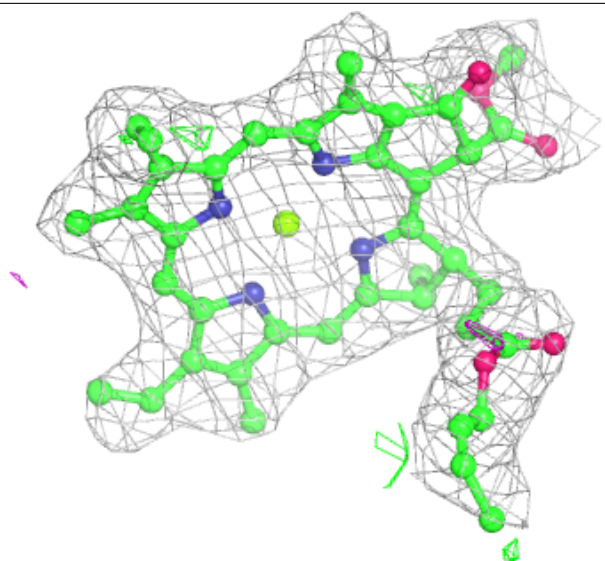
Electron density around CLA J 602:

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



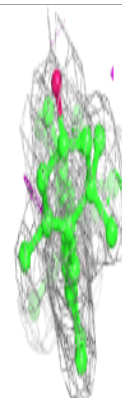
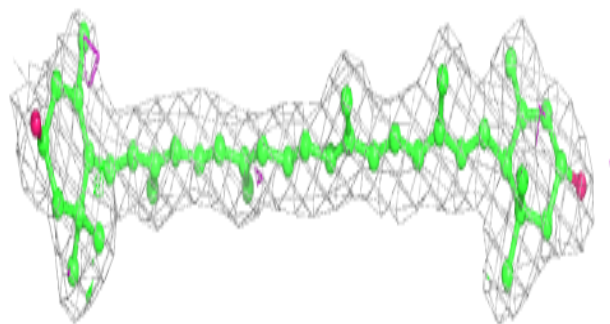
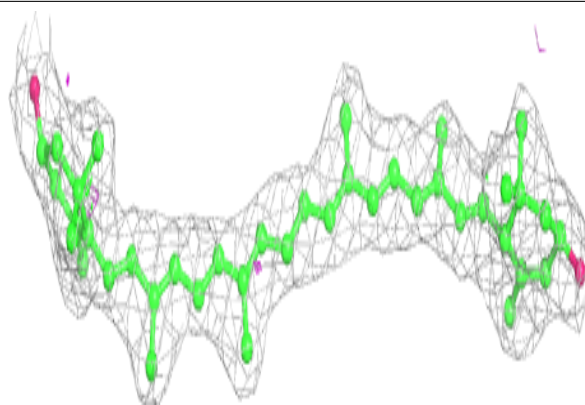
Electron density around CLA G 614:

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



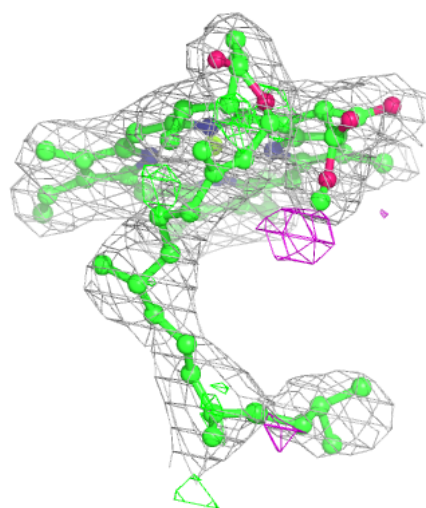
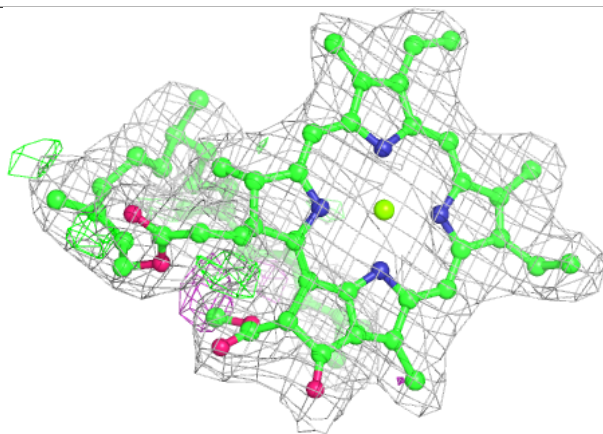
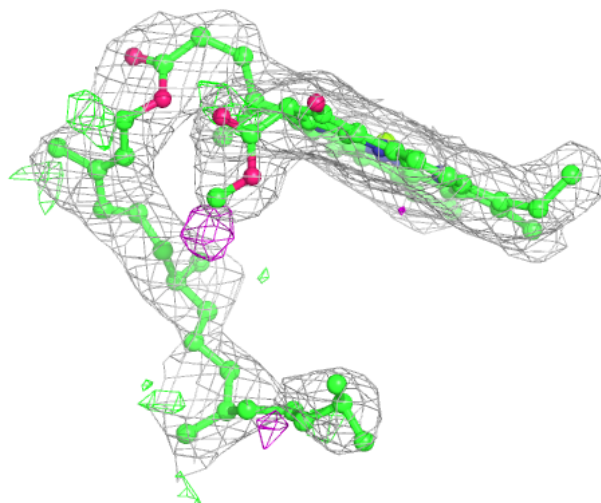
Electron density around LUT D 3621:

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



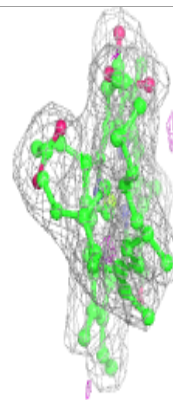
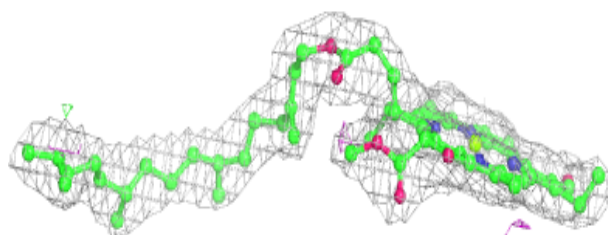
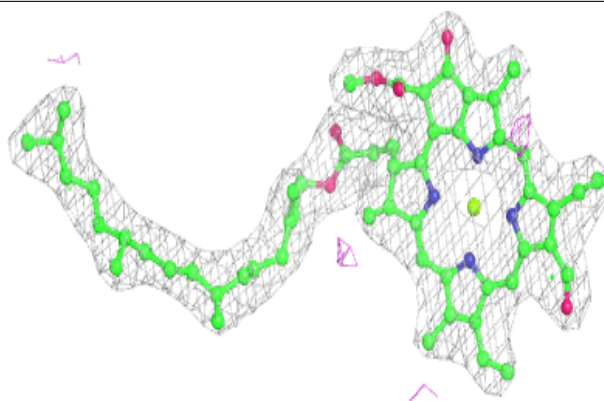
Electron density around CLA B 603:

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

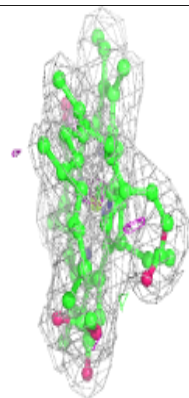
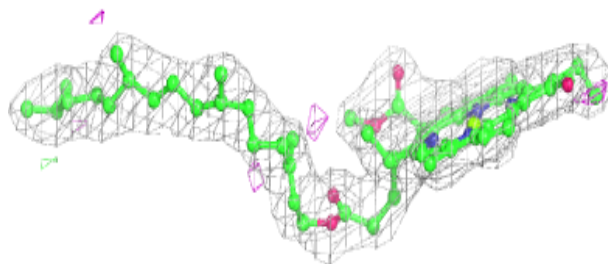
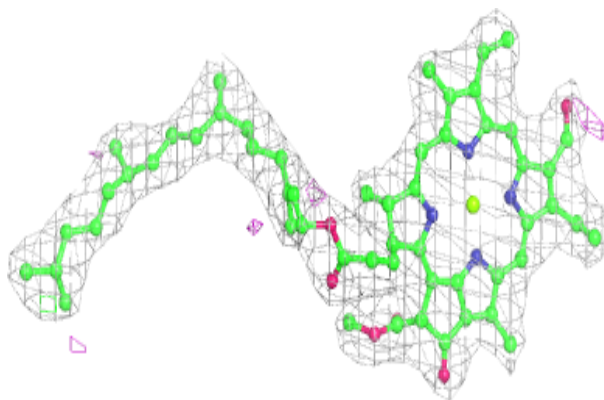


Electron density around CHL D 601:

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

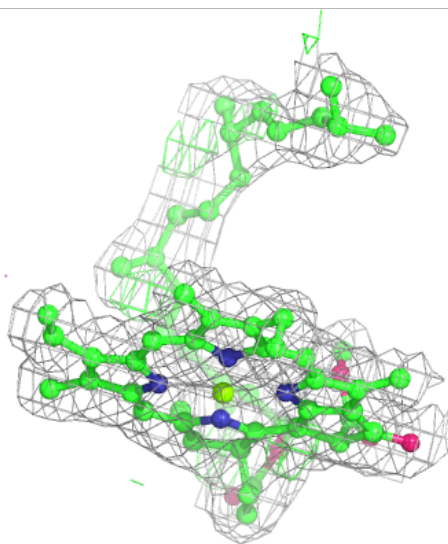
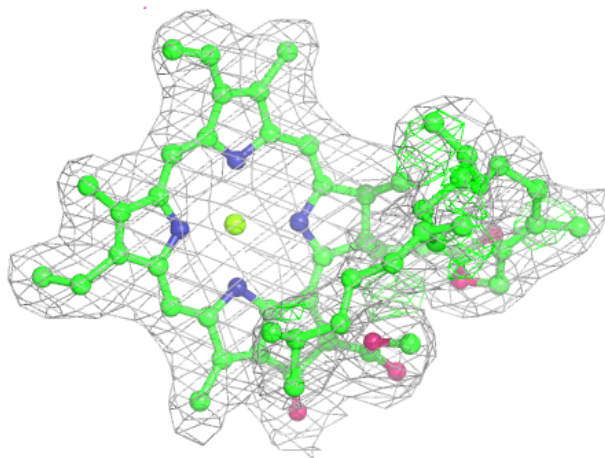
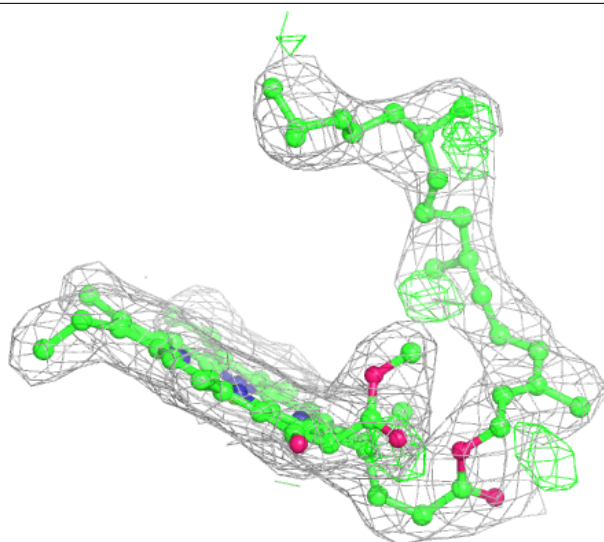
**Electron density around CHL F 601:**

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



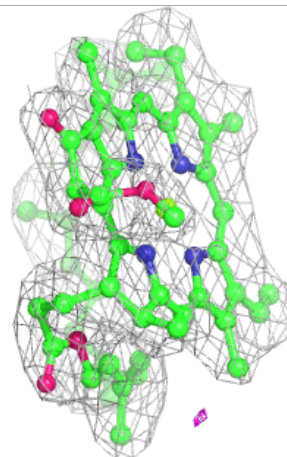
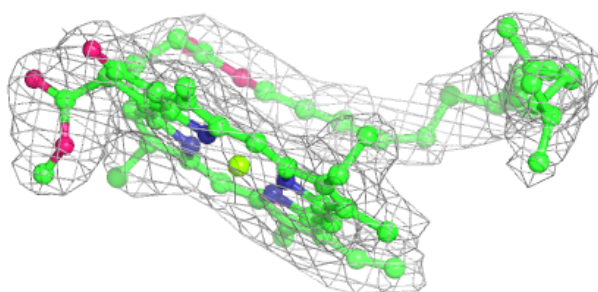
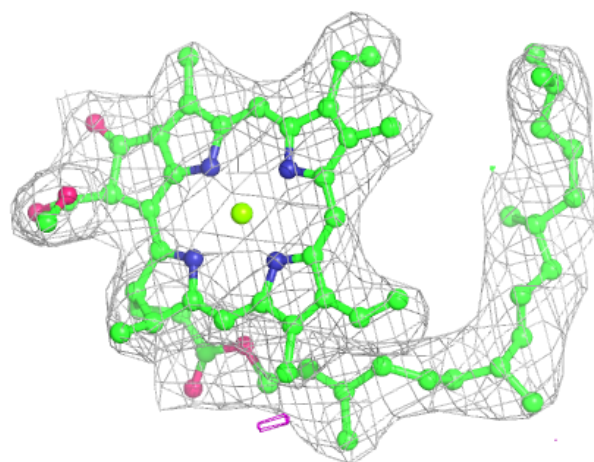
Electron density around CLA J 603:

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



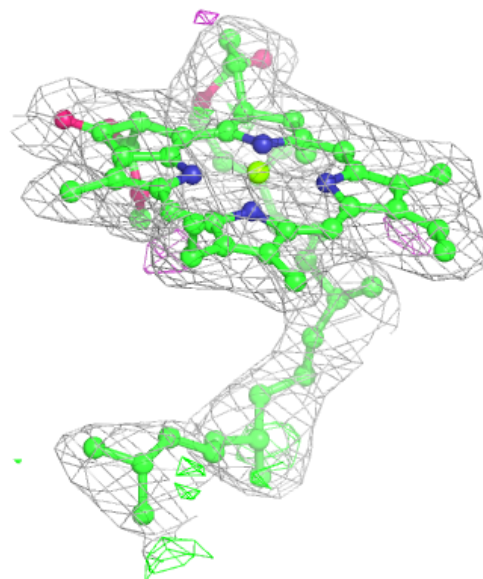
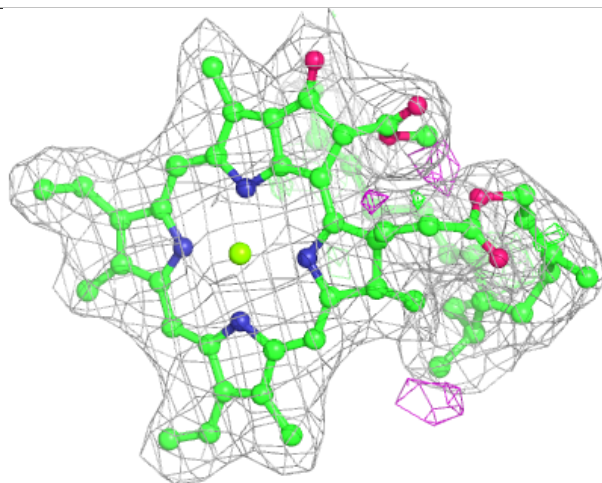
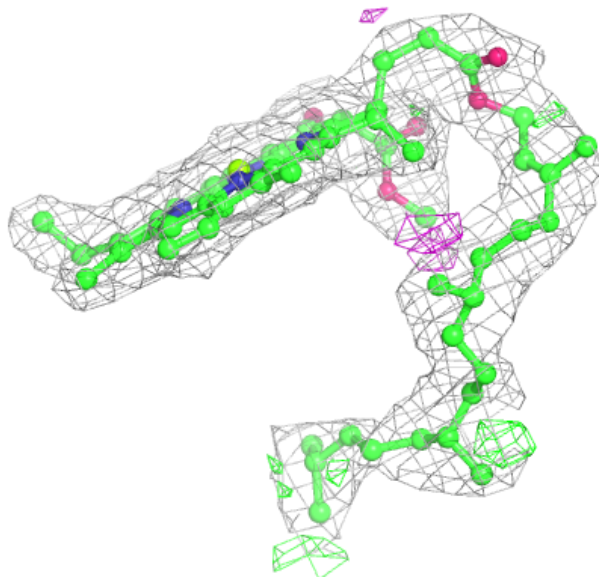
Electron density around CLA A 602:

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



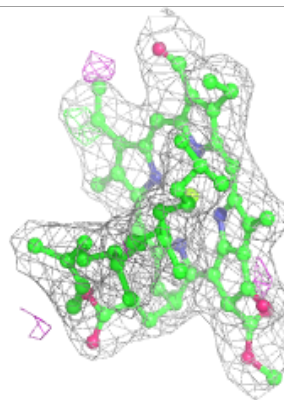
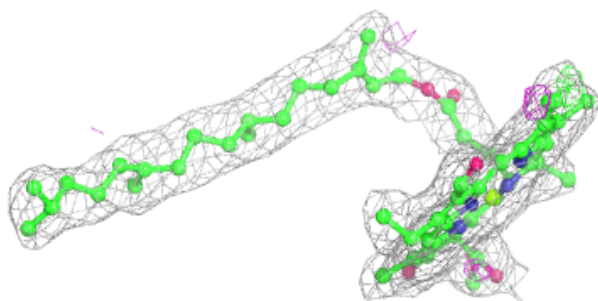
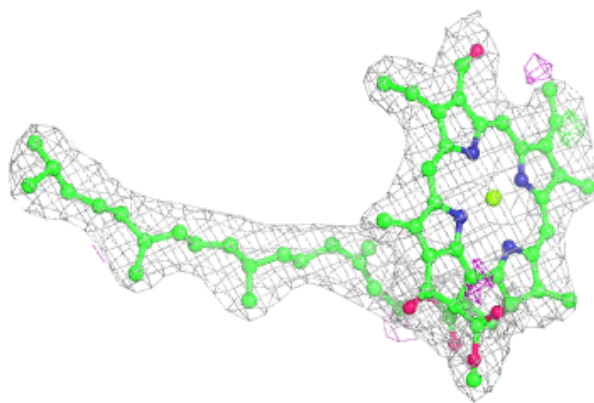
Electron density around CLA D 603:

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



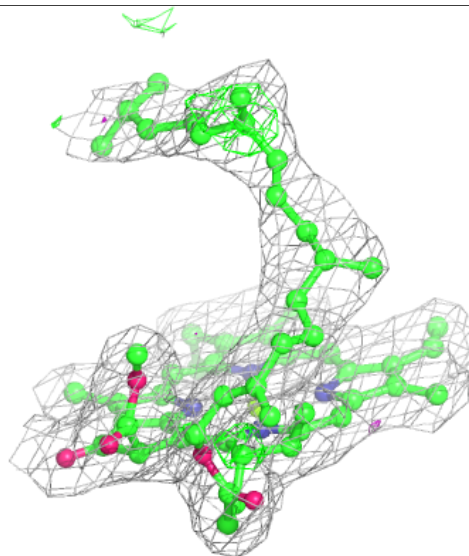
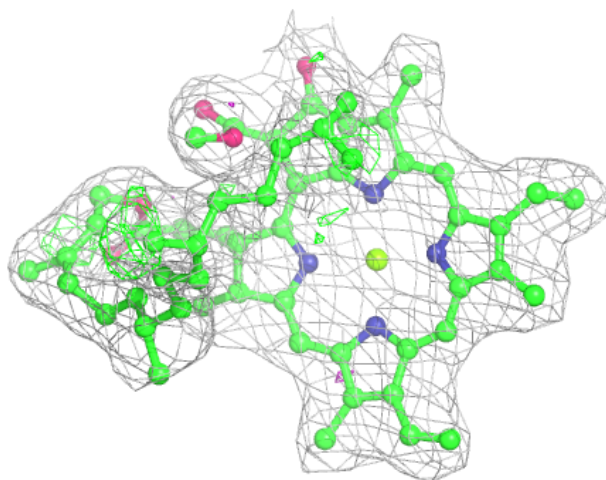
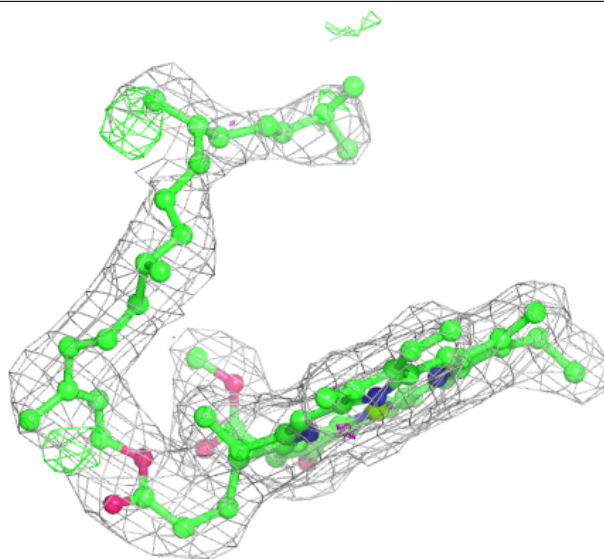
Electron density around CHL A 609:

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



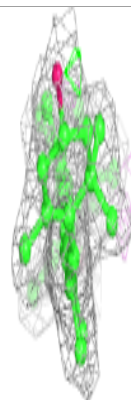
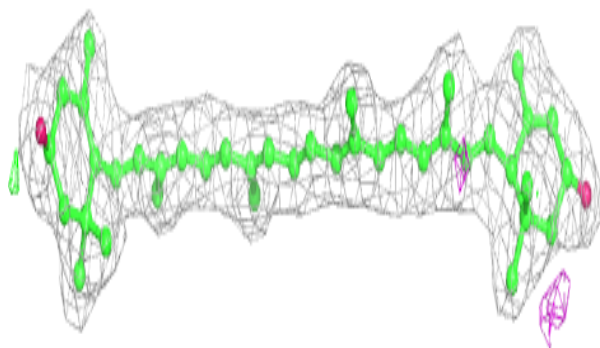
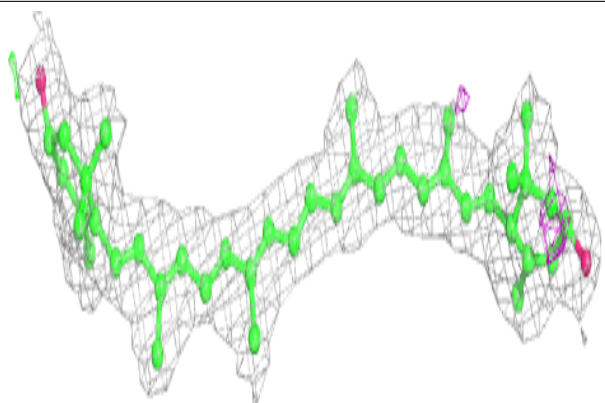
Electron density around CLA H 603:

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

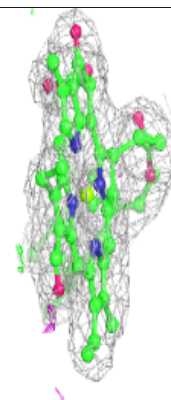
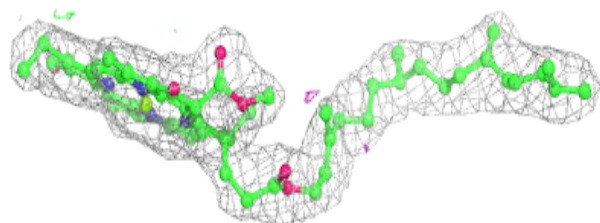
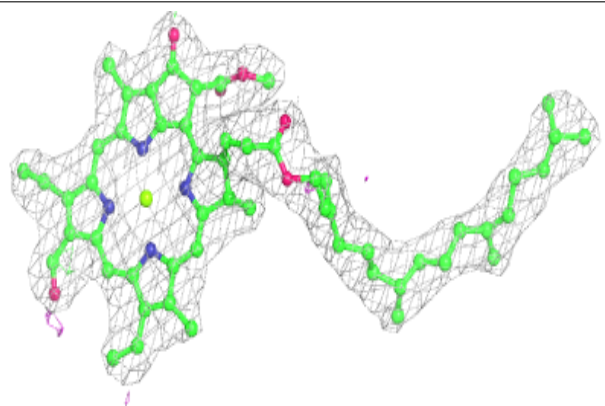


Electron density around LUT B 1621:

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

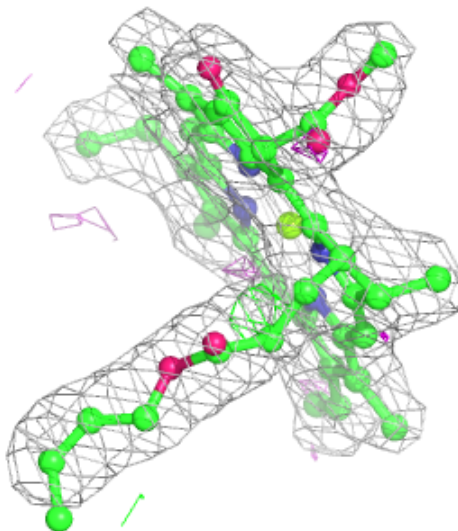
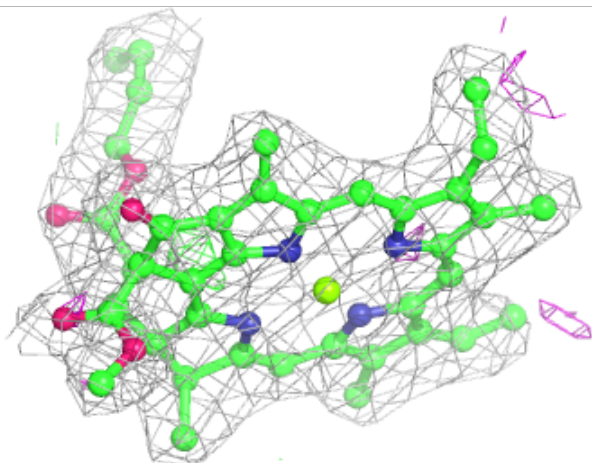
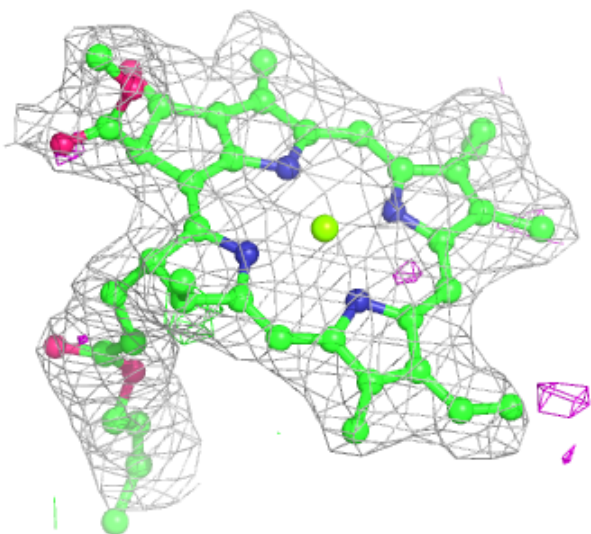
**Electron density around CHL C 601:**

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



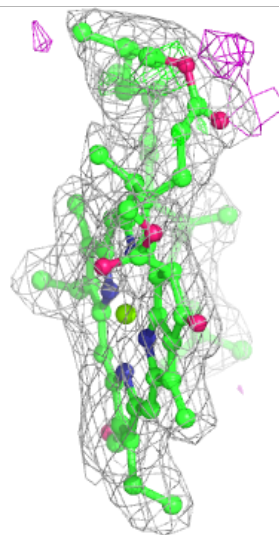
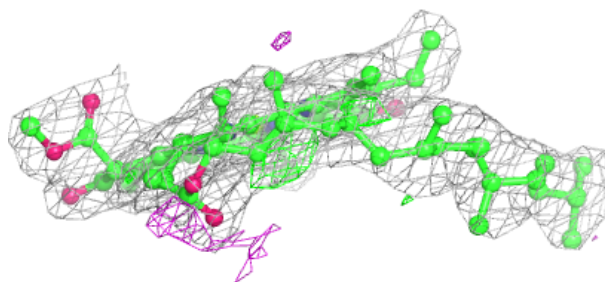
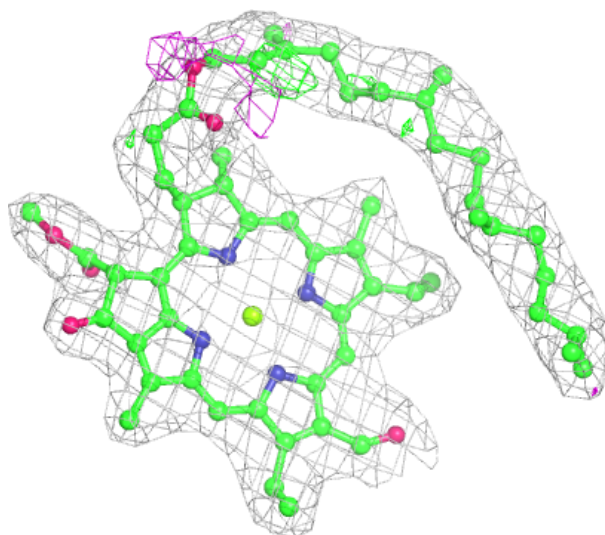
Electron density around CLA D 614:

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



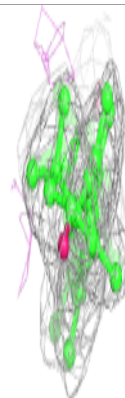
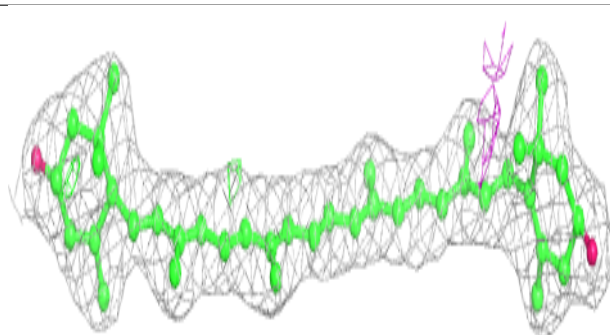
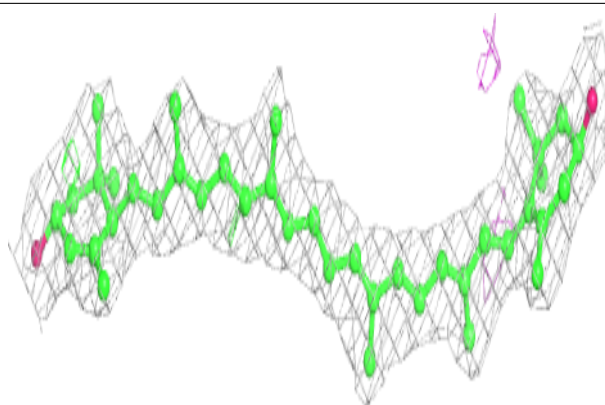
Electron density around CHL E 607:

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

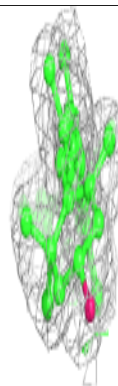
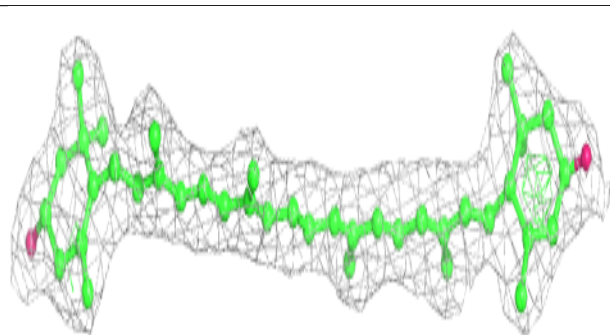
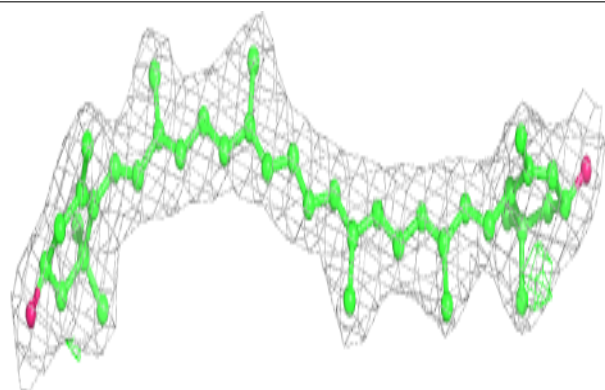


Electron density around LUT A 620:

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

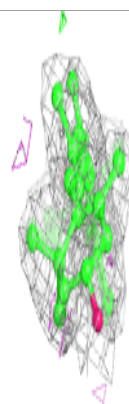
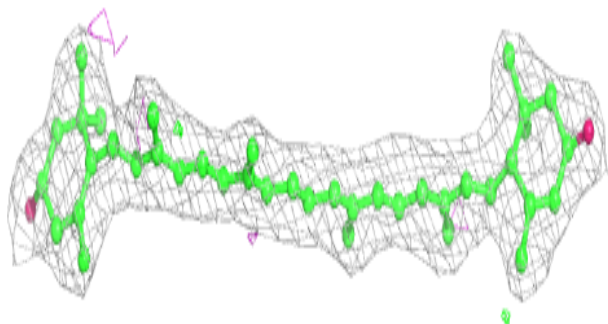
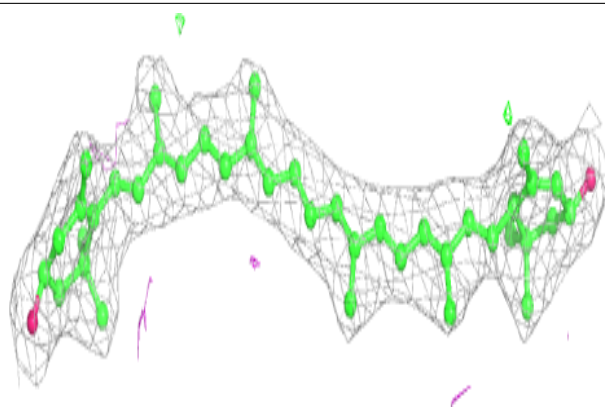
**Electron density around LUT H 7620:**

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

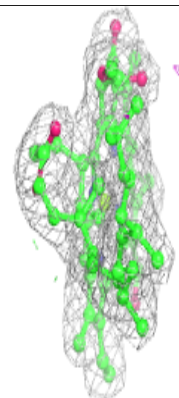
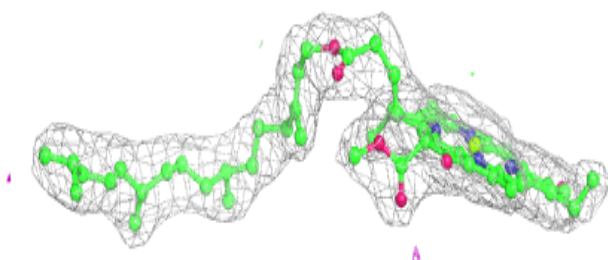
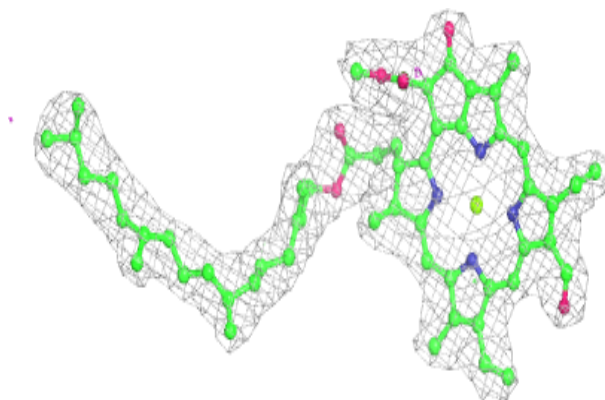


Electron density around LUT D 3620:

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

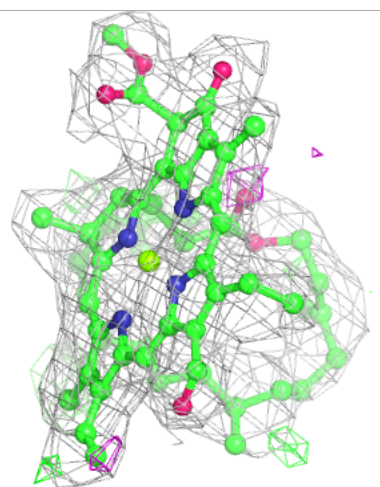
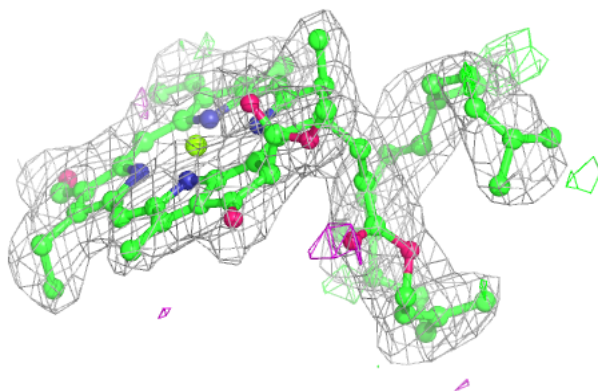
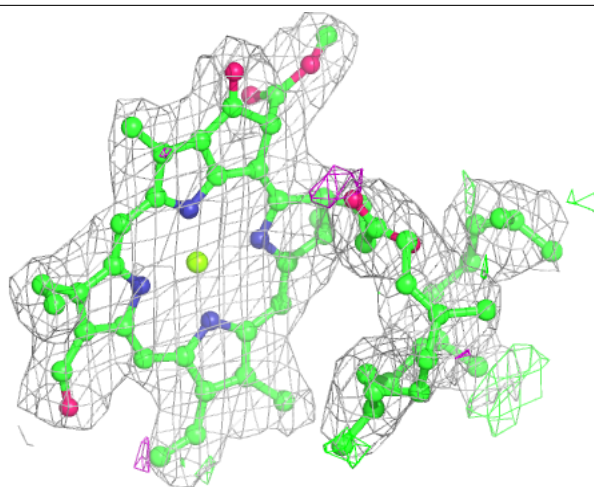
**Electron density around CHL J 601:**

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



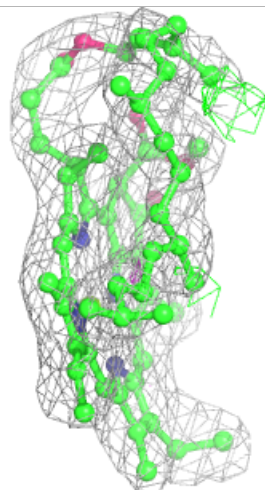
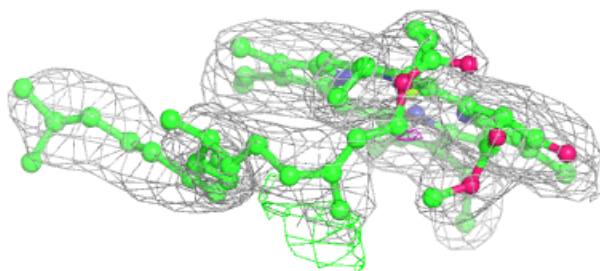
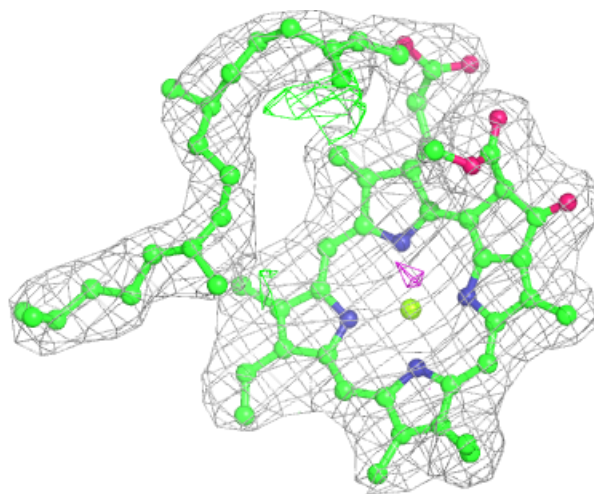
Electron density around CHL E 608:

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



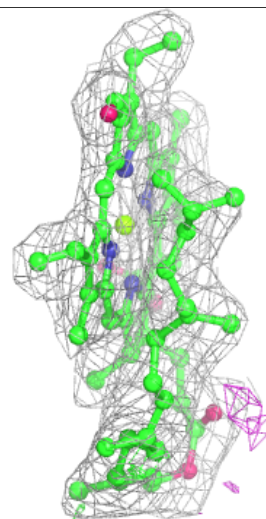
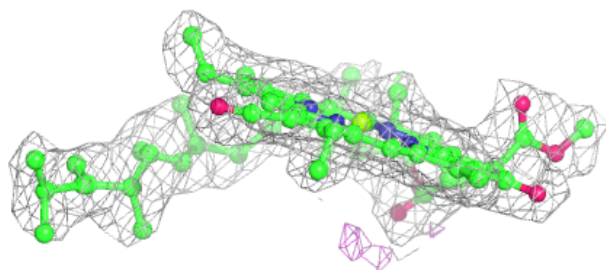
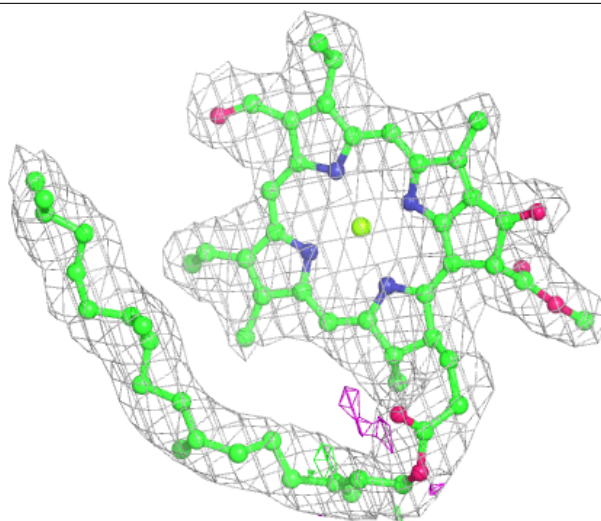
Electron density around CLA J 612:

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



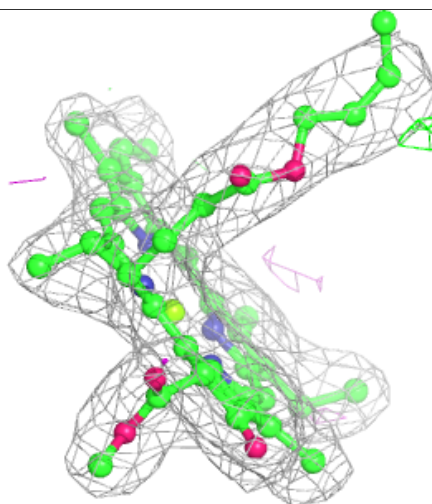
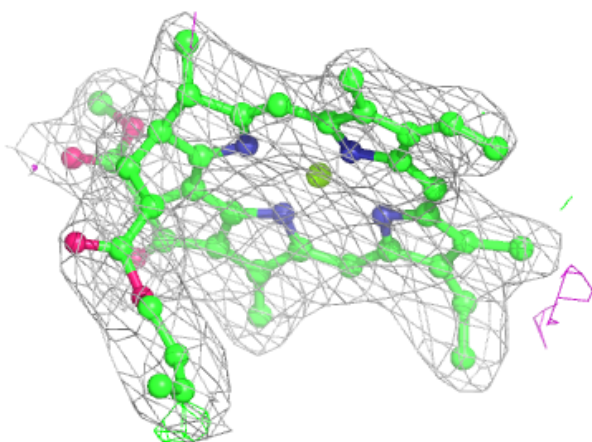
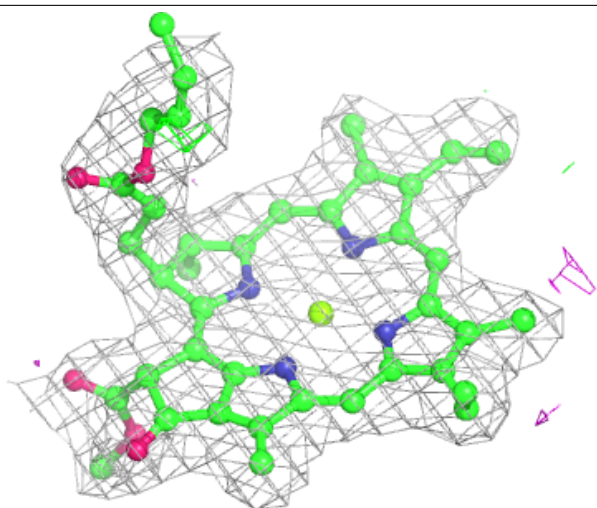
Electron density around CHL F 607:

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



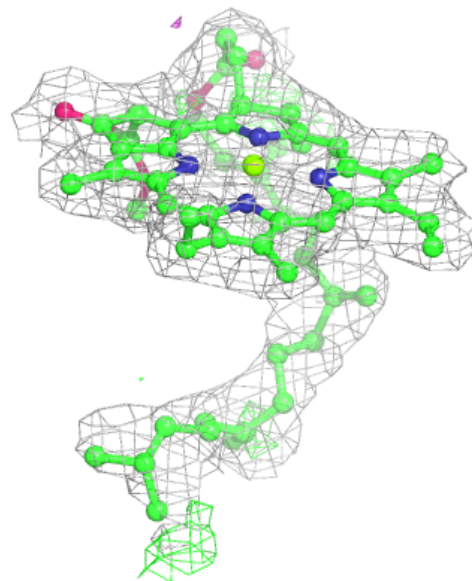
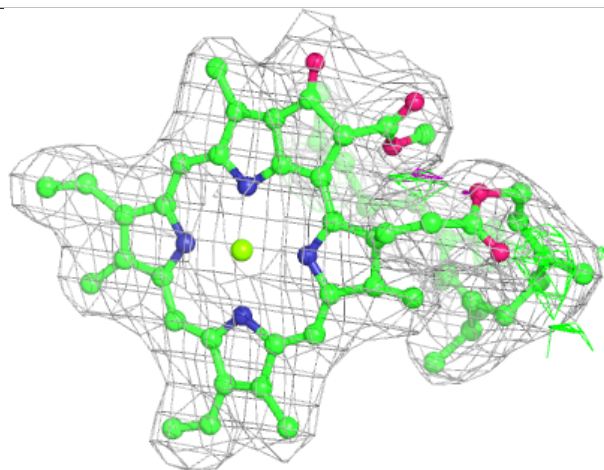
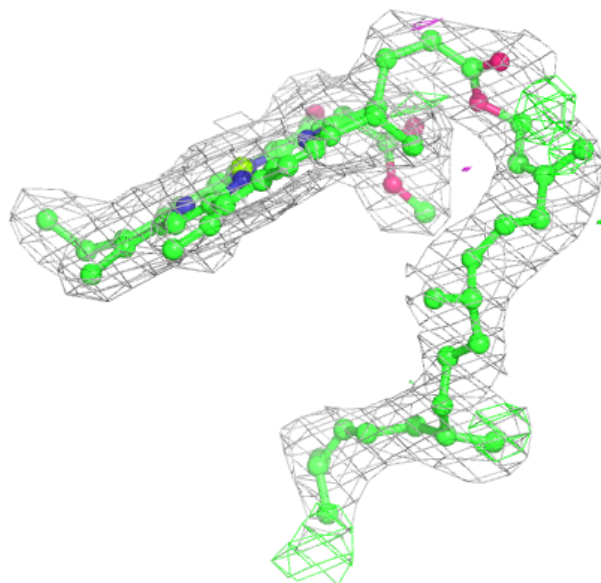
Electron density around CLA E 614:

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



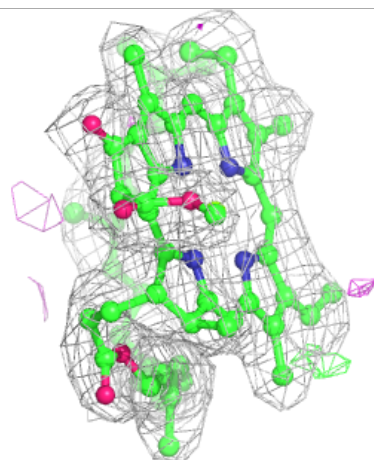
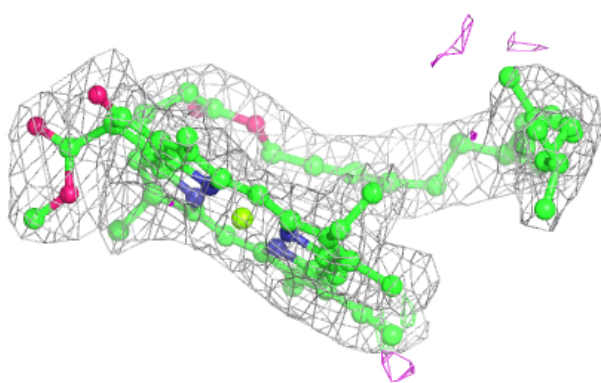
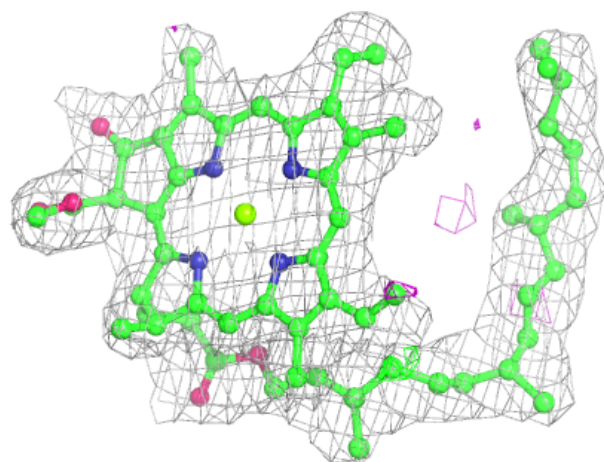
Electron density around CLA F 603:

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



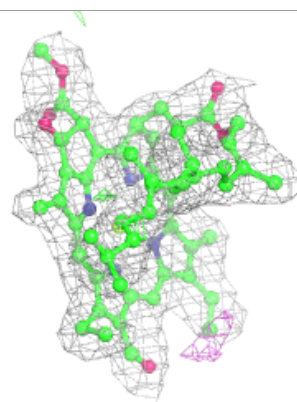
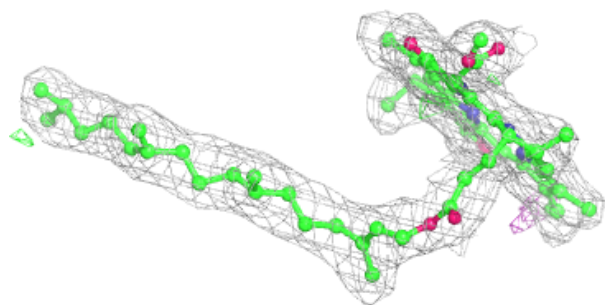
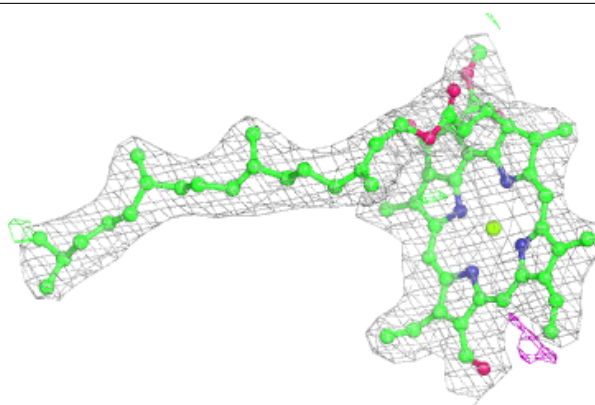
Electron density around CLA F 602:

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



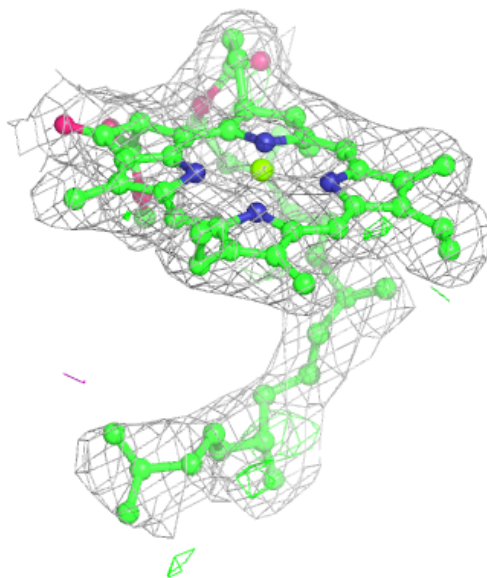
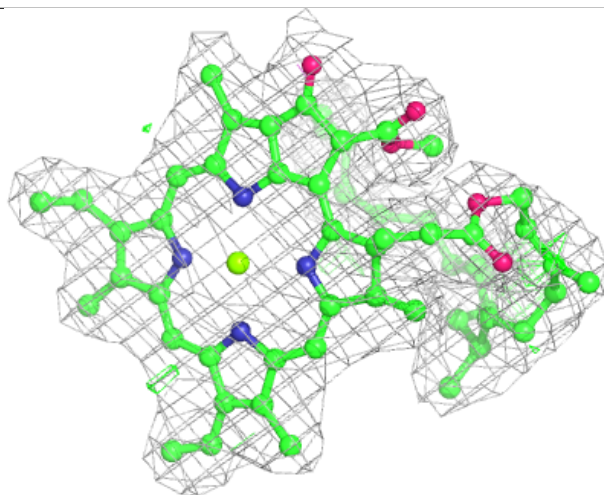
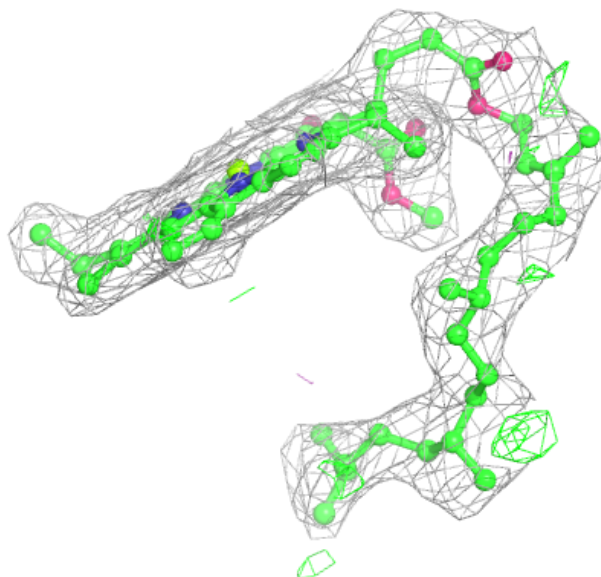
Electron density around CHL G 609:

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



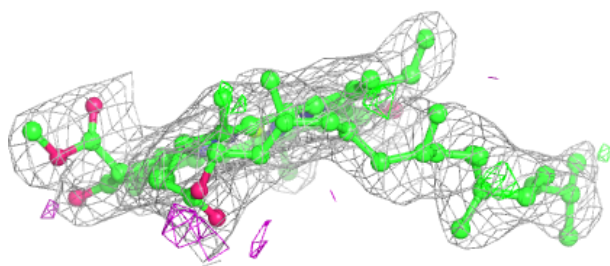
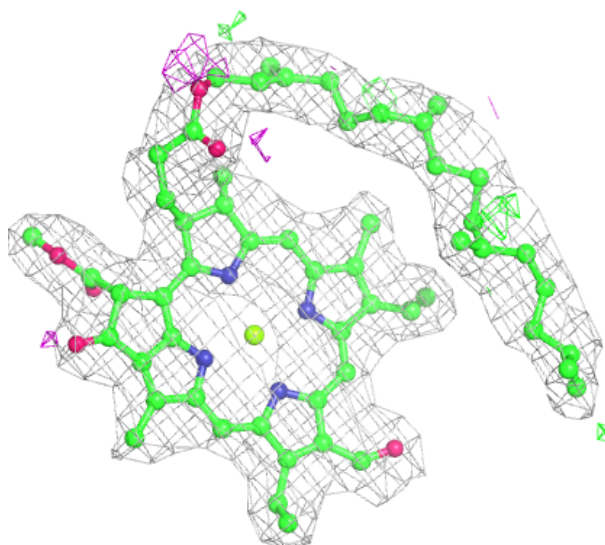
Electron density around CLA C 603:

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



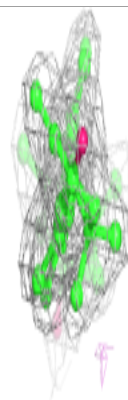
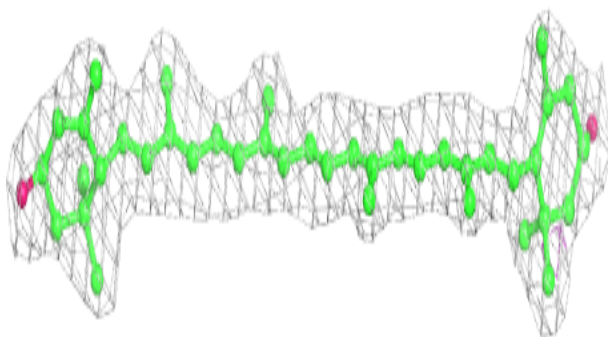
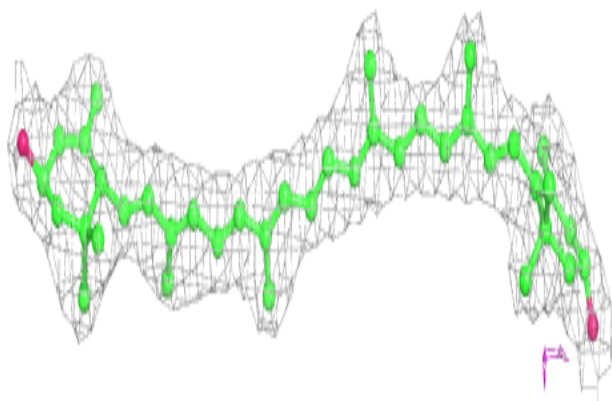
Electron density around CHL I 607:

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

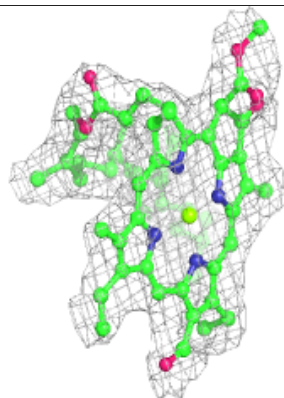
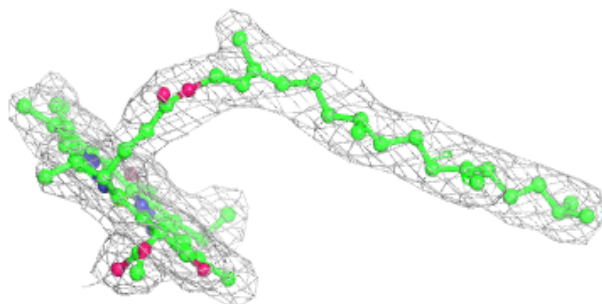
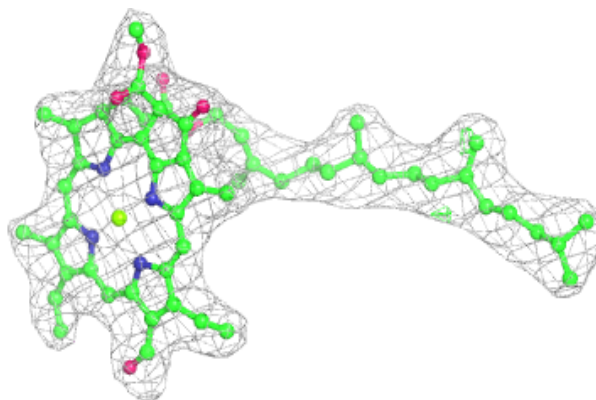


Electron density around LUT I 8621:

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

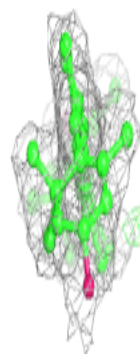
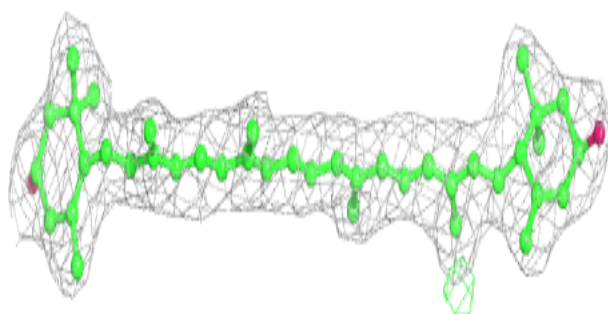
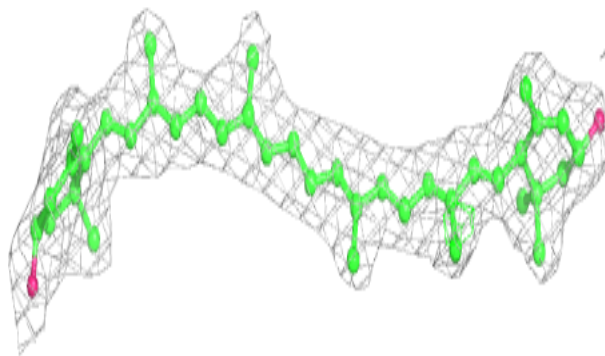
**Electron density around CHL D 609:**

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

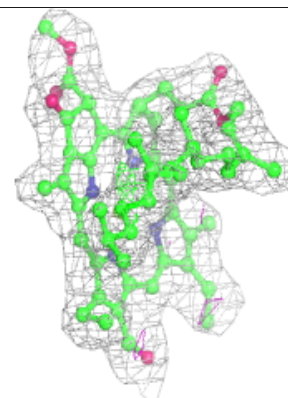
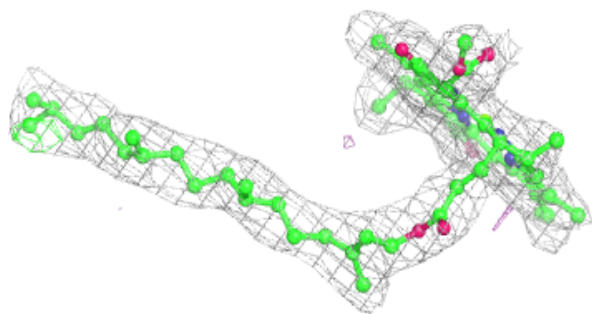
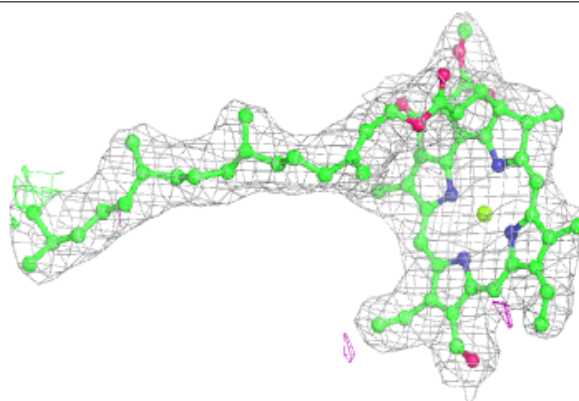


Electron density around LUT J 9621:

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

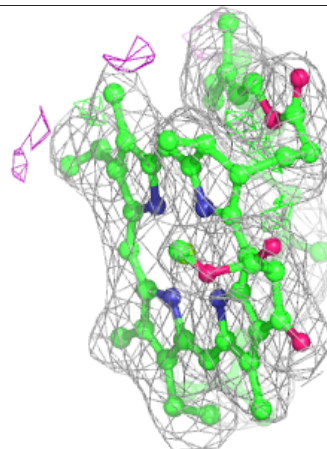
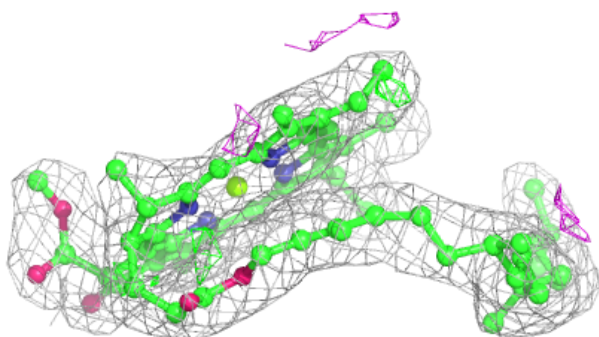
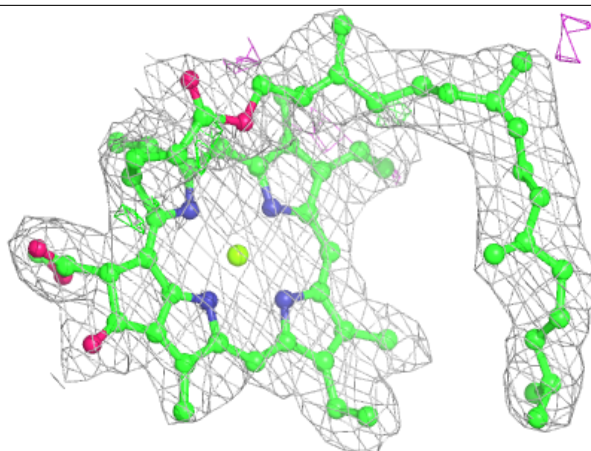
**Electron density around CHL F 609:**

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

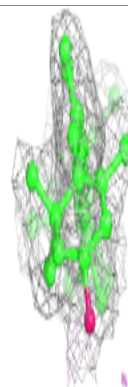
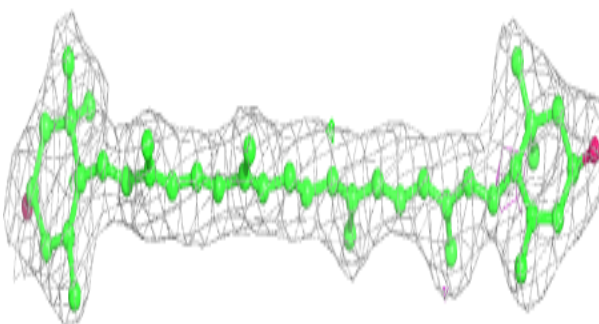
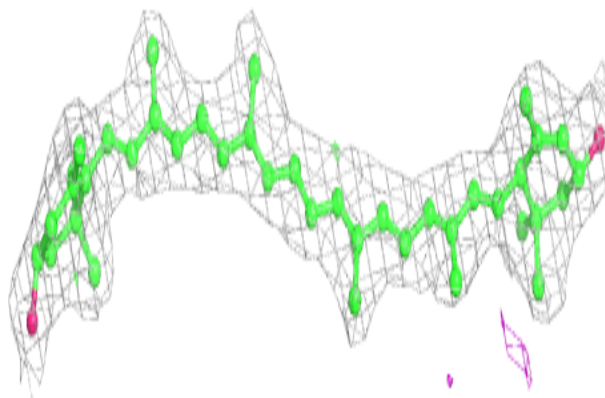


Electron density around CLA D 602:

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

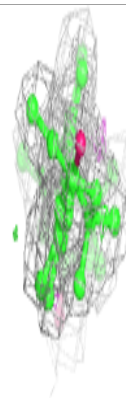
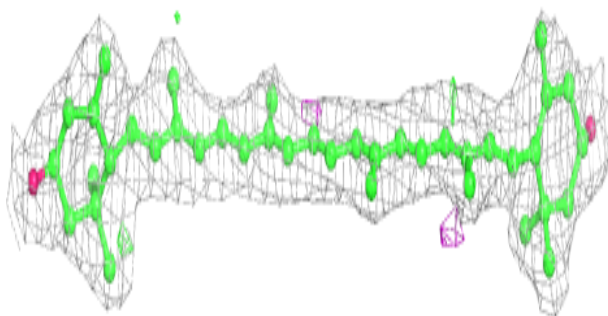
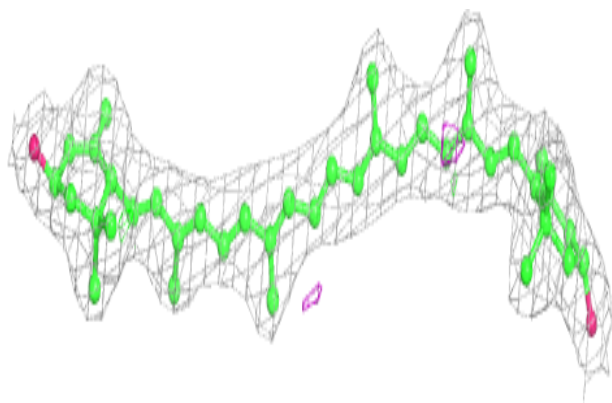
**Electron density around LUT F 5621:**

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



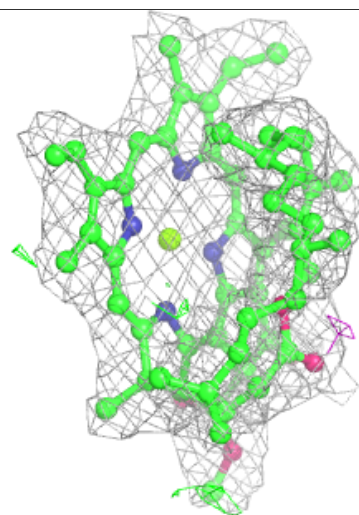
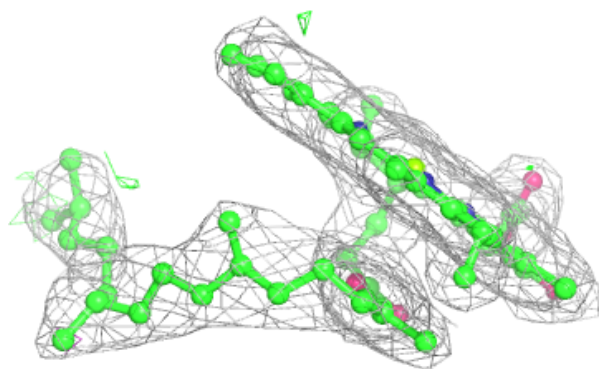
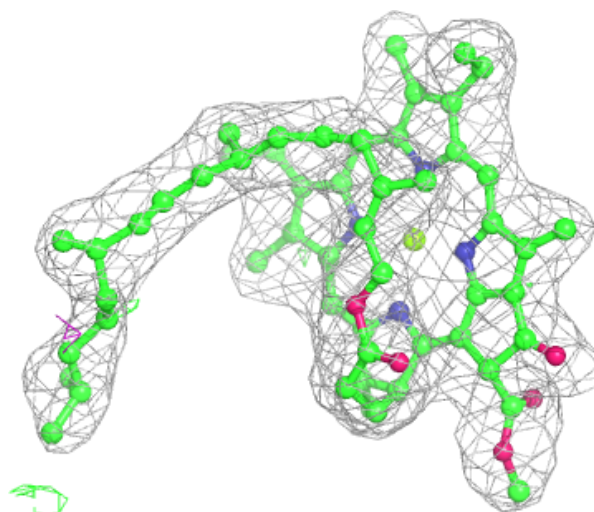
Electron density around LUT G 6621:

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



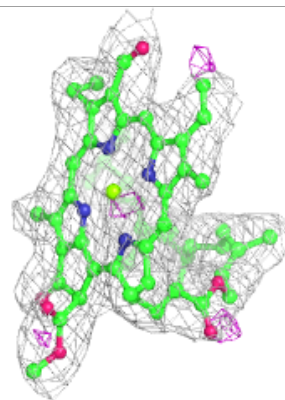
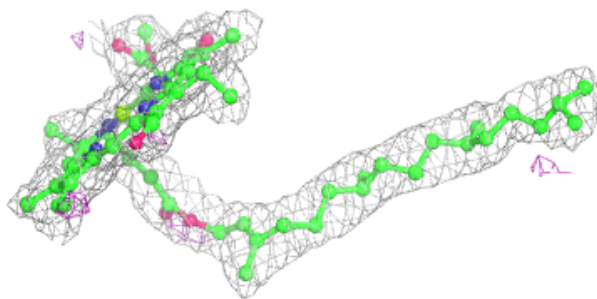
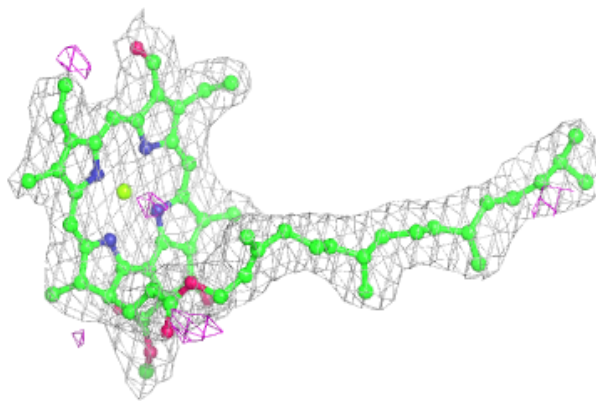
Electron density around CLA I 613:

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

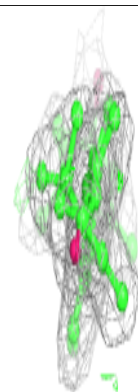
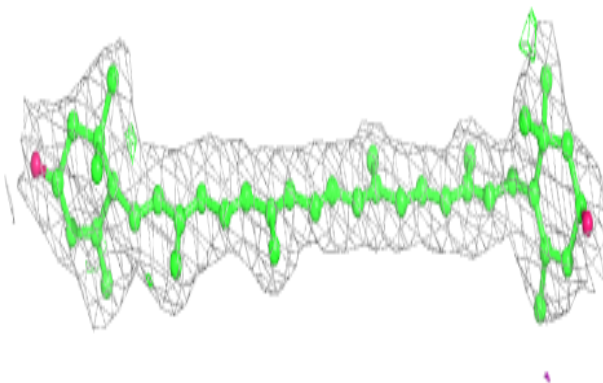
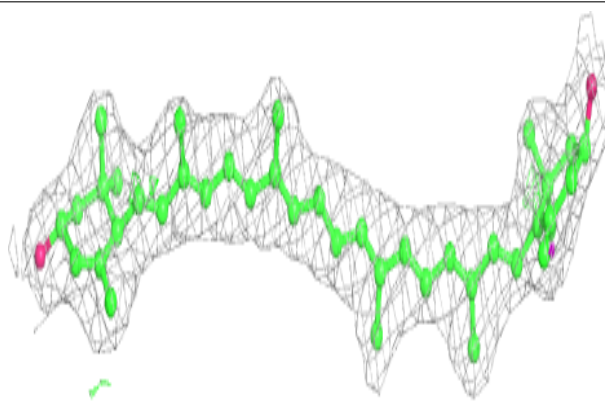


Electron density around CHL J 609:

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

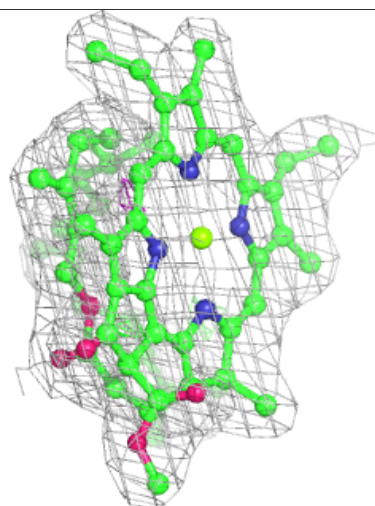
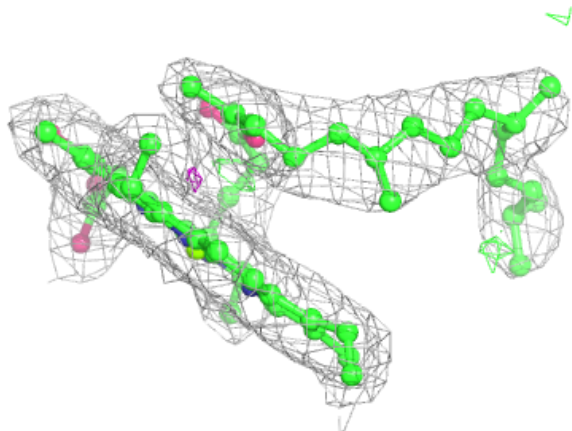
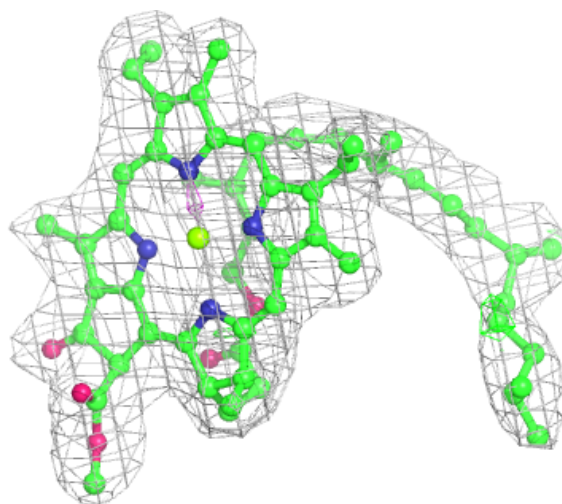
**Electron density around LUT H 7621:**

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



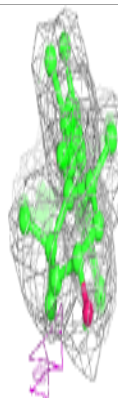
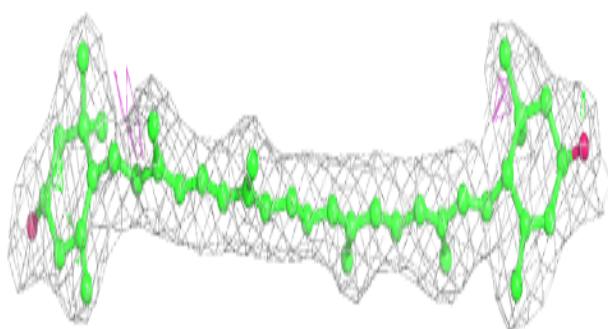
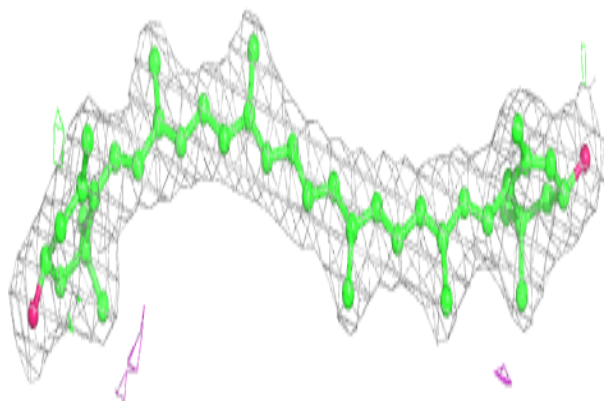
Electron density around CLA J 613:

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

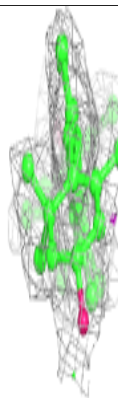
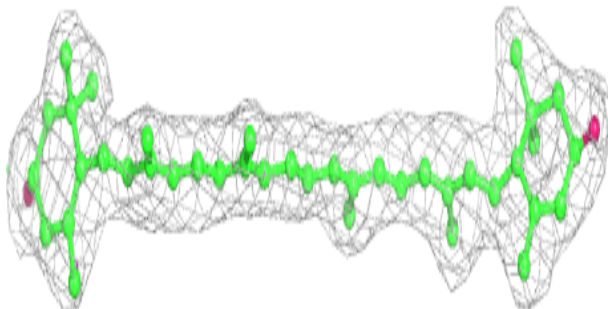
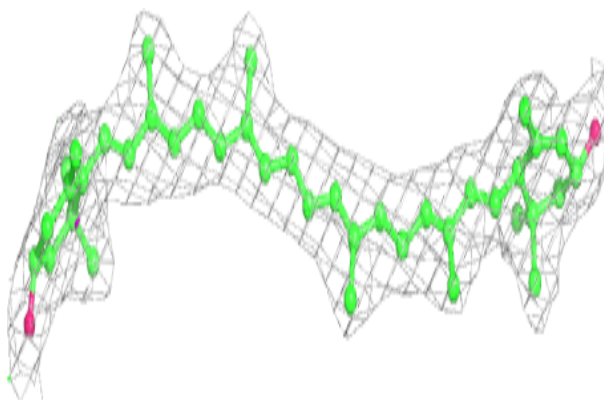


Electron density around LUT F 5620:

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

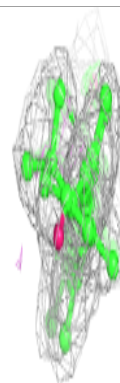
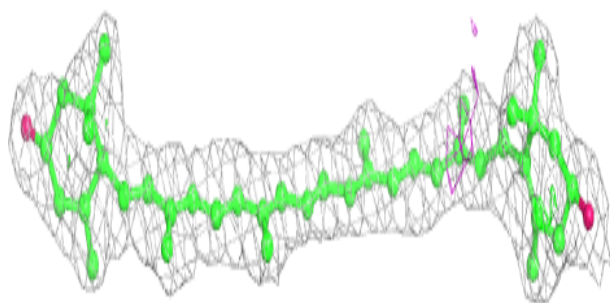
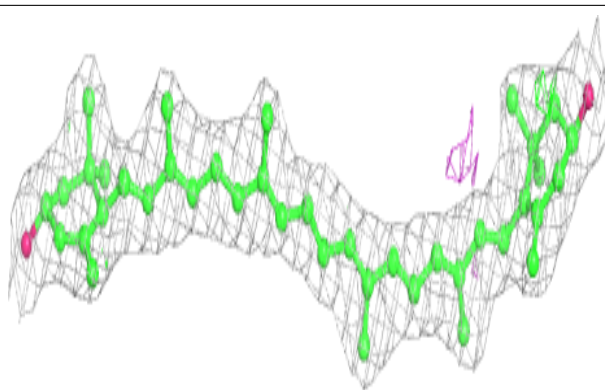
**Electron density around LUT C 2621:**

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



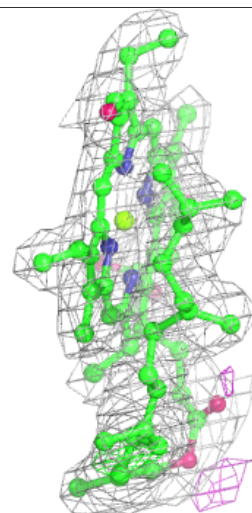
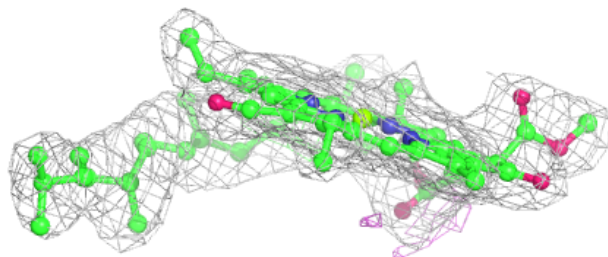
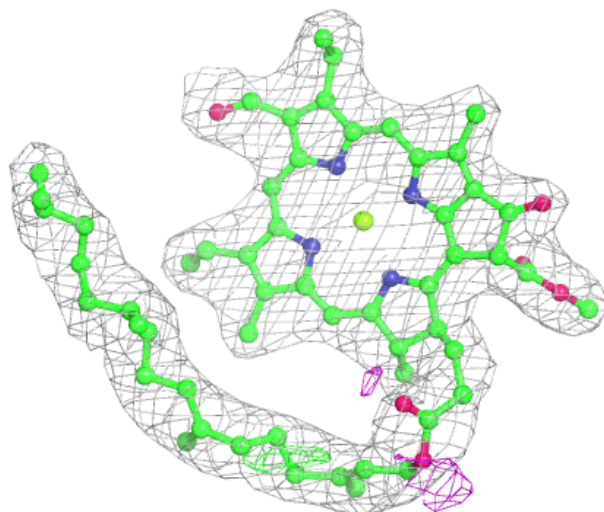
Electron density around LUT J 9620:

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



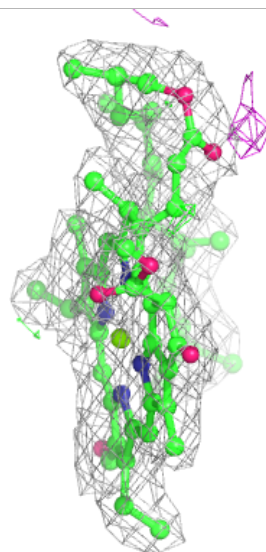
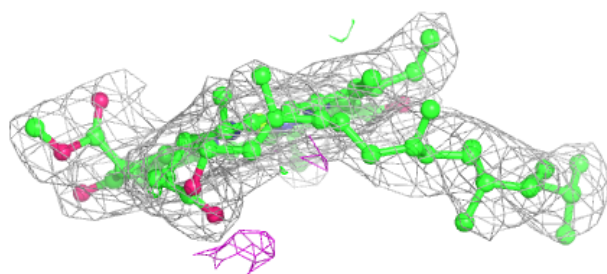
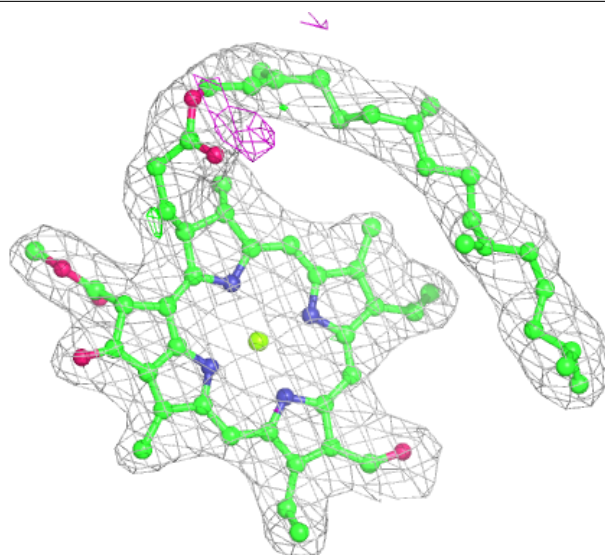
Electron density around CHL C 607:

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



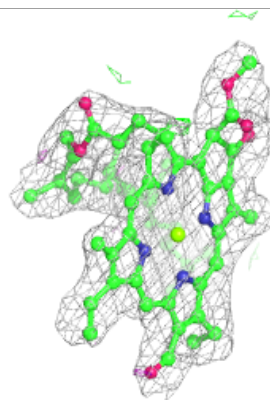
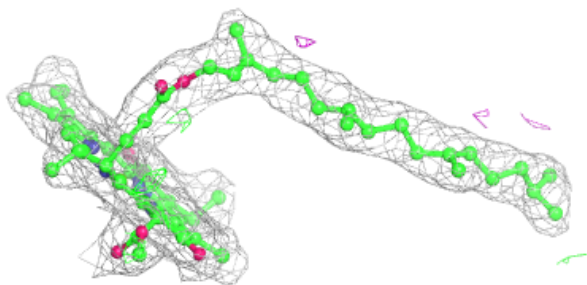
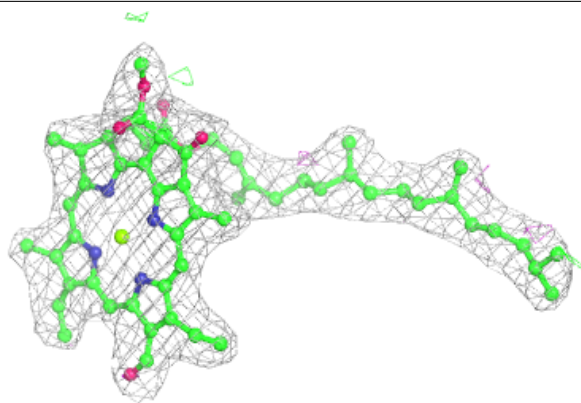
Electron density around CHL H 607:

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



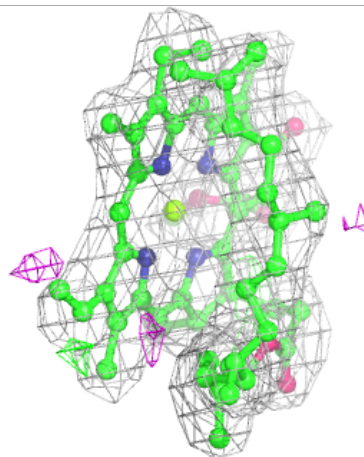
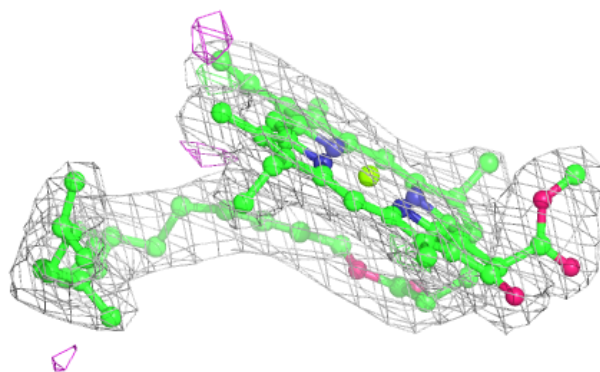
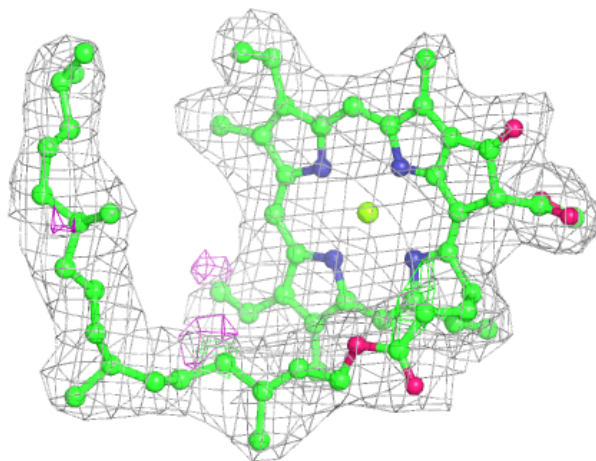
Electron density around CHL E 609:

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



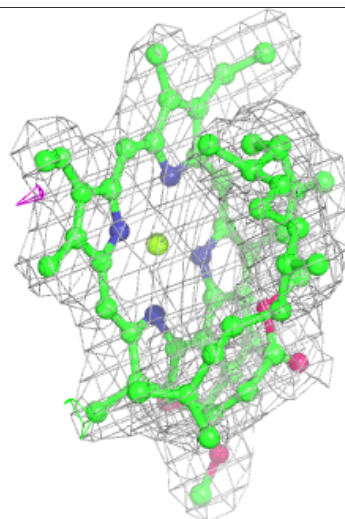
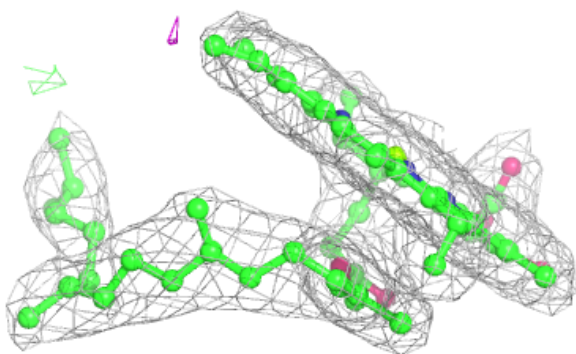
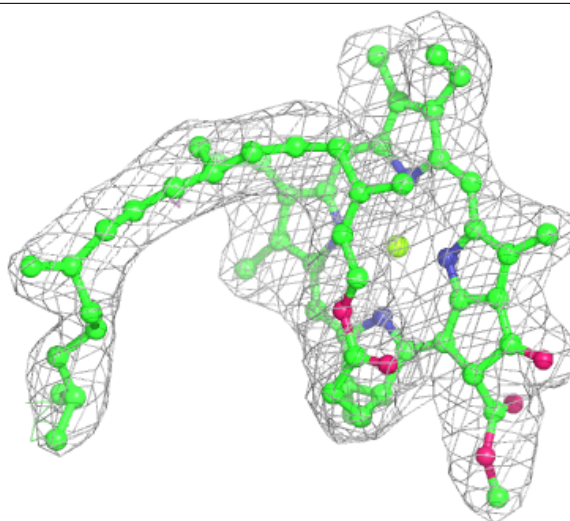
Electron density around CLA C 602:

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



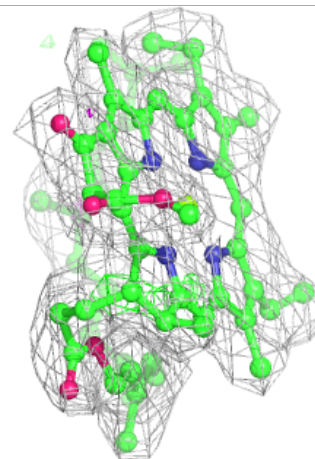
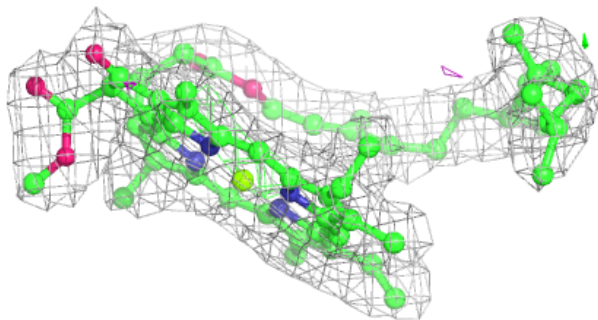
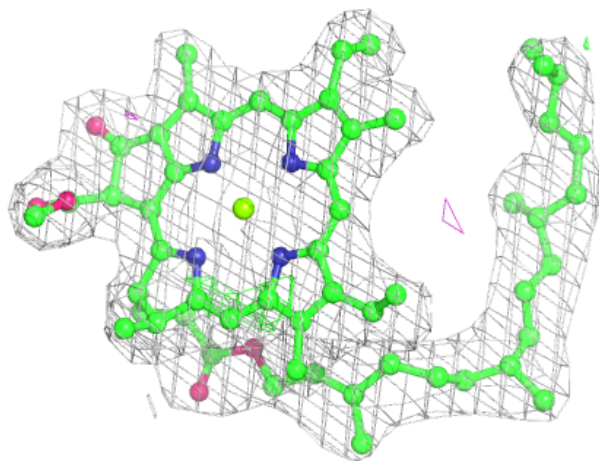
Electron density around CLA B 613:

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



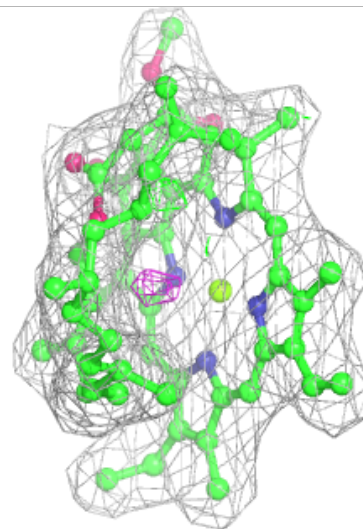
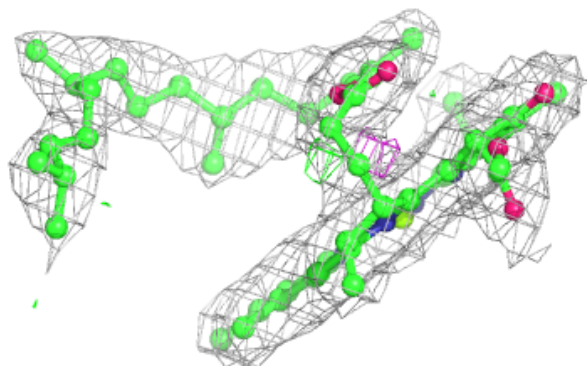
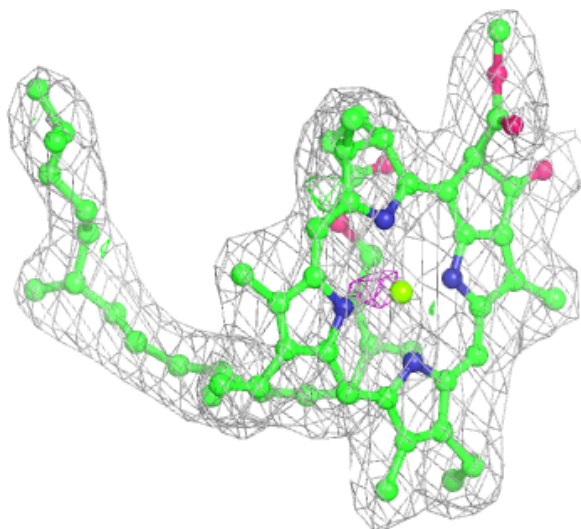
Electron density around CLA B 602:

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



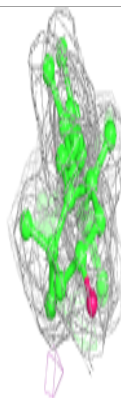
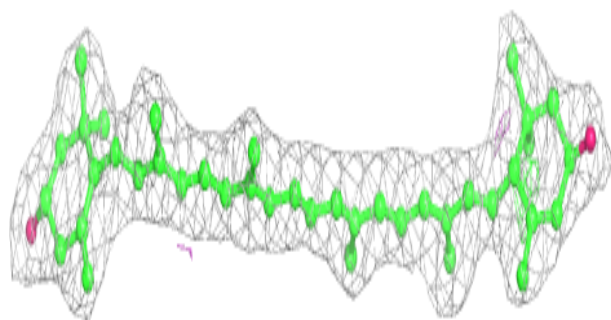
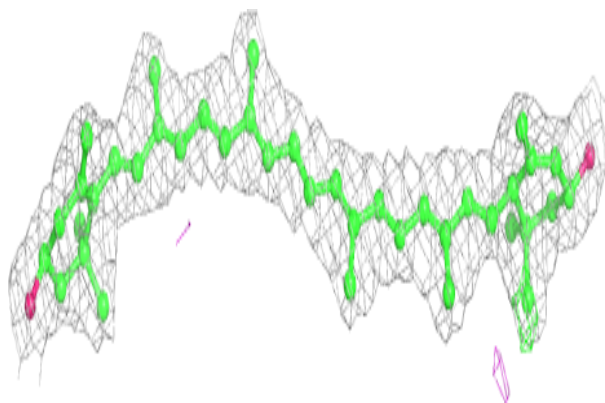
Electron density around CLA H 613:

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



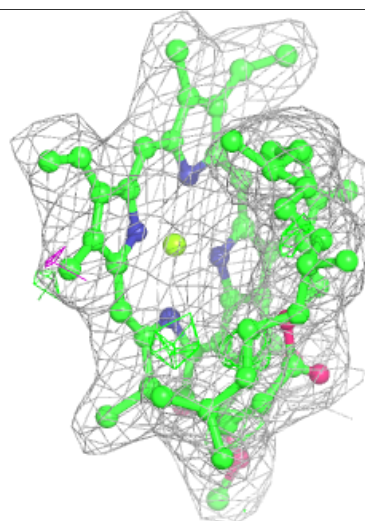
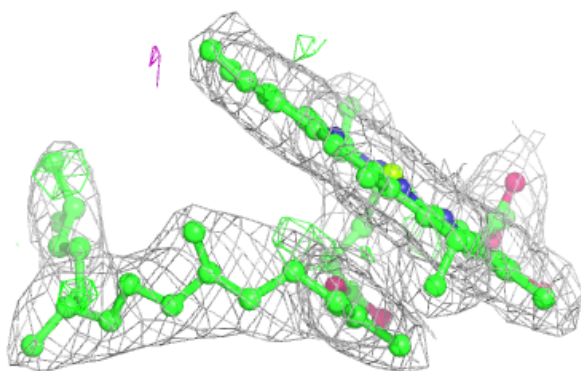
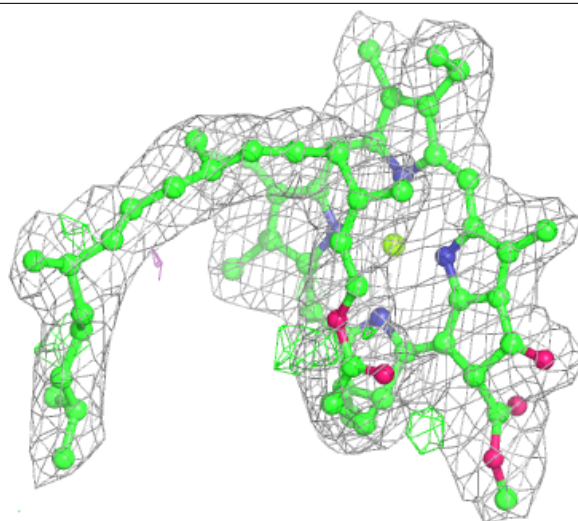
Electron density around LUT B 1620:

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



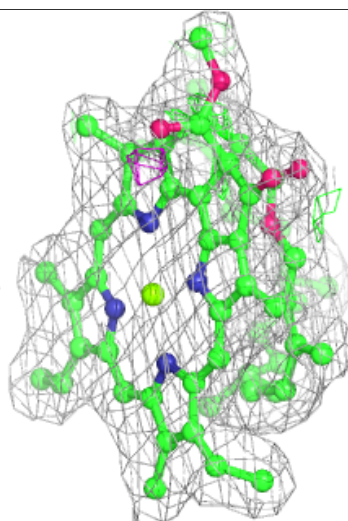
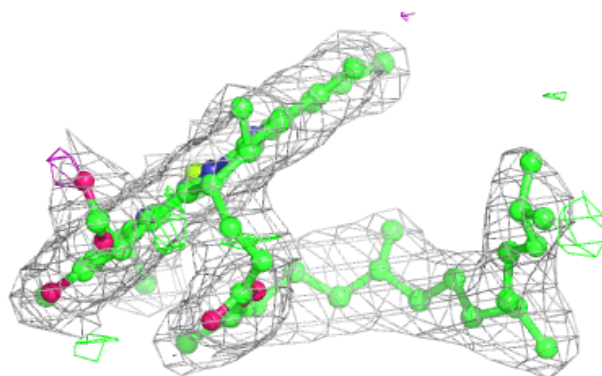
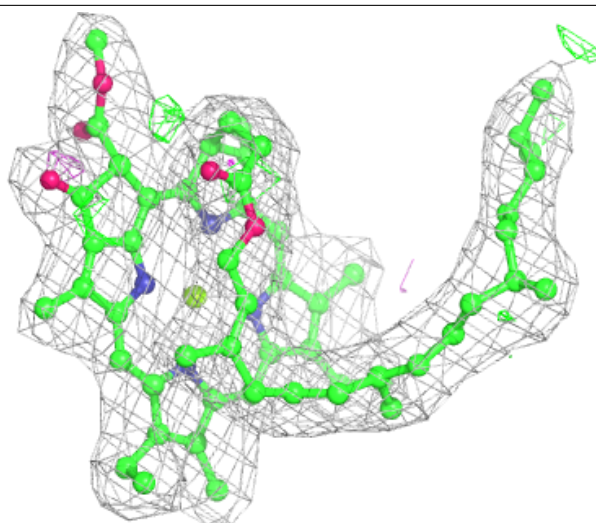
Electron density around CLA F 613:

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



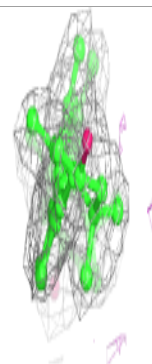
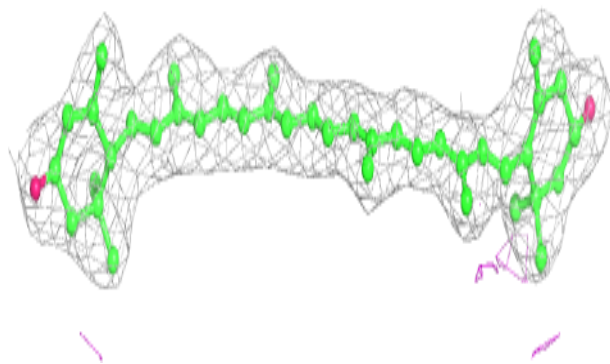
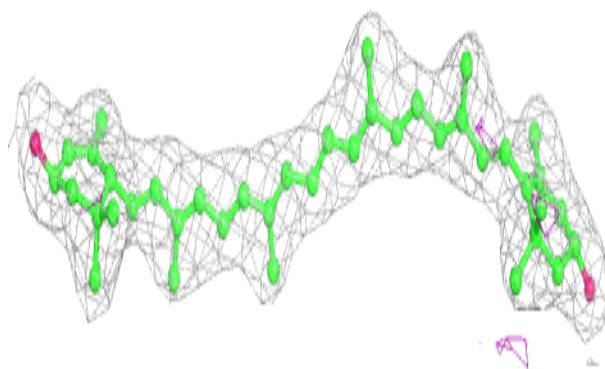
Electron density around CLA C 613:

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



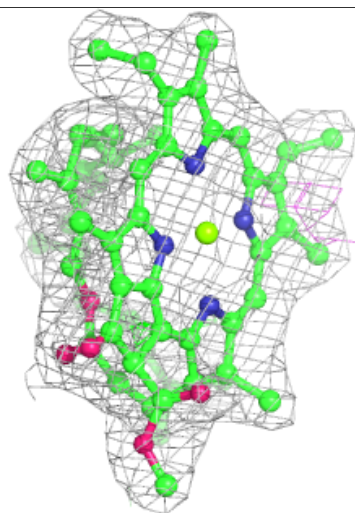
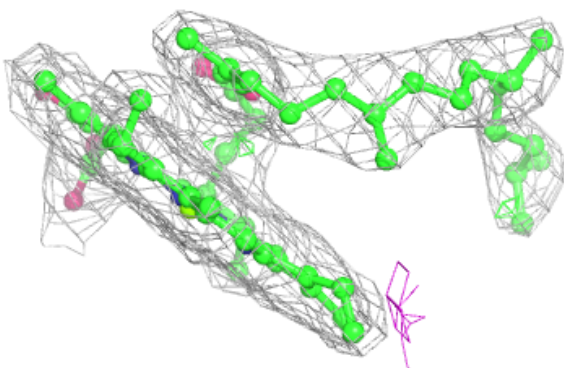
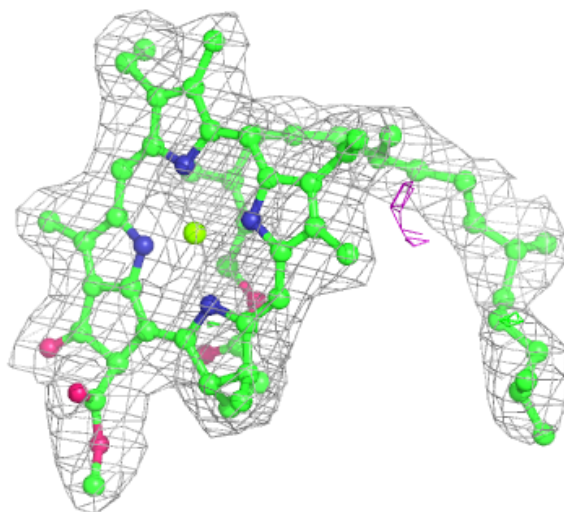
Electron density around LUT E 4620:

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



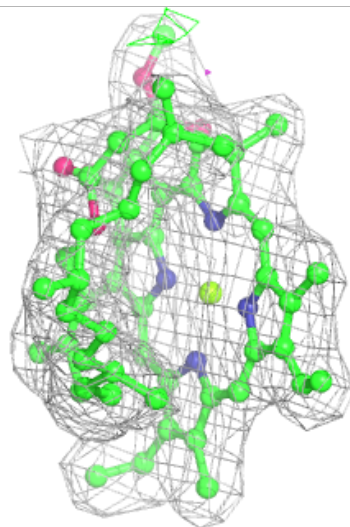
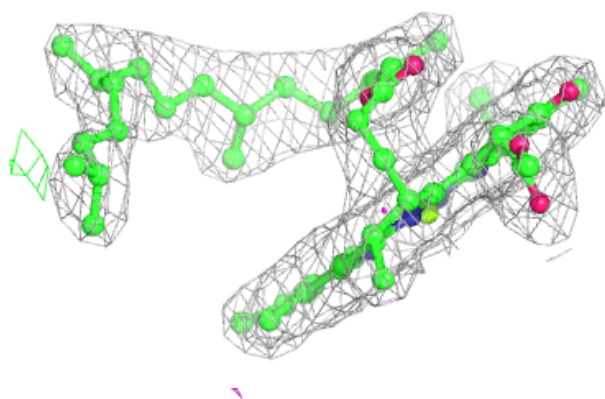
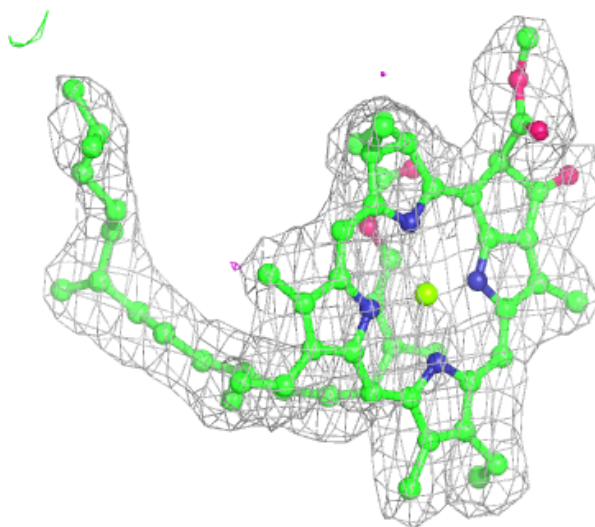
Electron density around CLA E 613:

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



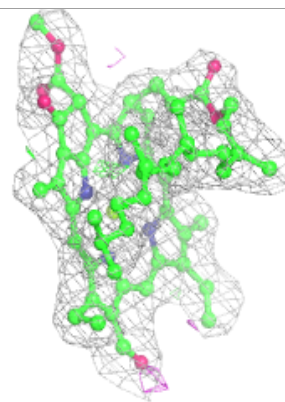
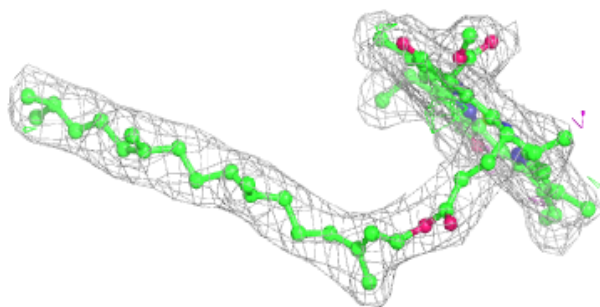
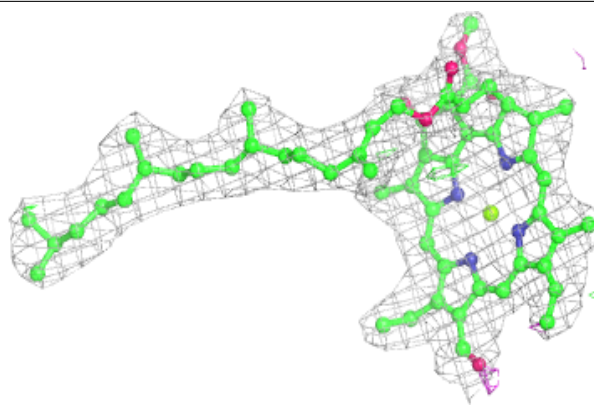
Electron density around CLA D 613:

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

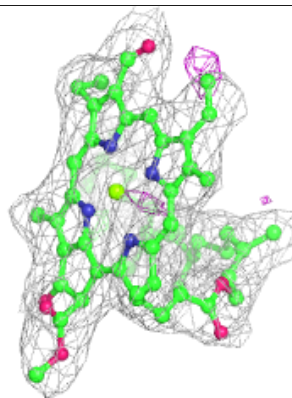
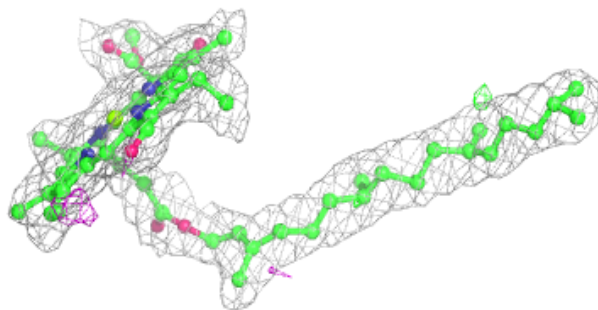
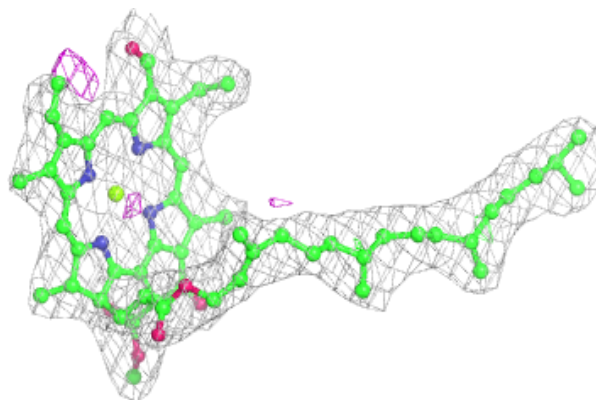


Electron density around CHL I 609:

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

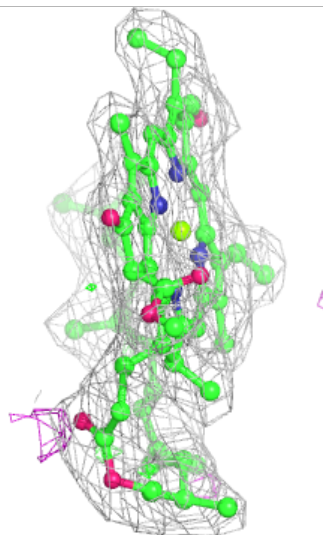
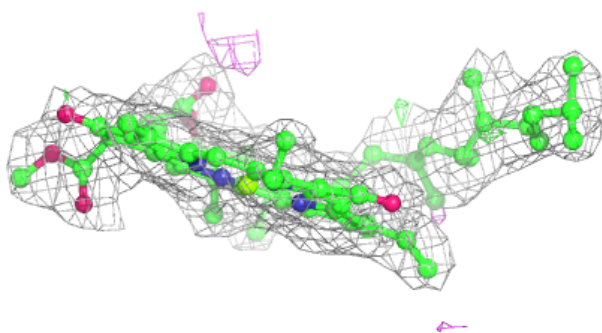
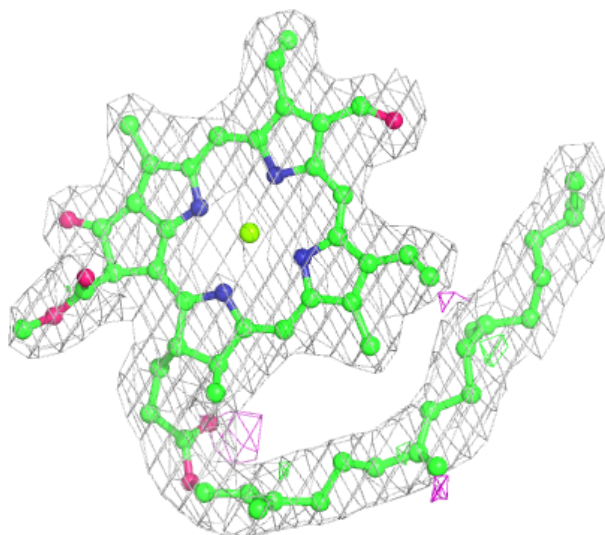
**Electron density around CHL C 609:**

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



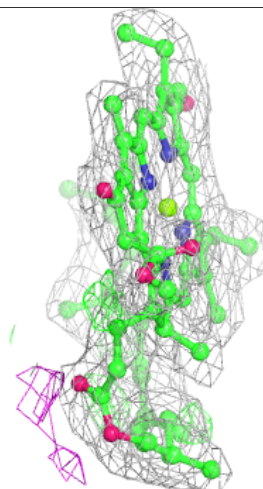
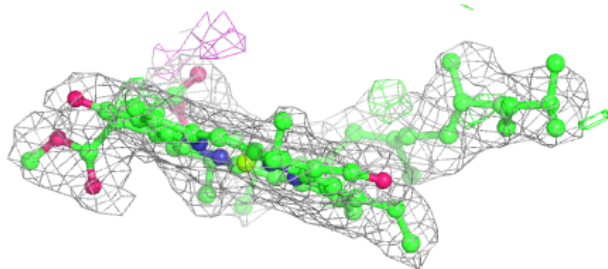
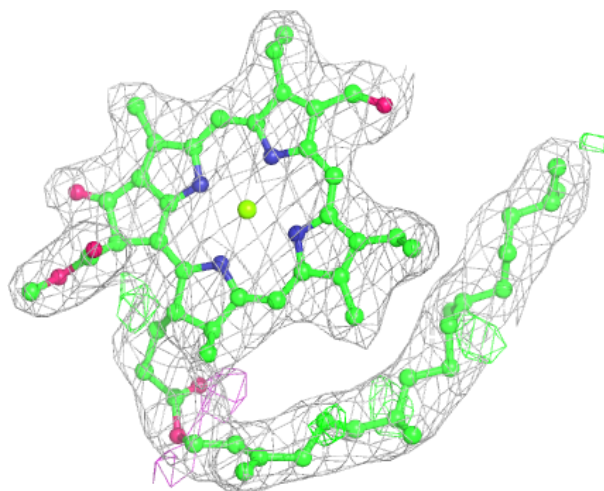
Electron density around CHL G 607:

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



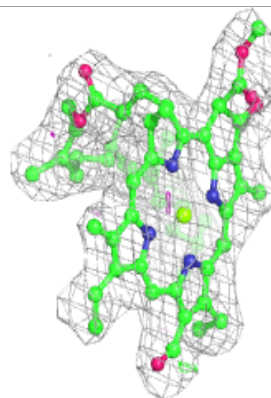
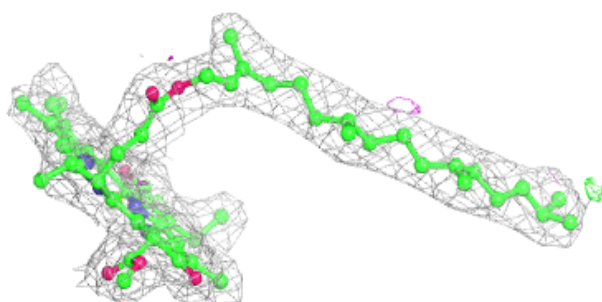
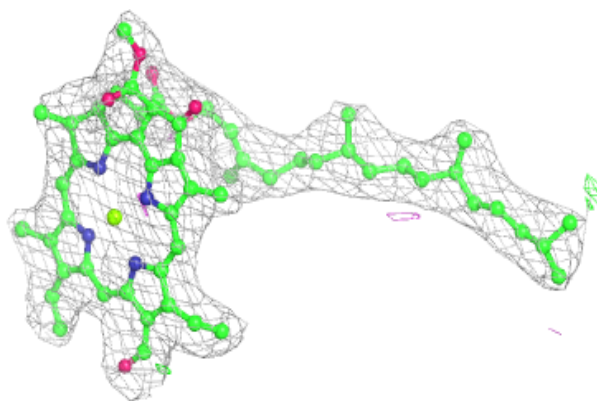
Electron density around CHL D 607:

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

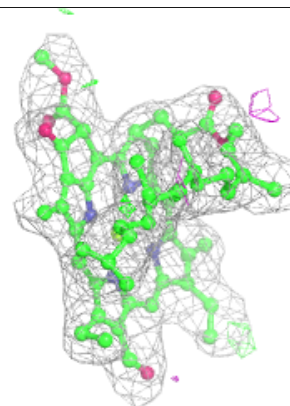
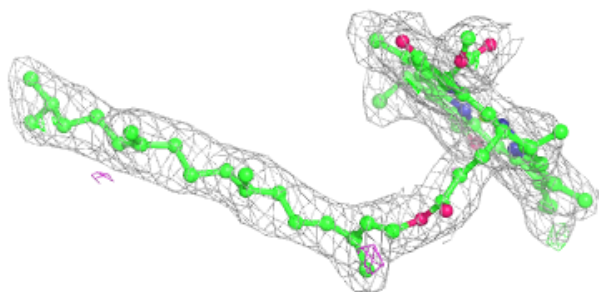
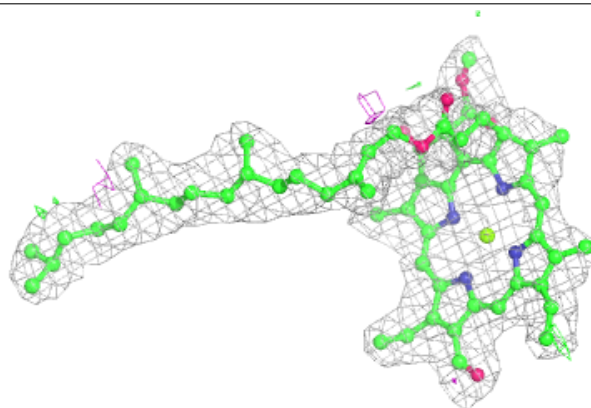


Electron density around CHL H 609:

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

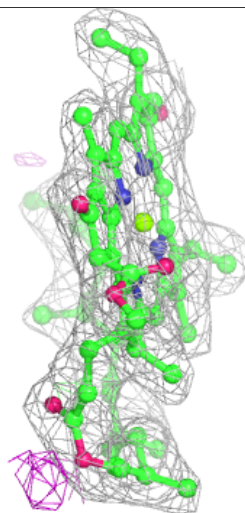
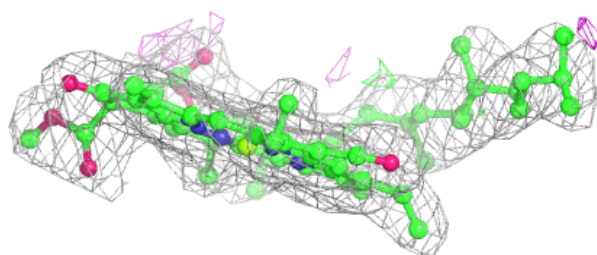
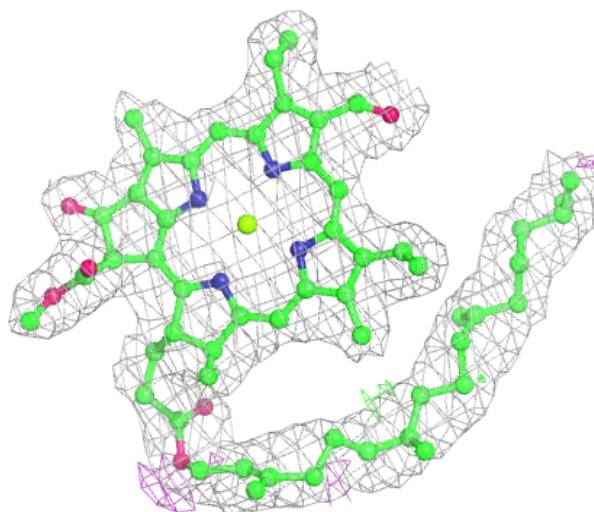
**Electron density around CHL B 609:**

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



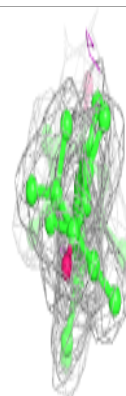
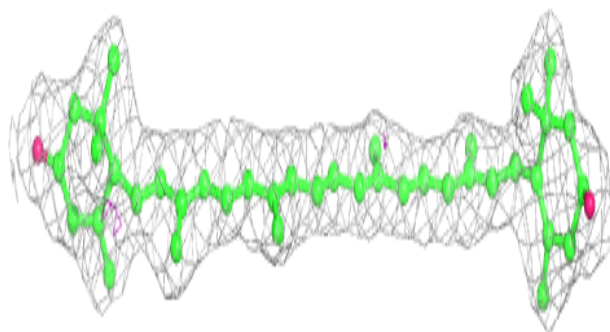
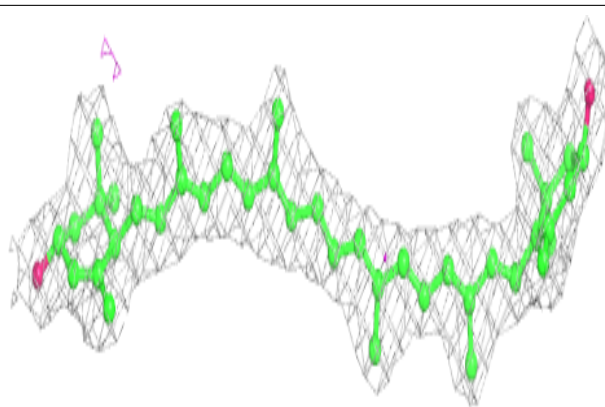
Electron density around CHL B 607:

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



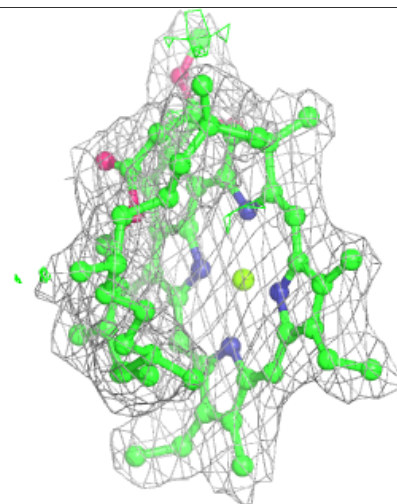
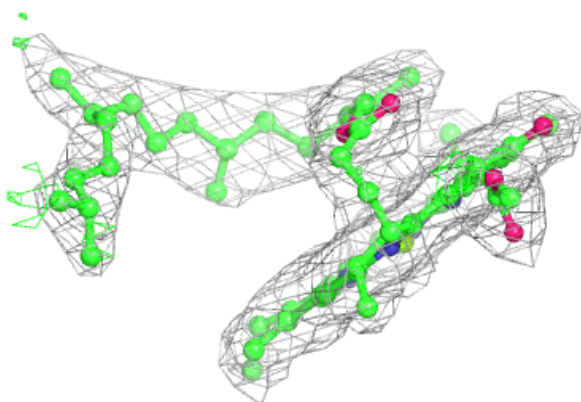
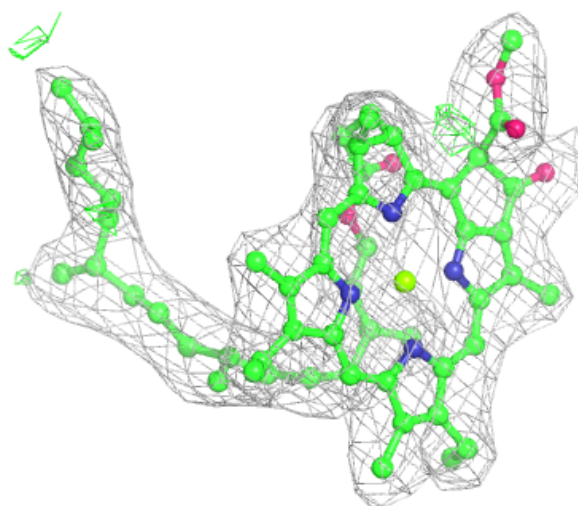
Electron density around LUT A 621:

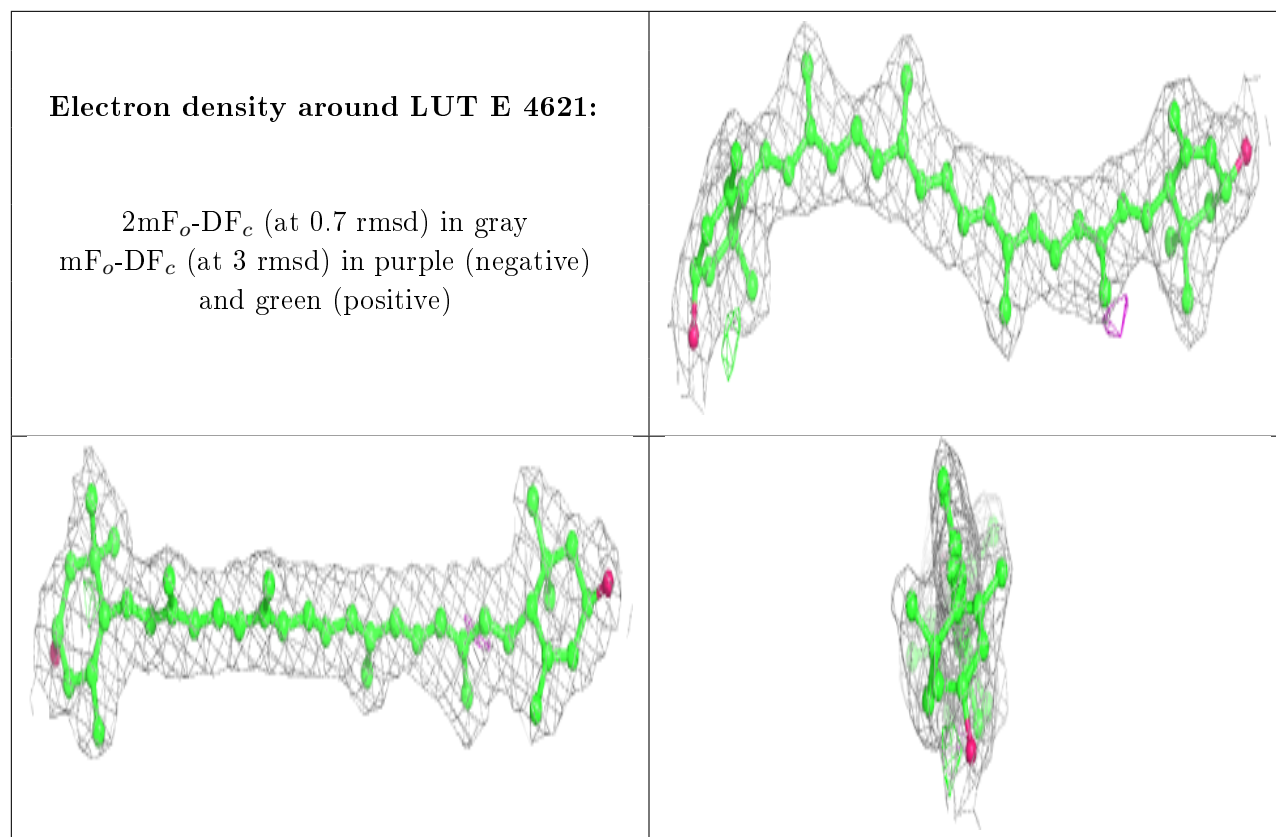
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.