



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2024 – 04:40 AM EST

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

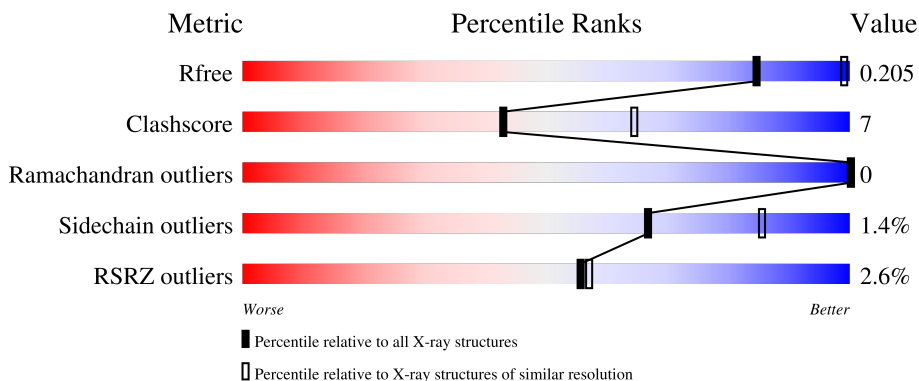
# 1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 2% 78% 16% 6%
1	B	232	 2% 74% 20% 6%
1	C	232	 3% 79% 15% 6%
1	D	232	 2% 80% 14% 6%
1	E	232	 2% 78% 16% 6%

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Mol	Chain	Length	Quality of chain
1	F	232	
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	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	I	613	X	-	-	-
10	CLA	I	614	X	-	-	-
10	CLA	J	602	X	-	-	-
10	CLA	J	603	X	-	-	-
10	CLA	J	604	X	-	-	-
10	CLA	J	610	X	-	-	-
10	CLA	J	611	X	-	-	-
10	CLA	J	612	X	-	-	-
10	CLA	J	613	X	-	-	-
10	CLA	J	614	X	-	-	-
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	-	-	-

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

## 2 Entry composition [i](#)

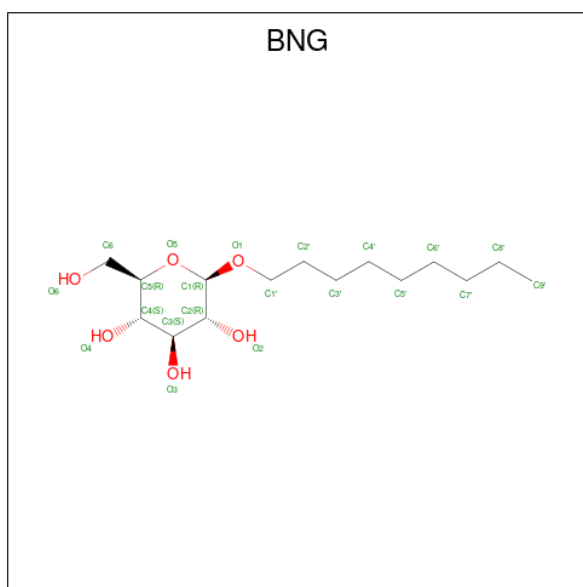
There are 11 unique types of molecules in this entry. The entry contains 29039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: C<sub>15</sub>H<sub>30</sub>O<sub>6</sub>).



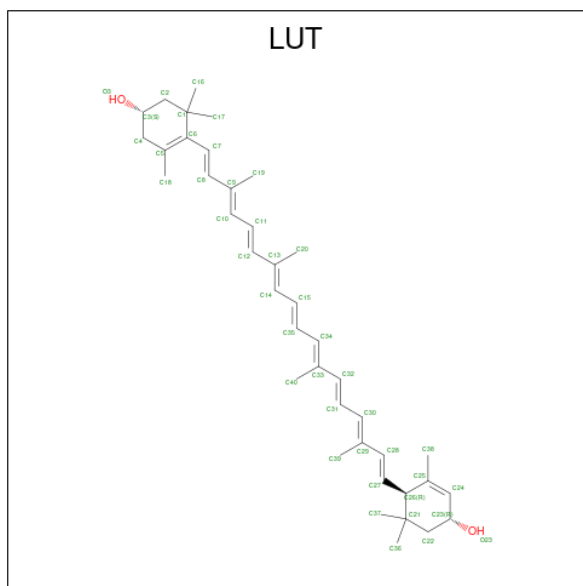
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			21	15 6		
2	B	1	Total	C O	0	0
			21	15 6		
2	C	1	Total	C O	0	0
			21	15 6		
2	D	1	Total	C O	0	0
			21	15 6		
2	E	1	Total	C O	0	0
			21	15 6		
2	F	1	Total	C O	0	0
			21	15 6		
2	G	1	Total	C O	0	0
			21	15 6		
2	H	1	Total	C O	0	0
			21	15 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: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



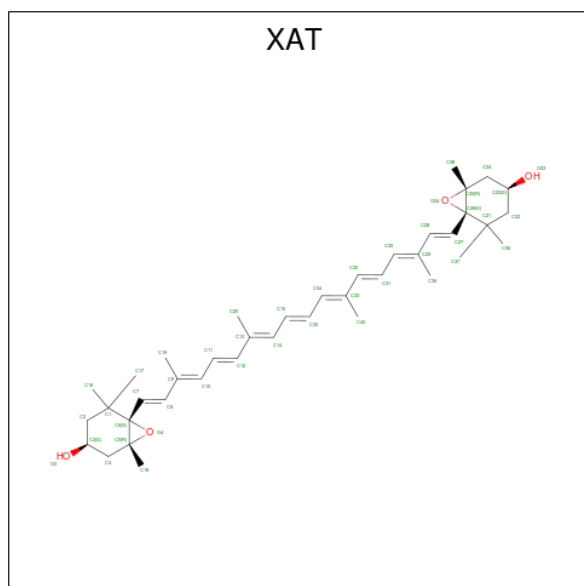
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 42 40 2	0	0
4	A	1	Total C O 42 40 2	0	0
4	B	1	Total C O 42 40 2	0	0
4	B	1	Total C O 42 40 2	0	0
4	C	1	Total C O 42 40 2	0	0
4	C	1	Total C O 42 40 2	0	0
4	D	1	Total C O 42 40 2	0	0
4	D	1	Total C O 42 40 2	0	0
4	E	1	Total C O 42 40 2	0	0
4	E	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	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: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



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		

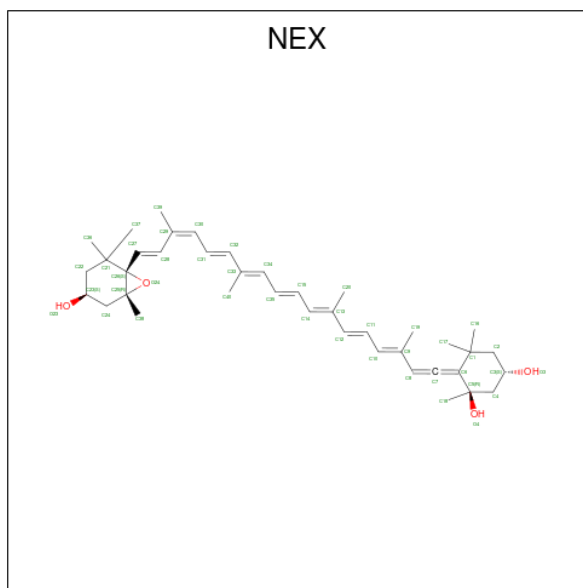
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			44	40	4		
5	E	1	Total	C	O	0	0
			44	40	4		
5	F	1	Total	C	O	0	0
			44	40	4		
5	H	1	Total	C	O	0	0
			44	40	4		
5	I	1	Total	C	O	0	0
			44	40	4		
5	J	1	Total	C	O	0	0
			44	40	4		

- 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-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



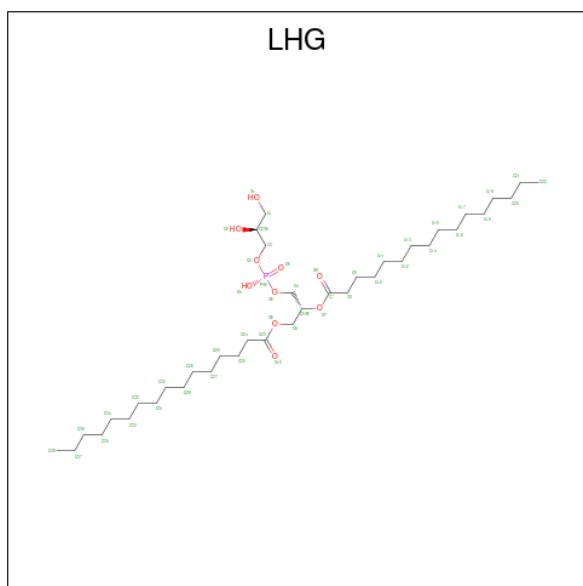
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			44	40	4		
6	B	1	Total	C	O	0	0
			44	40	4		
6	C	1	Total	C	O	0	0
			44	40	4		
6	D	1	Total	C	O	0	0
			44	40	4		

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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: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



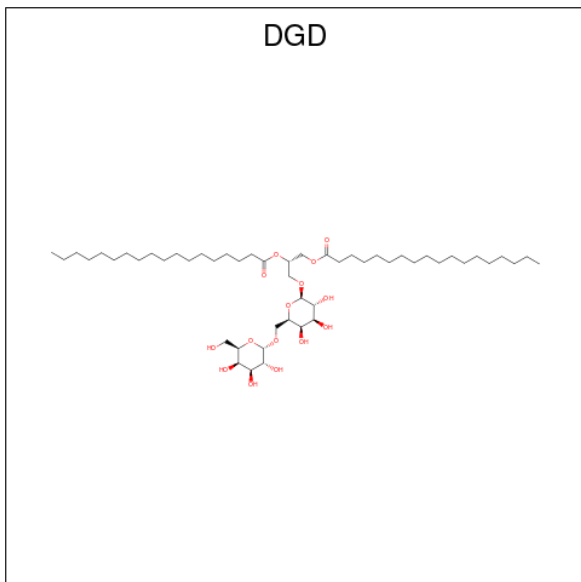
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			49	38	10	1		
7	B	1	Total	C	O	P	0	0
			49	38	10	1		
7	C	1	Total	C	O	P	0	0
			49	38	10	1		
7	D	1	Total	C	O	P	0	0
			49	38	10	1		
7	E	1	Total	C	O	P	0	0
			49	38	10	1		

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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:  $C_{51}H_{96}O_{15}$ ).



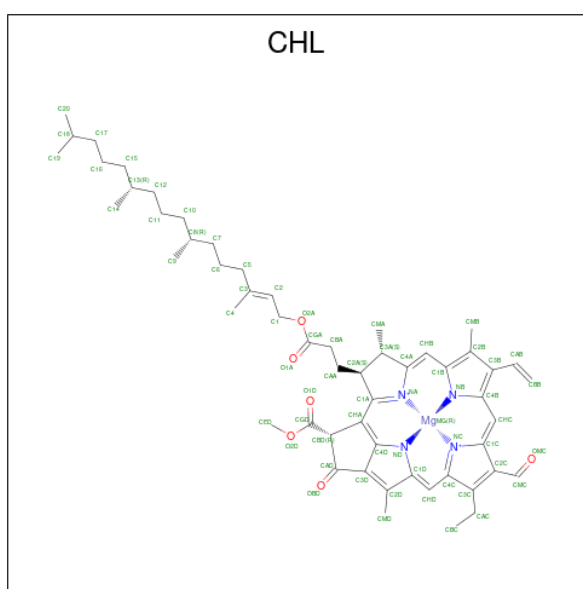
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			66	51	15		
8	B	1	Total	C	O	0	0
			66	51	15		
8	B	1	Total	C	O	0	0
			66	51	15		
8	D	1	Total	C	O	0	0
			66	51	15		
8	D	1	Total	C	O	0	0
			66	51	15		
8	E	1	Total	C	O	0	0
			66	51	15		

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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:  $C_{55}H_{70}MgN_4O_6$ ).



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

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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	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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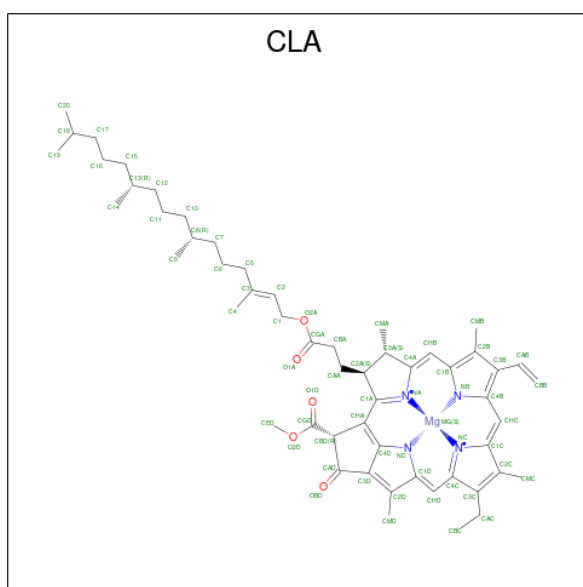
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F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

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

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



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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			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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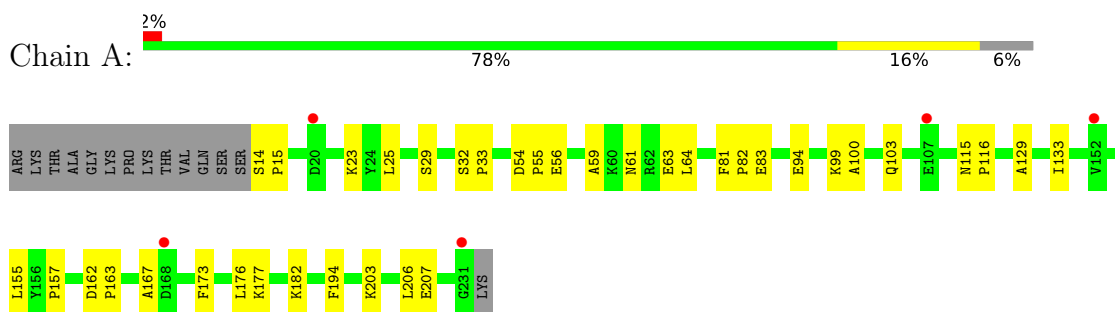
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
11	D	77	Total O 77 77	0	0
11	E	67	Total O 67 67	0	0
11	F	73	Total O 73 73	0	0
11	G	71	Total O 71 71	0	0
11	H	70	Total O 70 70	0	0
11	I	68	Total O 68 68	0	0
11	J	66	Total O 66 66	0	0

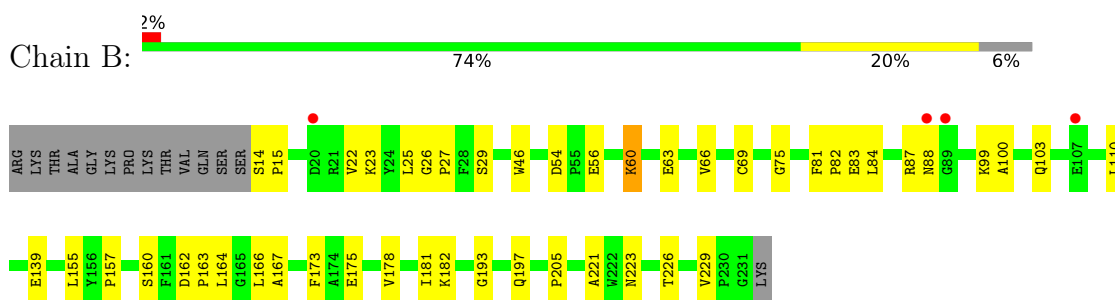
### 3 Residue-property plots [i](#)

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

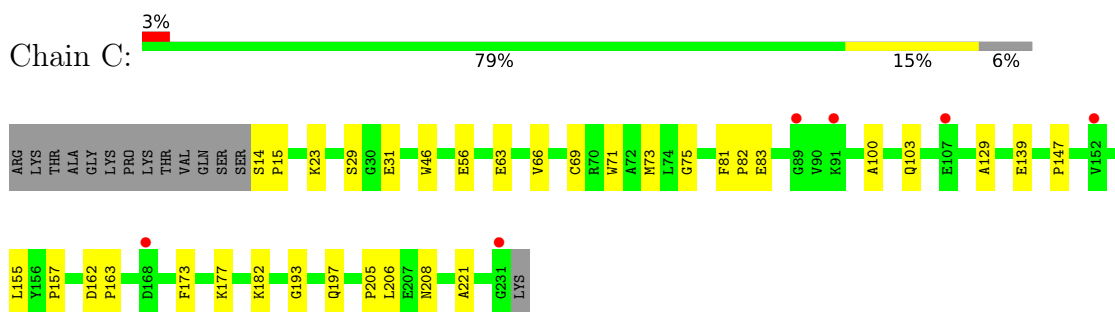
- Molecule 1: Chlorophyll A-B binding protein, chloroplast



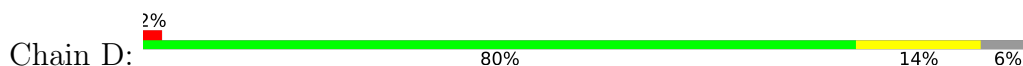
- Molecule 1: Chlorophyll A-B binding protein, chloroplast



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

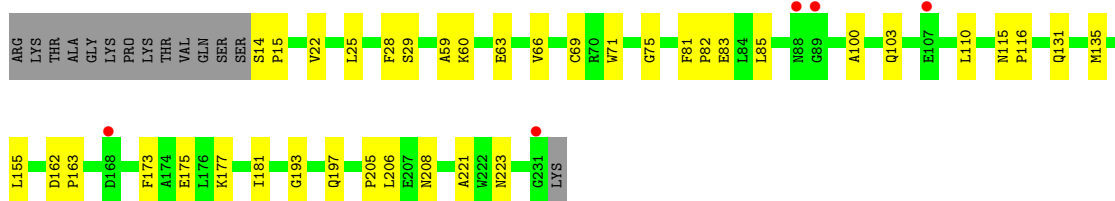
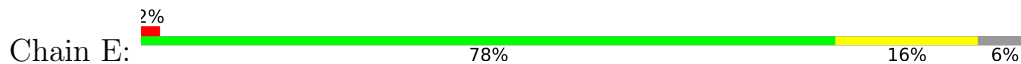


- Molecule 1: Chlorophyll A-B binding protein, chloroplast

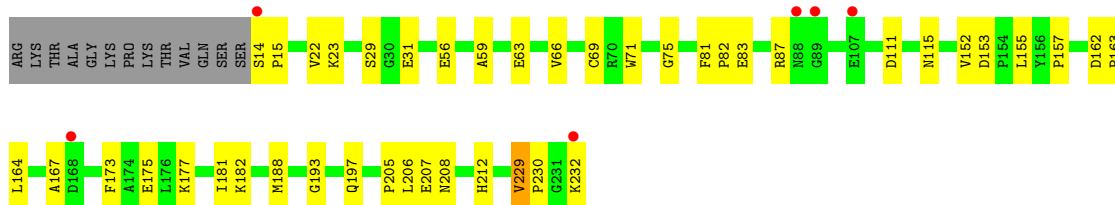
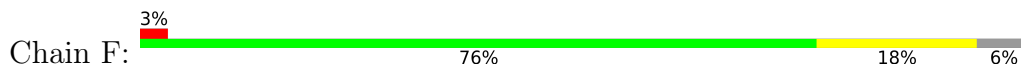




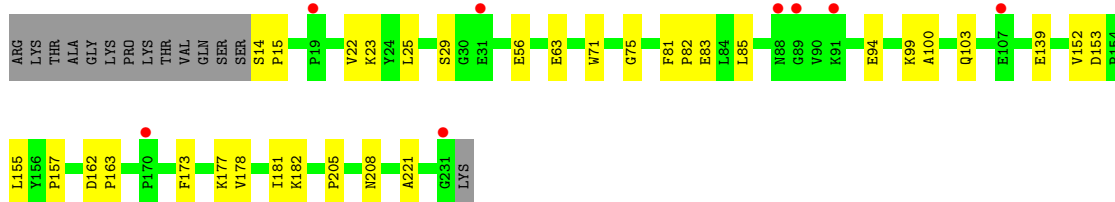
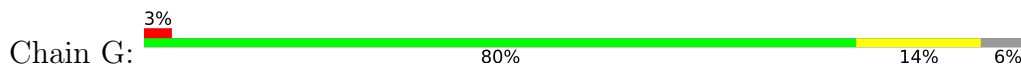
● Molecule 1: Chlorophyll A-B binding protein, chloroplast



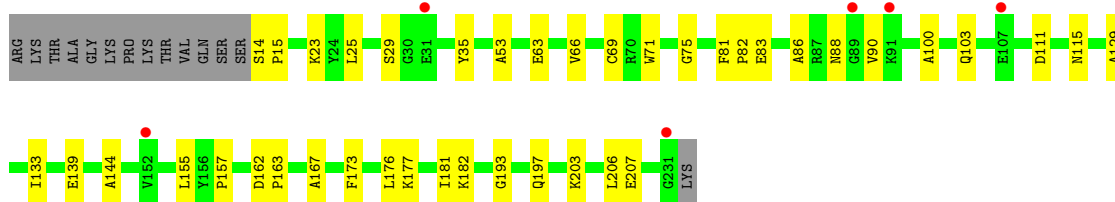
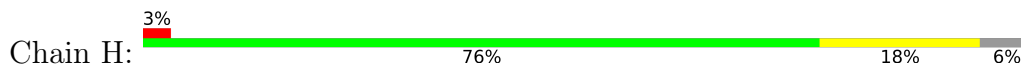
● Molecule 1: Chlorophyll A-B binding protein, chloroplast




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

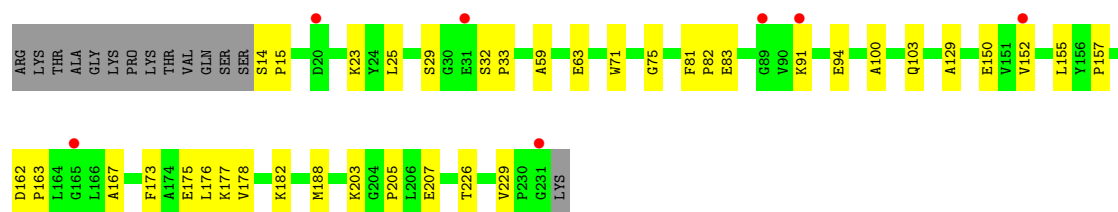


● Molecule 1: Chlorophyll A-B binding protein, chloroplast




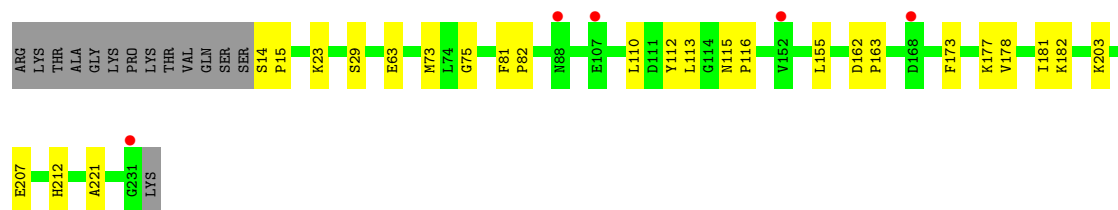
- Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain I: 



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

Chain J: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	261.79Å 261.79Å 660.50Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.04 (at 2.72Å)	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 <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 66.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1661	0	1592	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.

The worst 5 of 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:HA	1:E:60:LYS:HE2	1.66	0.77

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	216/232 (93%)	207 (96%)	9 (4%)	0	100   100
1	B	216/232 (93%)	210 (97%)	6 (3%)	0	100   100

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

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	168/180 (93%)	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
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

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	175	GLU
1	G	181	ILE
1	G	56	GLU
1	H	181	ILE
1	D	32	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	223	ASN
1	H	88	ASN
1	J	223	ASN
1	I	88	ASN
1	I	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	604	11	62,70,73	1.48	9 (14%)	72,109,113	2.32	18 (25%)
9	CHL	D	607	11	66,74,74	1.36	10 (15%)	73,114,114	1.96	13 (17%)
9	CHL	B	605	1	48,56,74	1.60	9 (18%)	51,92,114	1.84	8 (15%)
5	XAT	B	1622	-	39,47,47	0.67	0	54,74,74	1.36	4 (7%)
10	CLA	B	610	1	65,73,73	1.51	10 (15%)	76,113,113	1.68	11 (14%)
10	CLA	E	612	1	65,73,73	1.61	10 (15%)	76,113,113	1.70	12 (15%)
10	CLA	C	611	7	65,73,73	1.46	10 (15%)	76,113,113	1.92	12 (15%)
10	CLA	G	604	11	62,70,73	1.44	10 (16%)	72,109,113	2.14	15 (20%)
6	NEX	I	8623	-	38,46,46	0.98	2 (5%)	50,70,70	1.13	4 (8%)
9	CHL	A	601	1	66,74,74	1.36	9 (13%)	73,114,114	1.89	12 (16%)
4	LUT	I	8621	-	42,43,43	0.96	4 (9%)	51,60,60	1.53	7 (13%)
10	CLA	F	603	1	65,73,73	1.64	12 (18%)	76,113,113	1.80	14 (18%)
10	CLA	J	602	1	65,73,73	1.48	11 (16%)	76,113,113	2.11	20 (26%)
10	CLA	B	614	1	49,57,73	1.69	9 (18%)	55,93,113	2.11	9 (16%)
9	CHL	E	609	1	66,74,74	1.43	11 (16%)	73,114,114	1.78	9 (12%)
10	CLA	J	610	1	65,73,73	1.52	10 (15%)	76,113,113	1.74	15 (19%)
4	LUT	I	8620	-	42,43,43	0.87	4 (9%)	51,60,60	1.51	7 (13%)
9	CHL	B	609	1	66,74,74	1.50	12 (18%)	73,114,114	1.72	12 (16%)
9	CHL	H	609	1	66,74,74	1.44	10 (15%)	73,114,114	1.80	12 (16%)
10	CLA	A	602	1	65,73,73	1.49	10 (15%)	76,113,113	1.97	21 (27%)
6	NEX	B	1623	-	38,46,46	0.90	1 (2%)	50,70,70	1.17	5 (10%)
2	BNG	E	4633	-	21,21,21	0.53	0	26,26,26	0.75	1 (3%)
7	LHG	D	3630	10	48,48,48	0.85	3 (6%)	51,54,54	1.26	5 (9%)
9	CHL	I	608	11	66,74,74	1.45	9 (13%)	73,114,114	1.77	12 (16%)
10	CLA	D	603	1	65,73,73	1.50	10 (15%)	76,113,113	1.71	14 (18%)
10	CLA	F	610	1	65,73,73	1.63	10 (15%)	76,113,113	1.66	9 (11%)
10	CLA	H	613	1	65,73,73	1.44	8 (12%)	76,113,113	2.03	14 (18%)
4	LUT	C	2620	-	42,43,43	0.92	3 (7%)	51,60,60	1.43	6 (11%)
10	CLA	C	613	1	65,73,73	1.46	13 (20%)	76,113,113	1.94	11 (14%)
7	LHG	H	7630	10	48,48,48	0.92	3 (6%)	51,54,54	1.33	6 (11%)
10	CLA	G	602	1	65,73,73	1.52	13 (20%)	76,113,113	2.04	22 (28%)
10	CLA	E	603	1	65,73,73	1.59	12 (18%)	76,113,113	1.73	15 (19%)
10	CLA	A	604	11	62,70,73	1.50	10 (16%)	72,109,113	2.13	12 (16%)
10	CLA	J	604	11	62,70,73	1.47	9 (14%)	72,109,113	2.22	15 (20%)
6	NEX	E	4623	-	38,46,46	0.97	1 (2%)	50,70,70	1.11	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	CHL	G	606	11	51,59,74	1.83	10 (19%)	55,96,114	2.19	9 (16%)
8	DGD	D	3632	-	67,67,67	0.97	2 (2%)	81,81,81	1.00	8 (9%)
7	LHG	J	9630	10	48,48,48	0.97	3 (6%)	51,54,54	1.34	5 (9%)
10	CLA	D	602	1	65,73,73	1.56	13 (20%)	76,113,113	1.98	18 (23%)
9	CHL	H	608	11	66,74,74	1.49	11 (16%)	73,114,114	1.89	14 (19%)
9	CHL	H	605	1	48,56,74	1.69	9 (18%)	51,92,114	1.76	9 (17%)
7	LHG	C	2630	10	48,48,48	0.94	3 (6%)	51,54,54	1.34	5 (9%)
9	CHL	I	601	1	66,74,74	1.37	10 (15%)	73,114,114	1.84	10 (13%)
10	CLA	H	610	1	65,73,73	1.56	11 (16%)	76,113,113	1.74	17 (22%)
10	CLA	I	611	7	65,73,73	1.54	9 (13%)	76,113,113	1.82	17 (22%)
9	CHL	E	608	11	66,74,74	1.49	11 (16%)	73,114,114	1.86	14 (19%)
2	BNG	D	3633	-	21,21,21	0.51	0	26,26,26	0.84	1 (3%)
9	CHL	H	606	11	51,59,74	1.74	12 (23%)	55,96,114	2.21	10 (18%)
10	CLA	J	612	1	65,73,73	1.53	10 (15%)	76,113,113	1.79	17 (22%)
10	CLA	J	613	1	65,73,73	1.53	12 (18%)	76,113,113	1.79	13 (17%)
9	CHL	I	606	11	51,59,74	1.71	9 (17%)	55,96,114	2.27	9 (16%)
10	CLA	C	604	11	62,70,73	1.45	10 (16%)	72,109,113	2.24	12 (16%)
5	XAT	I	9622	-	39,47,47	0.75	1 (2%)	54,74,74	1.21	4 (7%)
9	CHL	C	601	1	66,74,74	1.40	10 (15%)	73,114,114	1.82	12 (16%)
6	NEX	A	623	-	38,46,46	1.03	2 (5%)	50,70,70	1.25	5 (10%)
10	CLA	C	610	1	65,73,73	1.62	11 (16%)	76,113,113	1.66	13 (17%)
7	LHG	B	1630	10	48,48,48	1.02	3 (6%)	51,54,54	1.32	5 (9%)
10	CLA	B	602	1	65,73,73	1.54	13 (20%)	76,113,113	2.08	18 (23%)
10	CLA	D	604	11	62,70,73	1.47	9 (14%)	72,109,113	2.30	15 (20%)
10	CLA	H	604	11	62,70,73	1.42	10 (16%)	72,109,113	2.19	17 (23%)
10	CLA	F	613	1	65,73,73	1.51	11 (16%)	76,113,113	1.92	10 (13%)
9	CHL	B	606	11	51,59,74	1.73	10 (19%)	55,96,114	2.15	9 (16%)
9	CHL	G	605	1	48,56,74	1.71	10 (20%)	51,92,114	1.77	7 (13%)
9	CHL	H	607	11	66,74,74	1.55	10 (15%)	73,114,114	2.02	15 (20%)
6	NEX	J	9623	-	38,46,46	1.02	2 (5%)	50,70,70	1.17	4 (8%)
10	CLA	C	612	1	65,73,73	1.50	9 (13%)	76,113,113	1.74	12 (15%)
10	CLA	A	611	7	65,73,73	1.51	10 (15%)	76,113,113	1.95	17 (22%)
10	CLA	G	613	1	65,73,73	1.46	11 (16%)	76,113,113	2.02	11 (14%)
8	DGD	E	4632	-	67,67,67	0.97	1 (1%)	81,81,81	1.05	8 (9%)
9	CHL	E	605	1	48,56,74	1.60	10 (20%)	51,92,114	1.89	8 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	F	614	1	49,57,73	1.69	7 (14%)	55,93,113	1.98	9 (16%)
9	CHL	F	607	11	66,74,74	1.54	7 (10%)	73,114,114	2.13	18 (24%)
4	LUT	G	6621	-	42,43,43	0.94	2 (4%)	51,60,60	1.37	7 (13%)
9	CHL	A	606	11	51,59,74	1.70	9 (17%)	55,96,114	2.22	14 (25%)
10	CLA	I	603	1	65,73,73	1.54	11 (16%)	76,113,113	1.67	13 (17%)
6	NEX	H	7623	-	38,46,46	0.96	2 (5%)	50,70,70	1.20	5 (10%)
8	DGD	H	6632	-	67,67,67	0.85	1 (1%)	81,81,81	1.01	7 (8%)
10	CLA	I	612	1	65,73,73	1.55	10 (15%)	76,113,113	1.75	12 (15%)
10	CLA	I	602	1	65,73,73	1.52	14 (21%)	76,113,113	2.14	21 (27%)
4	LUT	G	6620	-	42,43,43	0.94	4 (9%)	51,60,60	1.48	8 (15%)
9	CHL	I	605	1	48,56,74	1.69	8 (16%)	51,92,114	1.87	10 (19%)
9	CHL	F	601	1	66,74,74	1.40	9 (13%)	73,114,114	1.83	11 (15%)
2	BNG	I	8633	-	21,21,21	0.54	0	26,26,26	0.76	1 (3%)
10	CLA	H	602	1	65,73,73	1.58	11 (16%)	76,113,113	2.00	23 (30%)
4	LUT	B	1621	-	42,43,43	1.03	5 (11%)	51,60,60	1.36	4 (7%)
4	LUT	J	9620	-	42,43,43	0.99	4 (9%)	51,60,60	1.52	5 (9%)
8	DGD	I	8632	-	67,67,67	0.92	1 (1%)	81,81,81	1.00	8 (9%)
4	LUT	D	3621	-	42,43,43	1.08	4 (9%)	51,60,60	1.43	9 (17%)
4	LUT	E	4621	-	42,43,43	1.08	4 (9%)	51,60,60	1.41	6 (11%)
2	BNG	F	5633	-	21,21,21	0.54	0	26,26,26	0.79	1 (3%)
4	LUT	H	7621	-	42,43,43	0.98	4 (9%)	51,60,60	1.47	6 (11%)
2	BNG	G	6633	-	21,21,21	0.53	0	26,26,26	0.79	1 (3%)
10	CLA	B	612	1	65,73,73	1.59	12 (18%)	76,113,113	1.70	12 (15%)
5	XAT	H	4622	-	39,47,47	0.74	0	54,74,74	1.34	5 (9%)
9	CHL	J	605	1	48,56,74	1.70	9 (18%)	51,92,114	1.90	8 (15%)
9	CHL	J	601	1	66,74,74	1.44	12 (18%)	73,114,114	1.73	9 (12%)
9	CHL	J	606	11	51,59,74	1.77	10 (19%)	55,96,114	2.18	10 (18%)
10	CLA	I	614	1	49,57,73	1.66	10 (20%)	55,93,113	2.04	9 (16%)
10	CLA	G	612	1	65,73,73	1.54	11 (16%)	76,113,113	1.81	12 (15%)
5	XAT	E	2622	-	39,47,47	0.72	0	54,74,74	1.24	6 (11%)
2	BNG	A	633	-	21,21,21	0.56	0	26,26,26	0.79	1 (3%)
9	CHL	J	608	11	66,74,74	1.47	12 (18%)	73,114,114	1.76	11 (15%)
10	CLA	B	603	1	65,73,73	1.54	12 (18%)	76,113,113	1.82	13 (17%)
10	CLA	C	614	1	49,57,73	1.68	10 (20%)	55,93,113	2.12	12 (21%)
9	CHL	F	609	1	66,74,74	1.45	12 (18%)	73,114,114	1.80	15 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	CHL	F	605	1	48,56,74	1.69	7 (14%)	51,92,114	1.87	8 (15%)
6	NEX	G	6623	-	38,46,46	0.99	2 (5%)	50,70,70	1.27	6 (12%)
10	CLA	E	611	7	65,73,73	1.55	10 (15%)	76,113,113	1.89	15 (19%)
5	XAT	B	5622	-	39,47,47	0.72	0	54,74,74	1.22	5 (9%)
2	BNG	B	1633	-	21,21,21	0.50	0	26,26,26	0.81	1 (3%)
9	CHL	E	606	11	51,59,74	1.72	11 (21%)	55,96,114	2.34	13 (23%)
4	LUT	D	3620	-	42,43,43	0.91	3 (7%)	51,60,60	1.56	7 (13%)
9	CHL	C	608	11	66,74,74	1.48	12 (18%)	73,114,114	1.91	14 (19%)
8	DGD	B	2632	-	67,67,67	0.92	1 (1%)	81,81,81	1.05	8 (9%)
10	CLA	H	614	1	49,57,73	1.66	7 (14%)	55,93,113	2.12	11 (20%)
6	NEX	C	2623	-	38,46,46	1.01	2 (5%)	50,70,70	1.13	3 (6%)
10	CLA	B	611	7	65,73,73	1.50	9 (13%)	76,113,113	1.99	17 (22%)
4	LUT	A	620	-	42,43,43	0.93	4 (9%)	51,60,60	1.55	7 (13%)
10	CLA	G	611	7	65,73,73	1.49	10 (15%)	76,113,113	1.93	15 (19%)
4	LUT	E	4620	-	42,43,43	1.03	4 (9%)	51,60,60	1.55	6 (11%)
10	CLA	H	611	7	65,73,73	1.50	10 (15%)	76,113,113	1.89	15 (19%)
7	LHG	G	6630	10	48,48,48	0.98	3 (6%)	51,54,54	1.39	5 (9%)
10	CLA	E	613	1	65,73,73	1.54	10 (15%)	76,113,113	1.88	14 (18%)
9	CHL	F	608	11	66,74,74	1.46	11 (16%)	73,114,114	1.92	14 (19%)
10	CLA	A	603	1	65,73,73	1.56	11 (16%)	76,113,113	1.82	15 (19%)
5	XAT	A	622	-	39,47,47	0.62	0	54,74,74	1.18	3 (5%)
8	DGD	H	7632	-	67,67,67	0.94	2 (2%)	81,81,81	1.00	8 (9%)
9	CHL	A	609	1	66,74,74	1.50	10 (15%)	73,114,114	1.77	11 (15%)
9	CHL	F	606	11	51,59,74	1.80	10 (19%)	55,96,114	2.24	12 (21%)
9	CHL	D	605	1	48,56,74	1.73	9 (18%)	51,92,114	1.93	8 (15%)
10	CLA	D	610	1	65,73,73	1.60	9 (13%)	76,113,113	1.76	12 (15%)
10	CLA	F	612	1	65,73,73	1.65	11 (16%)	76,113,113	1.78	14 (18%)
7	LHG	I	8630	10	48,48,48	1.02	3 (6%)	51,54,54	1.38	5 (9%)
10	CLA	I	604	11	62,70,73	1.43	8 (12%)	72,109,113	2.21	14 (19%)
9	CHL	B	607	11	66,74,74	1.47	10 (15%)	73,114,114	2.11	16 (21%)
9	CHL	I	607	11	66,74,74	1.57	10 (15%)	73,114,114	2.08	16 (21%)
10	CLA	B	613	1	65,73,73	1.48	11 (16%)	76,113,113	1.99	12 (15%)
10	CLA	I	610	1	65,73,73	1.58	11 (16%)	76,113,113	1.64	12 (15%)
6	NEX	F	5623	-	38,46,46	0.97	2 (5%)	50,70,70	1.20	6 (12%)
10	CLA	A	610	1	65,73,73	1.53	10 (15%)	76,113,113	1.73	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	G	614	1	49,57,73	1.73	9 (18%)	55,93,113	2.02	10 (18%)
9	CHL	G	607	11	66,74,74	1.44	10 (15%)	73,114,114	2.08	16 (21%)
10	CLA	H	603	1	65,73,73	1.55	12 (18%)	76,113,113	1.73	11 (14%)
9	CHL	J	609	1	66,74,74	1.53	10 (15%)	73,114,114	1.73	12 (16%)
10	CLA	C	603	1	65,73,73	1.55	12 (18%)	76,113,113	1.83	13 (17%)
8	DGD	A	632	-	67,67,67	0.95	2 (2%)	81,81,81	0.97	8 (9%)
4	LUT	B	1620	-	42,43,43	0.95	3 (7%)	51,60,60	1.42	7 (13%)
7	LHG	F	5630	10	48,48,48	1.02	3 (6%)	51,54,54	1.32	5 (9%)
2	BNG	J	9633	-	21,21,21	0.52	0	26,26,26	0.80	1 (3%)
10	CLA	D	614	1	49,57,73	1.69	9 (18%)	55,93,113	2.01	9 (16%)
10	CLA	F	611	7	65,73,73	1.51	9 (13%)	76,113,113	1.84	14 (18%)
9	CHL	B	601	1	66,74,74	1.39	9 (13%)	73,114,114	1.79	12 (16%)
9	CHL	C	606	11	51,59,74	1.79	10 (19%)	55,96,114	2.28	13 (23%)
4	LUT	J	9621	-	42,43,43	1.02	4 (9%)	51,60,60	1.56	7 (13%)
9	CHL	B	608	11	66,74,74	1.49	10 (15%)	73,114,114	1.93	16 (21%)
8	DGD	G	9632	-	67,67,67	1.05	2 (2%)	81,81,81	1.07	8 (9%)
10	CLA	I	613	1	65,73,73	1.45	9 (13%)	76,113,113	1.99	11 (14%)
9	CHL	A	605	1	48,56,74	1.69	8 (16%)	51,92,114	1.84	9 (17%)
9	CHL	D	601	1	66,74,74	1.37	10 (15%)	73,114,114	1.85	13 (17%)
9	CHL	G	608	11	66,74,74	1.52	11 (16%)	73,114,114	1.74	10 (13%)
10	CLA	D	611	7	65,73,73	1.46	9 (13%)	76,113,113	1.95	16 (21%)
4	LUT	C	2621	-	42,43,43	1.20	5 (11%)	51,60,60	1.43	8 (15%)
10	CLA	C	602	1	65,73,73	1.55	9 (13%)	76,113,113	1.99	19 (25%)
7	LHG	E	4630	10	48,48,48	0.90	3 (6%)	51,54,54	1.32	5 (9%)
10	CLA	F	602	1	65,73,73	1.53	13 (20%)	76,113,113	2.04	20 (26%)
7	LHG	A	630	10	48,48,48	0.92	3 (6%)	51,54,54	1.41	6 (11%)
6	NEX	D	3623	-	38,46,46	1.00	2 (5%)	50,70,70	1.12	5 (10%)
8	DGD	B	1632	-	67,67,67	0.96	2 (2%)	81,81,81	1.04	8 (9%)
5	XAT	J	3622	-	39,47,47	0.72	1 (2%)	54,74,74	1.21	4 (7%)
10	CLA	A	612	1	65,73,73	1.60	10 (15%)	76,113,113	1.74	13 (17%)
9	CHL	C	605	1	48,56,74	1.71	10 (20%)	51,92,114	1.89	9 (17%)
10	CLA	A	613	1	65,73,73	1.49	13 (20%)	76,113,113	1.75	12 (15%)
10	CLA	J	611	7	65,73,73	1.45	9 (13%)	76,113,113	1.92	14 (18%)
10	CLA	E	602	1	65,73,73	1.53	12 (18%)	76,113,113	1.93	19 (25%)
10	CLA	G	603	1	65,73,73	1.53	12 (18%)	76,113,113	1.84	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	CHL	C	609	1	66,74,74	1.52	11 (16%)	73,114,114	1.81	10 (13%)
4	LUT	F	5620	-	42,43,43	0.86	3 (7%)	51,60,60	1.47	7 (13%)
4	LUT	H	7620	-	42,43,43	0.88	2 (4%)	51,60,60	1.52	6 (11%)
2	BNG	C	2633	-	21,21,21	0.54	0	26,26,26	0.79	1 (3%)
5	XAT	D	8622	-	39,47,47	0.71	1 (2%)	54,74,74	1.26	6 (11%)
5	XAT	F	6622	-	39,47,47	0.67	0	54,74,74	1.21	6 (11%)
9	CHL	G	609	1	66,74,74	1.43	12 (18%)	73,114,114	1.70	11 (15%)
10	CLA	A	614	1	49,57,73	1.66	9 (18%)	55,93,113	2.05	10 (18%)
9	CHL	A	607	11	66,74,74	1.46	10 (15%)	73,114,114	2.08	13 (17%)
8	DGD	D	5632	-	67,67,67	0.95	1 (1%)	81,81,81	1.09	9 (11%)
9	CHL	J	607	11	66,74,74	1.40	9 (13%)	73,114,114	2.03	15 (20%)
10	CLA	J	603	1	65,73,73	1.64	11 (16%)	76,113,113	1.85	15 (19%)
9	CHL	G	601	1	66,74,74	1.44	10 (15%)	73,114,114	1.89	10 (13%)
10	CLA	J	614	1	49,57,73	1.63	8 (16%)	55,93,113	1.98	9 (16%)
5	XAT	C	7622	-	39,47,47	0.76	1 (2%)	54,74,74	1.26	5 (9%)
9	CHL	D	609	1	66,74,74	1.44	10 (15%)	73,114,114	1.85	13 (17%)
10	CLA	E	604	11	62,70,73	1.46	11 (17%)	72,109,113	2.10	12 (16%)
9	CHL	C	607	11	66,74,74	1.50	11 (16%)	73,114,114	2.09	16 (21%)
4	LUT	A	621	-	42,43,43	1.15	5 (11%)	51,60,60	1.55	8 (15%)
2	BNG	H	7633	-	21,21,21	0.52	0	26,26,26	0.79	1 (3%)
9	CHL	E	601	1	66,74,74	1.50	11 (16%)	73,114,114	1.84	13 (17%)
9	CHL	A	608	11	66,74,74	1.49	10 (15%)	73,114,114	1.88	13 (17%)
9	CHL	D	606	11	51,59,74	1.79	11 (21%)	55,96,114	2.37	13 (23%)
9	CHL	E	607	11	66,74,74	1.45	10 (15%)	73,114,114	2.11	15 (20%)
10	CLA	E	614	1	49,57,73	1.70	8 (16%)	55,93,113	2.11	11 (20%)
9	CHL	H	601	1	66,74,74	1.46	10 (15%)	73,114,114	1.86	13 (17%)
9	CHL	I	609	1	66,74,74	1.56	11 (16%)	73,114,114	1.88	13 (17%)
4	LUT	F	5621	-	42,43,43	1.04	4 (9%)	51,60,60	1.56	8 (15%)
10	CLA	D	612	1	65,73,73	1.56	11 (16%)	76,113,113	1.81	15 (19%)
9	CHL	D	608	11	66,74,74	1.43	11 (16%)	73,114,114	1.84	11 (15%)
10	CLA	D	613	1	65,73,73	1.55	12 (18%)	76,113,113	2.03	12 (15%)
10	CLA	G	610	1	65,73,73	1.50	10 (15%)	76,113,113	1.76	13 (17%)
10	CLA	H	612	1	65,73,73	1.60	13 (20%)	76,113,113	1.75	13 (17%)
10	CLA	F	604	11	62,70,73	1.41	9 (14%)	72,109,113	2.21	18 (25%)
10	CLA	E	610	1	65,73,73	1.60	11 (16%)	76,113,113	1.69	12 (15%)

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	604	11	1/1/14/20	9/34/112/115	-
9	CHL	D	607	11	3/3/20/26	14/39/137/137	-
9	CHL	B	605	1	3/3/16/26	7/18/116/137	-
5	XAT	B	1622	-	-	1/31/93/93	0/4/4/4
10	CLA	B	610	1	1/1/15/20	3/37/115/115	-
10	CLA	E	612	1	1/1/15/20	15/37/115/115	-
10	CLA	C	611	7	1/1/15/20	17/37/115/115	-
10	CLA	G	604	11	1/1/14/20	16/34/112/115	-
6	NEX	I	8623	-	-	2/27/83/83	0/3/3/3
9	CHL	A	601	1	5/5/20/26	14/39/137/137	-
4	LUT	I	8621	-	-	2/29/67/67	0/2/2/2
10	CLA	F	603	1	2/2/15/20	15/37/115/115	-
10	CLA	J	602	1	2/2/15/20	14/37/115/115	-
10	CLA	B	614	1	1/1/11/20	5/18/96/115	-
9	CHL	E	609	1	5/5/20/26	17/39/137/137	-
10	CLA	J	610	1	1/1/15/20	5/37/115/115	-
9	CHL	H	609	1	5/5/20/26	15/39/137/137	-
9	CHL	B	609	1	5/5/20/26	16/39/137/137	-
4	LUT	I	8620	-	-	1/29/67/67	0/2/2/2
10	CLA	A	602	1	2/2/15/20	18/37/115/115	-
6	NEX	B	1623	-	-	3/27/83/83	0/3/3/3
2	BNG	E	4633	-	-	10/12/32/32	0/1/1/1
9	CHL	I	608	11	4/4/20/26	17/39/137/137	-
7	LHG	D	3630	10	-	32/53/53/53	-
10	CLA	D	603	1	2/2/15/20	17/37/115/115	-
10	CLA	F	610	1	1/1/15/20	7/37/115/115	-
10	CLA	H	613	1	1/1/15/20	13/37/115/115	-
4	LUT	C	2620	-	-	1/29/67/67	0/2/2/2
10	CLA	C	613	1	1/1/15/20	10/37/115/115	-
7	LHG	H	7630	10	-	34/53/53/53	-
10	CLA	G	602	1	2/2/15/20	14/37/115/115	-
10	CLA	E	603	1	2/2/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	604	11	1/1/14/20	11/34/112/115	-
10	CLA	J	604	11	1/1/14/20	9/34/112/115	-
6	NEX	E	4623	-	-	3/27/83/83	0/3/3/3
9	CHL	G	606	11	3/3/17/26	5/21/119/137	-
8	DGD	D	3632	-	2/2/13/13	27/55/95/95	0/2/2/2
10	CLA	D	602	1	2/2/15/20	17/37/115/115	-
7	LHG	J	9630	10	-	32/53/53/53	-
9	CHL	H	608	11	4/4/20/26	22/39/137/137	-
9	CHL	H	605	1	3/3/16/26	7/18/116/137	-
9	CHL	I	601	1	4/4/20/26	15/39/137/137	-
10	CLA	H	610	1	2/2/15/20	9/37/115/115	-
7	LHG	C	2630	10	-	35/53/53/53	-
10	CLA	I	611	7	1/1/15/20	20/37/115/115	-
9	CHL	E	608	11	4/4/20/26	17/39/137/137	-
9	CHL	H	606	11	3/3/17/26	6/21/119/137	-
2	BNG	D	3633	-	-	10/12/32/32	0/1/1/1
10	CLA	J	612	1	1/1/15/20	14/37/115/115	-
10	CLA	J	613	1	1/1/15/20	13/37/115/115	-
9	CHL	I	606	11	3/3/17/26	6/21/119/137	-
10	CLA	C	604	11	1/1/14/20	16/34/112/115	-
5	XAT	I	9622	-	-	0/31/93/93	0/4/4/4
9	CHL	C	601	1	4/4/20/26	17/39/137/137	-
10	CLA	C	610	1	1/1/15/20	4/37/115/115	-
6	NEX	A	623	-	-	3/27/83/83	0/3/3/3
10	CLA	B	602	1	2/2/15/20	17/37/115/115	-
7	LHG	B	1630	10	-	35/53/53/53	-
10	CLA	D	604	11	1/1/14/20	15/34/112/115	-
10	CLA	H	604	11	1/1/14/20	18/34/112/115	-
10	CLA	F	613	1	1/1/15/20	7/37/115/115	-
9	CHL	B	606	11	3/3/17/26	7/21/119/137	-
9	CHL	G	605	1	3/3/16/26	6/18/116/137	-
9	CHL	H	607	11	3/3/20/26	13/39/137/137	-
10	CLA	C	612	1	1/1/15/20	11/37/115/115	-
6	NEX	J	9623	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	611	7	1/1/15/20	19/37/115/115	-
10	CLA	G	613	1	1/1/15/20	12/37/115/115	-
8	DGD	E	4632	-	2/2/13/13	23/55/95/95	0/2/2/2
9	CHL	E	605	1	3/3/16/26	8/18/116/137	-
10	CLA	F	614	1	1/1/11/20	5/18/96/115	-
9	CHL	F	607	11	3/3/20/26	16/39/137/137	-
9	CHL	A	606	11	3/3/17/26	5/21/119/137	-
4	LUT	G	6621	-	-	2/29/67/67	0/2/2/2
10	CLA	I	603	1	2/2/15/20	16/37/115/115	-
6	NEX	H	7623	-	-	2/27/83/83	0/3/3/3
8	DGD	H	6632	-	2/2/13/13	33/55/95/95	0/2/2/2
10	CLA	I	612	1	1/1/15/20	14/37/115/115	-
10	CLA	I	602	1	2/2/15/20	13/37/115/115	-
9	CHL	I	605	1	3/3/16/26	9/18/116/137	-
4	LUT	G	6620	-	-	1/29/67/67	0/2/2/2
9	CHL	F	601	1	4/4/20/26	15/39/137/137	-
2	BNG	I	8633	-	-	9/12/32/32	0/1/1/1
10	CLA	H	602	1	2/2/15/20	18/37/115/115	-
8	DGD	I	8632	-	2/2/13/13	26/55/95/95	0/2/2/2
4	LUT	B	1621	-	-	2/29/67/67	0/2/2/2
4	LUT	J	9620	-	-	2/29/67/67	0/2/2/2
4	LUT	D	3621	-	-	2/29/67/67	0/2/2/2
4	LUT	E	4621	-	-	2/29/67/67	0/2/2/2
2	BNG	F	5633	-	-	9/12/32/32	0/1/1/1
4	LUT	H	7621	-	-	2/29/67/67	0/2/2/2
10	CLA	B	612	1	1/1/15/20	15/37/115/115	-
2	BNG	G	6633	-	-	9/12/32/32	0/1/1/1
5	XAT	H	4622	-	-	1/31/93/93	0/4/4/4
9	CHL	J	605	1	3/3/16/26	8/18/116/137	-
9	CHL	J	601	1	4/4/20/26	18/39/137/137	-
9	CHL	J	606	11	3/3/17/26	7/21/119/137	-
10	CLA	I	614	1	1/1/11/20	7/18/96/115	-
10	CLA	G	612	1	1/1/15/20	13/37/115/115	-
5	XAT	E	2622	-	-	1/31/93/93	0/4/4/4
2	BNG	A	633	-	-	11/12/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CHL	J	608	11	4/4/20/26	21/39/137/137	-
10	CLA	B	603	1	2/2/15/20	15/37/115/115	-
10	CLA	C	614	1	1/1/11/20	5/18/96/115	-
9	CHL	F	609	1	5/5/20/26	15/39/137/137	-
9	CHL	F	605	1	3/3/16/26	6/18/116/137	-
6	NEX	G	6623	-	-	2/27/83/83	0/3/3/3
10	CLA	E	611	7	1/1/15/20	19/37/115/115	-
5	XAT	B	5622	-	-	1/31/93/93	0/4/4/4
2	BNG	B	1633	-	-	11/12/32/32	0/1/1/1
9	CHL	E	606	11	3/3/17/26	5/21/119/137	-
4	LUT	D	3620	-	-	1/29/67/67	0/2/2/2
9	CHL	C	608	11	4/4/20/26	17/39/137/137	-
8	DGD	B	2632	-	2/2/13/13	29/55/95/95	0/2/2/2
10	CLA	H	614	1	1/1/11/20	5/18/96/115	-
6	NEX	C	2623	-	-	2/27/83/83	0/3/3/3
10	CLA	B	611	7	1/1/15/20	19/37/115/115	-
4	LUT	A	620	-	-	1/29/67/67	0/2/2/2
10	CLA	G	611	7	1/1/15/20	17/37/115/115	-
4	LUT	E	4620	-	-	1/29/67/67	0/2/2/2
10	CLA	H	611	7	1/1/15/20	16/37/115/115	-
7	LHG	G	6630	10	-	38/53/53/53	-
10	CLA	E	613	1	1/1/15/20	11/37/115/115	-
9	CHL	F	608	11	4/4/20/26	17/39/137/137	-
10	CLA	A	603	1	2/2/15/20	18/37/115/115	-
5	XAT	A	622	-	-	0/31/93/93	0/4/4/4
8	DGD	H	7632	-	2/2/13/13	30/55/95/95	0/2/2/2
9	CHL	A	609	1	5/5/20/26	18/39/137/137	-
9	CHL	F	606	11	3/3/17/26	7/21/119/137	-
9	CHL	D	605	1	3/3/16/26	7/18/116/137	-
10	CLA	D	610	1	1/1/15/20	9/37/115/115	-
10	CLA	F	612	1	1/1/15/20	15/37/115/115	-
7	LHG	I	8630	10	-	38/53/53/53	-
10	CLA	I	604	11	1/1/14/20	11/34/112/115	-
9	CHL	B	607	11	3/3/20/26	15/39/137/137	-
9	CHL	I	607	11	3/3/20/26	13/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	B	613	1	1/1/15/20	8/37/115/115	-
10	CLA	I	610	1	2/2/15/20	8/37/115/115	-
10	CLA	H	603	1	2/2/15/20	14/37/115/115	-
10	CLA	A	610	1	1/1/15/20	5/37/115/115	-
10	CLA	G	614	1	1/1/11/20	5/18/96/115	-
9	CHL	G	607	11	3/3/20/26	14/39/137/137	-
6	NEX	F	5623	-	-	2/27/83/83	0/3/3/3
9	CHL	J	609	1	5/5/20/26	21/39/137/137	-
10	CLA	C	603	1	2/2/15/20	15/37/115/115	-
8	DGD	A	632	-	2/2/13/13	26/55/95/95	0/2/2/2
4	LUT	B	1620	-	-	1/29/67/67	0/2/2/2
7	LHG	F	5630	10	-	32/53/53/53	-
2	BNG	J	9633	-	-	10/12/32/32	0/1/1/1
10	CLA	D	614	1	1/1/11/20	5/18/96/115	-
10	CLA	F	611	7	1/1/15/20	20/37/115/115	-
9	CHL	B	601	1	4/4/20/26	13/39/137/137	-
9	CHL	C	606	11	3/3/17/26	7/21/119/137	-
4	LUT	J	9621	-	-	2/29/67/67	0/2/2/2
9	CHL	B	608	11	4/4/20/26	21/39/137/137	-
8	DGD	G	9632	-	2/2/13/13	28/55/95/95	0/2/2/2
10	CLA	I	613	1	1/1/15/20	11/37/115/115	-
9	CHL	A	605	1	3/3/16/26	6/18/116/137	-
9	CHL	D	601	1	4/4/20/26	17/39/137/137	-
9	CHL	G	608	11	4/4/20/26	18/39/137/137	-
10	CLA	D	611	7	1/1/15/20	18/37/115/115	-
4	LUT	C	2621	-	-	2/29/67/67	0/2/2/2
10	CLA	C	602	1	2/2/15/20	14/37/115/115	-
10	CLA	F	602	1	2/2/15/20	16/37/115/115	-
7	LHG	E	4630	10	-	35/53/53/53	-
7	LHG	A	630	10	-	39/53/53/53	-
6	NEX	D	3623	-	-	2/27/83/83	0/3/3/3
8	DGD	B	1632	-	2/2/13/13	30/55/95/95	0/2/2/2
5	XAT	J	3622	-	-	0/31/93/93	0/4/4/4
10	CLA	A	612	1	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CHL	C	605	1	3/3/16/26	8/18/116/137	-
10	CLA	A	613	1	1/1/15/20	7/37/115/115	-
10	CLA	J	611	7	1/1/15/20	18/37/115/115	-
10	CLA	E	602	1	2/2/15/20	15/37/115/115	-
10	CLA	G	603	1	2/2/15/20	14/37/115/115	-
9	CHL	C	609	1	5/5/20/26	14/39/137/137	-
4	LUT	F	5620	-	-	1/29/67/67	0/2/2/2
4	LUT	H	7620	-	-	1/29/67/67	0/2/2/2
9	CHL	G	609	1	5/5/20/26	17/39/137/137	-
2	BNG	C	2633	-	-	9/12/32/32	0/1/1/1
5	XAT	D	8622	-	-	1/31/93/93	0/4/4/4
5	XAT	F	6622	-	-	1/31/93/93	0/4/4/4
10	CLA	A	614	1	1/1/11/20	7/18/96/115	-
9	CHL	A	607	11	3/3/20/26	14/39/137/137	-
8	DGD	D	5632	-	2/2/13/13	27/55/95/95	0/2/2/2
9	CHL	J	607	11	3/3/20/26	11/39/137/137	-
10	CLA	J	603	1	2/2/15/20	13/37/115/115	-
9	CHL	G	601	1	4/4/20/26	13/39/137/137	-
10	CLA	J	614	1	1/1/11/20	8/18/96/115	-
5	XAT	C	7622	-	-	0/31/93/93	0/4/4/4
9	CHL	D	609	1	5/5/20/26	17/39/137/137	-
10	CLA	E	604	11	1/1/14/20	6/34/112/115	-
9	CHL	C	607	11	3/3/20/26	15/39/137/137	-
4	LUT	A	621	-	-	2/29/67/67	0/2/2/2
2	BNG	H	7633	-	-	10/12/32/32	0/1/1/1
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	D	606	11	3/3/17/26	7/21/119/137	-
9	CHL	E	607	11	3/3/20/26	13/39/137/137	-
10	CLA	E	614	1	1/1/11/20	5/18/96/115	-
9	CHL	H	601	1	4/4/20/26	8/39/137/137	-
9	CHL	I	609	1	5/5/20/26	16/39/137/137	-
10	CLA	D	612	1	1/1/15/20	13/37/115/115	-
10	CLA	D	613	1	1/1/15/20	10/37/115/115	-
9	CHL	D	608	11	4/4/20/26	14/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	G	610	1	1/1/15/20	7/37/115/115	-
10	CLA	H	612	1	1/1/15/20	14/37/115/115	-
4	LUT	F	5621	-	-	2/29/67/67	0/2/2/2
10	CLA	F	604	11	1/1/14/20	15/34/112/115	-
10	CLA	E	610	1	1/1/15/20	3/37/115/115	-

The worst 5 of 1577 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

The worst 5 of 2196 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

5 of 343 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	632	DGD	C2D
8	A	632	DGD	C5D
8	B	1632	DGD	C2D
8	B	1632	DGD	C5D
8	B	2632	DGD	C2D

5 of 2523 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	9633	BNG	C2-C1-O1-C1'
2	J	9633	BNG	O5-C1-O1-C1'
5	D	8622	XAT	O24-C26-C27-C28
5	H	4622	XAT	O24-C26-C27-C28
7	A	630	LHG	O1-C1-C2-O2

There are no ring outliers.

139 monomers are involved in 193 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	604	CLA	1	0
9	B	605	CHL	2	0
5	B	1622	XAT	1	0
10	B	610	CLA	2	0
10	E	612	CLA	2	0
10	C	611	CLA	3	0
10	G	604	CLA	1	0
9	A	601	CHL	2	0
4	I	8621	LUT	1	0
10	F	603	CLA	3	0
10	J	602	CLA	2	0
9	E	609	CHL	1	0
10	J	610	CLA	1	0
4	I	8620	LUT	2	0
9	B	609	CHL	1	0
9	H	609	CHL	2	0
10	A	602	CLA	3	0
7	D	3630	LHG	1	0
10	D	603	CLA	1	0
10	F	610	CLA	1	0
10	H	613	CLA	1	0
10	C	613	CLA	1	0
7	H	7630	LHG	2	0
10	G	602	CLA	2	0
10	E	603	CLA	4	0
10	A	604	CLA	1	0
10	J	604	CLA	1	0
9	G	606	CHL	1	0
10	D	602	CLA	2	0
9	H	608	CHL	1	0
9	H	605	CHL	1	0
7	C	2630	LHG	1	0
9	I	601	CHL	2	0
10	H	610	CLA	2	0
10	I	611	CLA	2	0
2	D	3633	BNG	1	0
10	J	612	CLA	2	0
10	J	613	CLA	1	0
9	I	606	CHL	1	0
10	C	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	9622	XAT	1	0
9	C	601	CHL	1	0
10	C	610	CLA	1	0
7	B	1630	LHG	3	0
10	B	602	CLA	2	0
10	D	604	CLA	2	0
10	F	613	CLA	2	0
9	B	606	CHL	1	0
10	C	612	CLA	2	0
10	A	611	CLA	3	0
10	G	613	CLA	1	0
9	E	605	CHL	1	0
4	G	6621	LUT	1	0
10	I	603	CLA	3	0
8	H	6632	DGD	1	0
10	I	612	CLA	1	0
10	I	602	CLA	2	0
9	I	605	CHL	1	0
9	F	601	CHL	3	0
10	H	602	CLA	3	0
4	B	1621	LUT	2	0
8	I	8632	DGD	1	0
4	D	3621	LUT	1	0
4	E	4621	LUT	1	0
4	H	7621	LUT	2	0
10	B	612	CLA	2	0
5	H	4622	XAT	1	0
9	J	605	CHL	2	0
10	G	612	CLA	2	0
5	E	2622	XAT	2	0
10	B	603	CLA	4	0
10	C	614	CLA	1	0
9	F	609	CHL	1	0
6	G	6623	NEX	1	0
10	E	611	CLA	1	0
9	C	608	CHL	2	0
10	B	611	CLA	3	0
4	A	620	LUT	2	0
10	G	611	CLA	4	0
4	E	4620	LUT	2	0
10	H	611	CLA	3	0
7	G	6630	LHG	2	0

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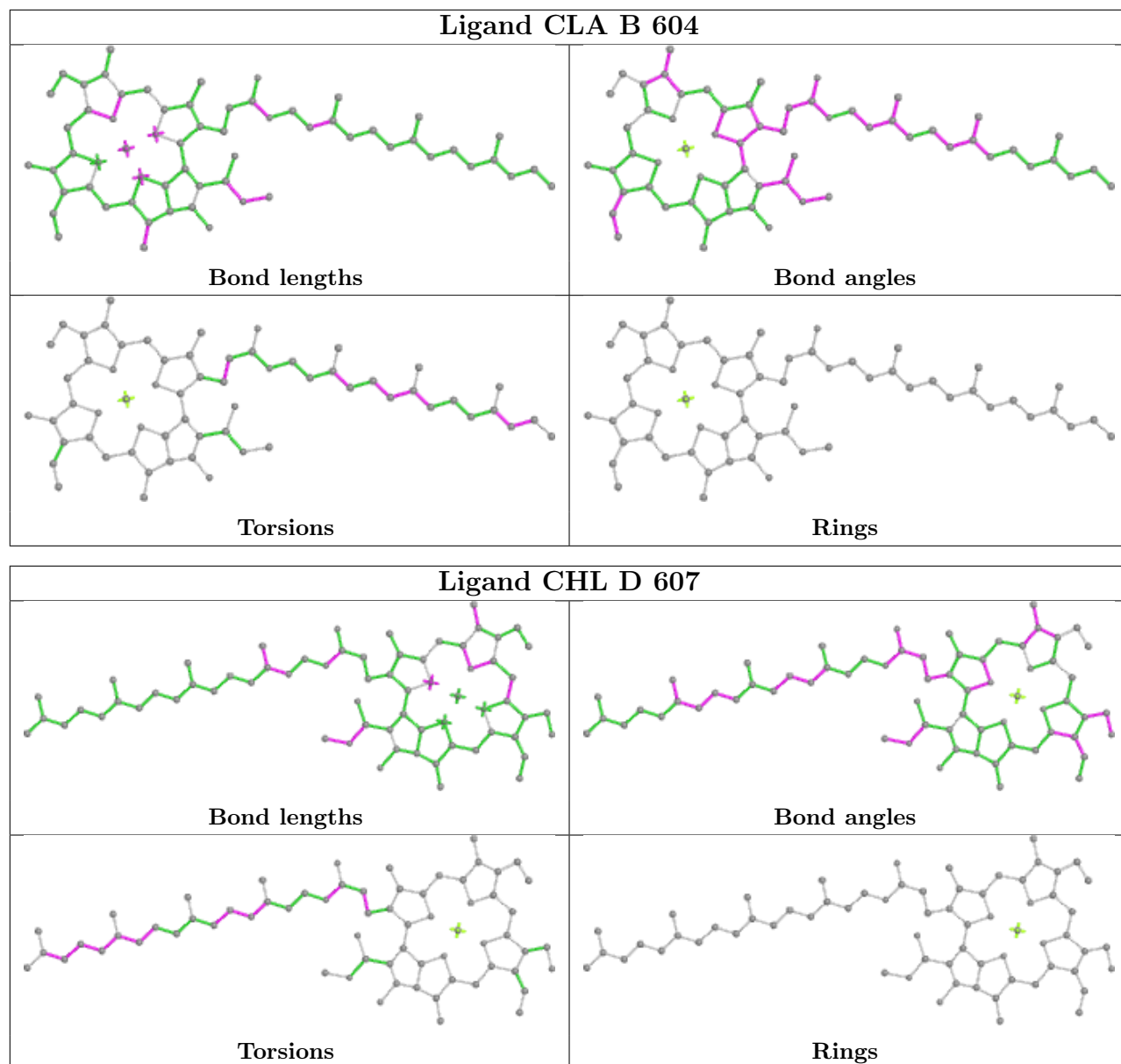
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	613	CLA	1	0
9	F	608	CHL	1	0
10	A	603	CLA	3	0
10	D	610	CLA	1	0
7	I	8630	LHG	3	0
10	I	604	CLA	1	0
10	B	613	CLA	1	0
10	I	610	CLA	2	0
10	A	610	CLA	2	0
9	G	607	CHL	1	0
10	H	603	CLA	4	0
10	C	603	CLA	4	0
8	A	632	DGD	1	0
4	B	1620	LUT	2	0
7	F	5630	LHG	3	0
10	F	611	CLA	1	0
9	B	601	CHL	3	0
4	J	9621	LUT	1	0
9	B	608	CHL	1	0
10	I	613	CLA	1	0
9	A	605	CHL	1	0
9	D	601	CHL	1	0
9	G	608	CHL	2	0
10	D	611	CLA	2	0
4	C	2621	LUT	2	0
10	C	602	CLA	3	0
7	E	4630	LHG	1	0
10	F	602	CLA	3	0
7	A	630	LHG	2	0
5	J	3622	XAT	1	0
10	A	612	CLA	2	0
10	J	611	CLA	3	0
10	E	602	CLA	2	0
10	G	603	CLA	3	0
9	C	609	CHL	2	0
4	F	5620	LUT	1	0
5	F	6622	XAT	1	0
9	G	609	CHL	2	0
8	D	5632	DGD	1	0
10	J	603	CLA	3	0
9	G	601	CHL	3	0
10	J	614	CLA	1	0

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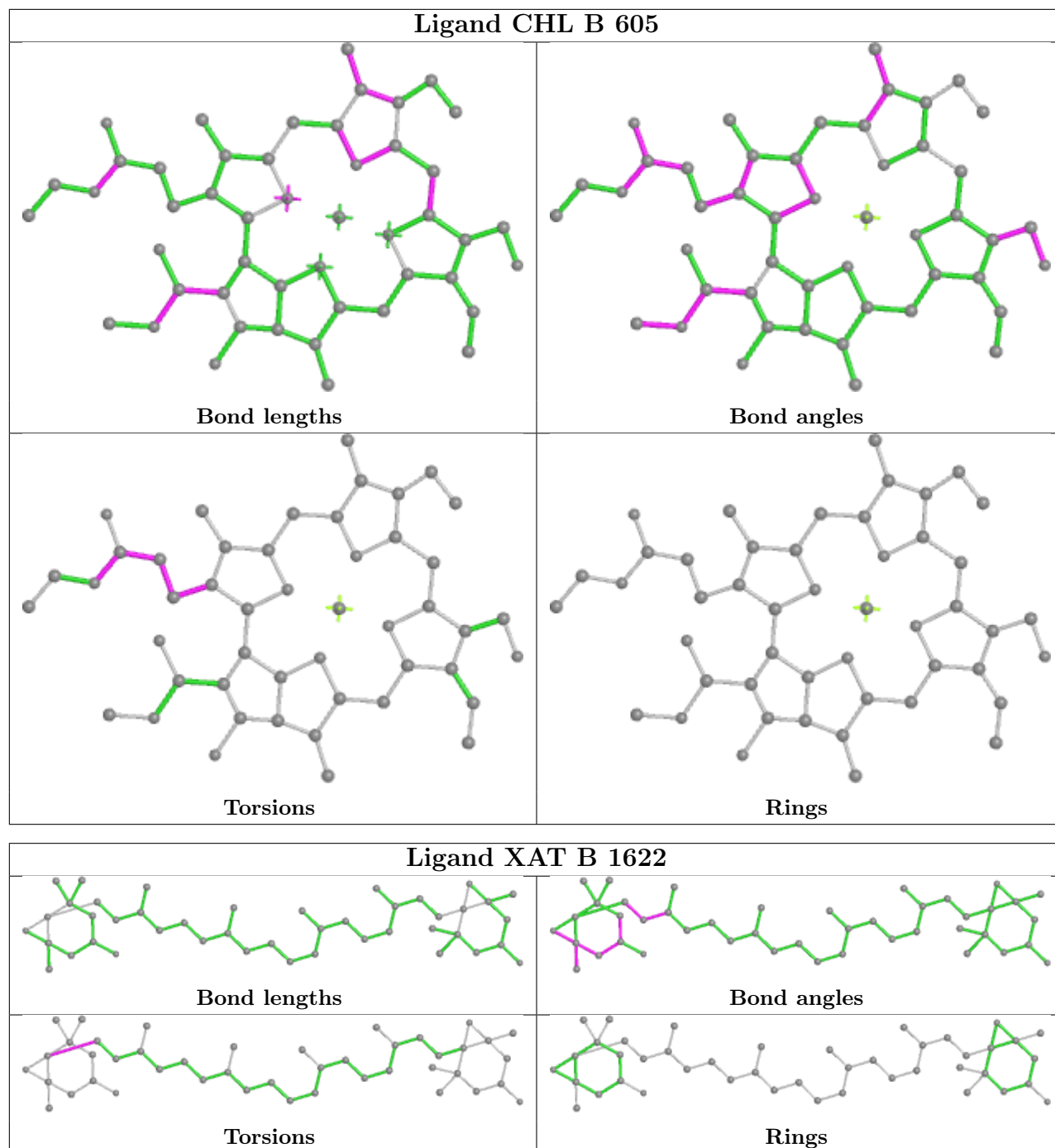
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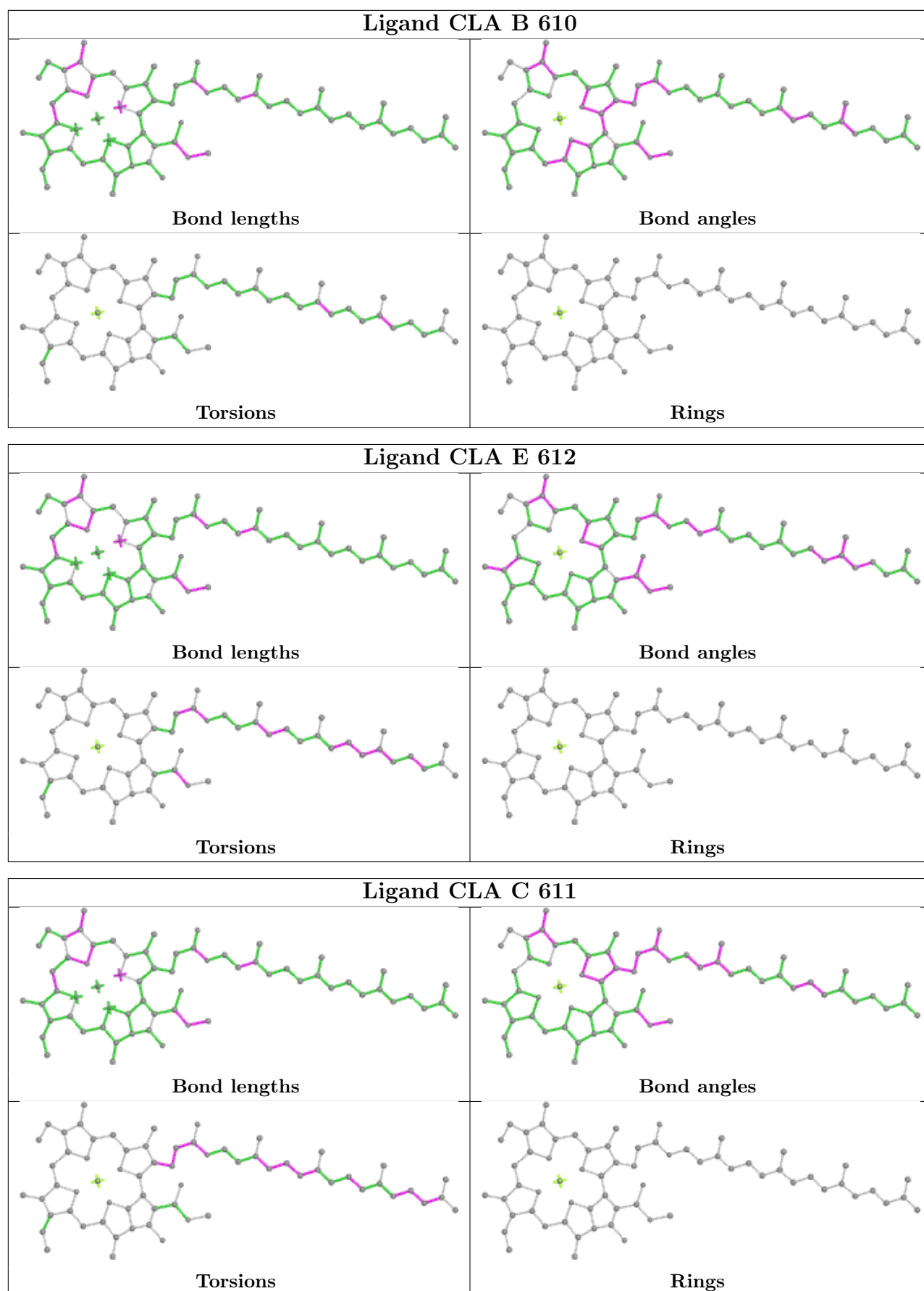
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	609	CHL	1	0
10	E	604	CLA	1	0
4	A	621	LUT	1	0
9	E	601	CHL	1	0
9	A	608	CHL	1	0
10	E	614	CLA	1	0
9	H	601	CHL	1	0
9	I	609	CHL	1	0
4	F	5621	LUT	1	0
10	D	612	CLA	2	0
10	D	613	CLA	1	0
10	G	610	CLA	1	0
10	H	612	CLA	2	0
10	F	604	CLA	1	0
10	E	610	CLA	1	0

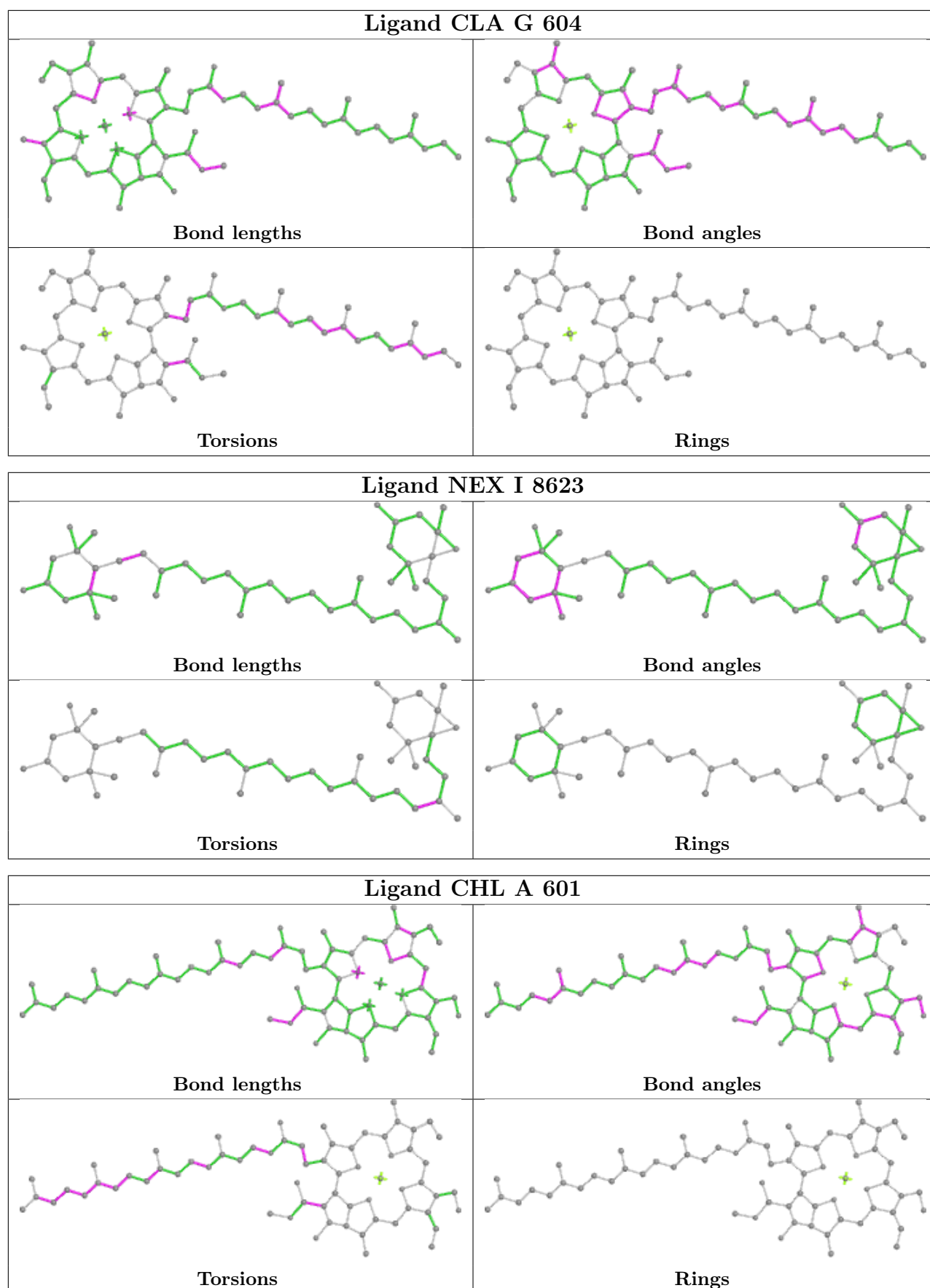
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

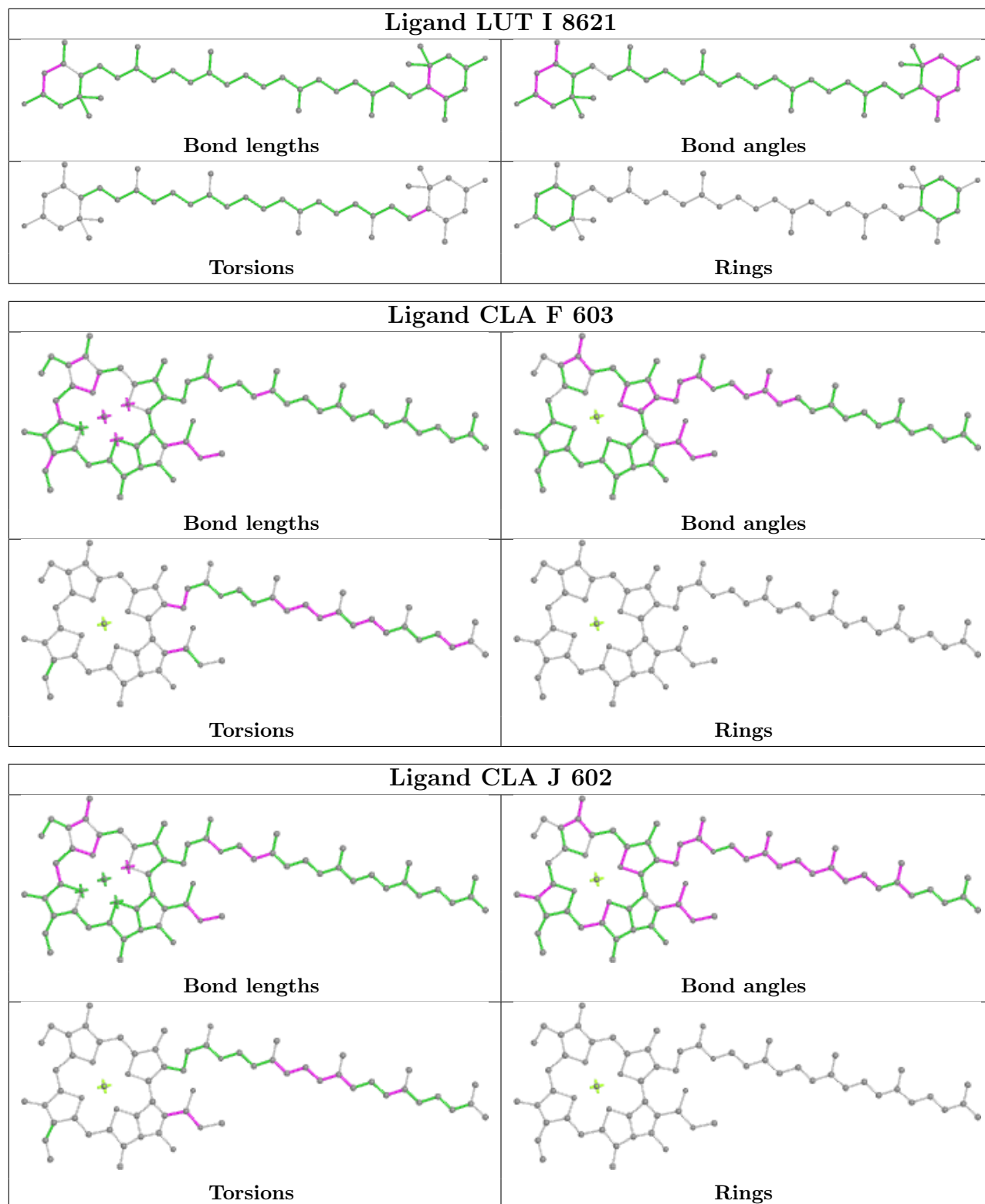


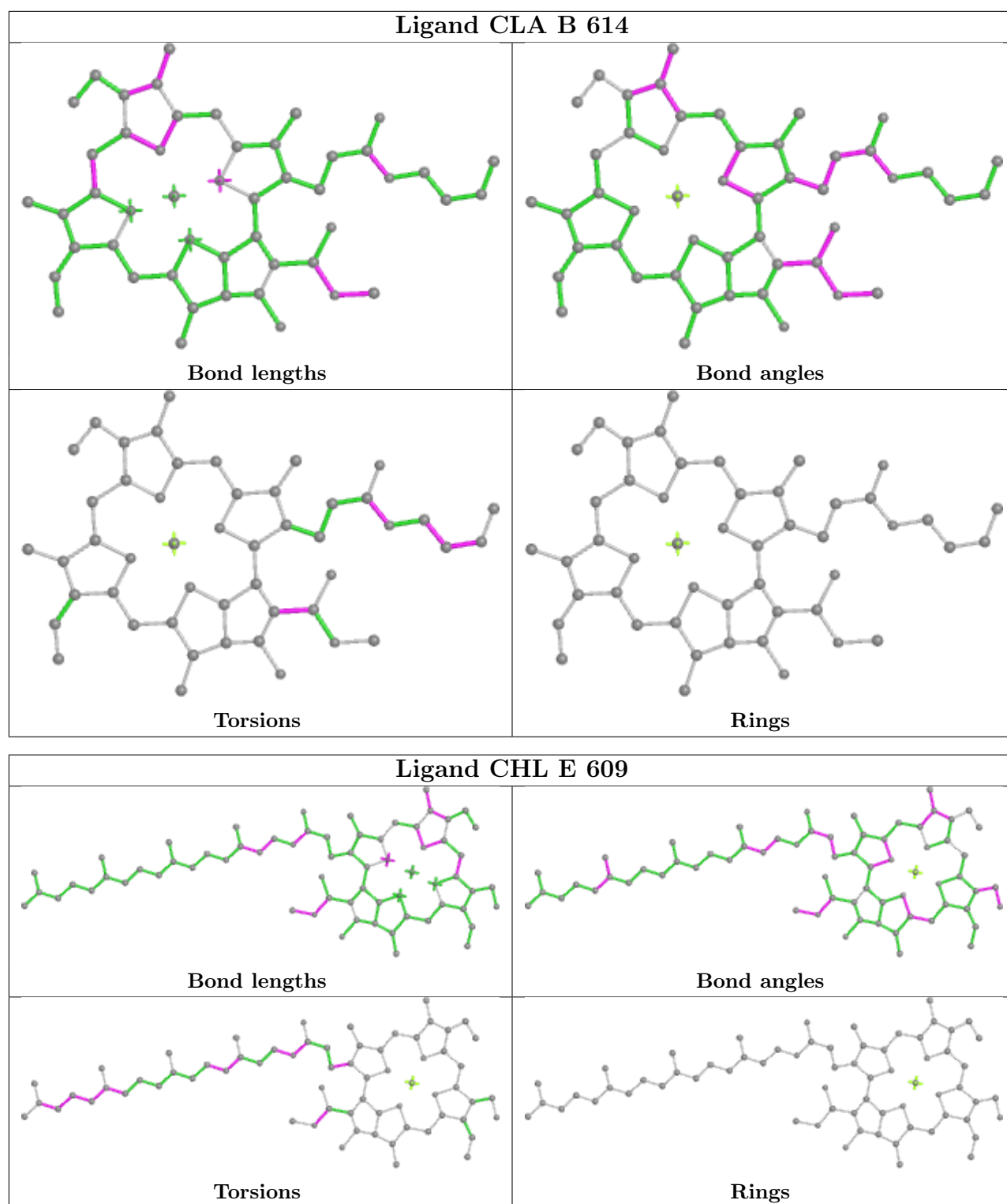


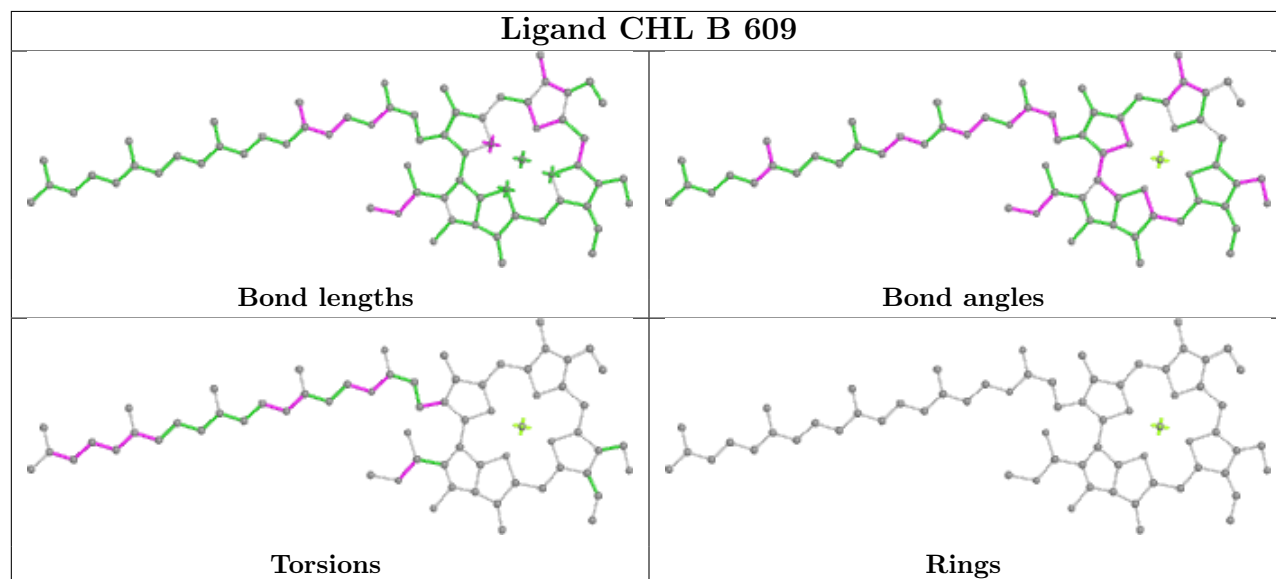
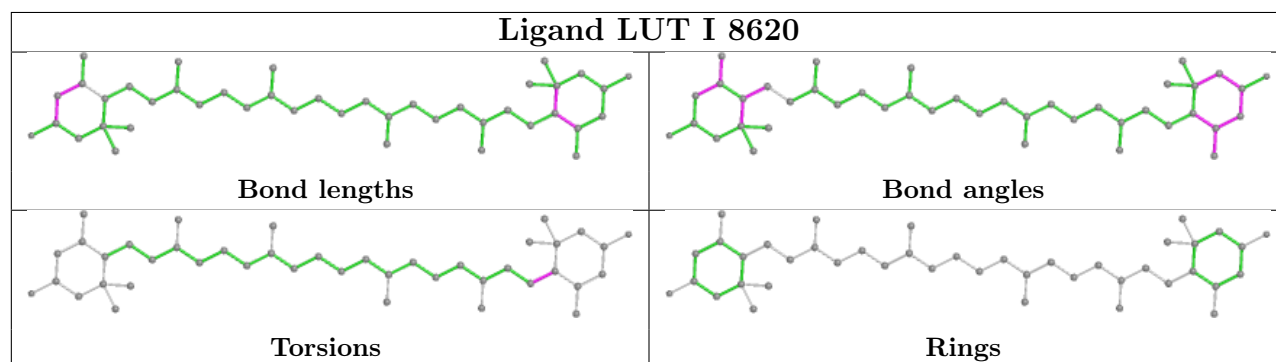
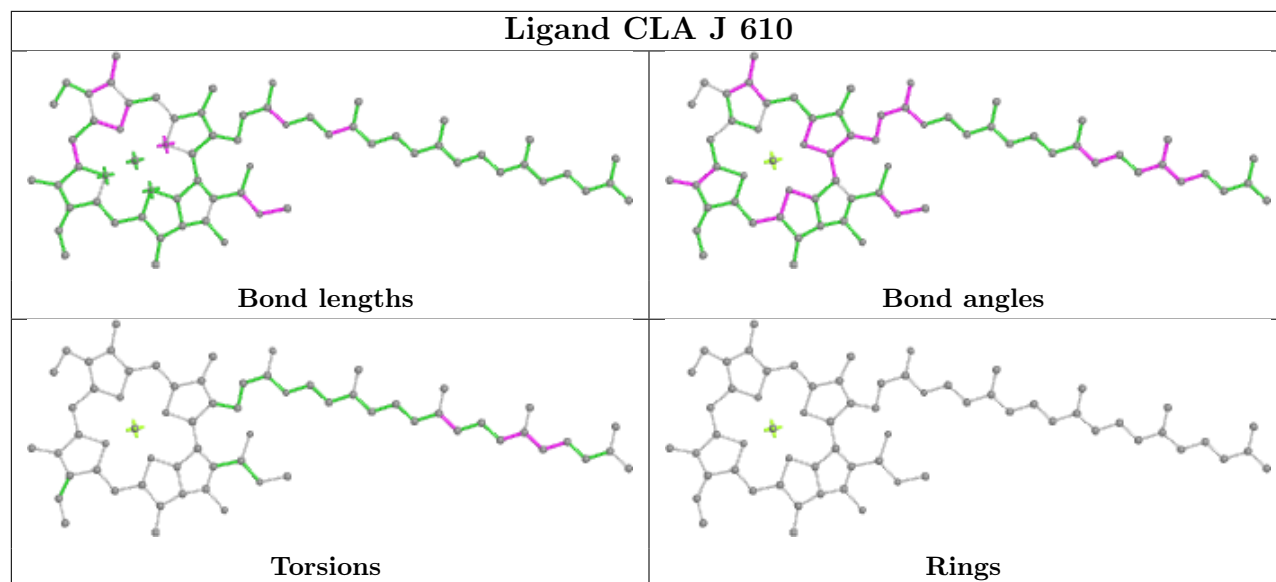


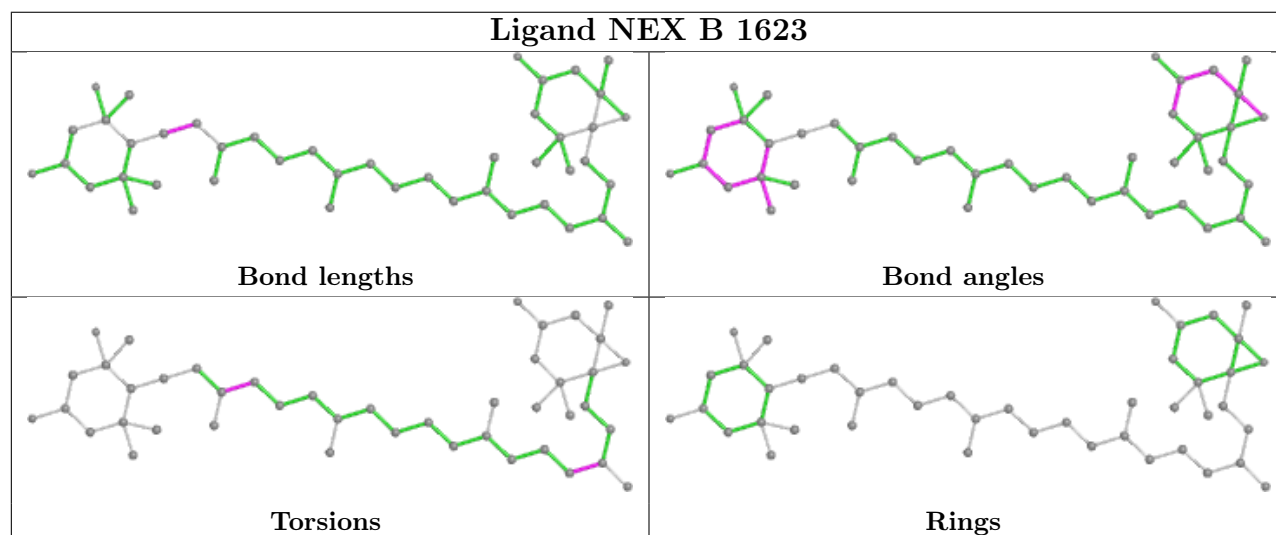
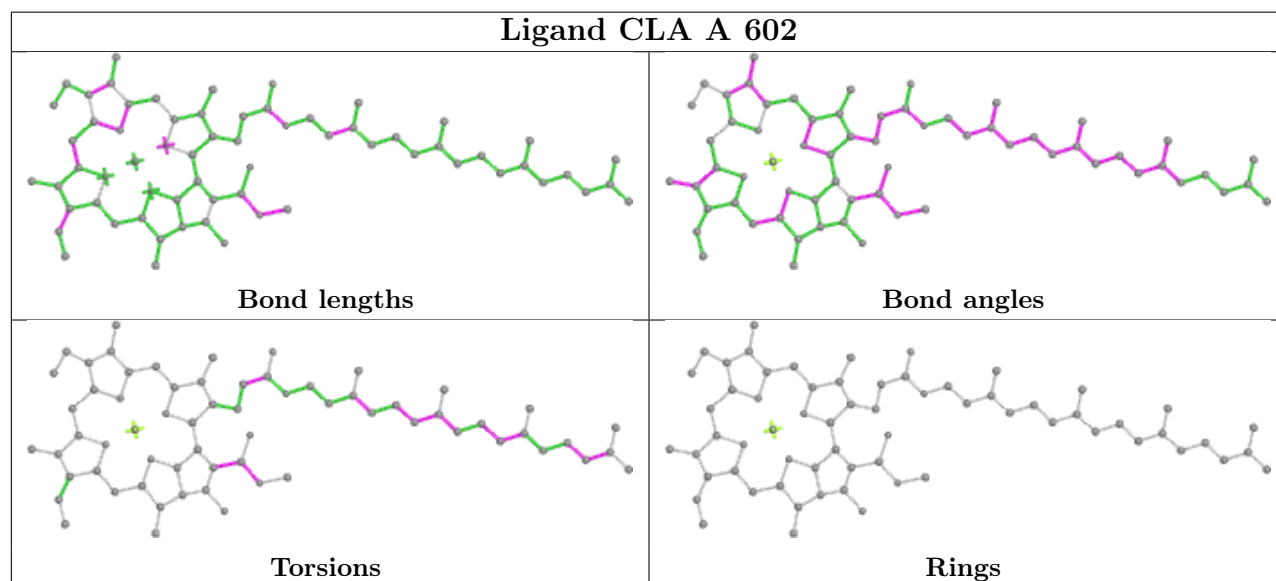
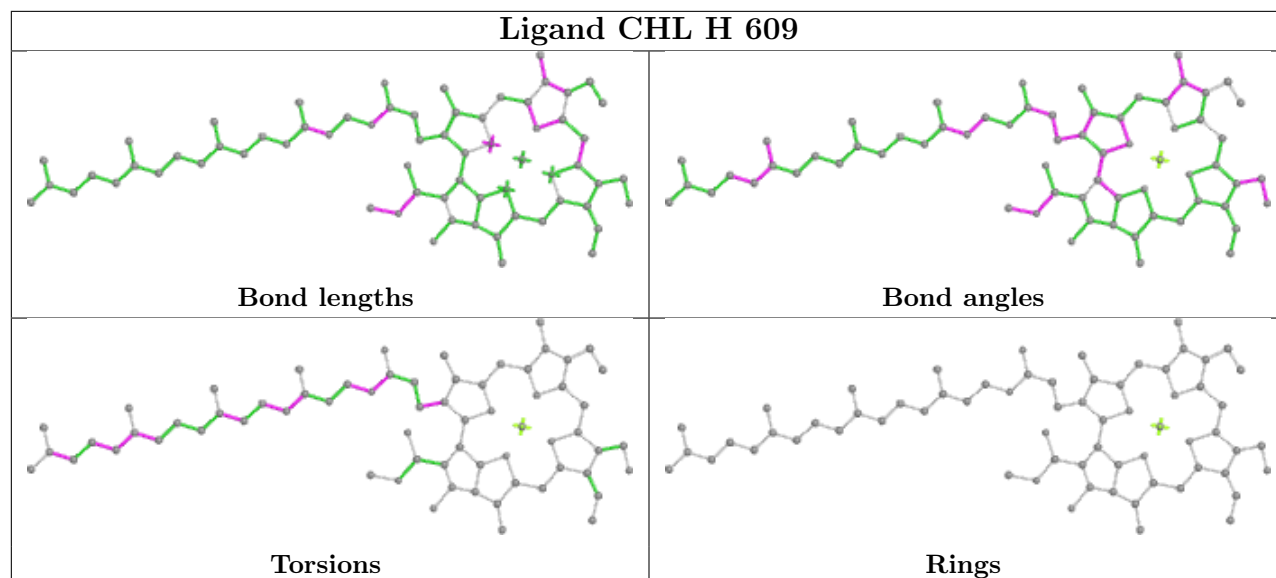


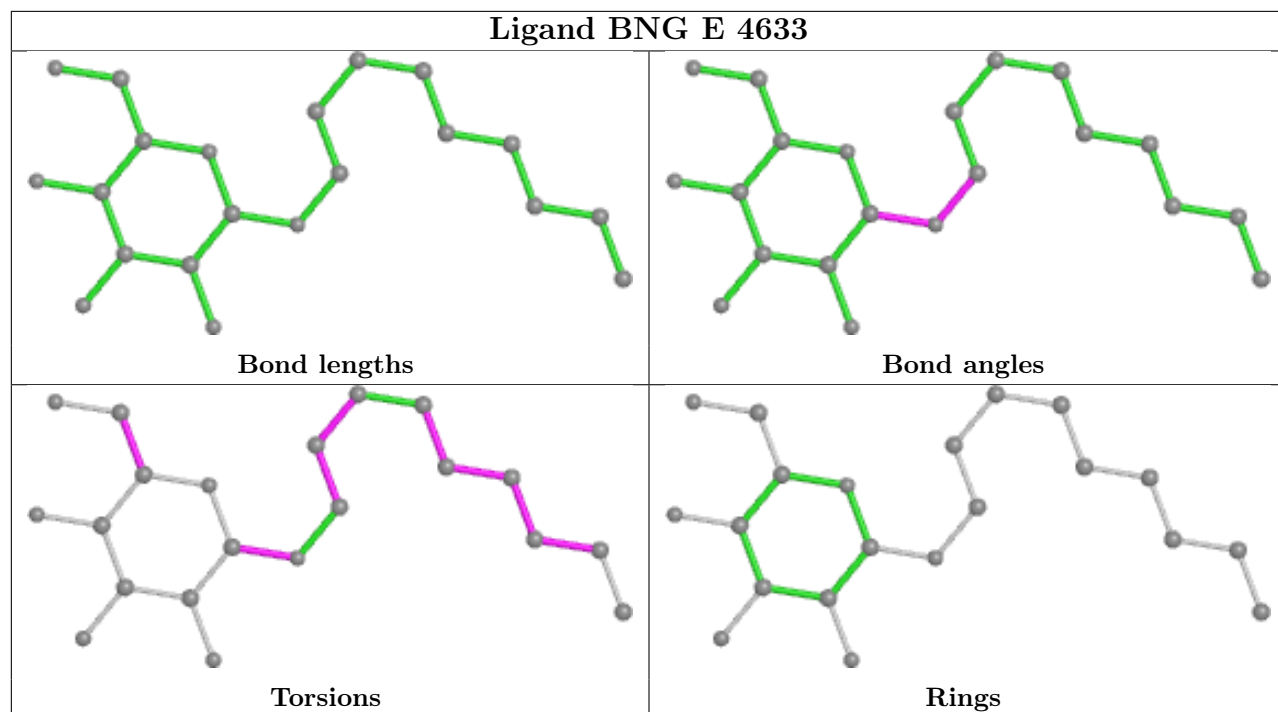




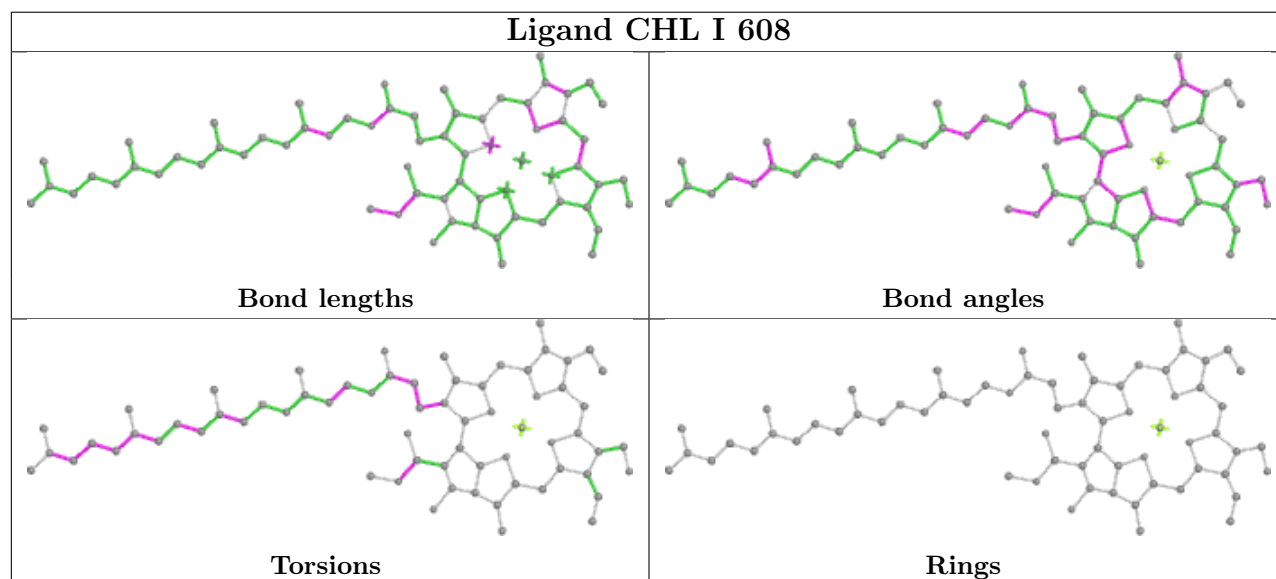
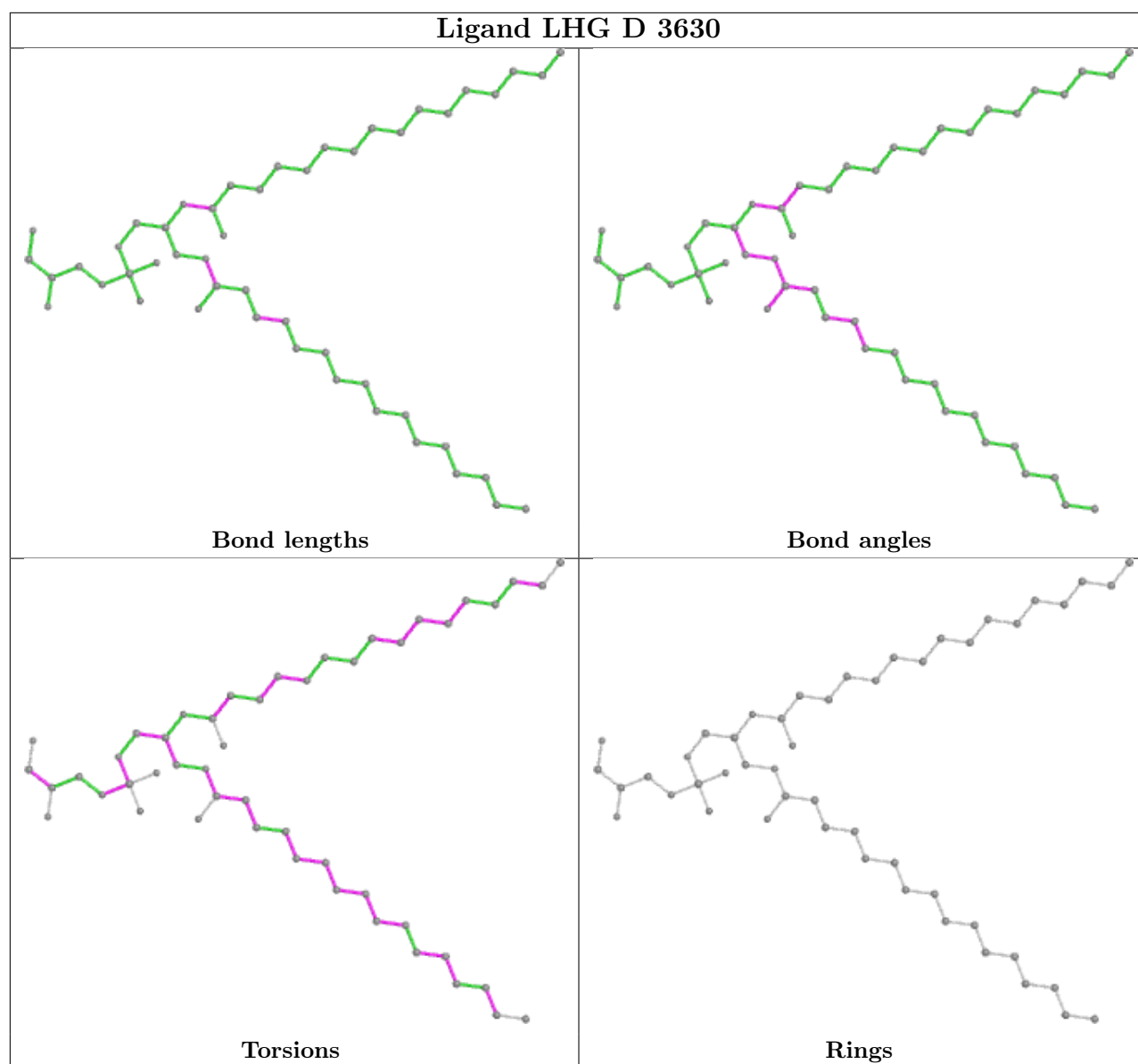


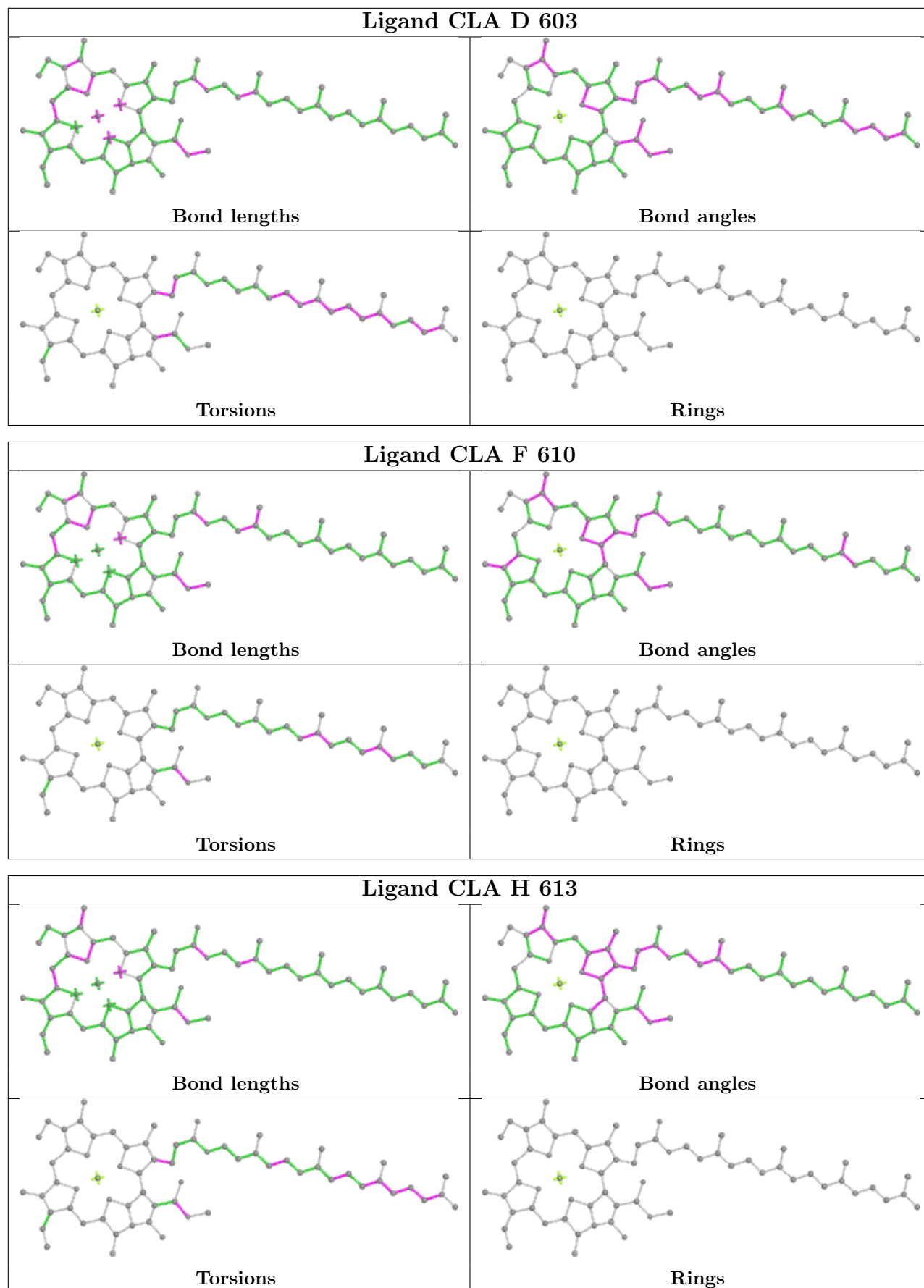


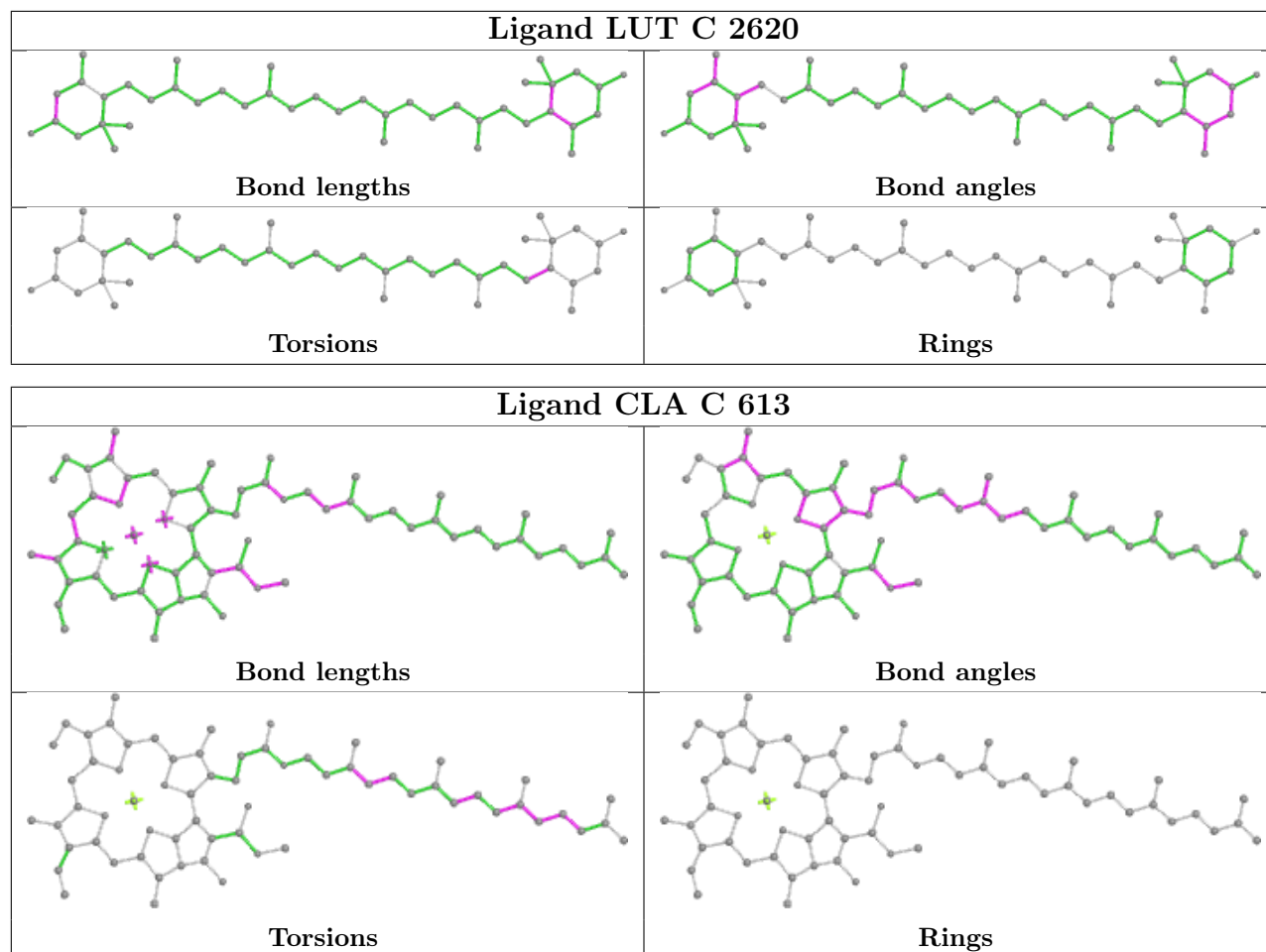


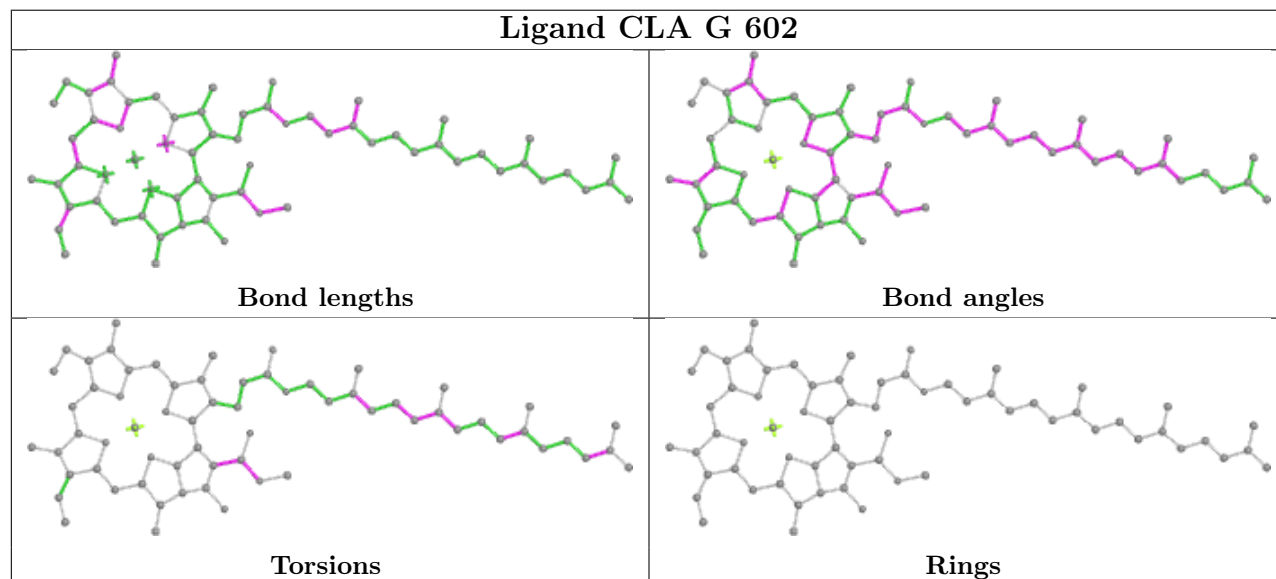
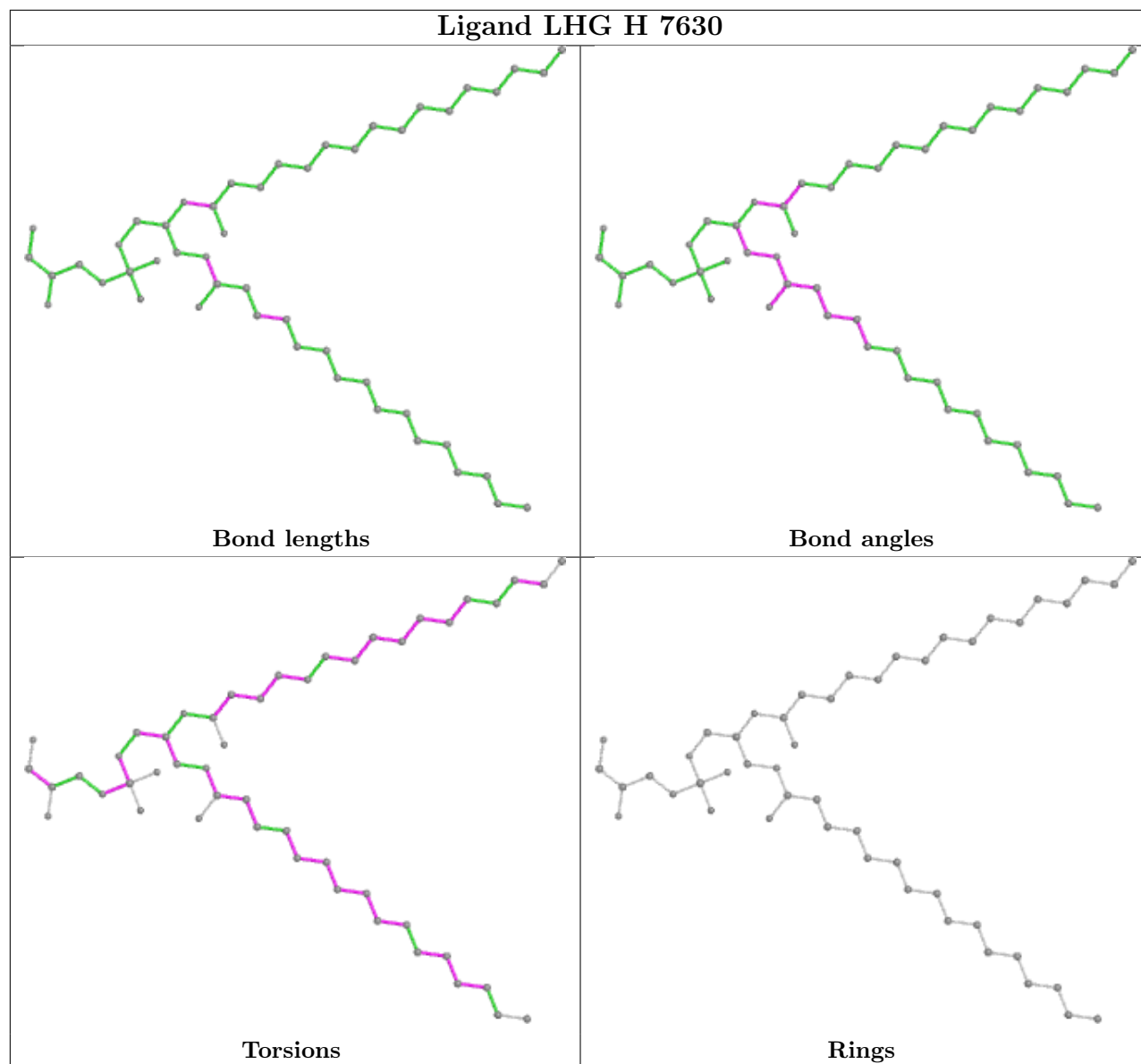


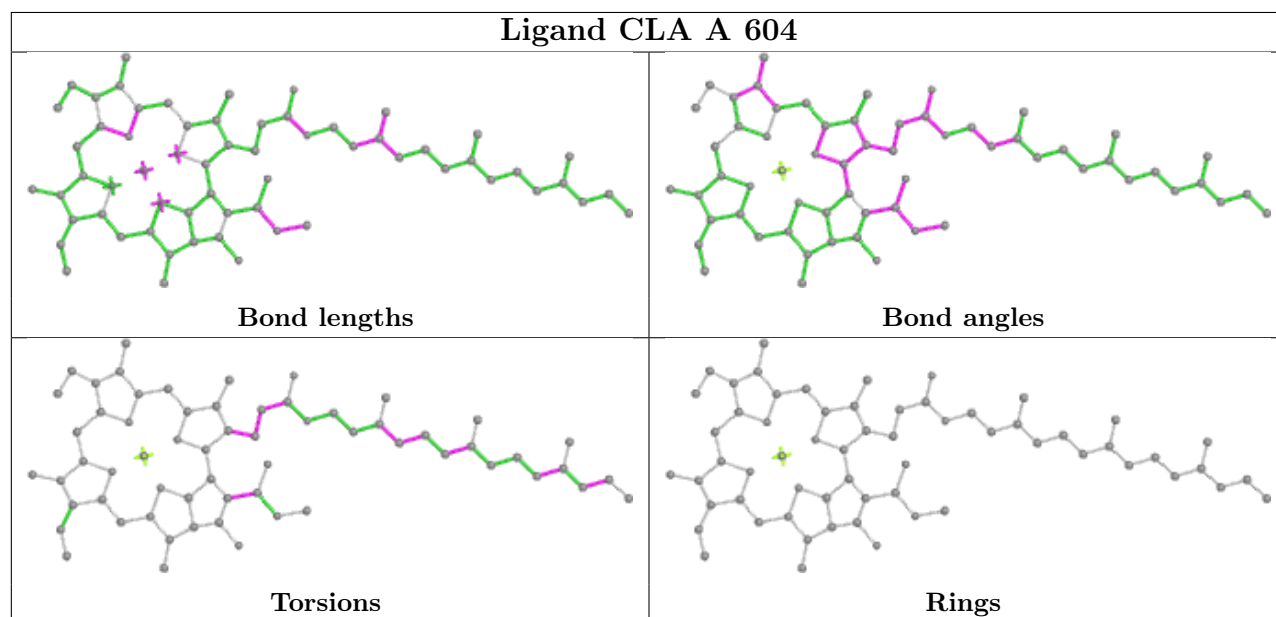
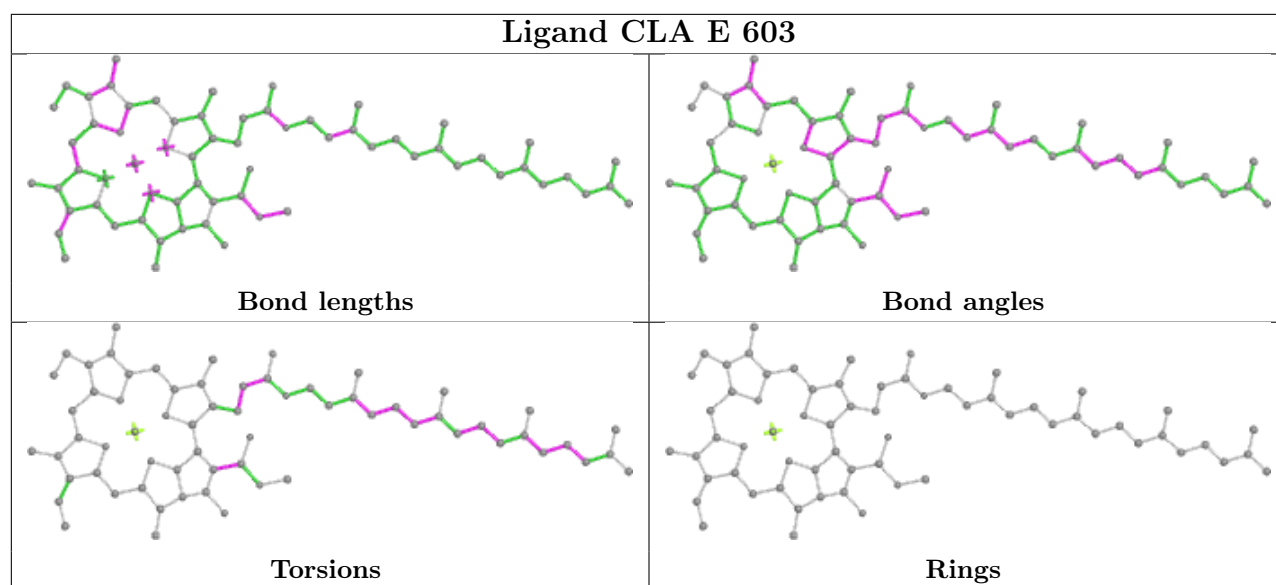


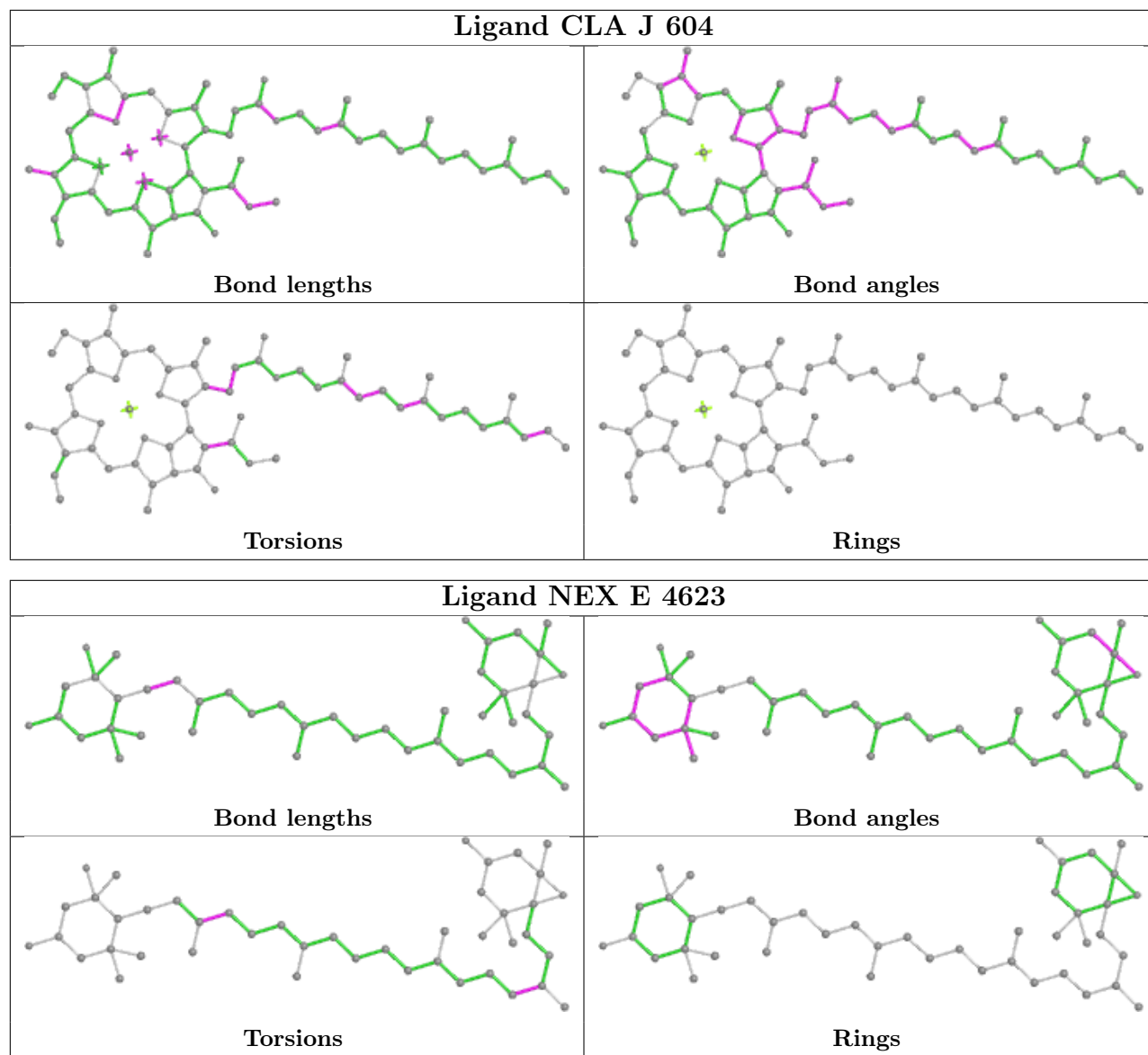


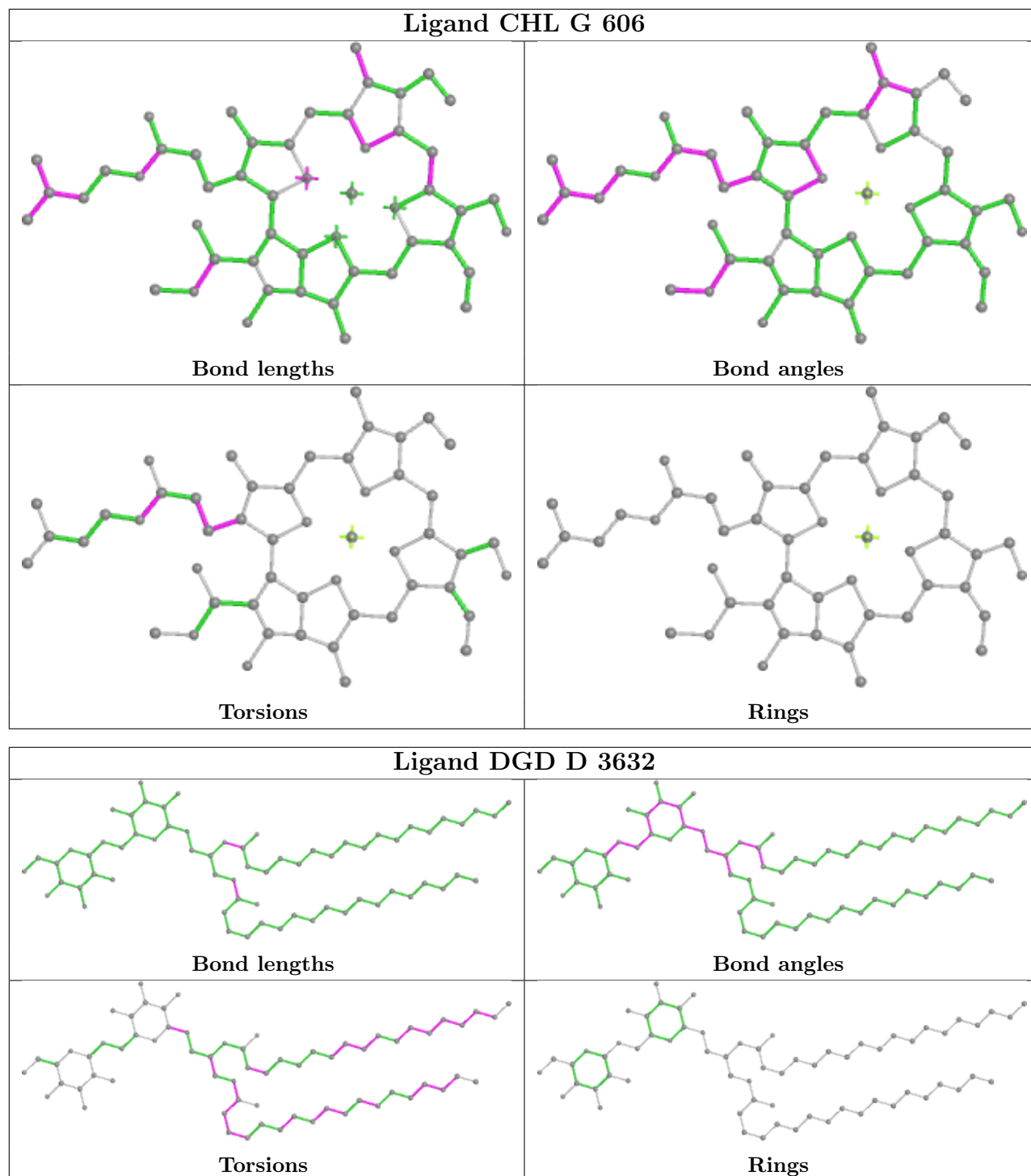


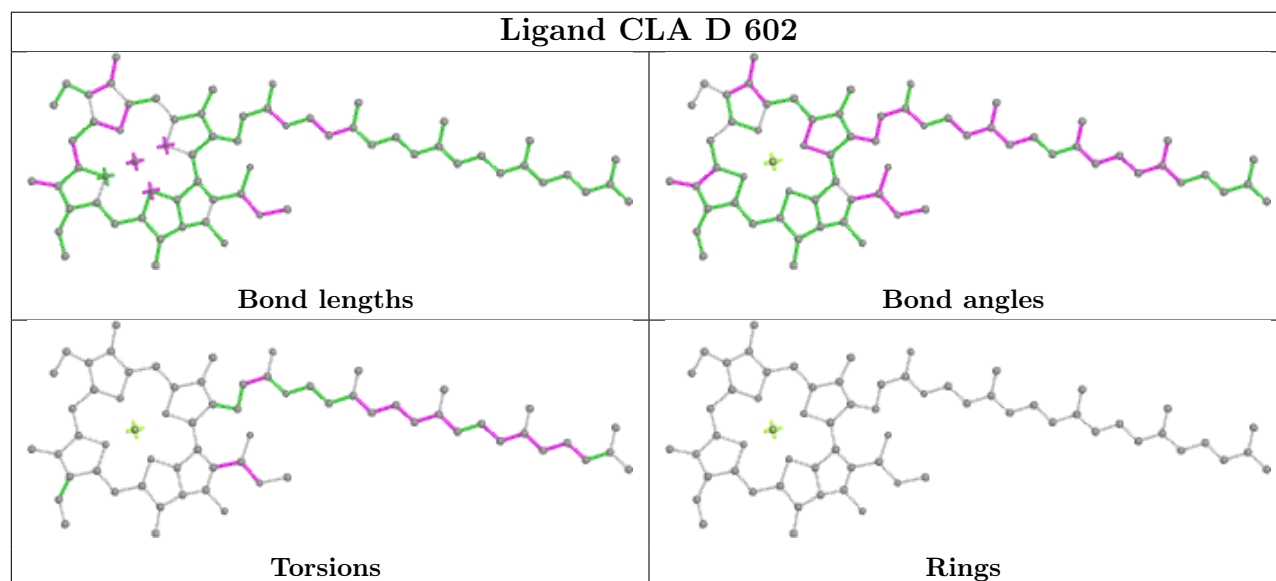
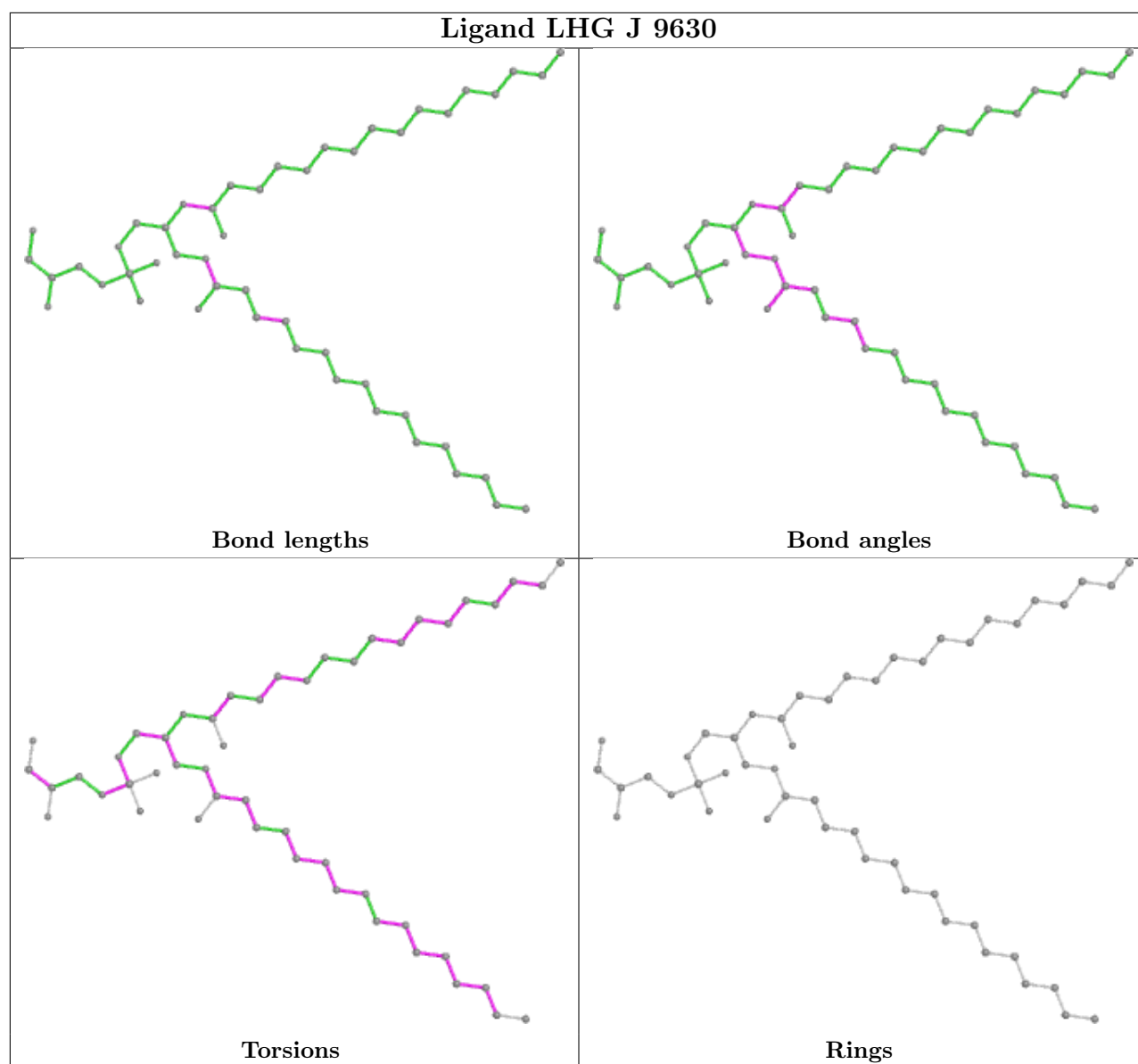




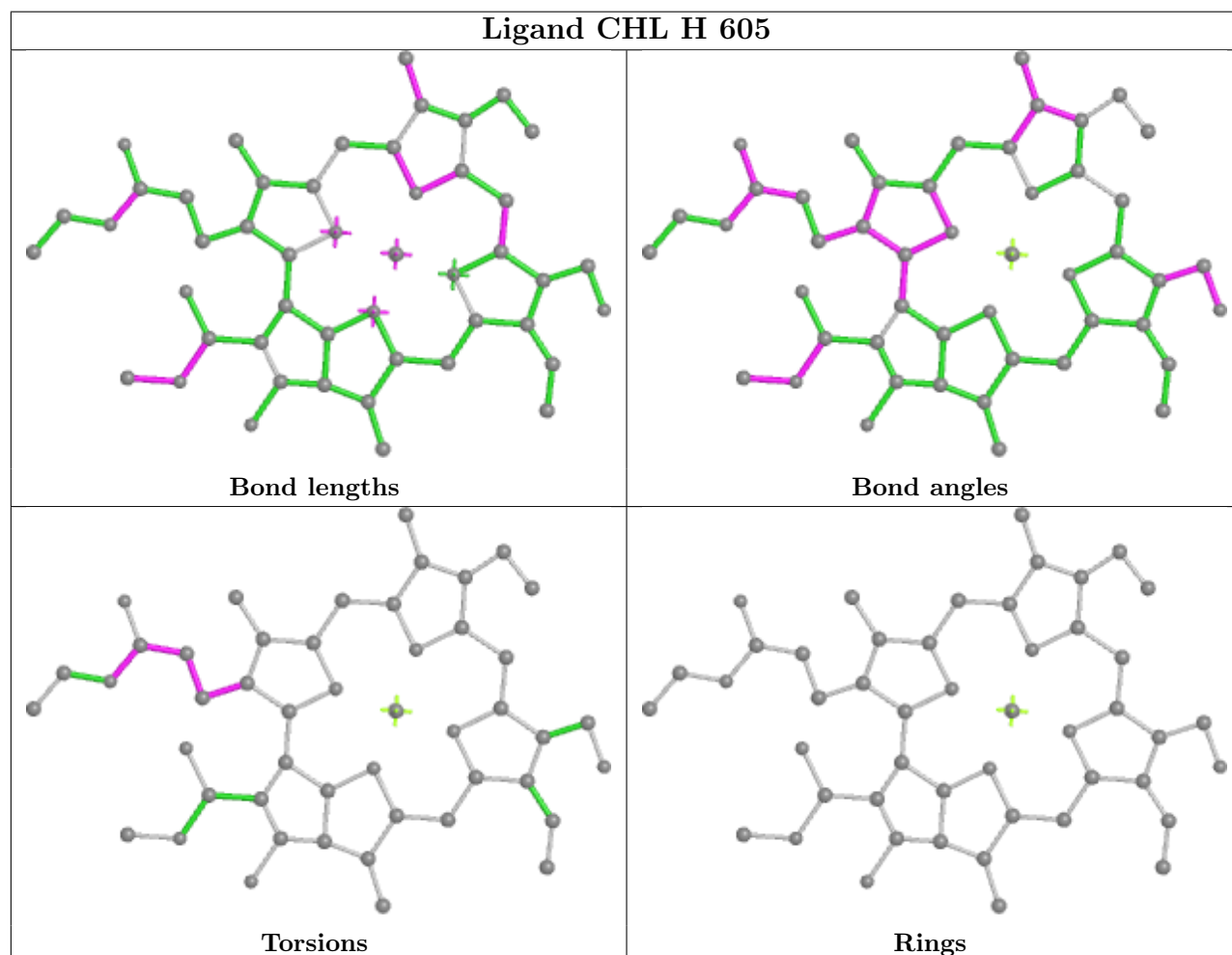
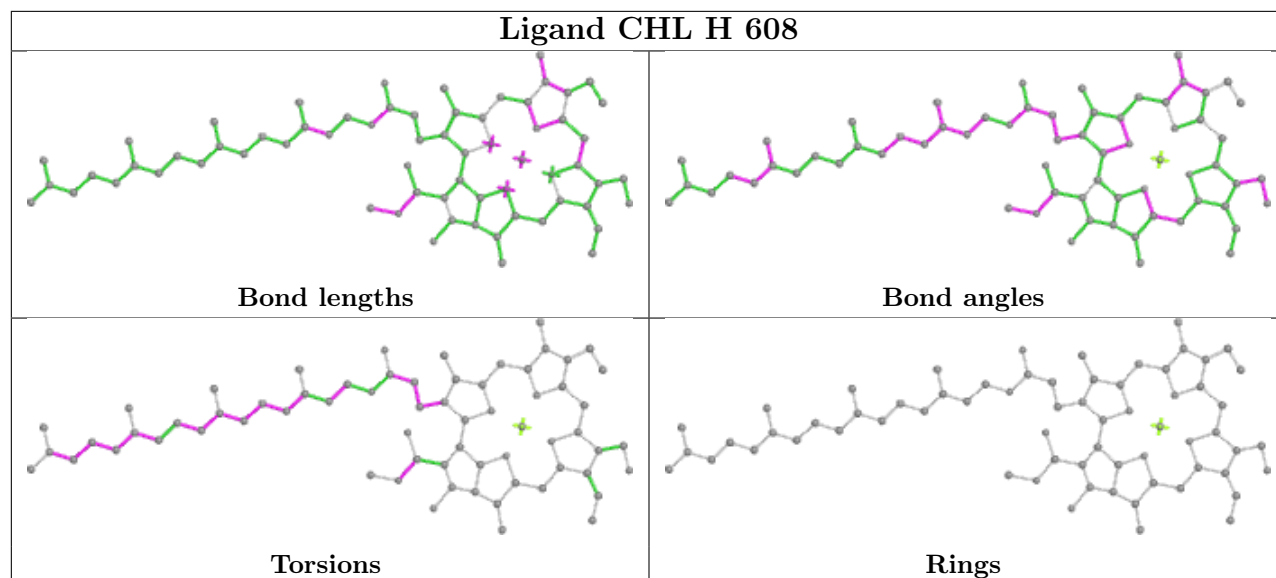


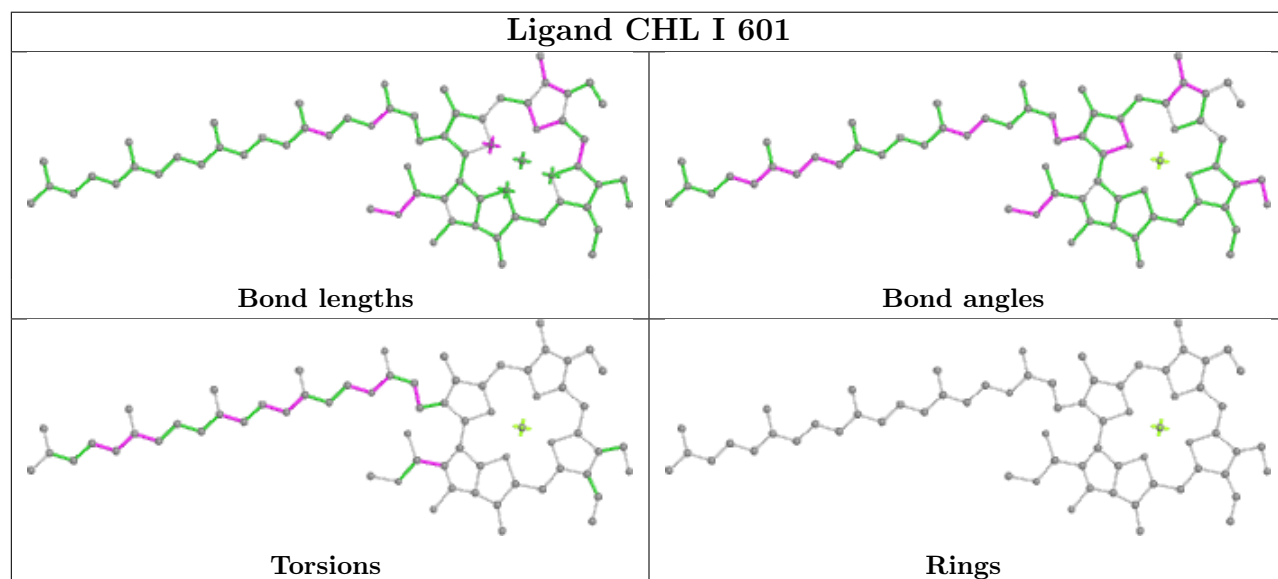
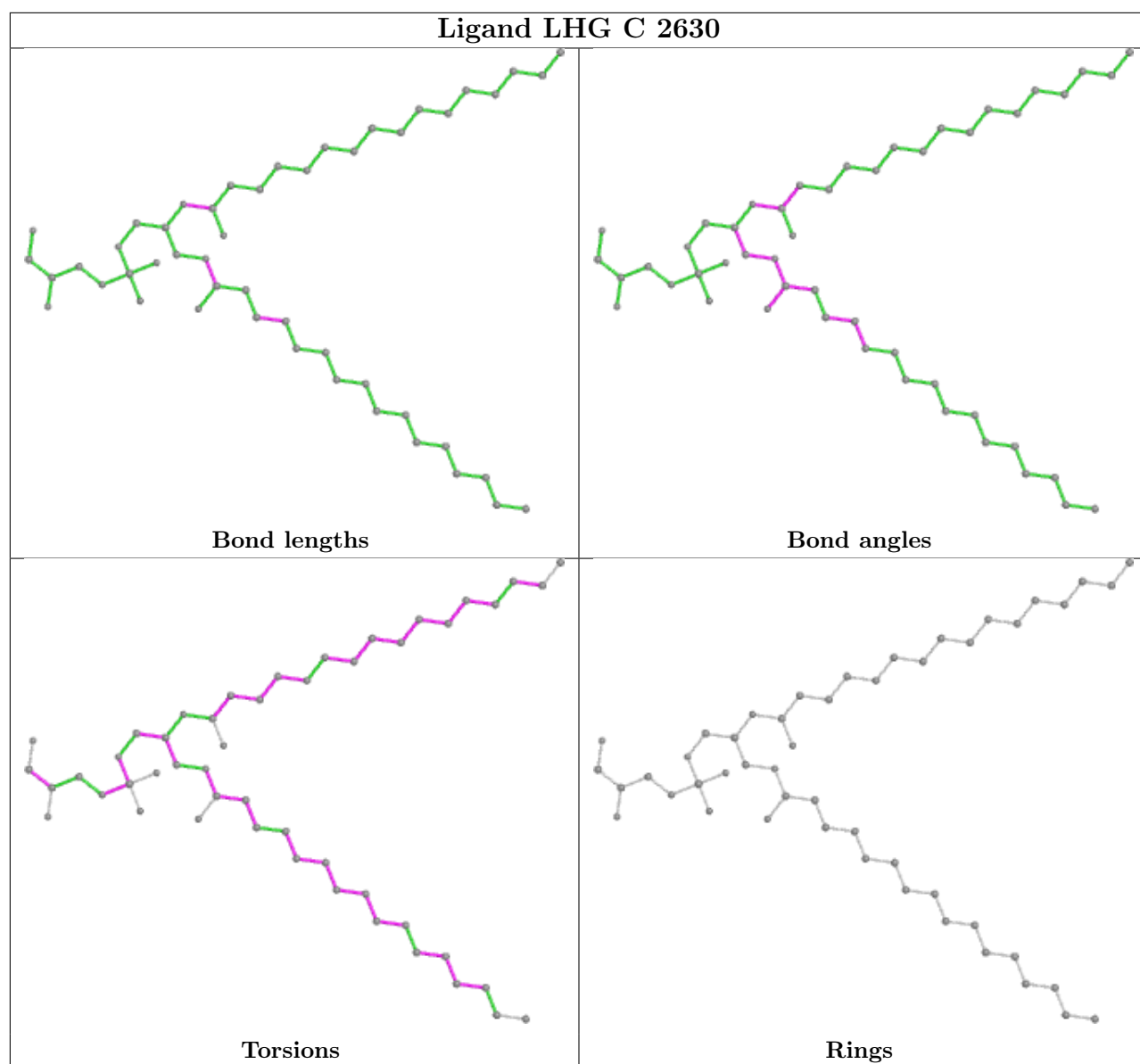


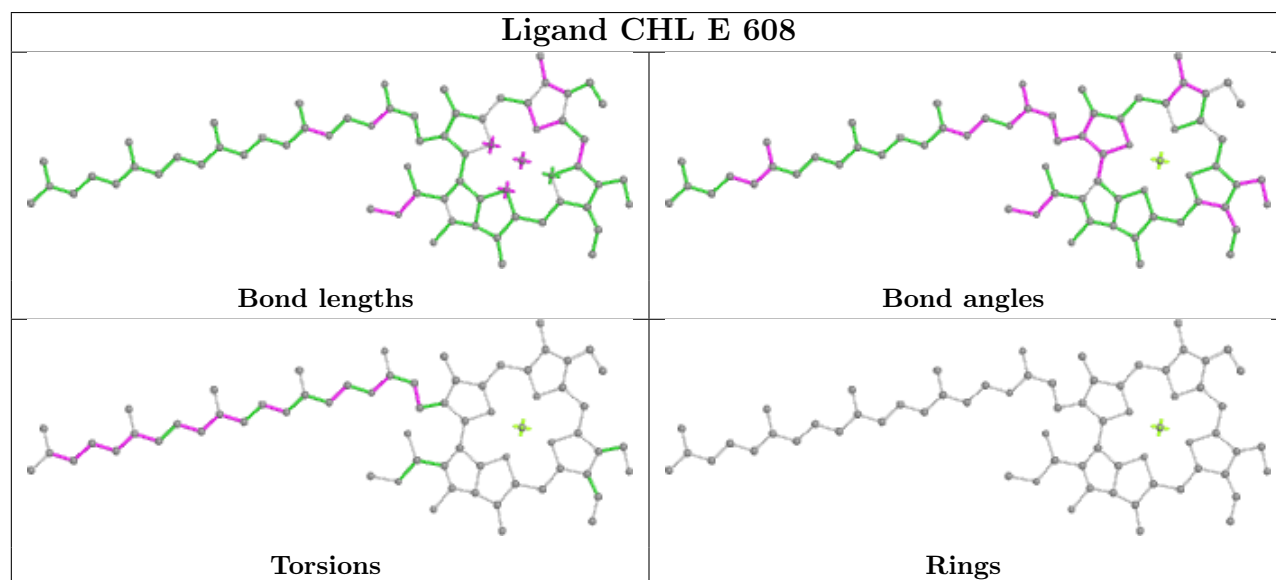
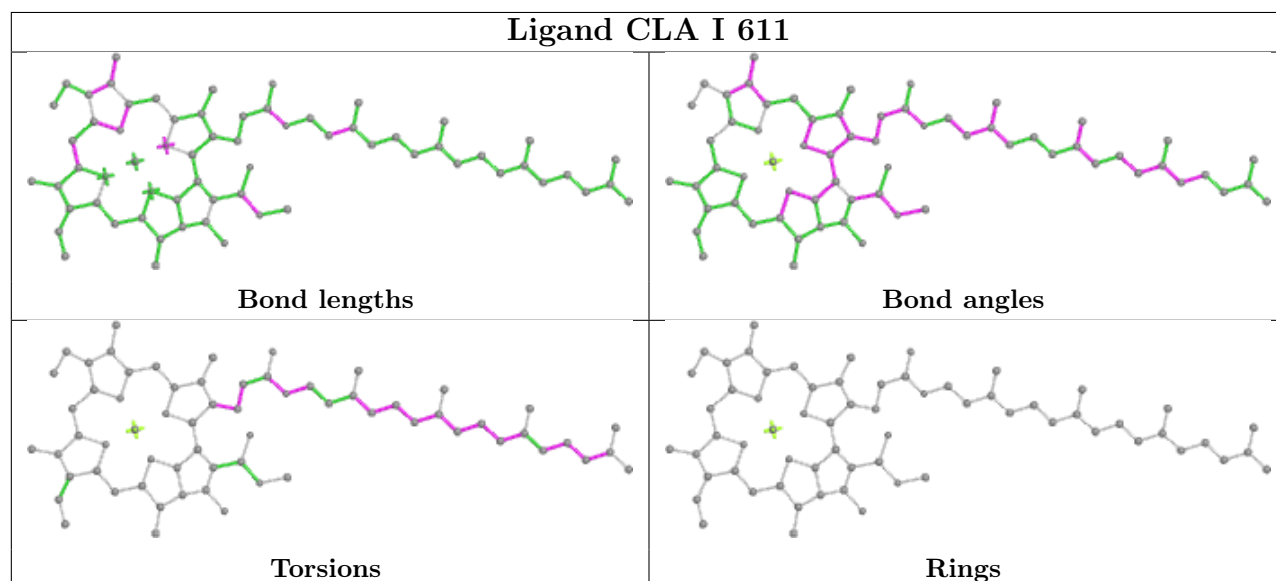
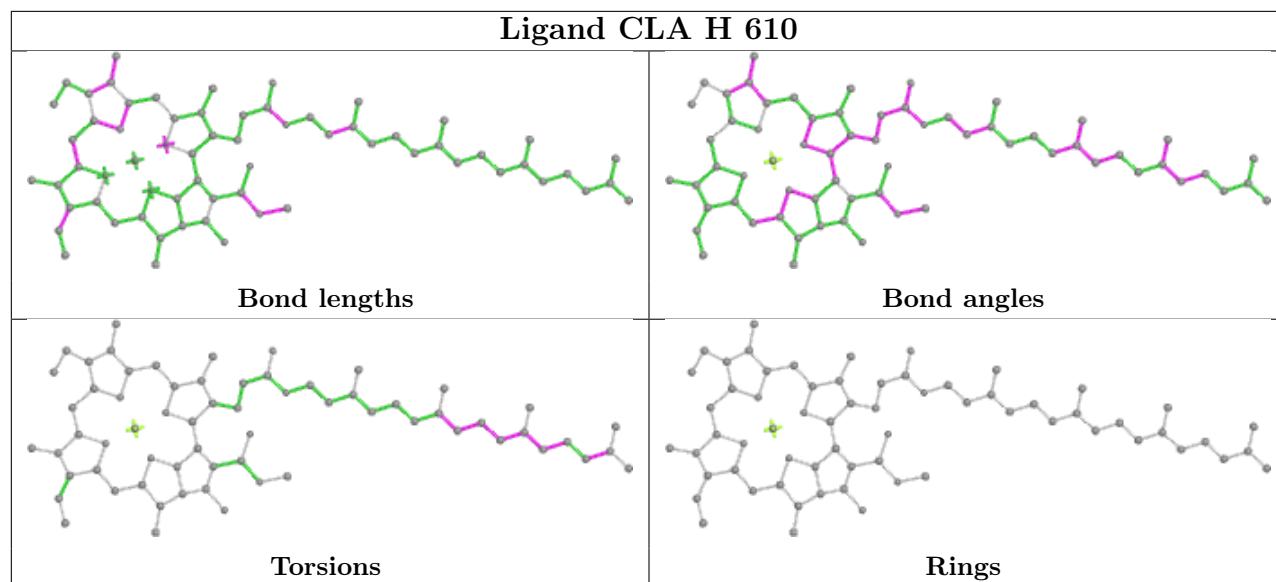


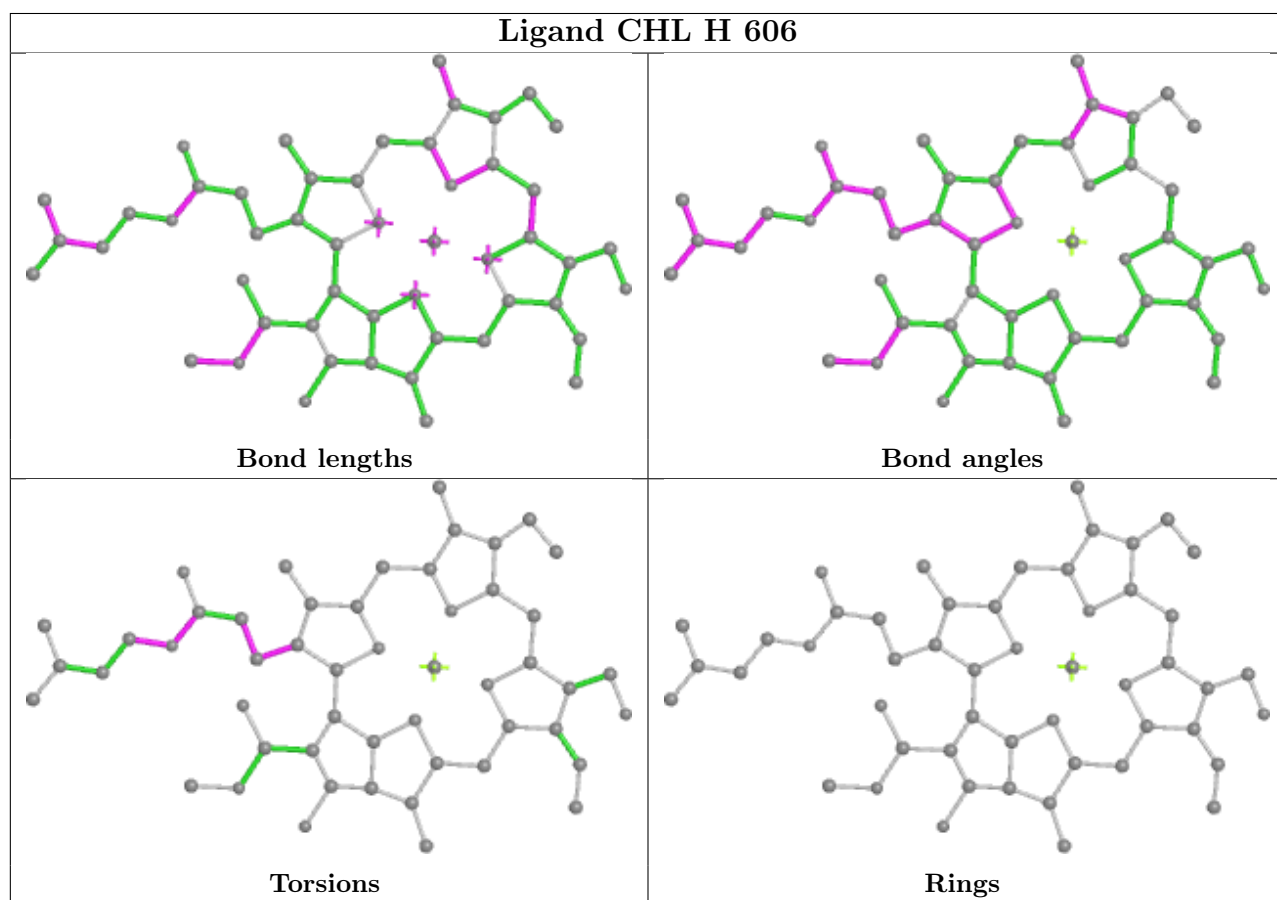
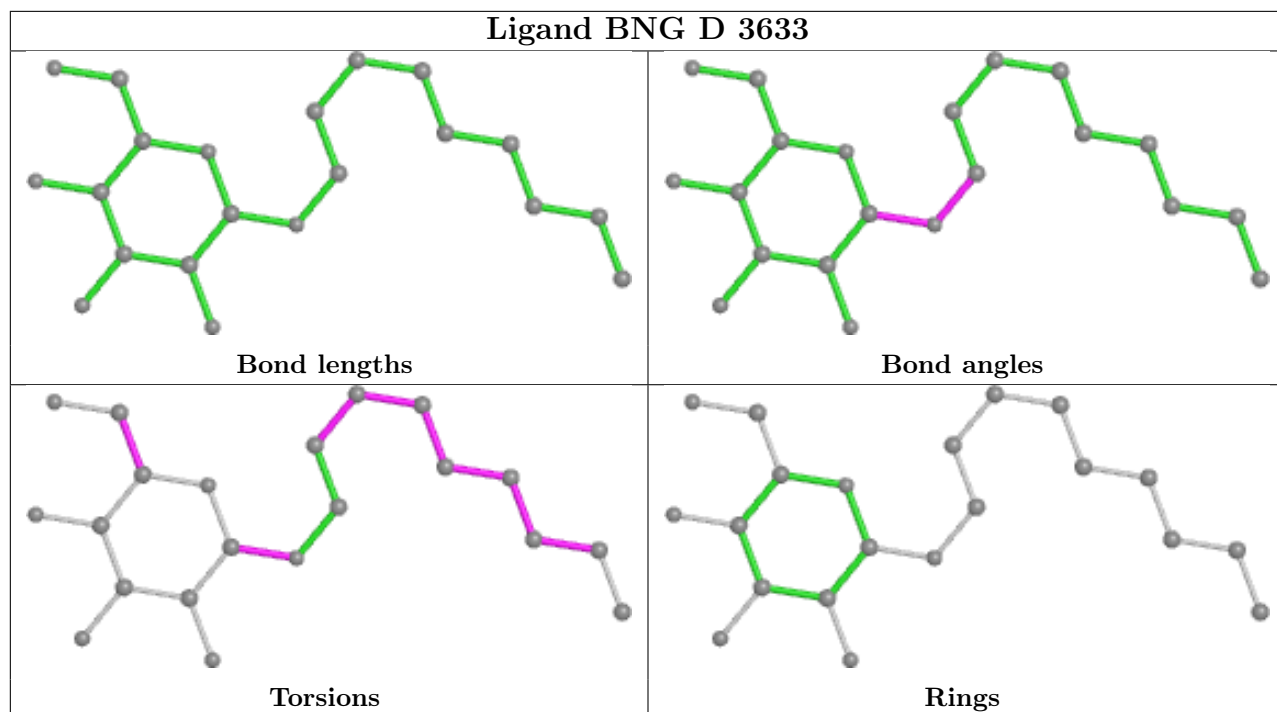


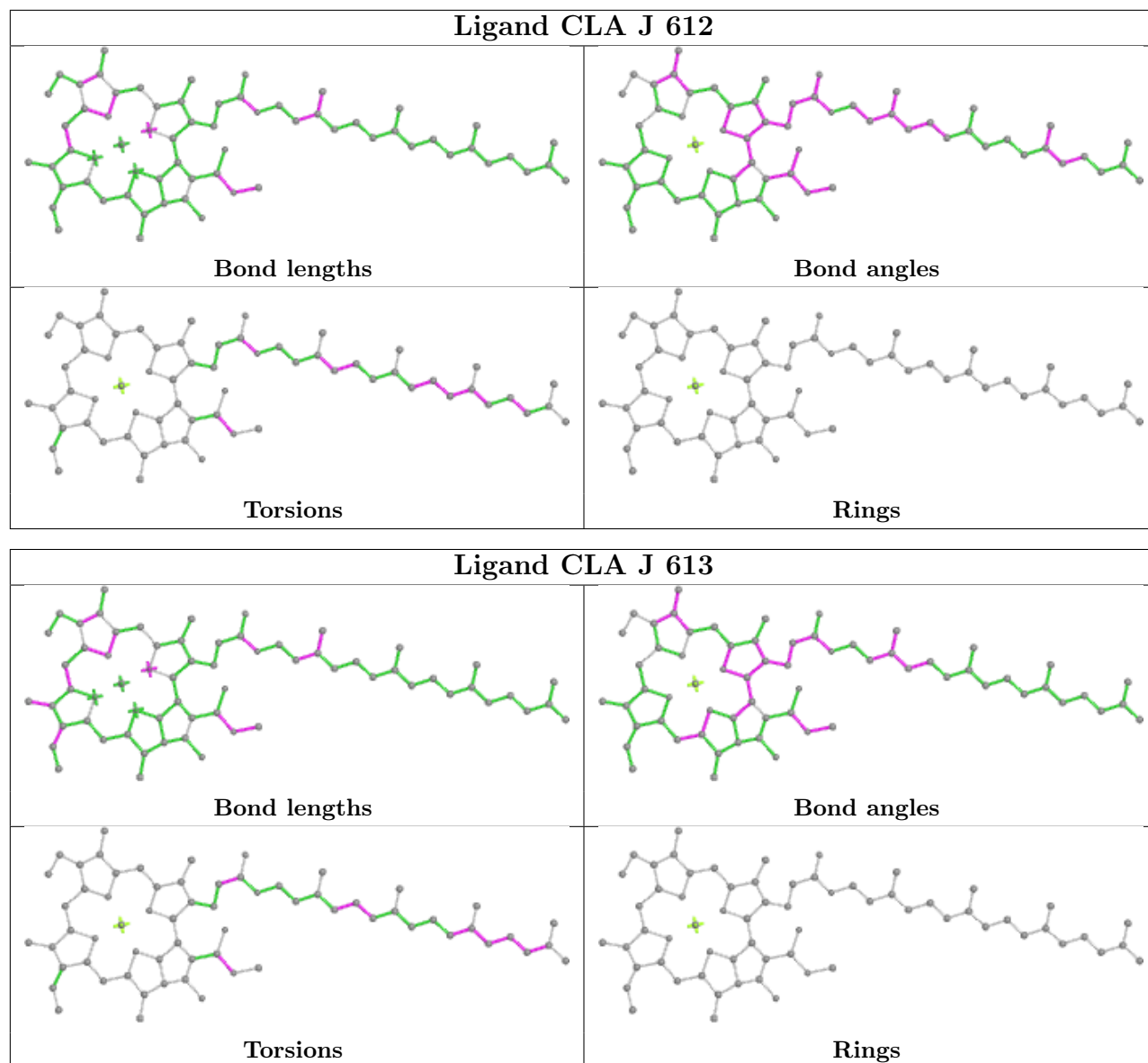


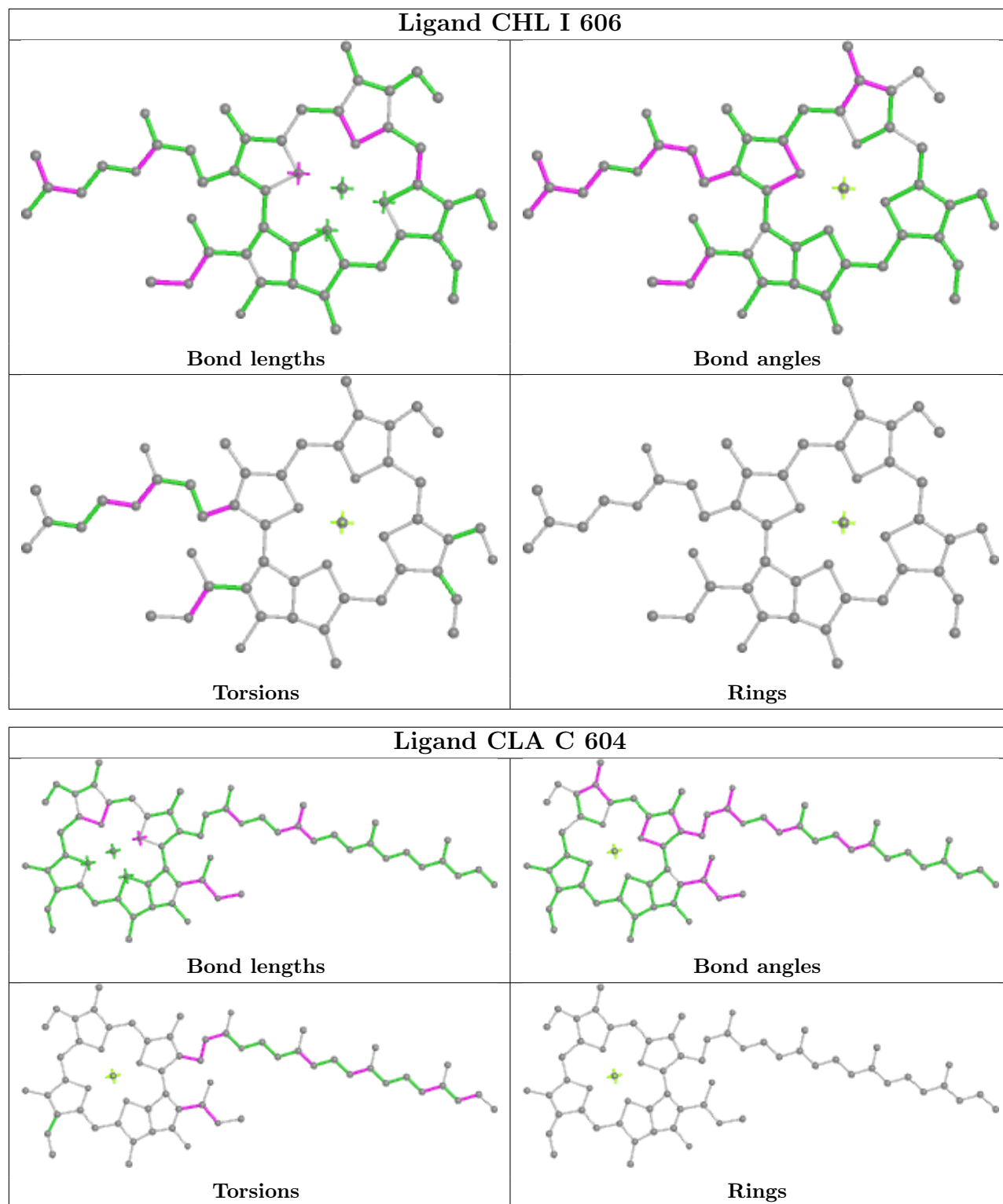


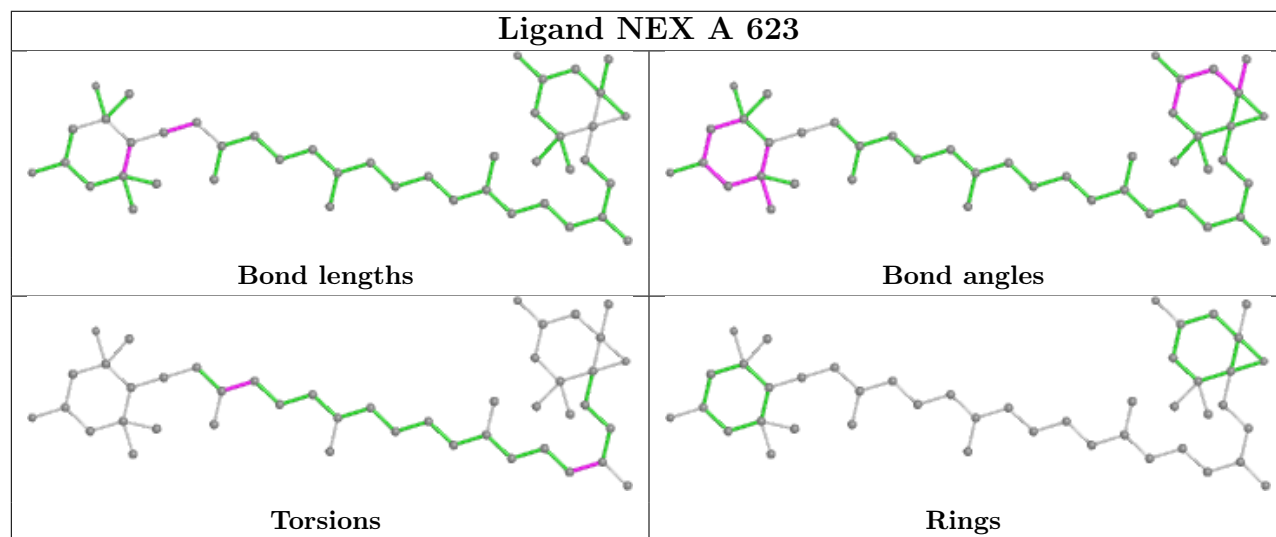
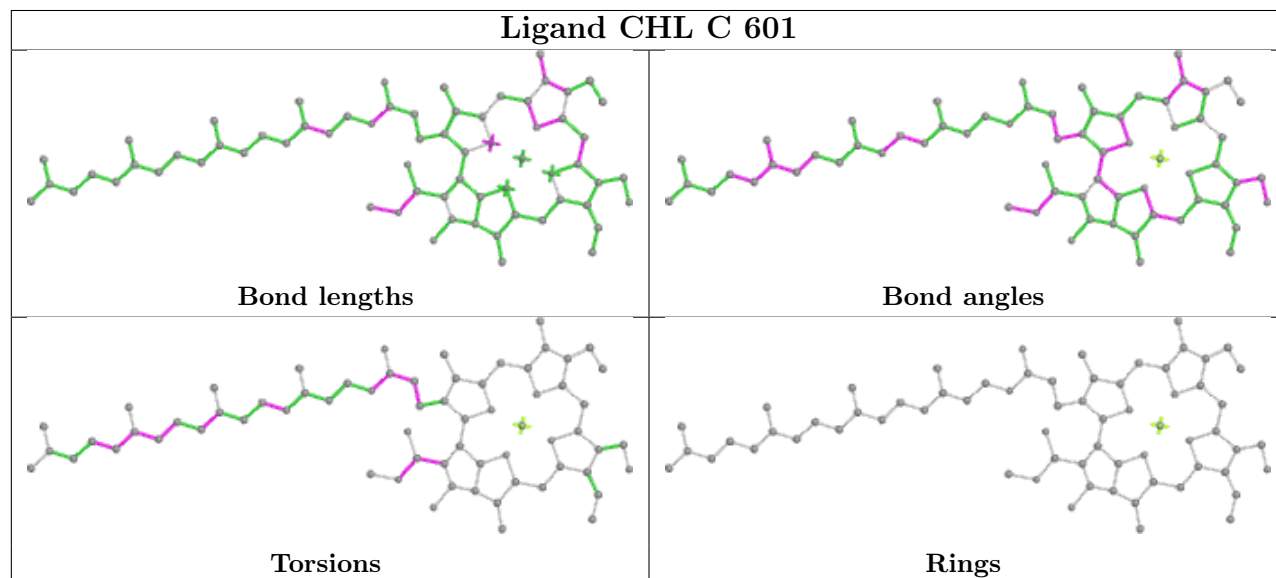
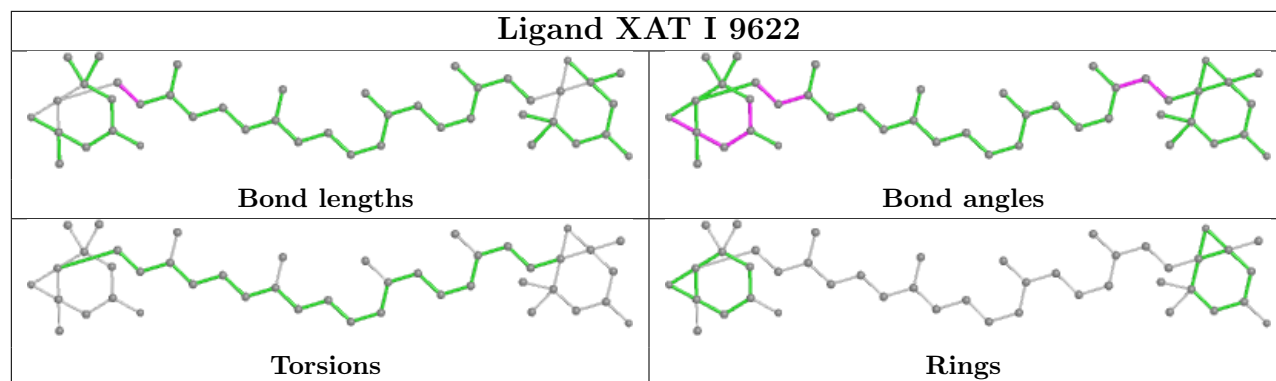


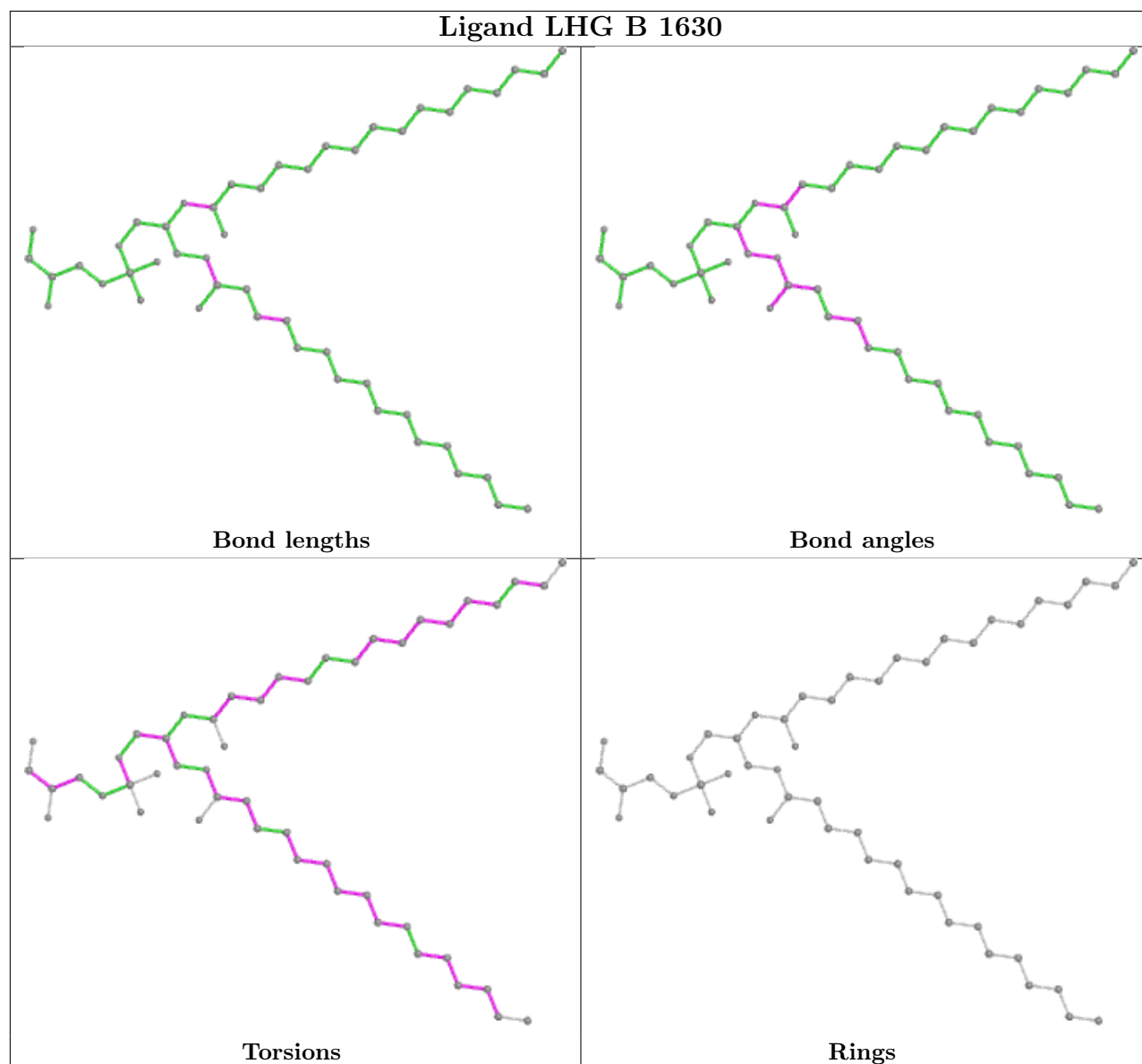
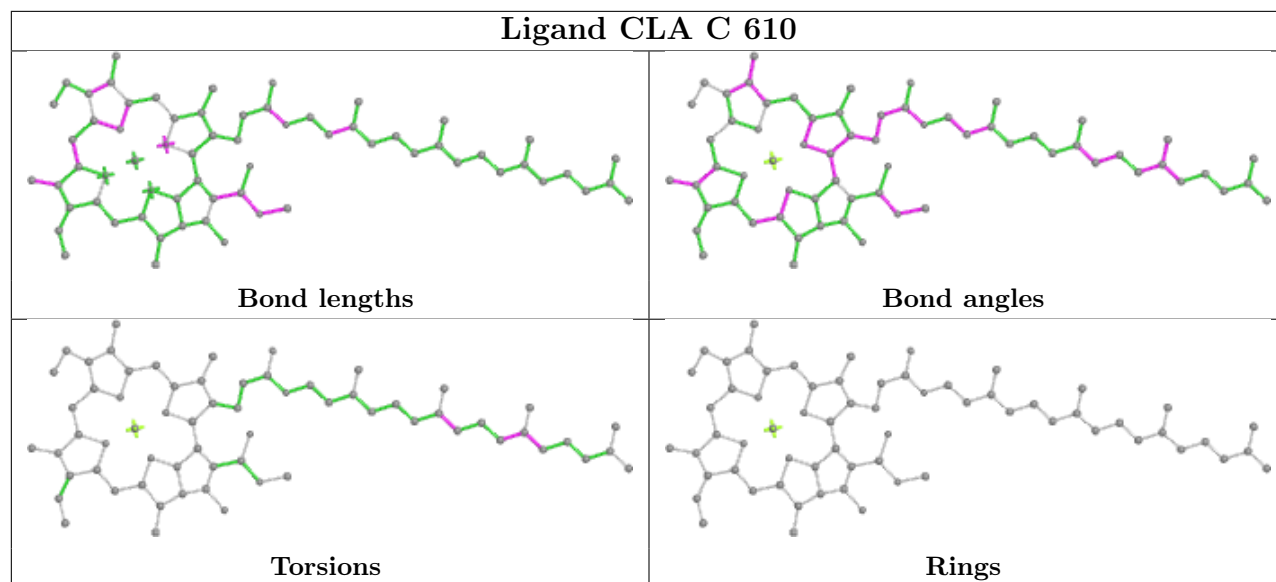




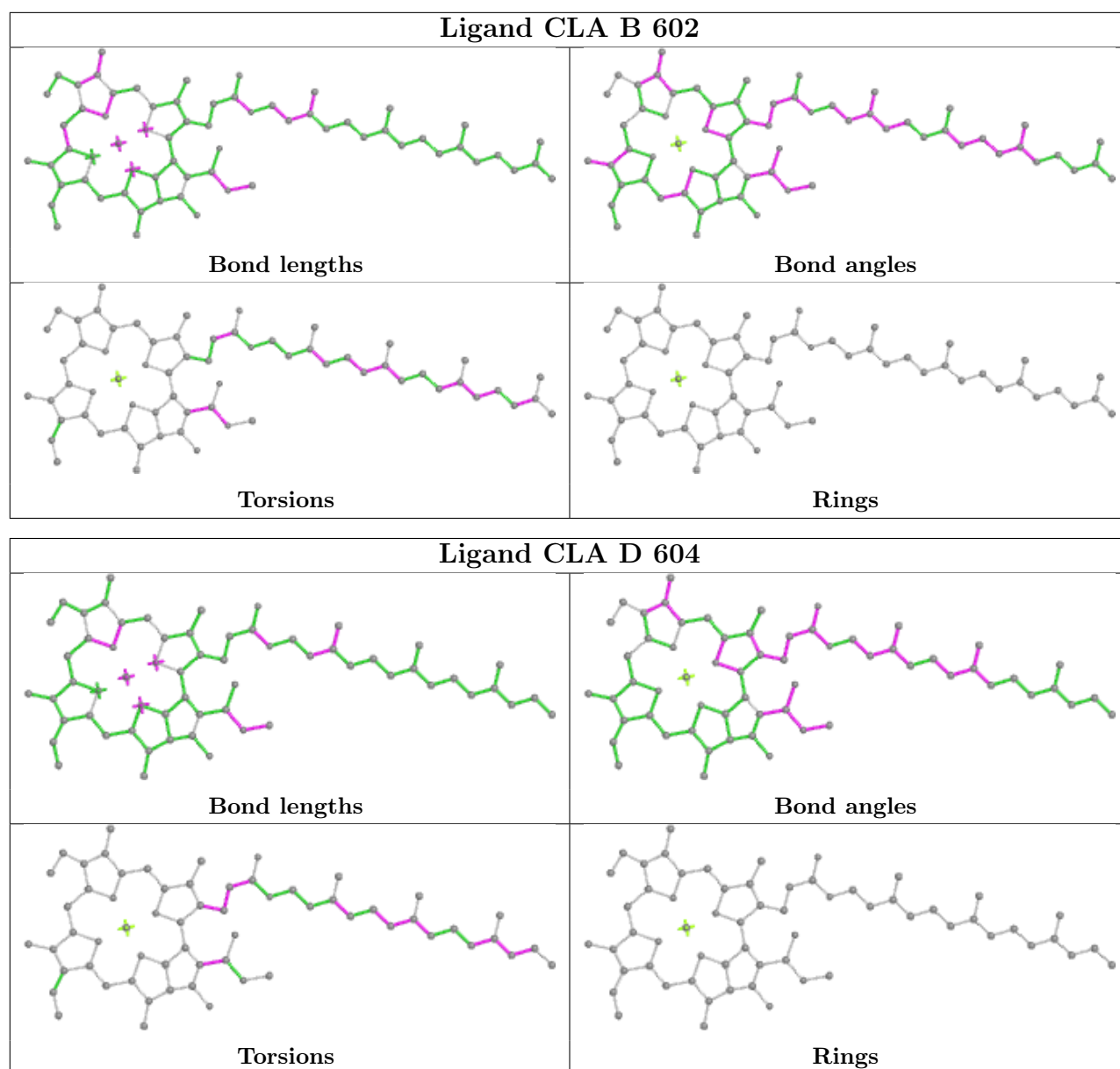


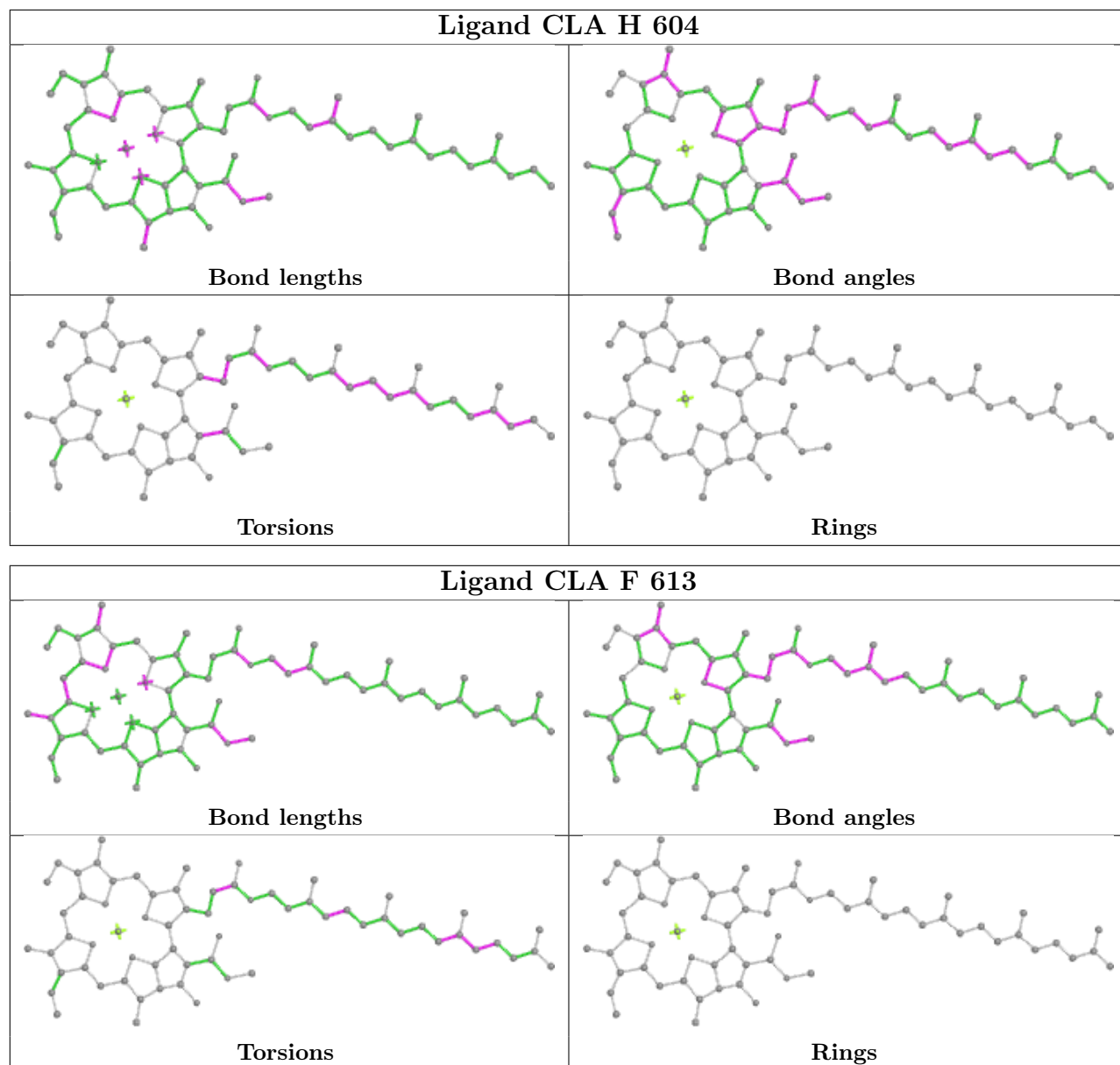


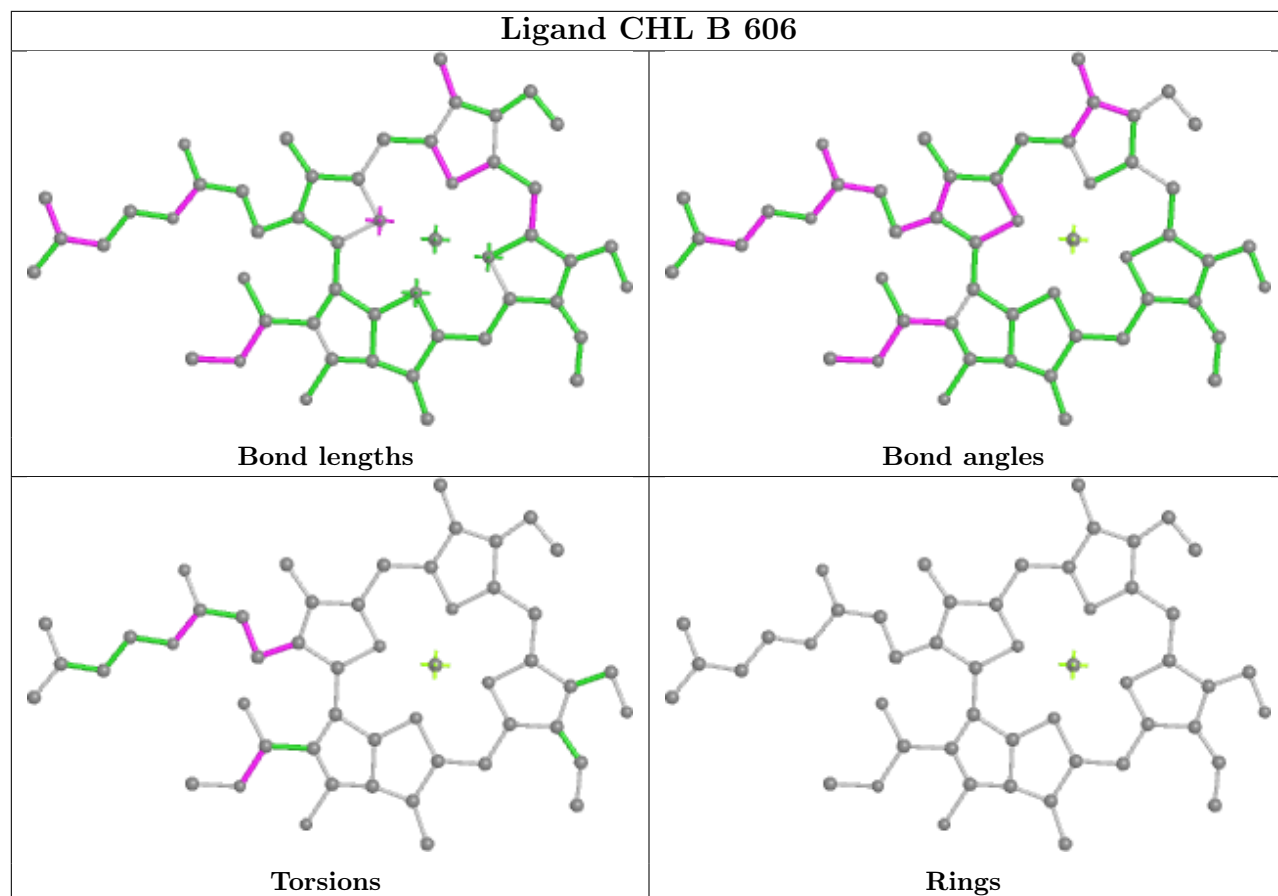


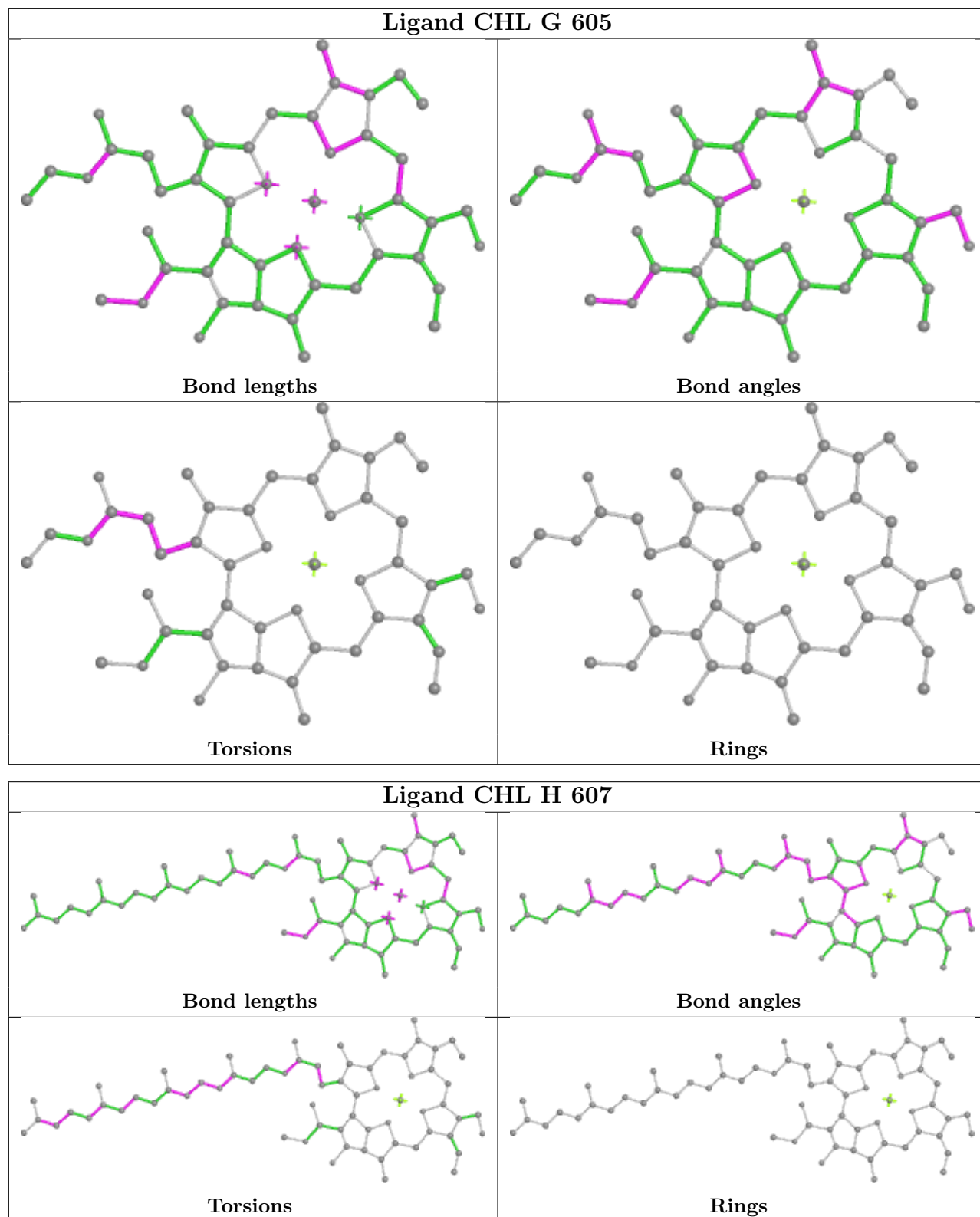


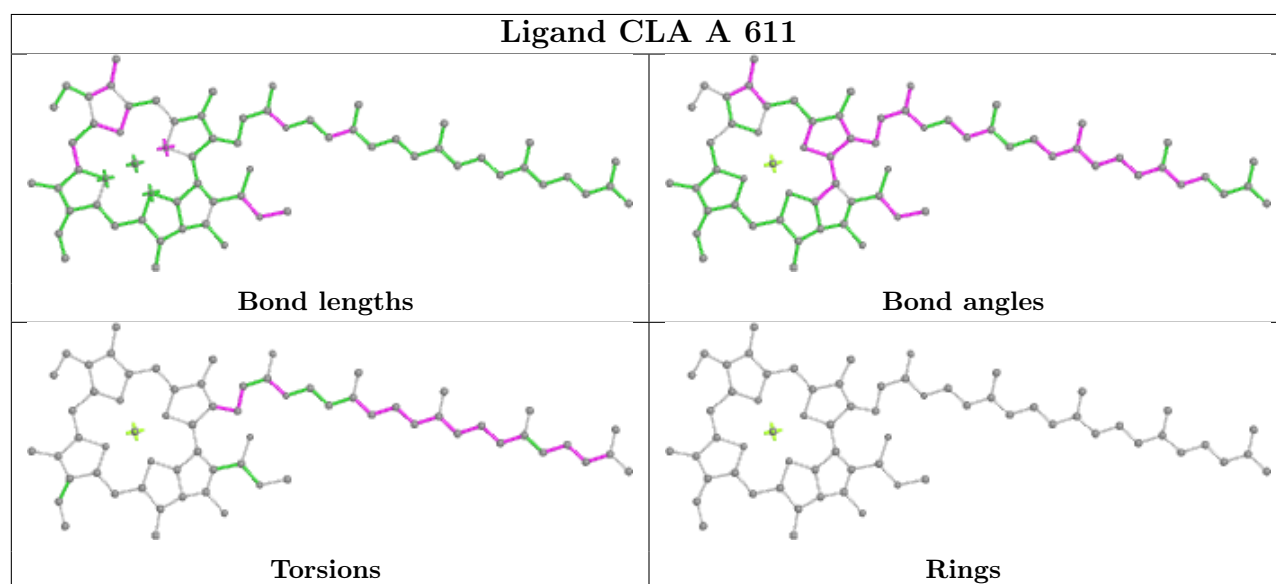
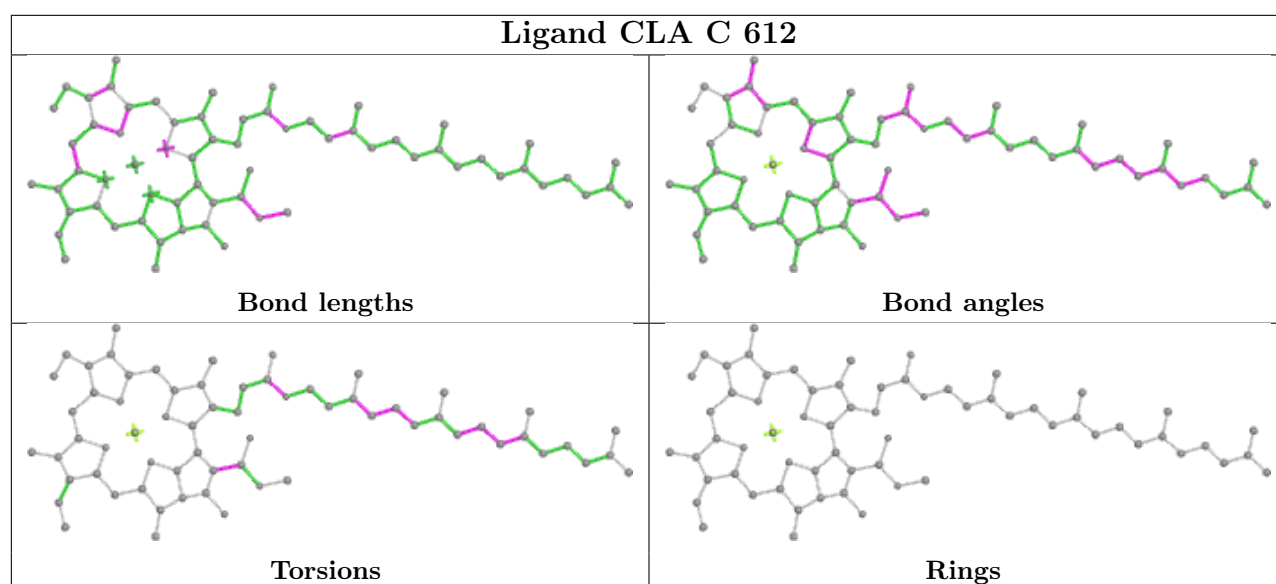
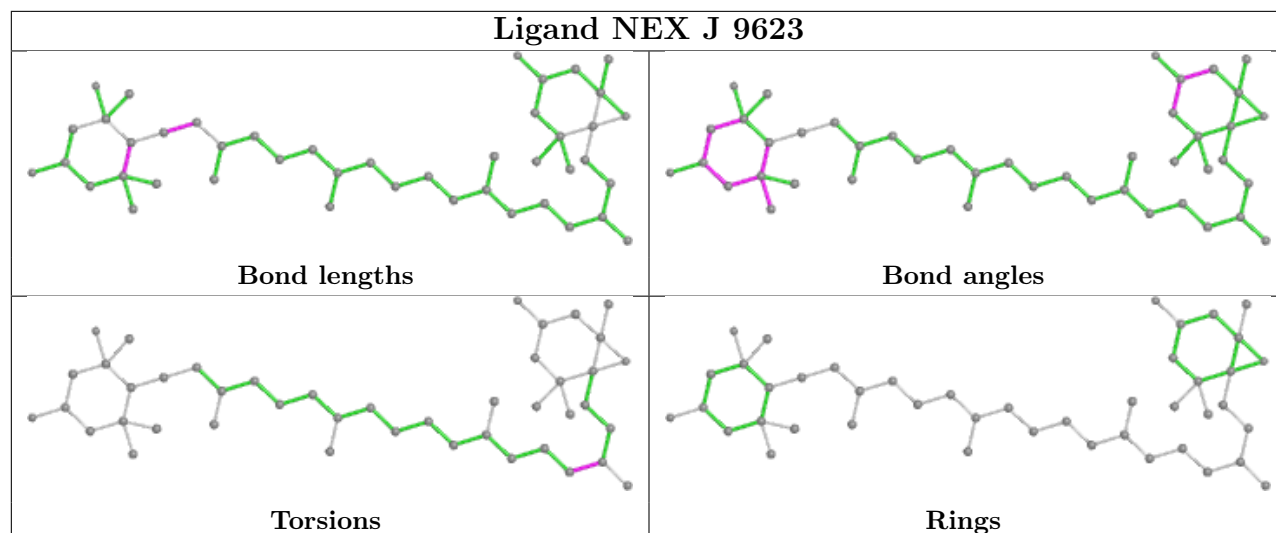


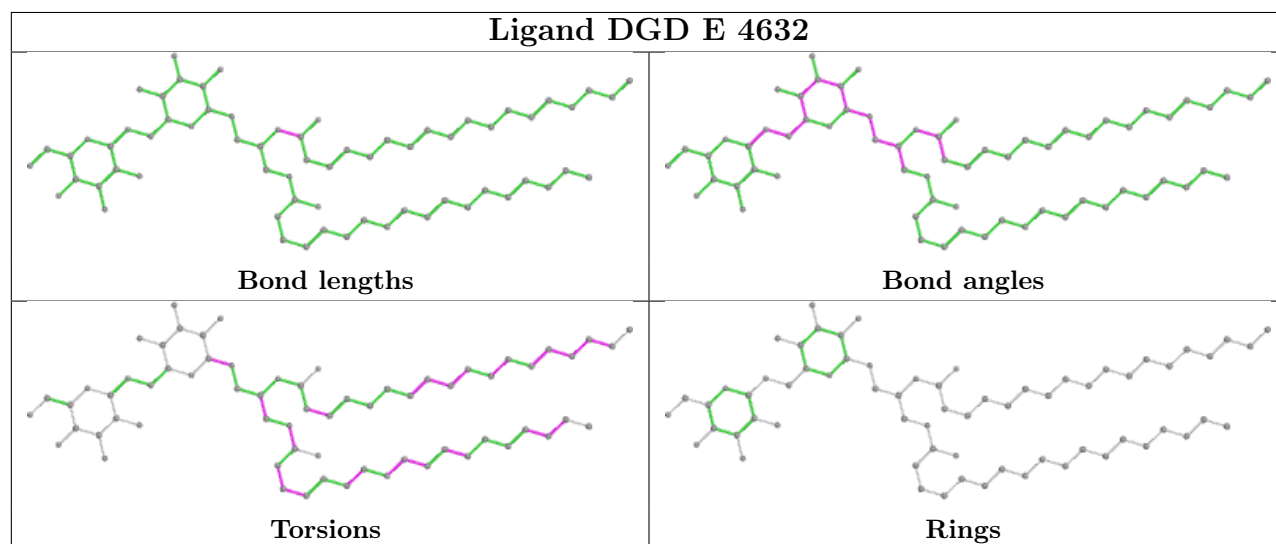
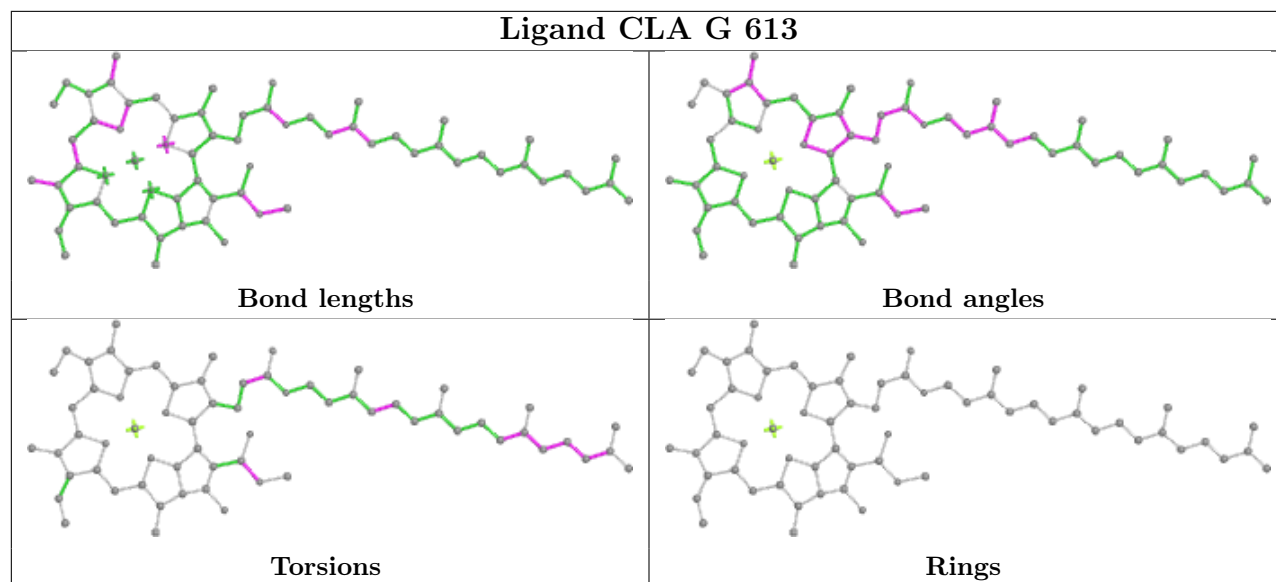


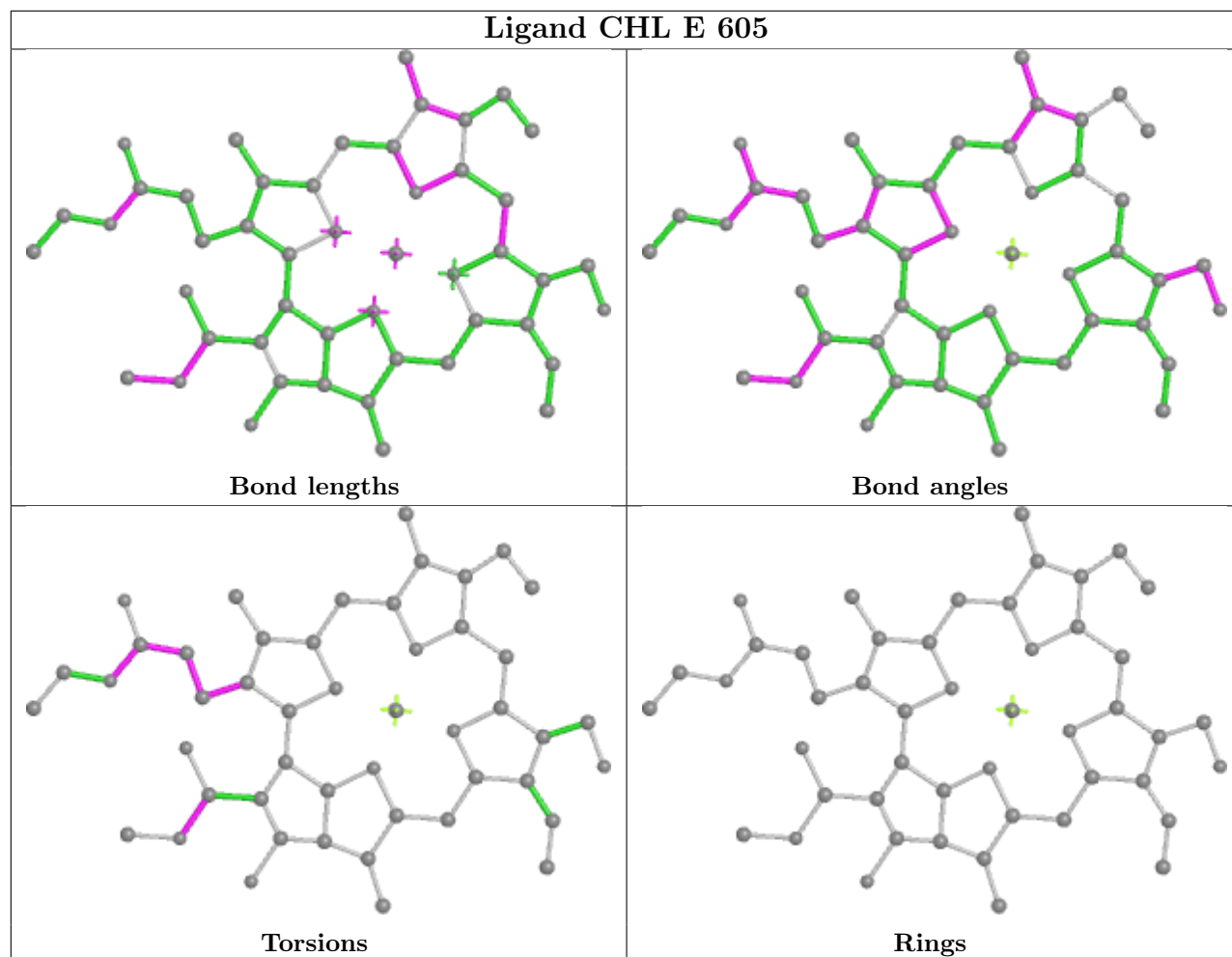


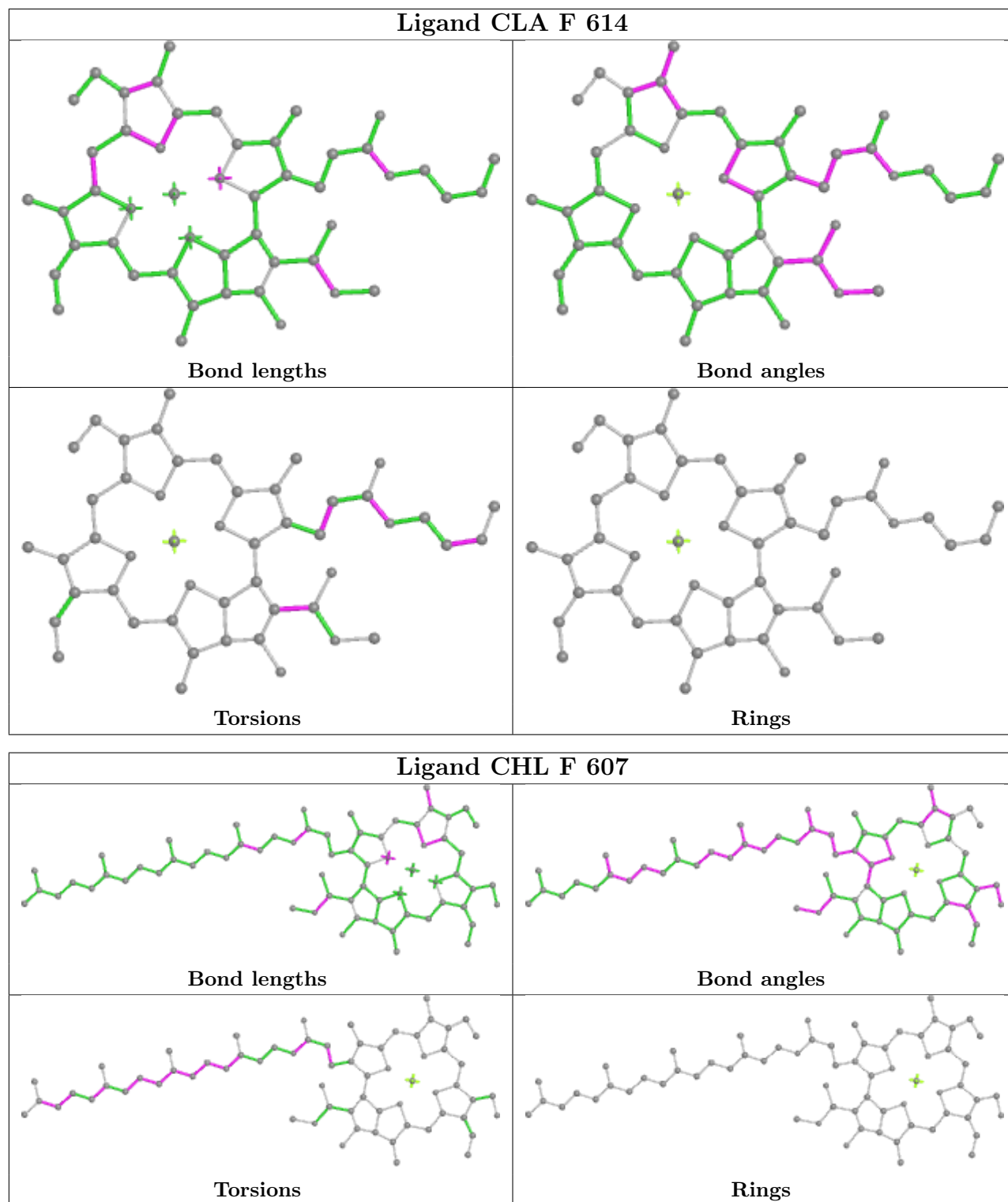




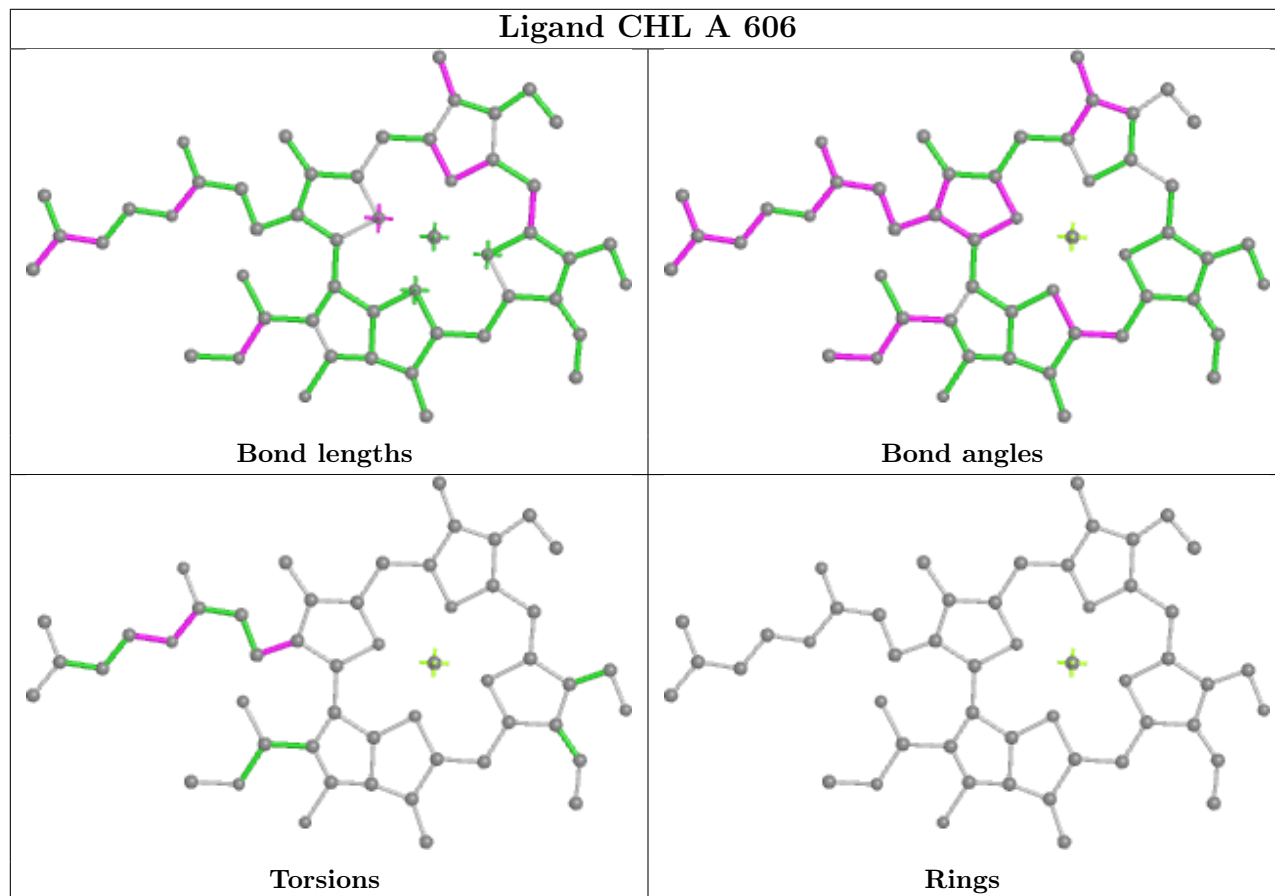
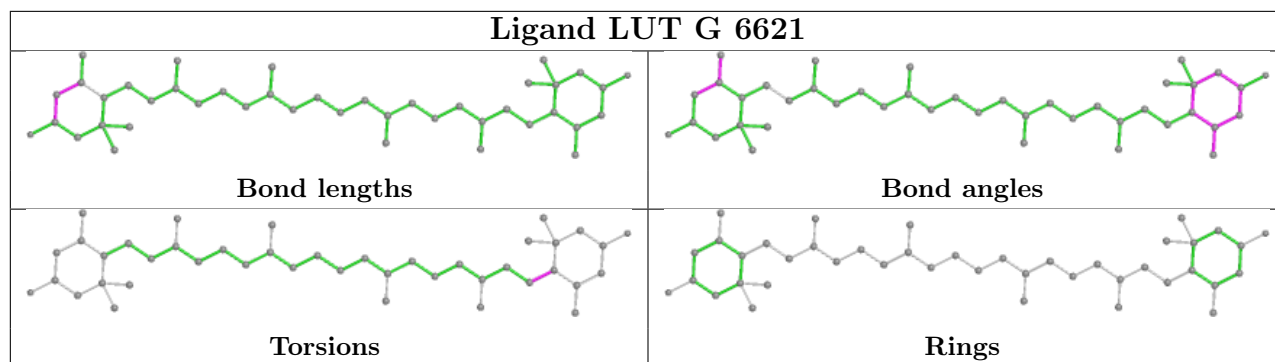


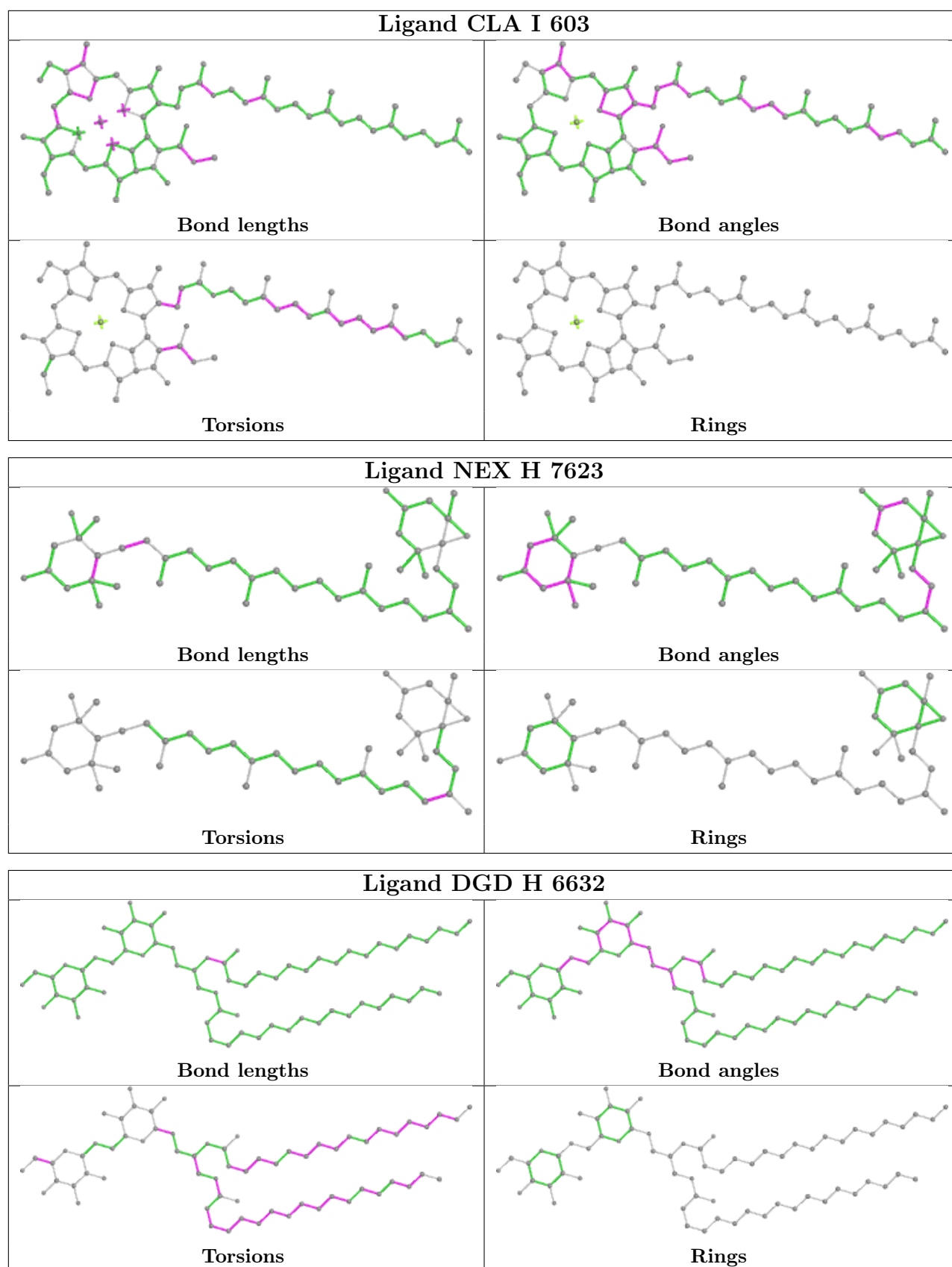


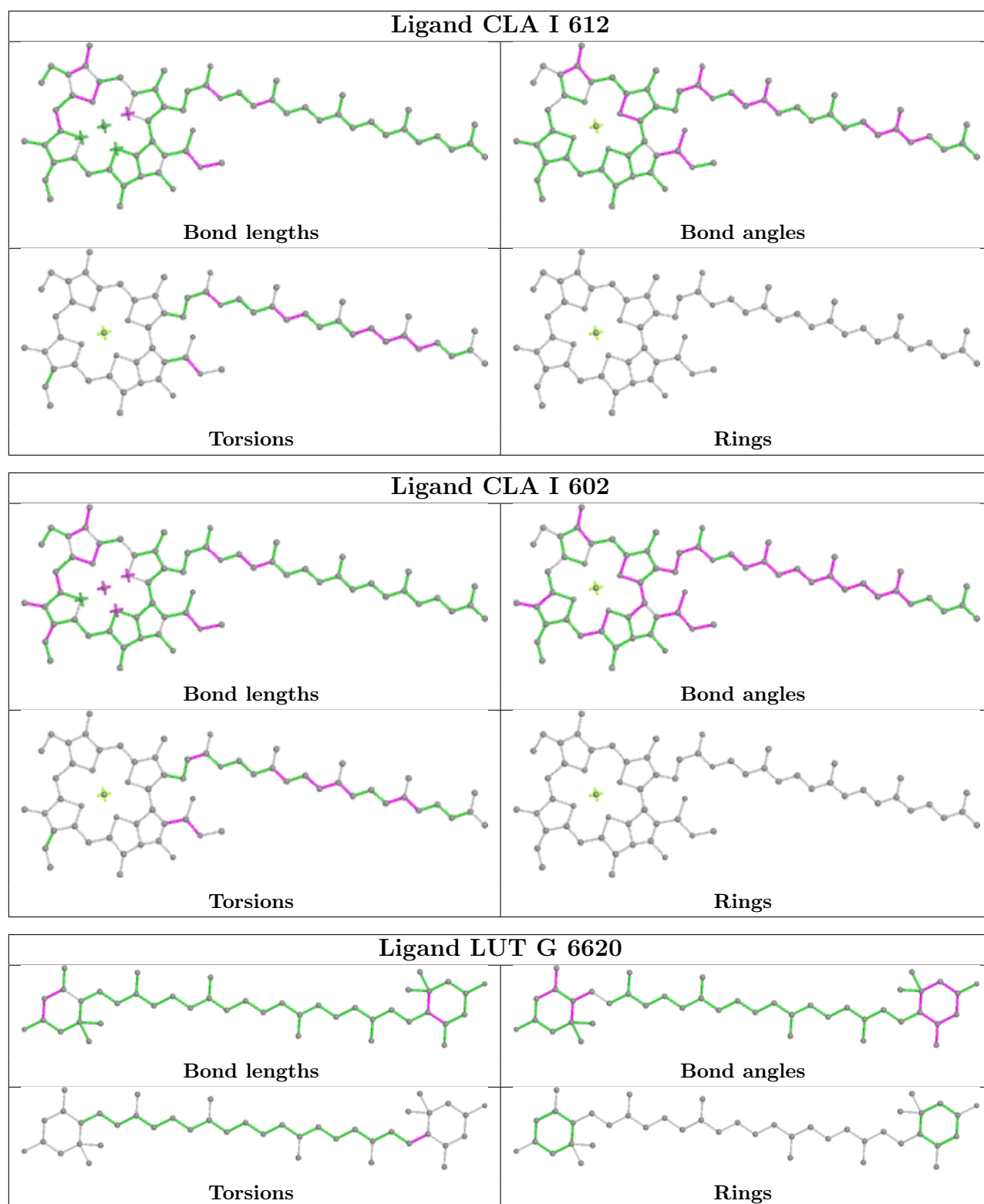


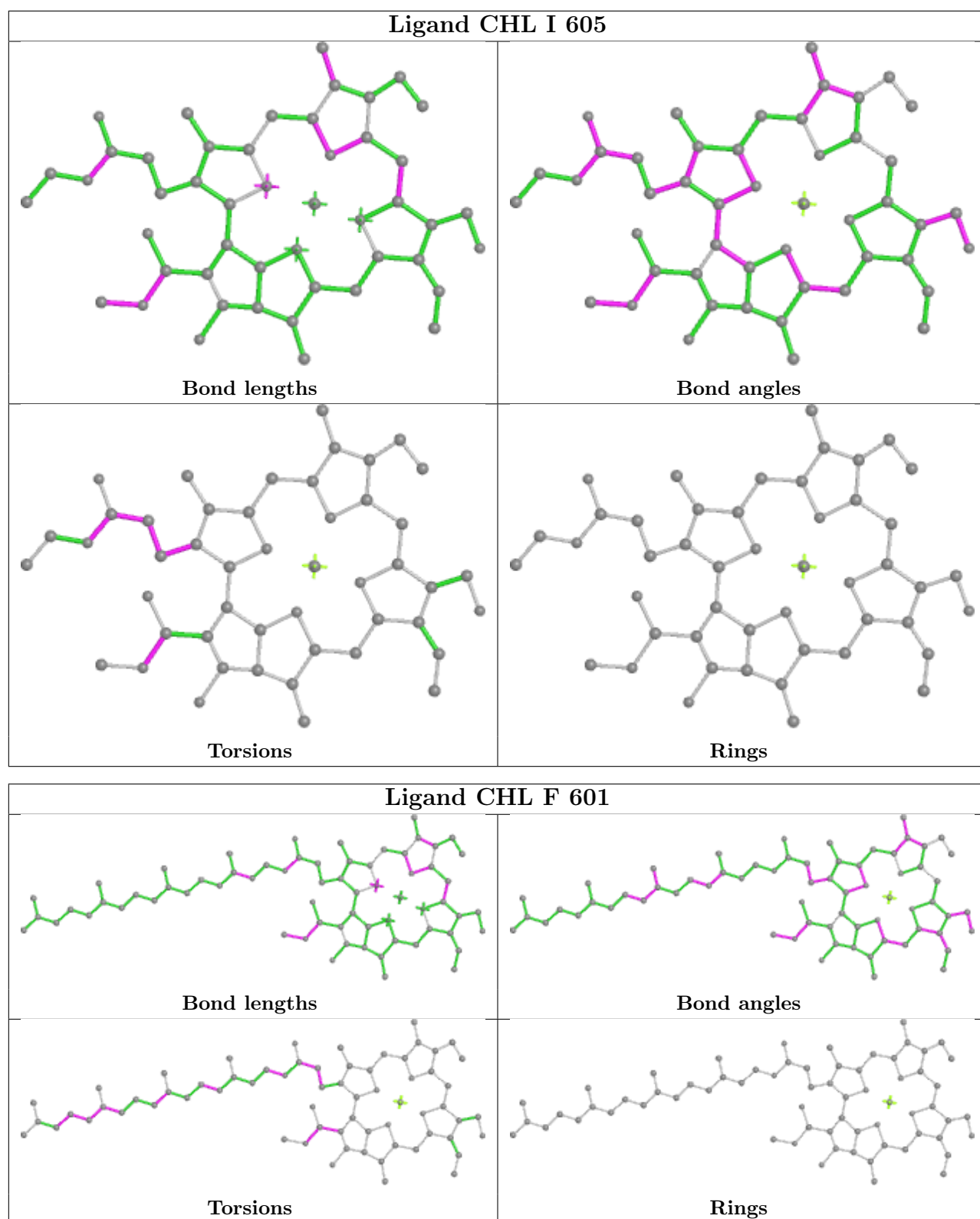


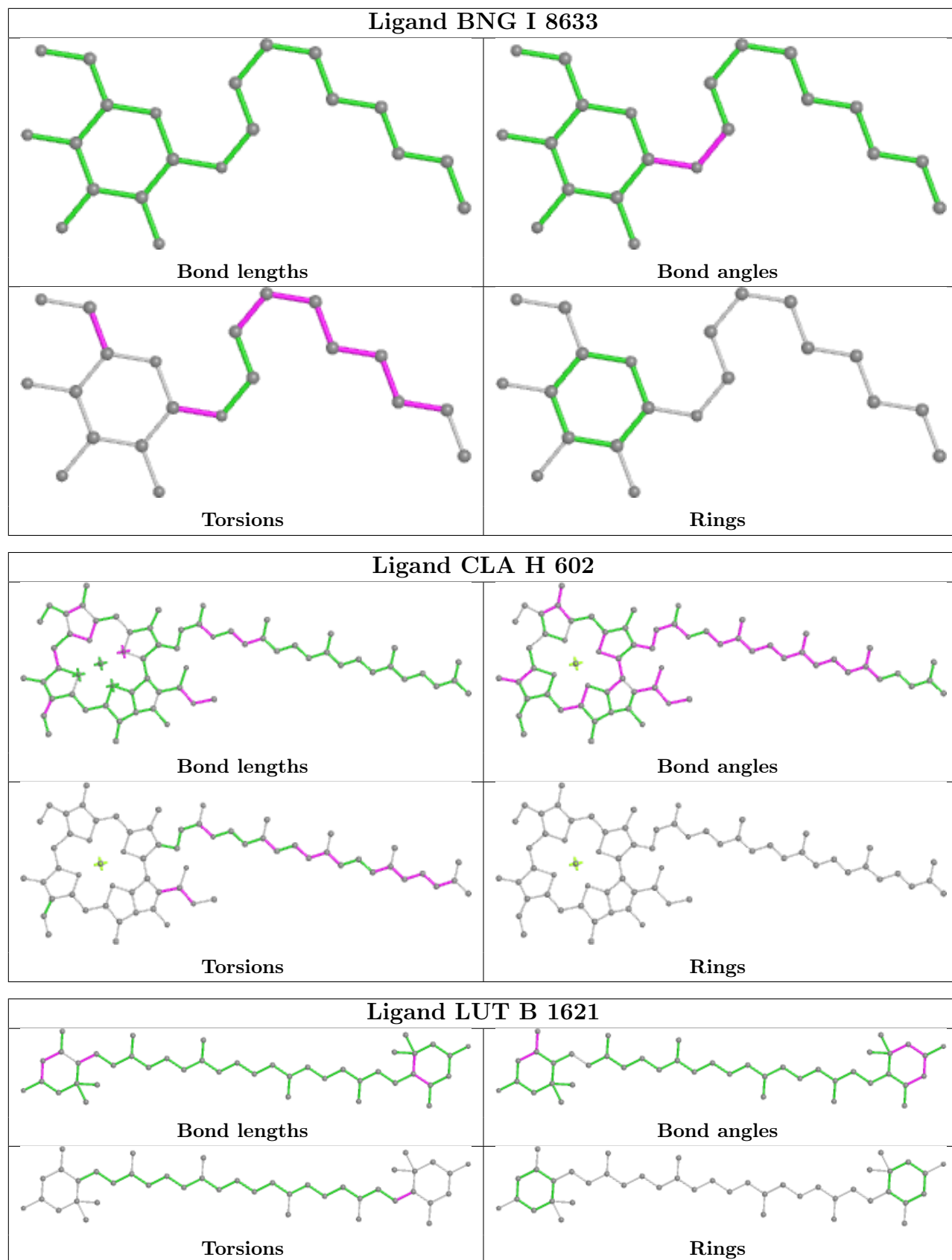


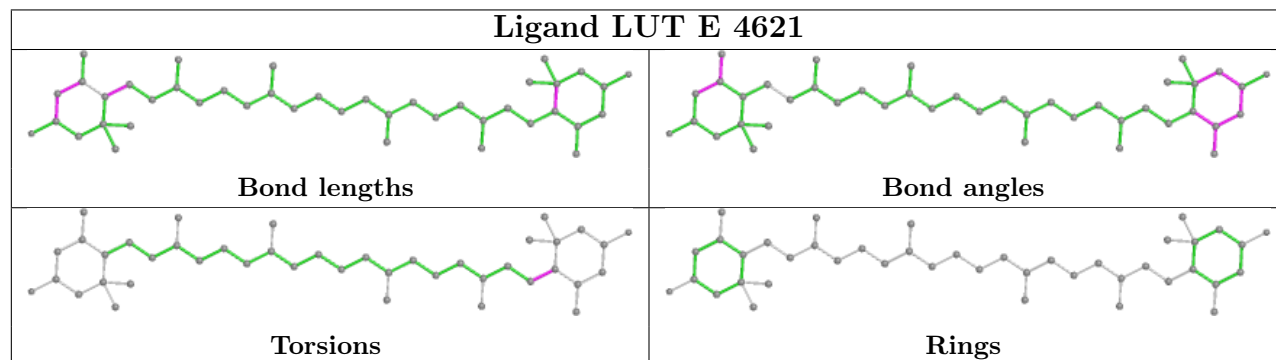
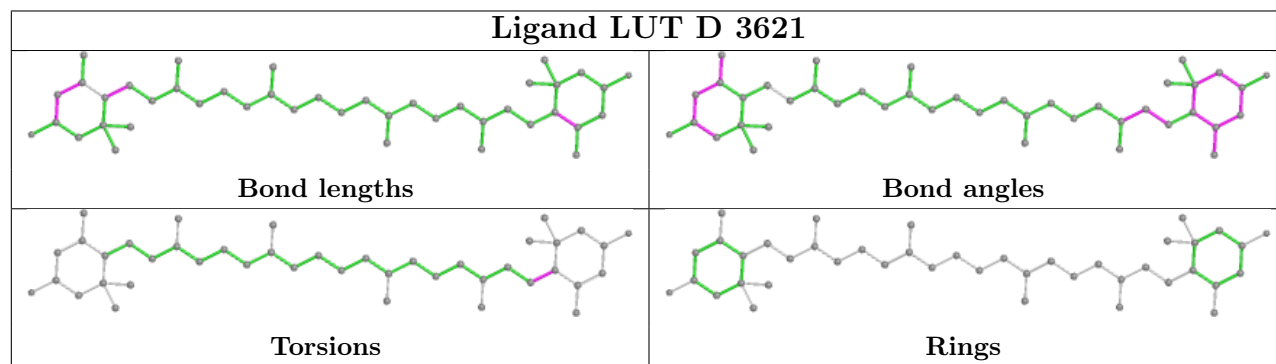
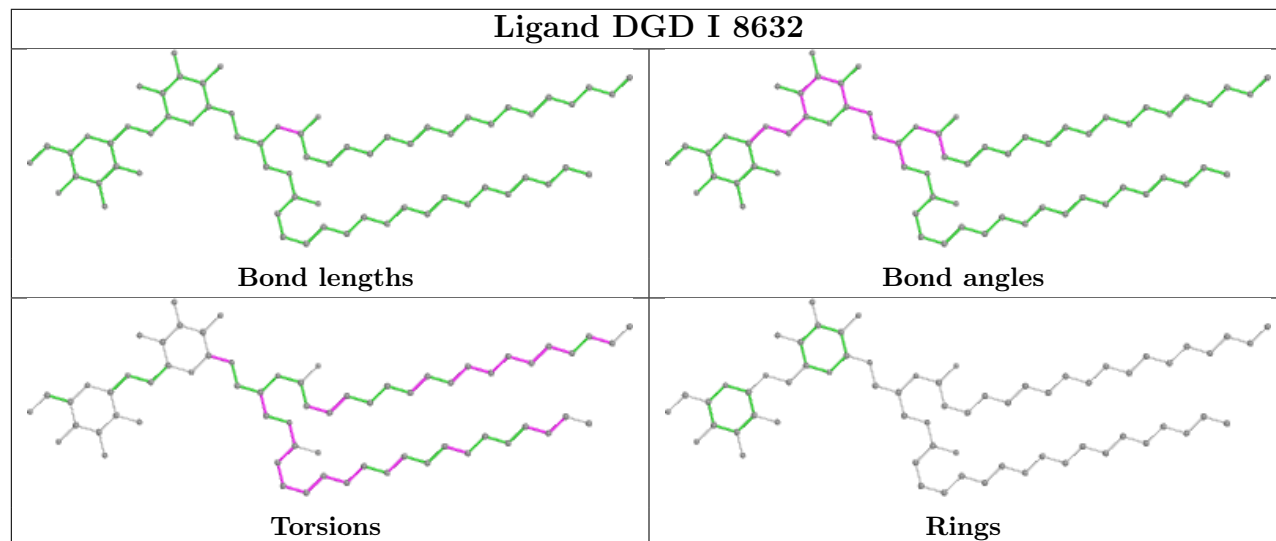
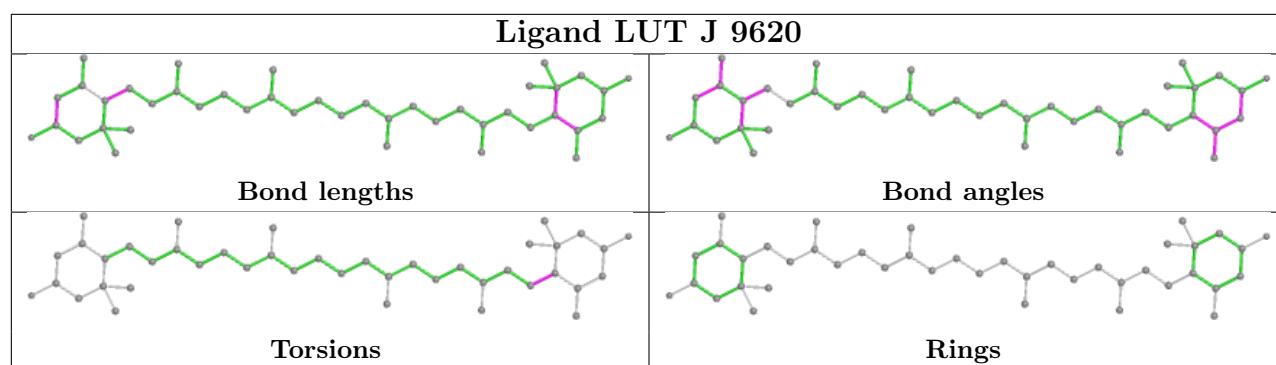


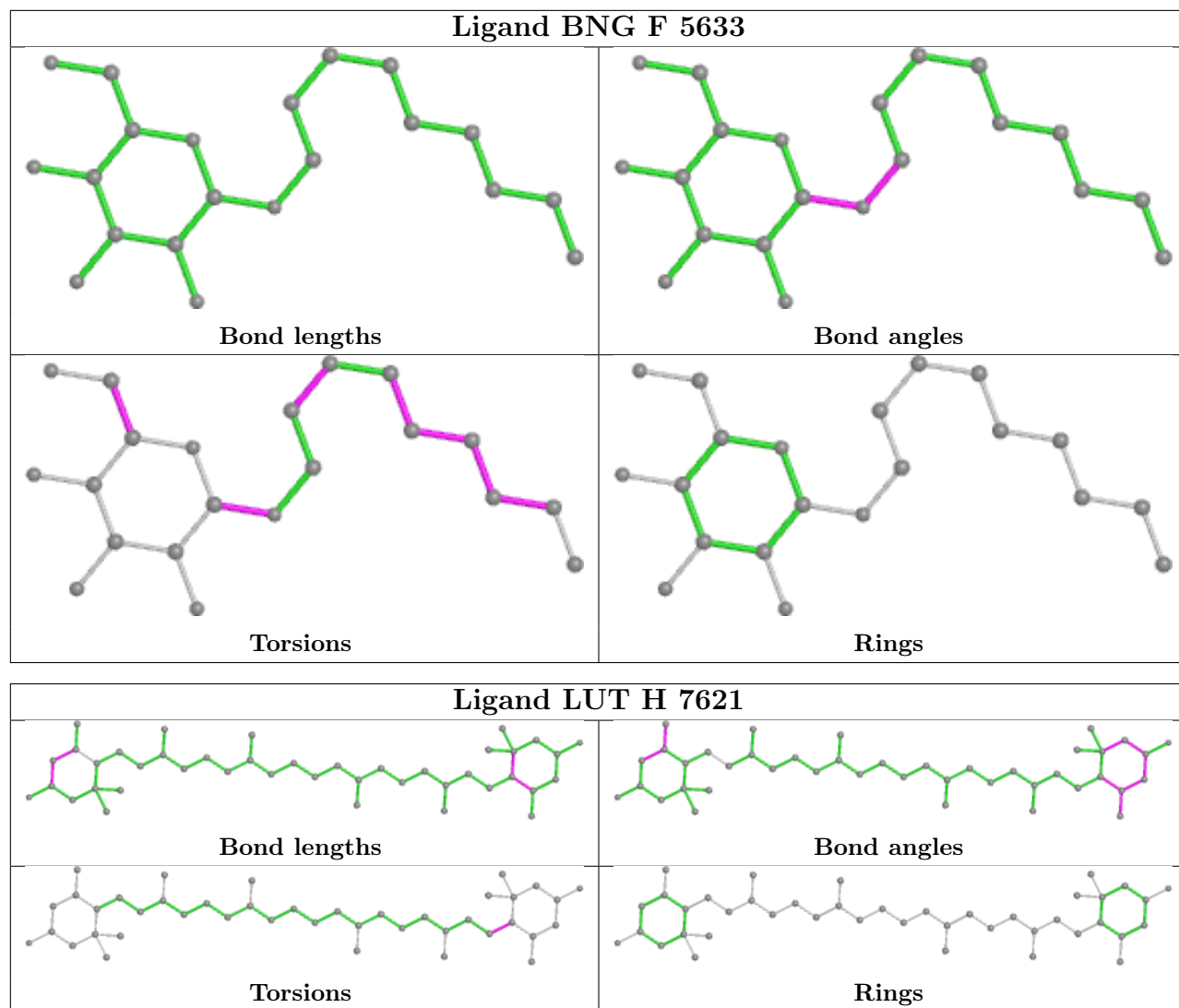


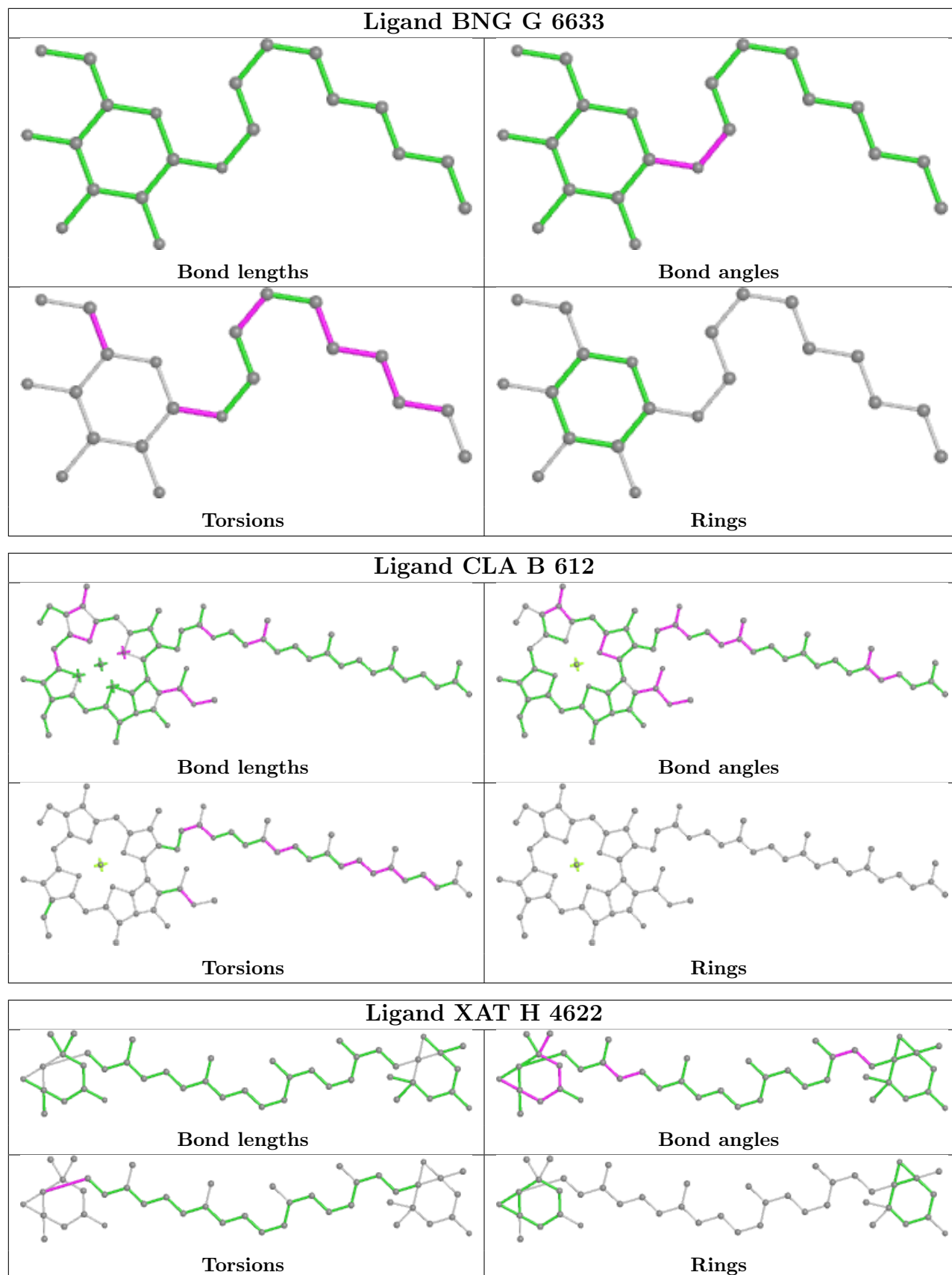




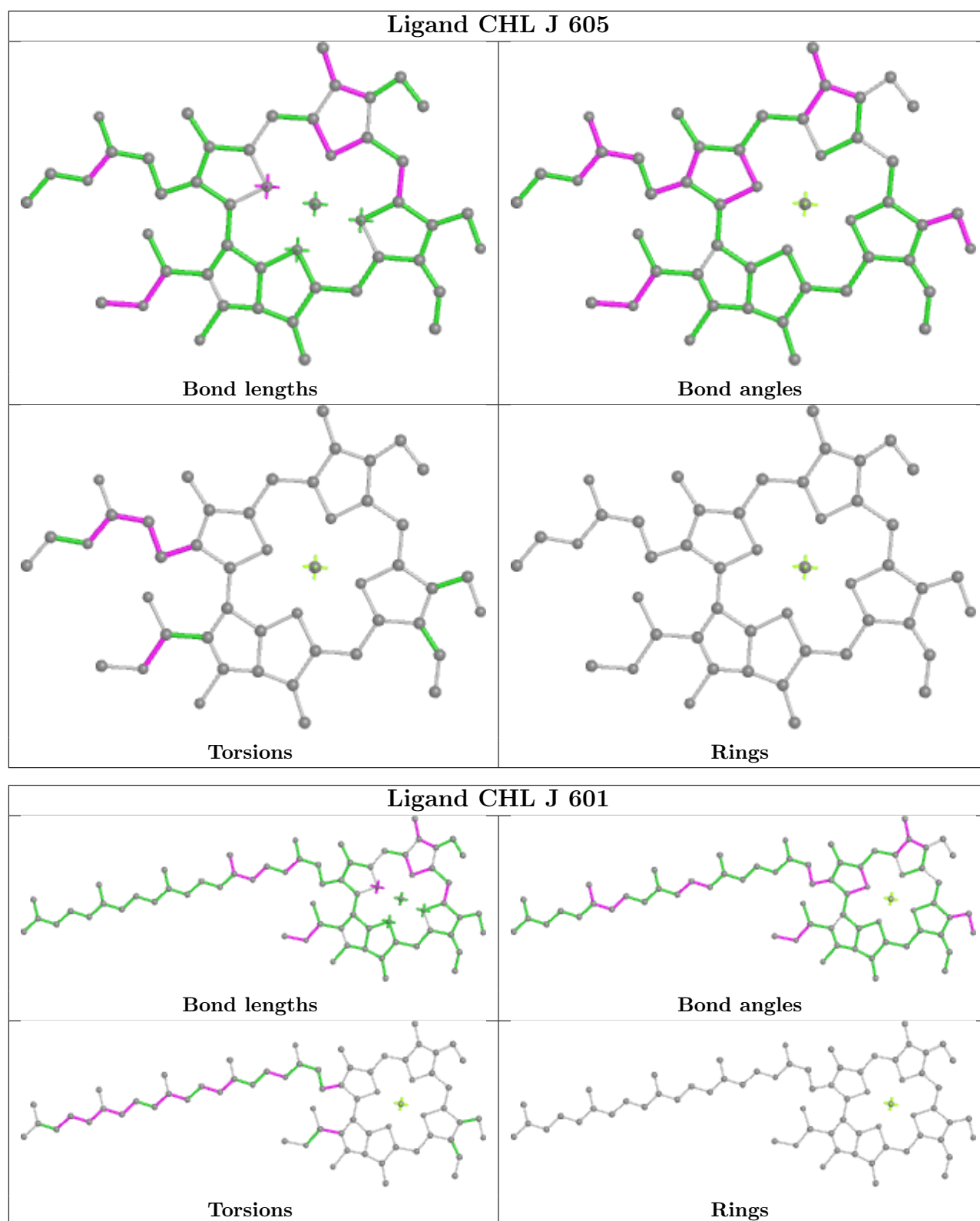


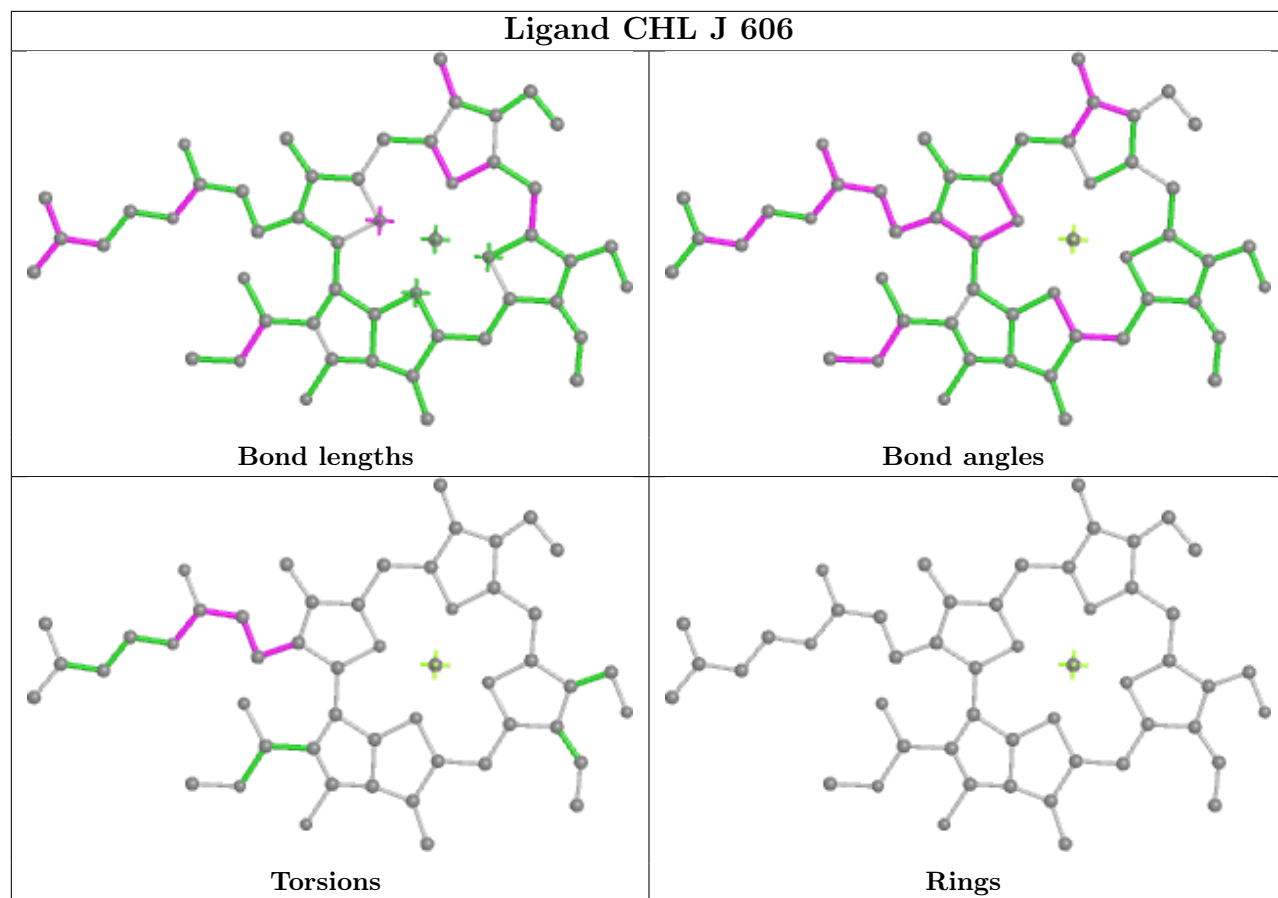


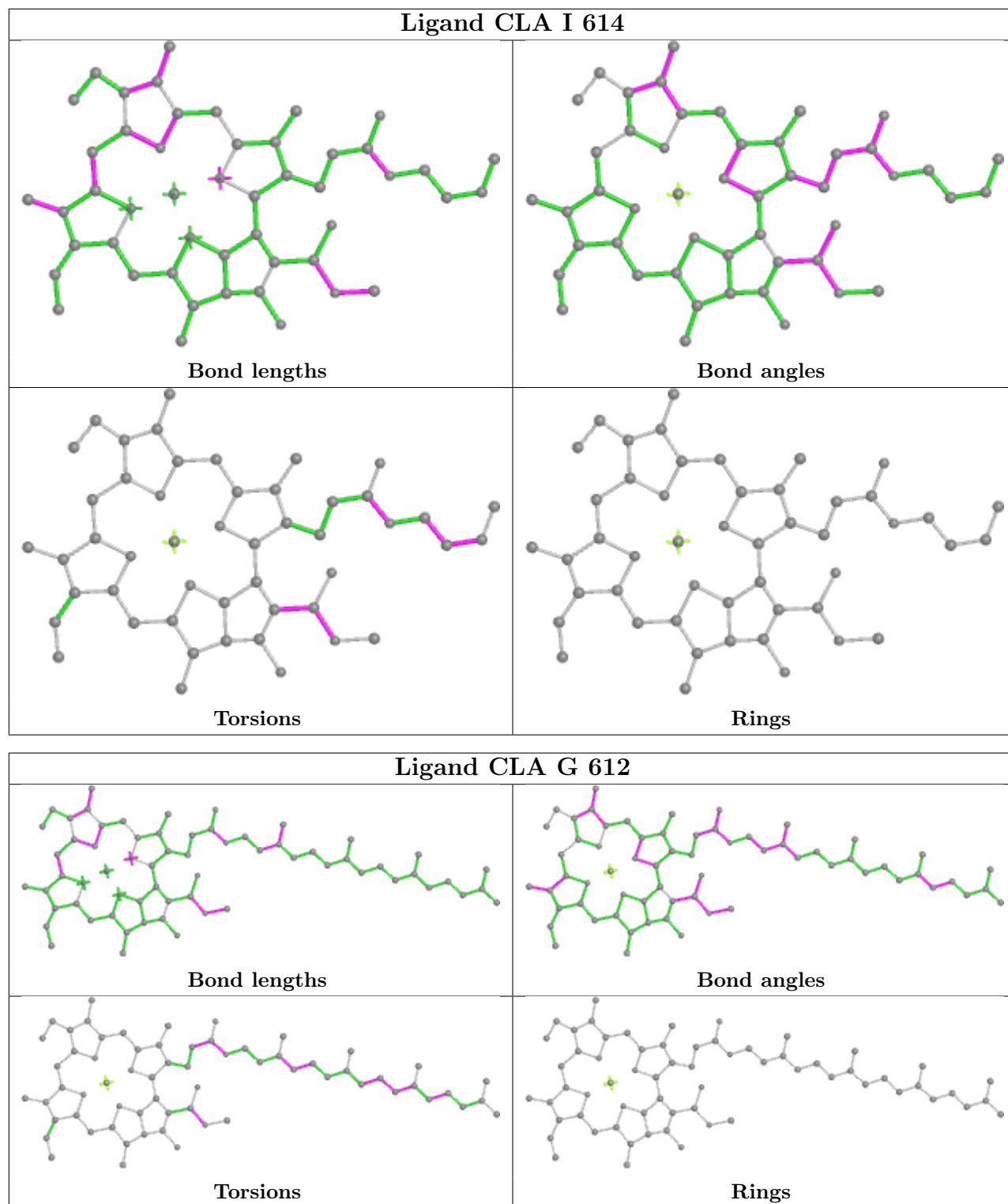


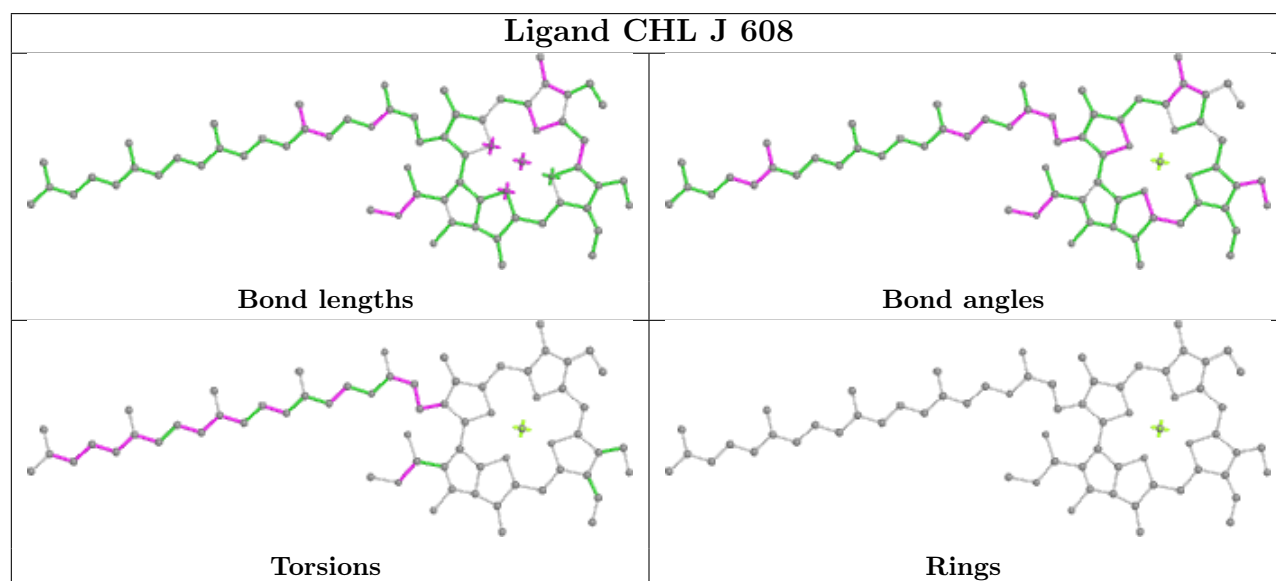
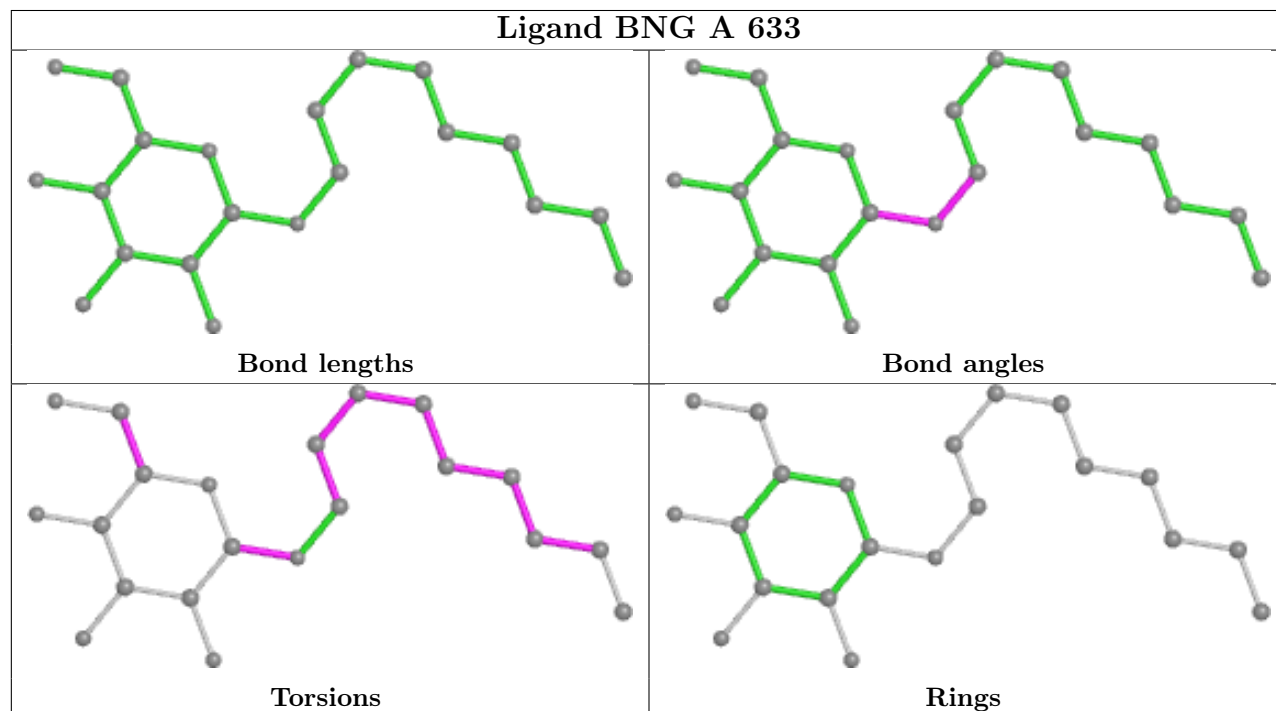
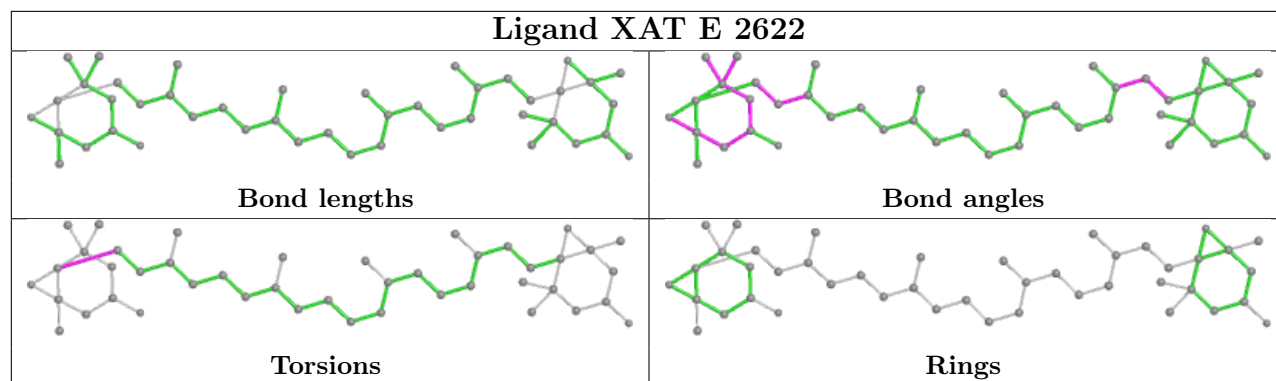


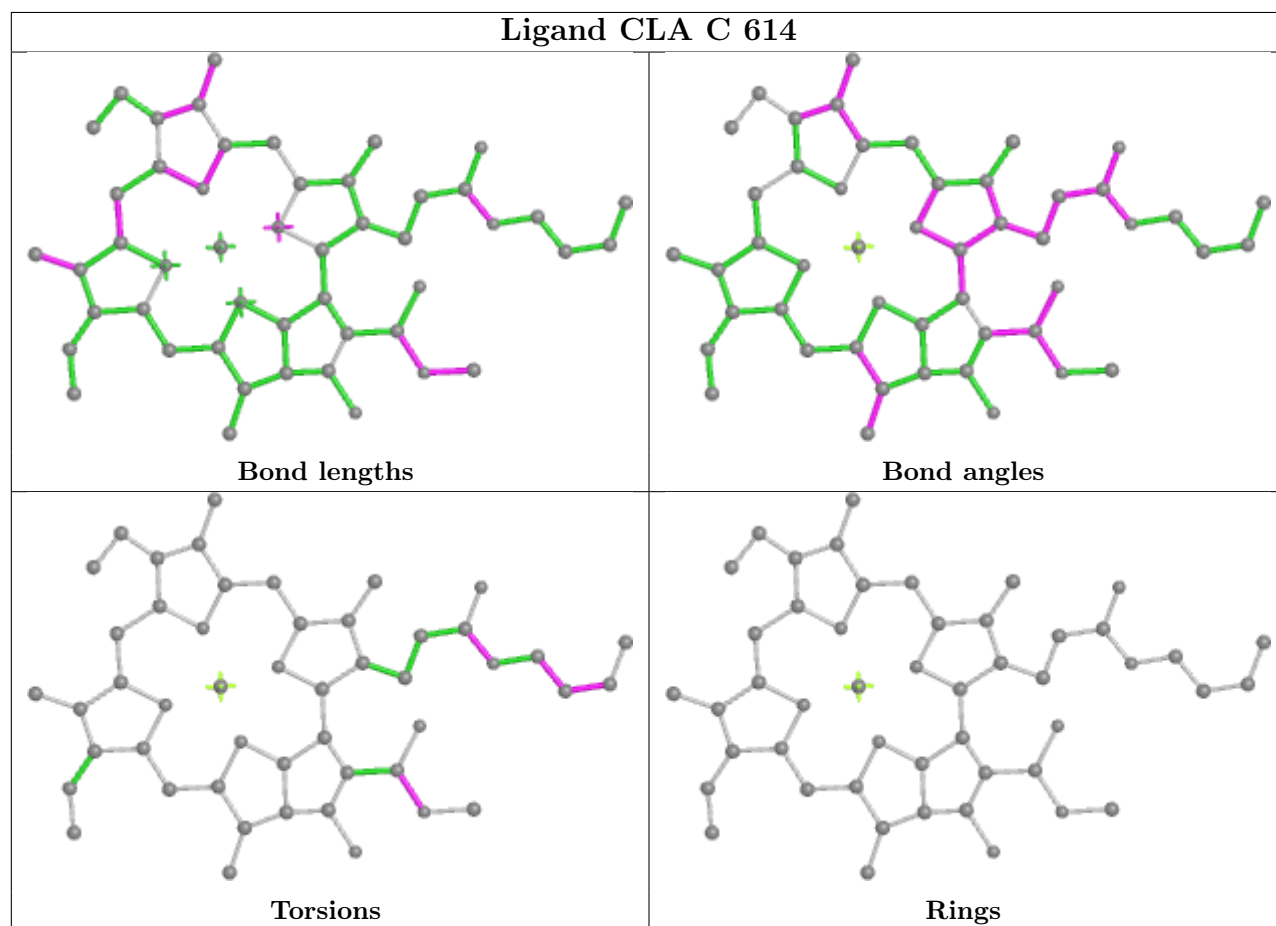
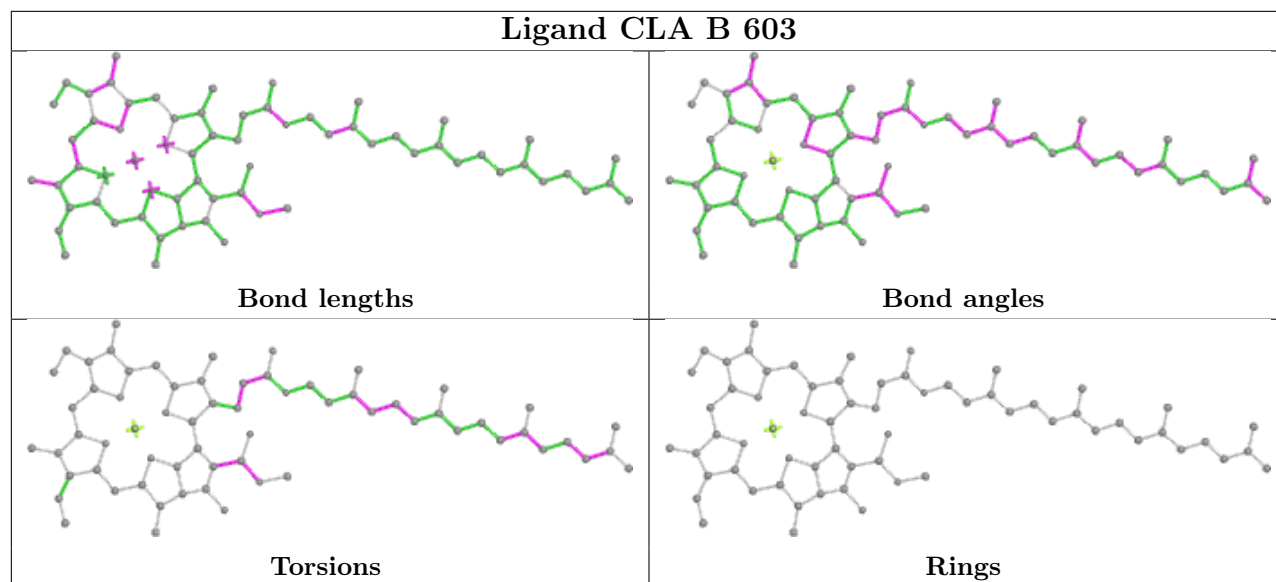


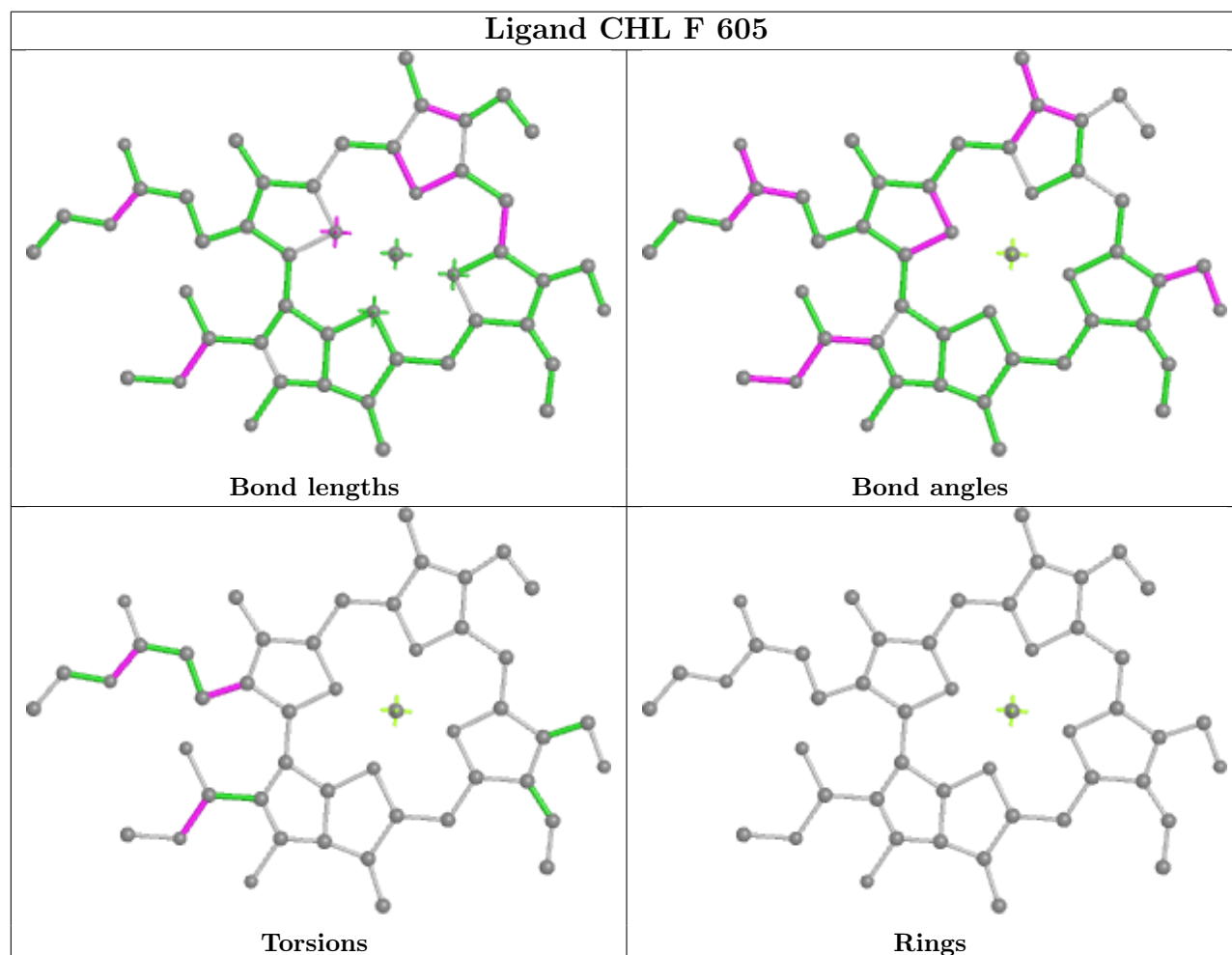
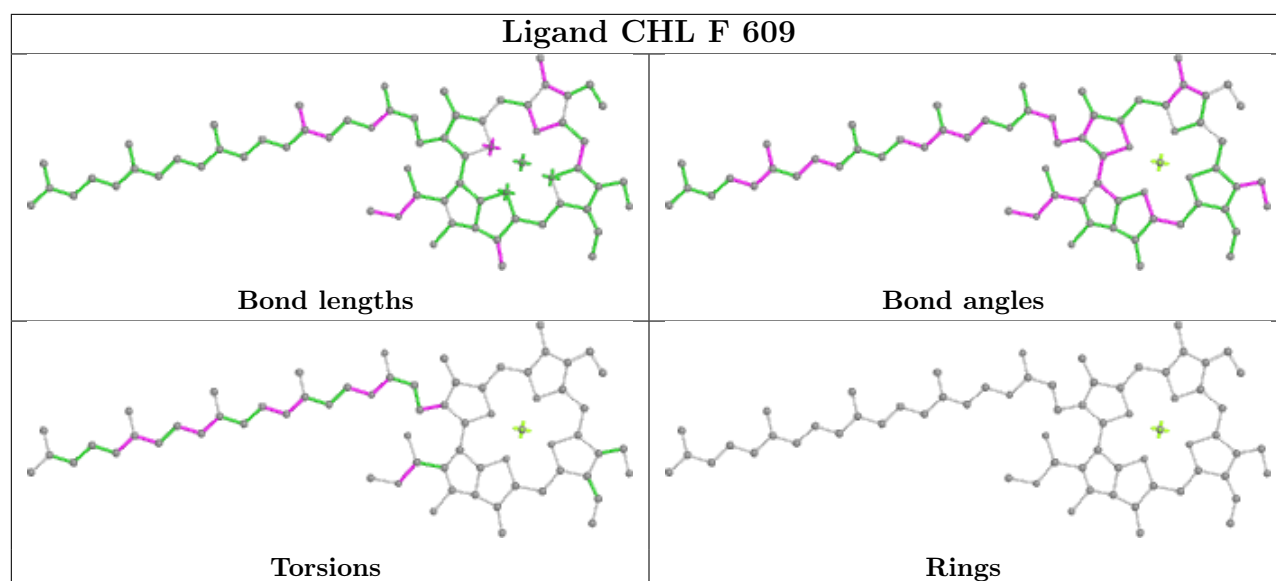


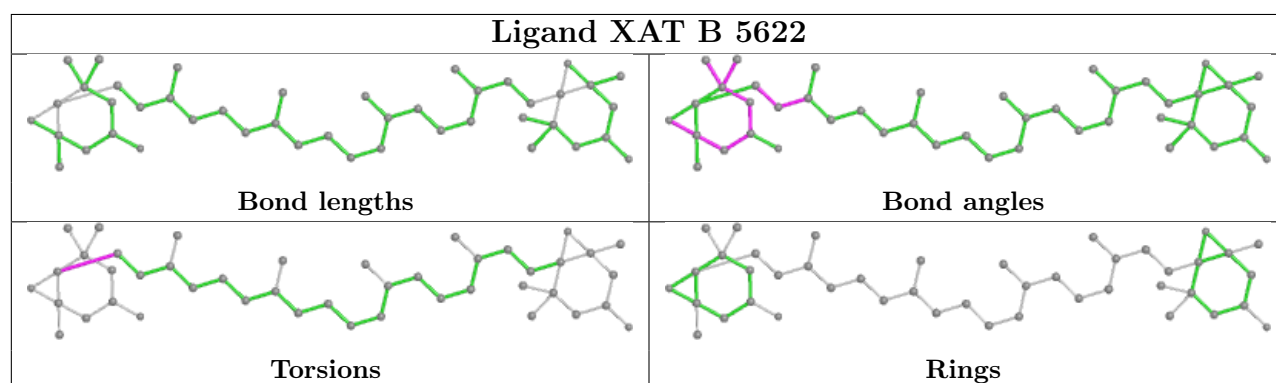
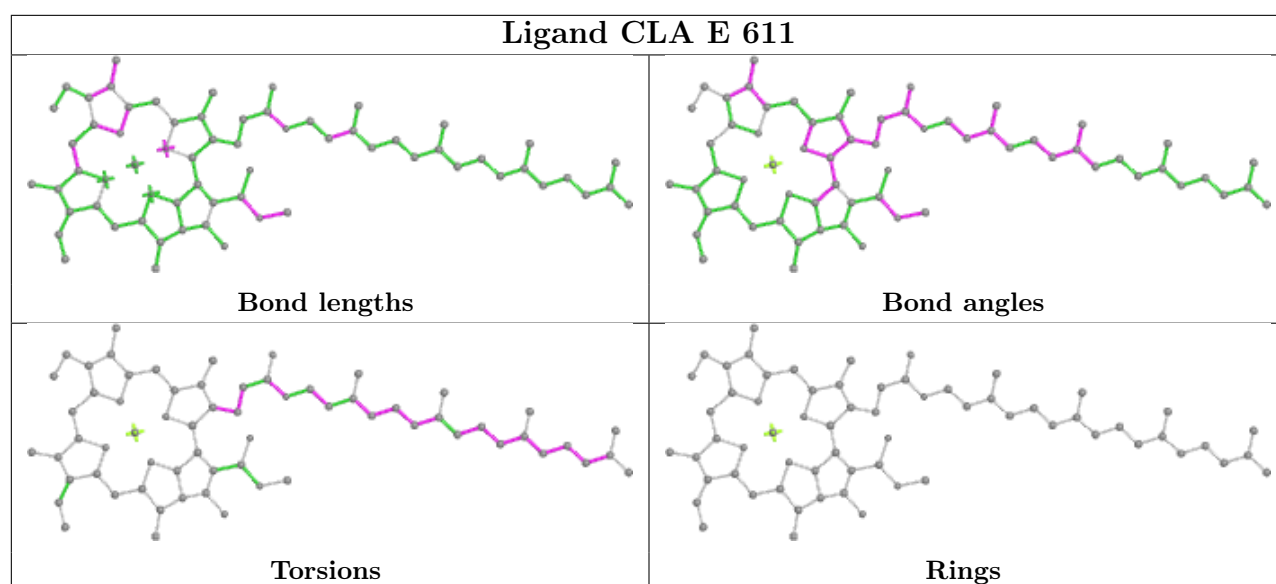
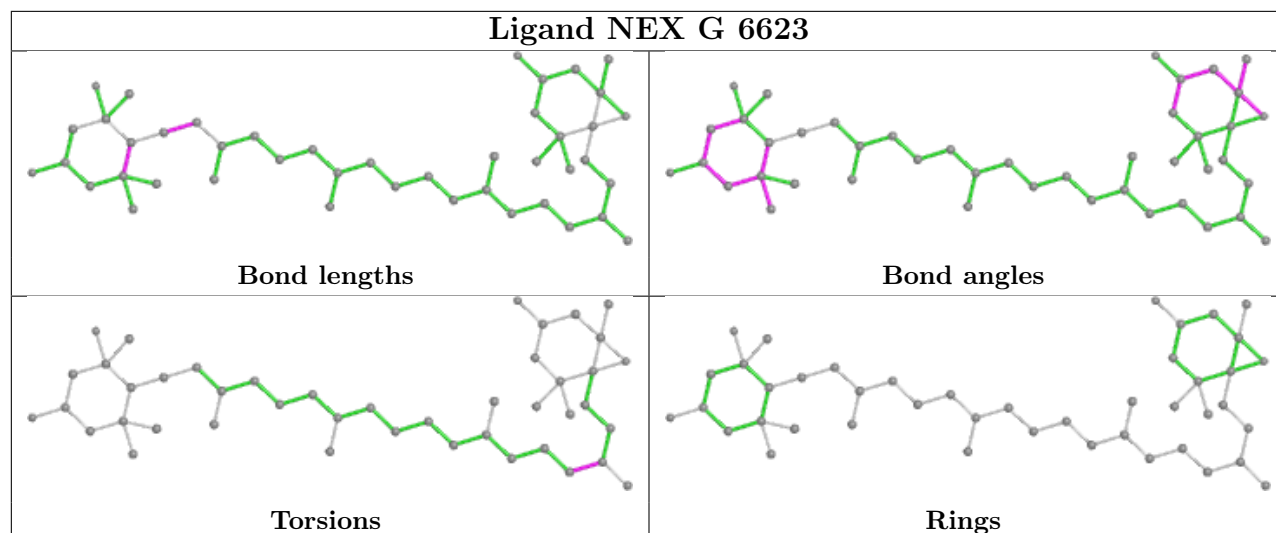


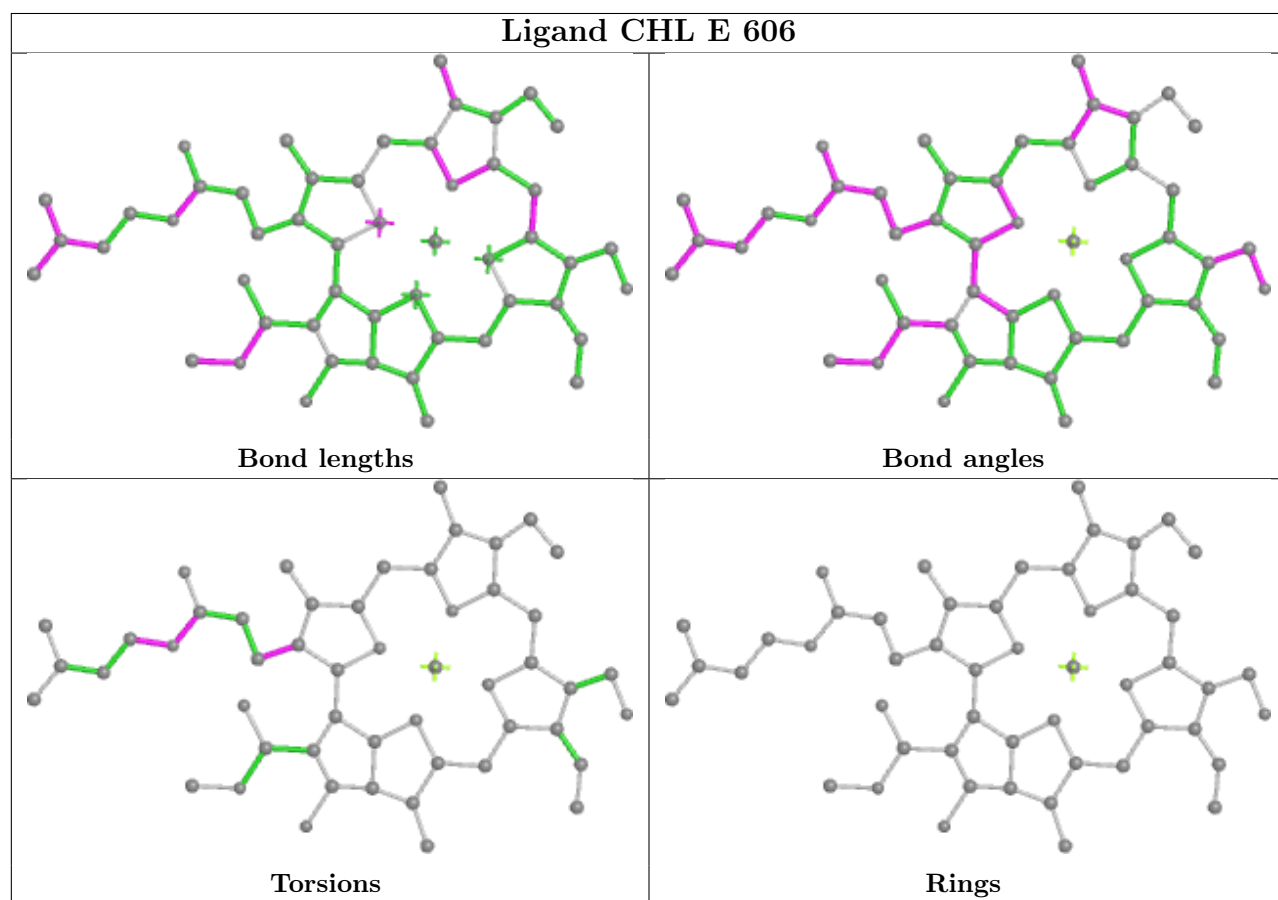
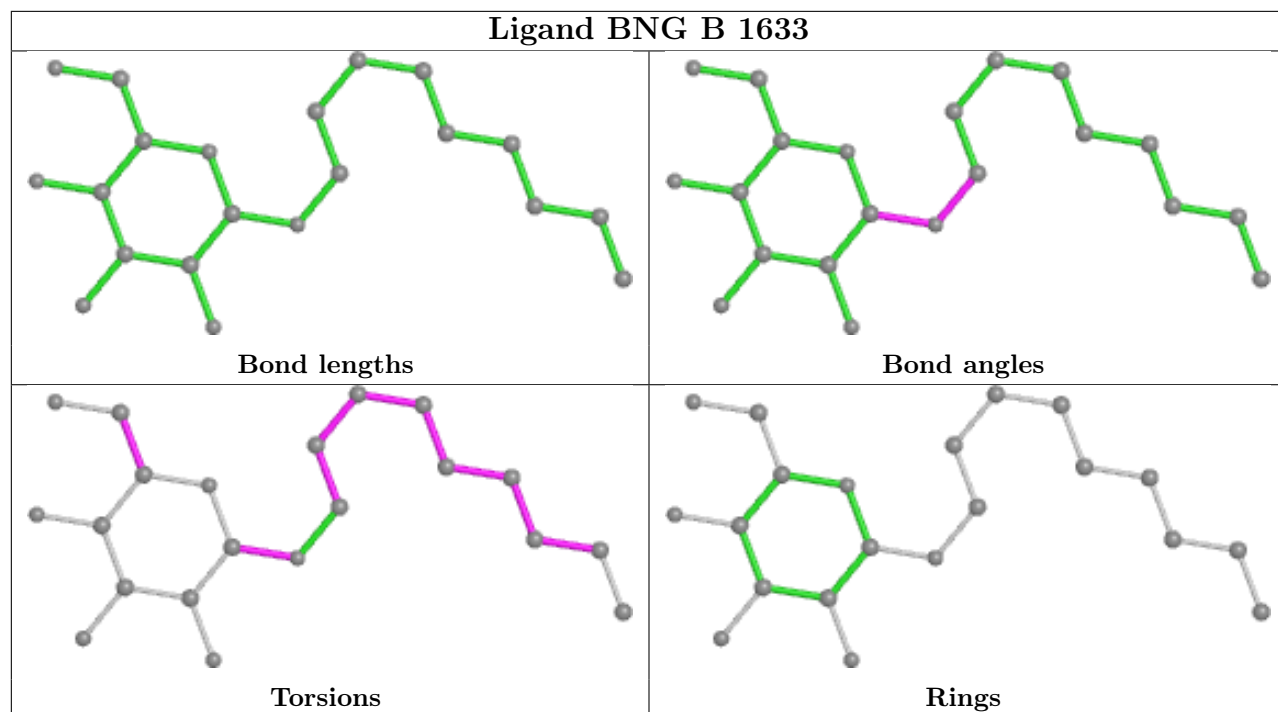




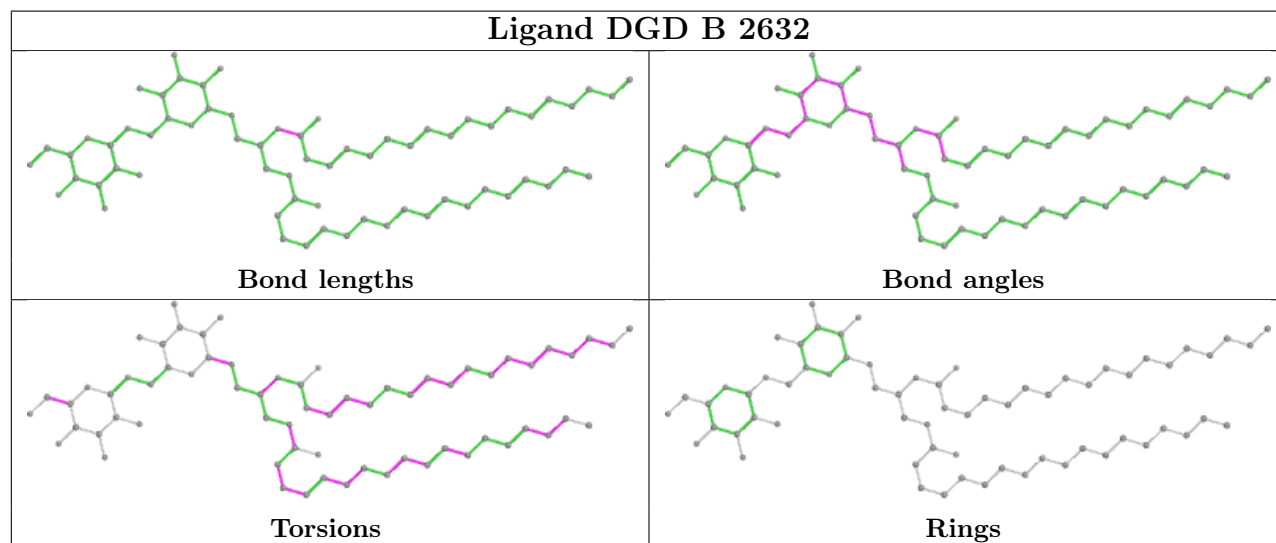
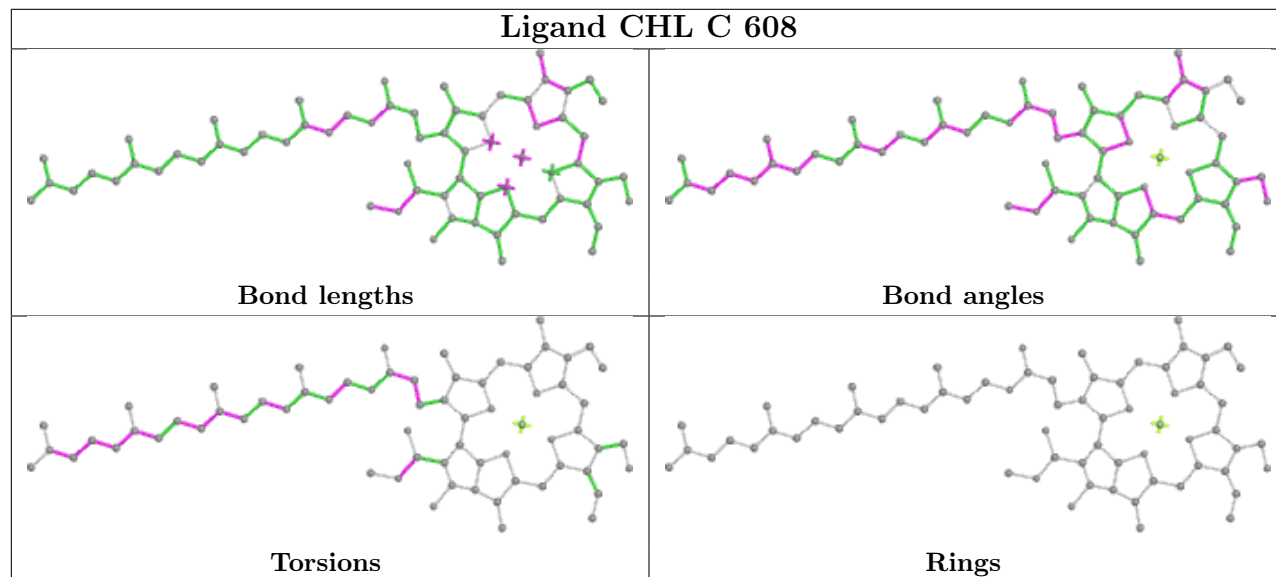
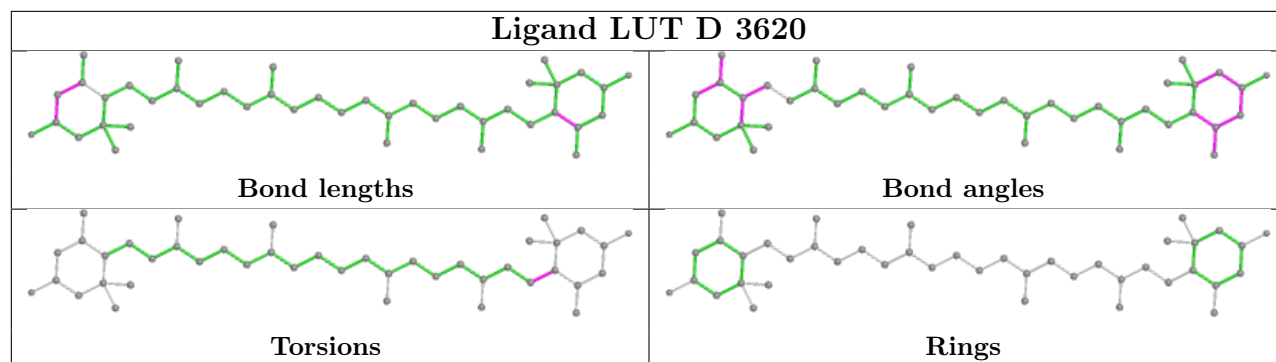


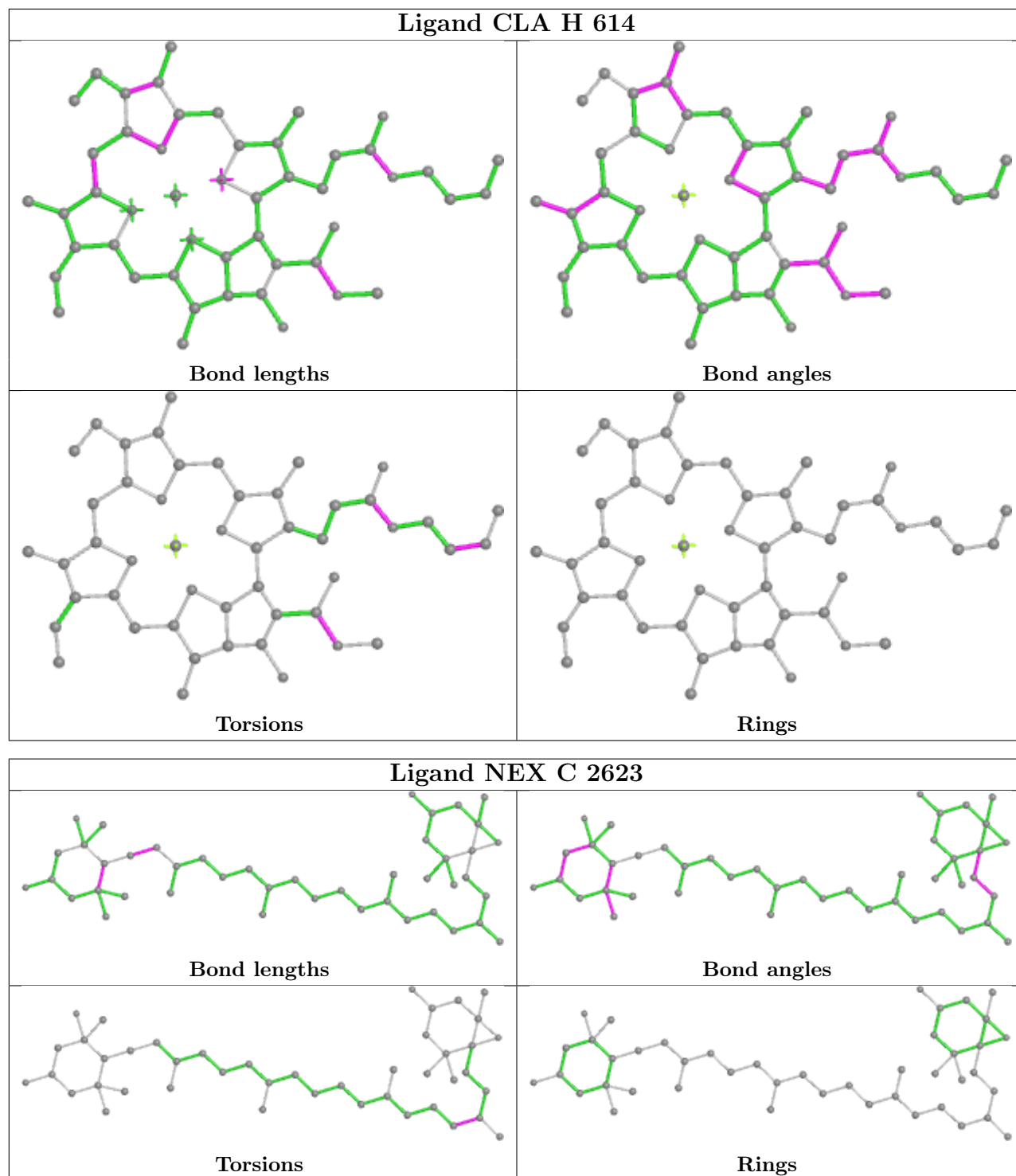


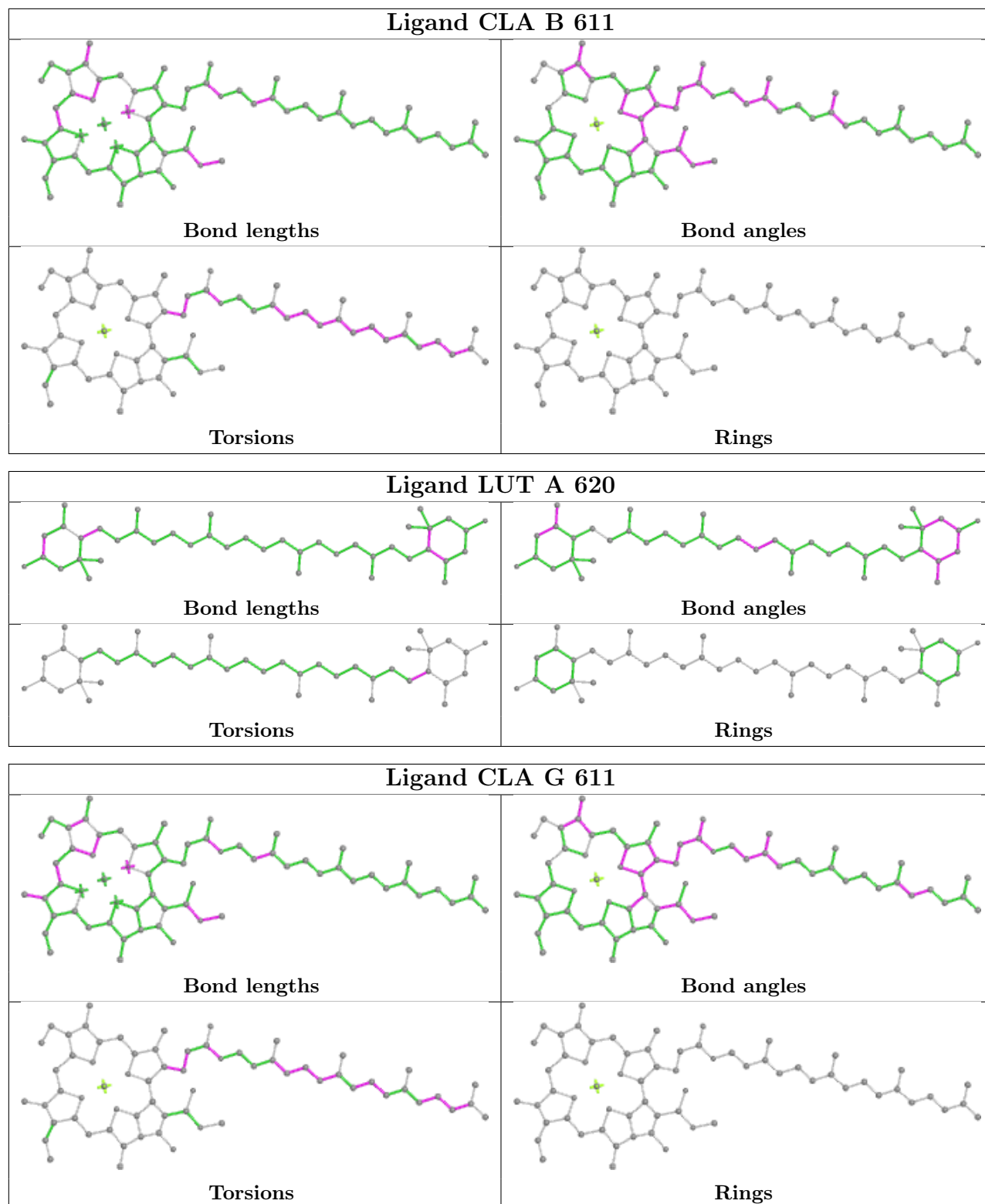


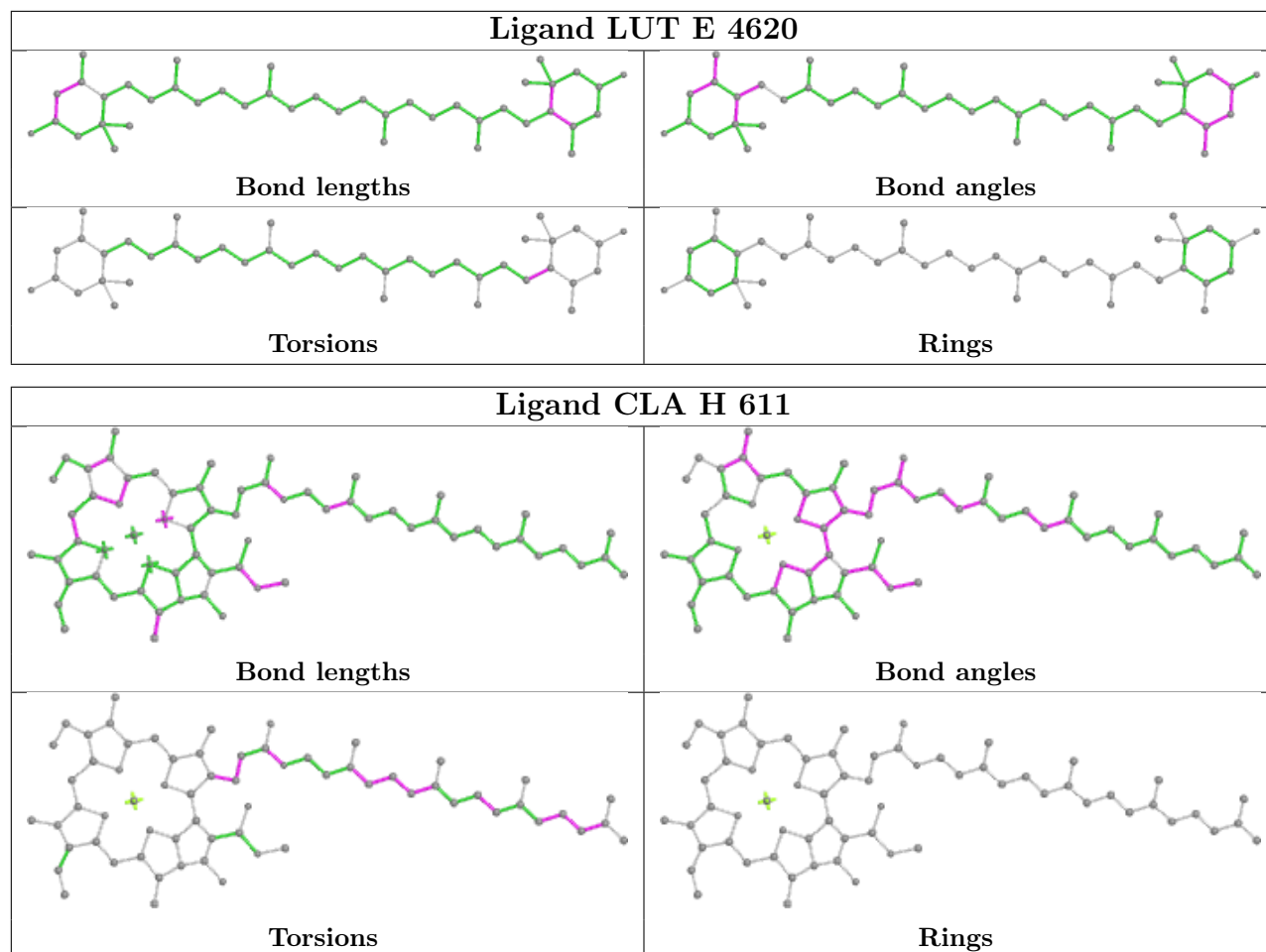


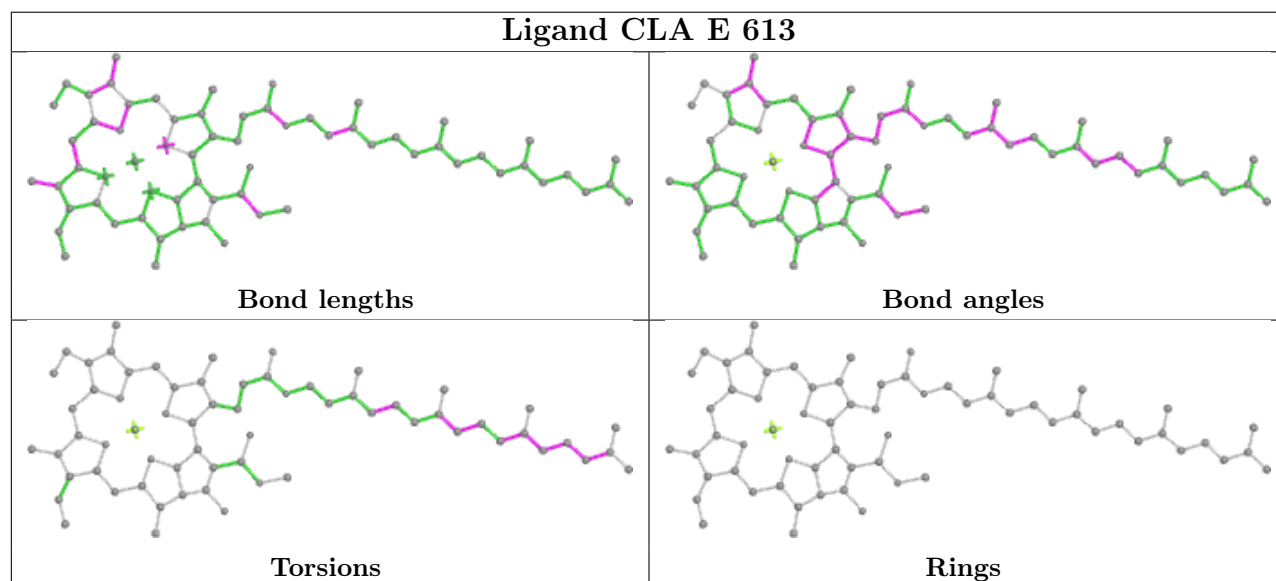
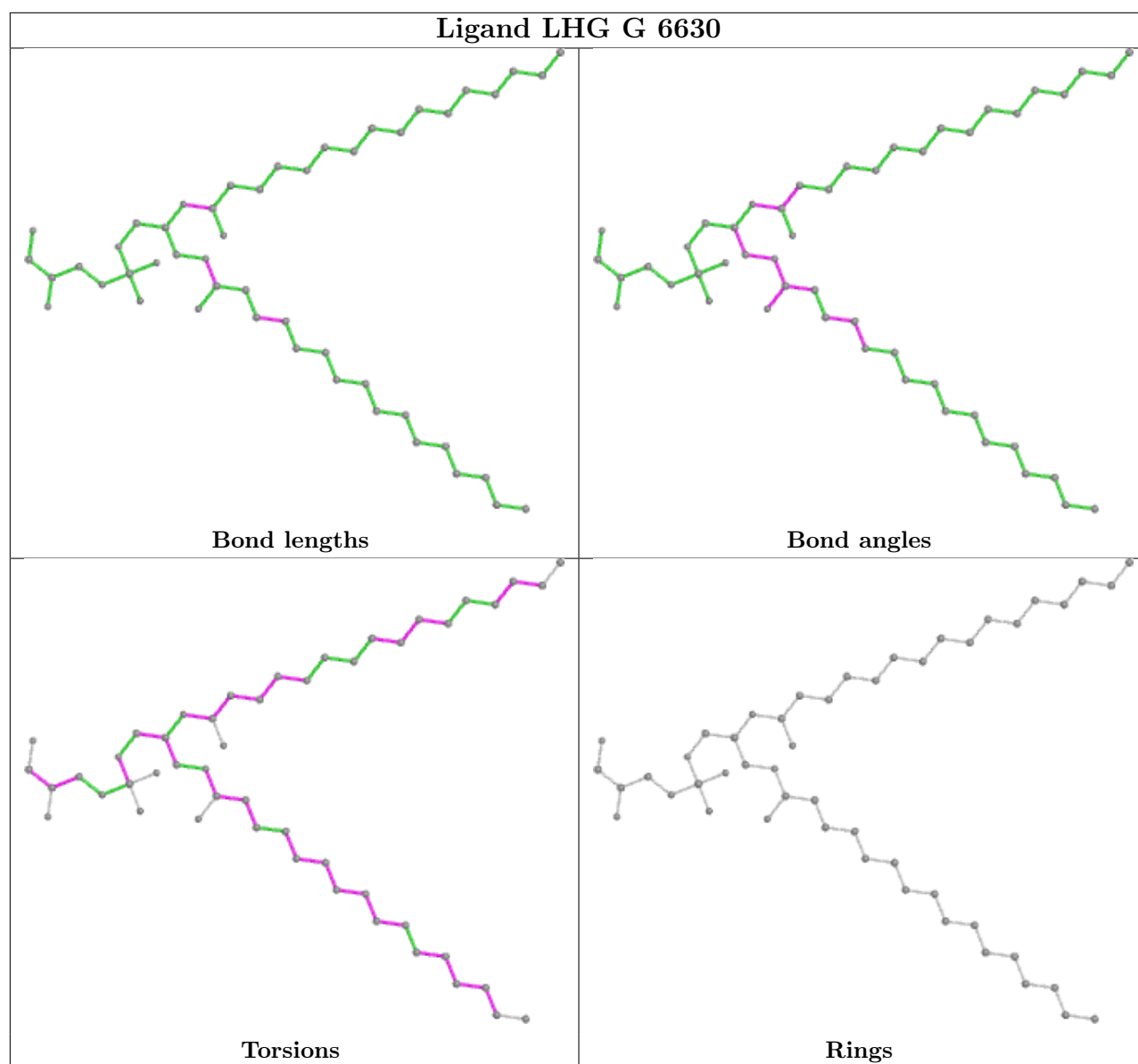


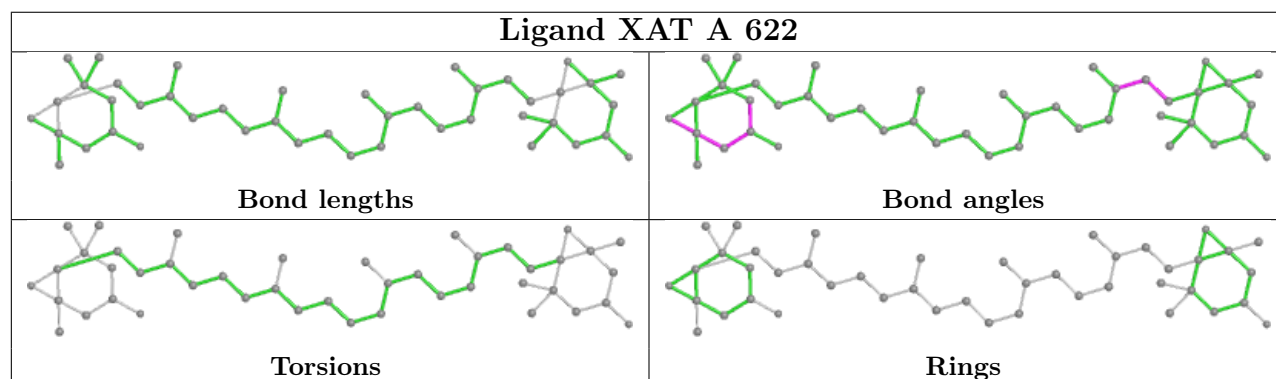
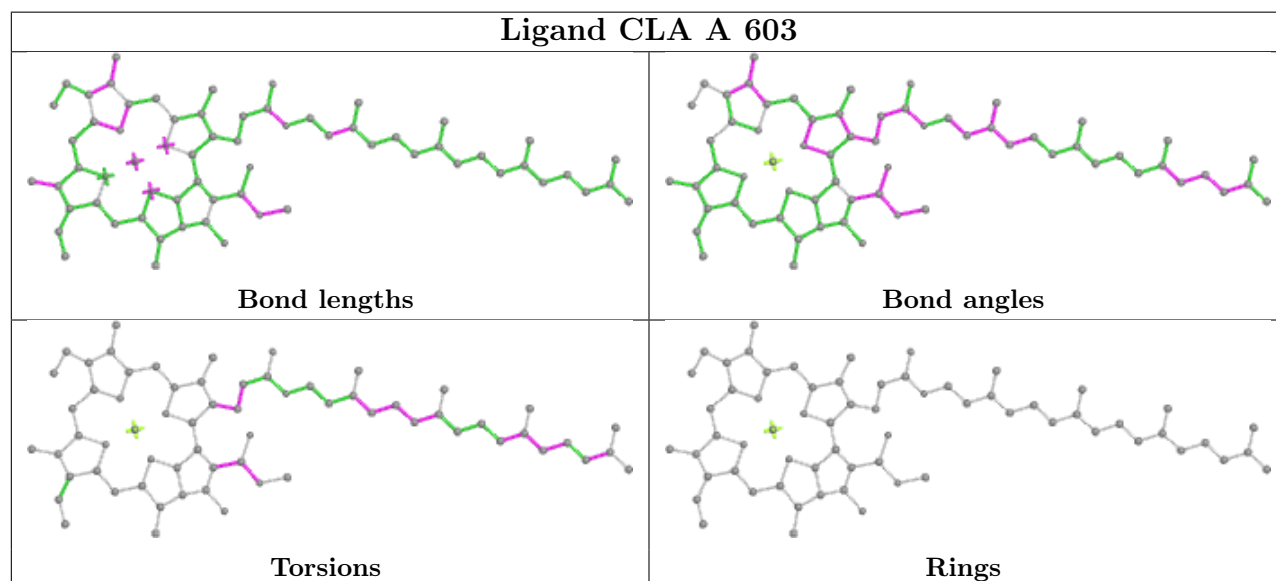
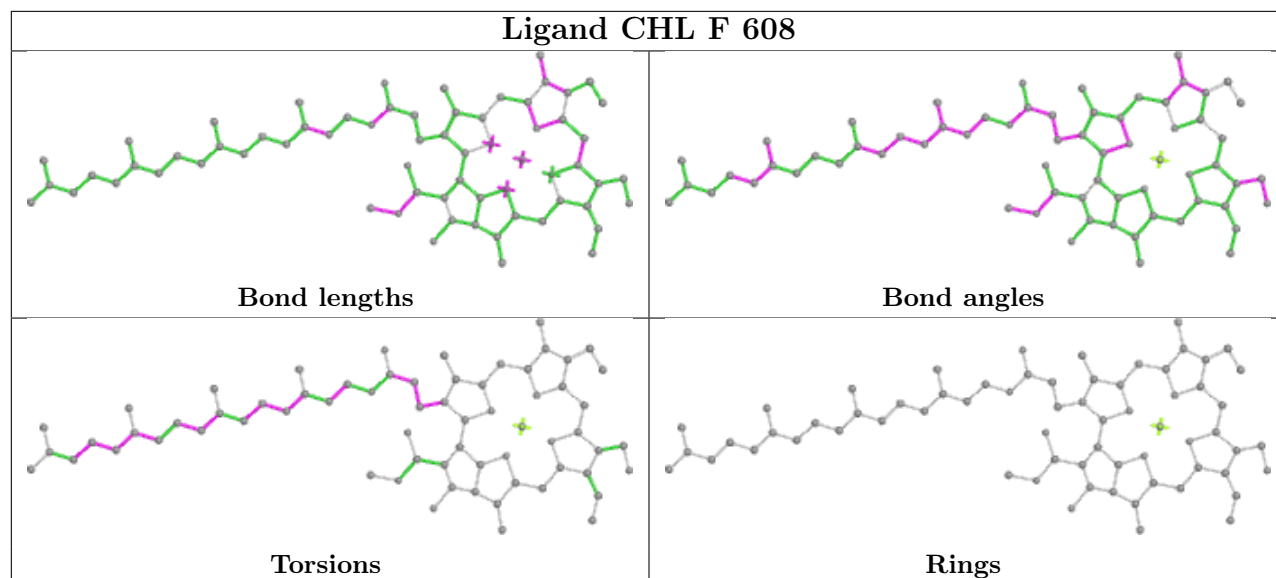


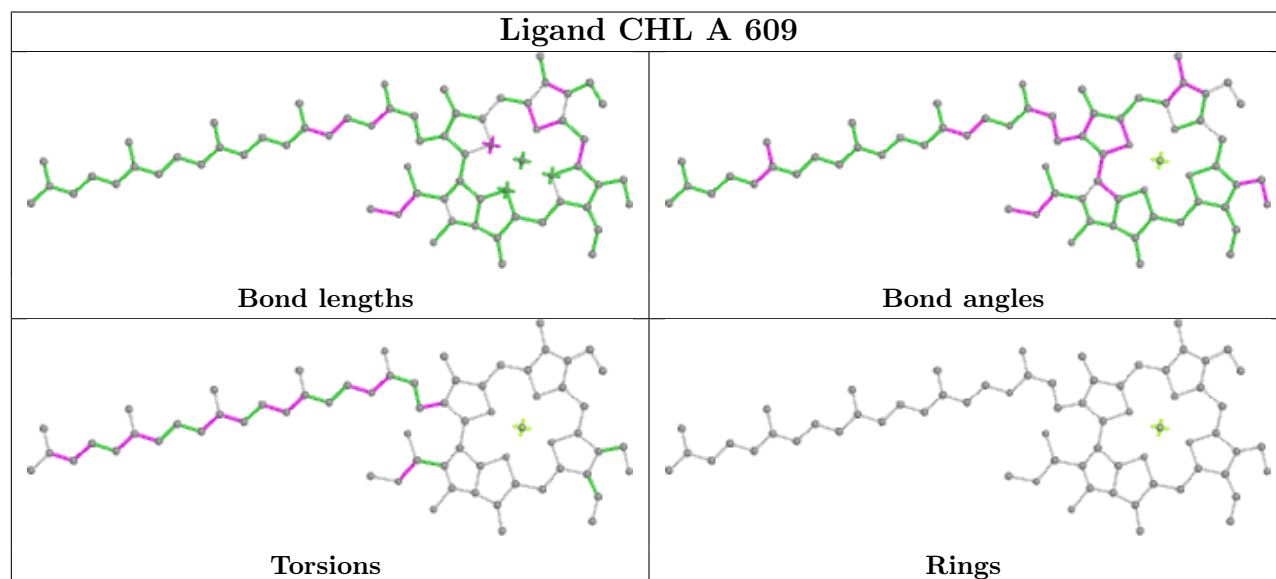
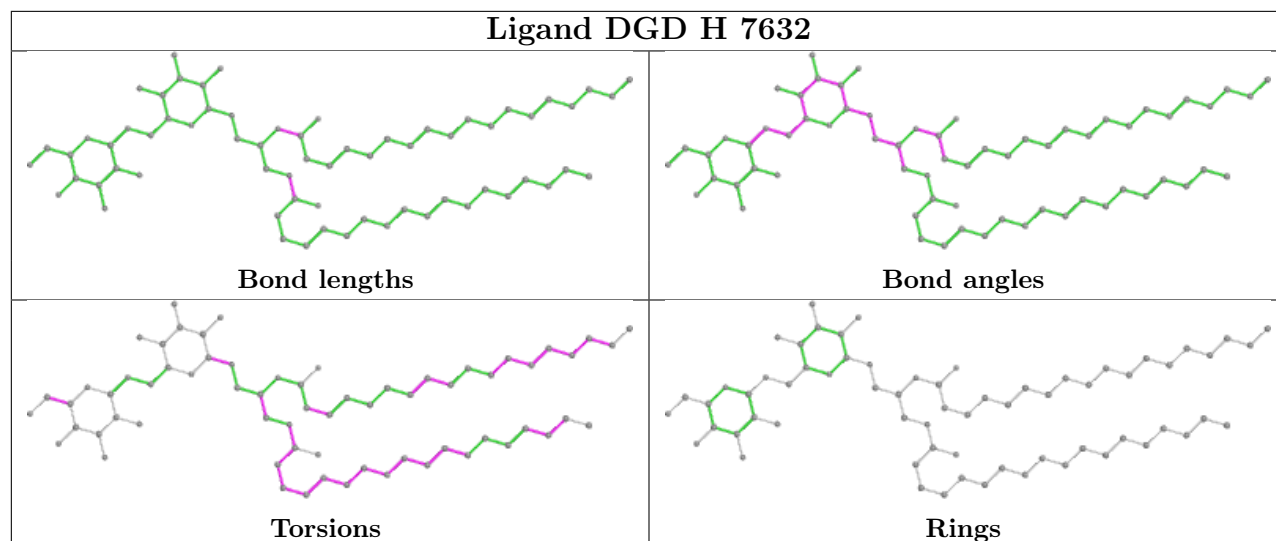


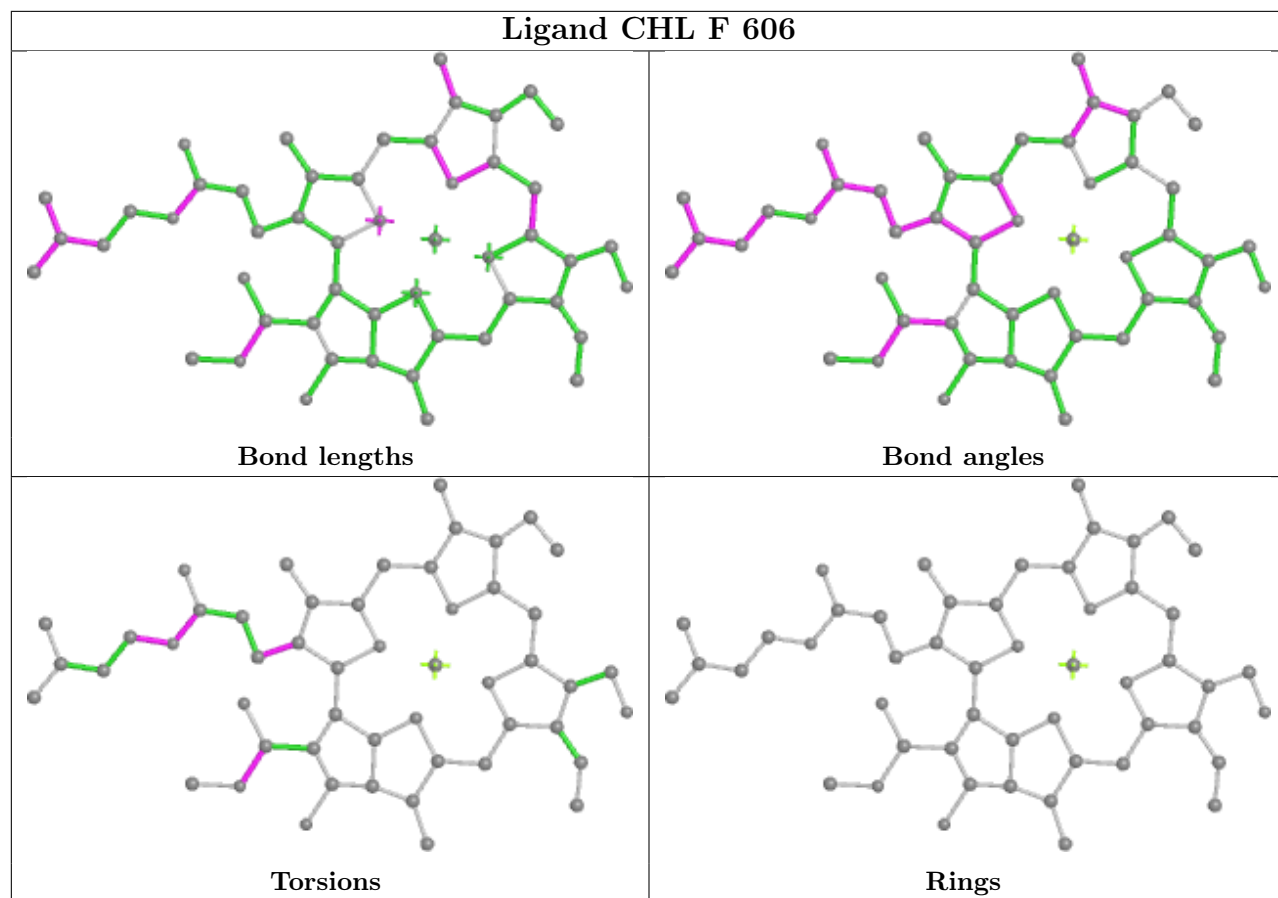




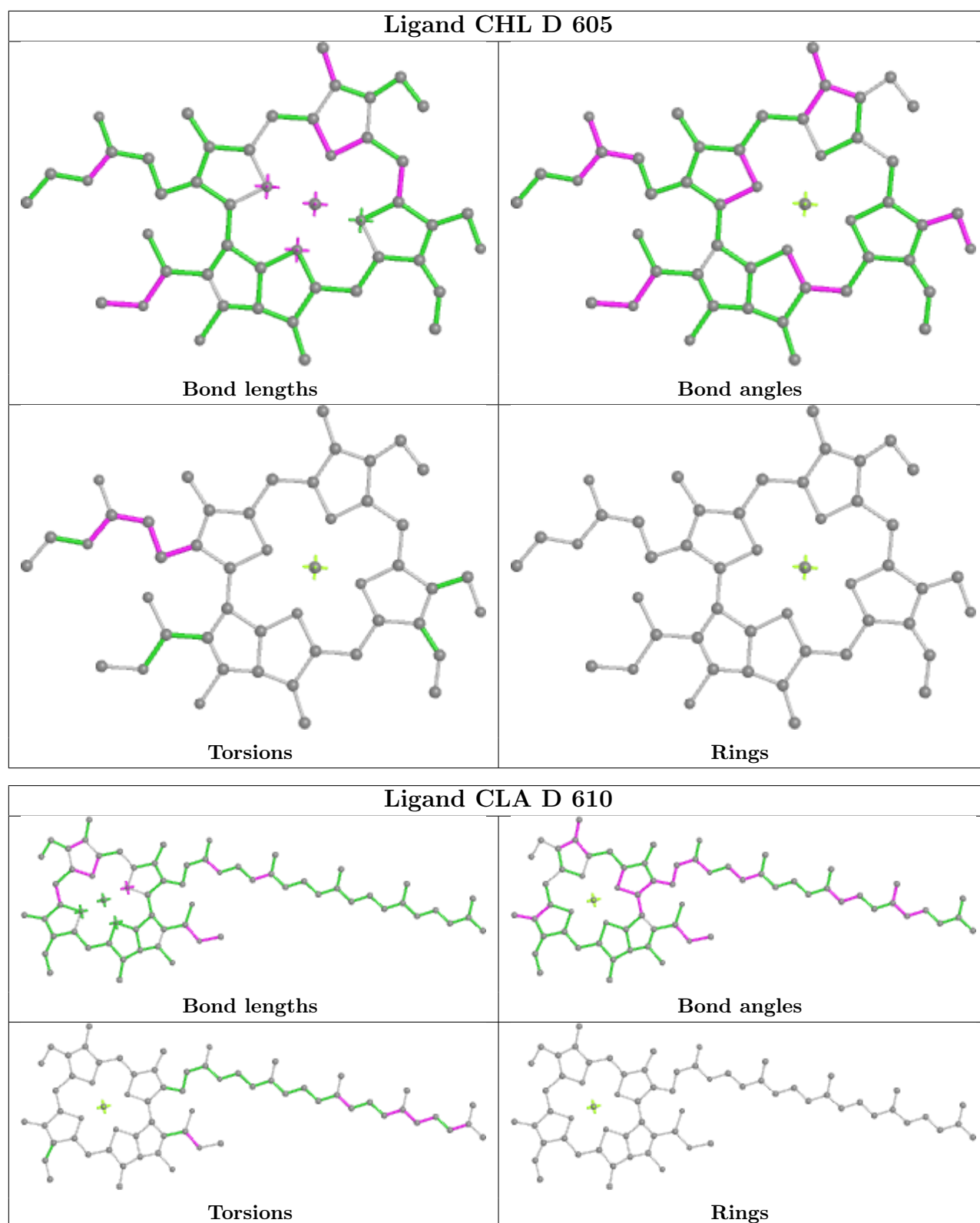


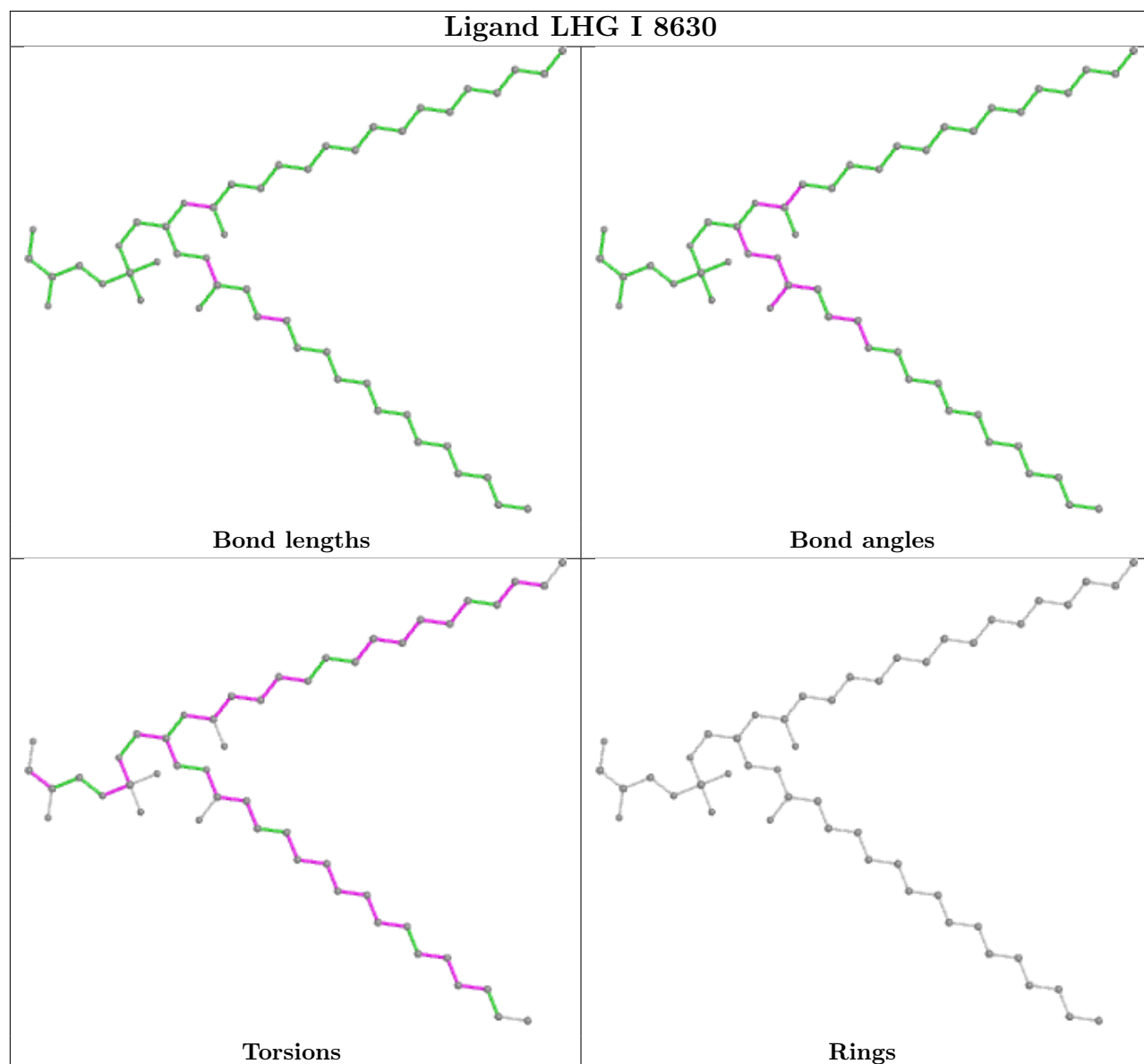
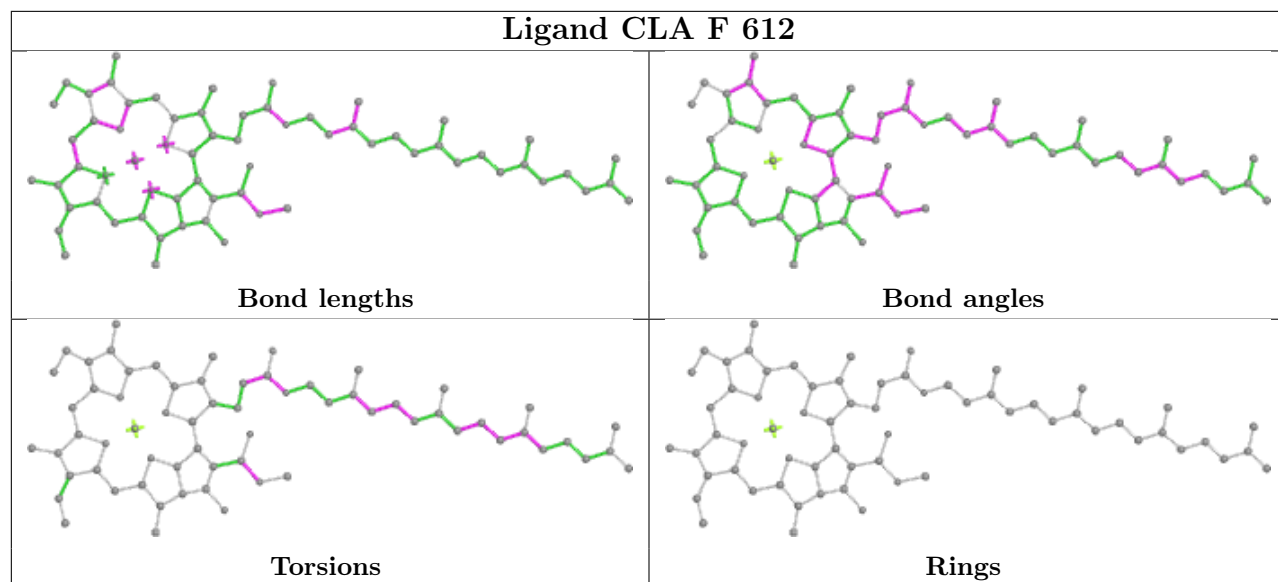


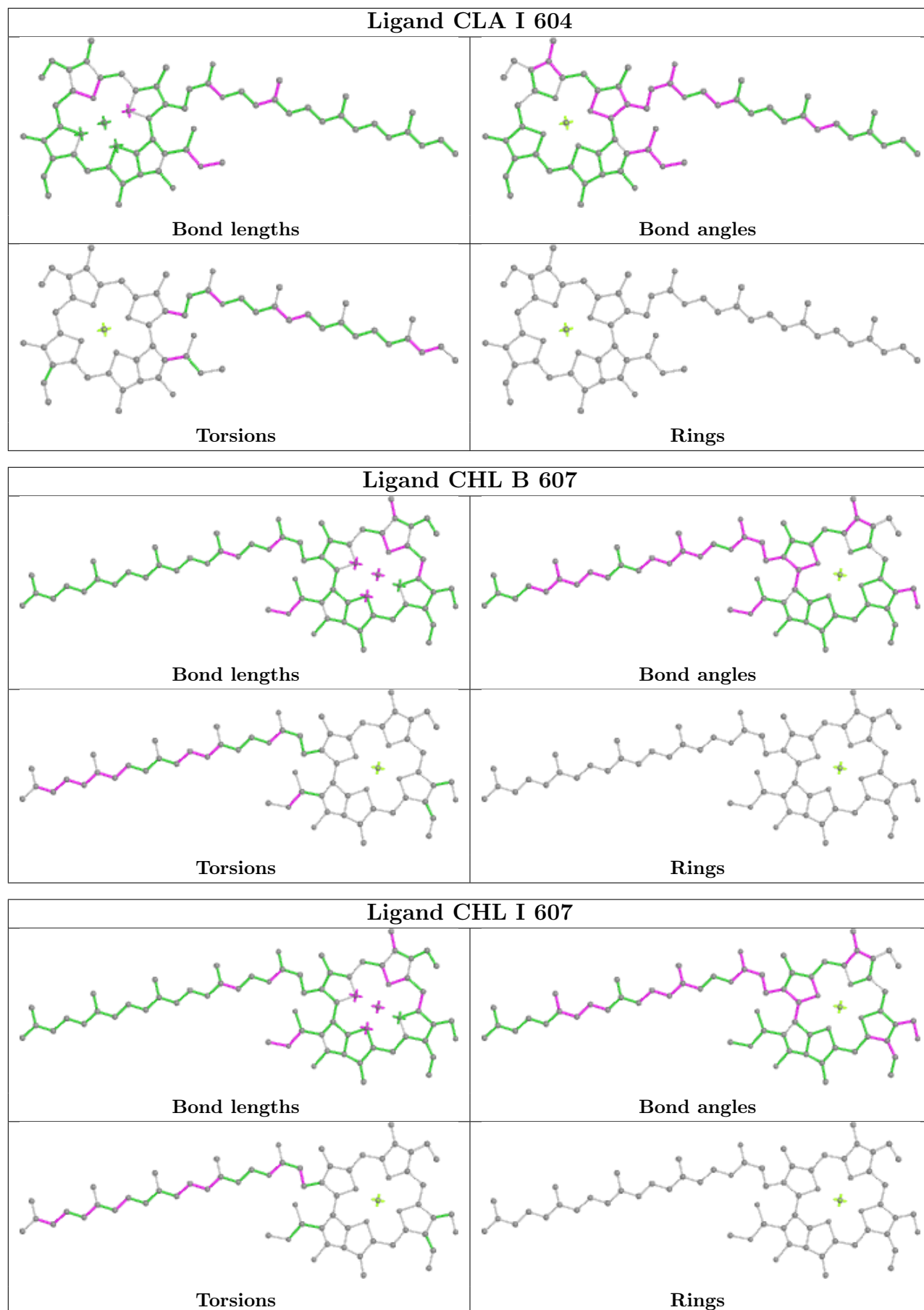


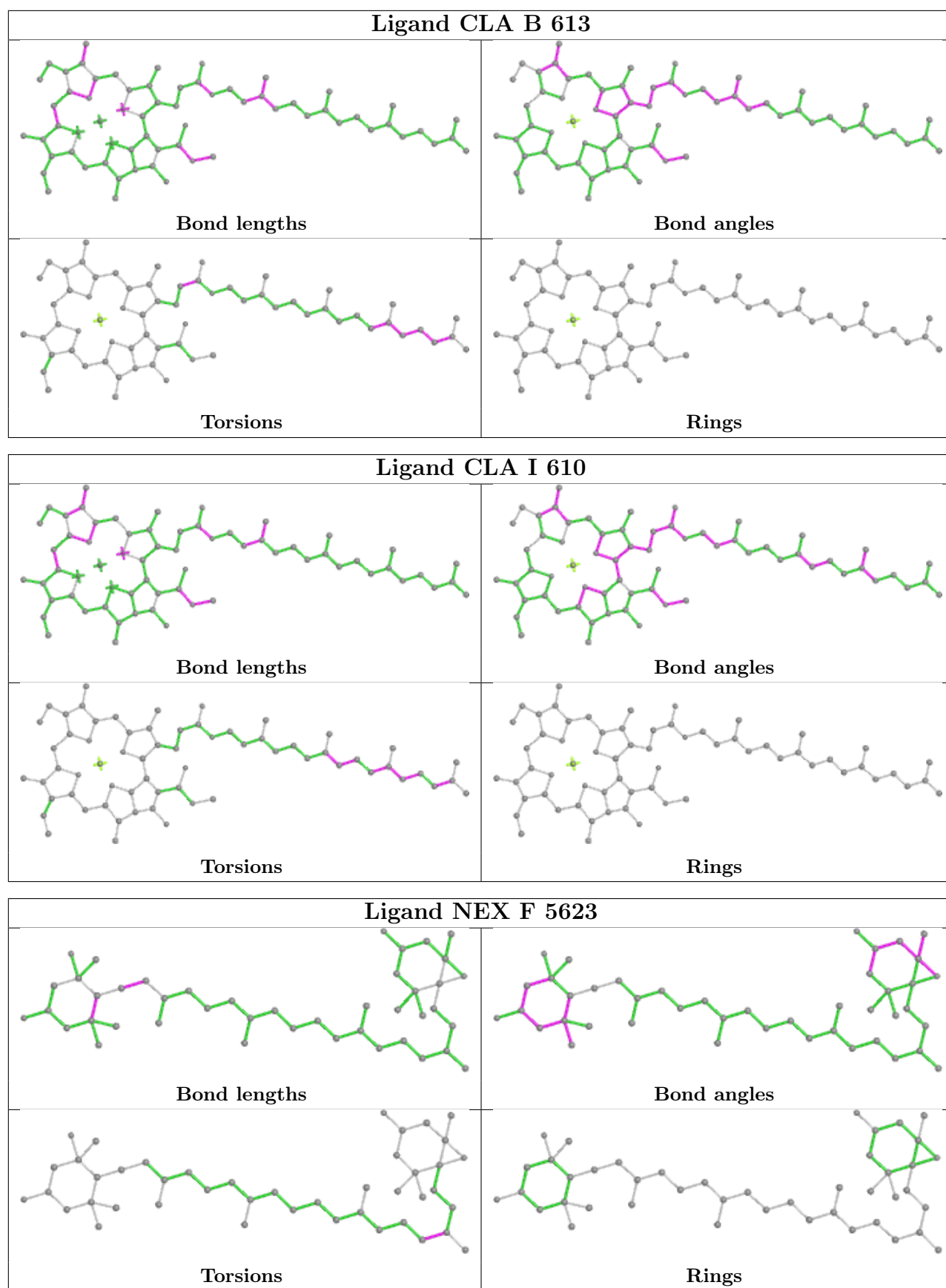


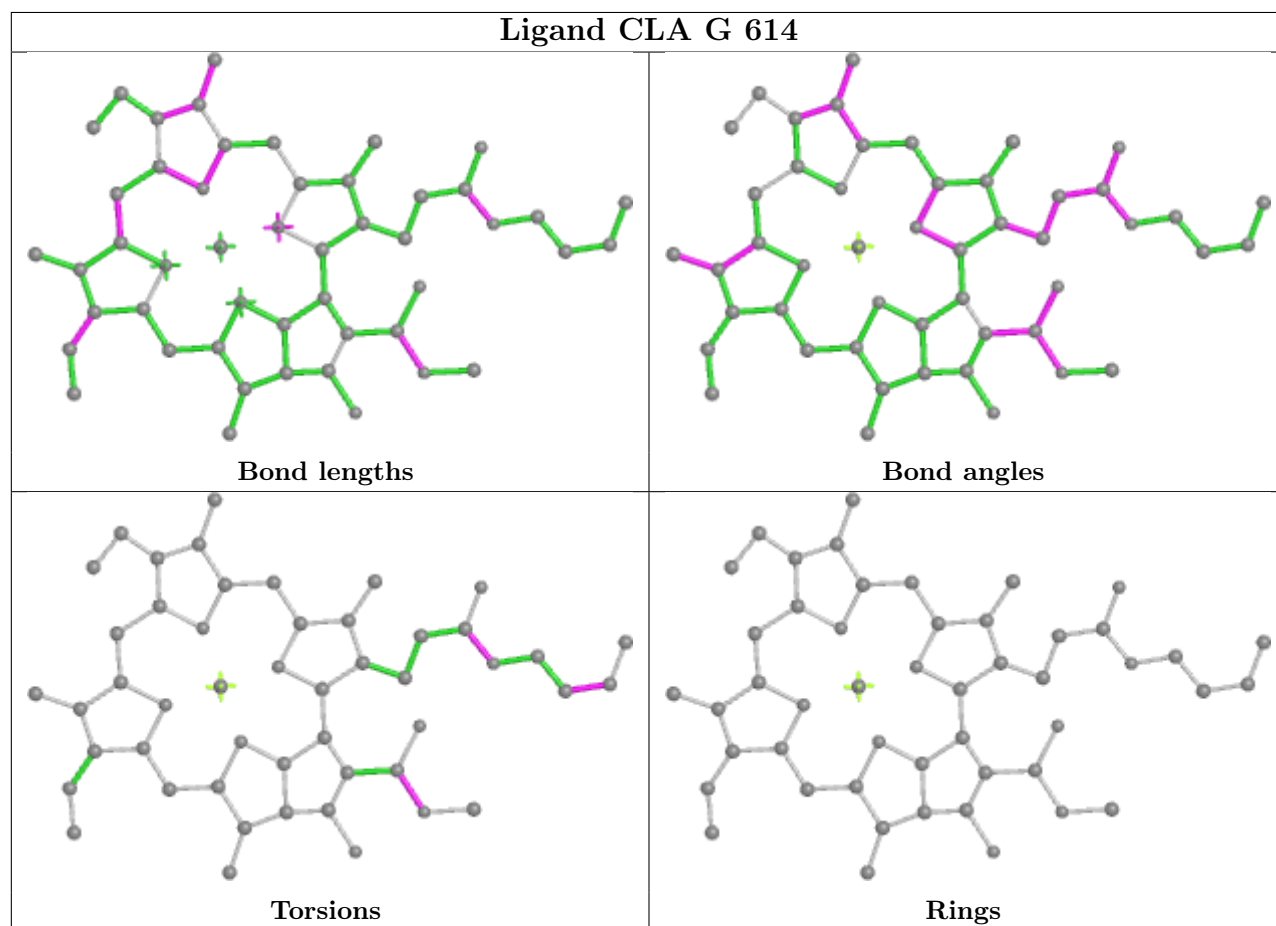
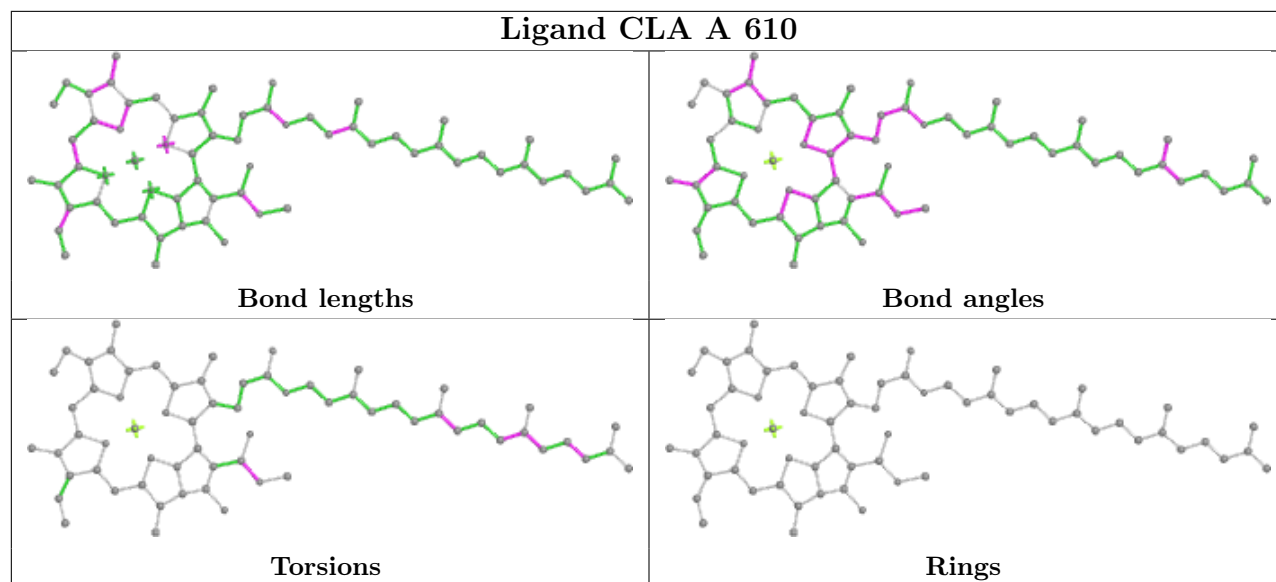


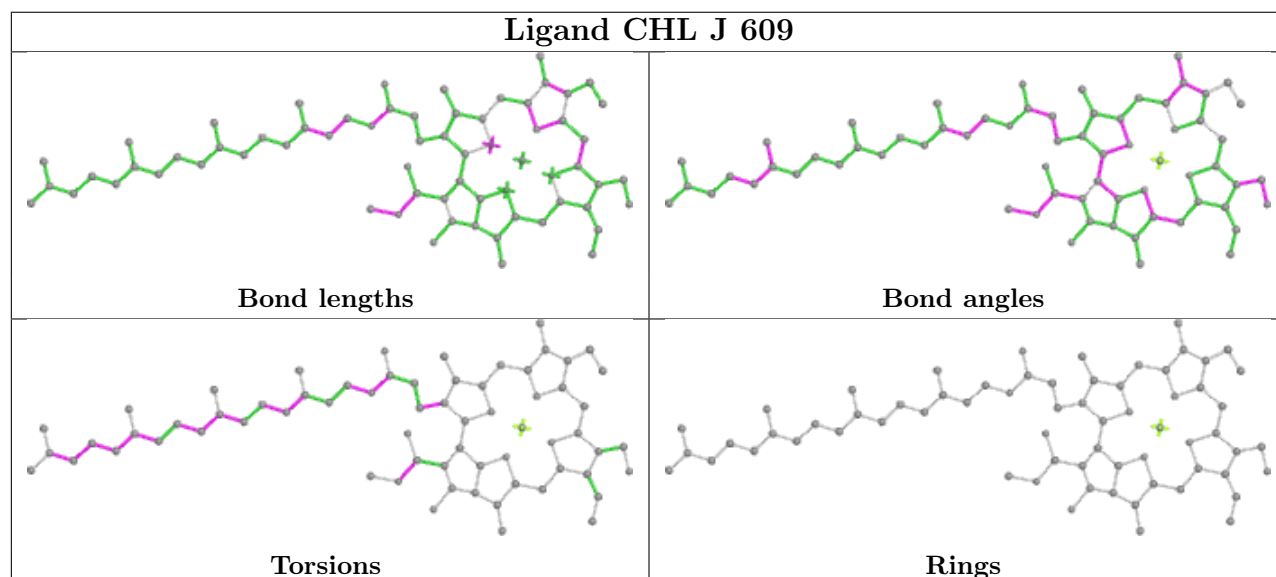
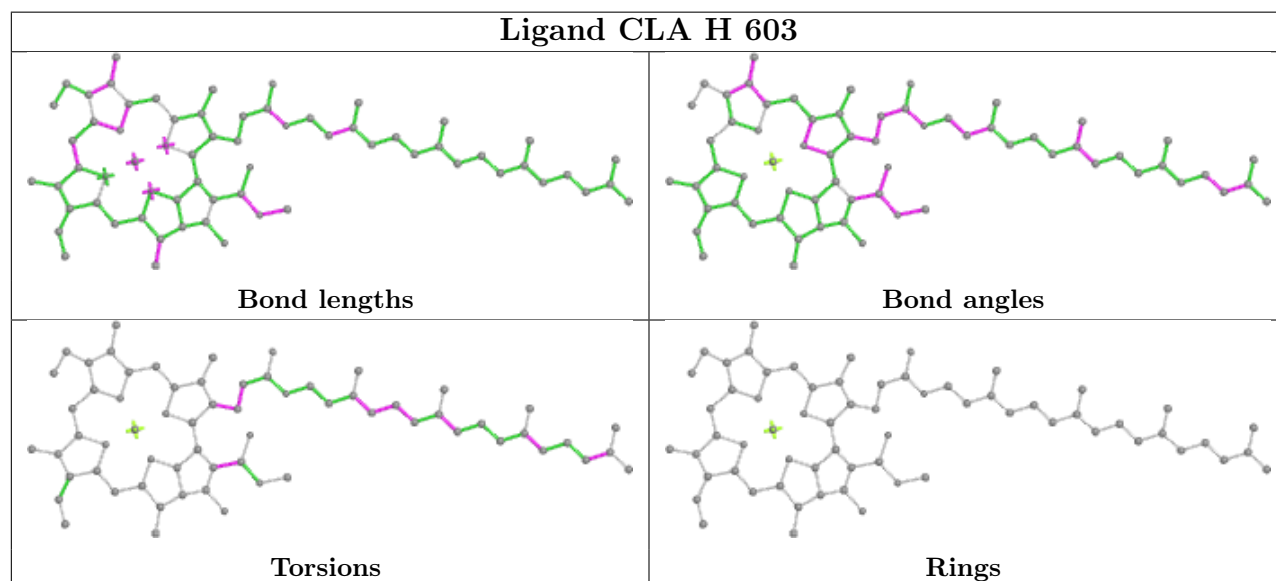
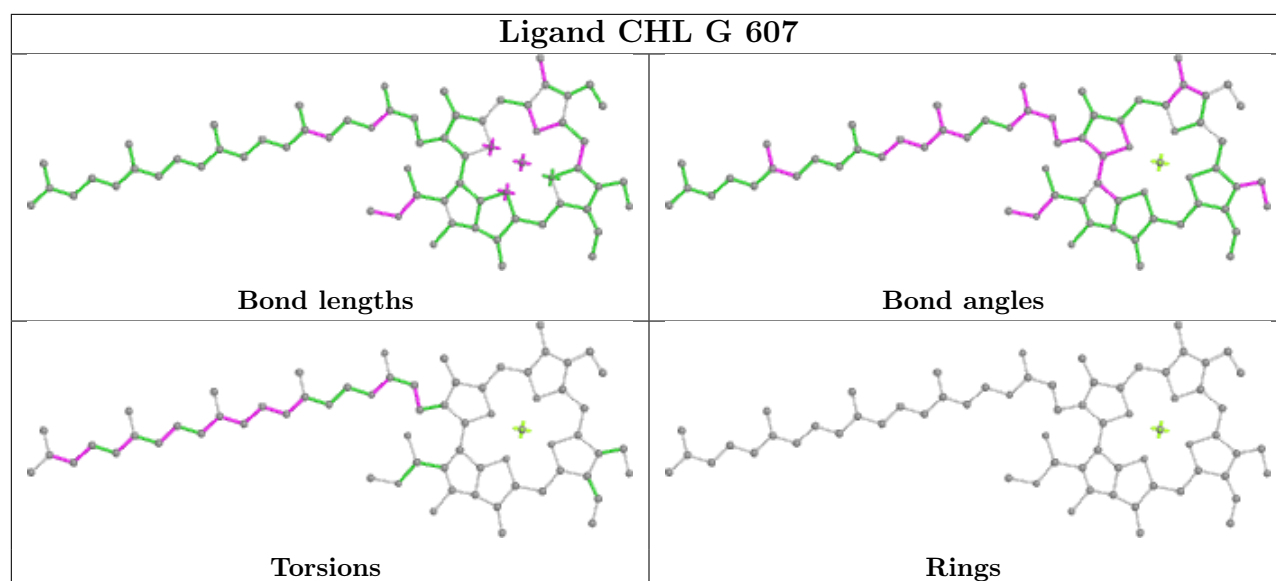


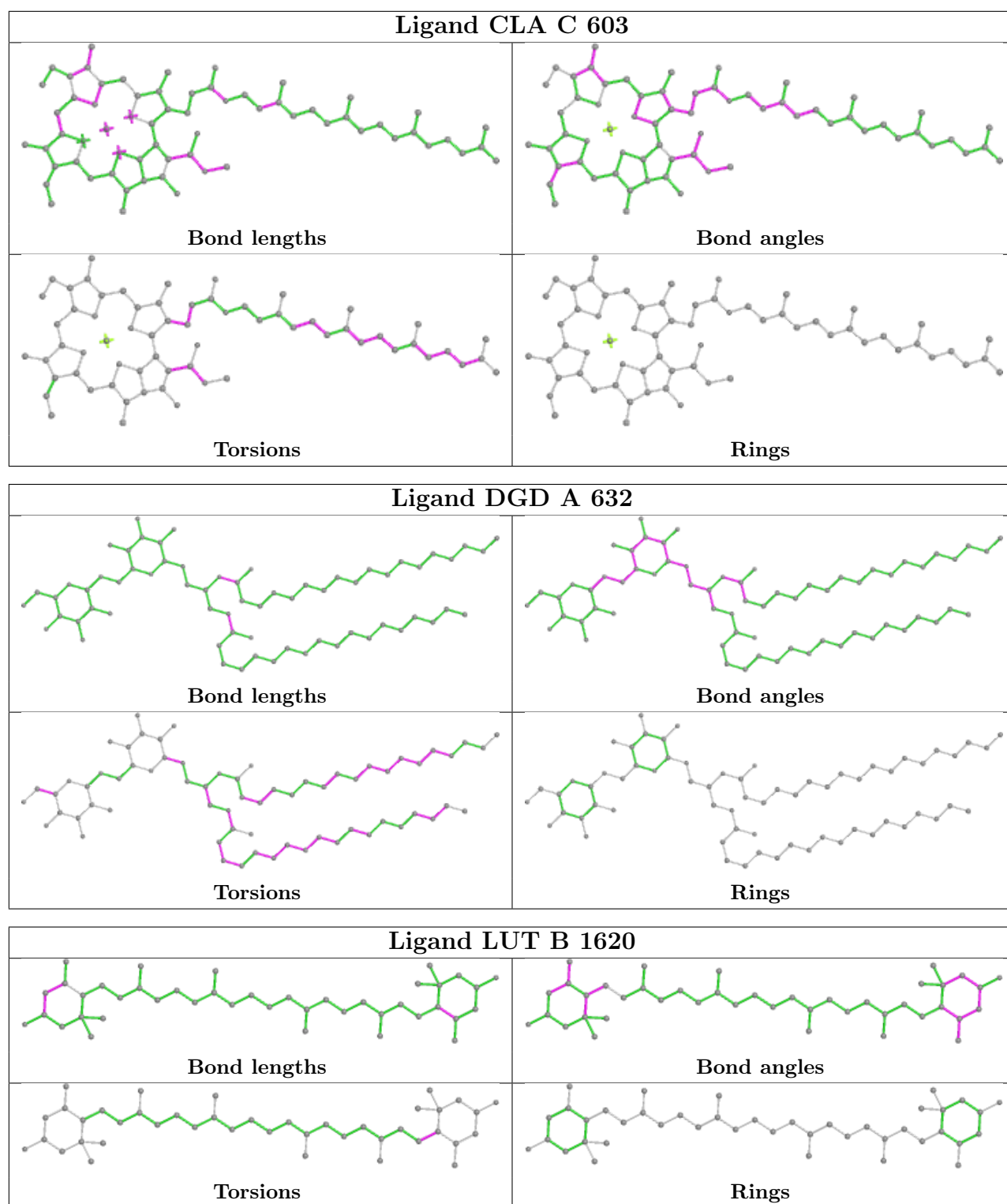


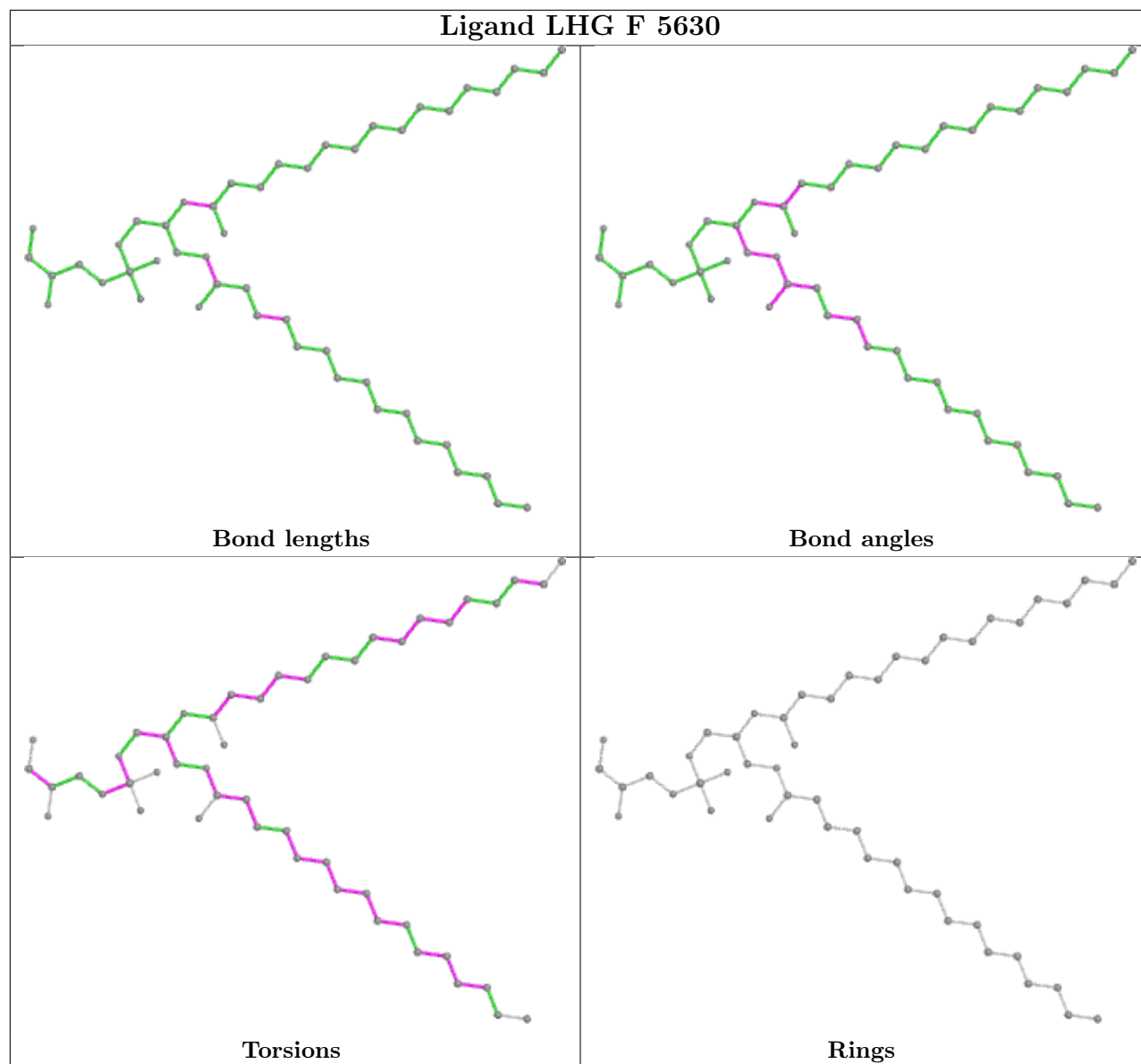




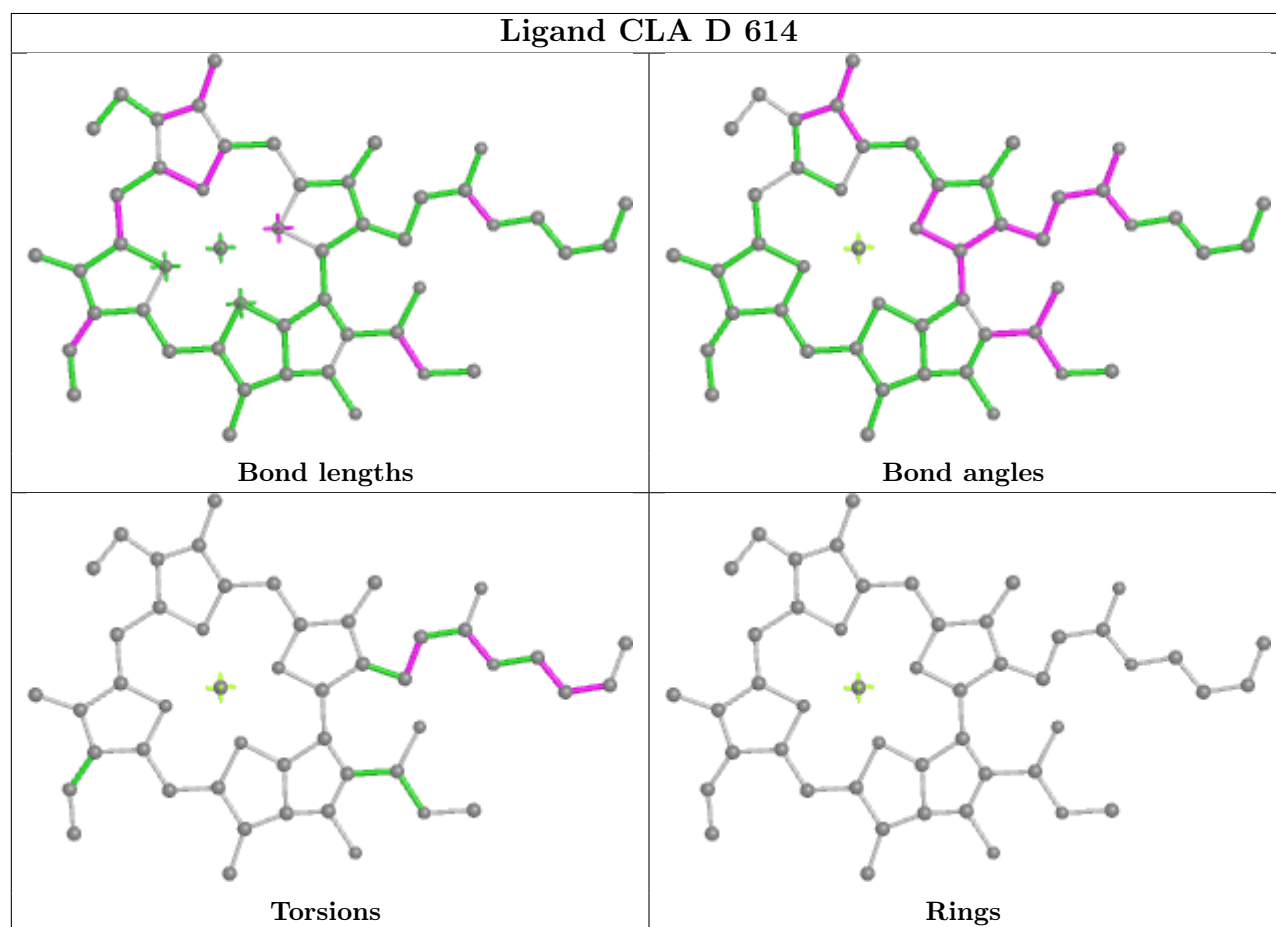
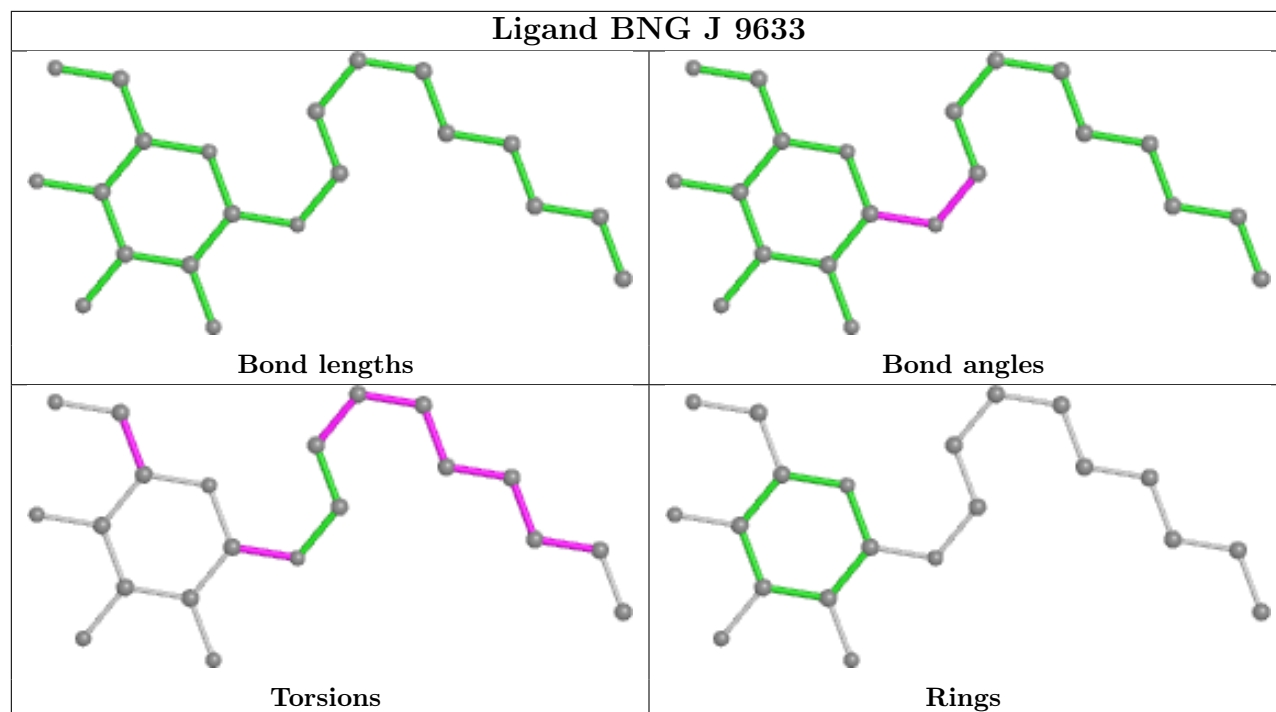


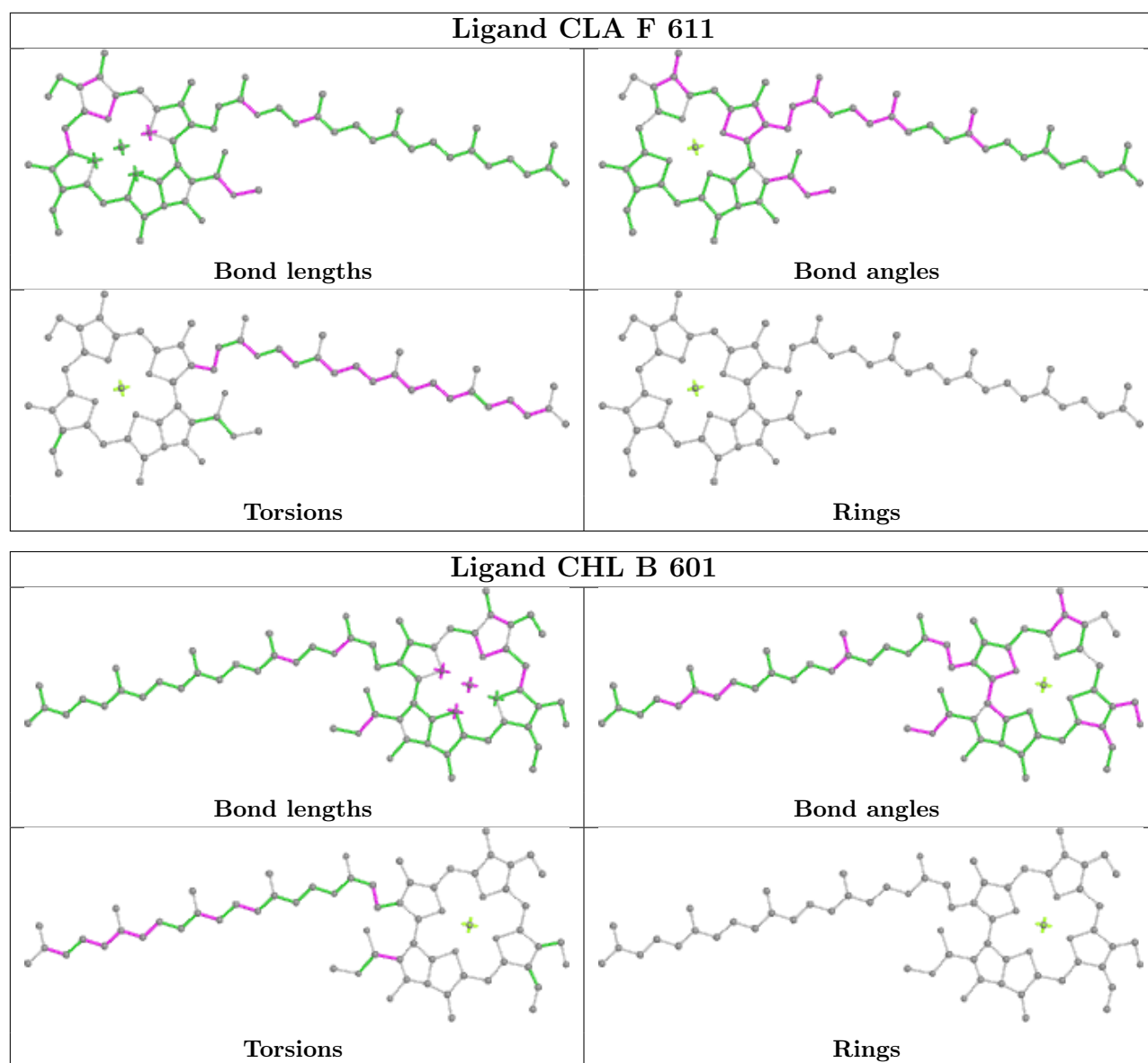


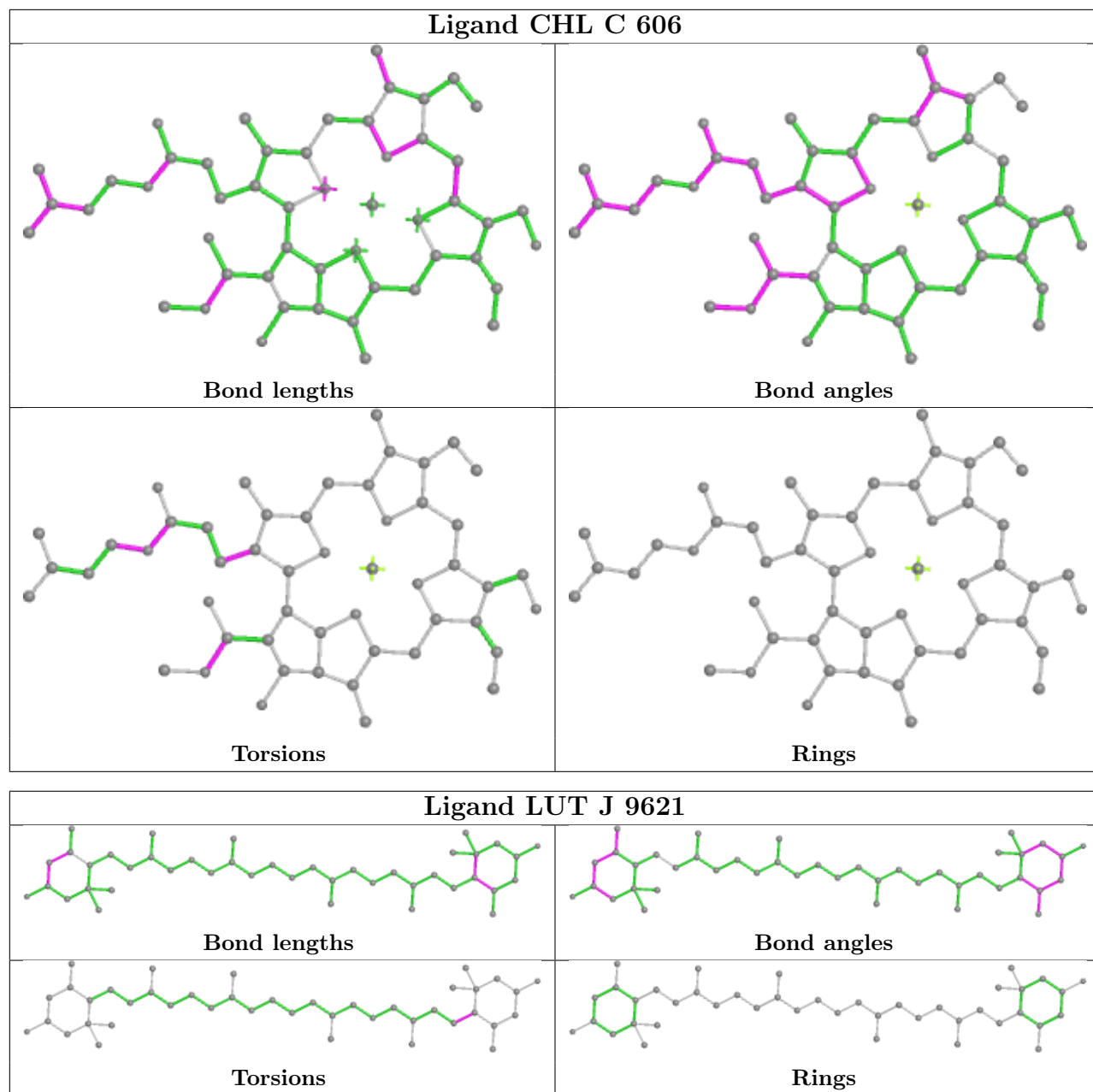


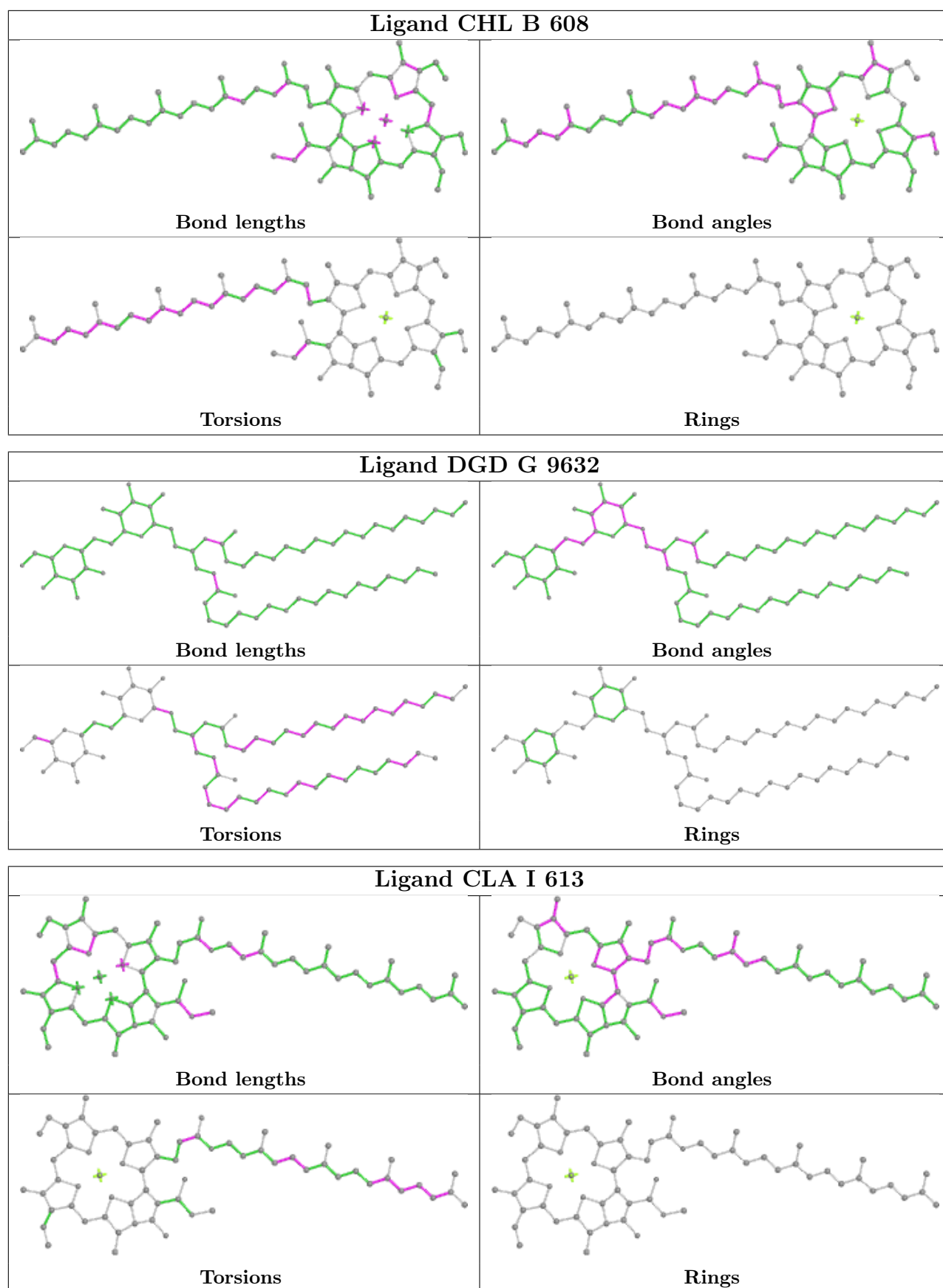


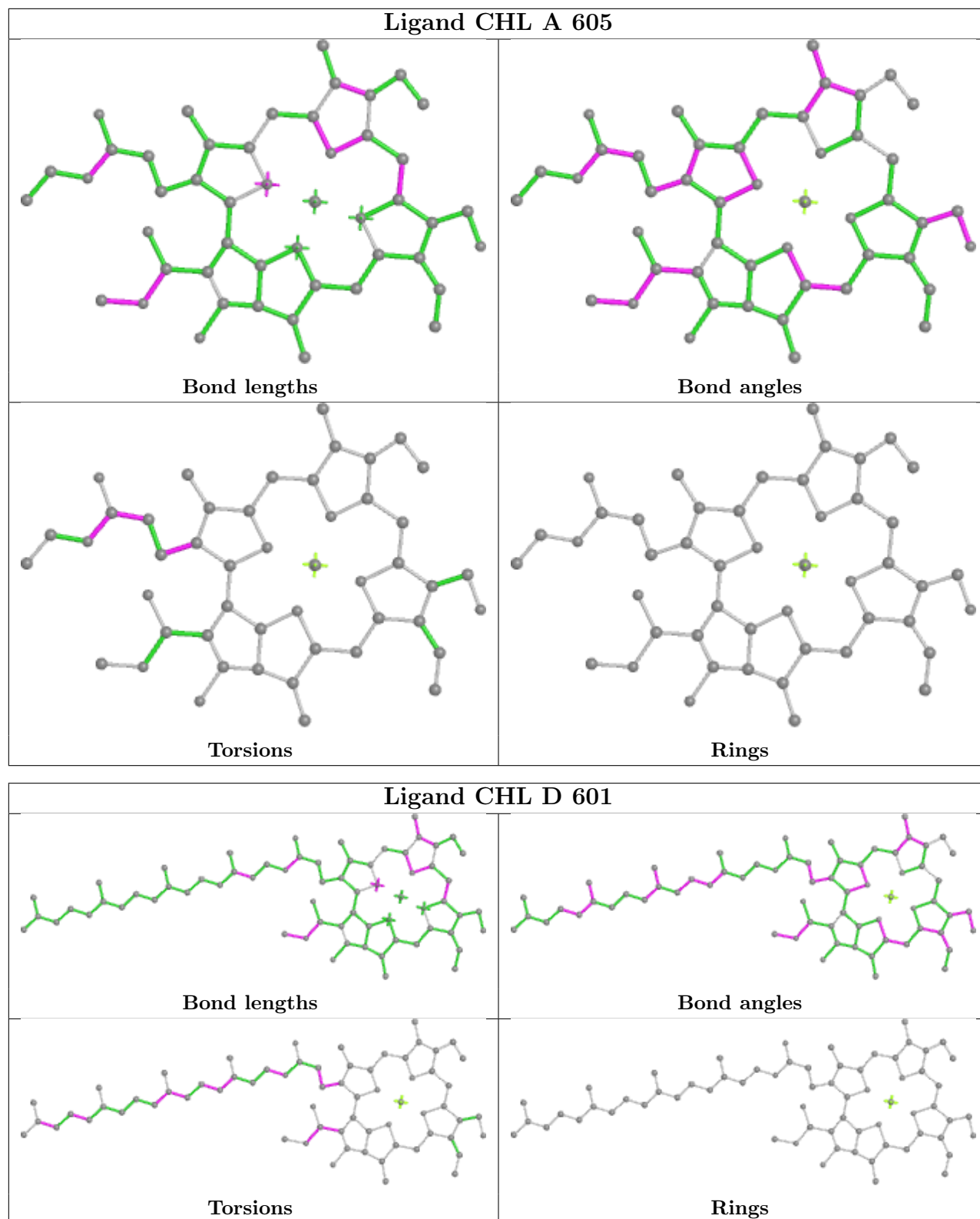


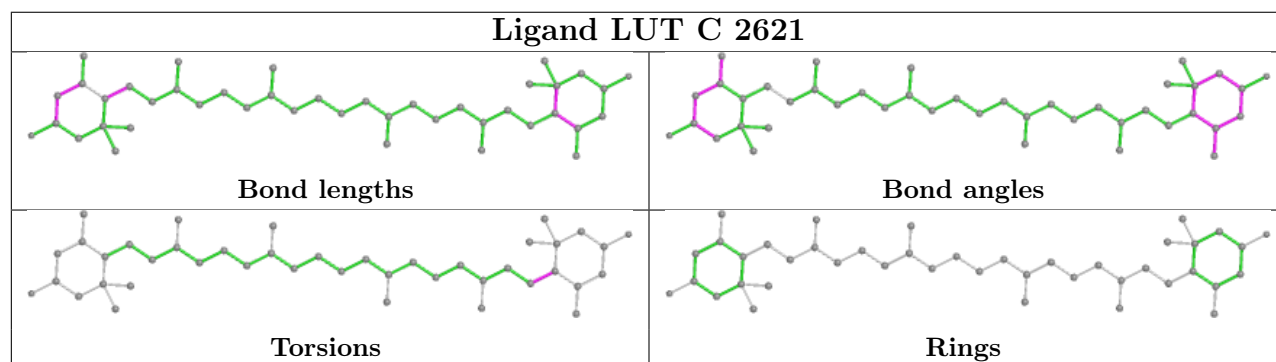
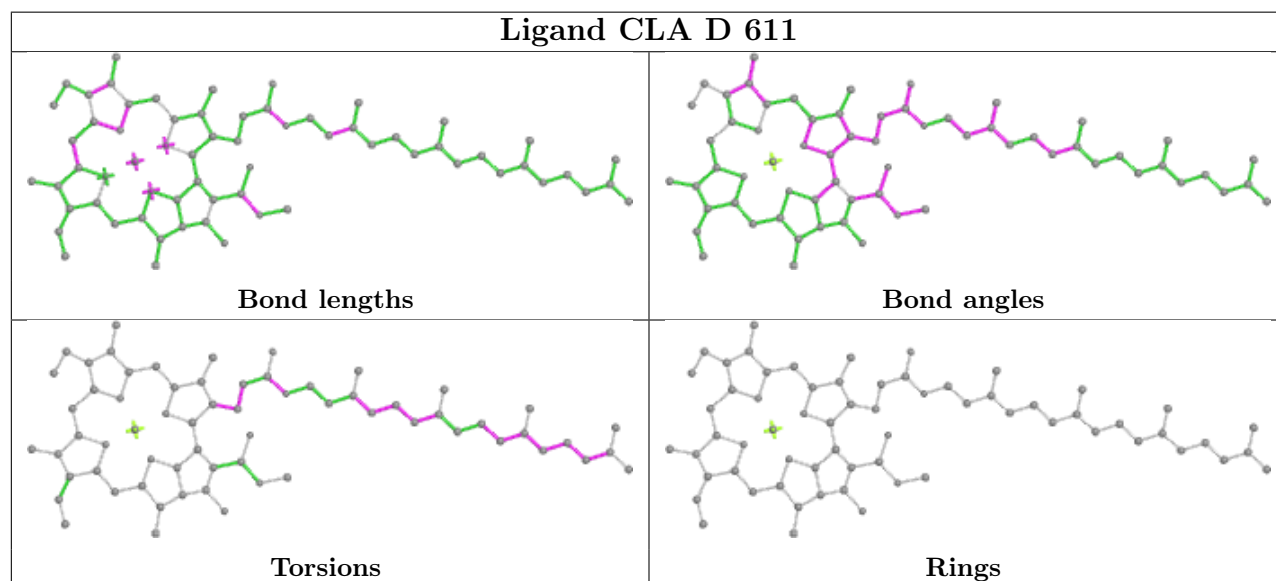
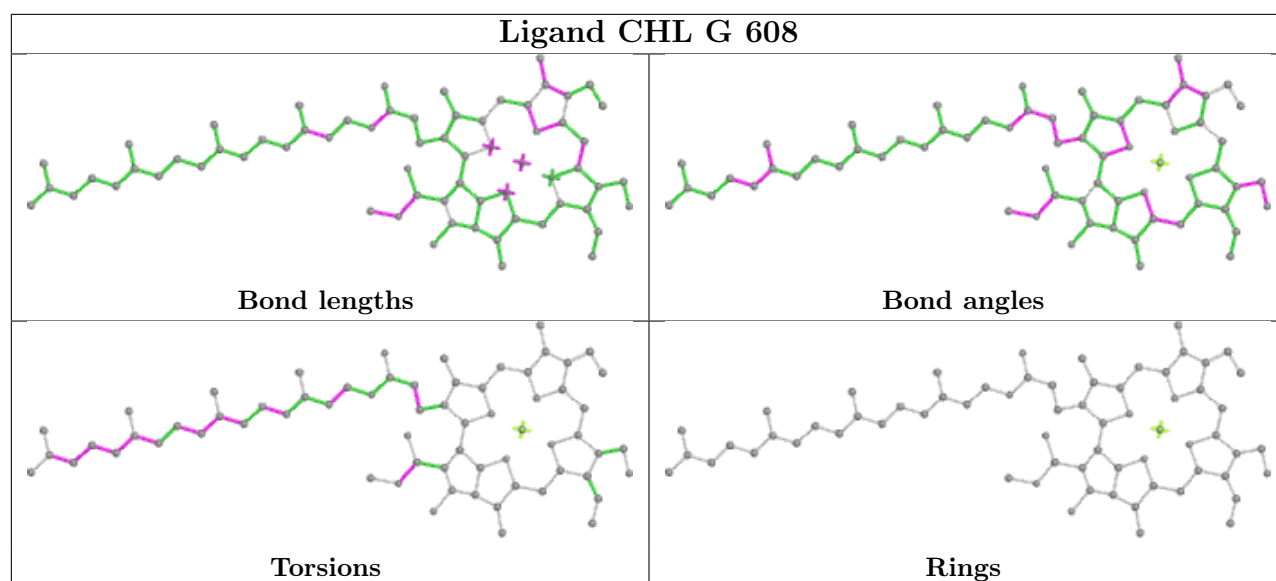


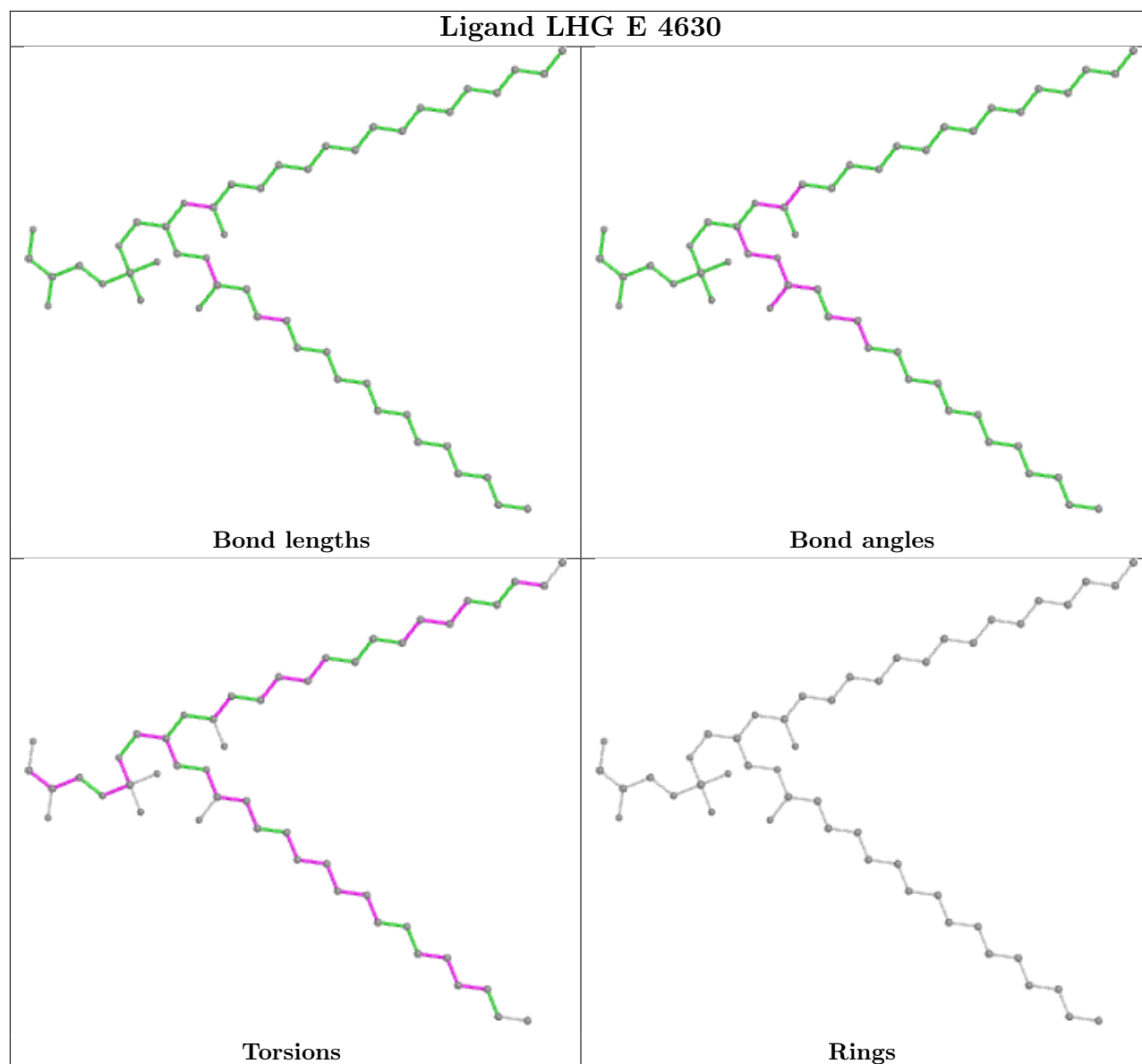
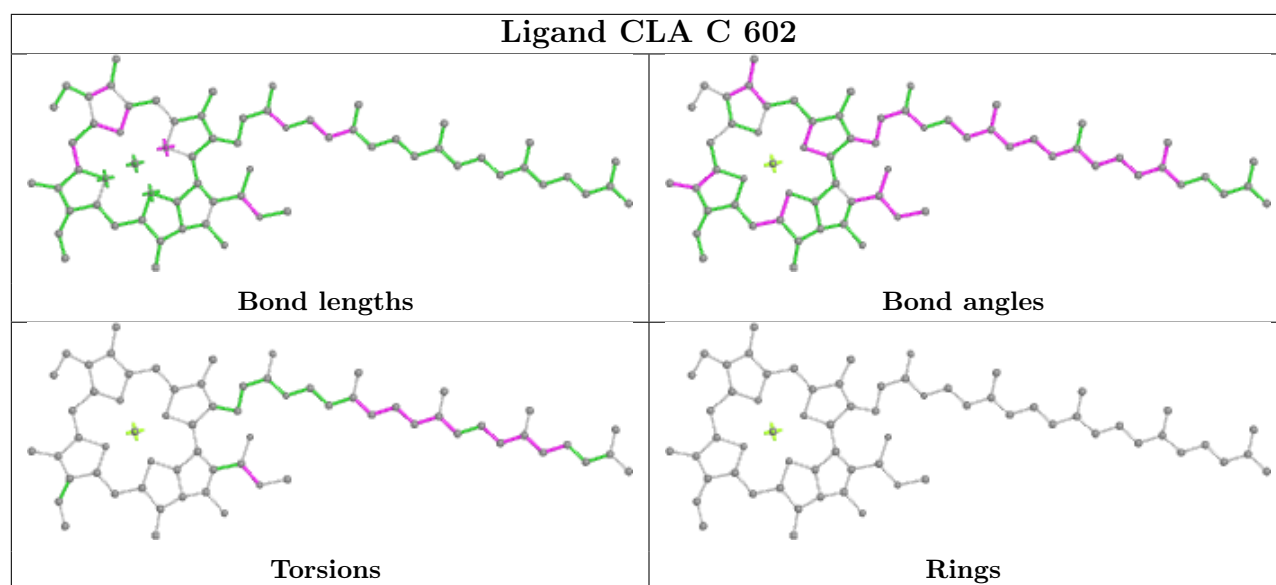


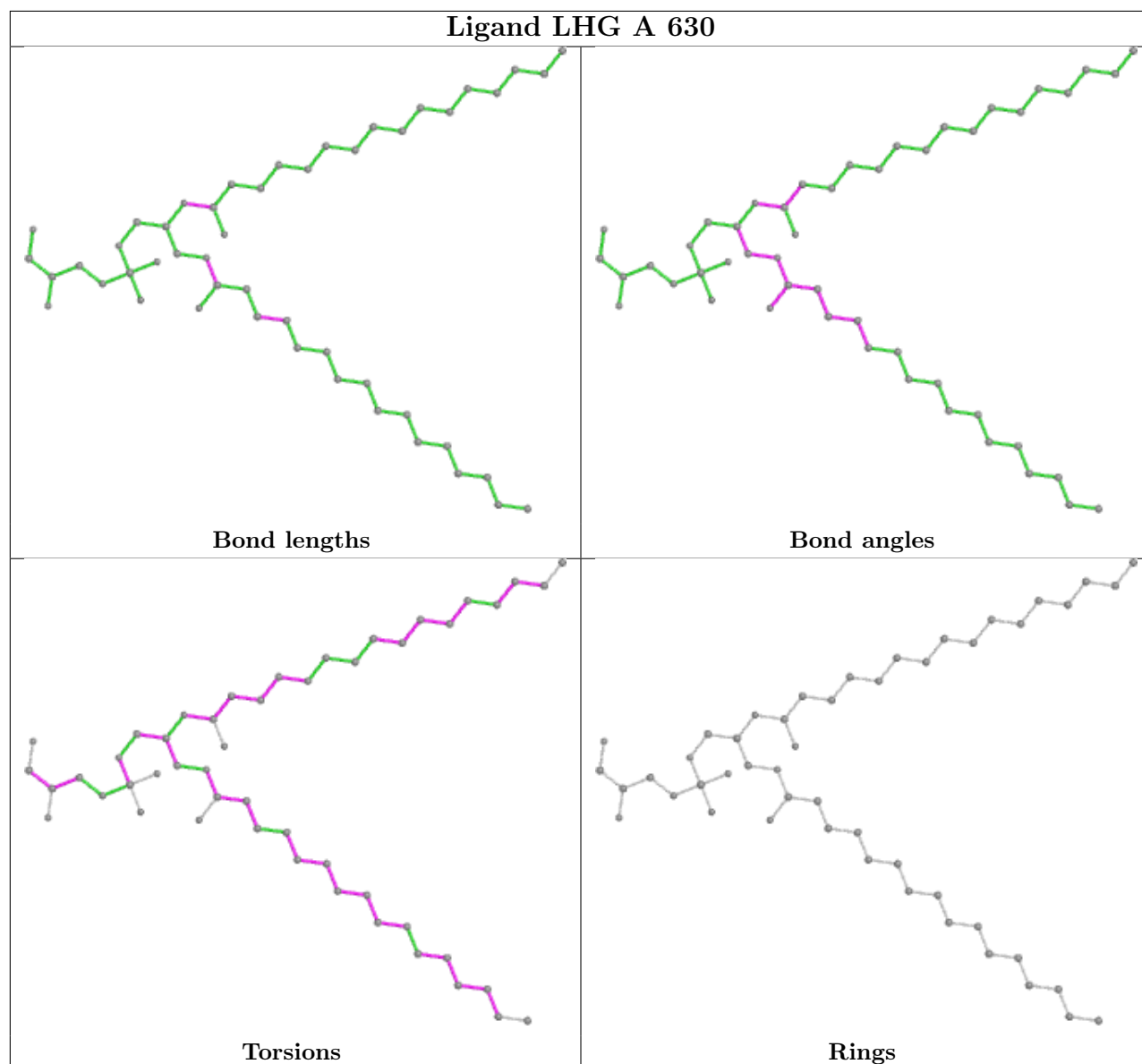
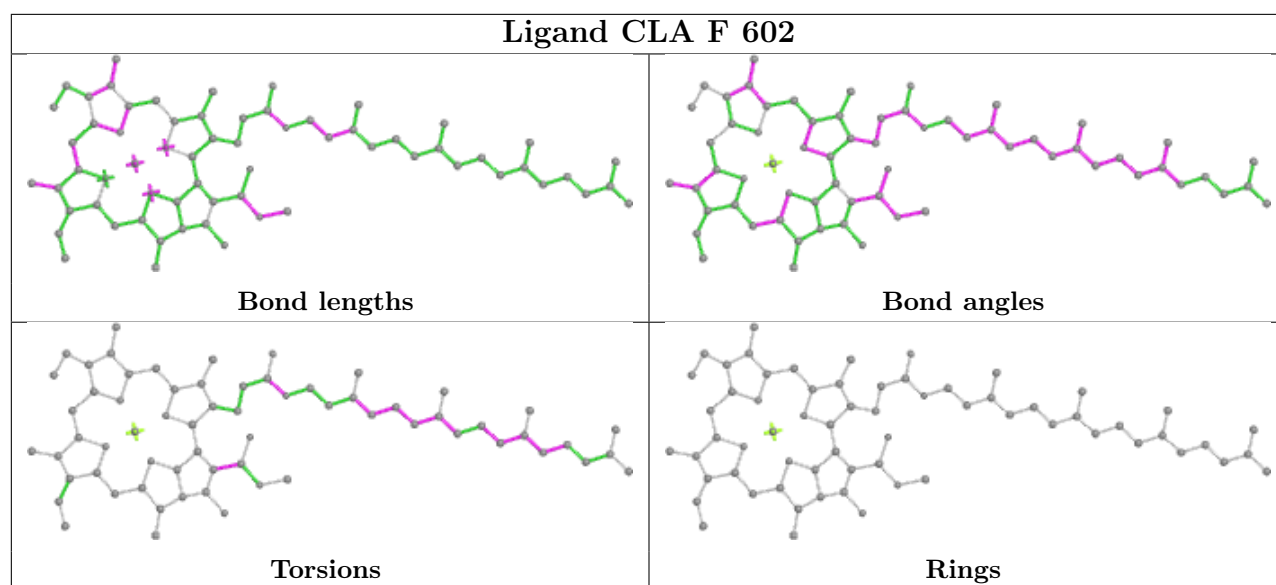




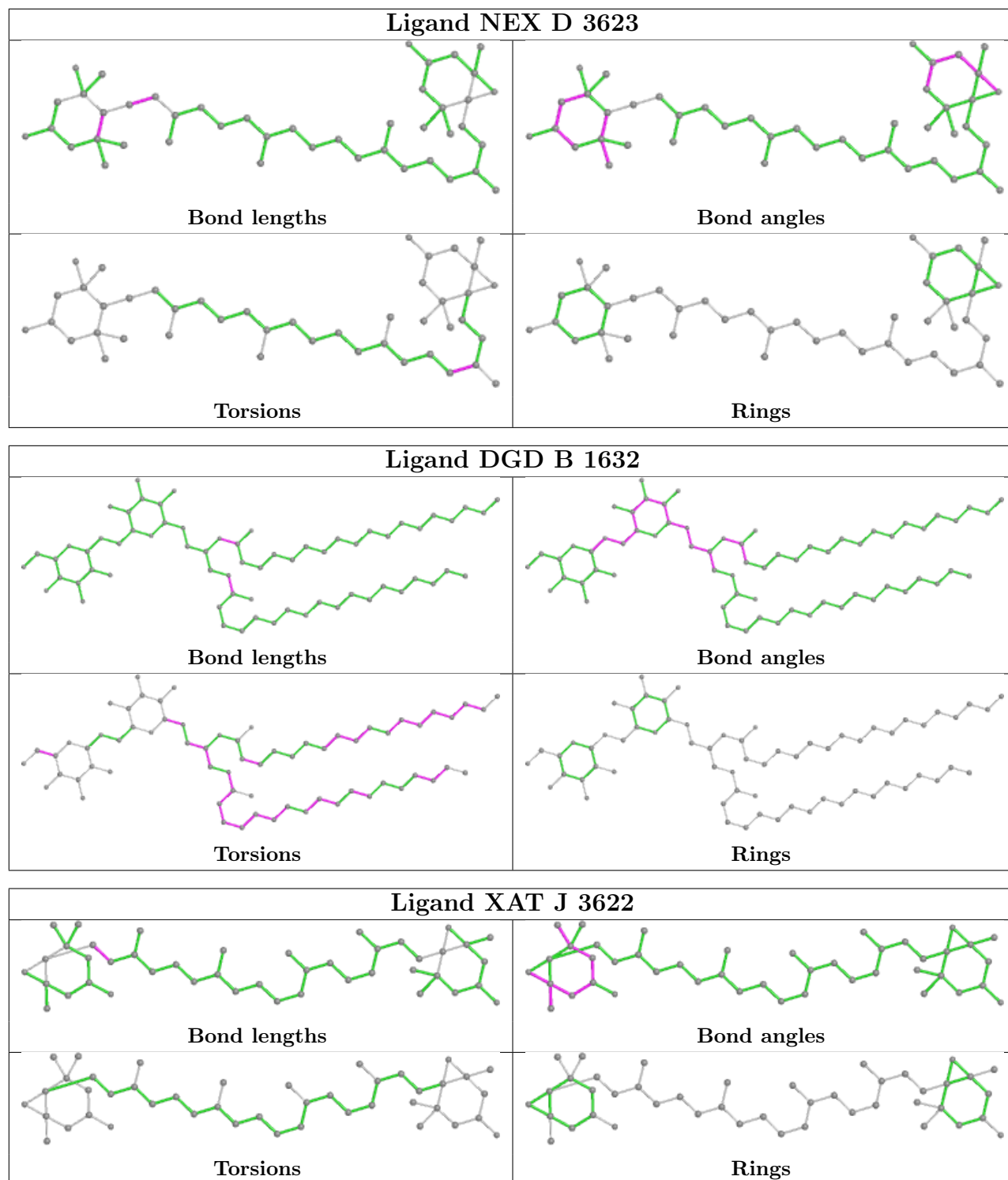


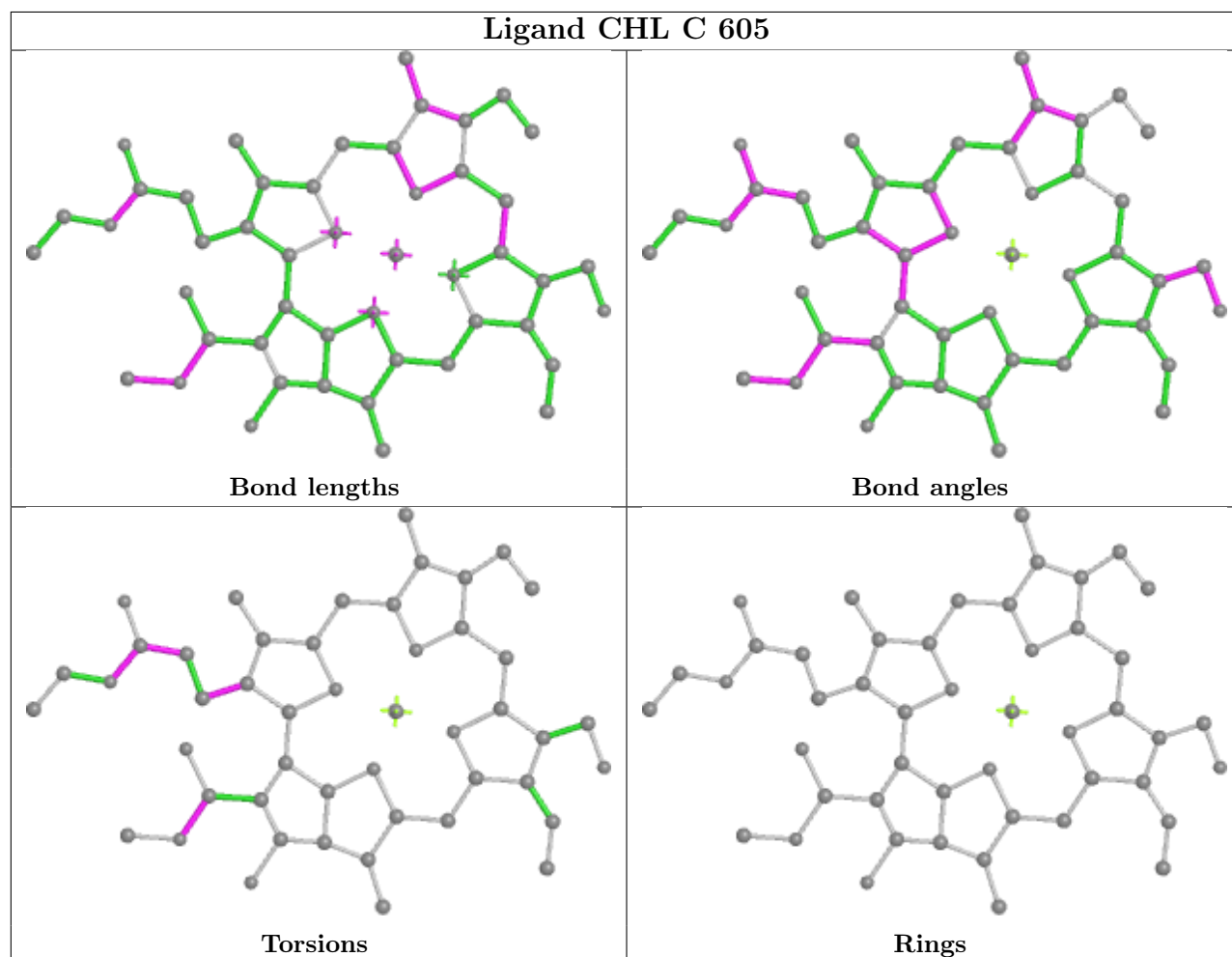
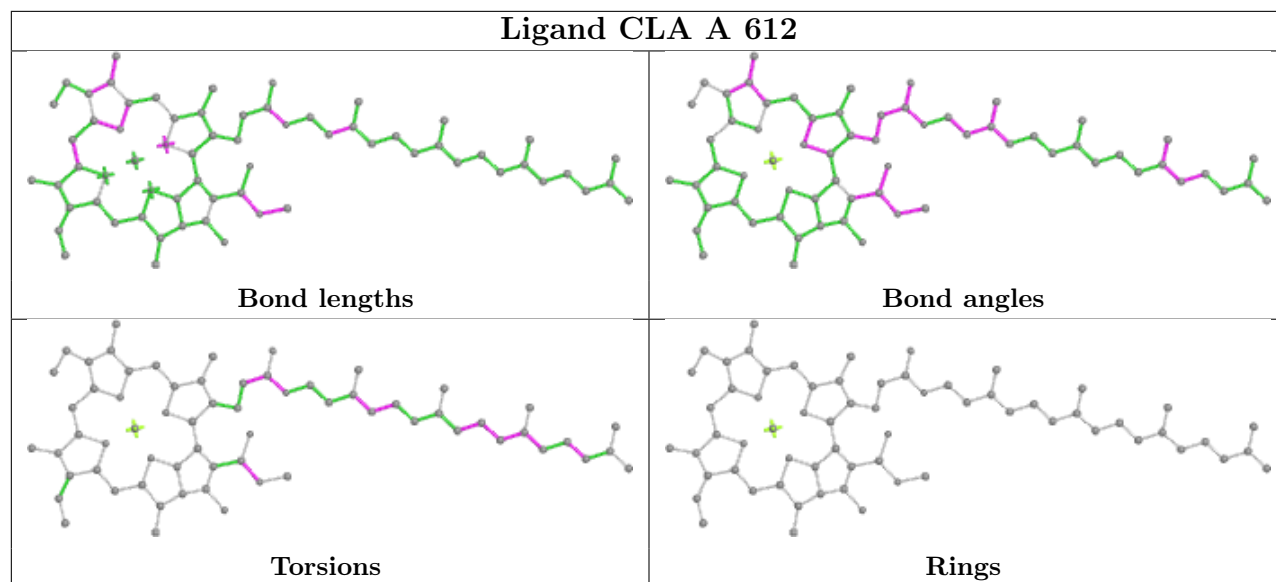


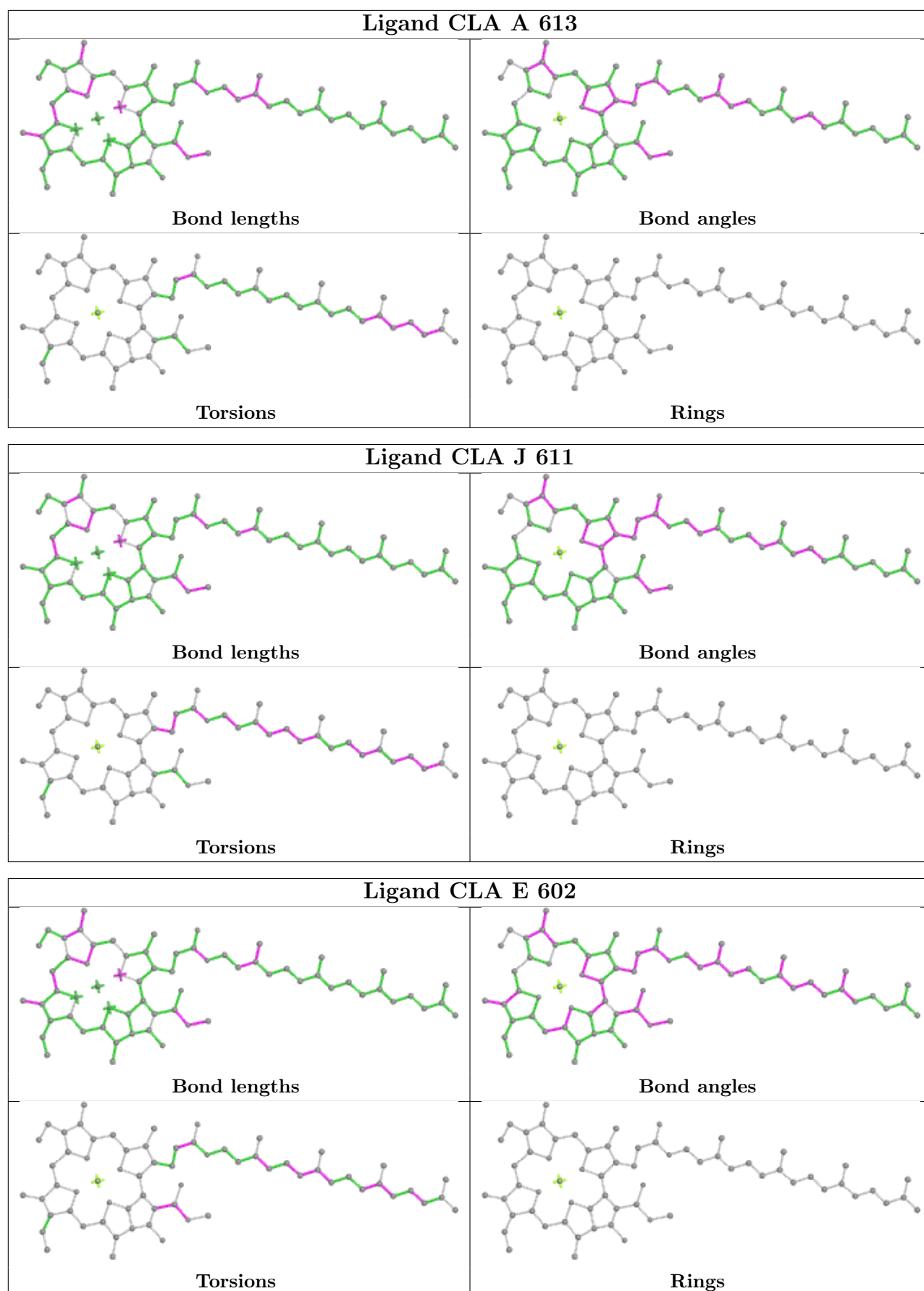


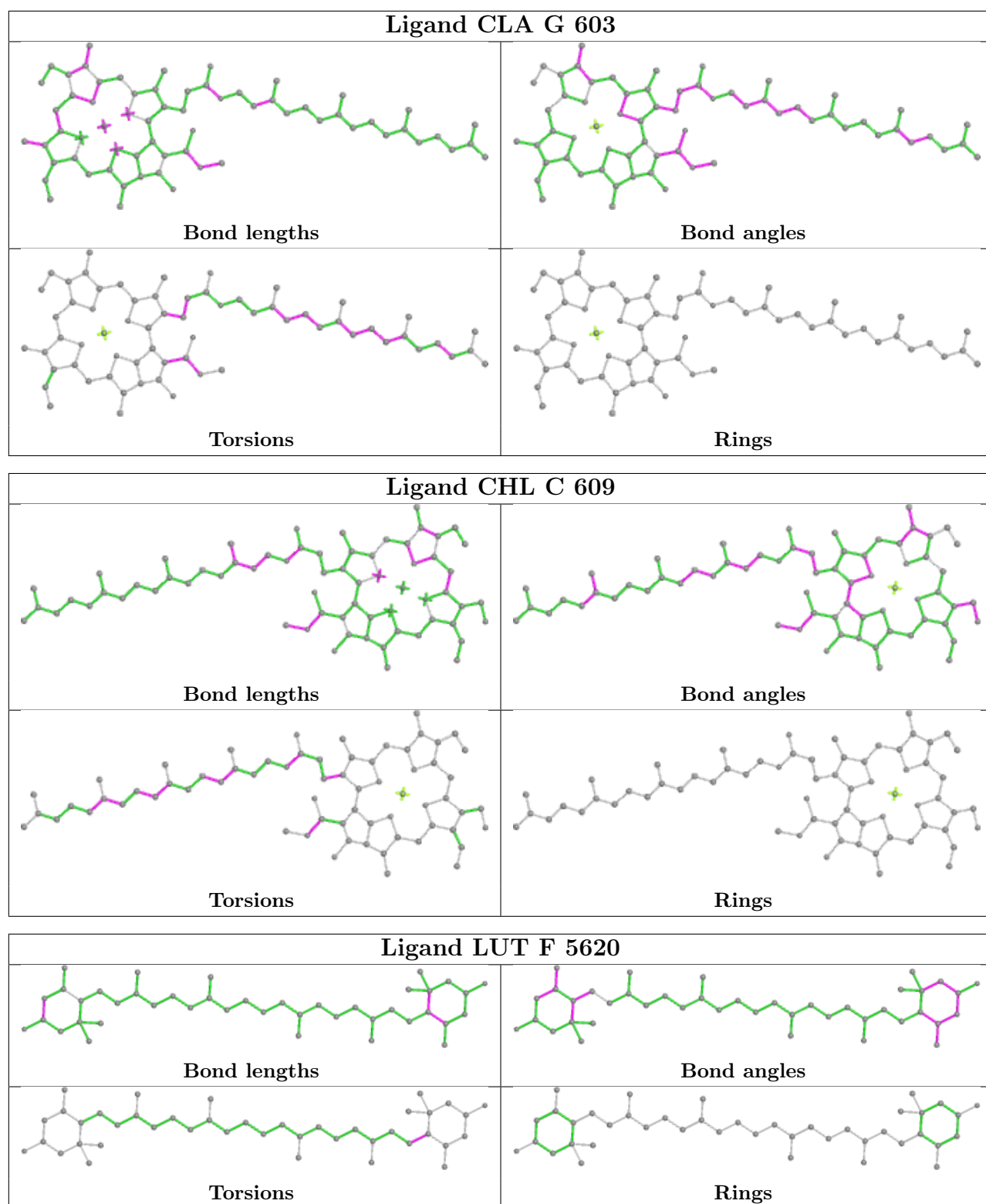


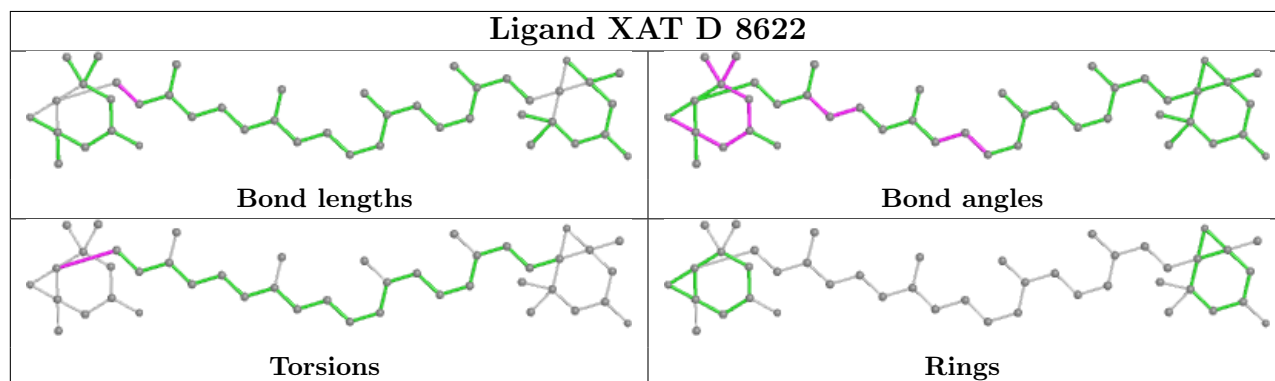
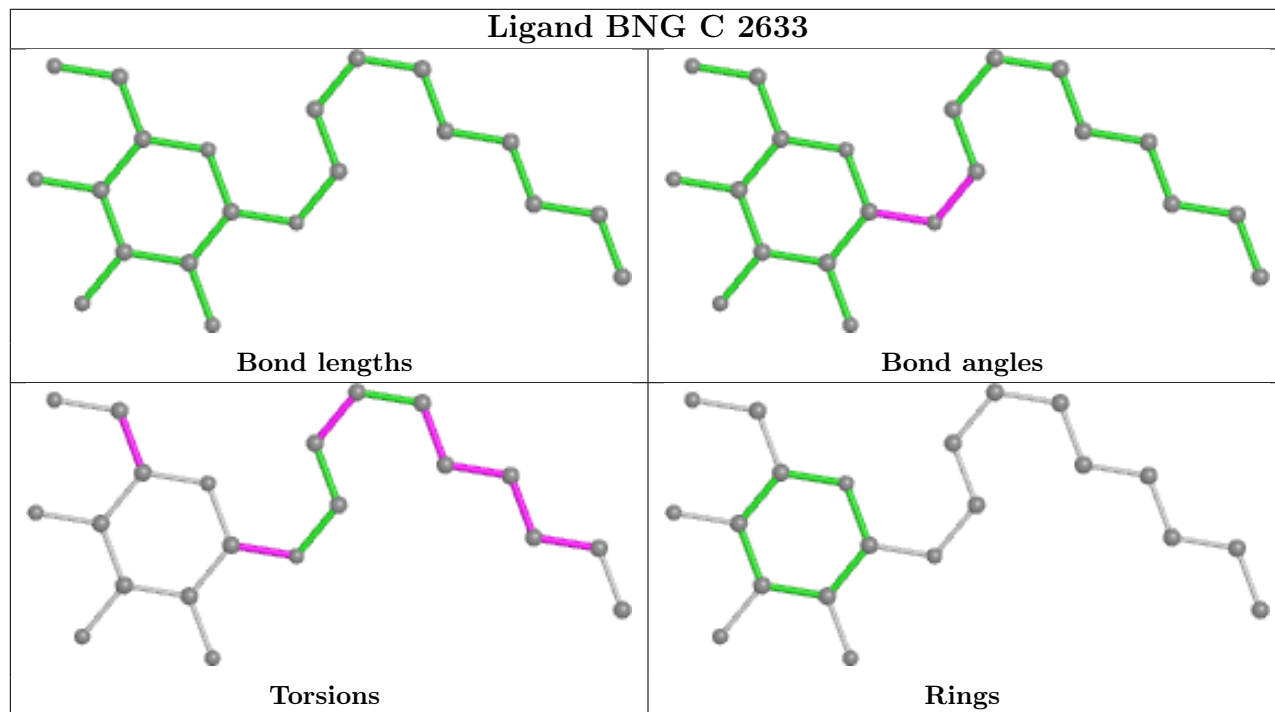
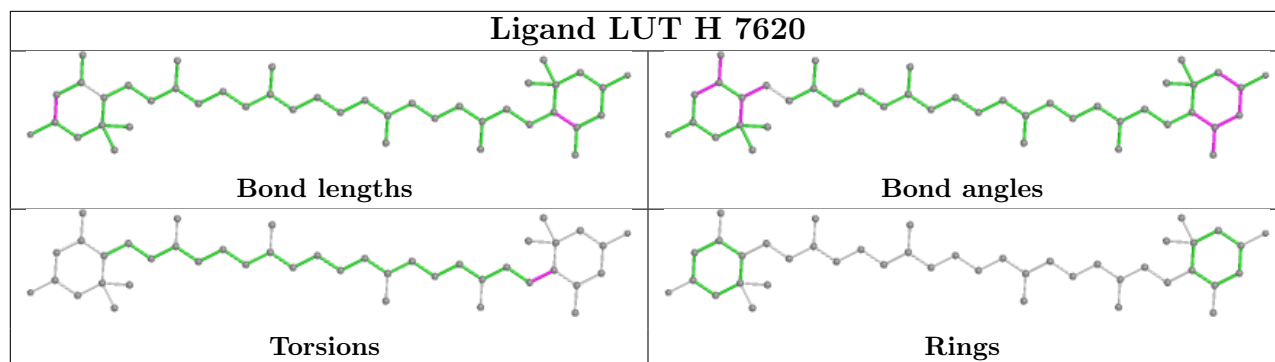


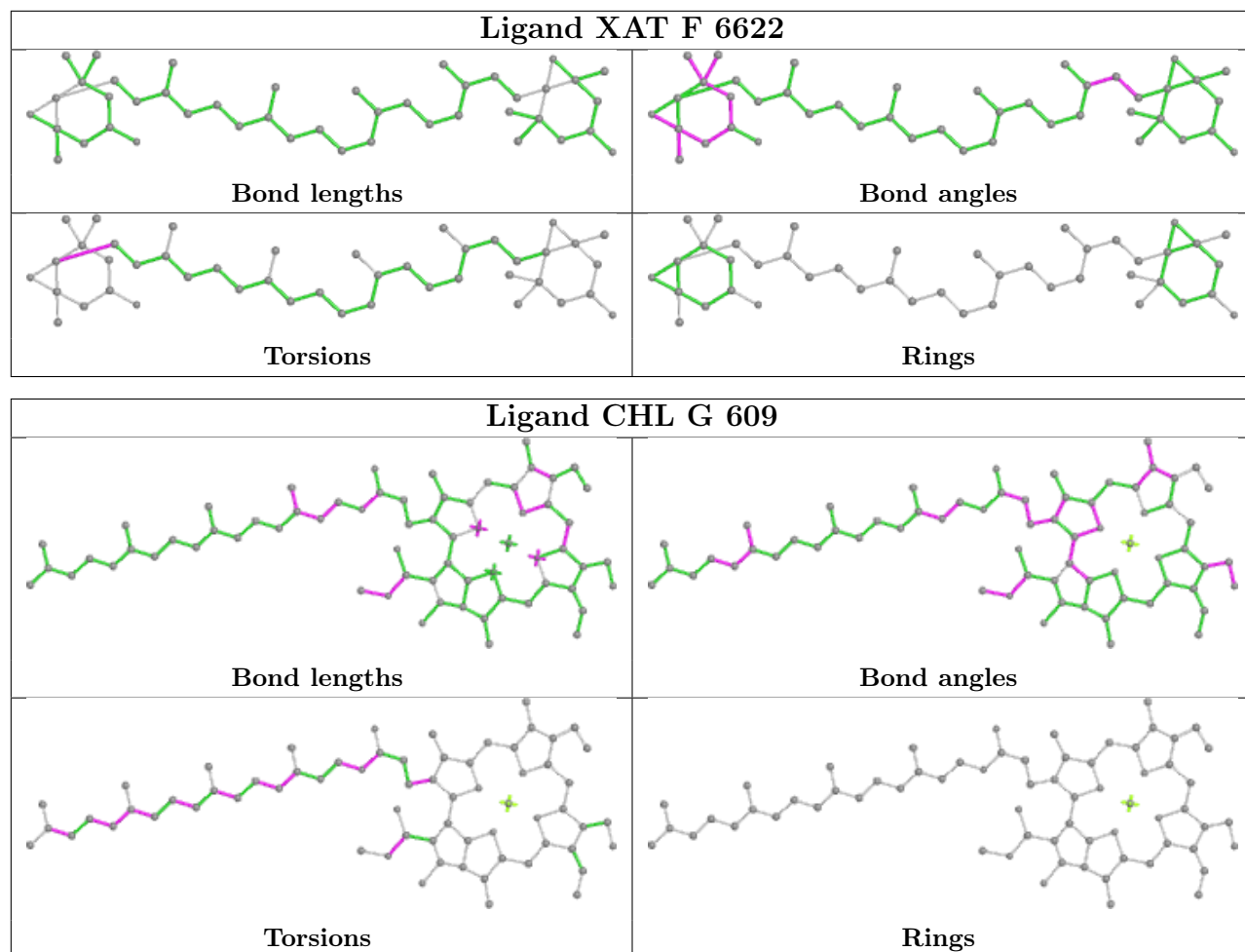


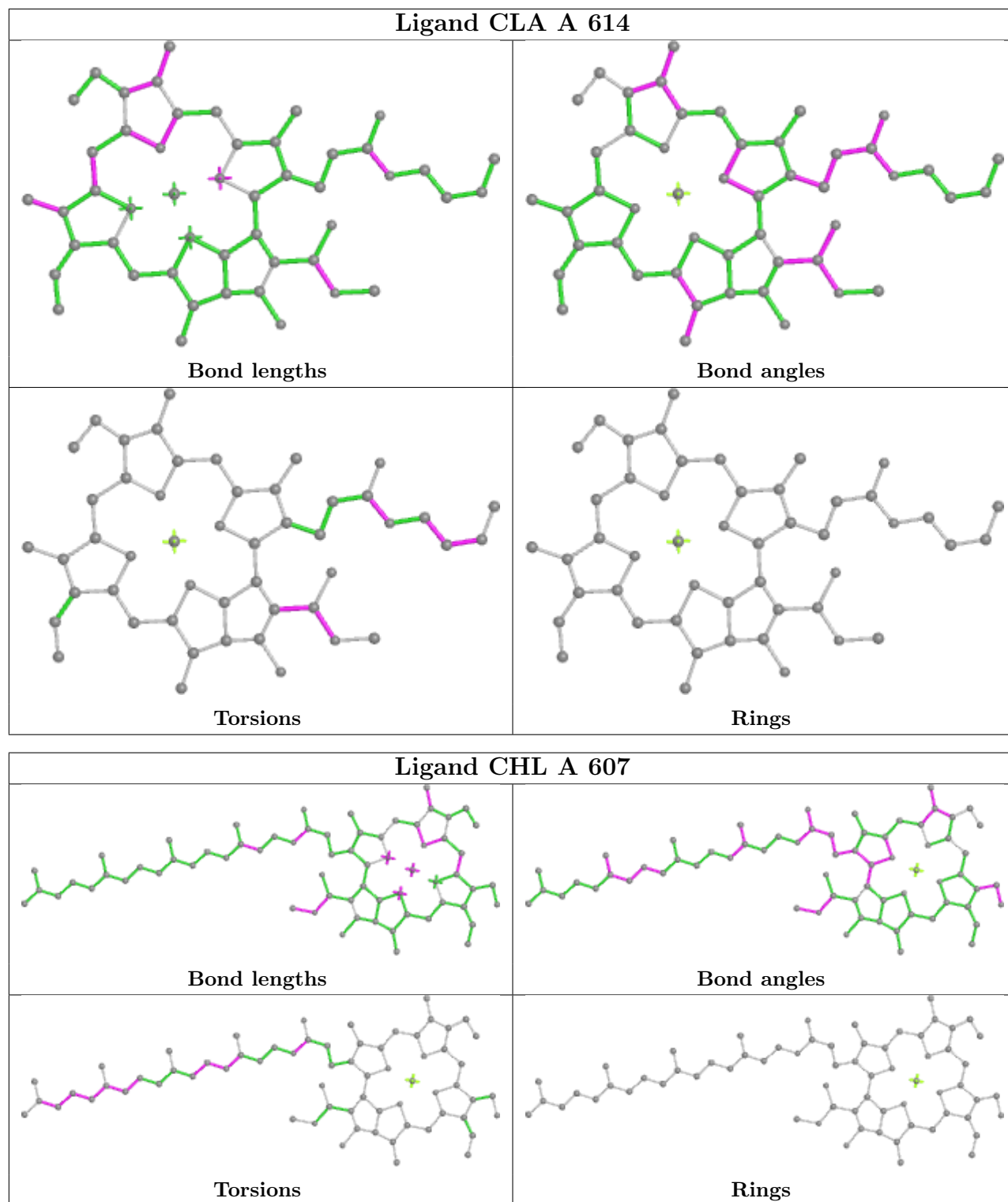


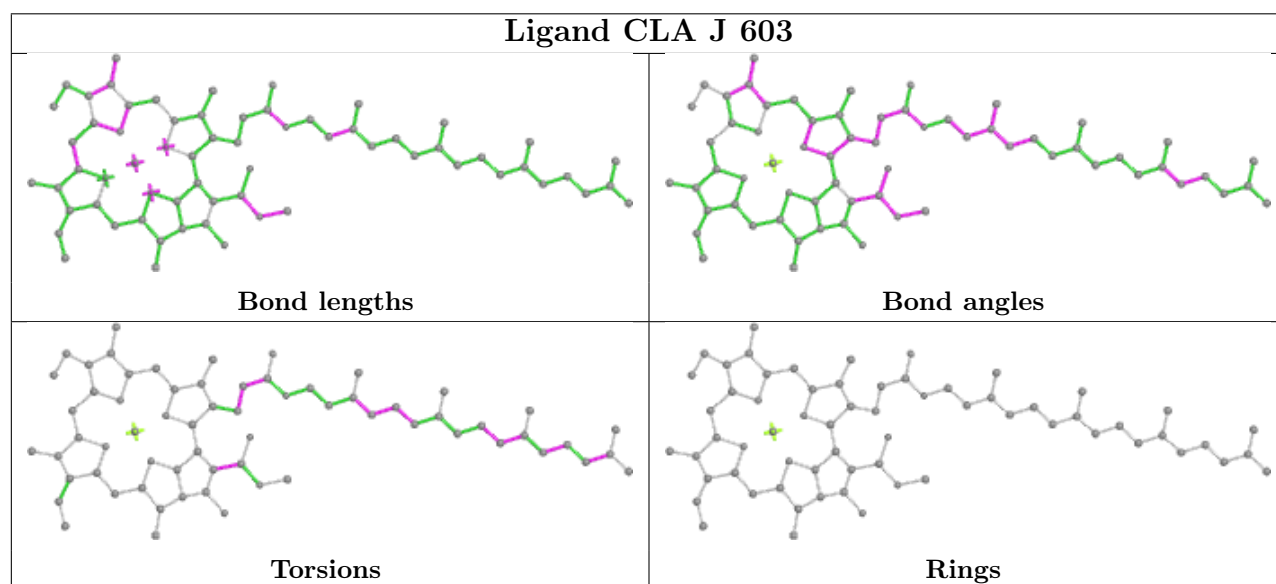
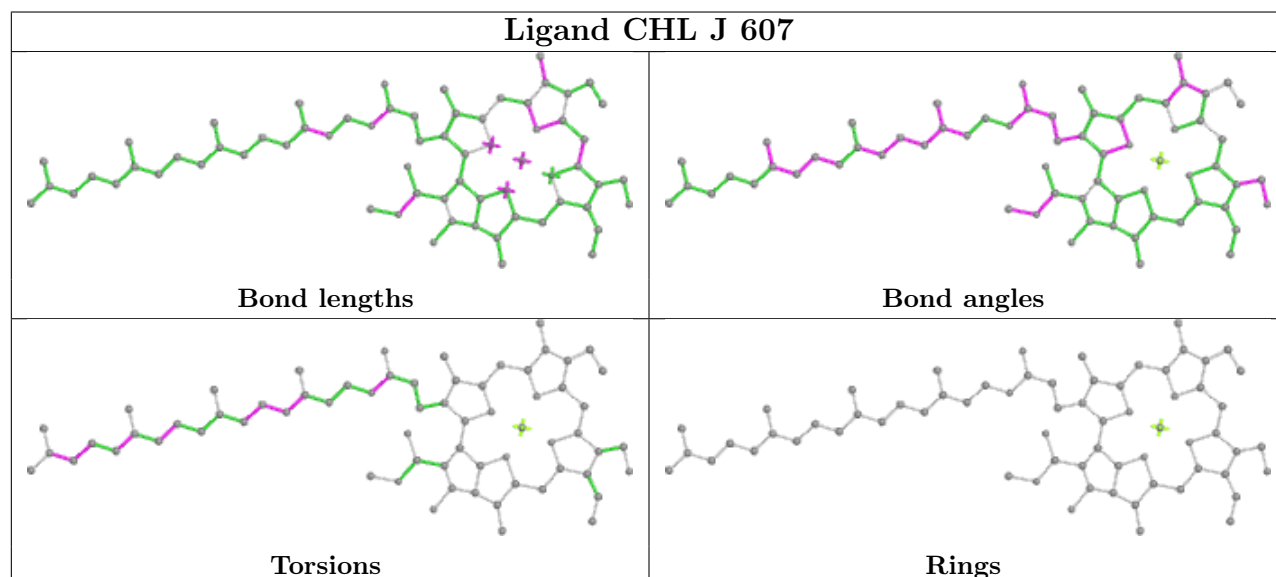
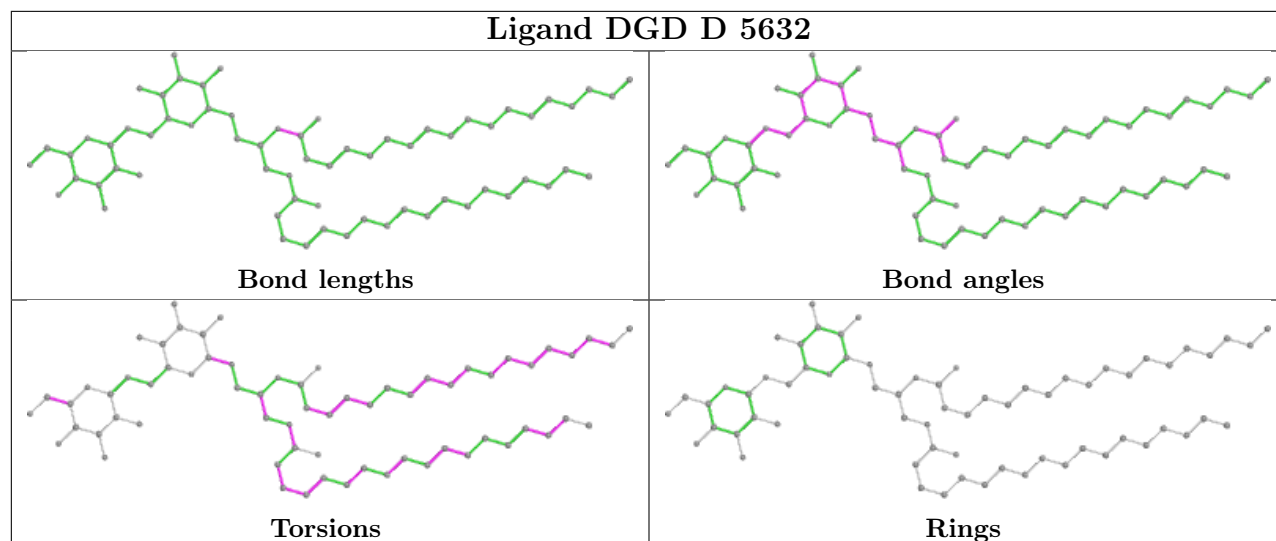




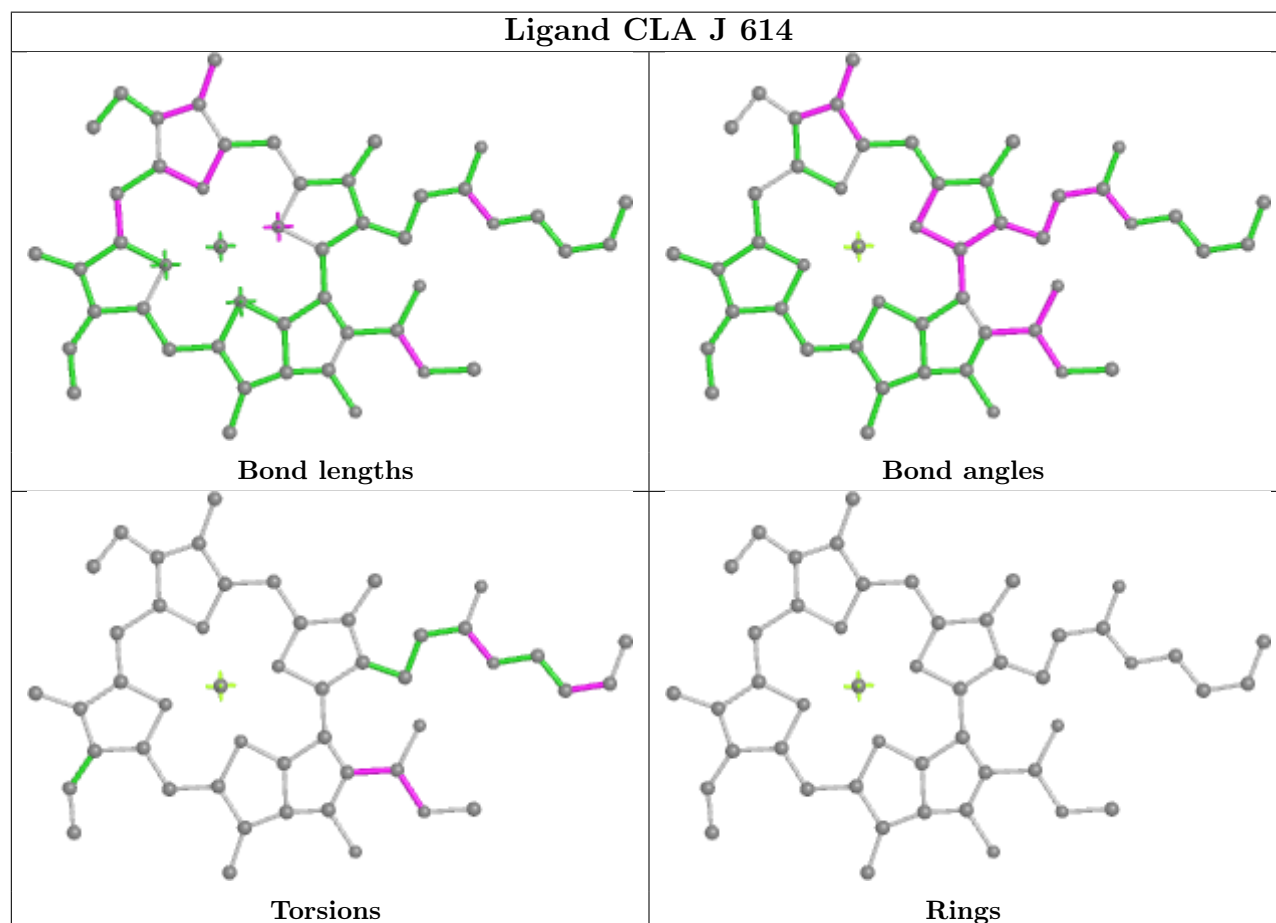
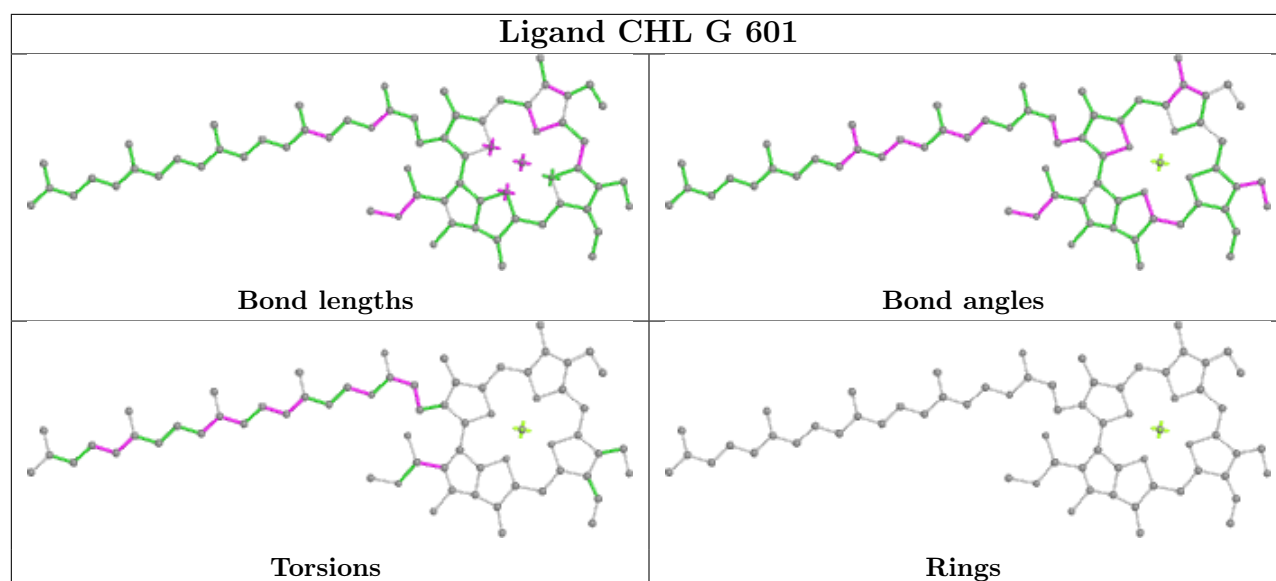


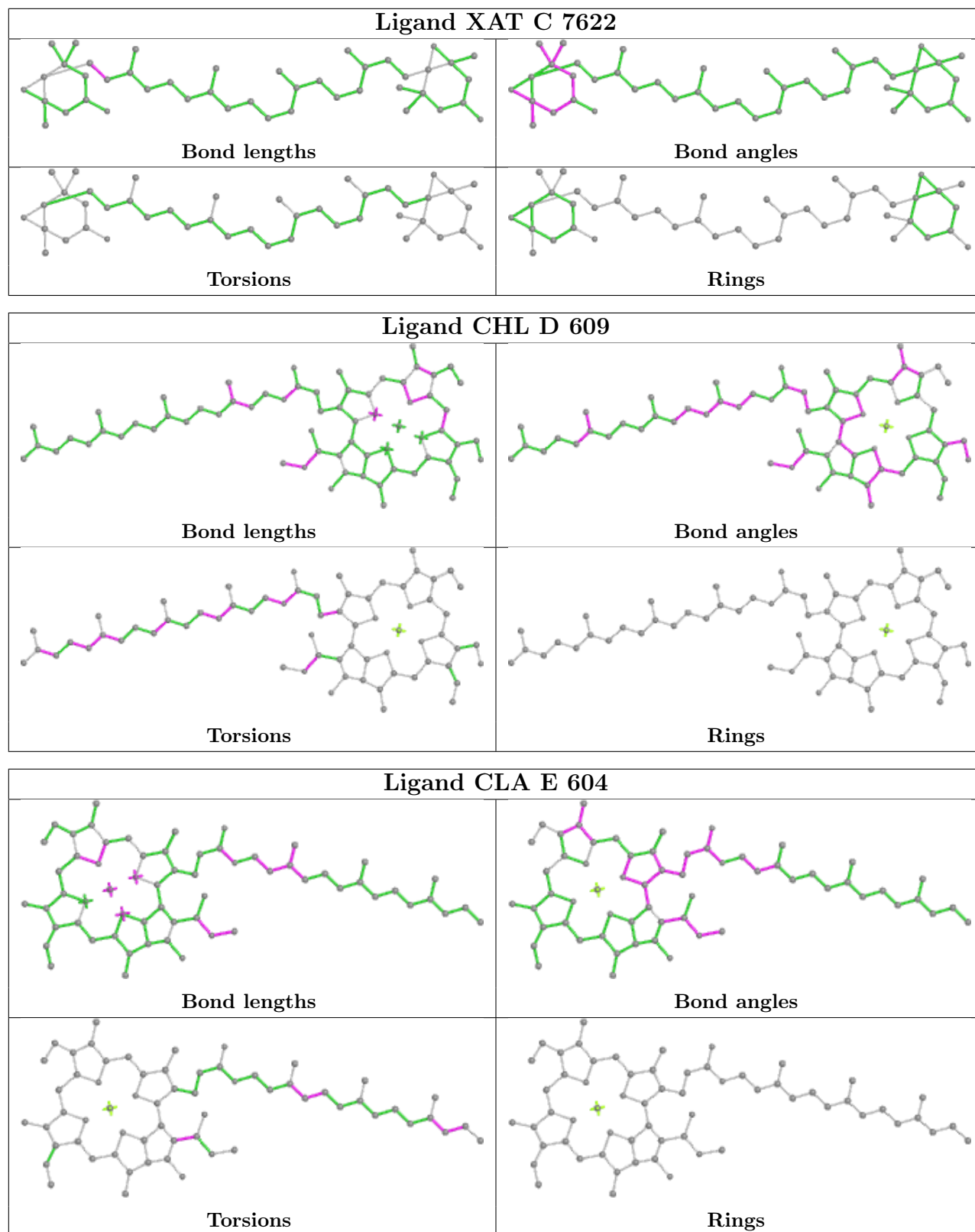


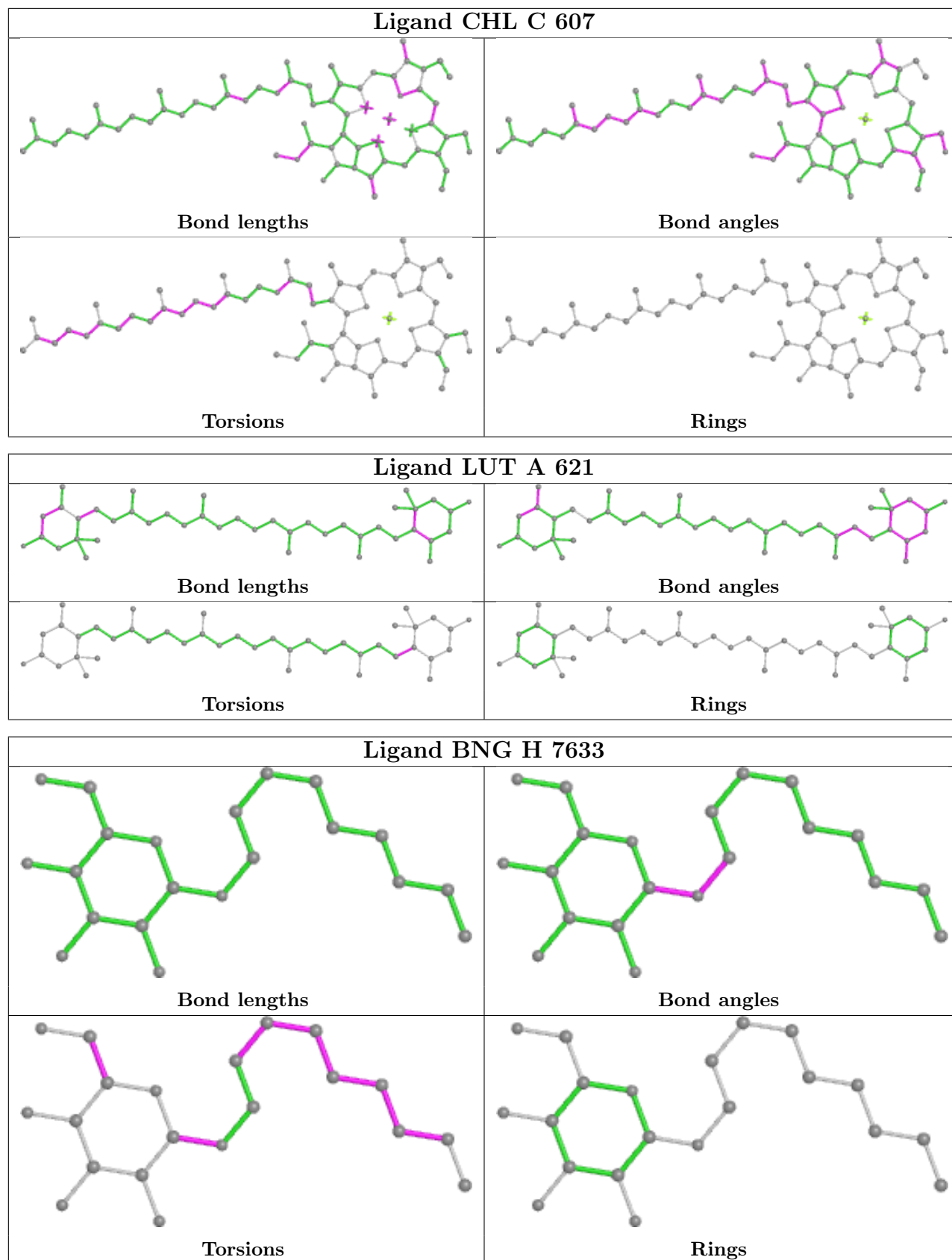


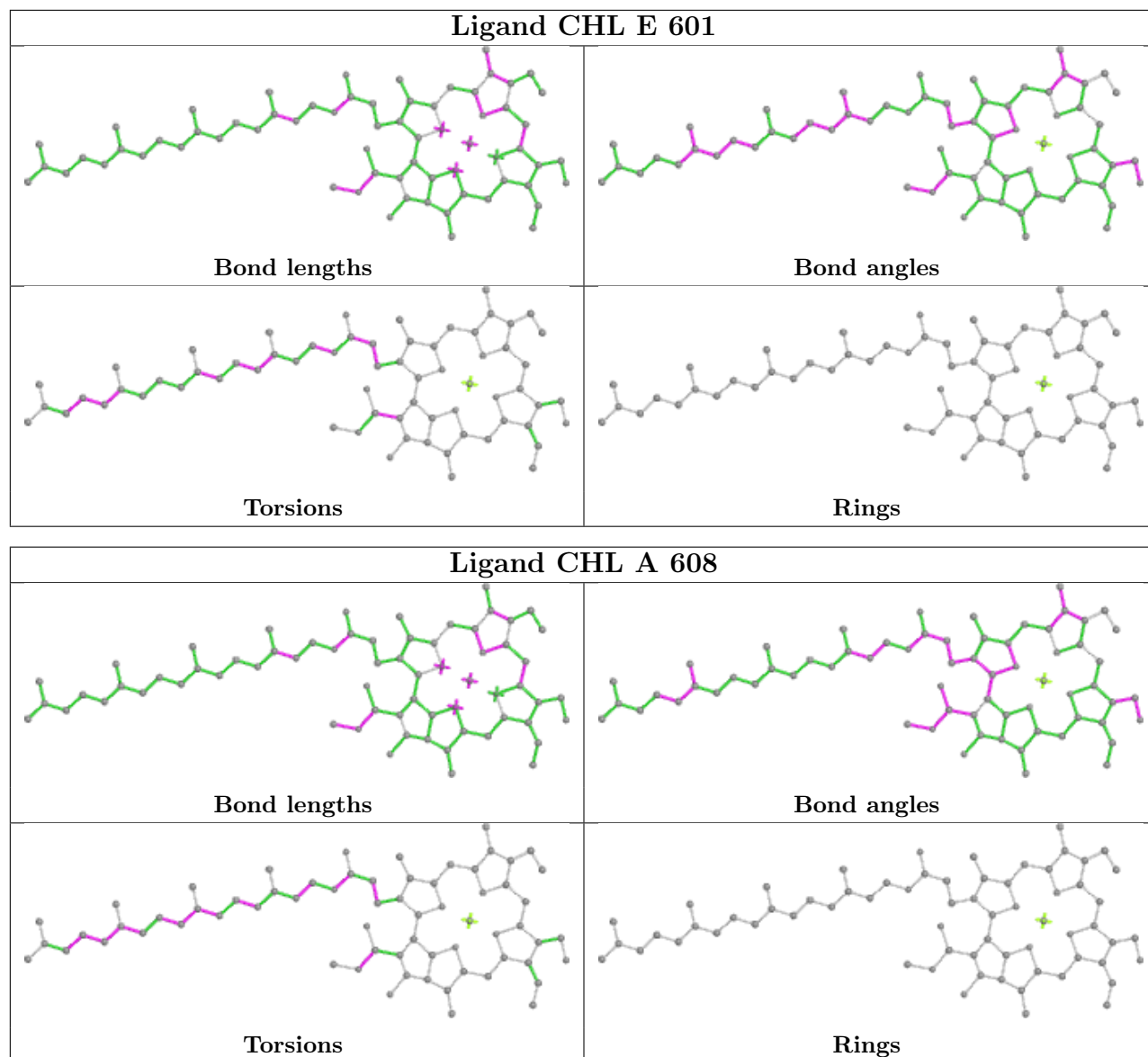


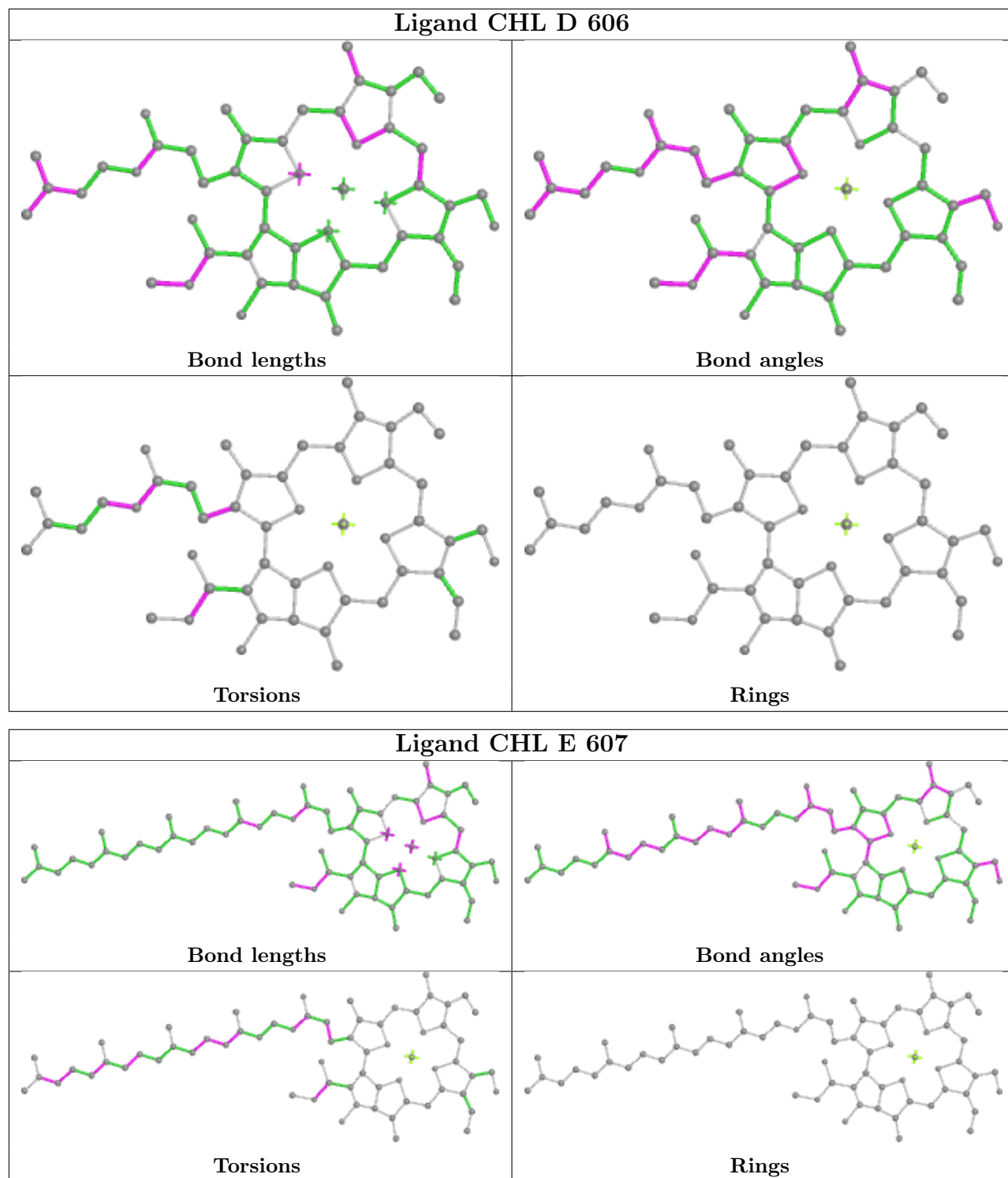


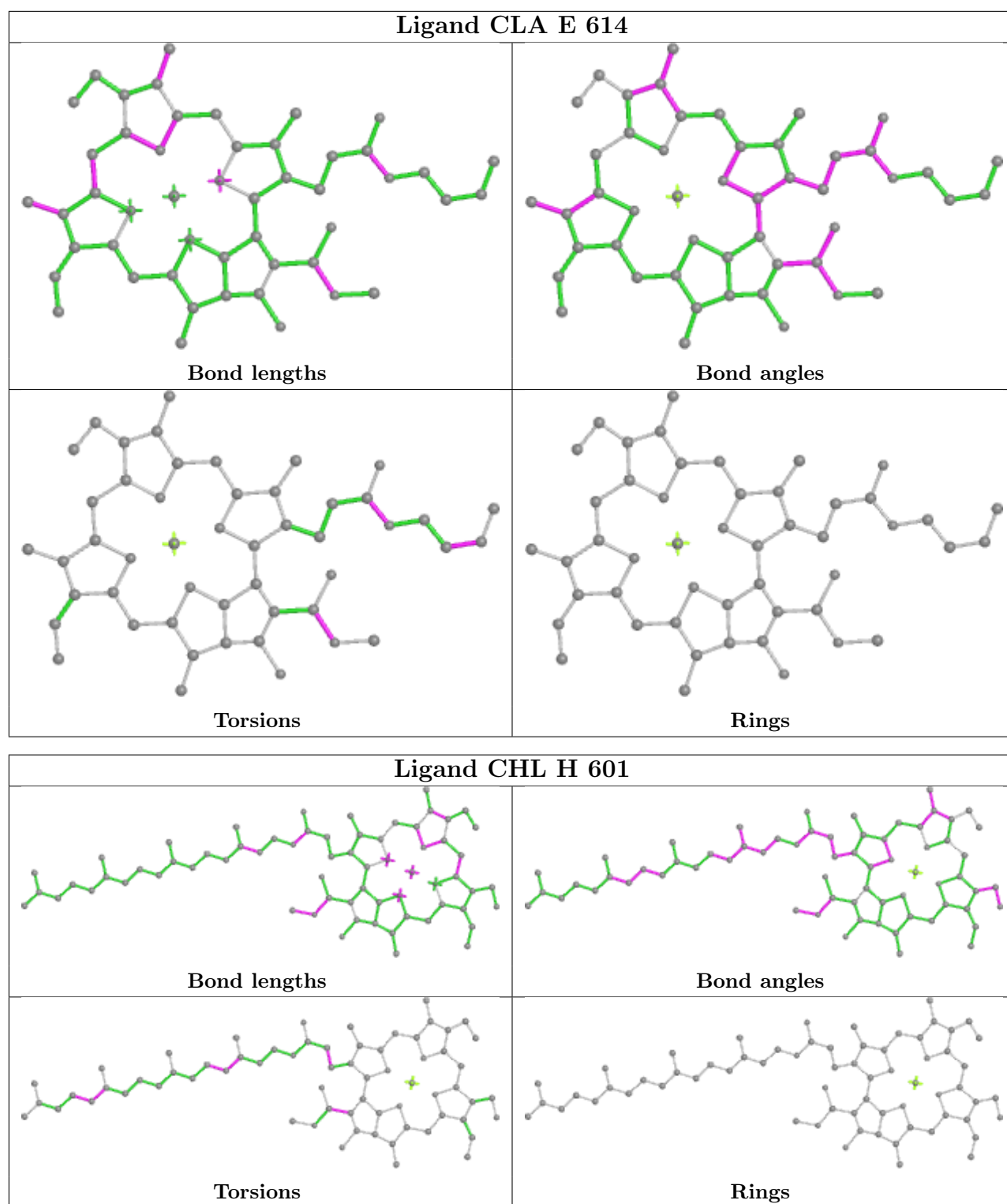


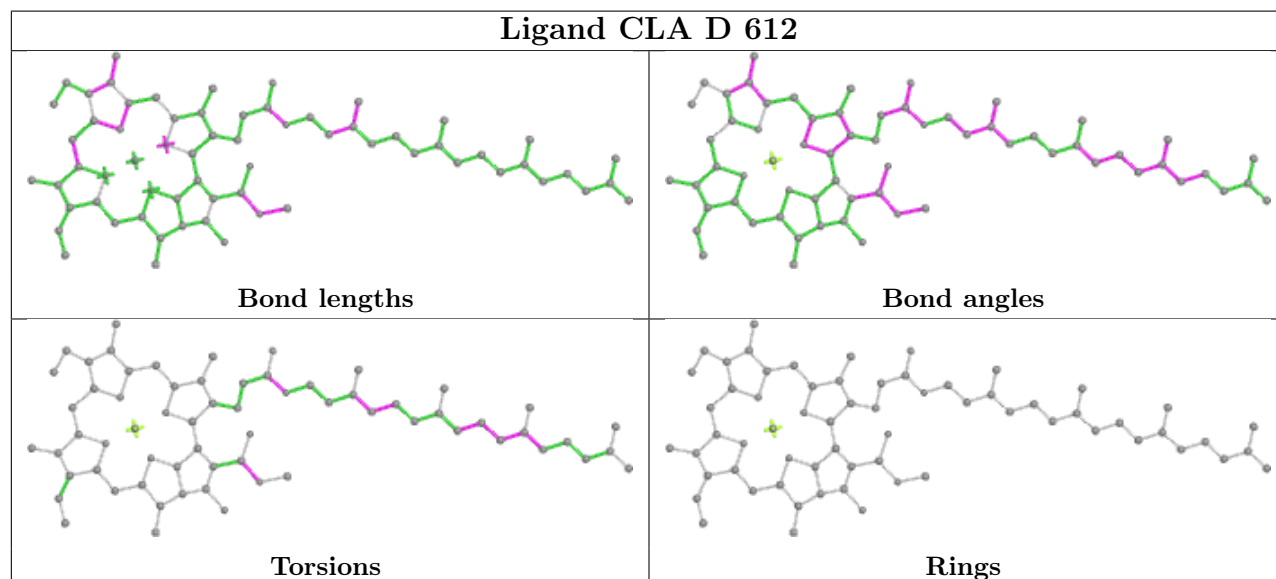
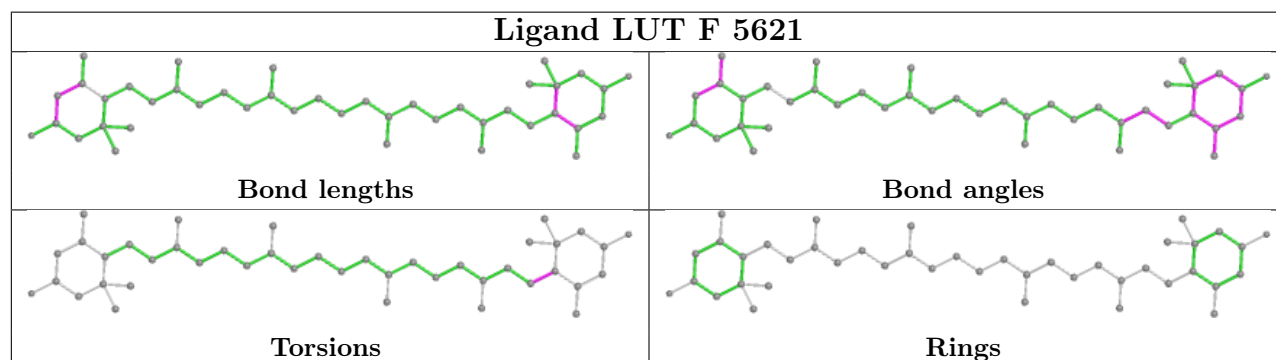
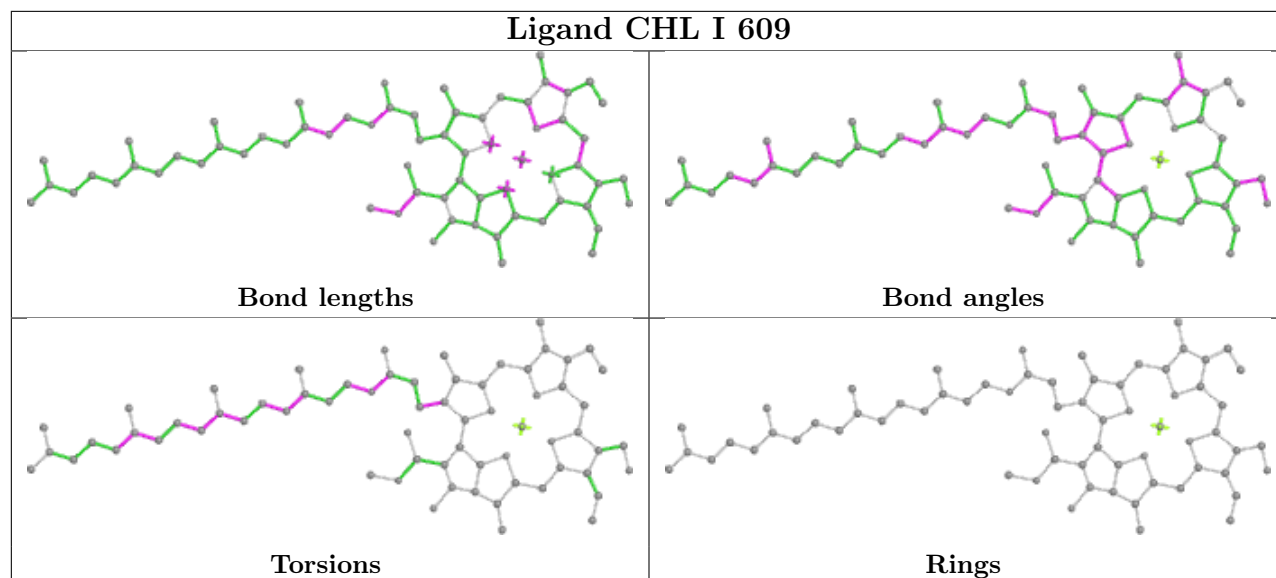


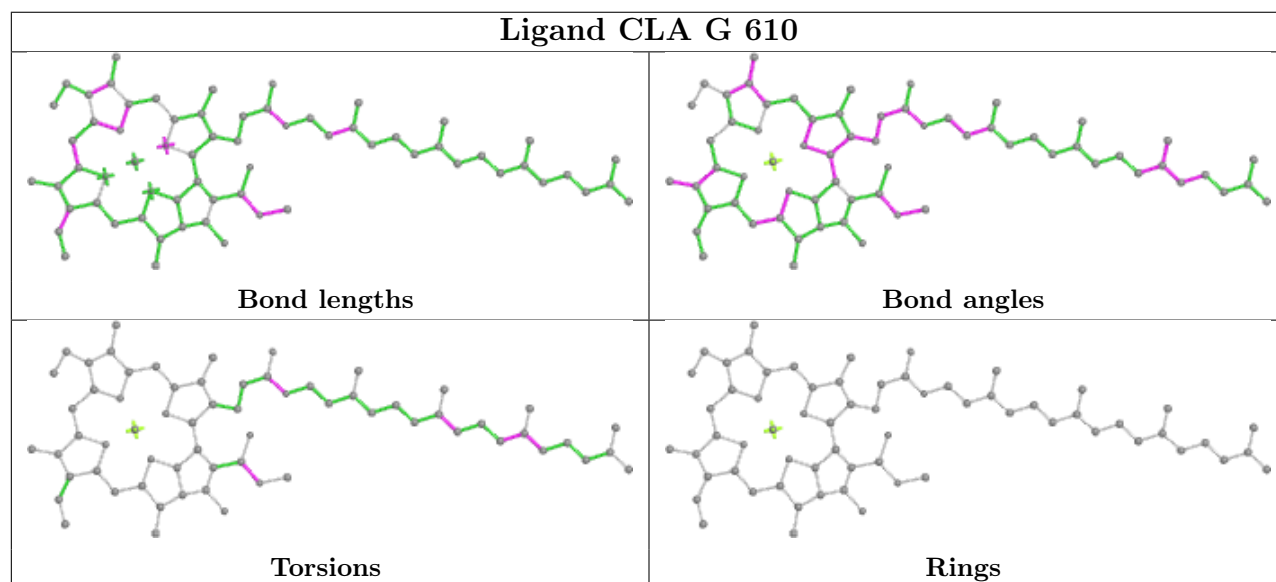
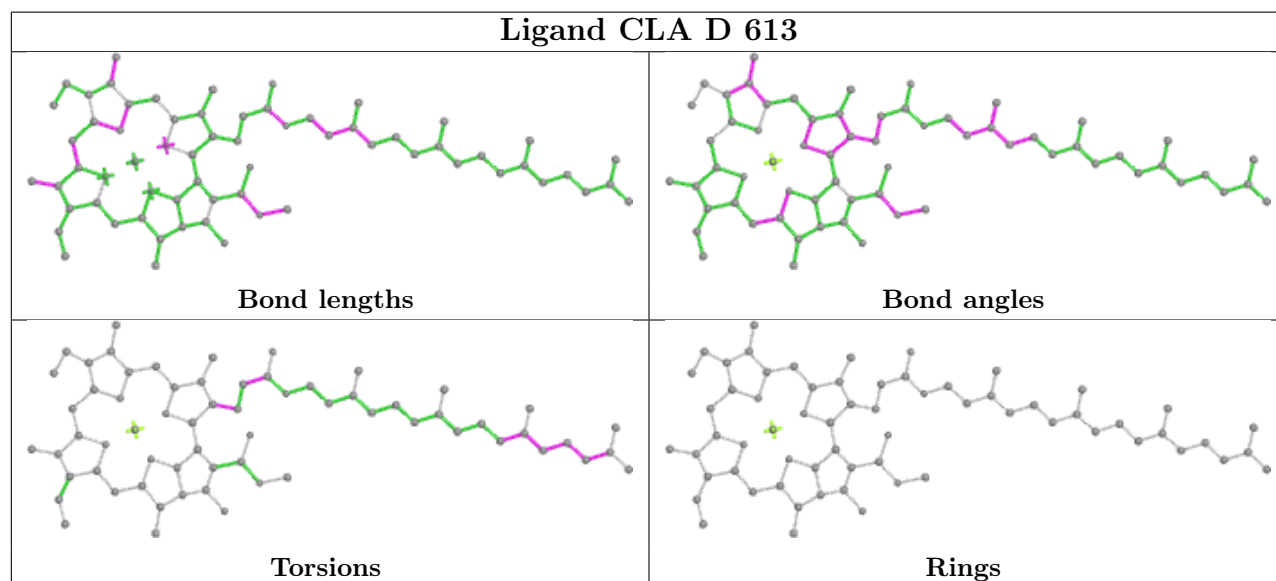
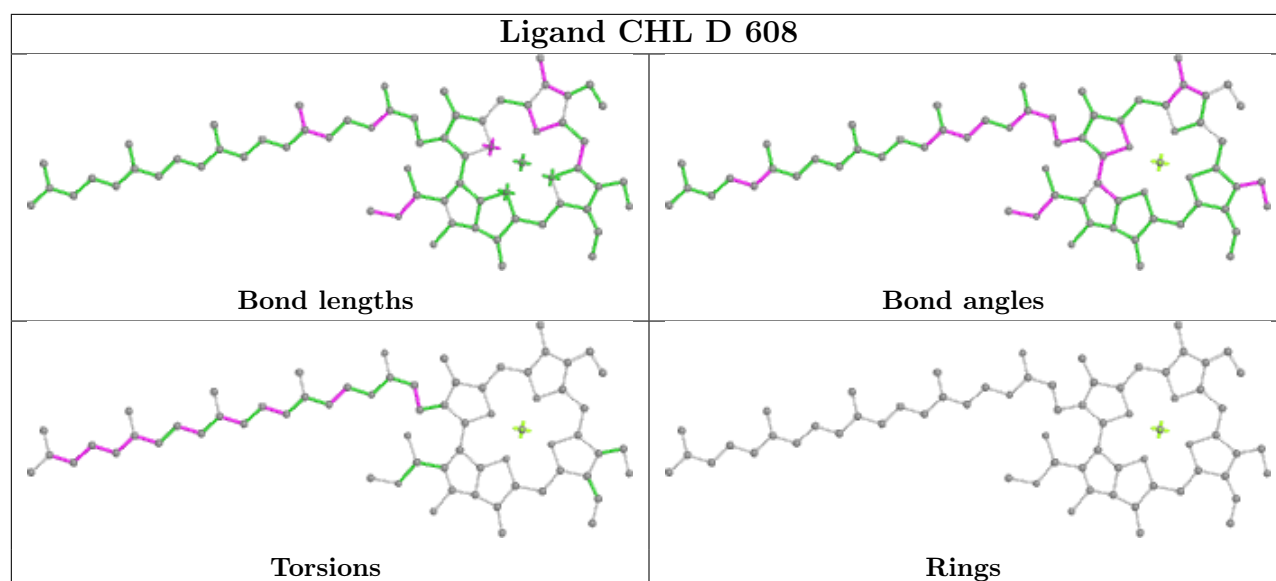




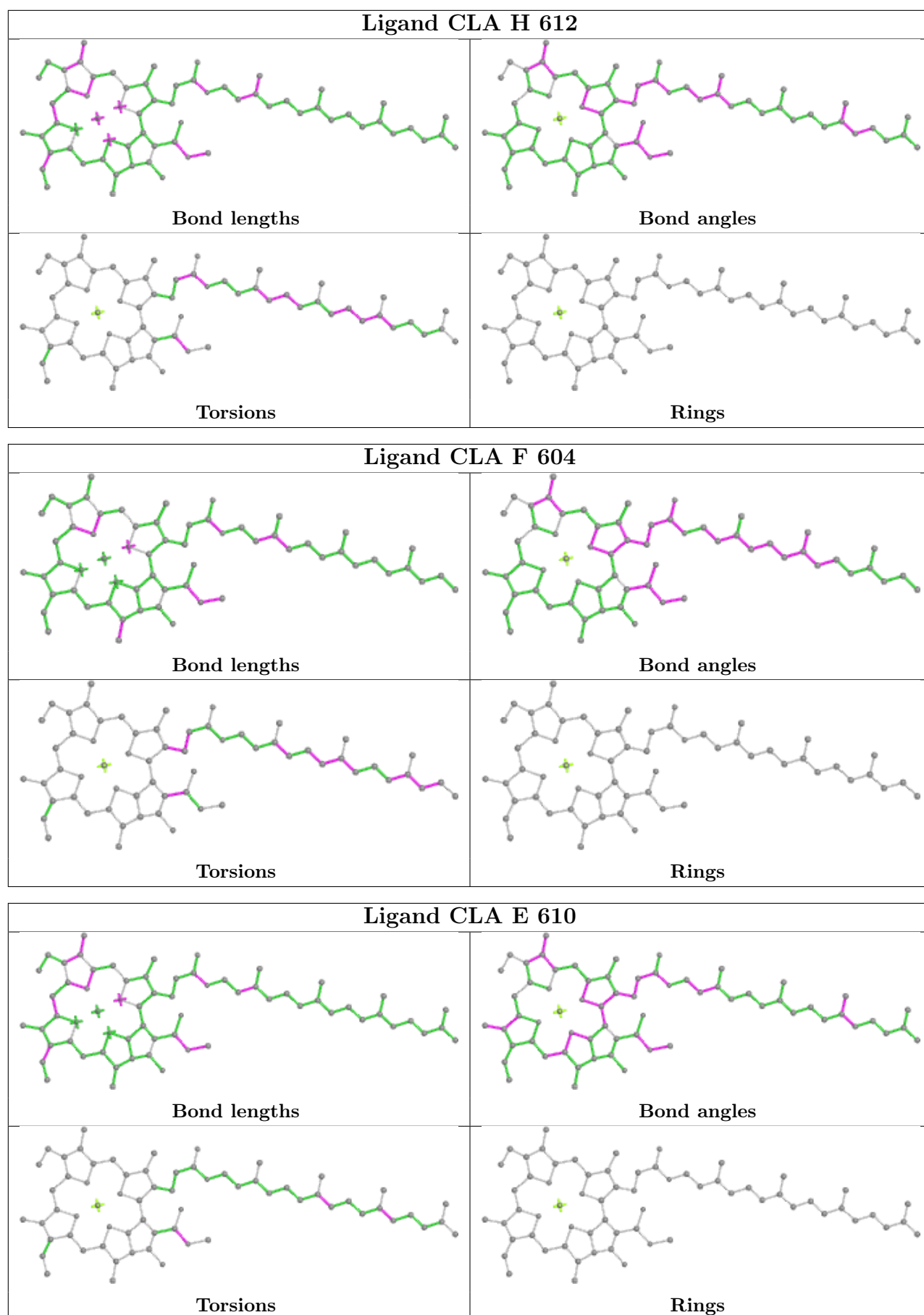












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	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

The worst 5 of 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

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	BNG	D	3633	21/21	0.61	0.41	61,86,92,92	0
2	BNG	G	6633	21/21	0.61	0.43	75,96,102,104	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	H	7633	21/21	0.64	0.38	71,90,97,99	0
2	BNG	J	9633	21/21	0.64	0.36	63,83,92,93	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	A	623	44/44	0.80	0.25	27,53,90,91	0
6	NEX	E	4623	44/44	0.80	0.25	16,30,74,76	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	G	9632	66/66	0.88	0.22	23,48,83,86	0
8	DGD	H	7632	66/66	0.88	0.22	30,50,82,83	0
8	DGD	D	5632	66/66	0.89	0.23	23,43,89,91	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
8	DGD	B	2632	66/66	0.89	0.22	21,44,77,79	0
8	DGD	I	8632	66/66	0.89	0.24	24,49,85,86	0
5	XAT	E	2622	44/44	0.90	0.16	16,22,27,30	0
5	XAT	A	622	44/44	0.90	0.17	16,26,34,38	0
8	DGD	D	3632	66/66	0.90	0.21	20,47,77,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	CLA	A	611	65/65	0.90	0.19	40,48,78,78	0
7	LHG	B	1630	49/49	0.91	0.21	32,40,55,60	0
5	XAT	B	5622	44/44	0.91	0.17	12,22,27,31	0
7	LHG	A	630	49/49	0.91	0.22	39,47,61,63	0
10	CLA	B	611	65/65	0.91	0.17	24,31,69,69	0
10	CLA	D	611	65/65	0.91	0.18	25,34,65,66	0
10	CLA	G	611	65/65	0.91	0.18	33,39,75,77	0
10	CLA	H	611	65/65	0.91	0.17	33,39,71,72	0
10	CLA	I	611	65/65	0.91	0.16	27,33,71,72	0
7	LHG	D	3630	49/49	0.92	0.18	30,36,55,60	0
7	LHG	E	4630	49/49	0.92	0.21	28,37,52,55	0
7	LHG	G	6630	49/49	0.92	0.20	31,38,57,61	0
7	LHG	I	8630	49/49	0.92	0.19	29,34,55,57	0
5	XAT	C	7622	44/44	0.92	0.15	17,23,31,34	0
5	XAT	D	8622	44/44	0.92	0.15	18,23,30,33	0
10	CLA	C	611	65/65	0.92	0.19	28,33,76,77	0
3	NA	A	634	1/1	0.92	0.34	1,1,1,1	1
10	CLA	E	611	65/65	0.92	0.17	26,32,70,72	0
5	XAT	F	6622	44/44	0.92	0.15	15,22,29,32	0
5	XAT	H	4622	44/44	0.92	0.15	20,24,30,34	0
5	XAT	I	9622	44/44	0.92	0.15	15,22,29,32	0
9	CHL	F	606	51/66	0.93	0.15	13,21,61,62	0
9	CHL	G	605	48/66	0.93	0.15	24,27,59,75	0
9	CHL	J	606	51/66	0.93	0.16	16,22,60,62	0
10	CLA	A	610	65/65	0.93	0.14	27,36,73,78	0
5	XAT	B	1622	44/44	0.93	0.14	17,23,28,30	0
10	CLA	B	604	62/65	0.93	0.17	19,22,75,78	0
7	LHG	J	9630	49/49	0.93	0.20	26,35,54,59	0
5	XAT	J	3622	44/44	0.93	0.14	17,24,29,31	0
7	LHG	F	5630	49/49	0.93	0.19	25,33,48,52	0
7	LHG	C	2630	49/49	0.93	0.18	24,30,48,50	0
10	CLA	F	611	65/65	0.93	0.15	20,26,73,75	0
7	LHG	H	7630	49/49	0.93	0.20	30,37,57,62	0
9	CHL	A	601	66/66	0.93	0.16	31,36,39,43	0
9	CHL	A	606	51/66	0.93	0.15	19,24,66,67	0
10	CLA	J	604	62/65	0.93	0.16	15,22,72,76	0
10	CLA	J	611	65/65	0.93	0.15	20,26,68,69	0
9	CHL	E	606	51/66	0.94	0.15	18,21,60,62	0
10	CLA	A	612	65/65	0.94	0.16	33,38,86,88	0
9	CHL	F	605	48/66	0.94	0.13	26,29,59,72	0
9	CHL	B	605	48/66	0.94	0.16	23,26,58,74	0
10	CLA	C	604	62/65	0.94	0.15	15,21,70,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CHL	C	605	48/66	0.94	0.15	25,29,58,72	0
10	CLA	C	612	65/65	0.94	0.15	20,31,82,85	0
9	CHL	G	608	66/66	0.94	0.14	27,31,67,68	0
10	CLA	E	604	62/65	0.94	0.16	18,23,75,79	0
9	CHL	H	605	48/66	0.94	0.14	24,30,60,73	0
10	CLA	F	604	62/65	0.94	0.16	17,21,76,81	0
9	CHL	H	606	51/66	0.94	0.14	17,22,67,69	0
10	CLA	F	612	65/65	0.94	0.15	22,28,79,81	0
10	CLA	G	604	62/65	0.94	0.15	17,24,75,79	0
9	CHL	I	605	48/66	0.94	0.15	29,32,60,73	0
10	CLA	G	612	65/65	0.94	0.16	22,33,89,91	0
10	CLA	H	604	62/65	0.94	0.16	18,25,69,74	0
10	CLA	H	610	65/65	0.94	0.15	24,32,69,74	0
9	CHL	I	606	51/66	0.94	0.14	15,19,62,64	0
10	CLA	H	612	65/65	0.94	0.17	24,34,86,87	0
10	CLA	I	604	62/65	0.94	0.17	20,25,77,81	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
10	CLA	I	612	65/65	0.94	0.15	23,30,87,90	0
10	CLA	A	604	62/65	0.94	0.16	18,25,74,79	0
9	CHL	D	606	51/66	0.94	0.16	16,22,60,61	0
9	CHL	F	608	66/66	0.95	0.13	22,28,63,65	0
10	CLA	B	612	65/65	0.95	0.13	18,27,88,89	0
10	CLA	B	614	49/65	0.95	0.11	10,22,59,69	0
9	CHL	G	601	66/66	0.95	0.14	27,32,36,40	0
10	CLA	C	610	65/65	0.95	0.13	15,21,65,70	0
9	CHL	B	608	66/66	0.95	0.12	16,22,63,63	0
9	CHL	G	606	51/66	0.95	0.14	15,23,59,60	0
10	CLA	D	604	62/65	0.95	0.16	20,25,66,70	0
4	LUT	G	6620	42/42	0.95	0.14	16,25,36,37	0
10	CLA	D	612	65/65	0.95	0.14	22,30,83,85	0
9	CHL	H	601	66/66	0.95	0.14	28,31,32,36	0
10	CLA	E	610	65/65	0.95	0.13	17,25,59,66	0
9	CHL	A	607	66/66	0.95	0.13	17,20,48,49	0
10	CLA	E	612	65/65	0.95	0.12	19,25,80,82	0
9	CHL	C	608	66/66	0.95	0.13	23,28,60,61	0
10	CLA	F	610	65/65	0.95	0.12	15,20,63,68	0
9	CHL	H	608	66/66	0.95	0.15	28,31,69,72	0
9	CHL	I	601	66/66	0.95	0.14	22,26,34,35	0
10	CLA	G	603	65/65	0.95	0.12	17,22,69,71	0
9	CHL	D	605	48/66	0.95	0.15	23,29,57,71	0
10	CLA	G	610	65/65	0.95	0.14	24,31,73,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CHL	A	608	66/66	0.95	0.12	30,35,67,68	0
9	CHL	I	608	66/66	0.95	0.13	21,26,66,67	0
9	CHL	J	605	48/66	0.95	0.13	20,26,59,71	0
9	CHL	D	608	66/66	0.95	0.14	24,29,65,67	0
9	CHL	J	608	66/66	0.95	0.14	19,26,67,68	0
10	CLA	A	603	65/65	0.95	0.11	20,26,77,78	0
10	CLA	H	614	49/65	0.95	0.12	16,26,60,68	0
9	CHL	E	601	66/66	0.95	0.14	23,28,31,33	0
9	CHL	E	605	48/66	0.95	0.15	20,25,58,71	0
9	CHL	B	601	66/66	0.95	0.14	22,26,37,38	0
9	CHL	A	605	48/66	0.95	0.15	19,25,57,71	0
10	CLA	I	614	49/65	0.95	0.14	20,23,58,67	0
10	CLA	A	614	49/65	0.95	0.13	20,27,59,66	0
10	CLA	J	610	65/65	0.95	0.12	18,24,64,67	0
9	CHL	B	606	51/66	0.95	0.14	11,20,60,62	0
10	CLA	J	614	49/65	0.95	0.13	14,22,57,67	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
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
4	LUT	I	8620	42/42	0.96	0.13	15,23,35,36	0
9	CHL	C	601	66/66	0.96	0.13	17,22,32,33	0
10	CLA	B	603	65/65	0.96	0.12	10,19,74,76	0
9	CHL	E	607	66/66	0.96	0.13	16,20,51,51	0
10	CLA	F	614	49/65	0.96	0.11	12,20,57,68	0
10	CLA	G	602	65/65	0.96	0.14	17,21,44,46	0
10	CLA	B	610	65/65	0.96	0.12	19,25,62,68	0
9	CHL	E	608	66/66	0.96	0.12	14,19,67,69	0
9	CHL	F	601	66/66	0.96	0.14	22,24,32,33	0
4	LUT	B	1621	42/42	0.96	0.14	8,14,23,25	0
4	LUT	C	2620	42/42	0.96	0.14	18,23,28,29	0
10	CLA	G	613	65/65	0.96	0.13	14,17,55,56	0
10	CLA	G	614	49/65	0.96	0.12	12,22,58,67	0
10	CLA	H	602	65/65	0.96	0.16	20,23,47,48	0
10	CLA	H	603	65/65	0.96	0.11	15,19,78,79	0
9	CHL	J	601	66/66	0.96	0.14	19,23,29,33	0
9	CHL	F	607	66/66	0.96	0.12	13,19,41,43	0
4	LUT	D	3620	42/42	0.96	0.13	18,24,35,36	0
10	CLA	C	614	49/65	0.96	0.11	14,18,54,65	0
10	CLA	D	603	65/65	0.96	0.10	14,21,74,75	0
10	CLA	I	602	65/65	0.96	0.15	17,21,52,57	0
10	CLA	I	603	65/65	0.96	0.11	16,20,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CHL	J	607	66/66	0.96	0.12	12,17,45,47	0
10	CLA	D	610	65/65	0.96	0.12	21,26,64,69	0
9	CHL	D	601	66/66	0.96	0.13	22,27,30,32	0
10	CLA	A	602	65/65	0.96	0.15	20,30,52,54	0
10	CLA	D	614	49/65	0.96	0.12	10,21,54,64	0
10	CLA	J	602	65/65	0.96	0.16	12,17,47,48	0
10	CLA	J	603	65/65	0.96	0.11	13,20,71,72	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
9	CHL	A	609	66/66	0.96	0.12	23,27,50,54	0
10	CLA	J	612	65/65	0.96	0.14	18,25,79,82	0
4	LUT	D	3621	42/42	0.96	0.17	11,19,23,23	0
10	CLA	F	602	65/65	0.97	0.14	9,17,42,48	0
9	CHL	G	607	66/66	0.97	0.13	15,17,49,51	0
10	CLA	A	613	65/65	0.97	0.13	15,19,46,49	0
4	LUT	F	5620	42/42	0.97	0.12	15,22,26,26	0
10	CLA	B	602	65/65	0.97	0.14	16,21,51,54	0
9	CHL	G	609	66/66	0.97	0.12	18,25,42,46	0
10	CLA	F	613	65/65	0.97	0.12	14,17,45,48	0
9	CHL	D	607	66/66	0.97	0.12	11,14,52,57	0
4	LUT	F	5621	42/42	0.97	0.14	11,19,22,24	0
9	CHL	D	609	66/66	0.97	0.10	18,23,42,46	0
9	CHL	H	607	66/66	0.97	0.12	12,18,49,50	0
10	CLA	B	613	65/65	0.97	0.13	13,17,52,56	0
4	LUT	C	2621	42/42	0.97	0.14	13,18,21,22	0
10	CLA	C	602	65/65	0.97	0.15	10,19,38,39	0
10	CLA	C	603	65/65	0.97	0.11	12,18,76,78	0
9	CHL	H	609	66/66	0.97	0.11	21,26,45,51	0
4	LUT	G	6621	42/42	0.97	0.15	16,21,23,25	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	C	613	65/65	0.97	0.11	13,15,43,47	0
9	CHL	I	607	66/66	0.97	0.11	11,17,53,56	0
10	CLA	D	602	65/65	0.97	0.14	13,20,45,46	0
10	CLA	H	613	65/65	0.97	0.12	10,17,55,57	0
9	CHL	B	609	66/66	0.97	0.11	14,20,43,47	0
9	CHL	I	609	66/66	0.97	0.12	17,20,45,50	0
9	CHL	E	609	66/66	0.97	0.11	16,19,40,43	0
4	LUT	H	7621	42/42	0.97	0.15	13,20,24,25	0
4	LUT	B	1620	42/42	0.97	0.11	13,19,30,30	0
10	CLA	D	613	65/65	0.97	0.12	15,18,50,52	0
4	LUT	I	8621	42/42	0.97	0.14	12,20,22,24	0

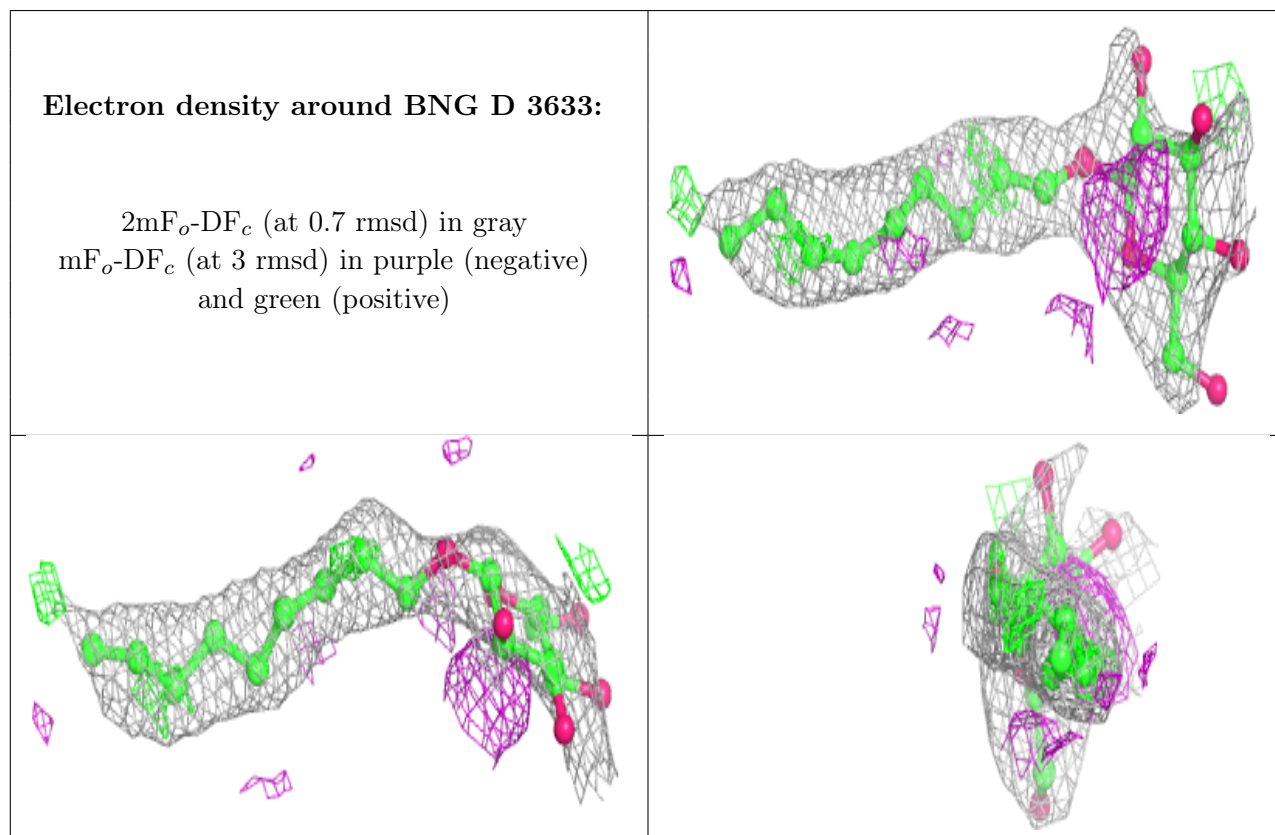
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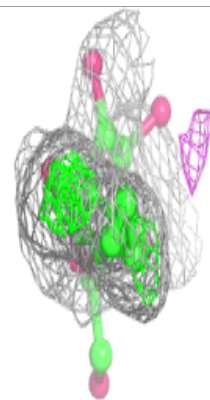
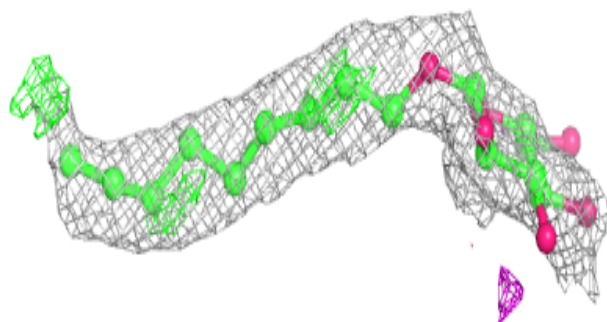
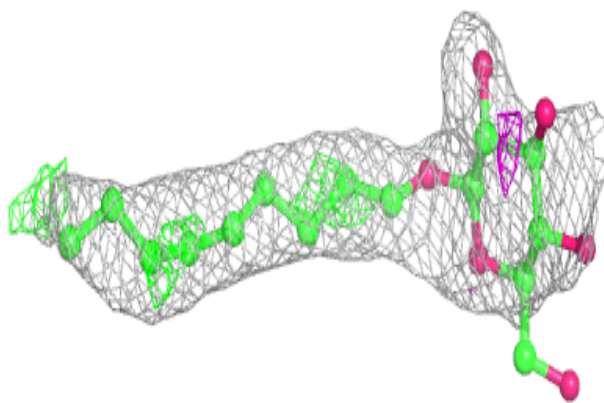
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	CLA	I	613	65/65	0.97	0.12	15,19,49,51	0
9	CHL	C	607	66/66	0.97	0.12	15,18,46,49	0
9	CHL	J	609	66/66	0.97	0.11	13,19,39,43	0
4	LUT	J	9620	42/42	0.97	0.10	11,18,34,35	0
9	CHL	F	609	66/66	0.97	0.11	14,22,43,47	0
9	CHL	C	609	66/66	0.97	0.10	15,22,41,42	0
4	LUT	J	9621	42/42	0.97	0.14	14,19,21,24	0
10	CLA	E	613	65/65	0.97	0.12	15,18,54,57	0
10	CLA	J	613	65/65	0.97	0.12	11,17,56,59	0
4	LUT	E	4620	42/42	0.97	0.10	16,21,29,30	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.

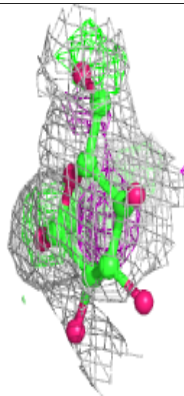
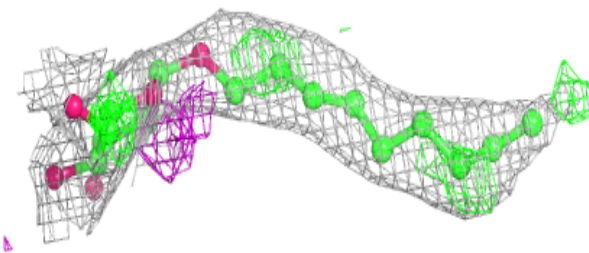
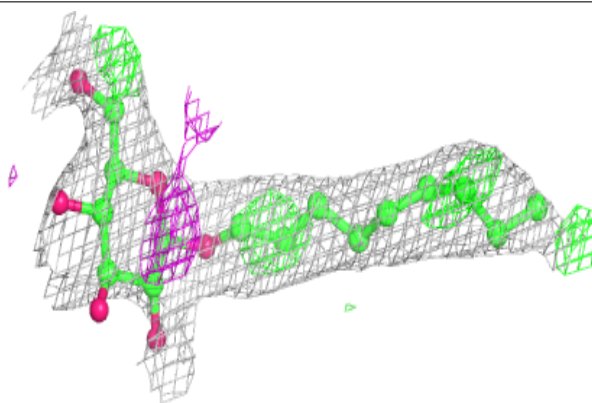


**Electron density around BNG G 6633:**

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

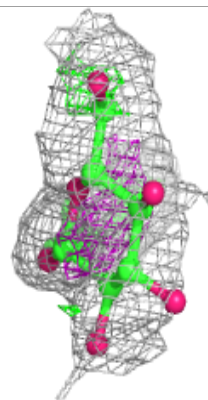
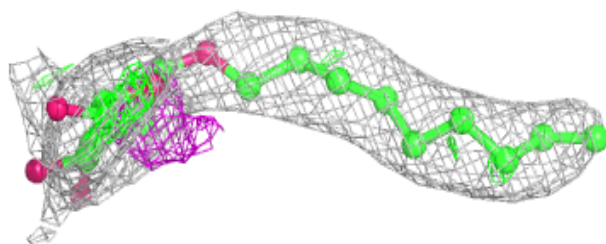
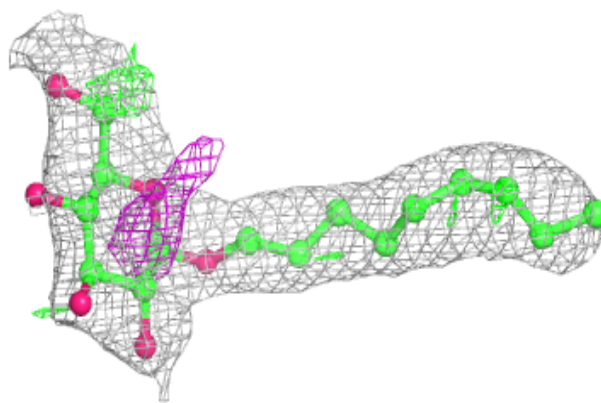
**Electron density around BNG C 2633:**

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

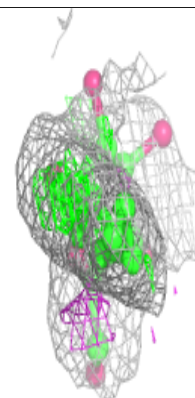
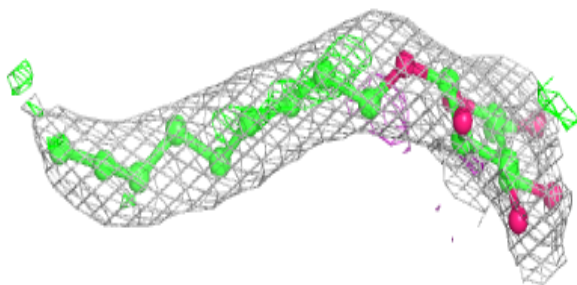
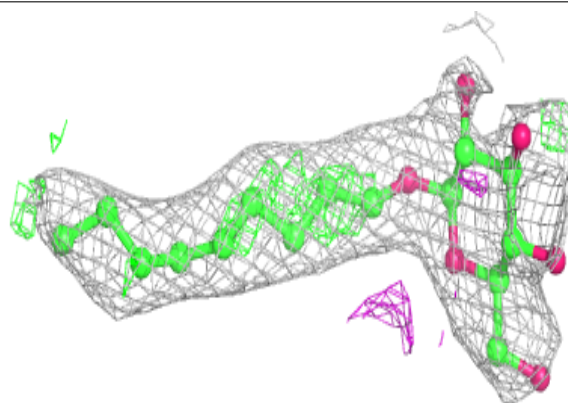


**Electron density around BNG A 633:**

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

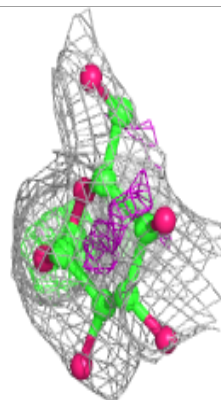
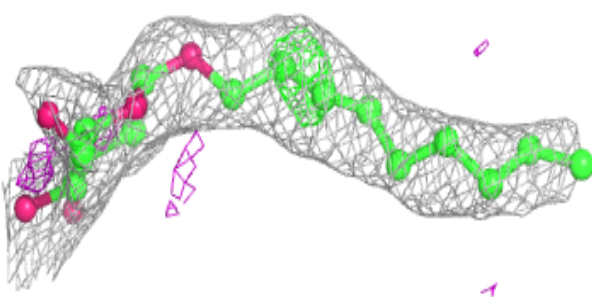
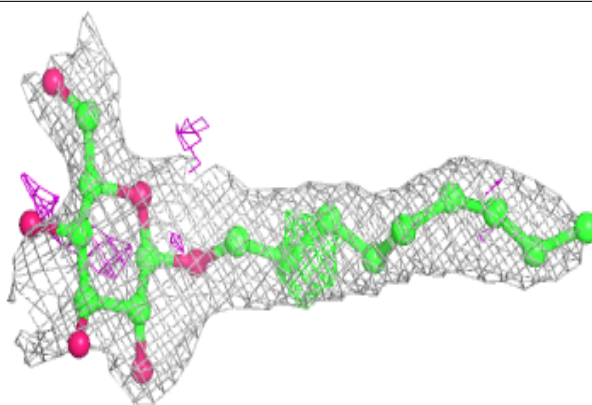
**Electron density around BNG E 4633:**

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

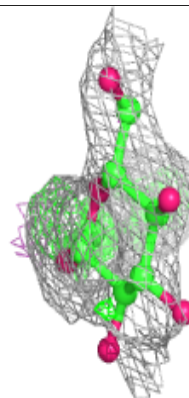
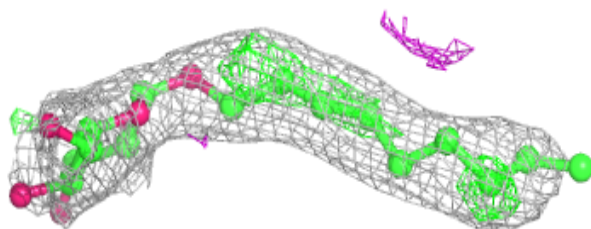
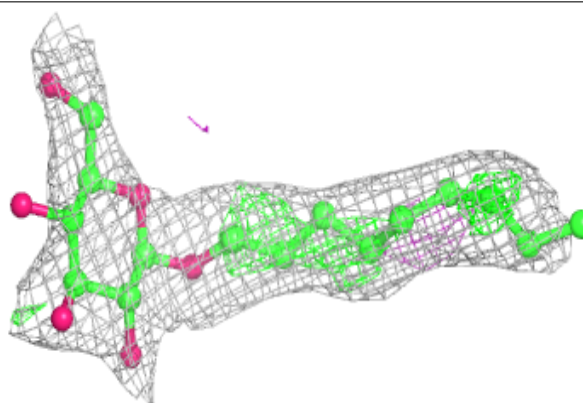


**Electron density around BNG H 7633:**

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

**Electron density around BNG J 9633:**

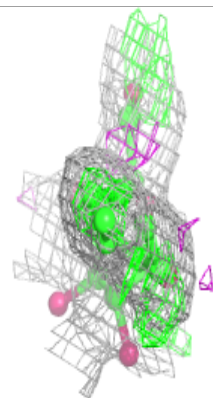
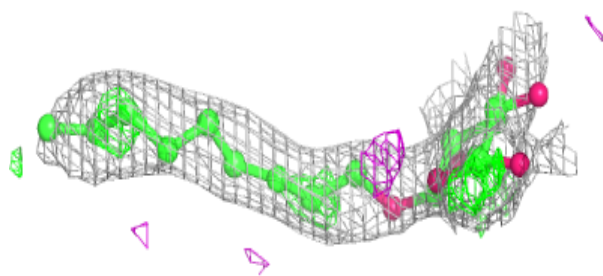
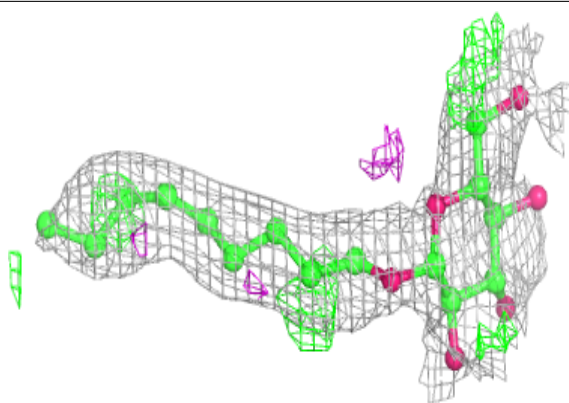
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



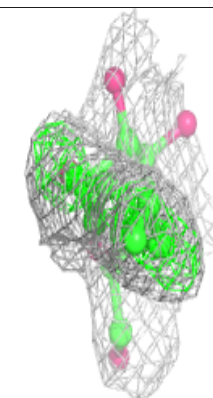
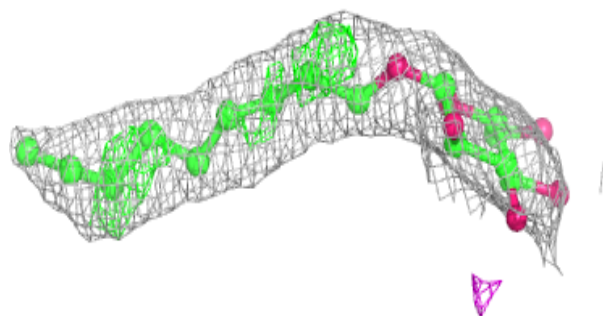
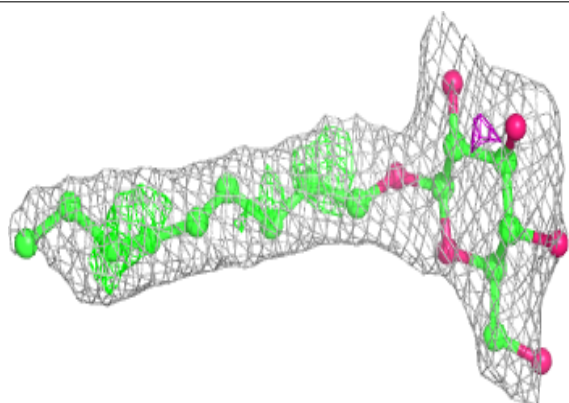


**Electron density around BNG B 1633:**

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

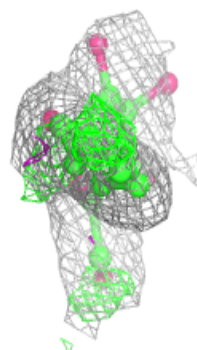
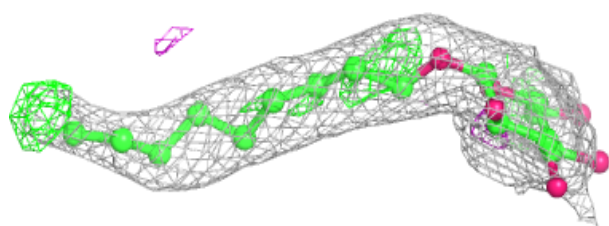
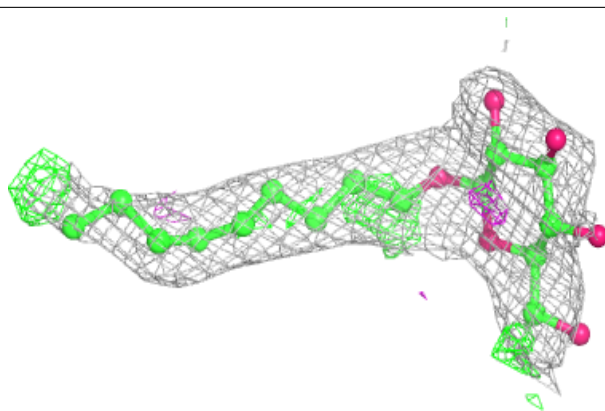
**Electron density around BNG F 5633:**

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

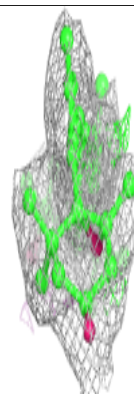
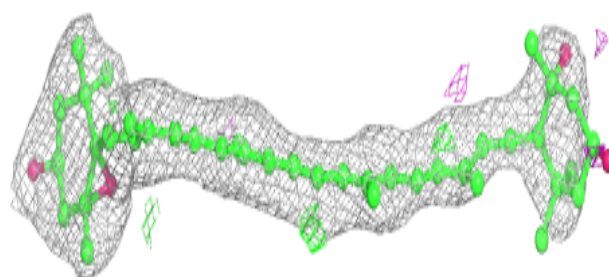
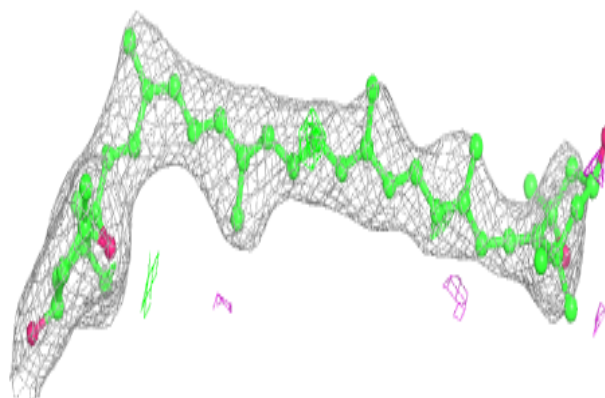


**Electron density around BNG I 8633:**

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

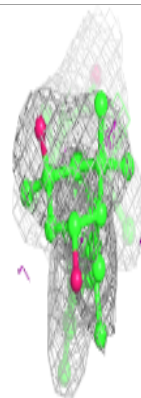
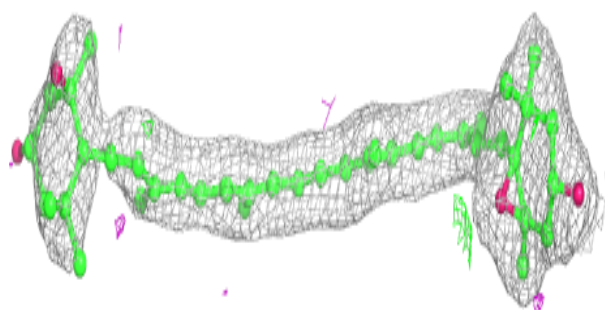
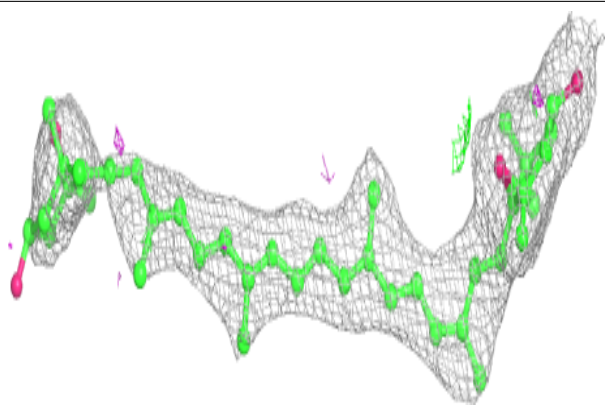
**Electron density around NEX H 7623:**

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

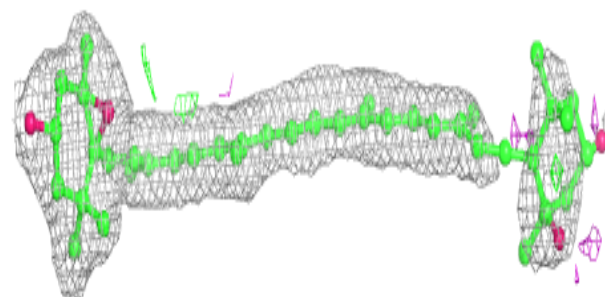
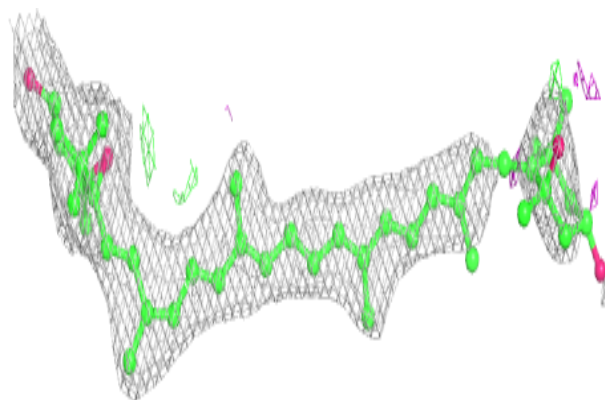


**Electron density around NEX G 6623:**

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

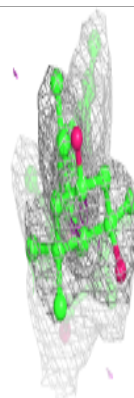
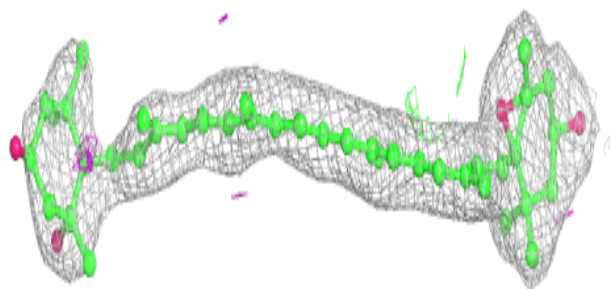
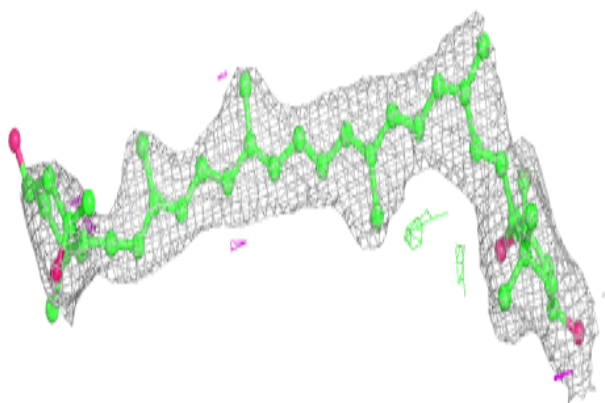
**Electron density around NEX J 9623:**

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

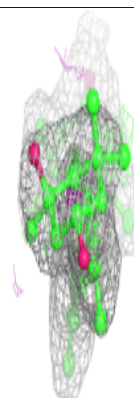
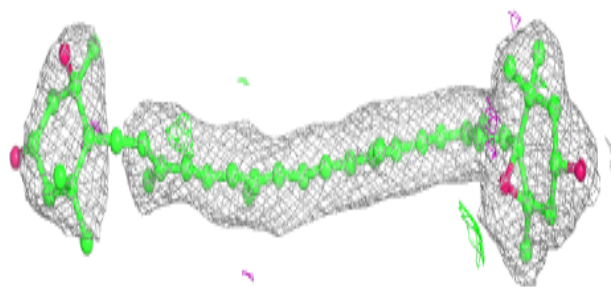
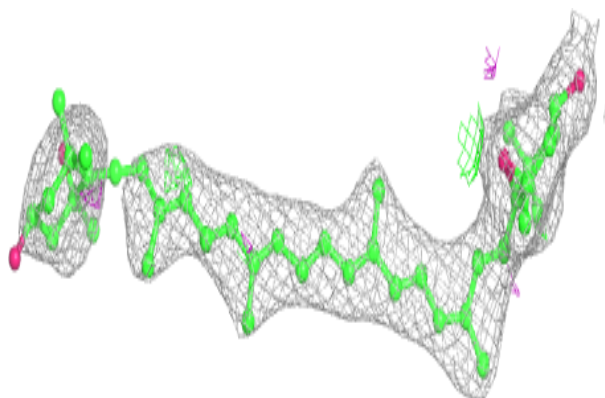


**Electron density around NEX I 8623:**

$2mF_o-DF_c$  (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:**

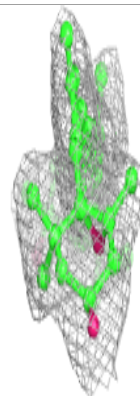
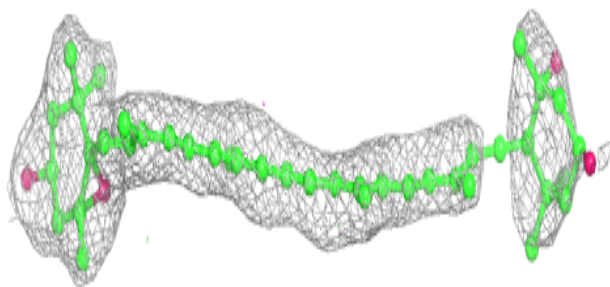
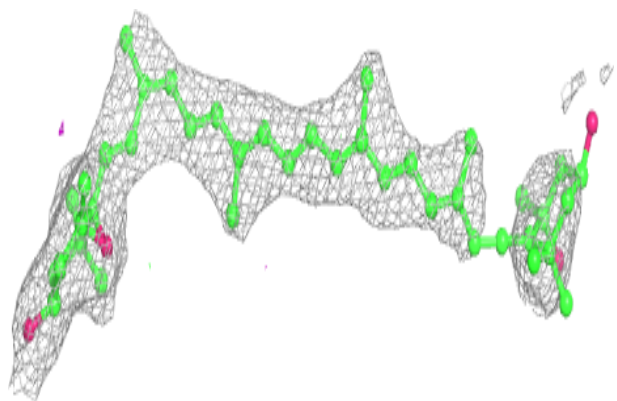
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



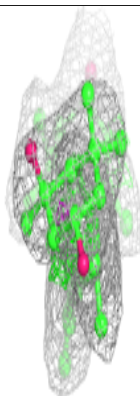
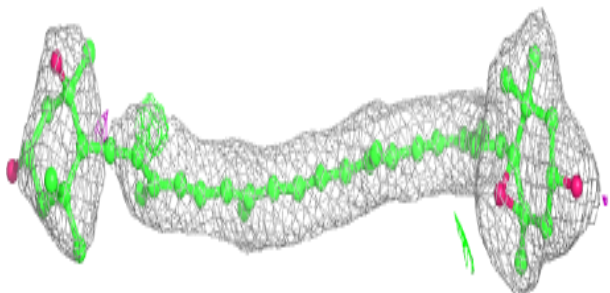
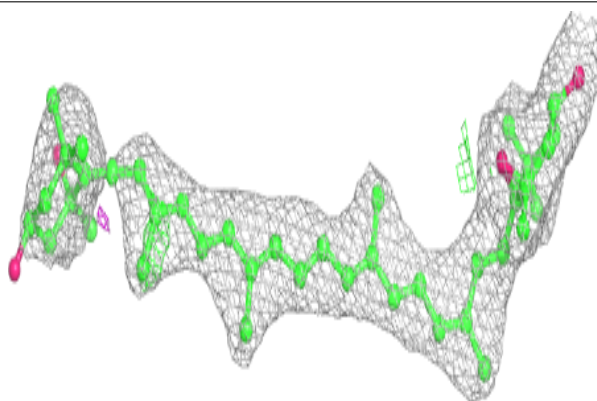


**Electron density around NEX A 623:**

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

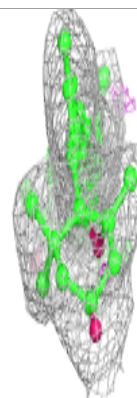
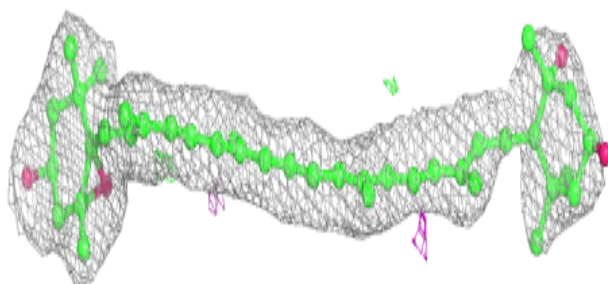
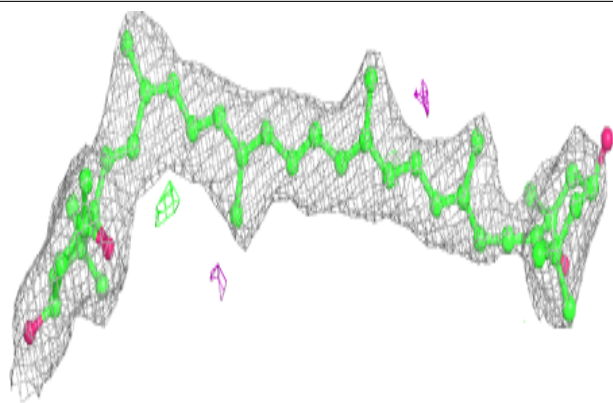
**Electron density around NEX E 4623:**

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

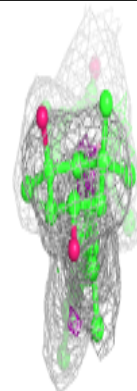
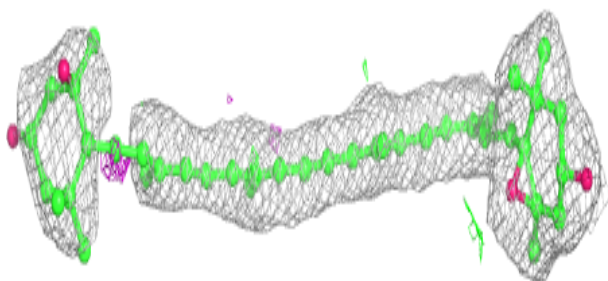
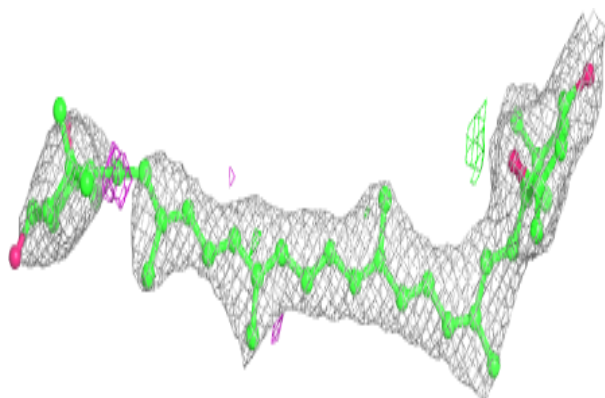


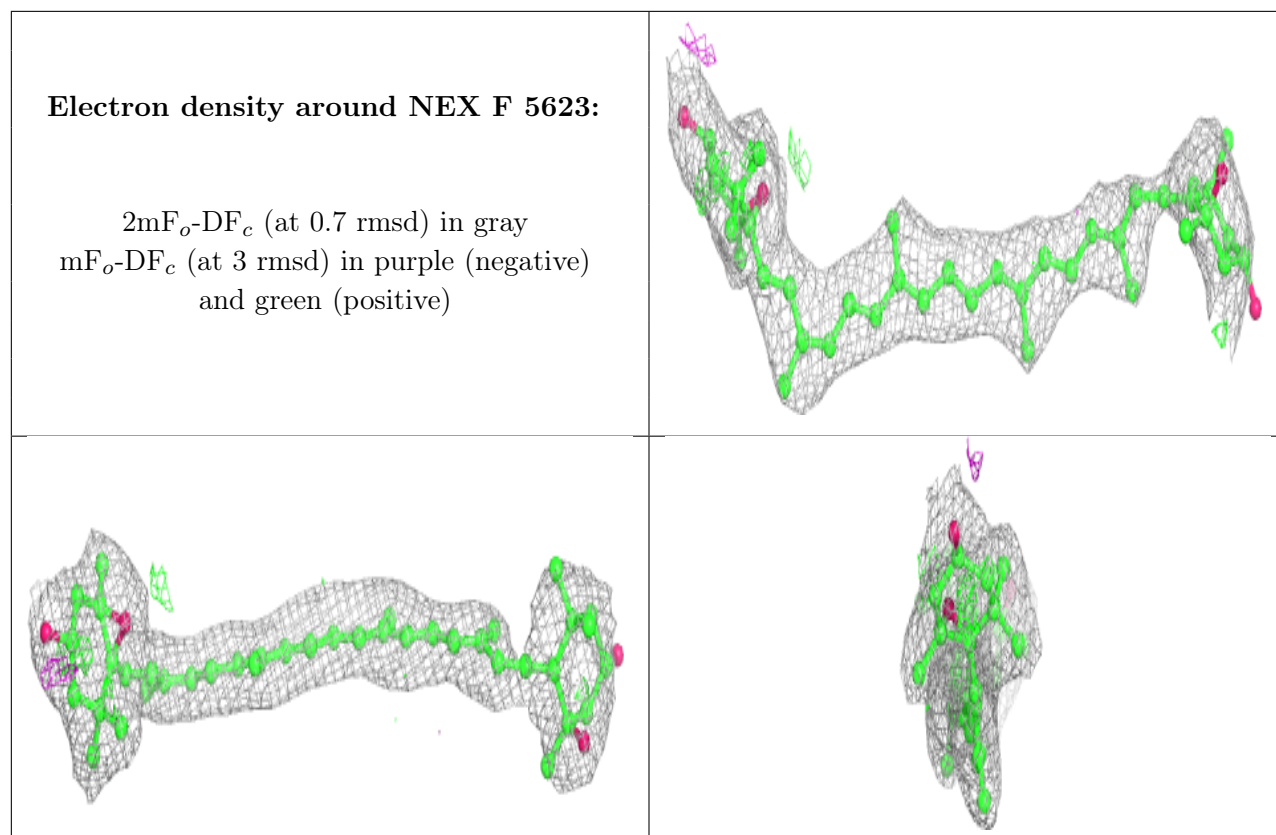
**Electron density around NEX B 1623:**

$2mF_o-DF_c$  (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:**

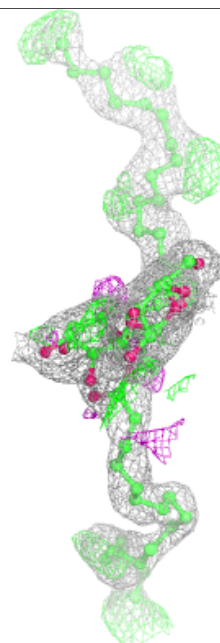
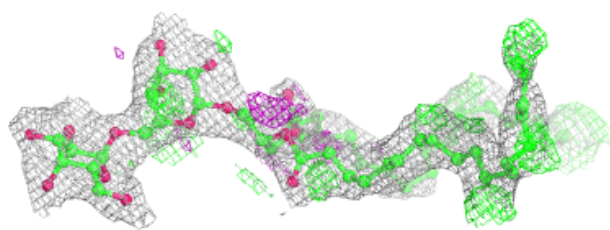
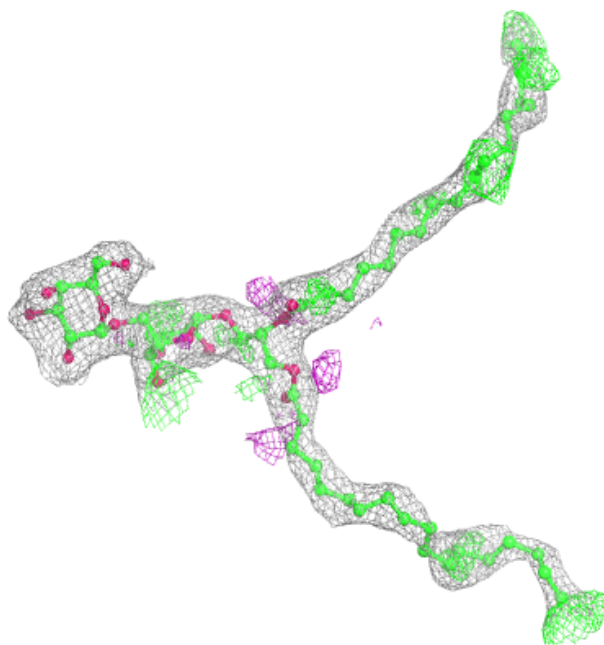
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





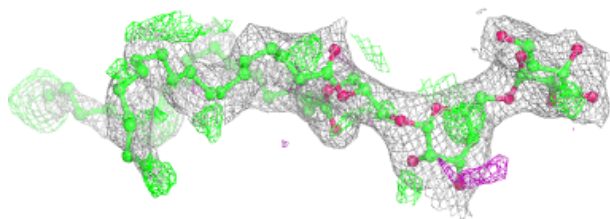
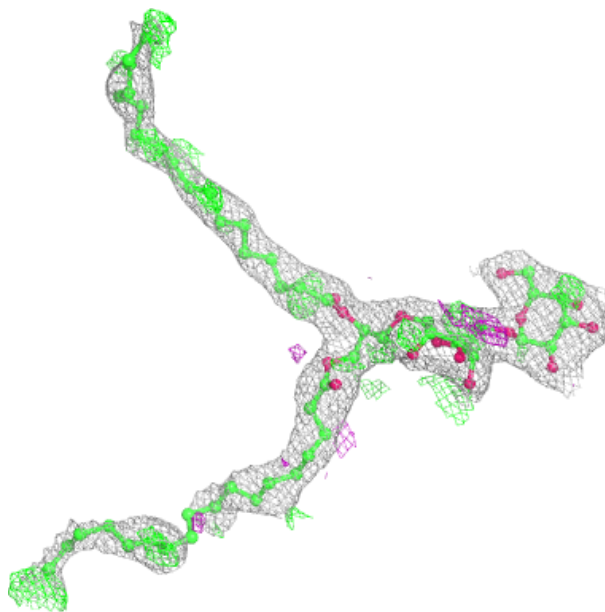
**Electron density around DGD A 632:**

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



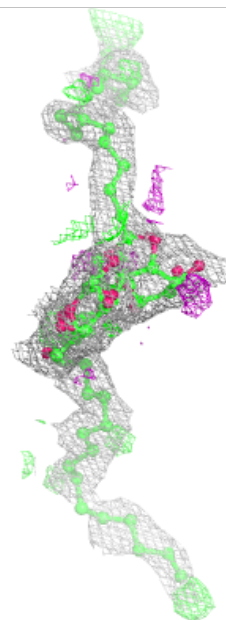
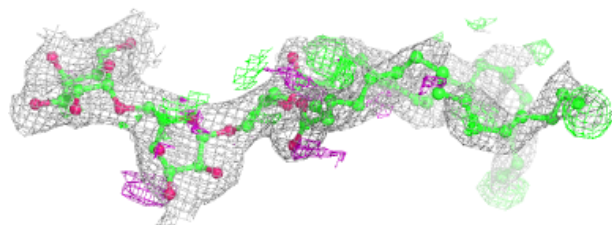
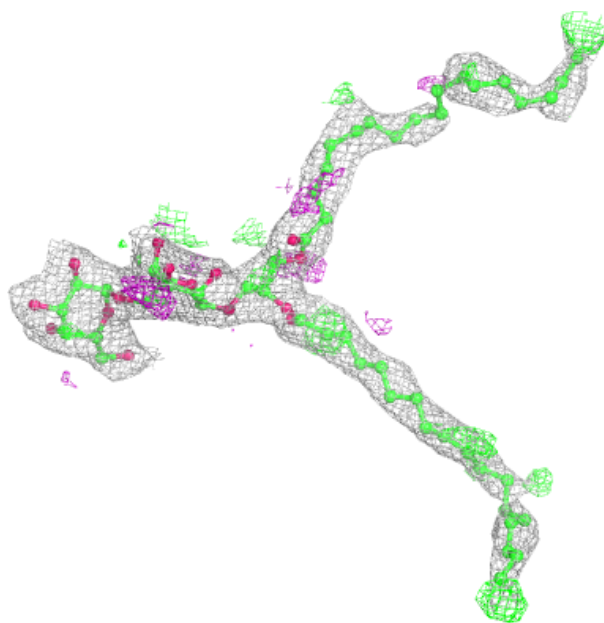
**Electron density around DGD G 9632:**

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



**Electron density around DGD H 7632:**

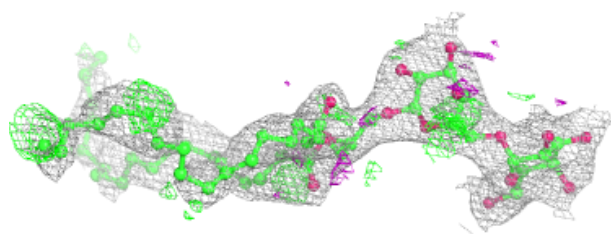
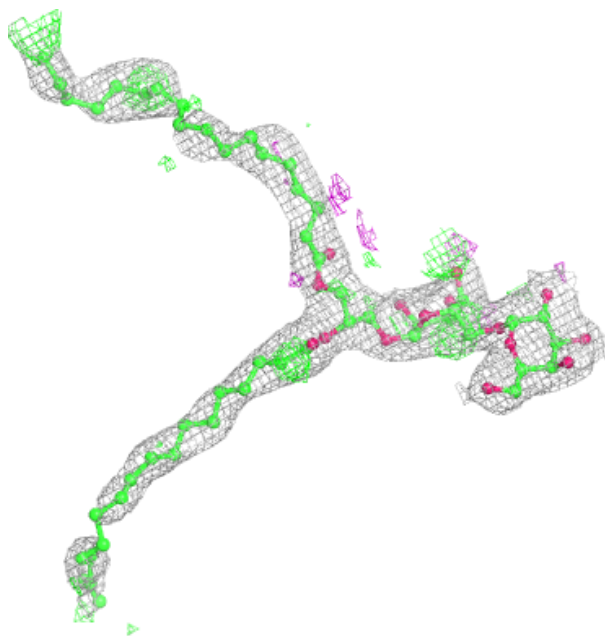
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





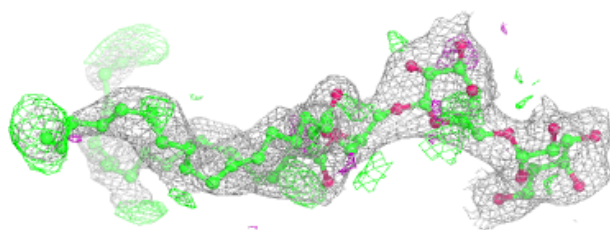
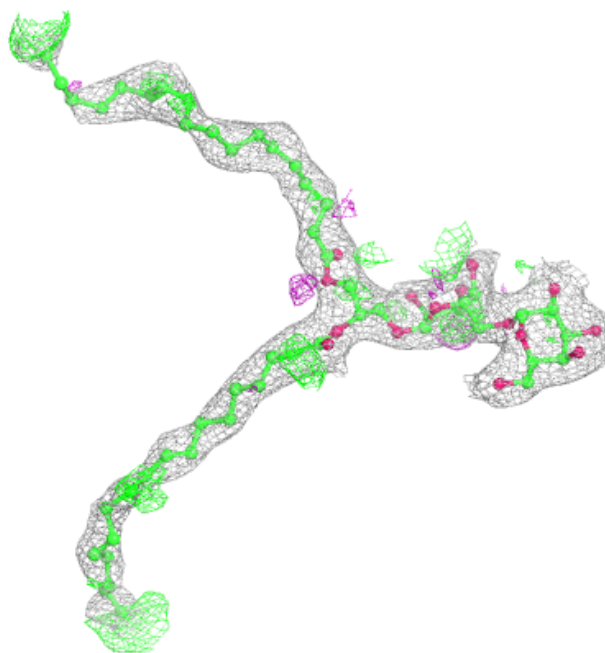
**Electron density around DGD D 5632:**

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



**Electron density around DGD E 4632:**

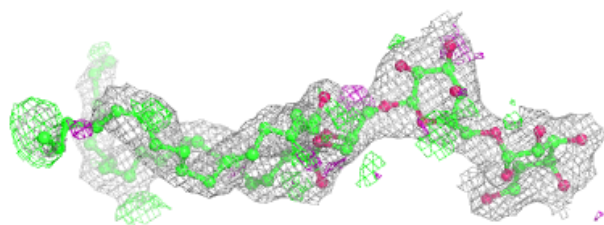
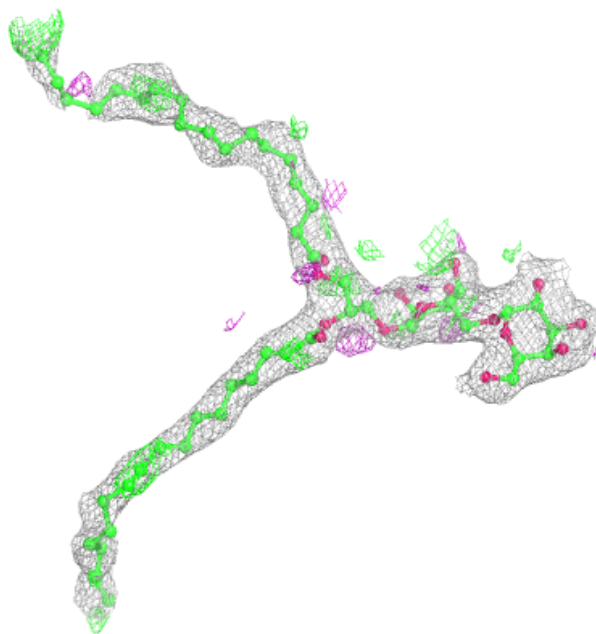
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





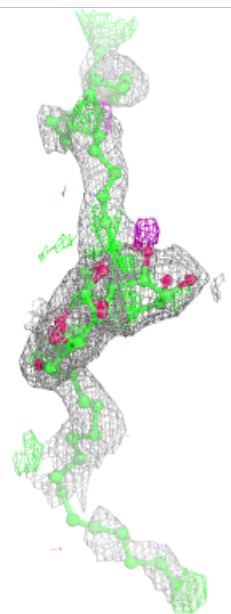
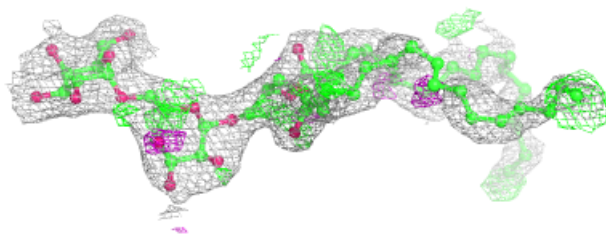
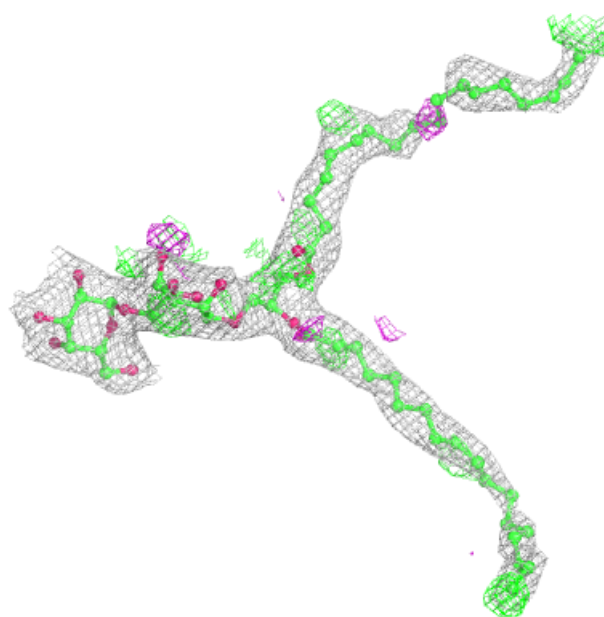
**Electron density around DGD B 1632:**

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



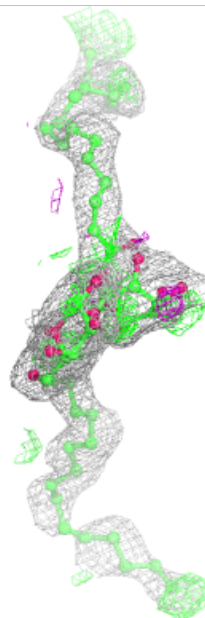
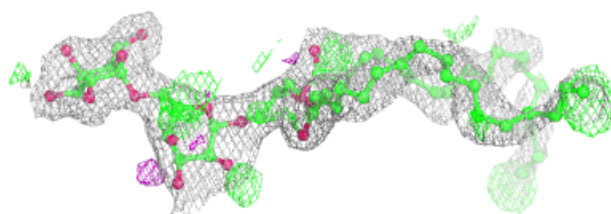
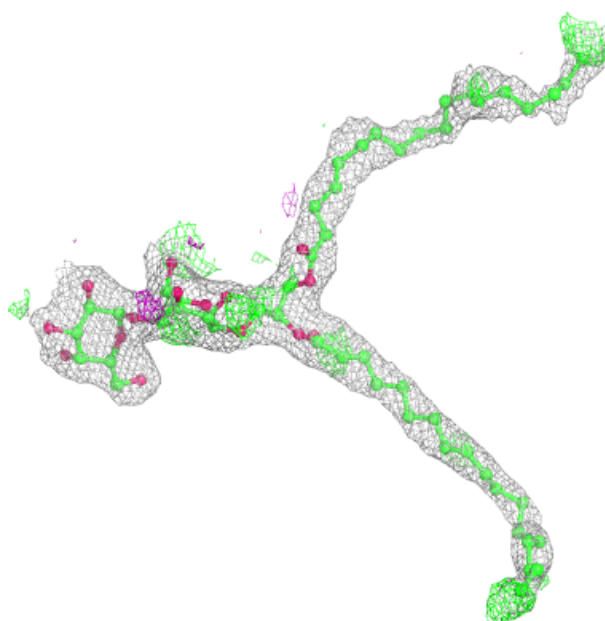
**Electron density around DGD H 6632:**

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



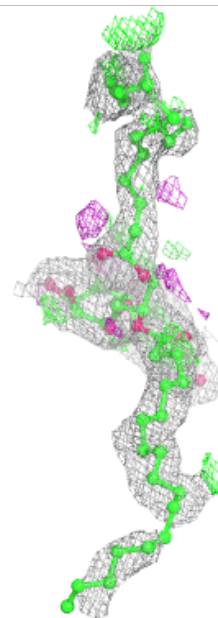
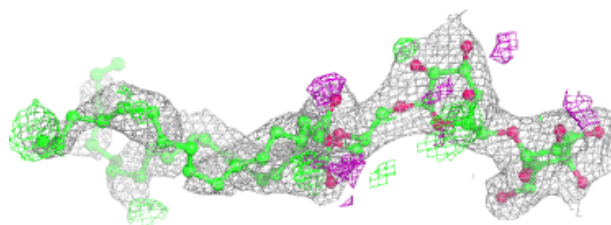
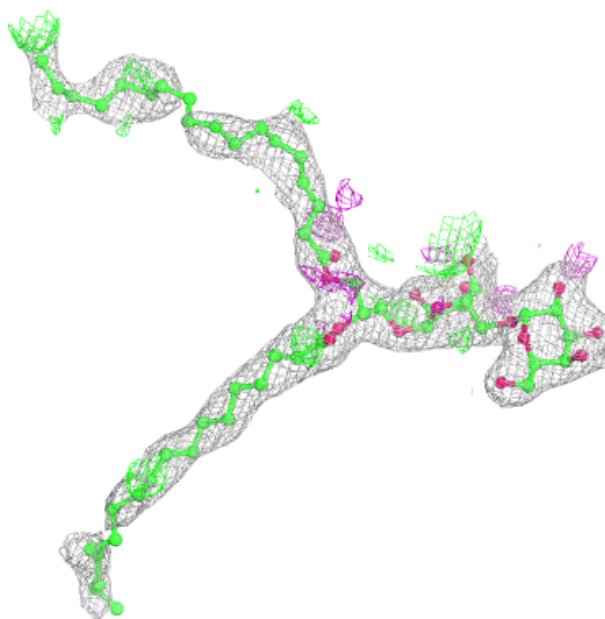
**Electron density around DGD B 2632:**

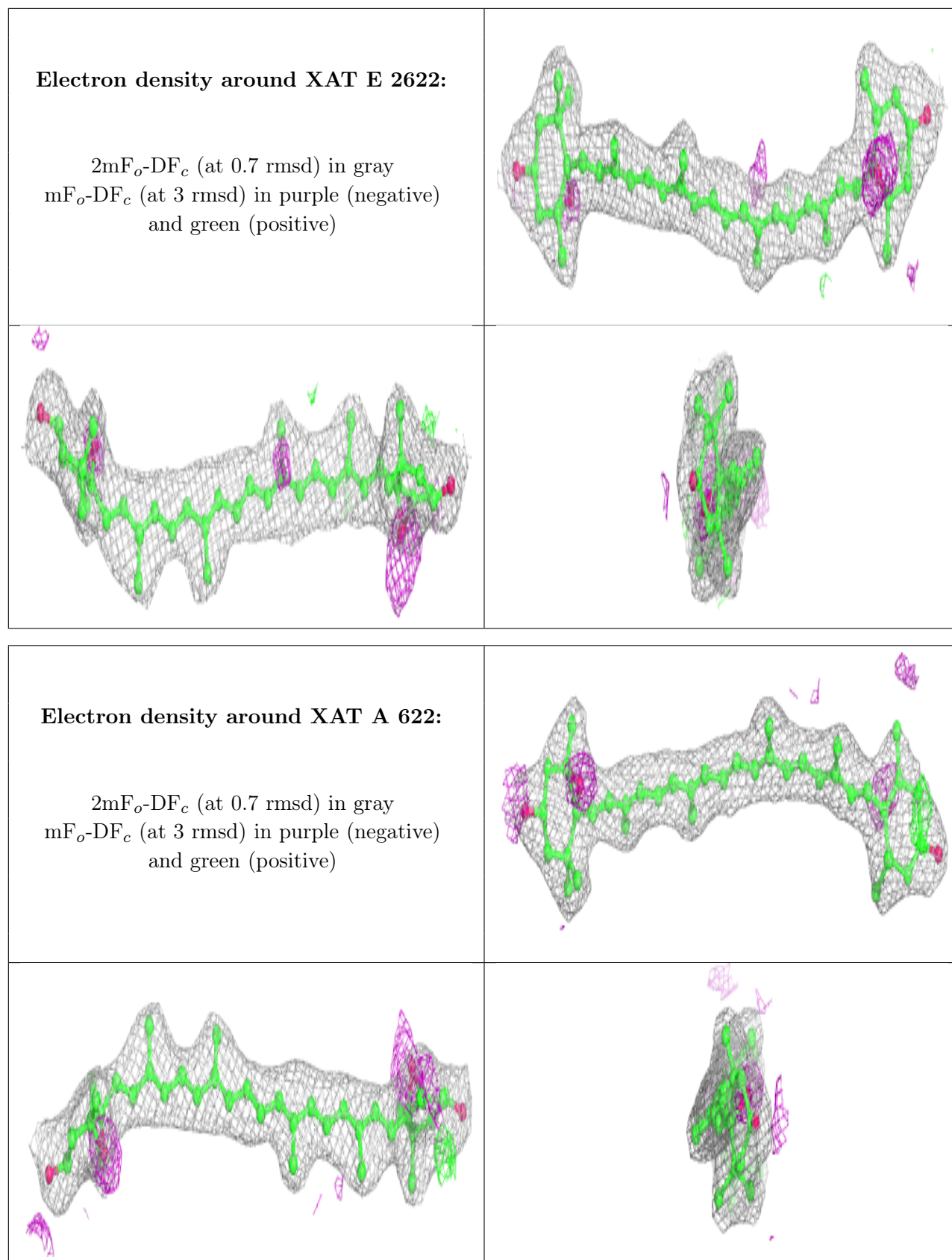
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around DGD I 8632:**

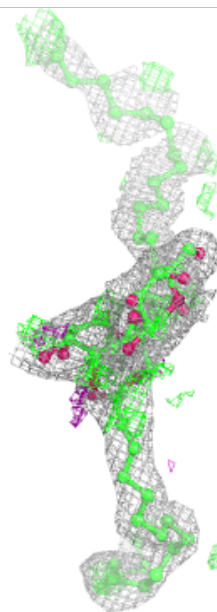
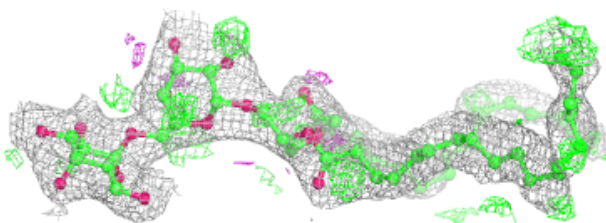
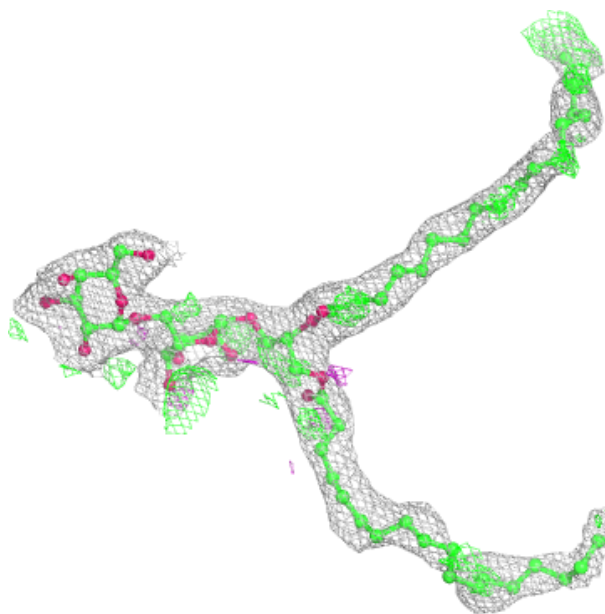
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around DGD D 3632:**

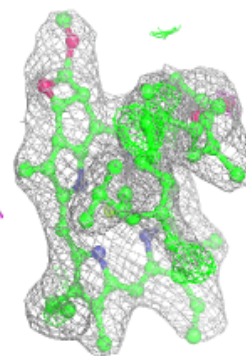
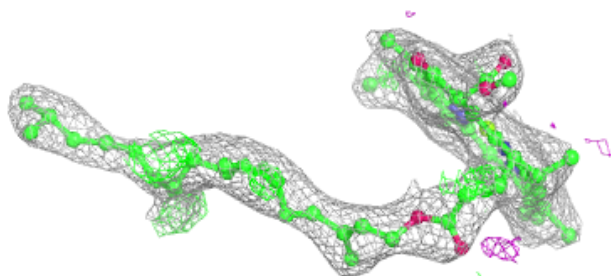
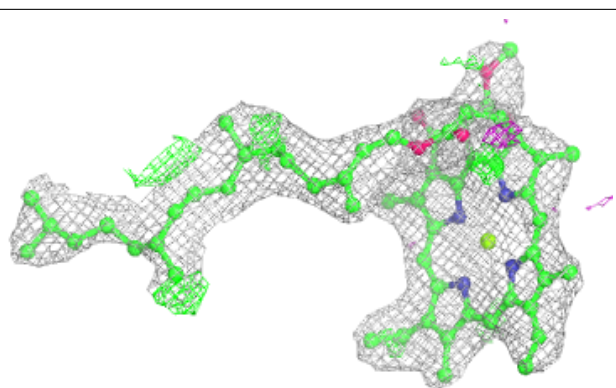
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



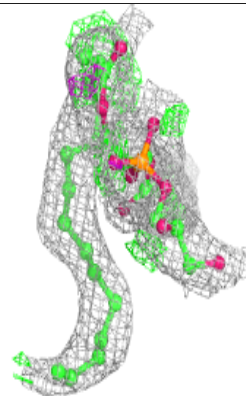
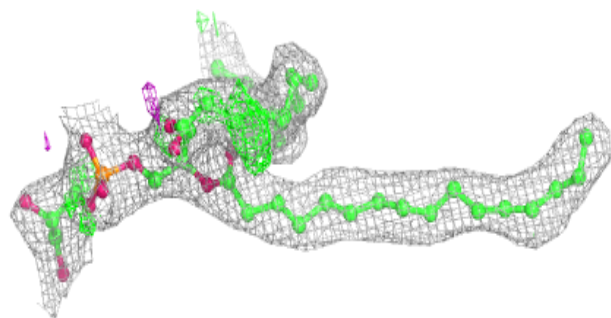
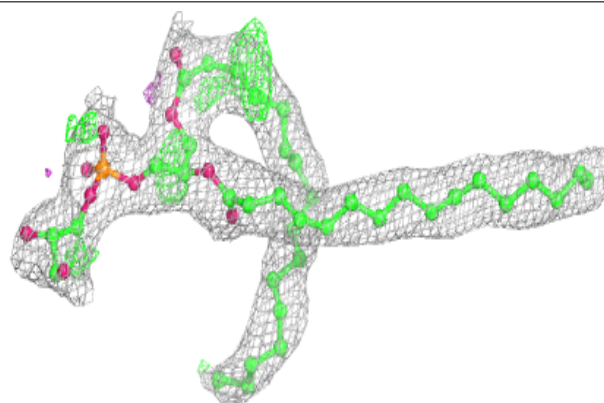


**Electron density around CLA A 611:**

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

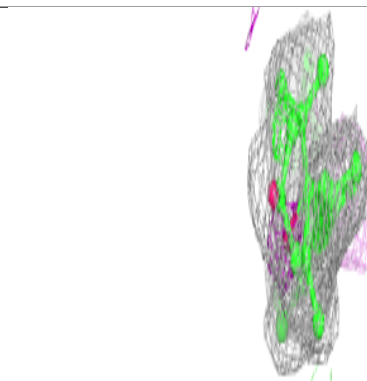
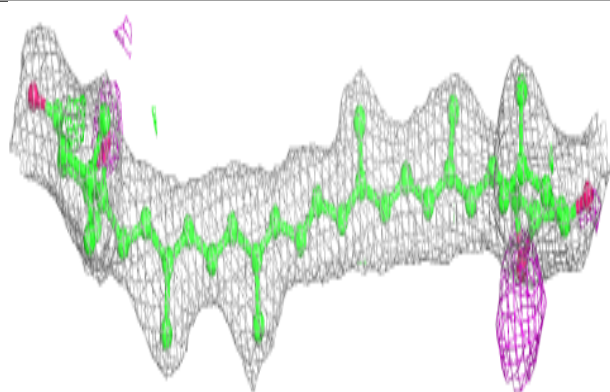
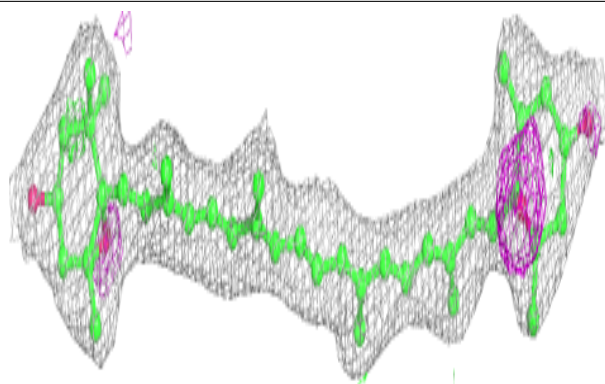
**Electron density around LHG B 1630:**

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

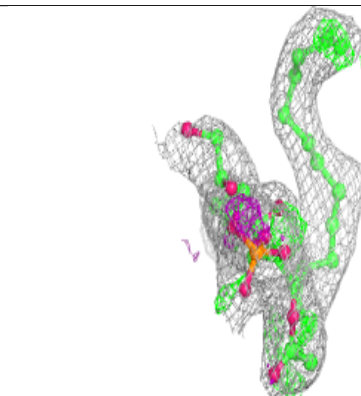
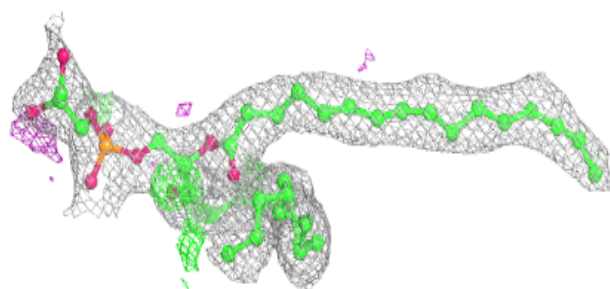
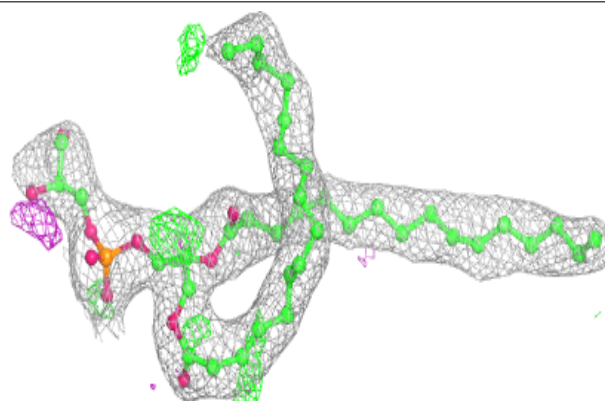


**Electron density around XAT B 5622:**

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

**Electron density around LHG A 630:**

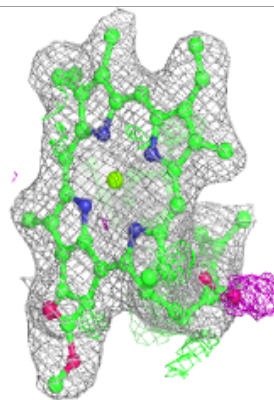
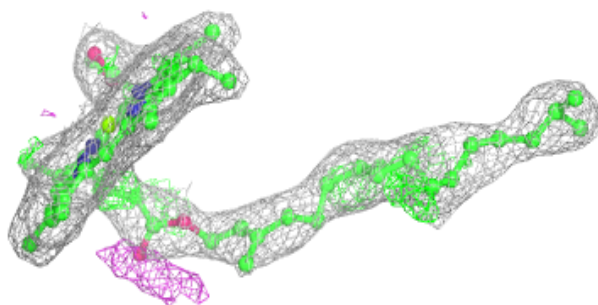
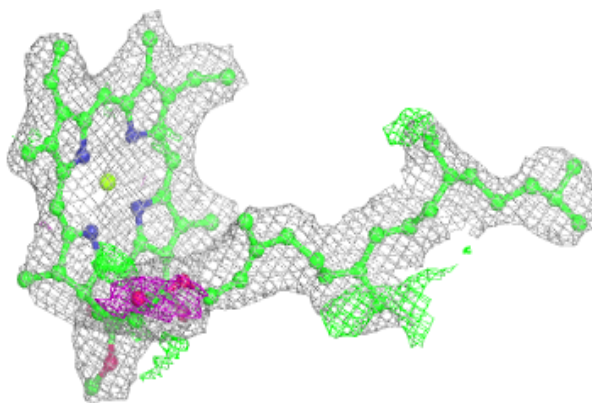
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



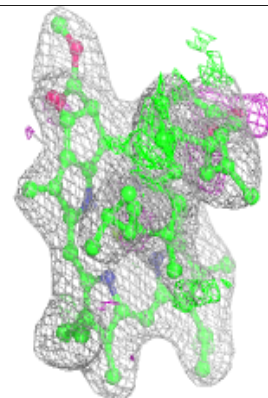
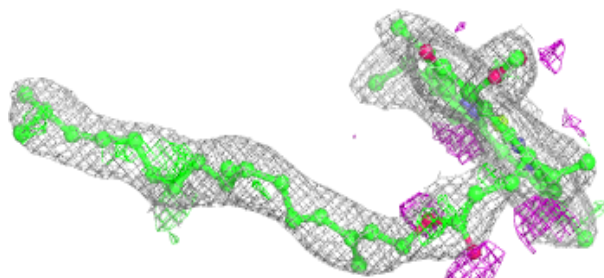
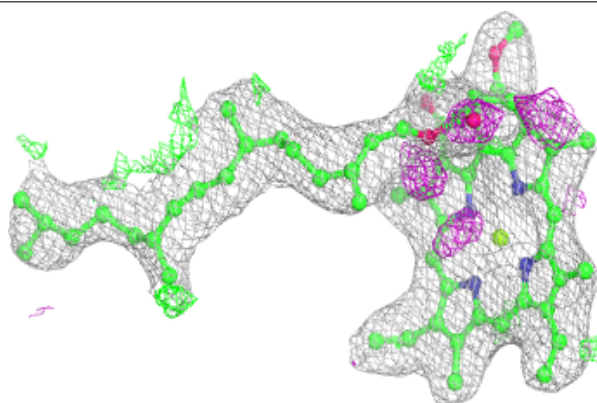


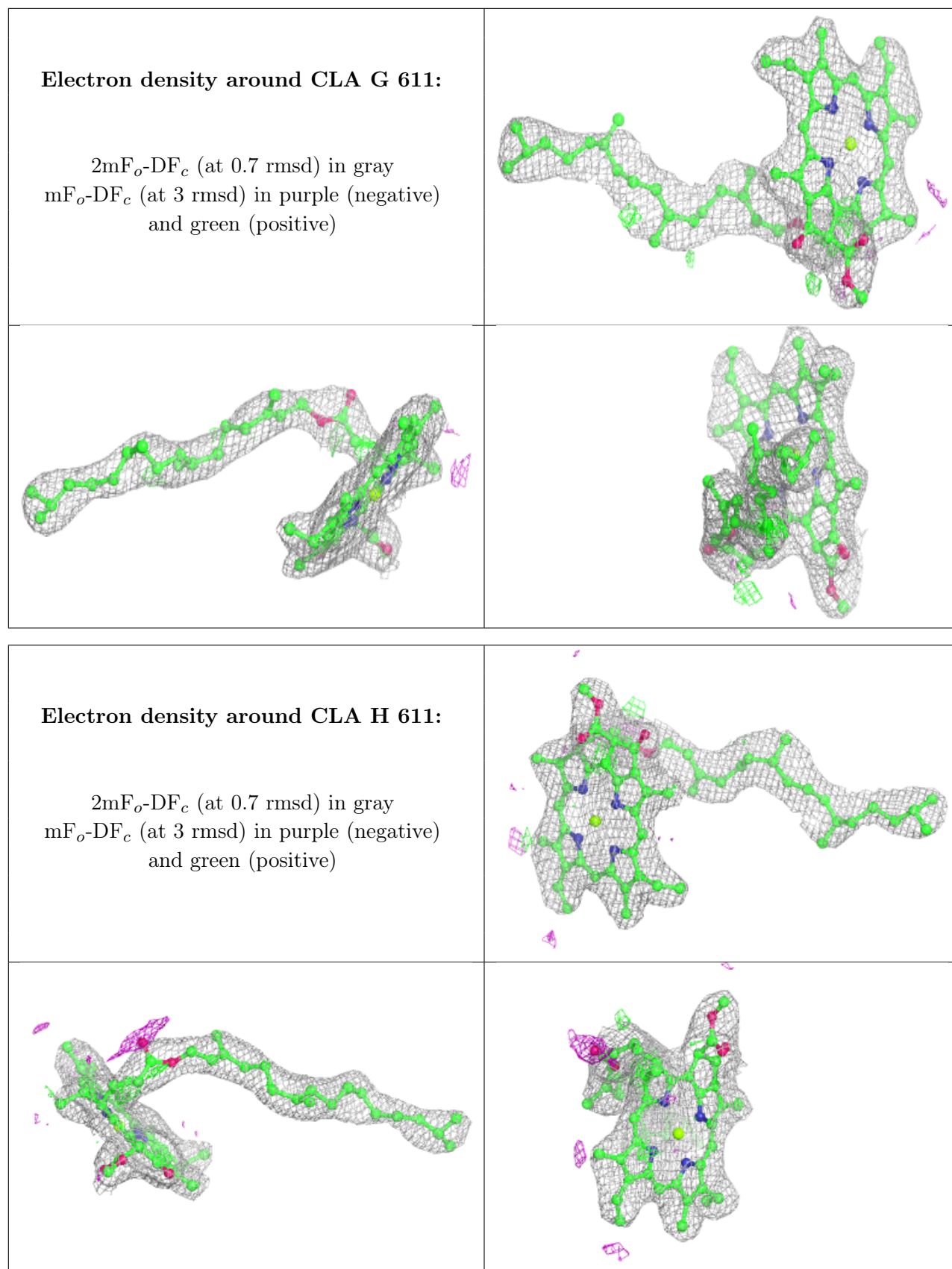
**Electron density around CLA B 611:**

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

**Electron density around CLA D 611:**

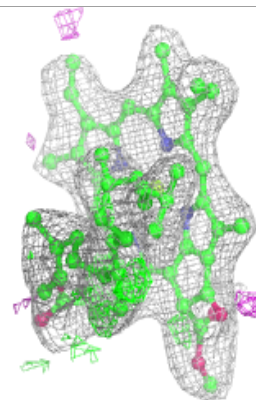
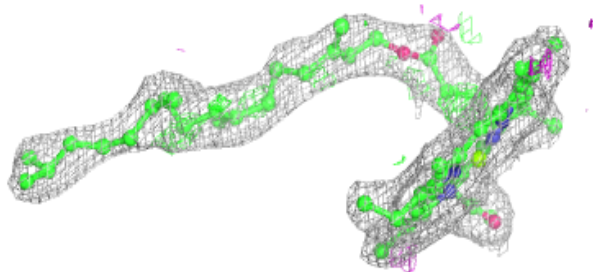
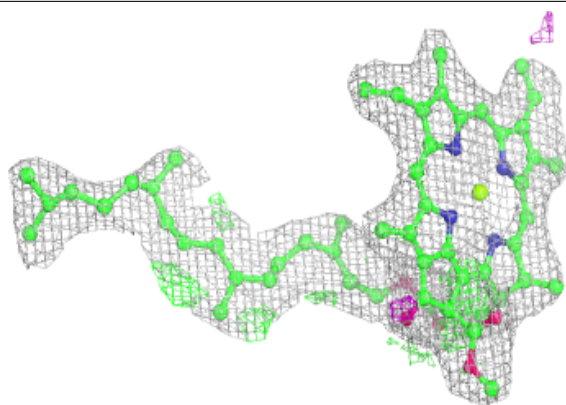
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



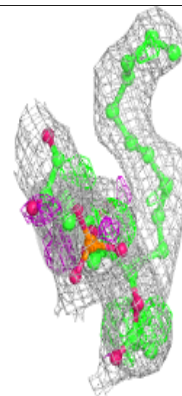
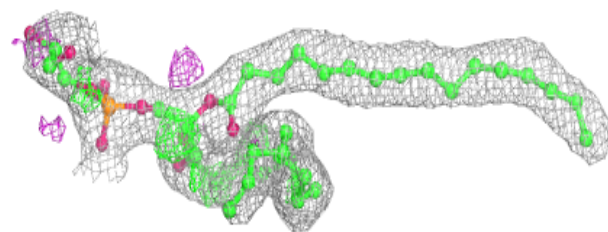
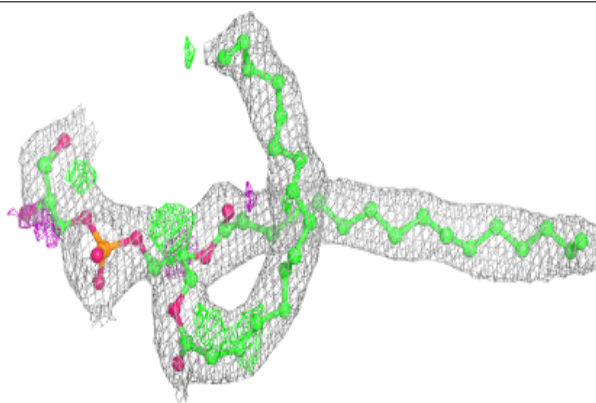


**Electron density around CLA I 611:**

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

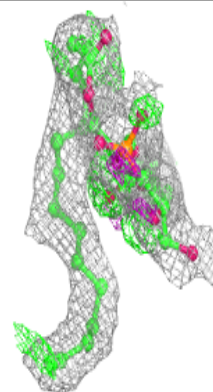
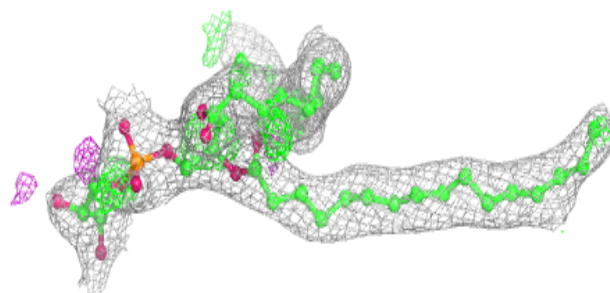
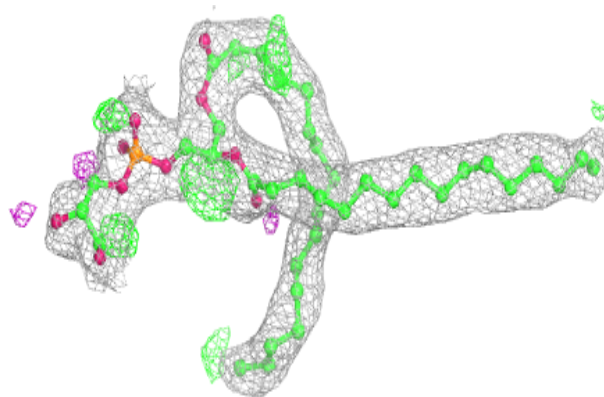
**Electron density around LHG D 3630:**

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

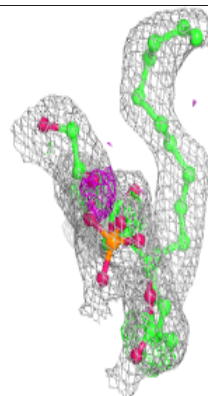
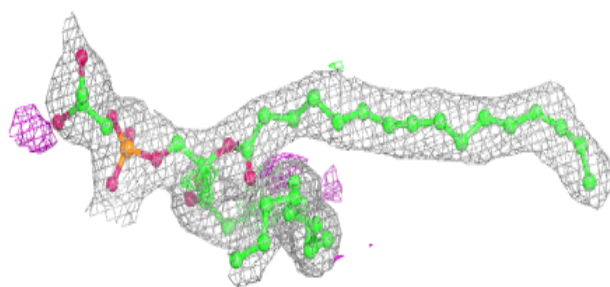
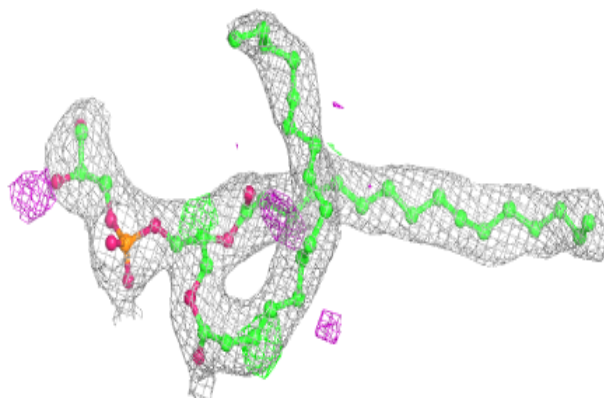


**Electron density around LHG E 4630:**

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

**Electron density around LHG G 6630:**

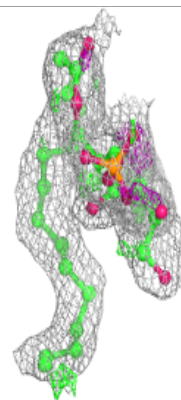
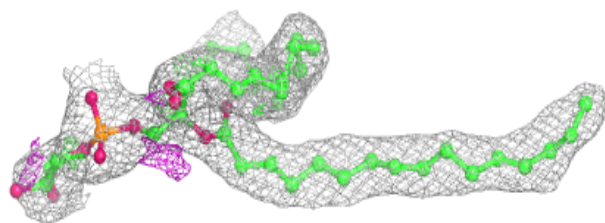
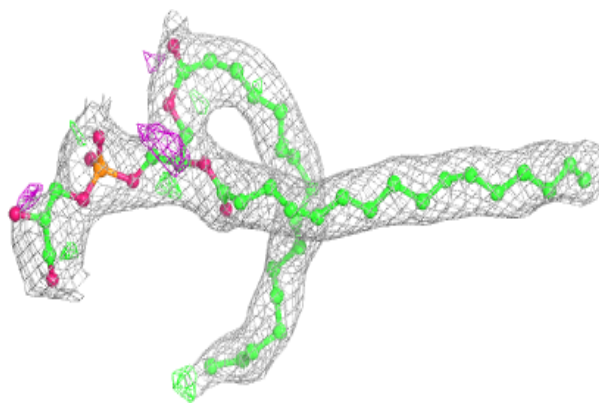
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



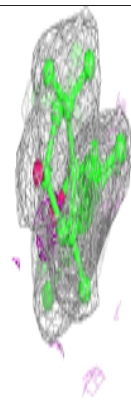
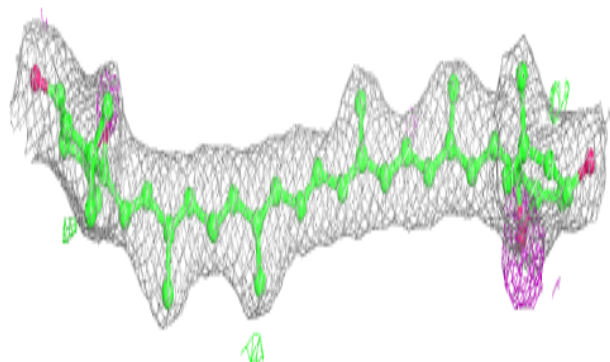
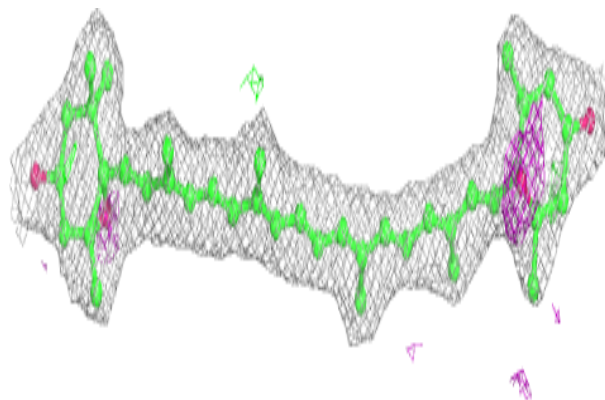


**Electron density around LHG I 8630:**

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

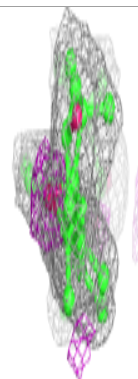
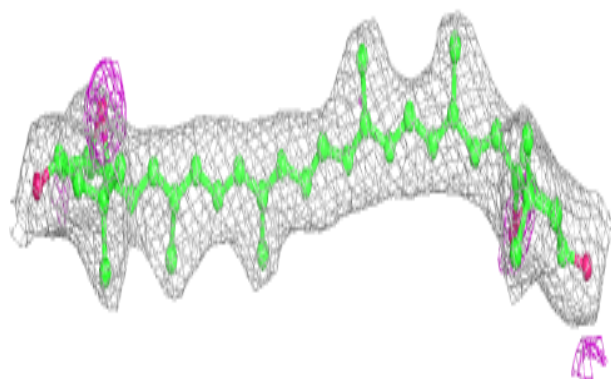
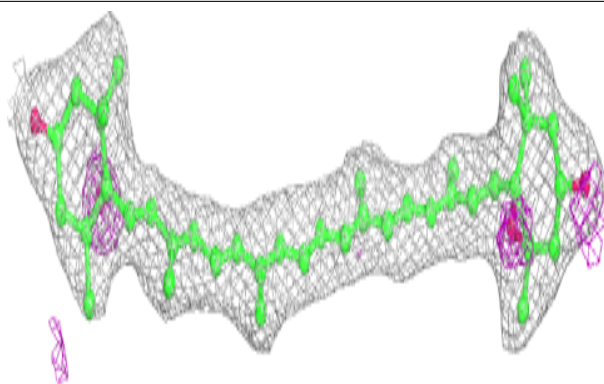
**Electron density around XAT C 7622:**

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

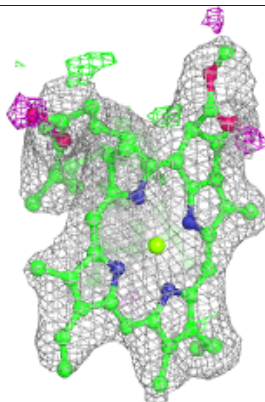
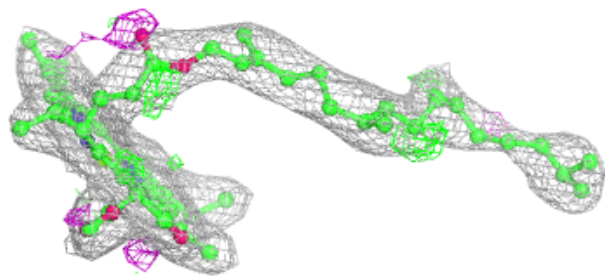
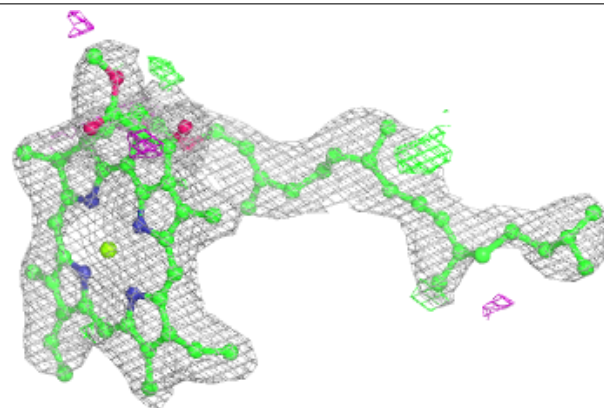


**Electron density around XAT D 8622:**

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

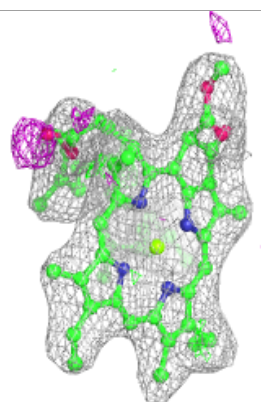
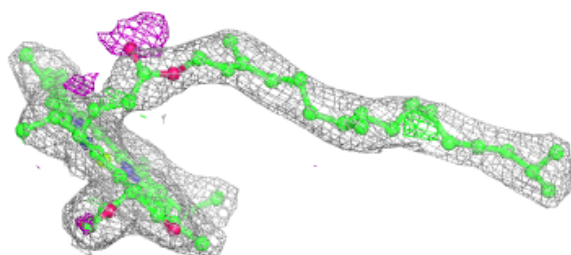
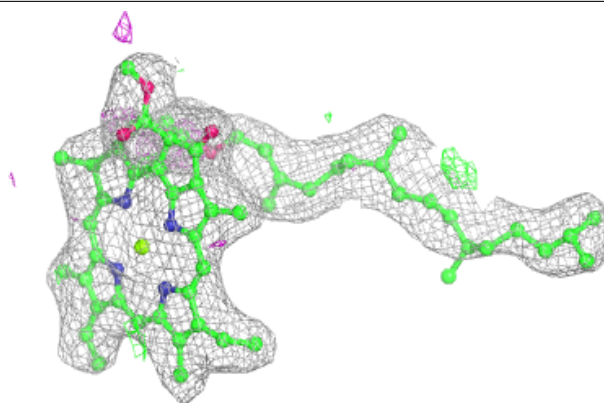
**Electron density around CLA C 611:**

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

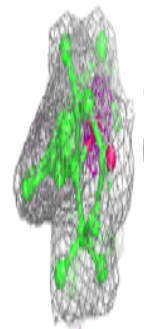
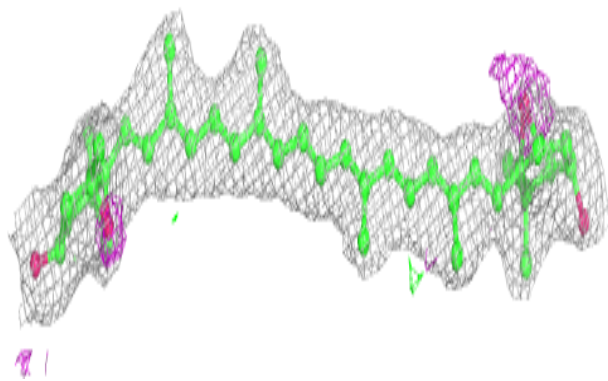
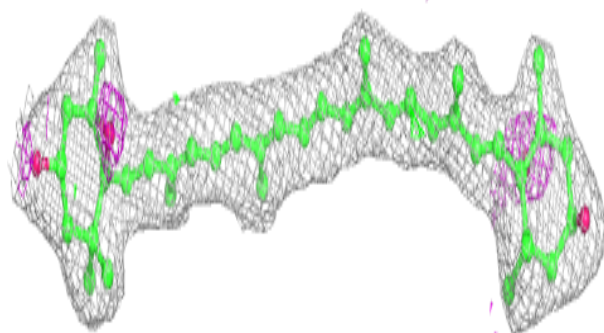


**Electron density around CLA E 611:**

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

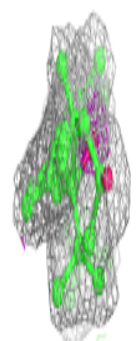
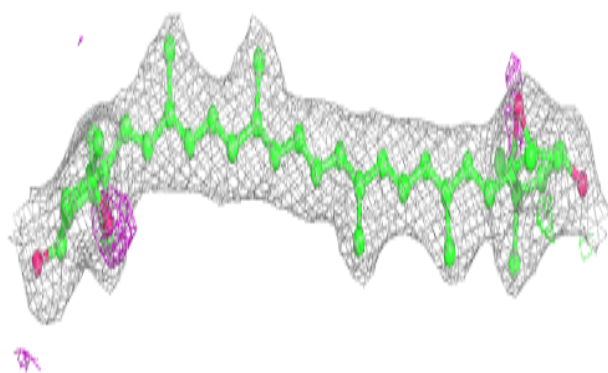
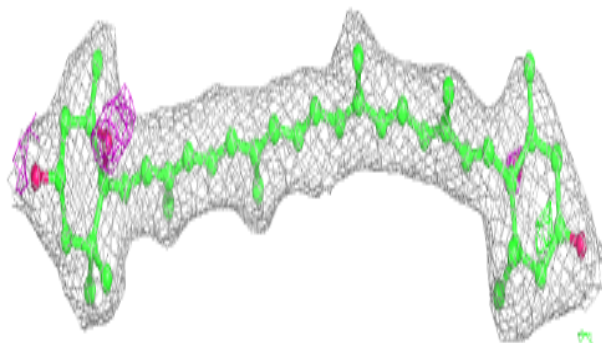
**Electron density around XAT F 6622:**

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

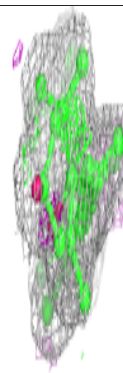
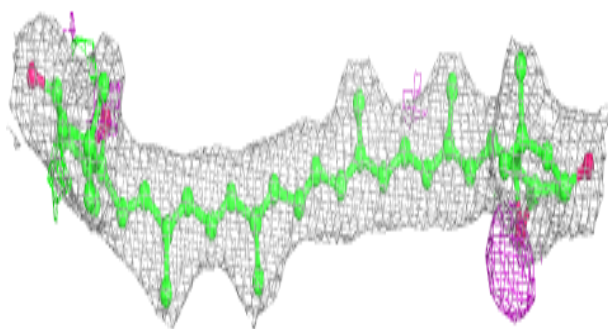
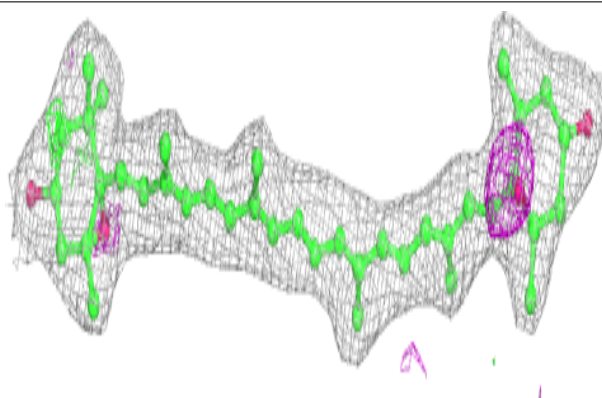


**Electron density around XAT H 4622:**

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

**Electron density around XAT I 9622:**

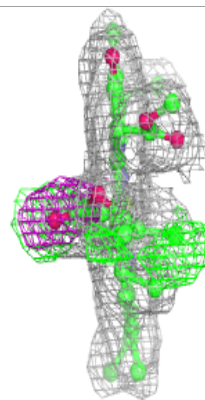
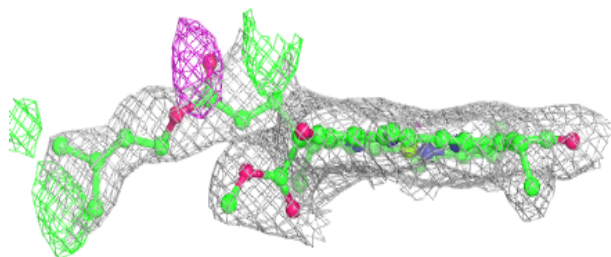
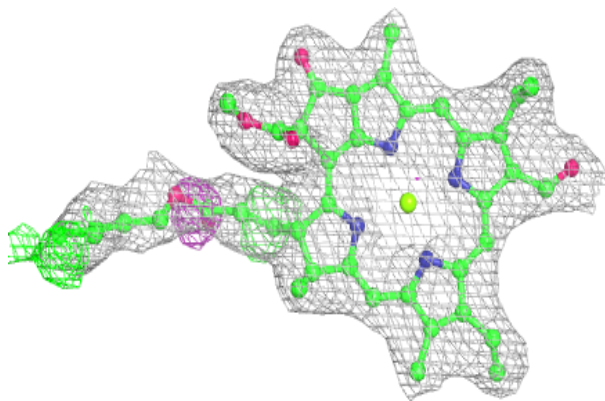
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



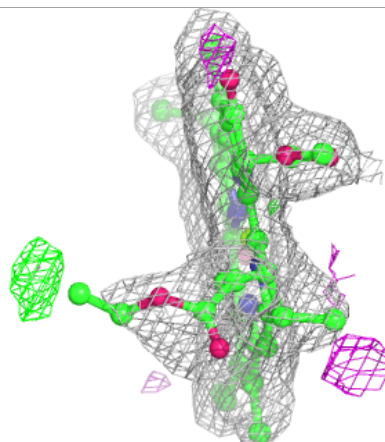
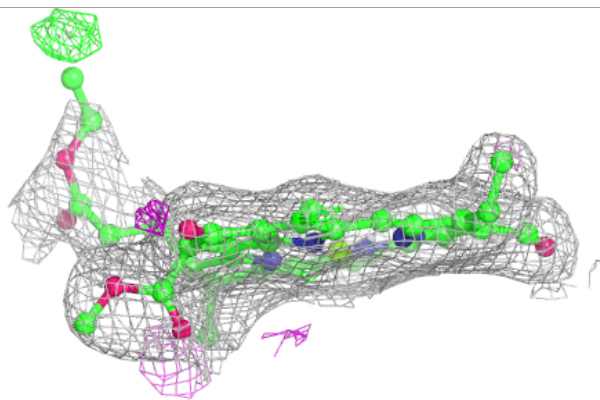
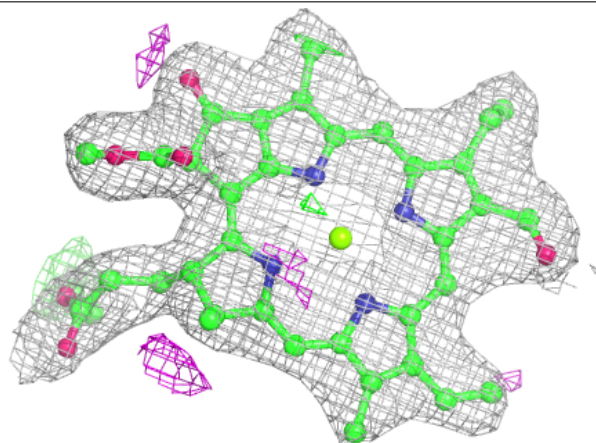


**Electron density around CHL F 606:**

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

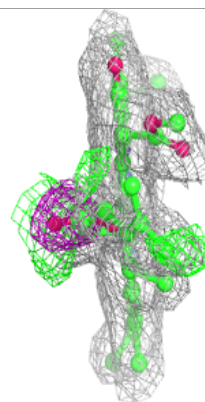
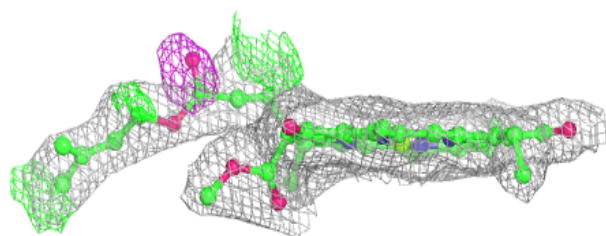
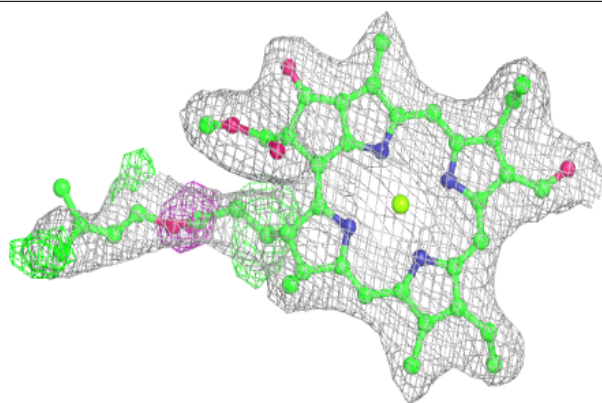
**Electron density around CHL G 605:**

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

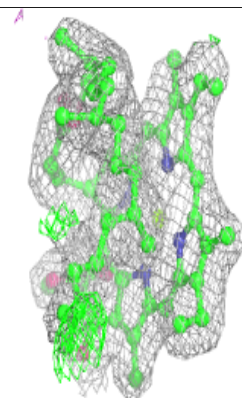
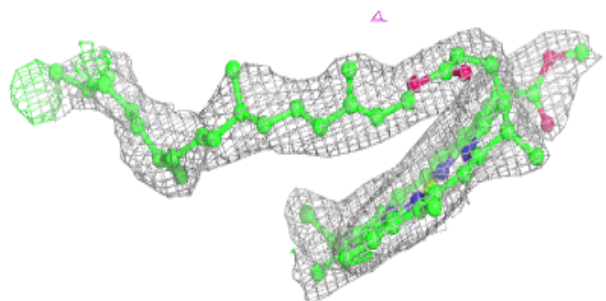
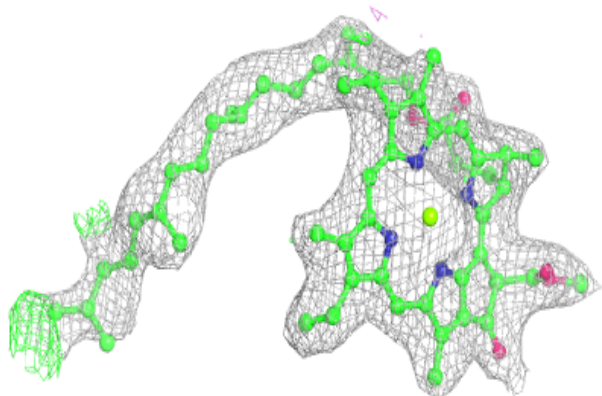


**Electron density around CHL J 606:**

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

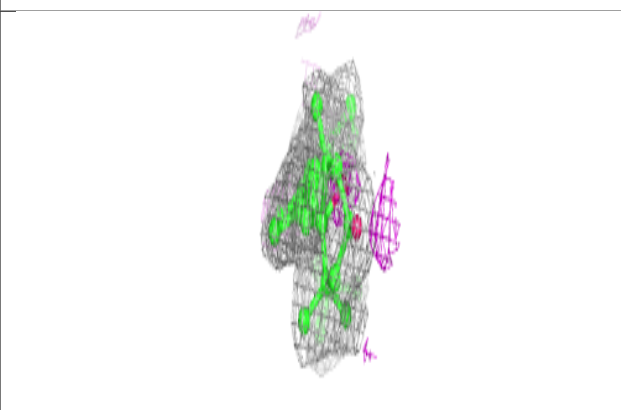
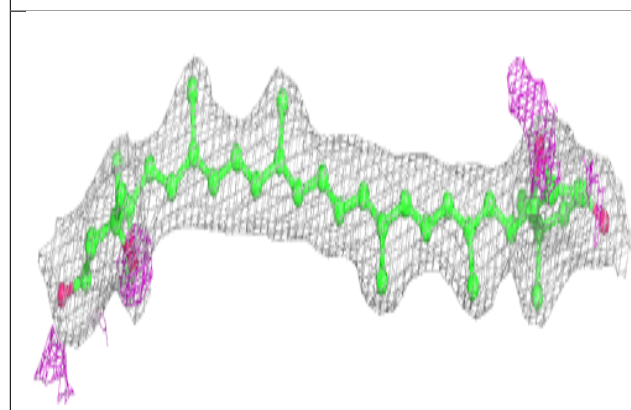
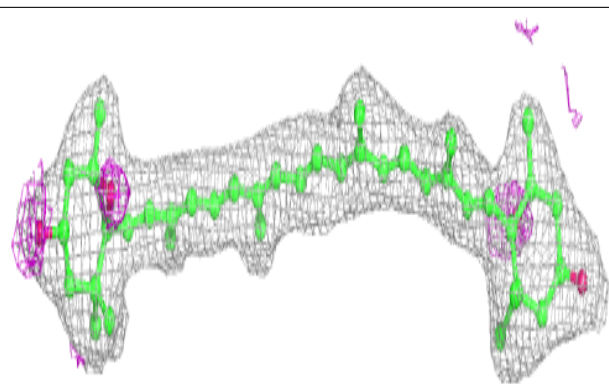
**Electron density around CLA A 610:**

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

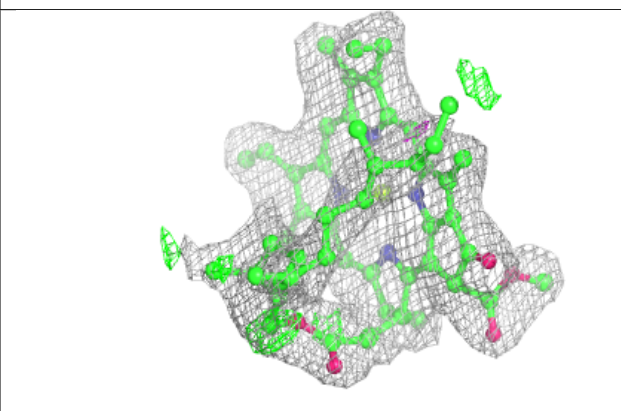
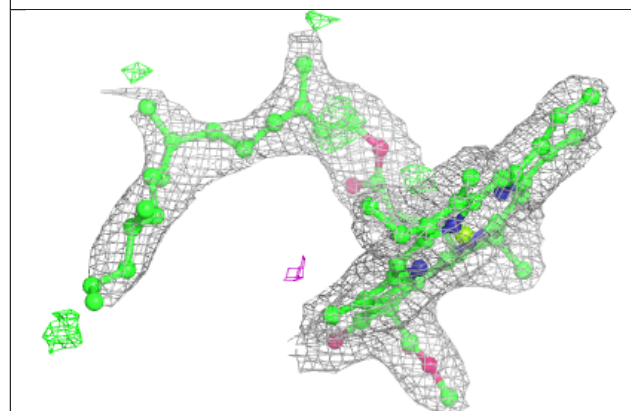
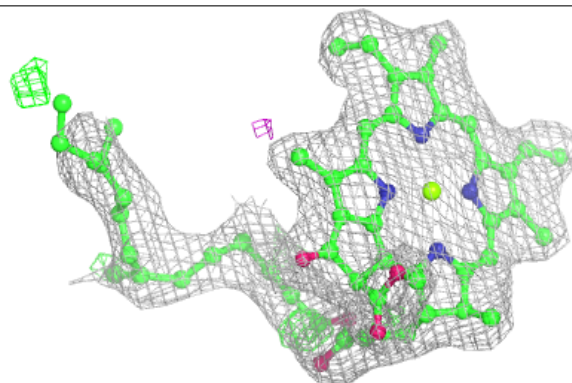


**Electron density around XAT B 1622:**

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

**Electron density around CLA B 604:**

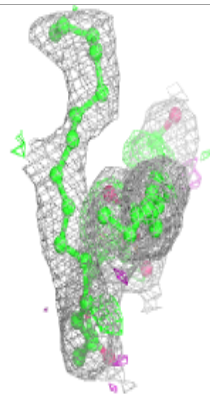
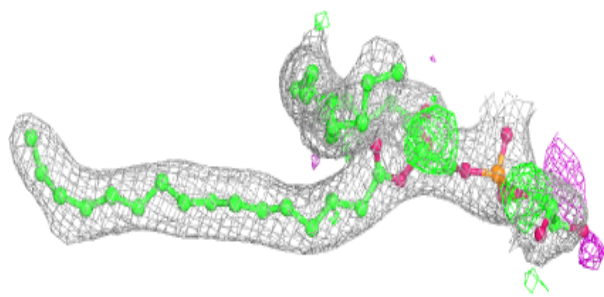
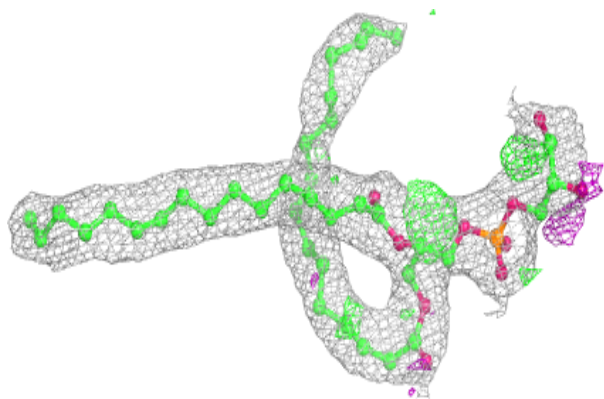
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



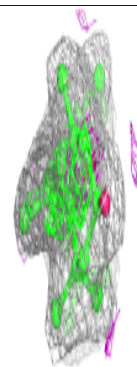
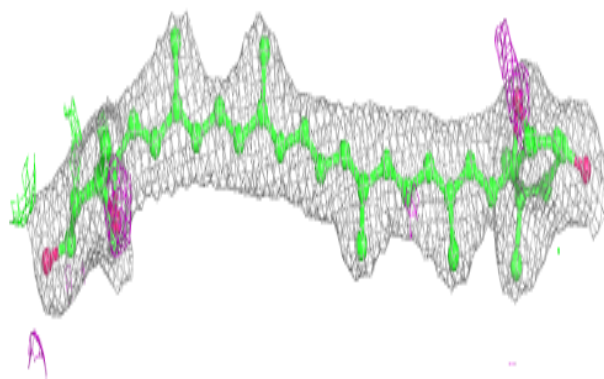
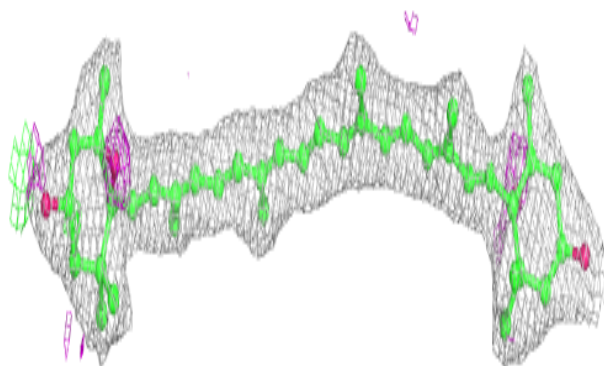


**Electron density around LHG J 9630:**

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

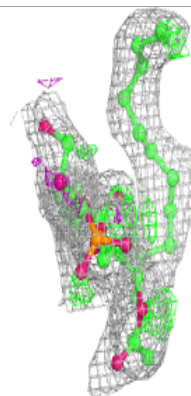
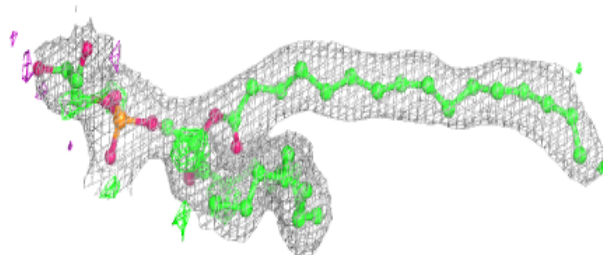
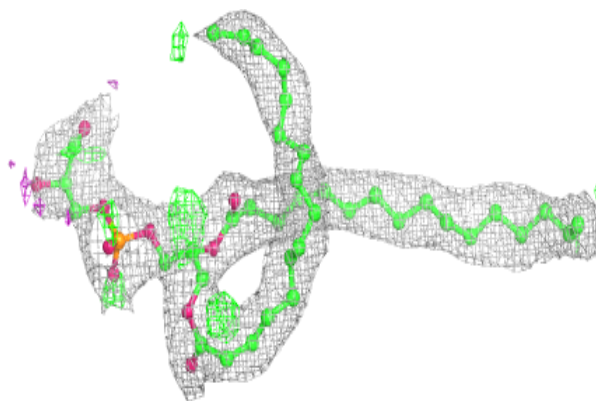
**Electron density around XAT J 3622:**

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

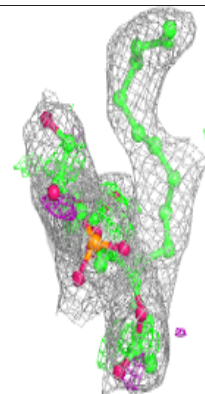
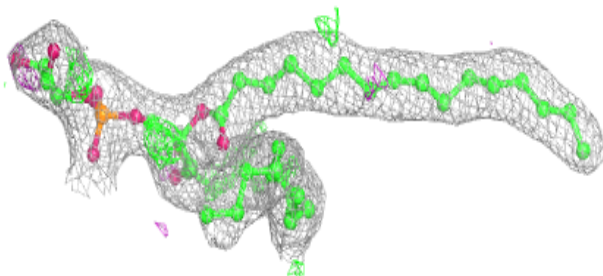
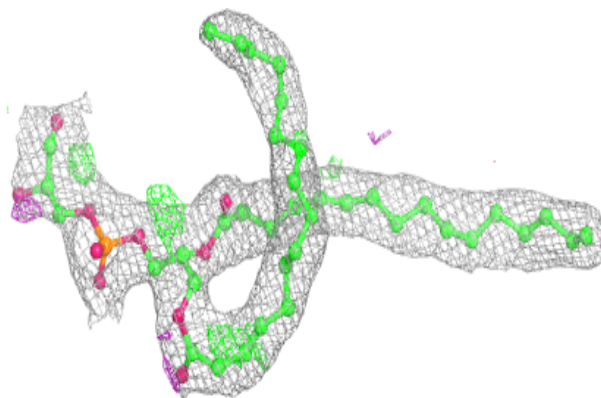


**Electron density around LHG F 5630:**

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

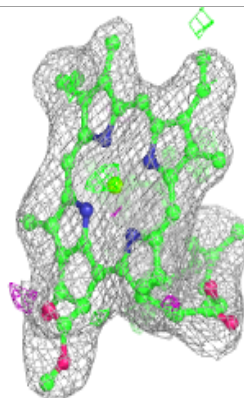
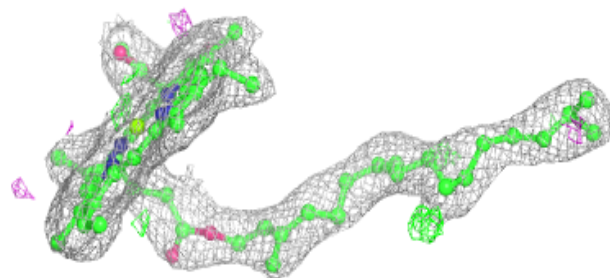
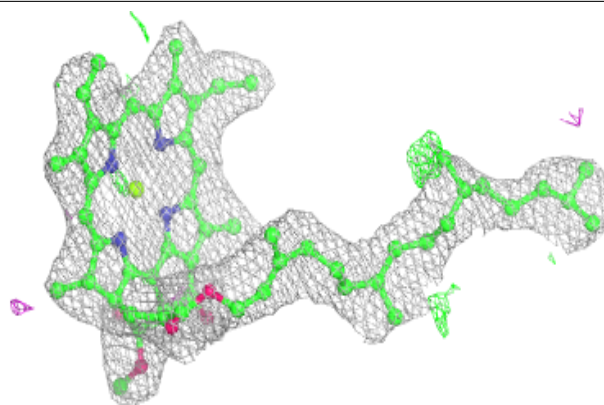
**Electron density around LHG C 2630:**

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

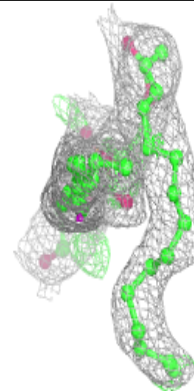
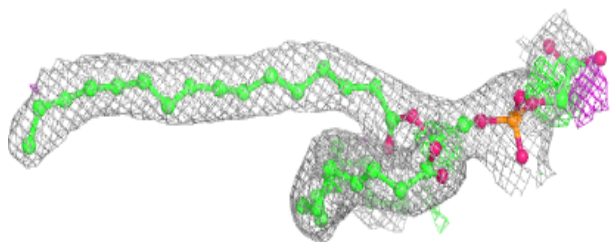
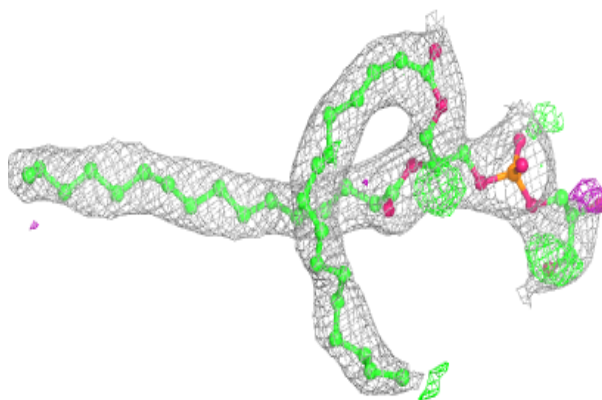


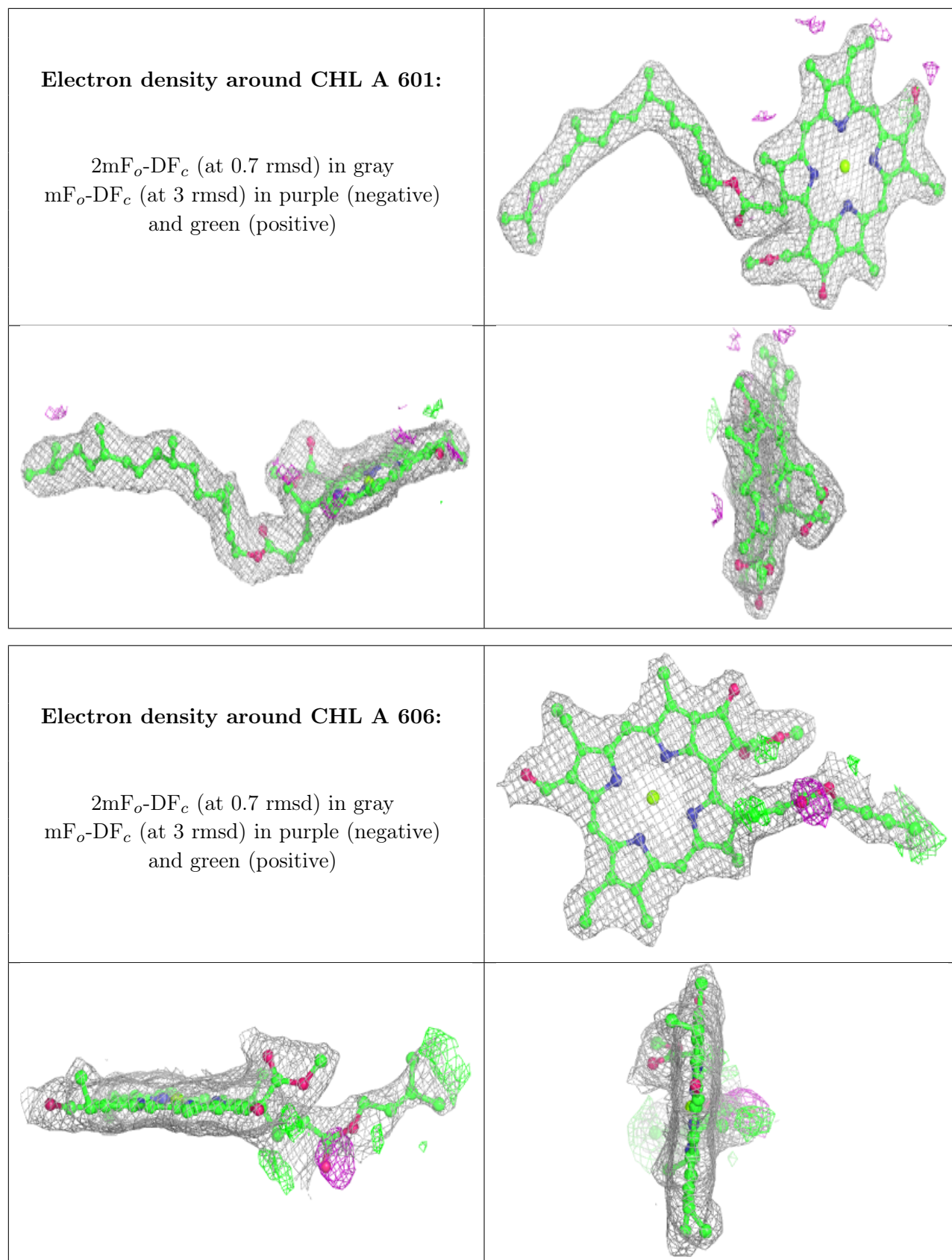
**Electron density around CLA F 611:**

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

**Electron density around LHG H 7630:**

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

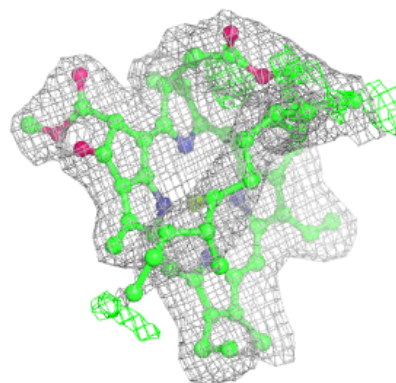
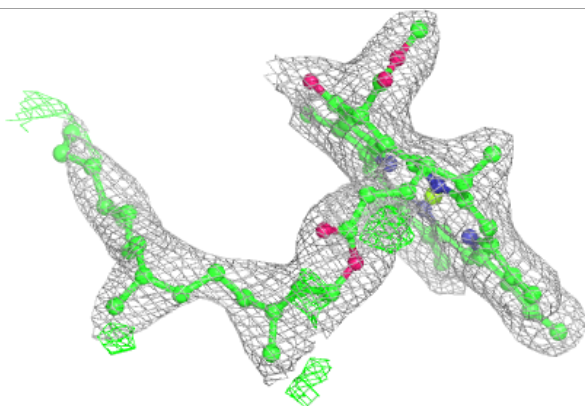
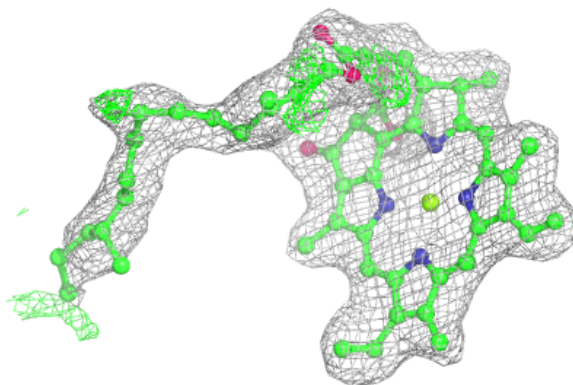




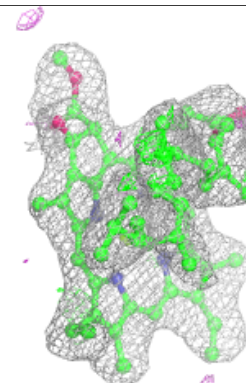
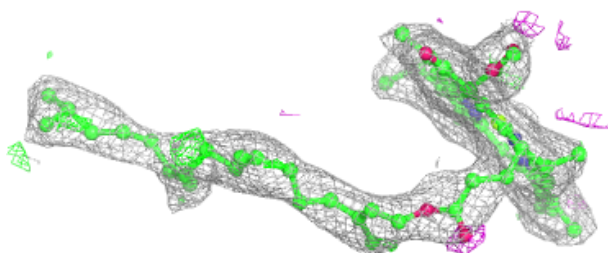
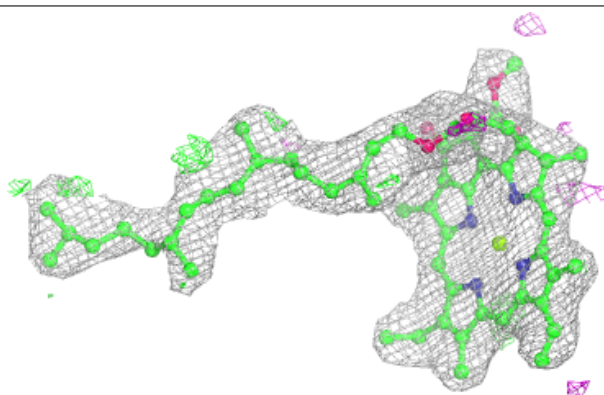


**Electron density around CLA J 604:**

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

**Electron density around CLA J 611:**

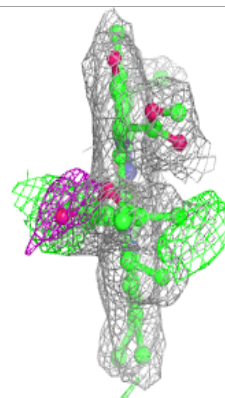
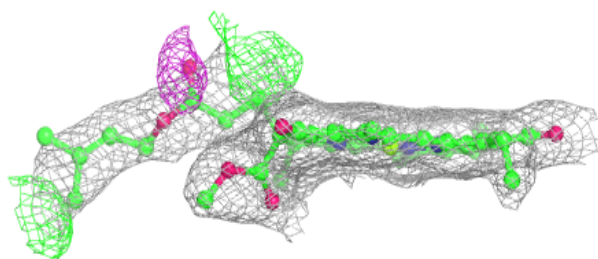
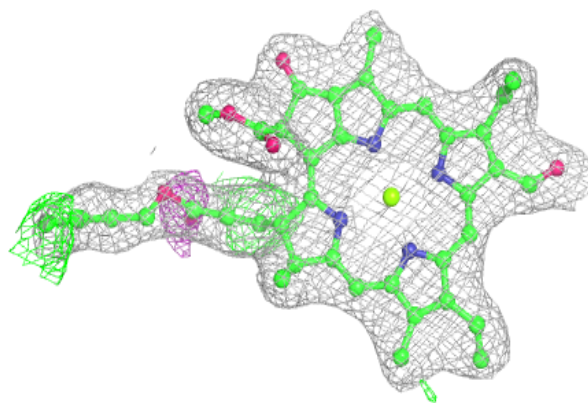
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





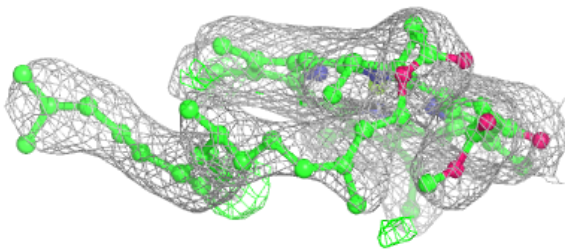
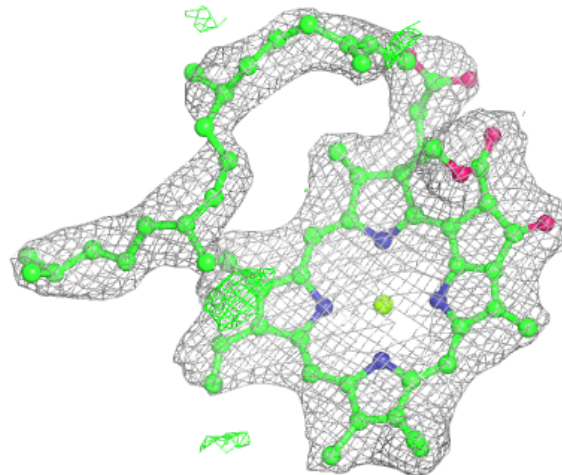
**Electron density around CHL E 606:**

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



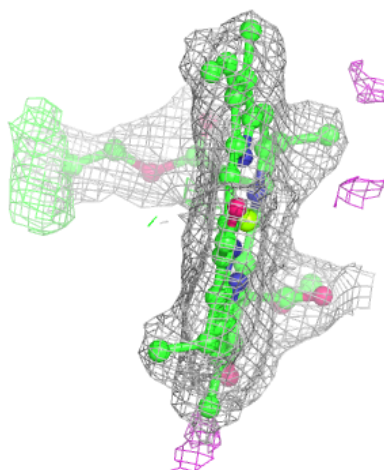
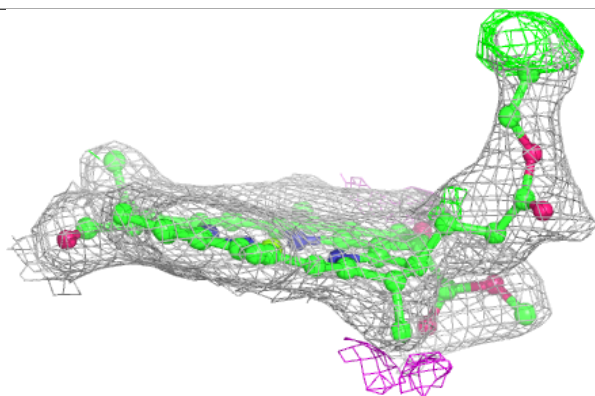
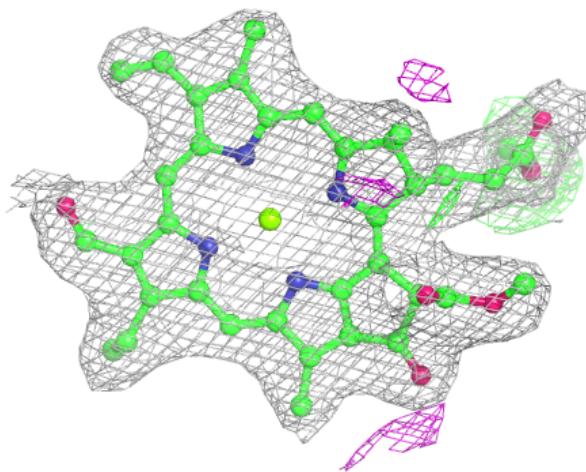
**Electron density around CLA A 612:**

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



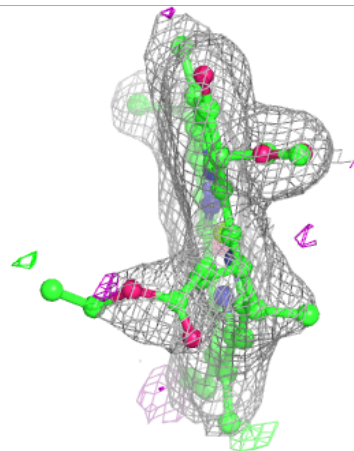
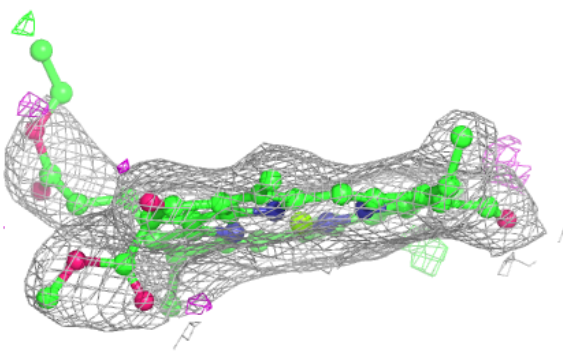
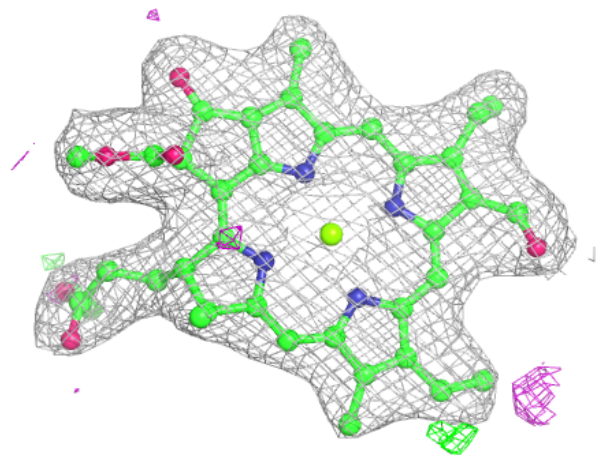
**Electron density around CHL F 605:**

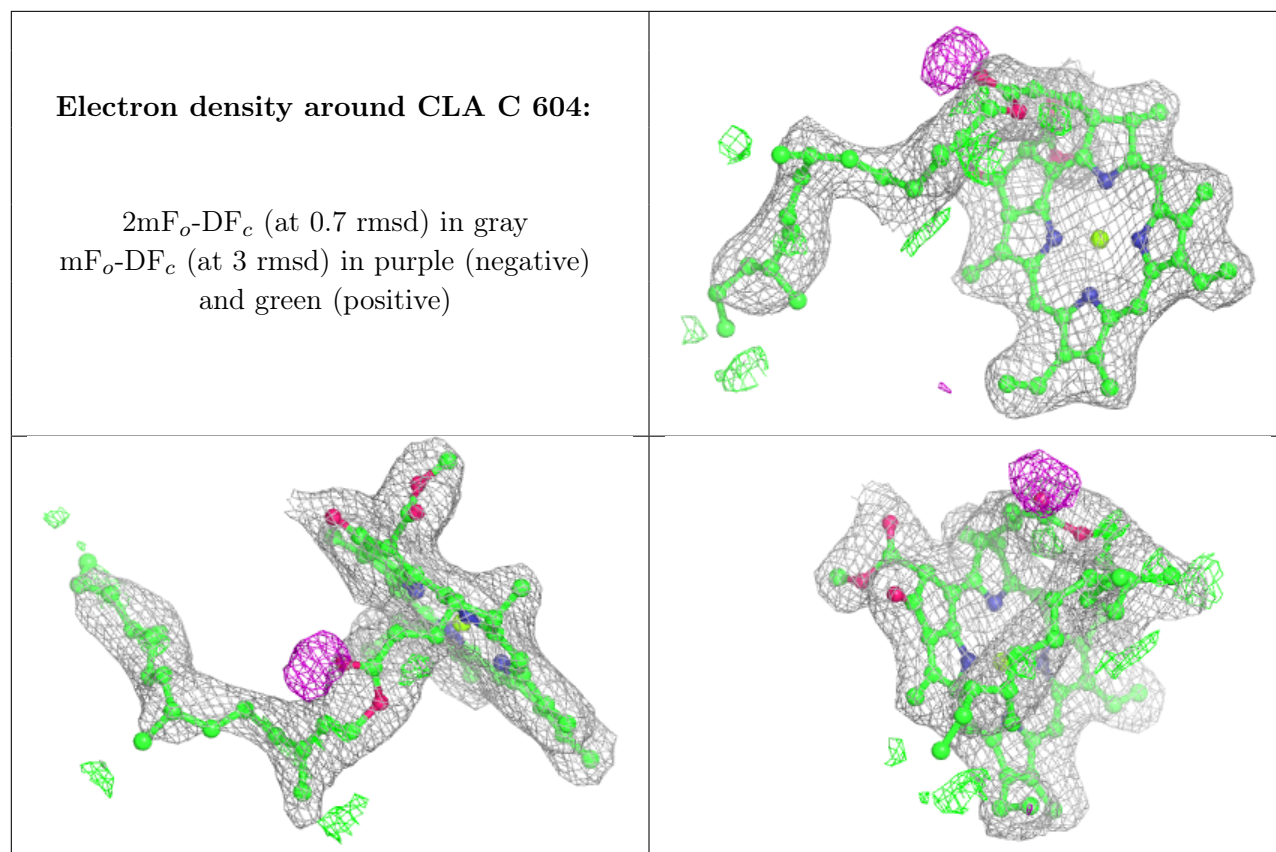
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CHL B 605:**

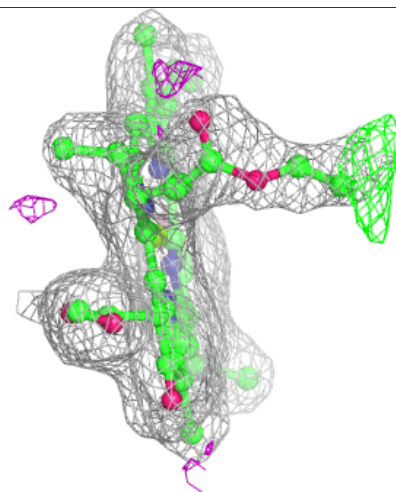
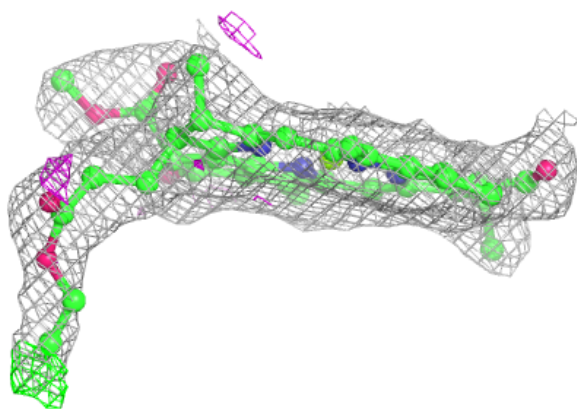
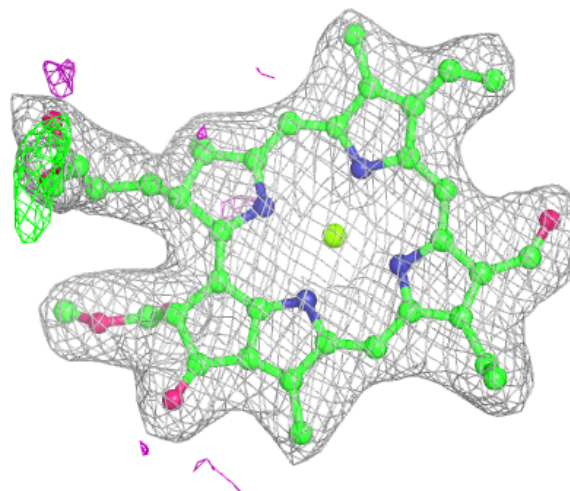
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CHL C 605:**

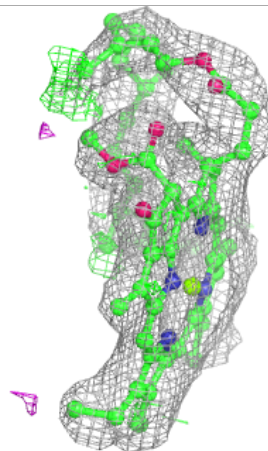
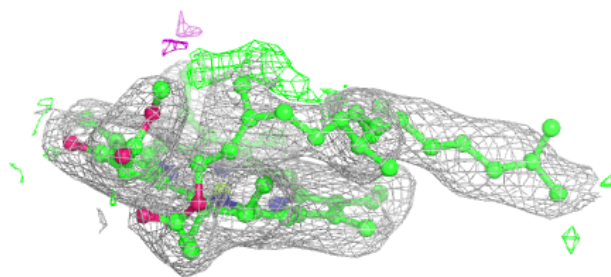
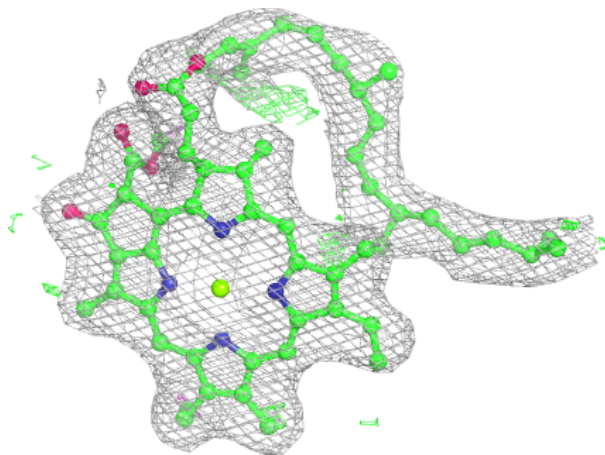
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





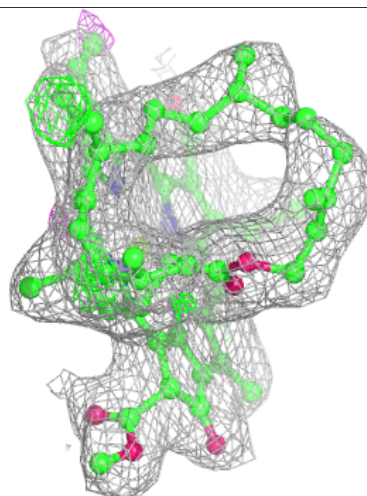
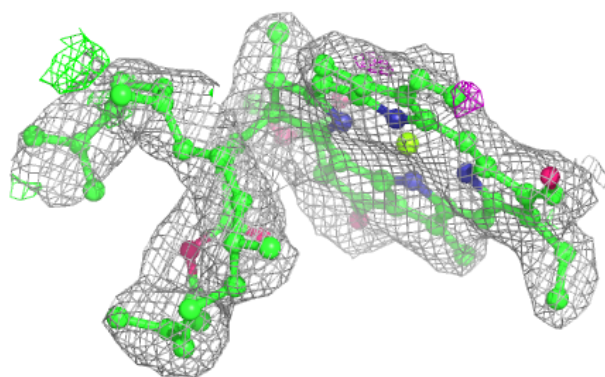
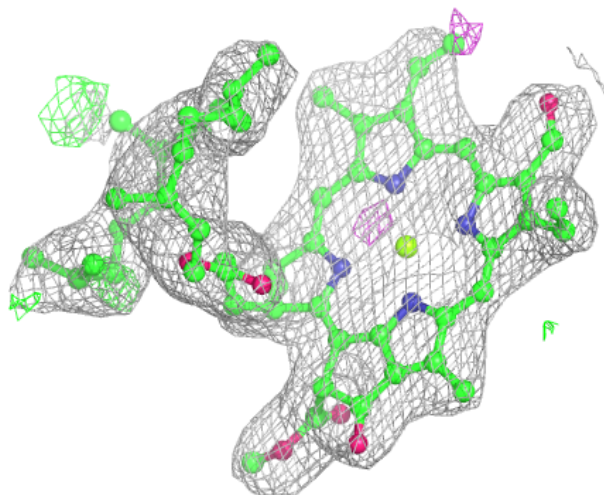
**Electron density around CLA C 612:**

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



**Electron density around CHL G 608:**

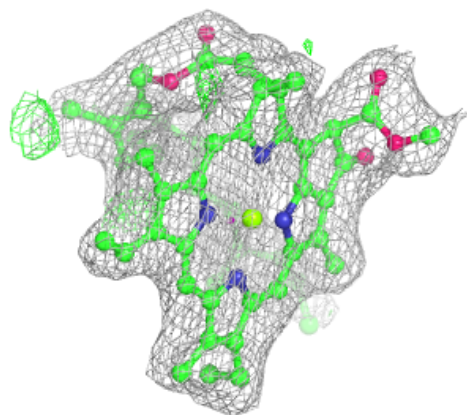
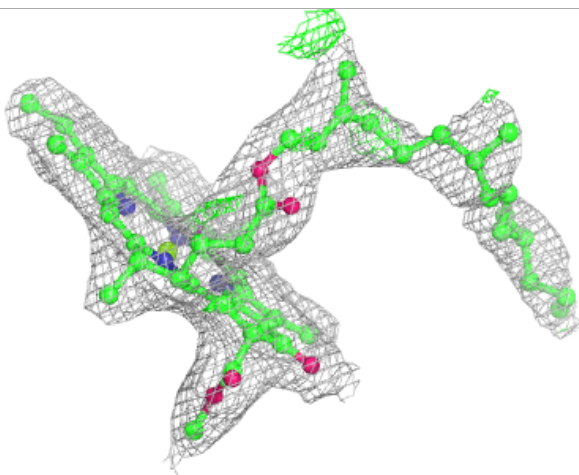
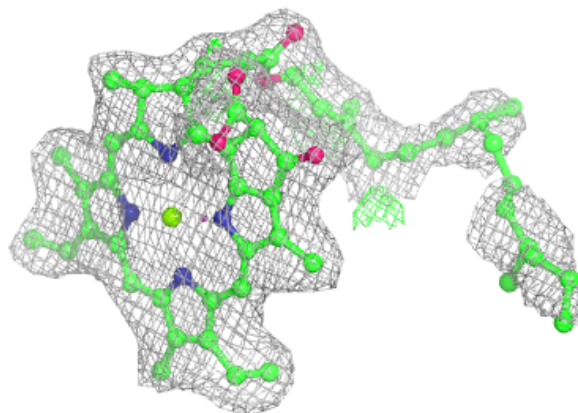
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





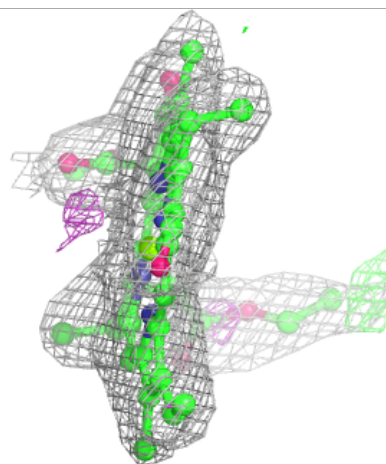
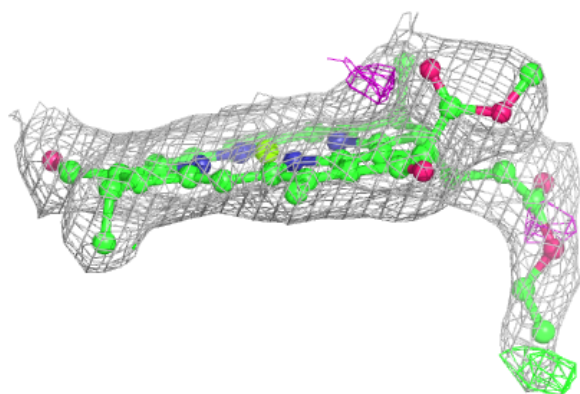
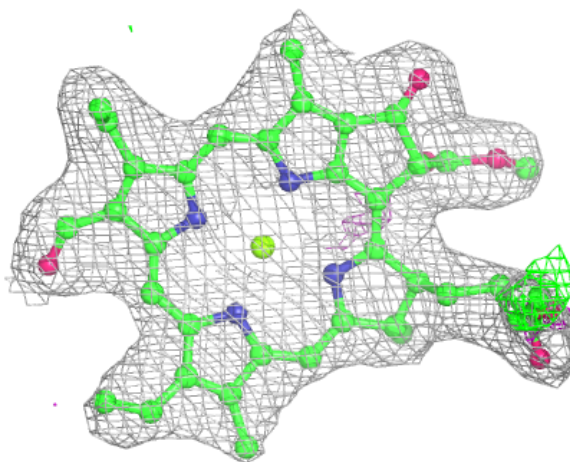
**Electron density around CLA E 604:**

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



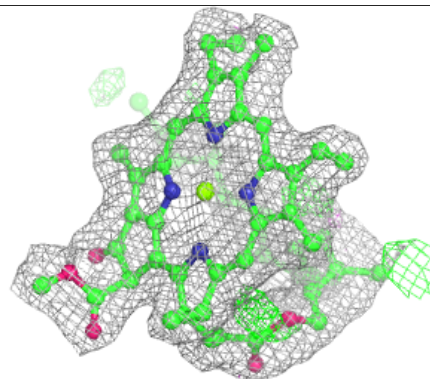
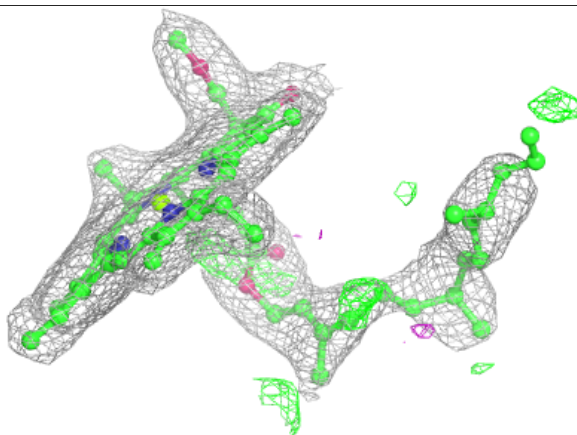
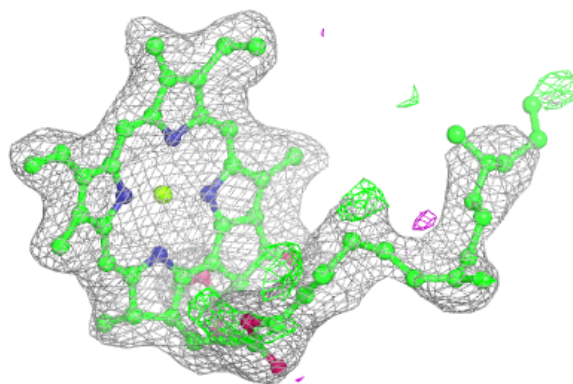
**Electron density around CHL H 605:**

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

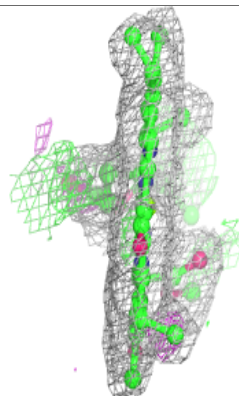
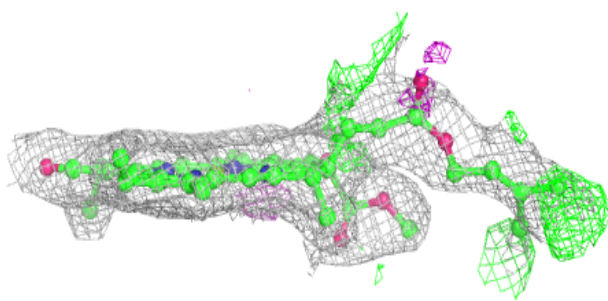
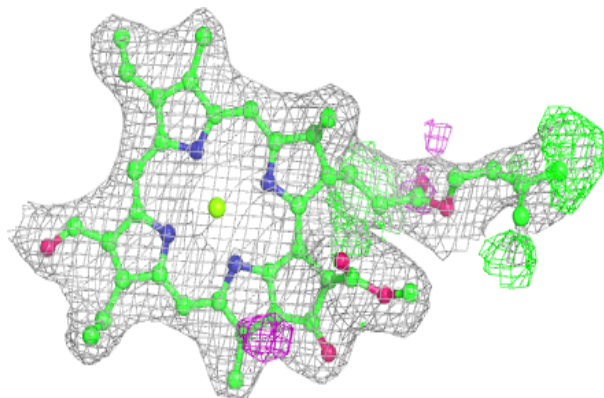


**Electron density around CLA F 604:**

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

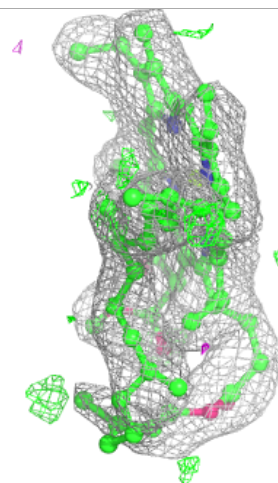
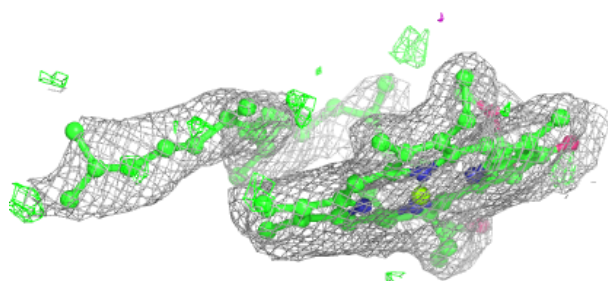
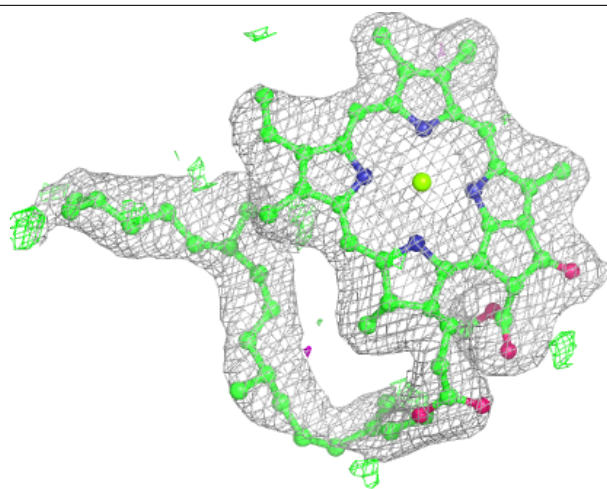
**Electron density around CHL H 606:**

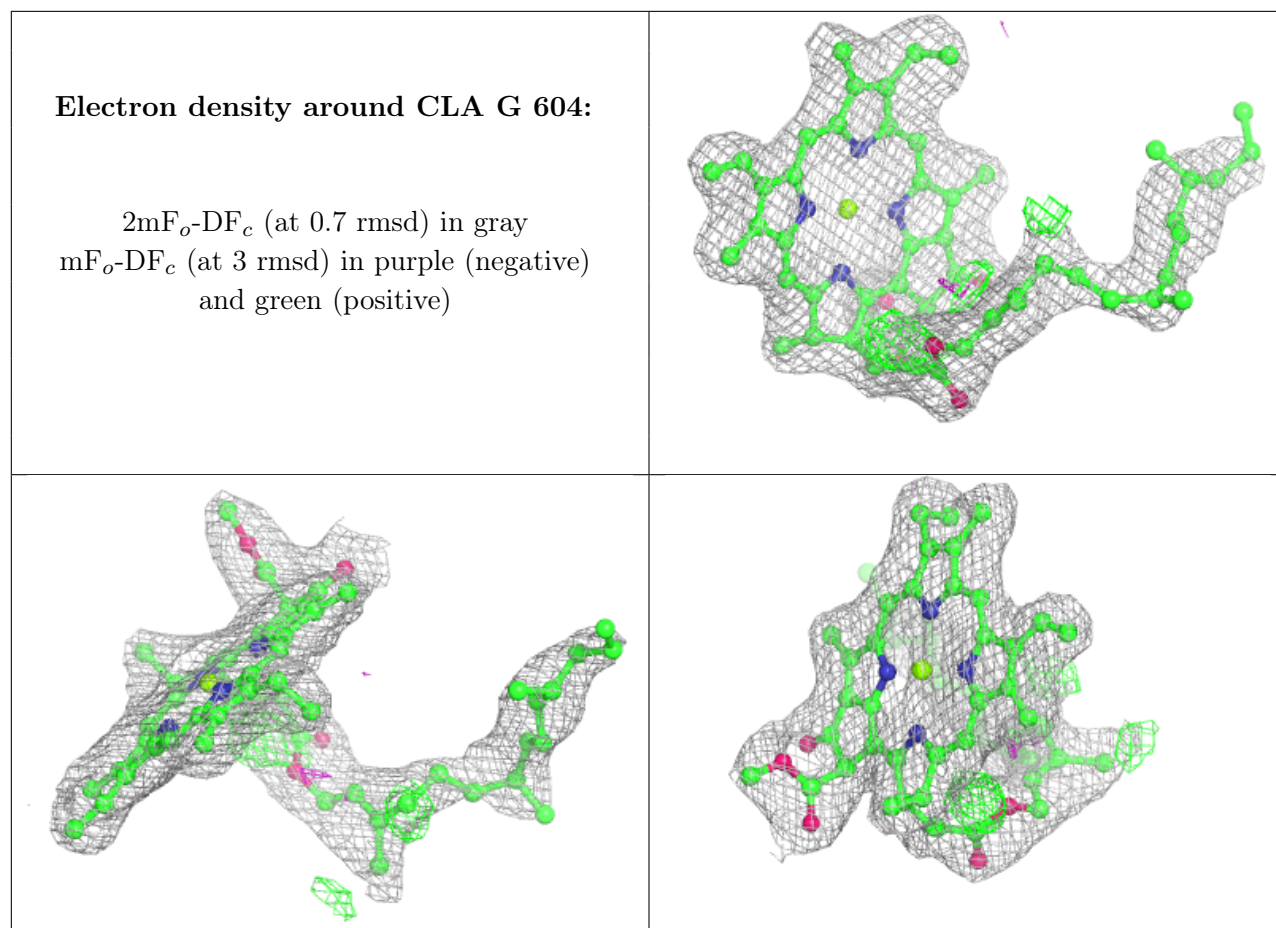
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA F 612:**

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

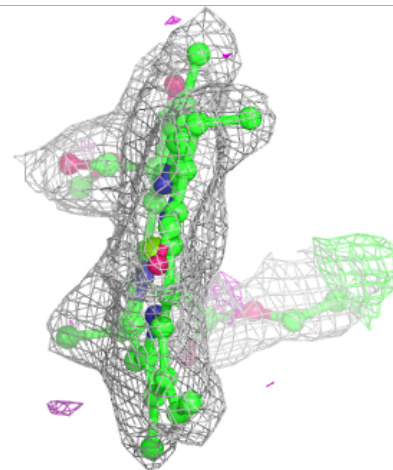
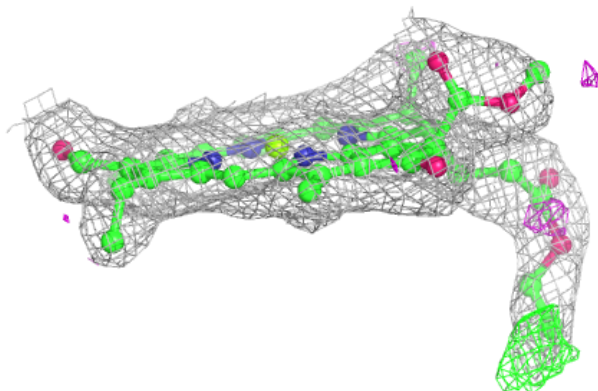
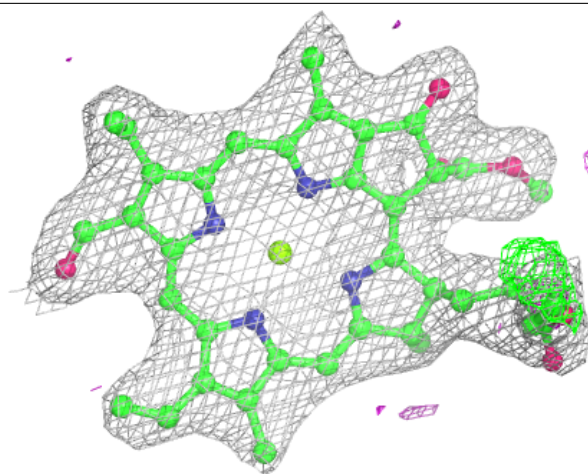


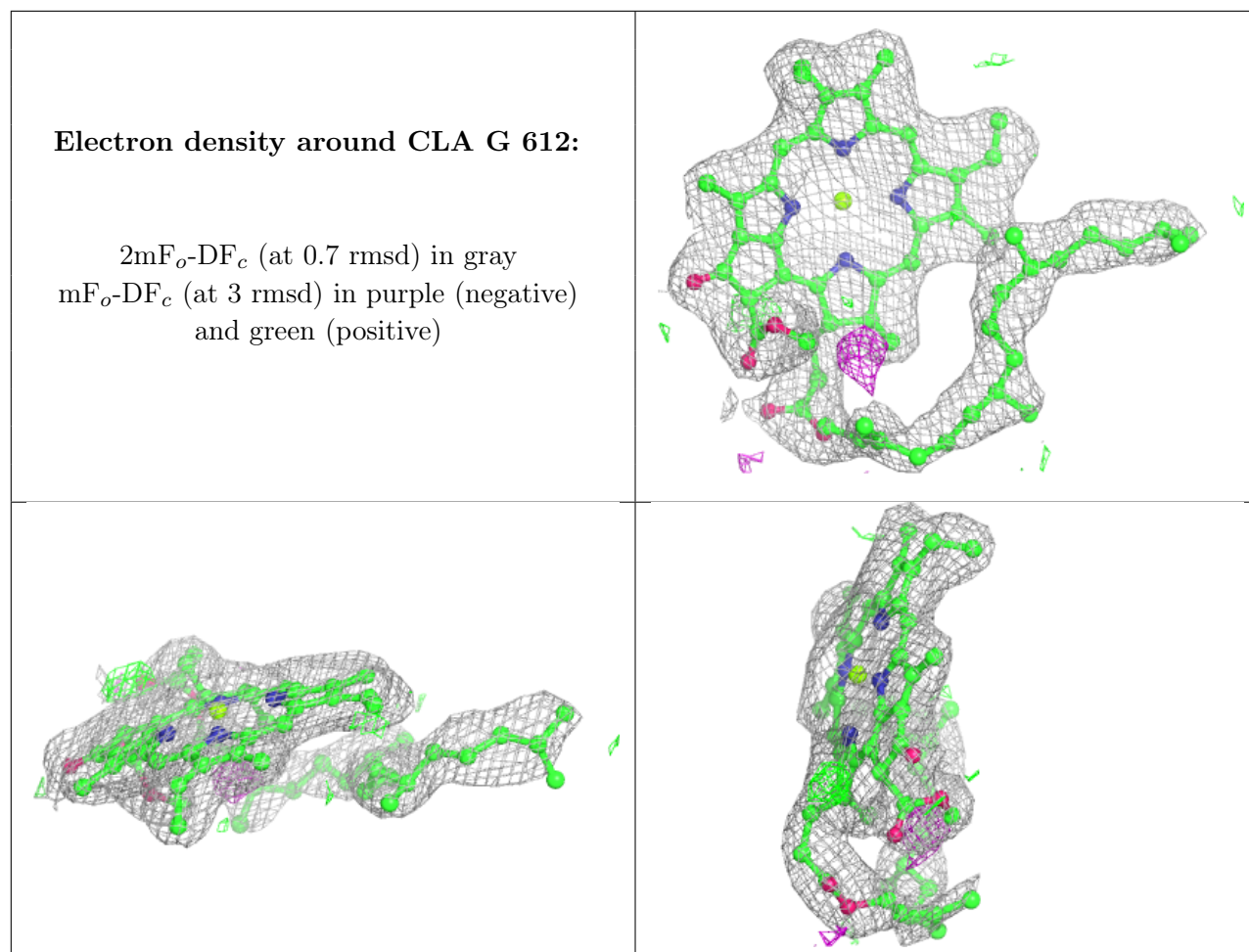




**Electron density around CHL I 605:**

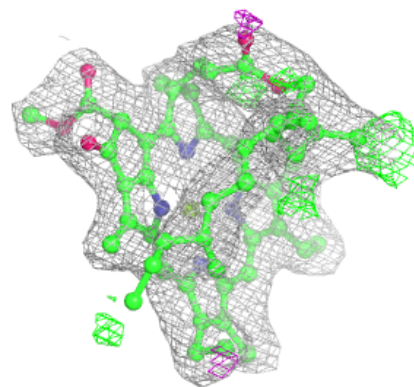
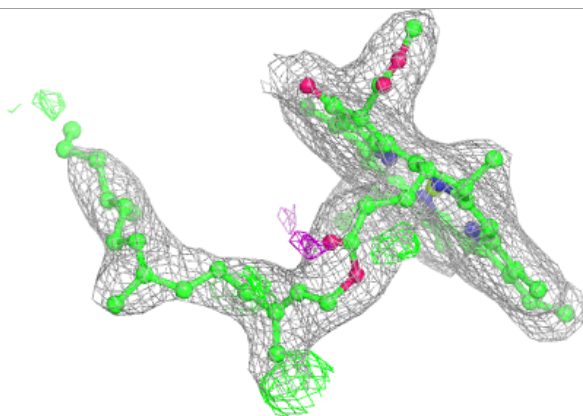
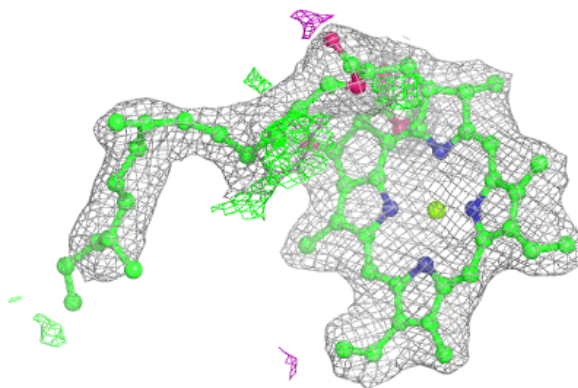
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



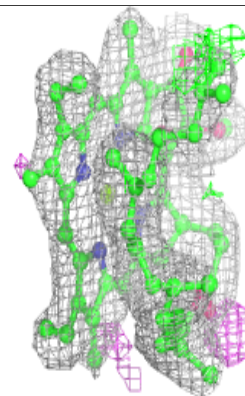
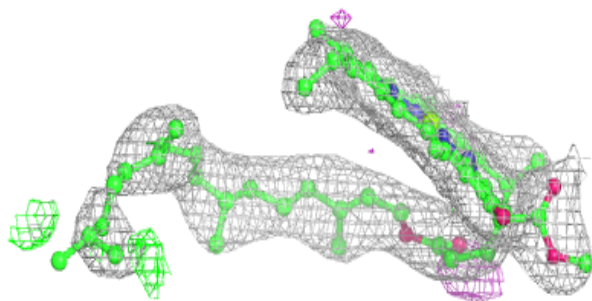
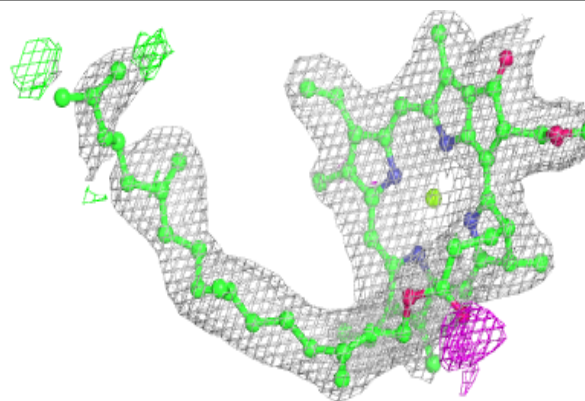


**Electron density around CLA H 604:**

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

**Electron density around CLA H 610:**

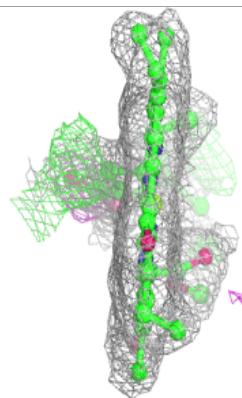
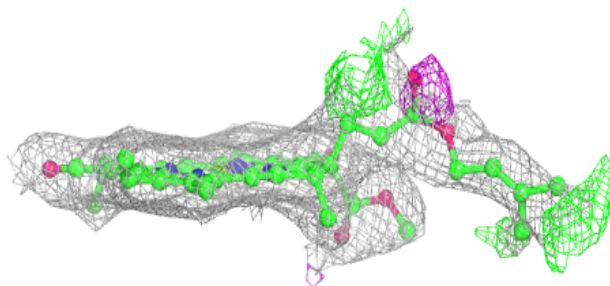
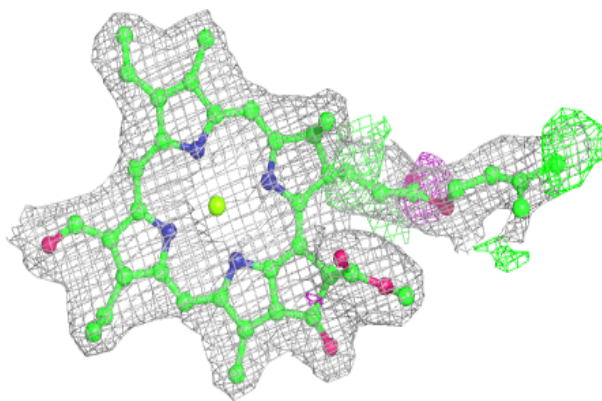
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

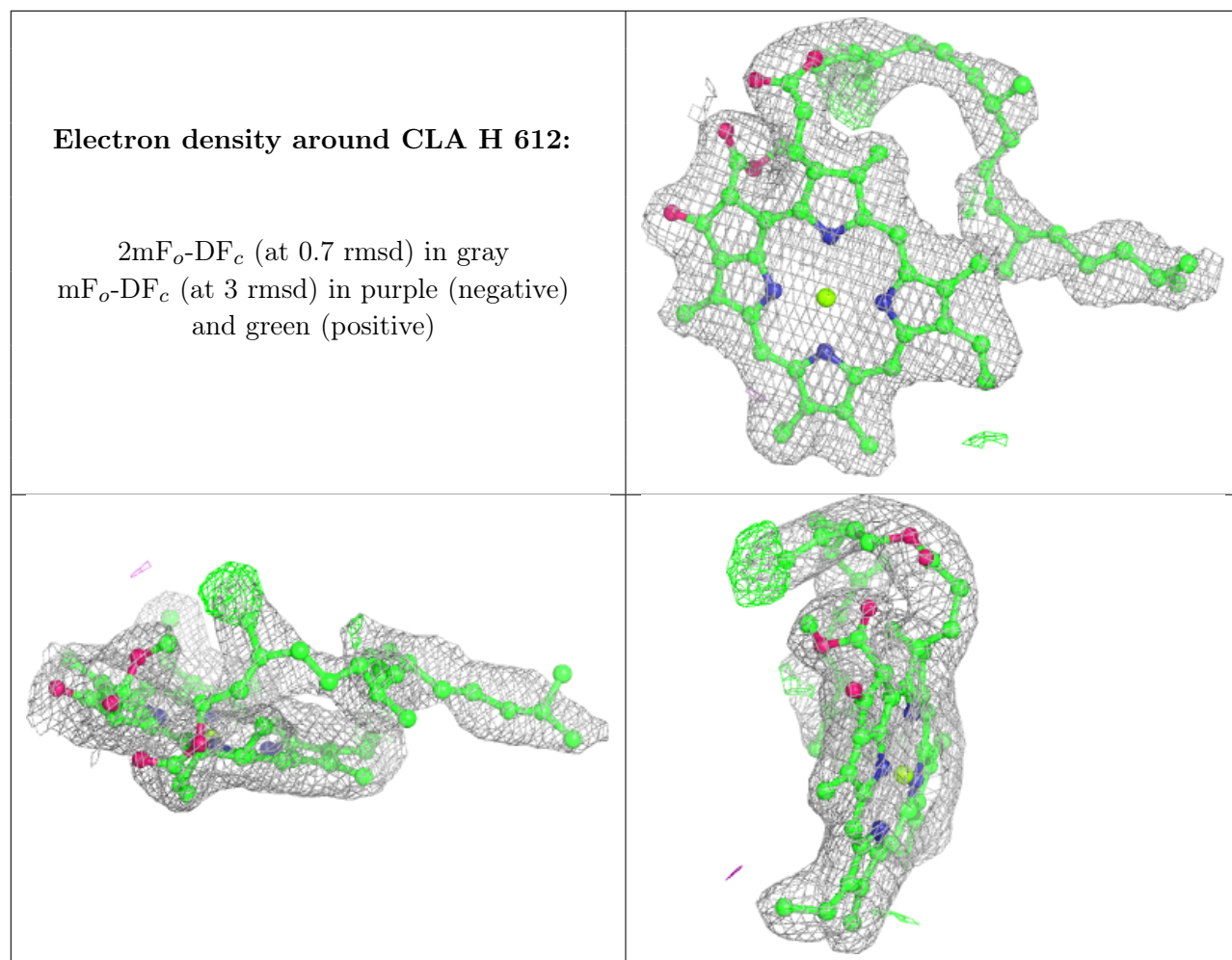




**Electron density around CHL I 606:**

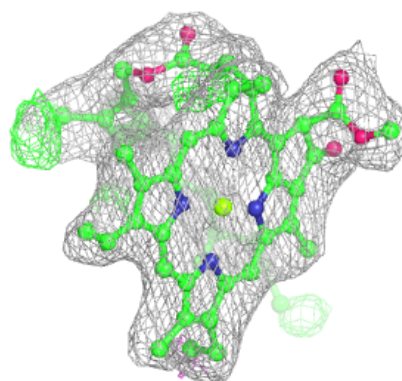
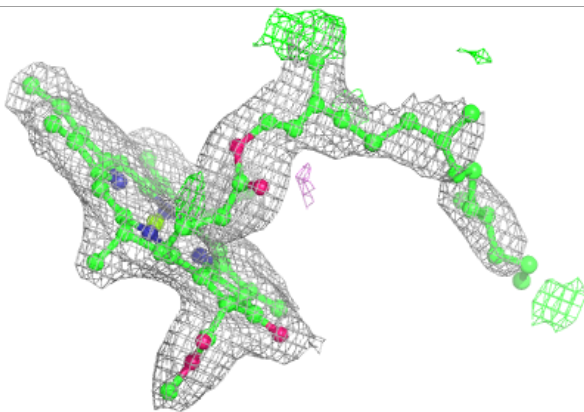
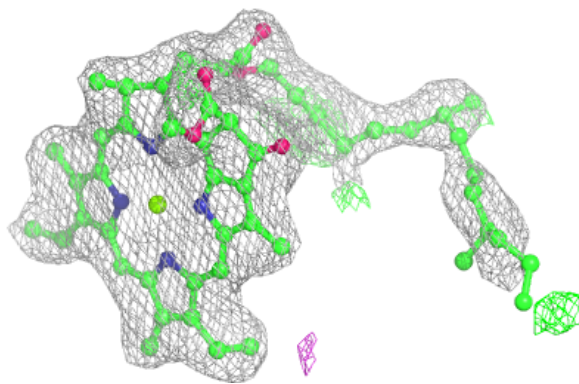
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



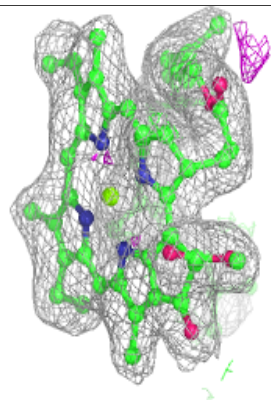
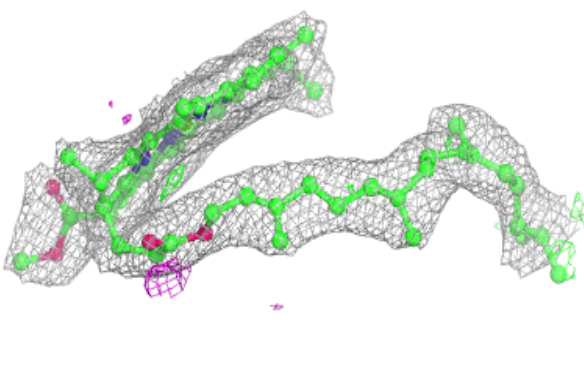
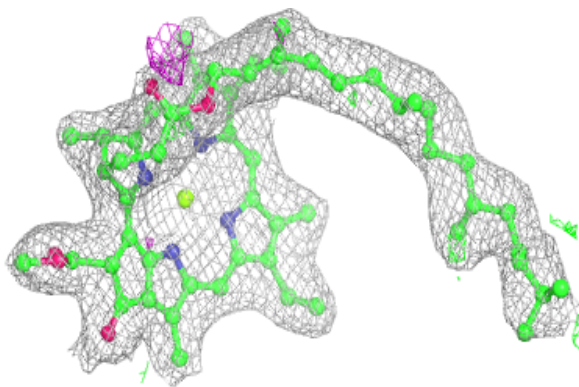


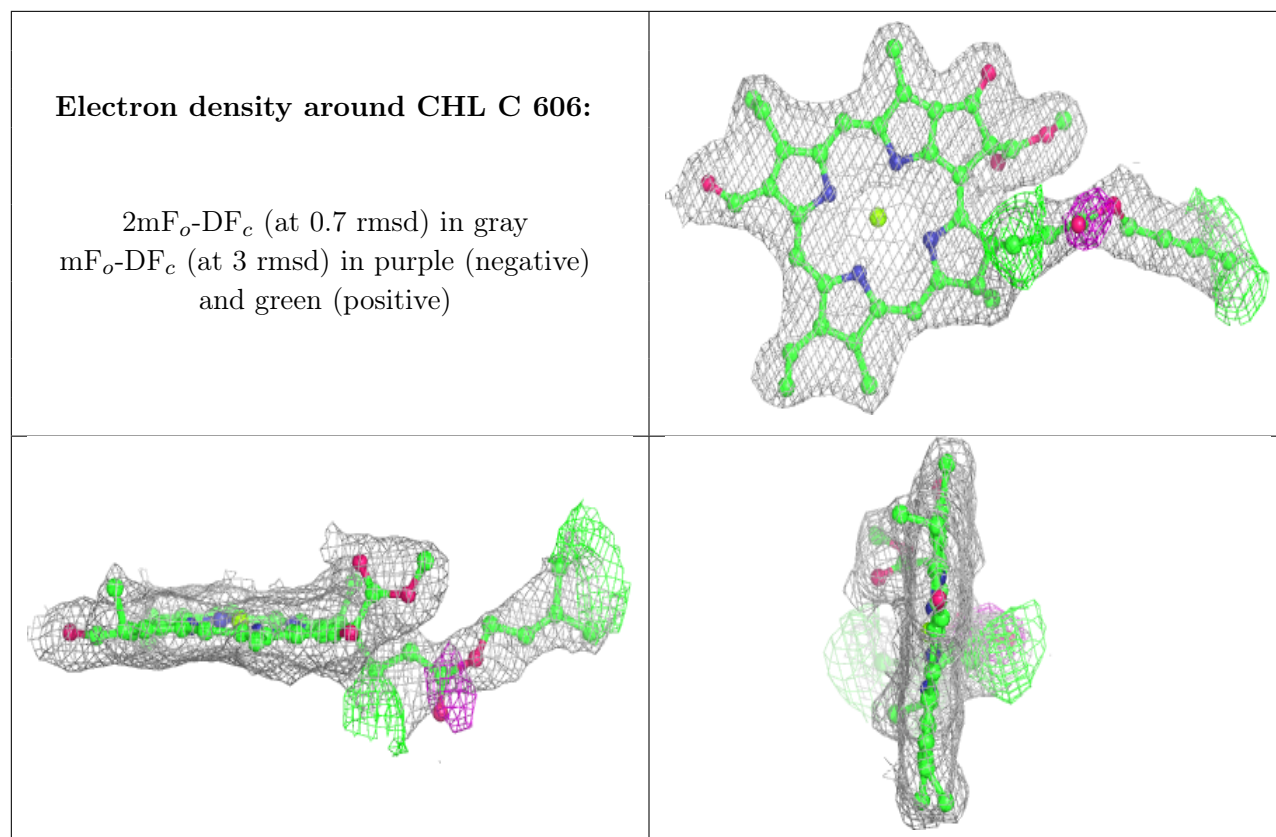
**Electron density around CLA I 604:**

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

**Electron density around CLA I 610:**

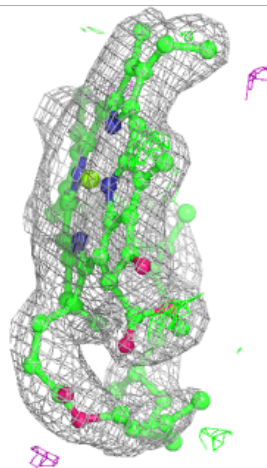
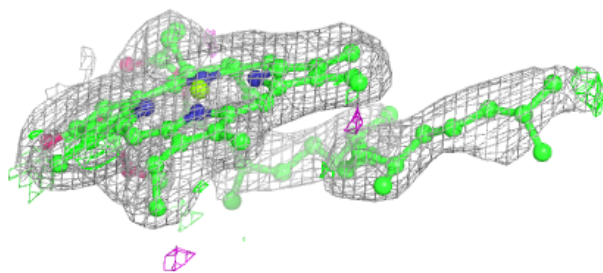
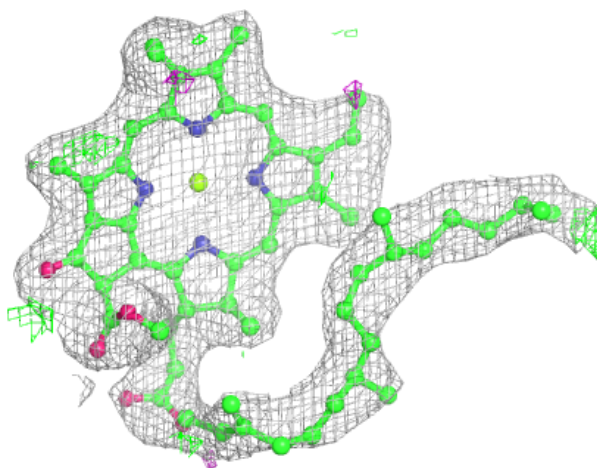
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA I 612:**

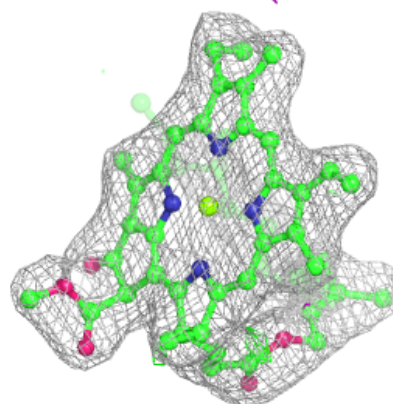
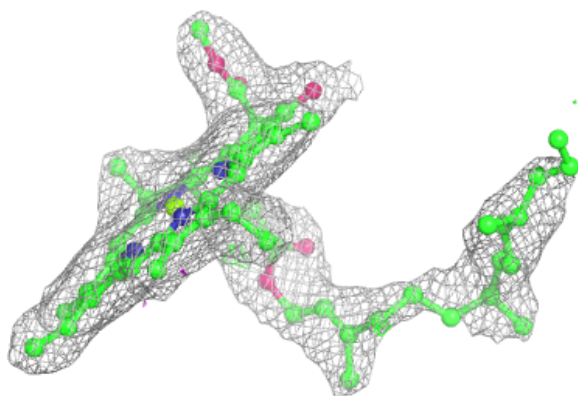
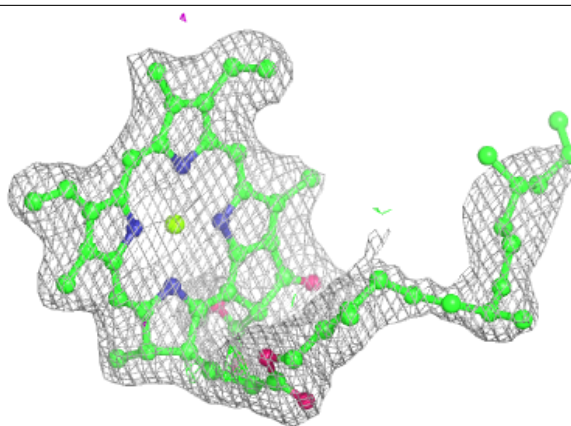
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



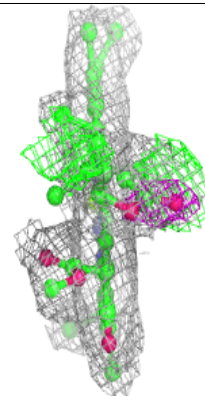
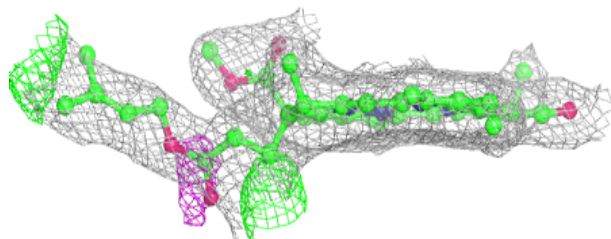
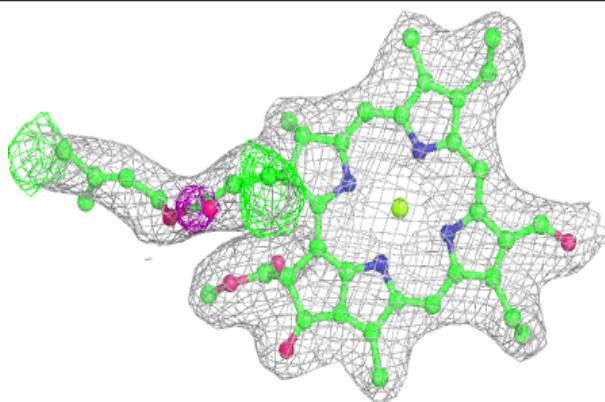


**Electron density around CLA A 604:**

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

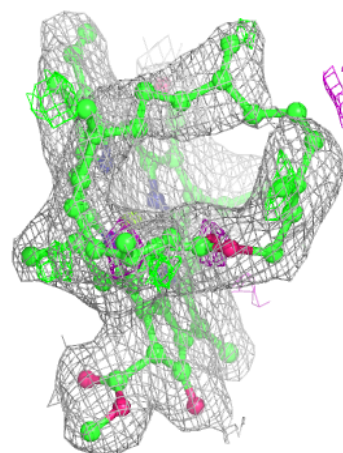
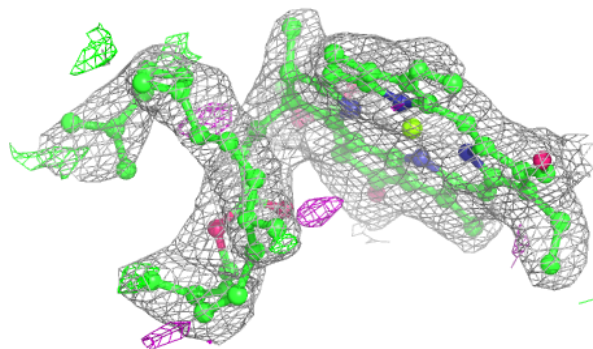
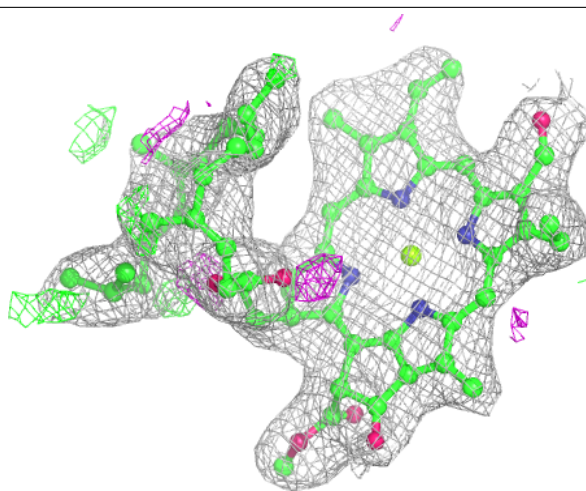
**Electron density around CHL D 606:**

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



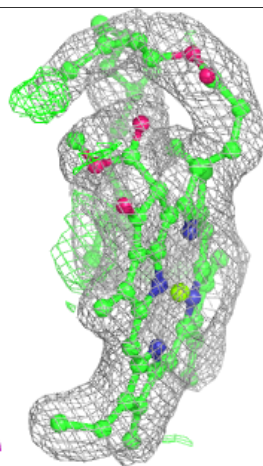
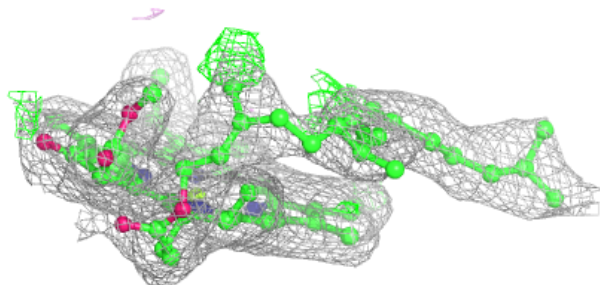
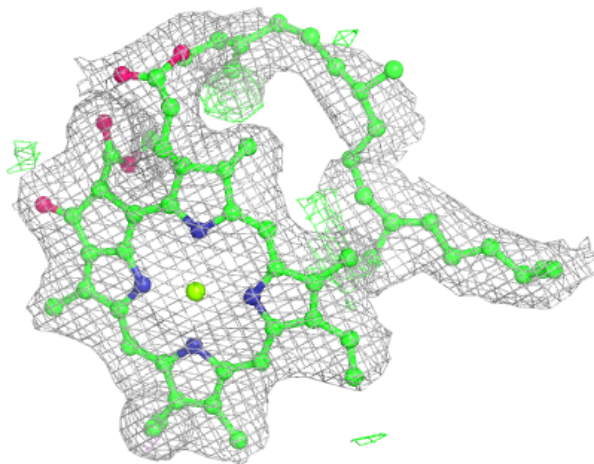
**Electron density around CHL F 608:**

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



**Electron density around CLA B 612:**

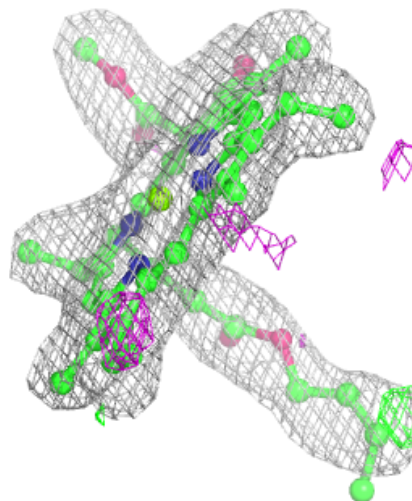
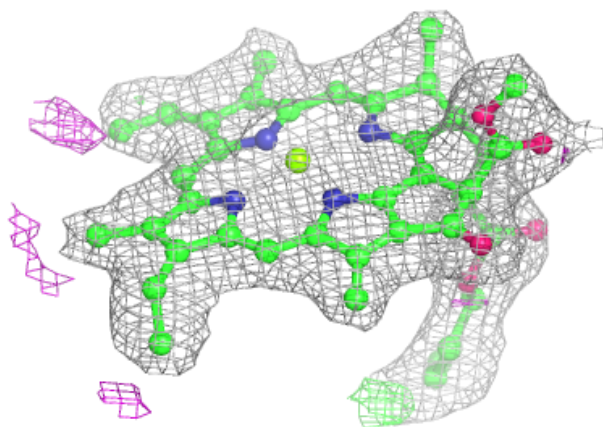
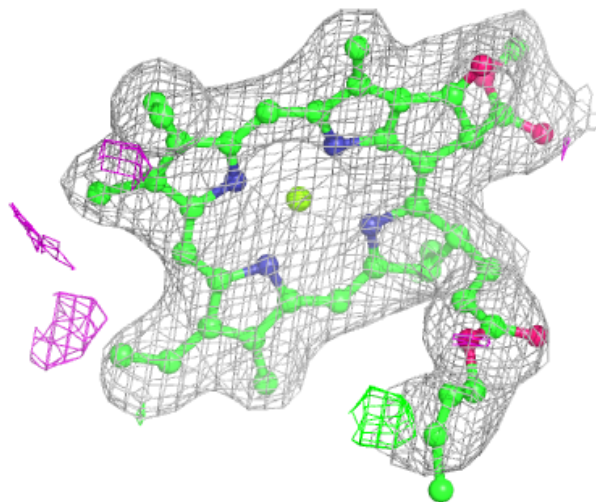
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

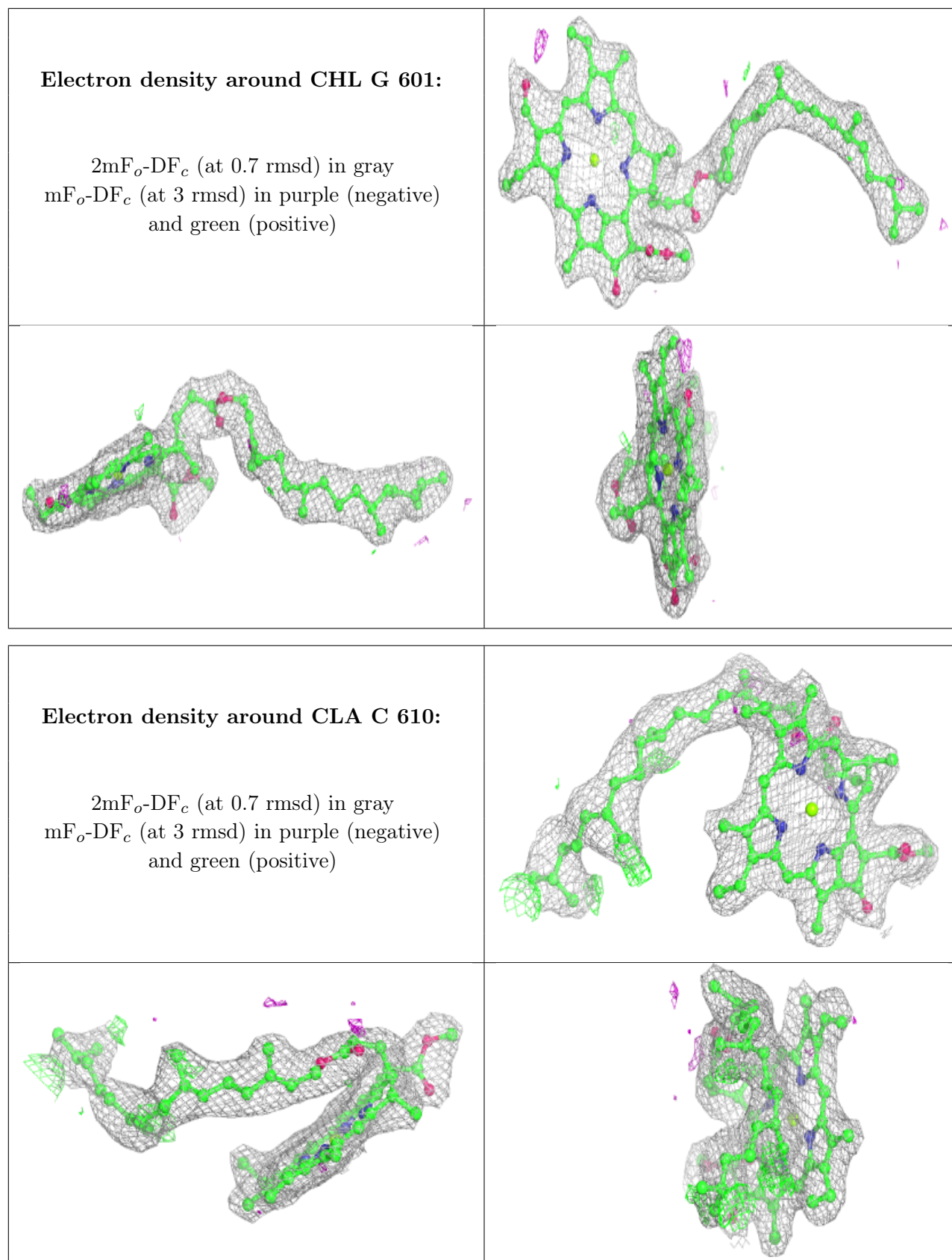




**Electron density around CLA B 614:**

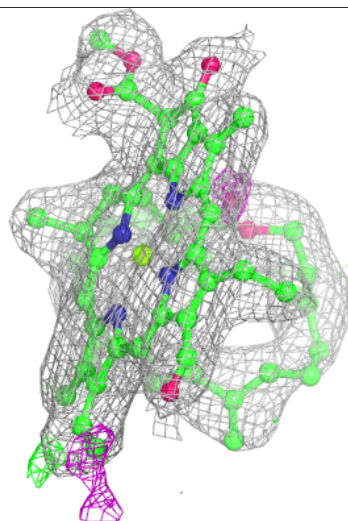
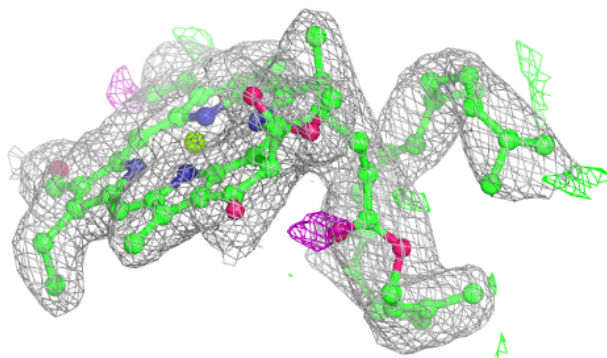
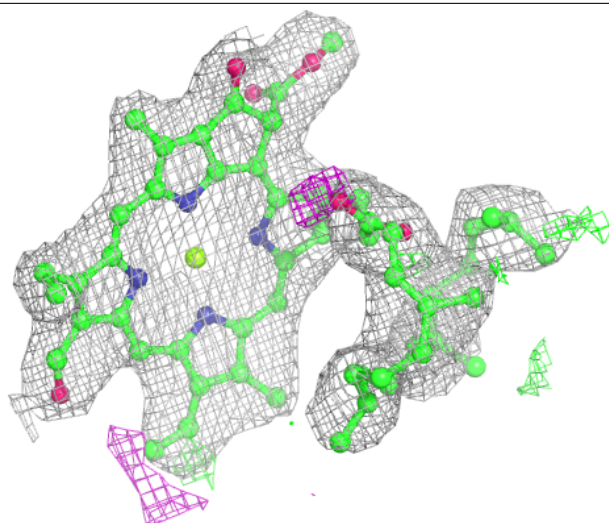
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

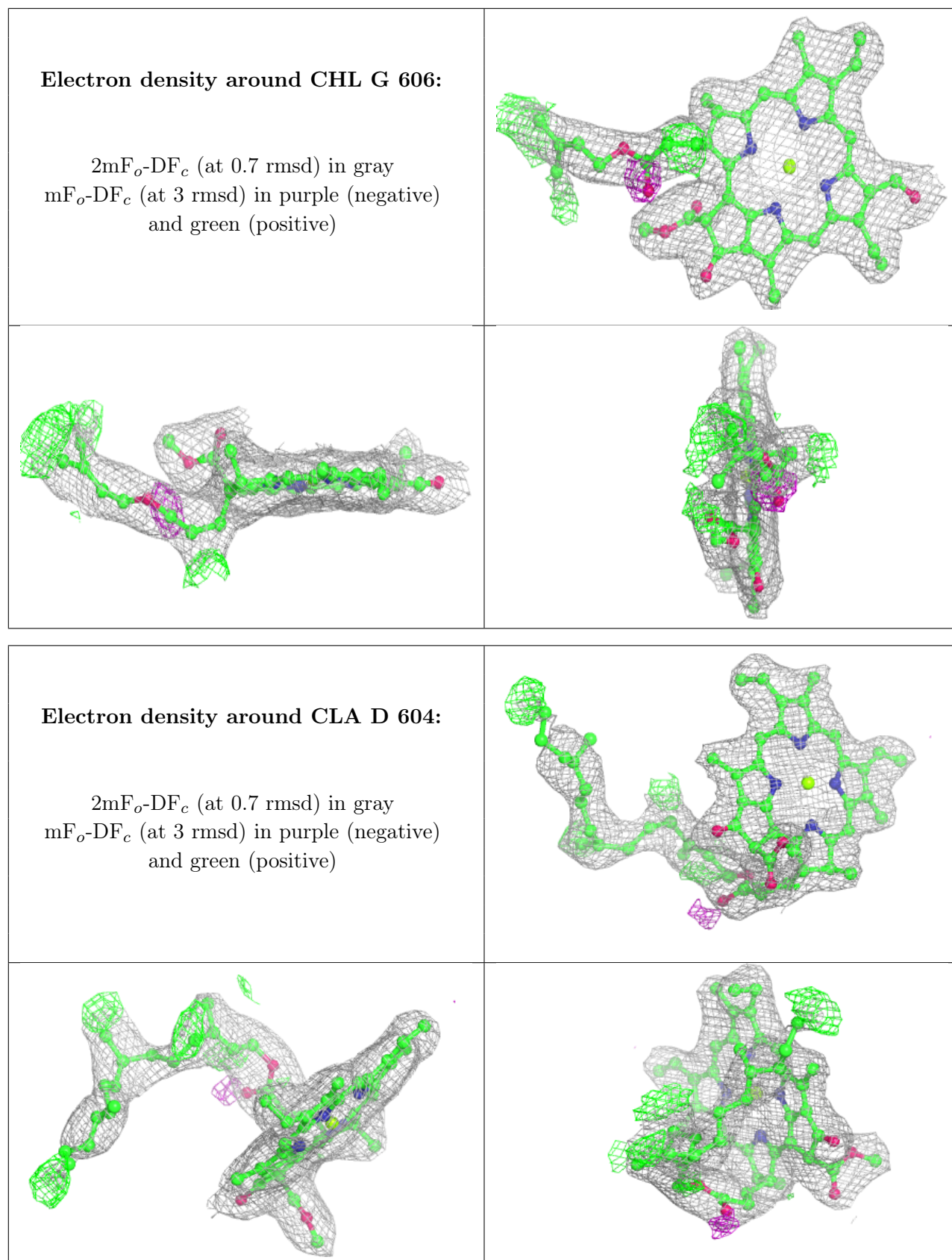




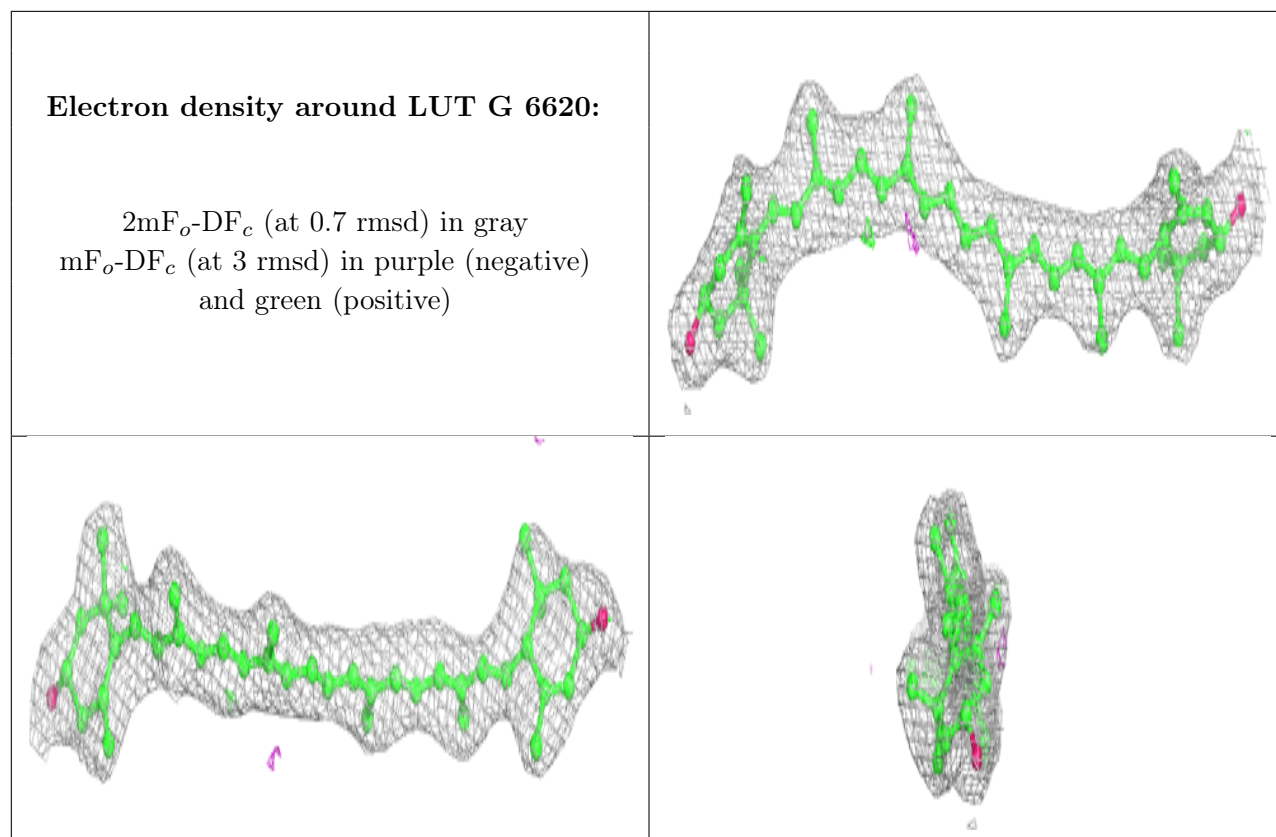
**Electron density around CHL B 608:**

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



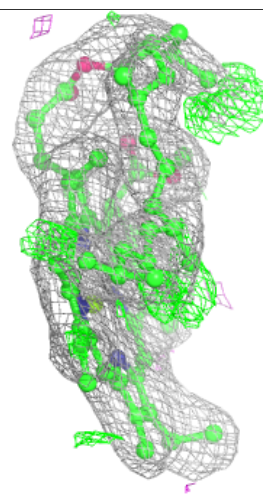
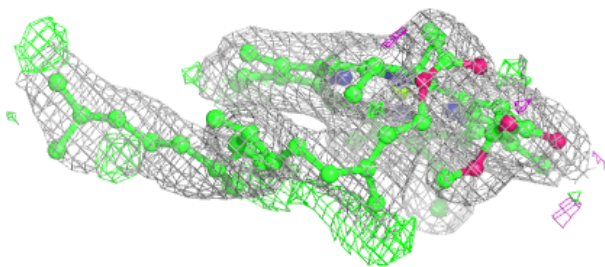
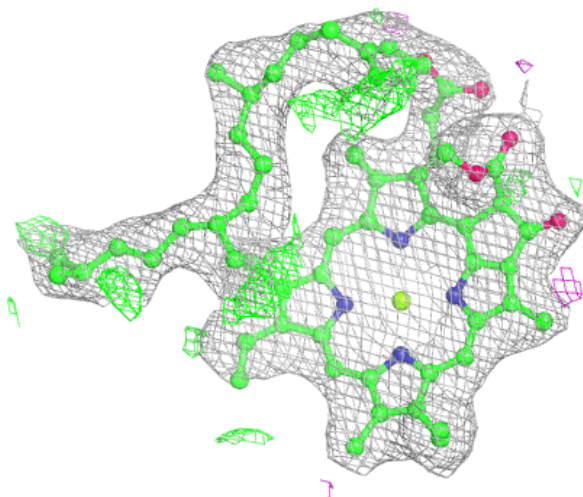


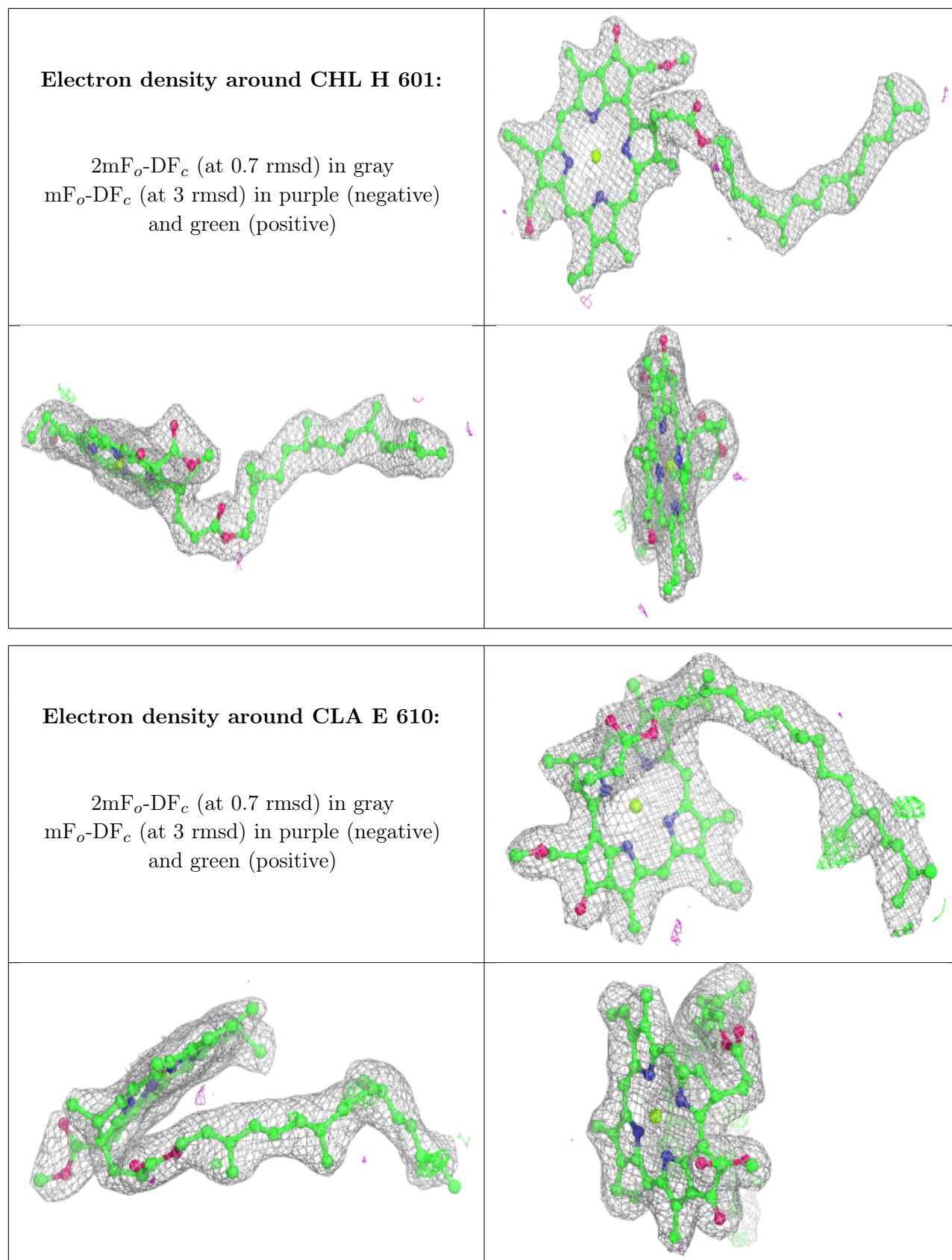


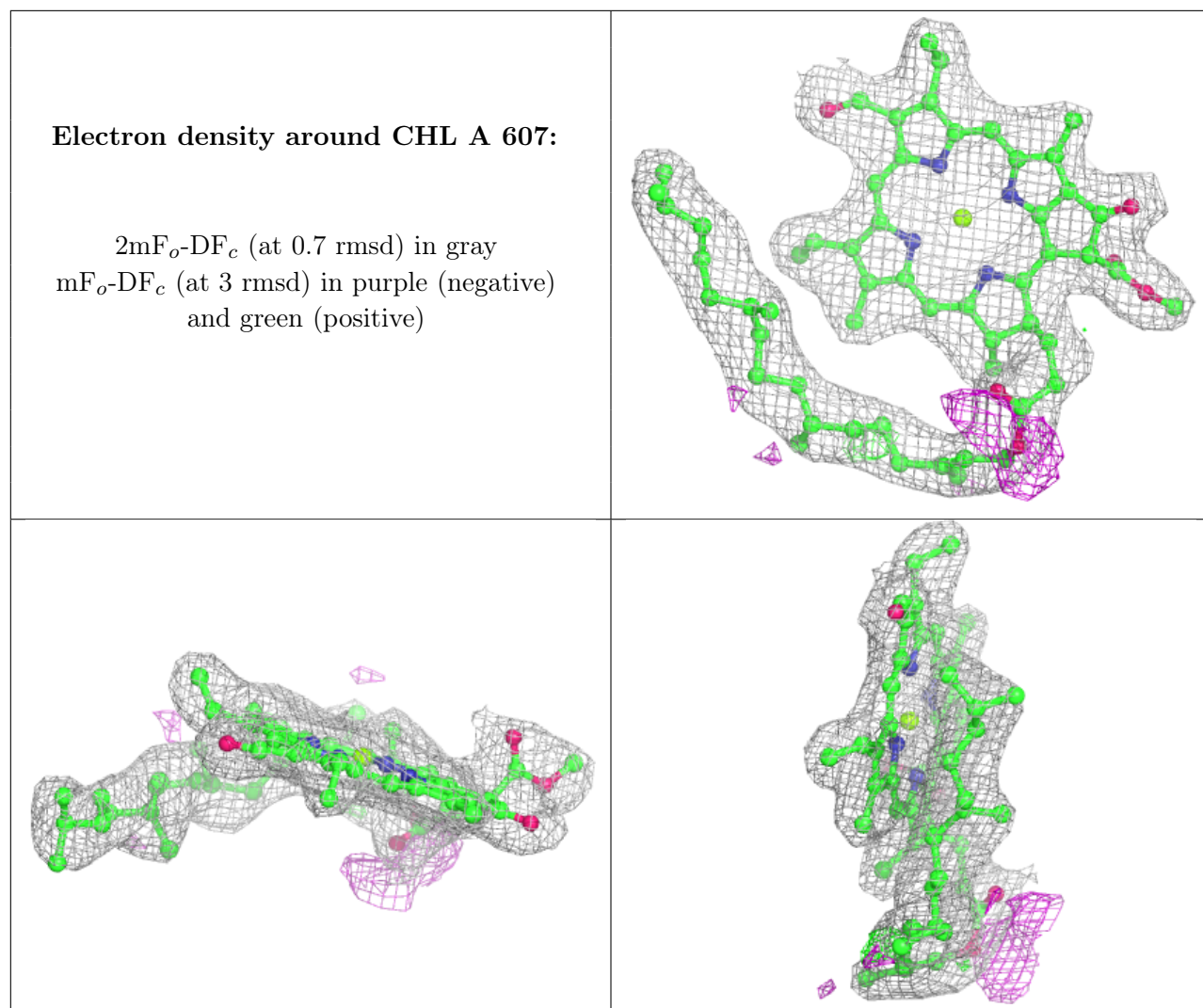


**Electron density around CLA D 612:**

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



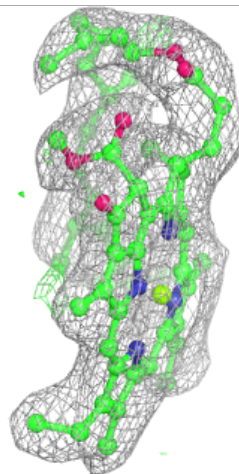
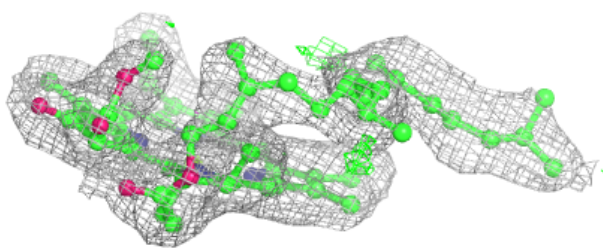
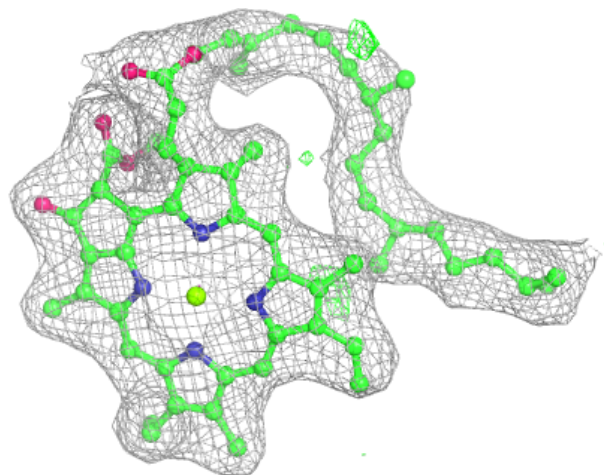






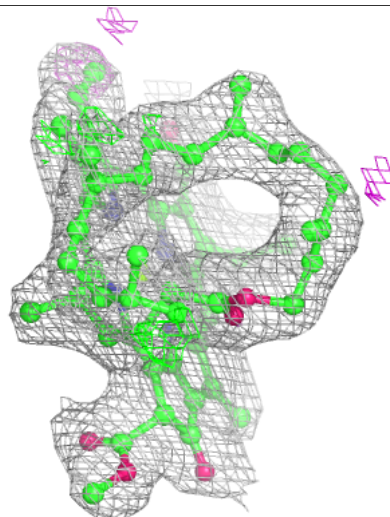
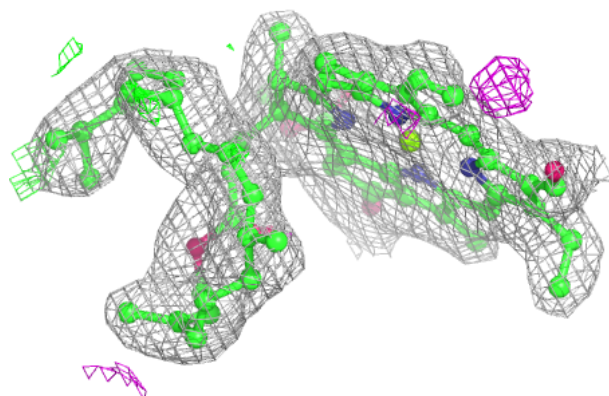
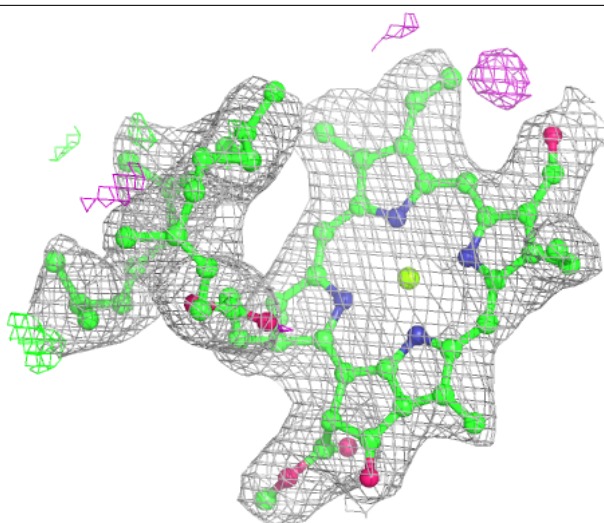
**Electron density around CLA E 612:**

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



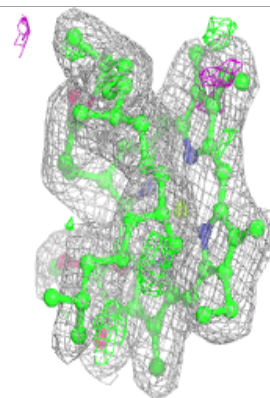
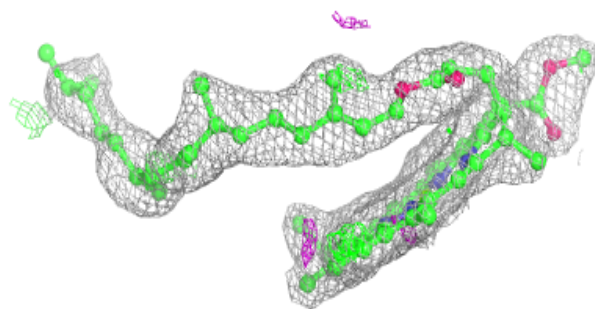
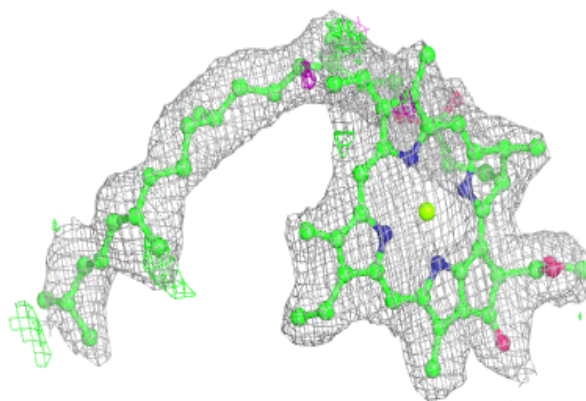
**Electron density around CHL C 608:**

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



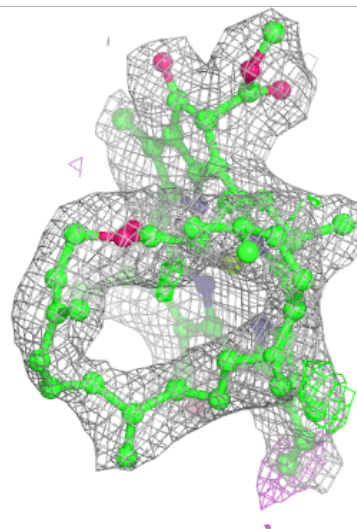
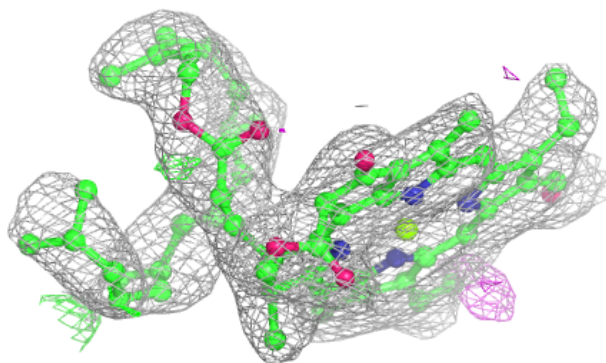
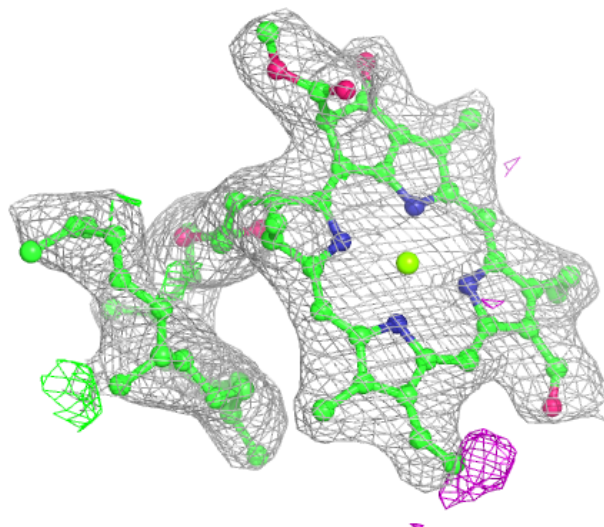
**Electron density around CLA F 610:**

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



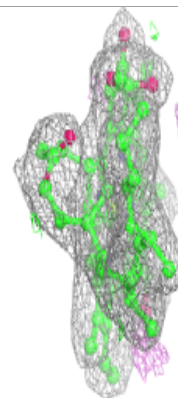
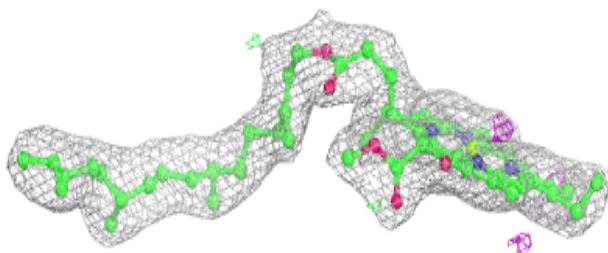
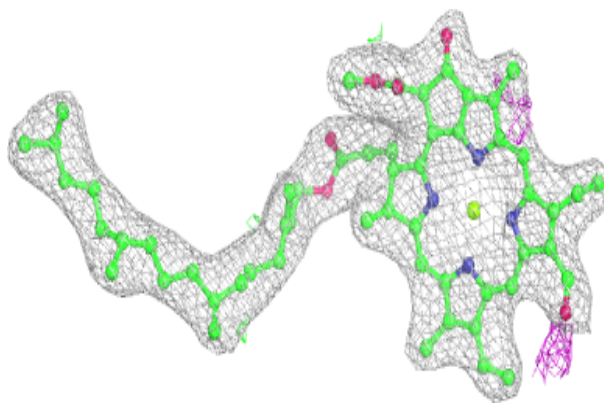
**Electron density around CHL H 608:**

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

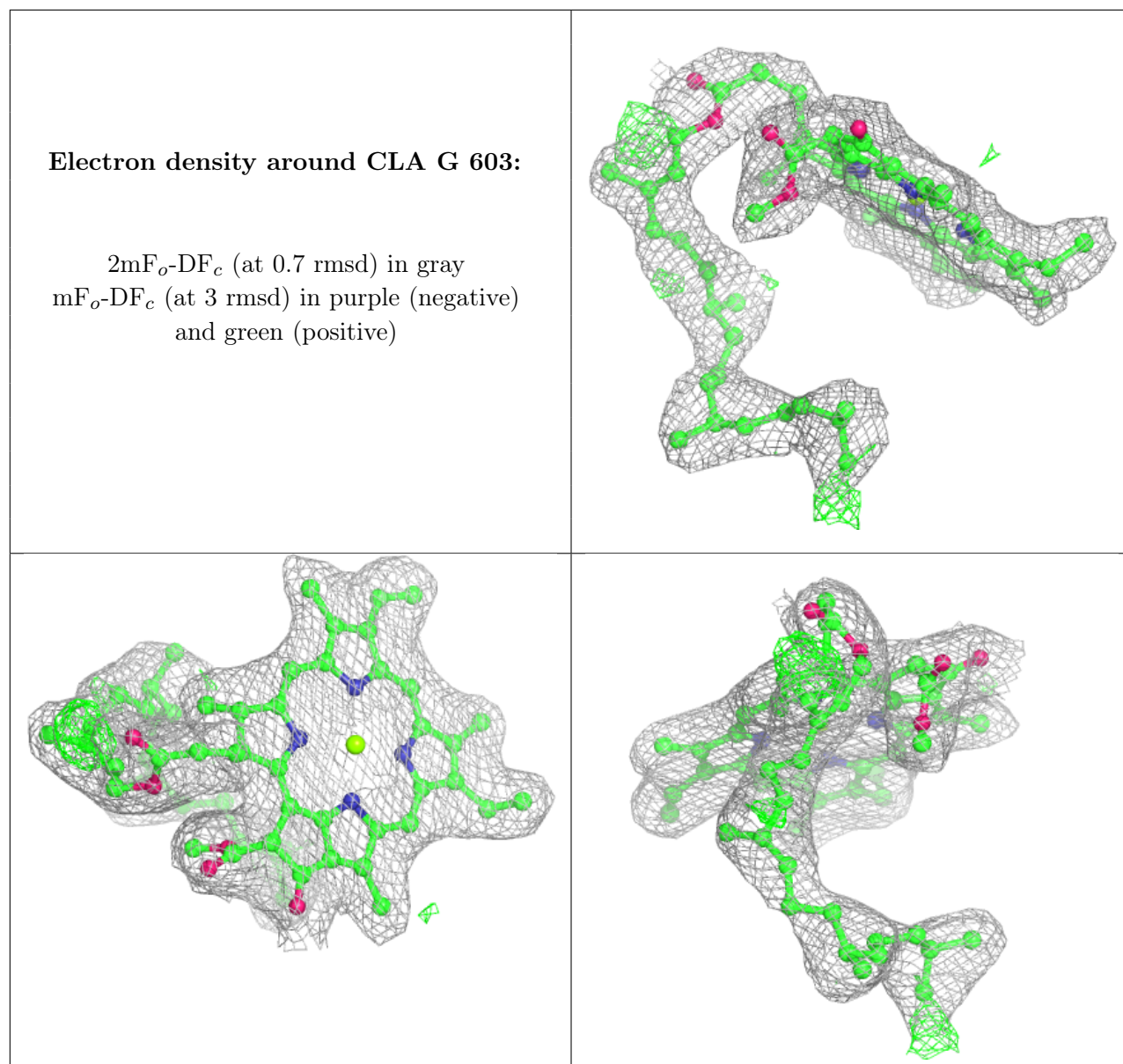


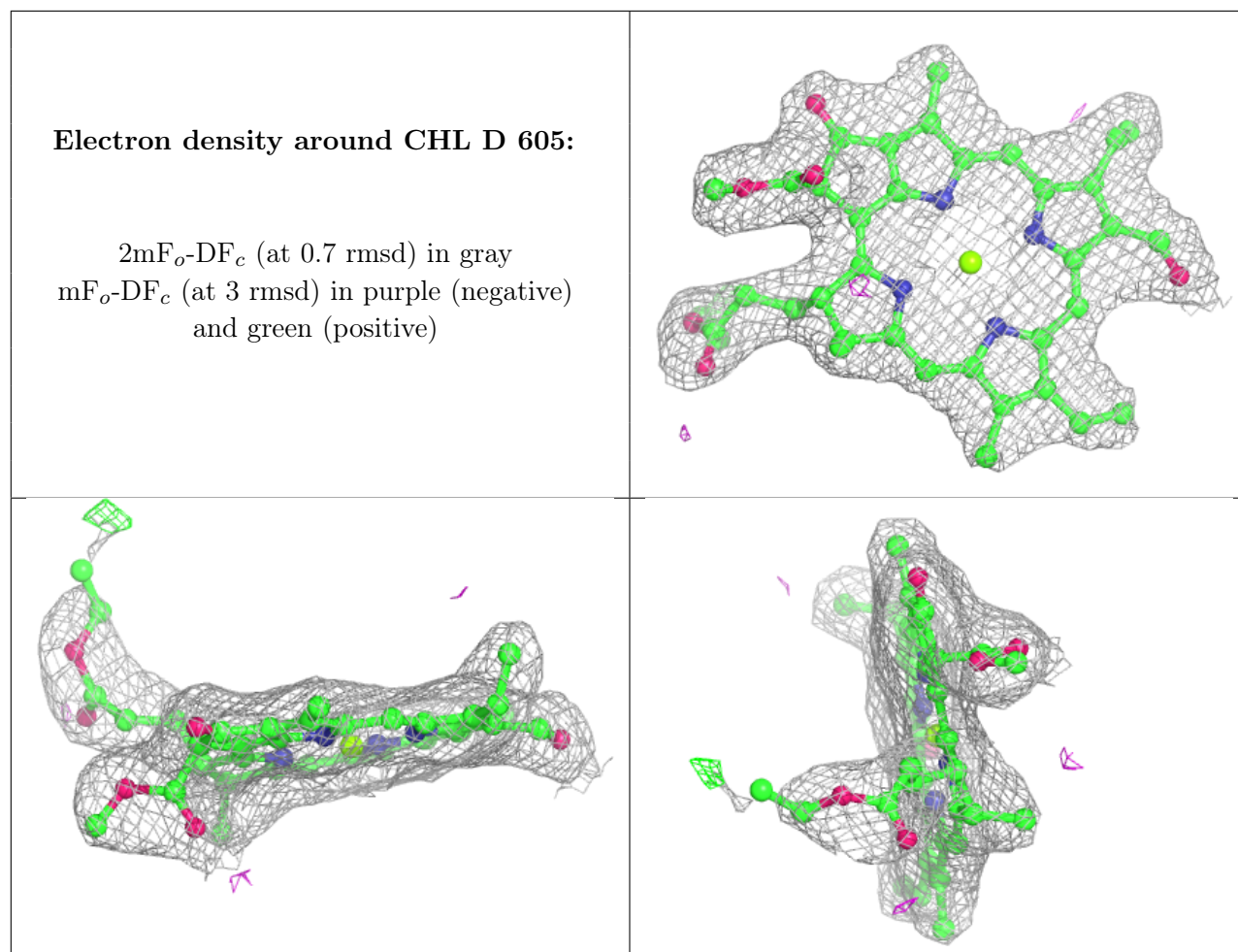
**Electron density around CHL I 601:**

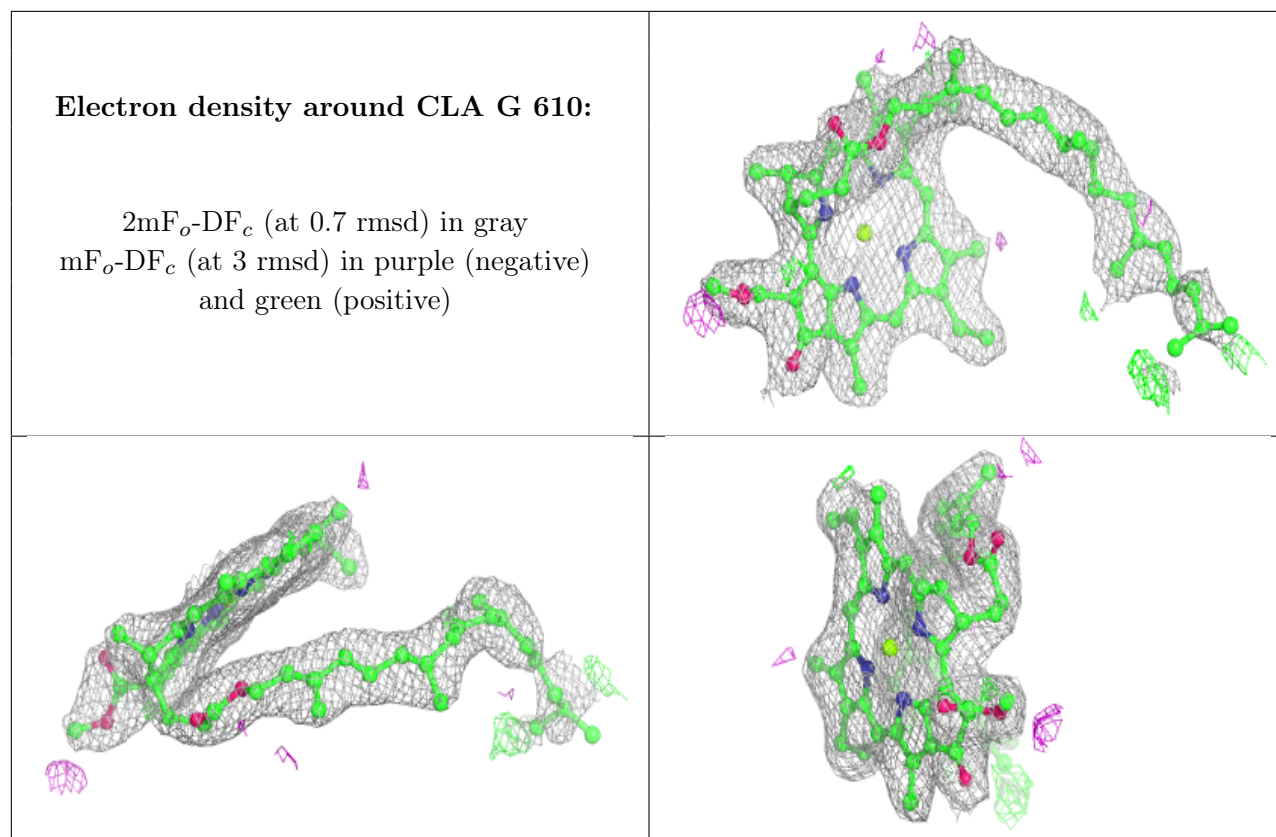
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



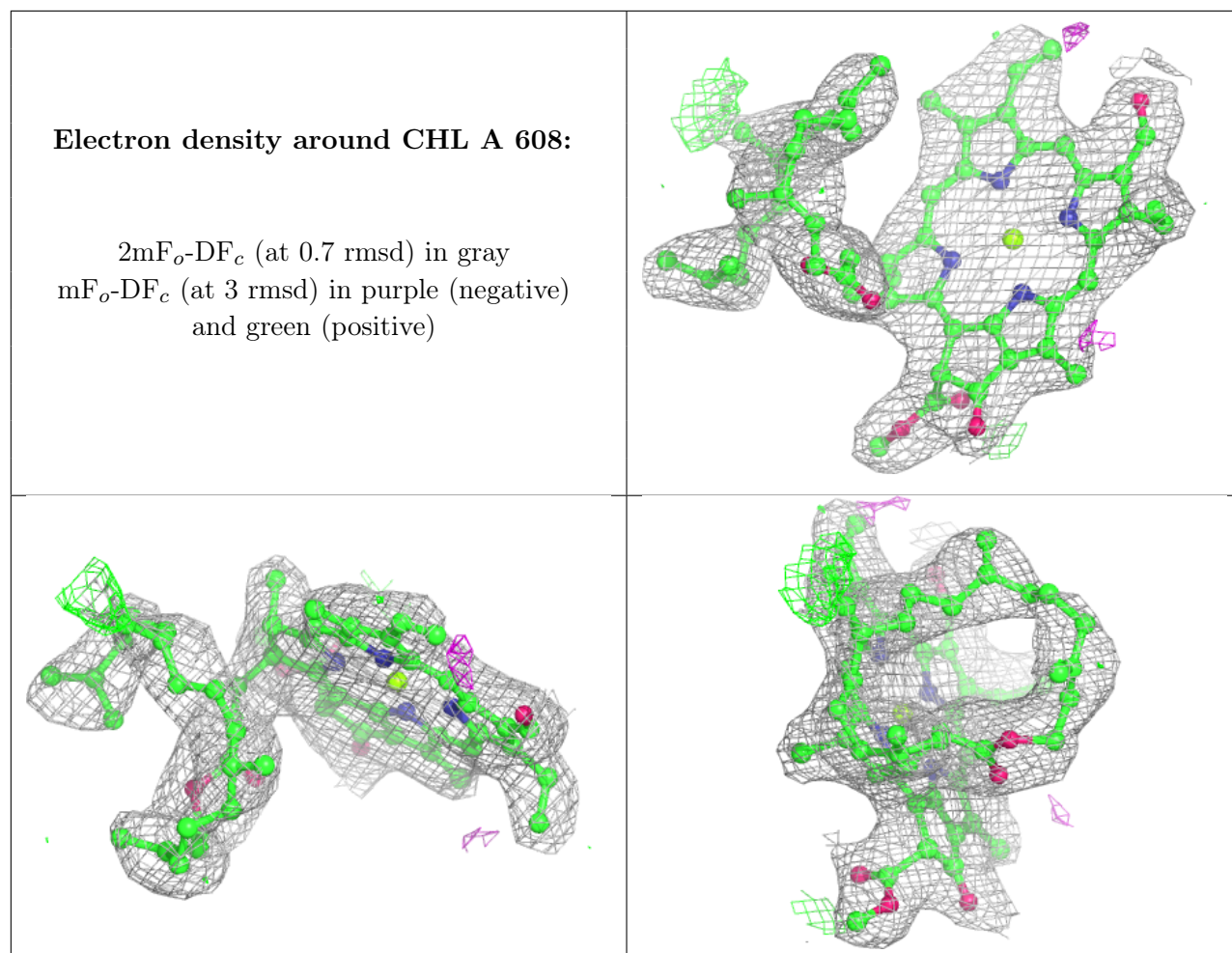






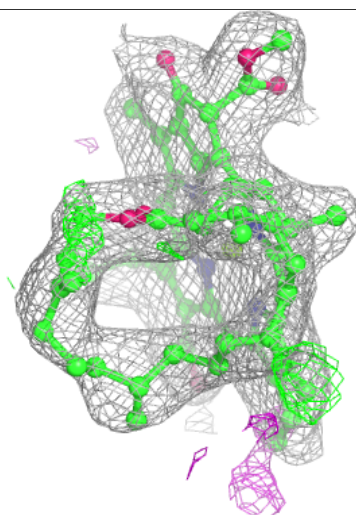
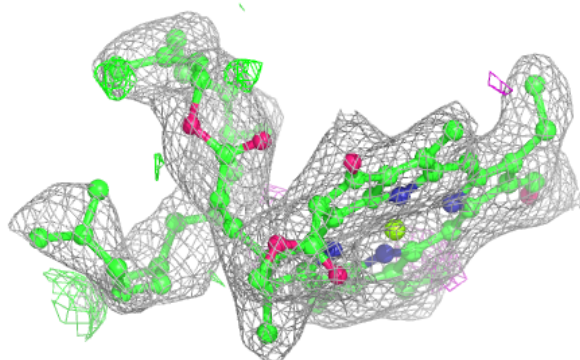
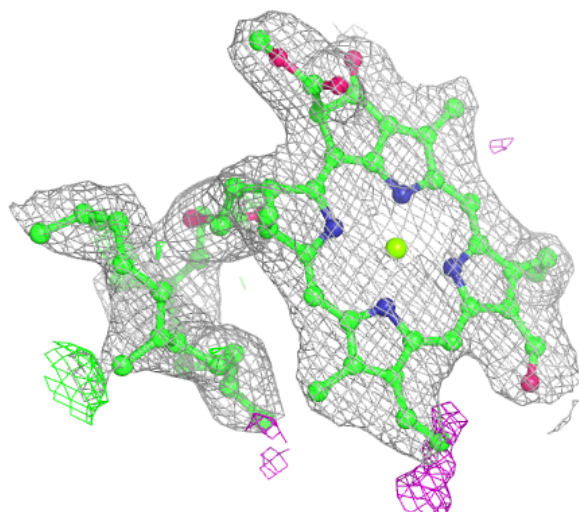






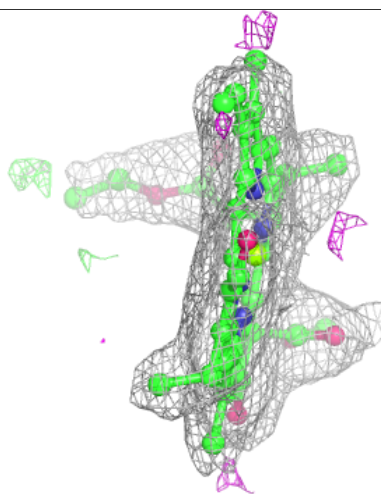
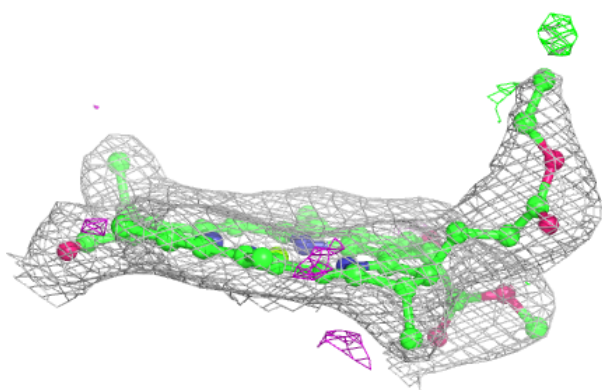
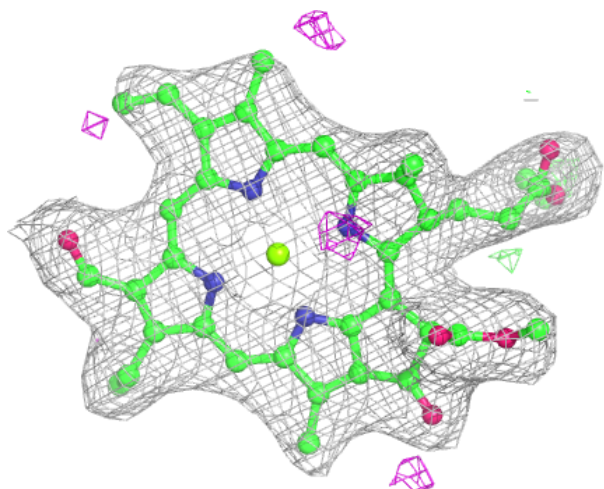
**Electron density around CHL I 608:**

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



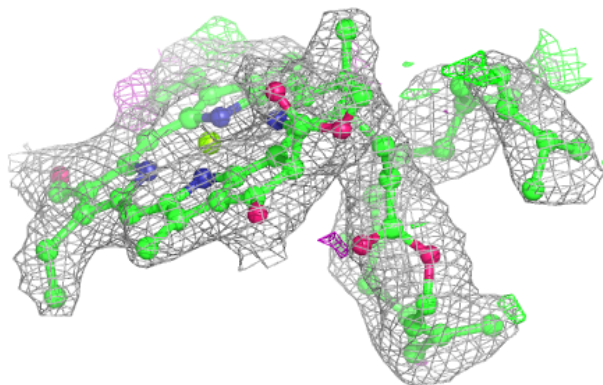
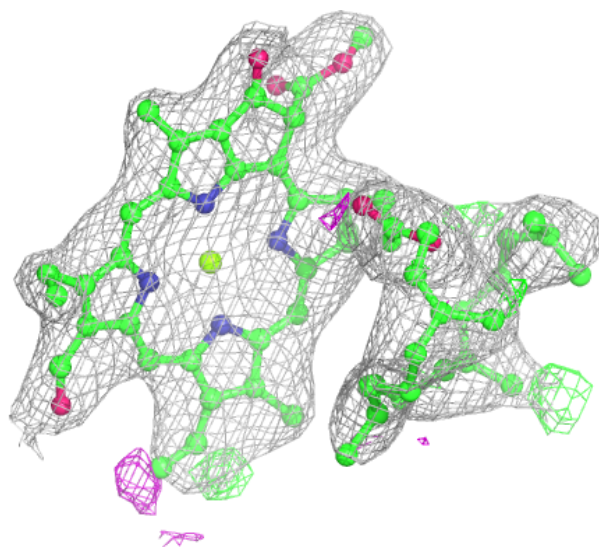
**Electron density around CHL J 605:**

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



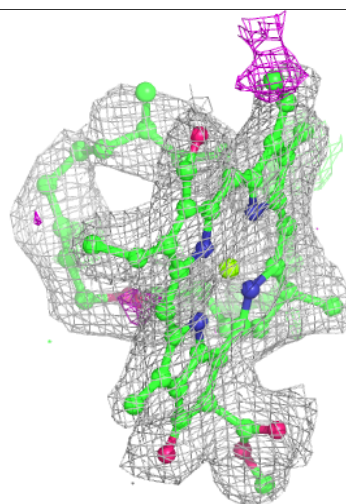
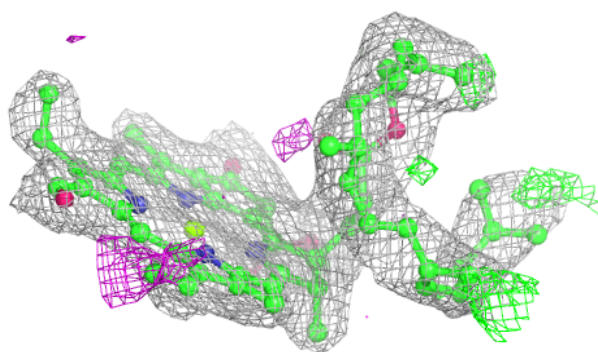
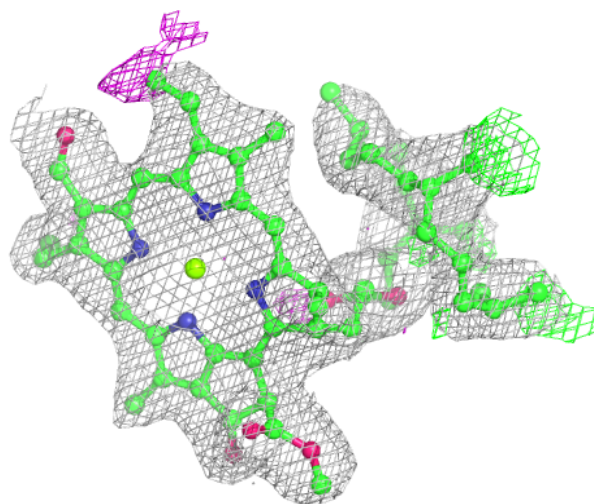
**Electron density around CHL D 608:**

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



**Electron density around CHL J 608:**

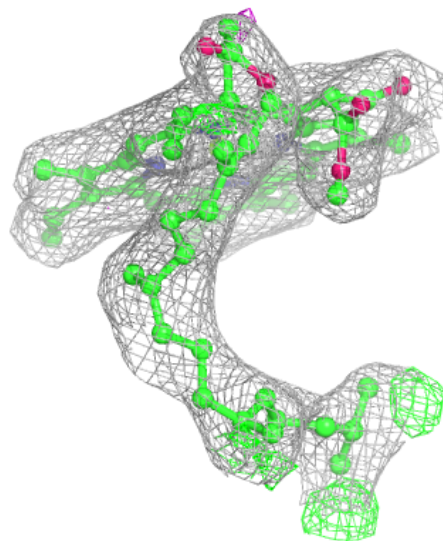
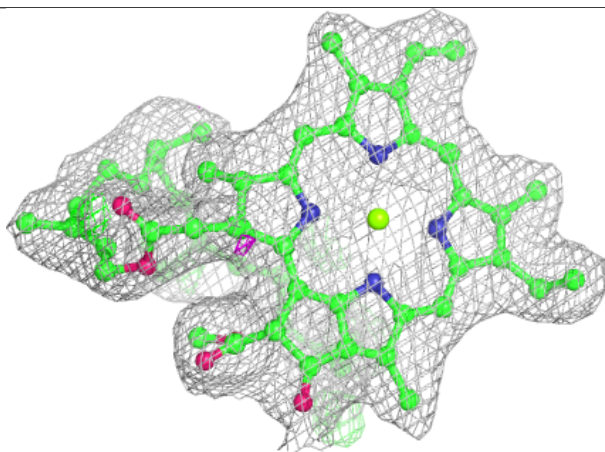
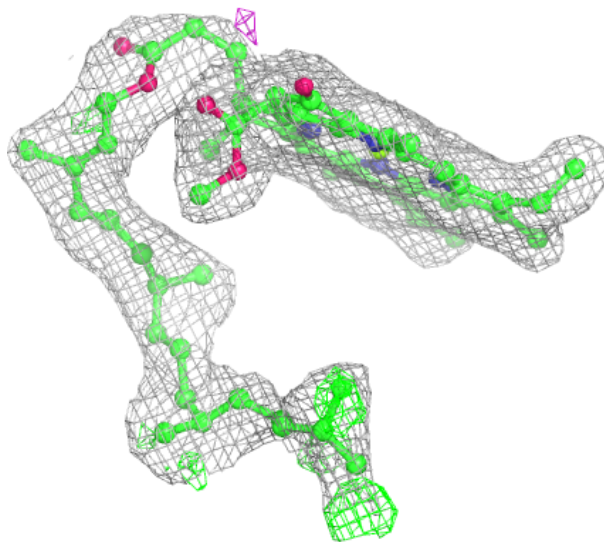
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

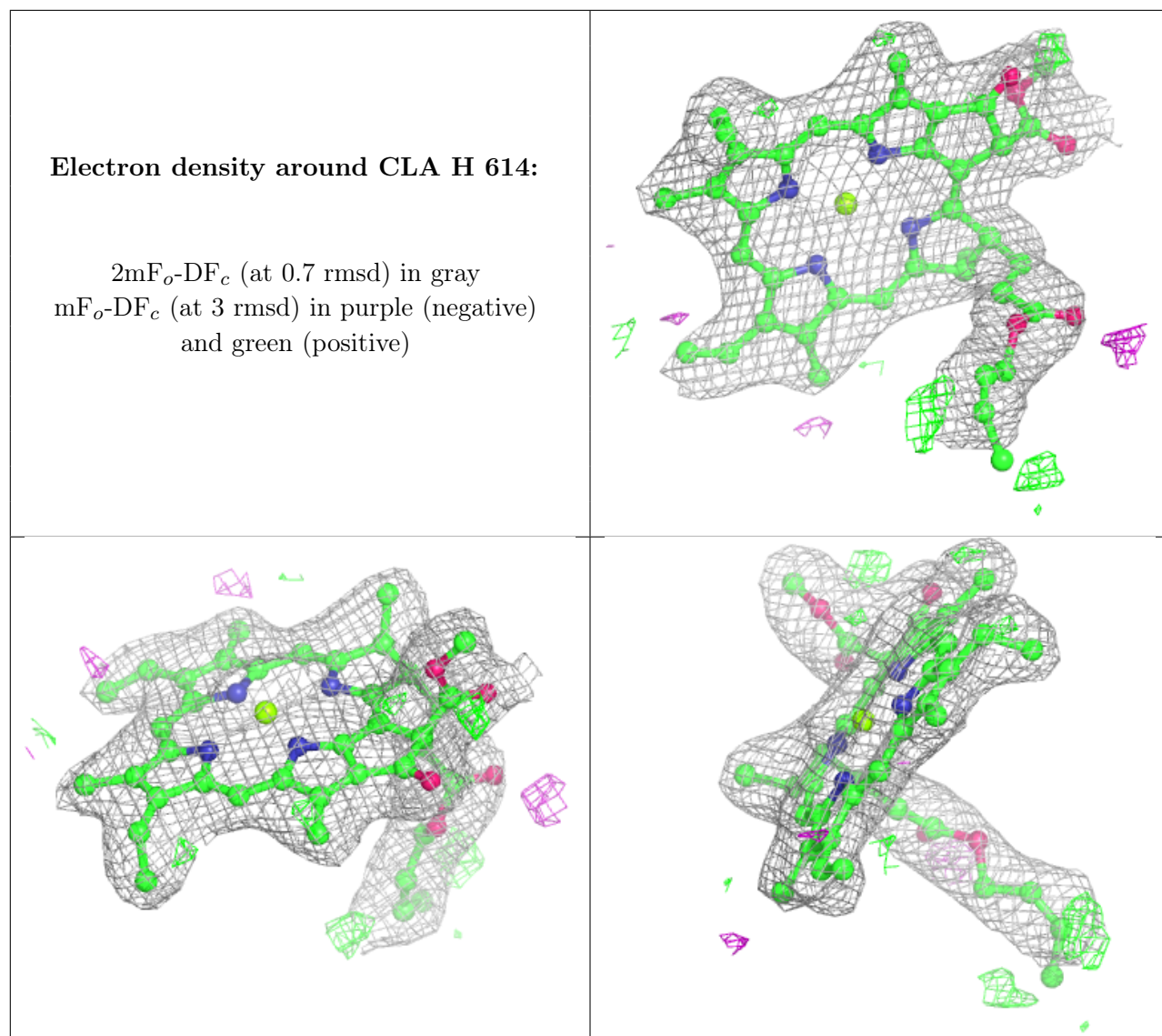




**Electron density around CLA A 603:**

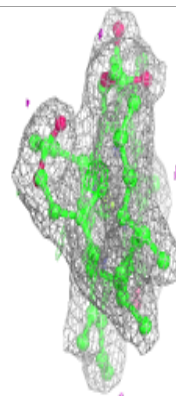
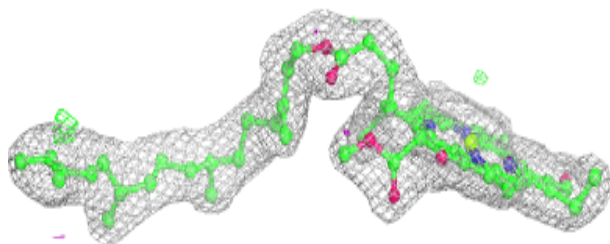
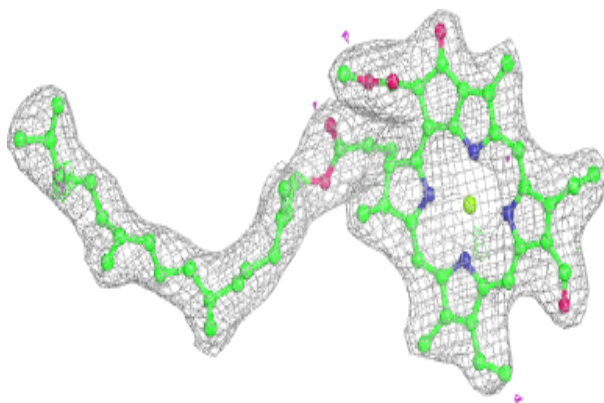
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CHL E 601:**

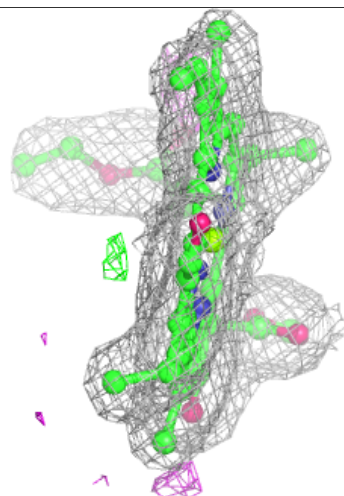
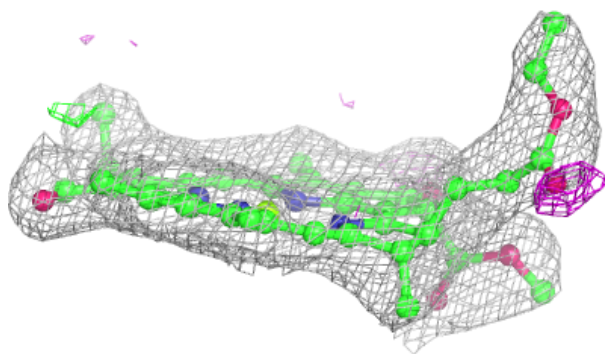
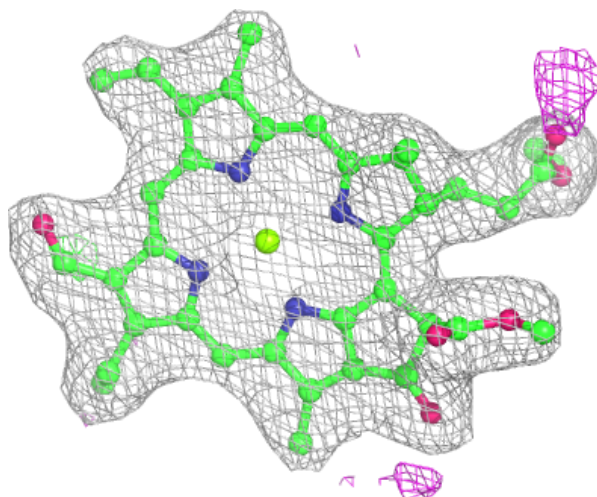
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

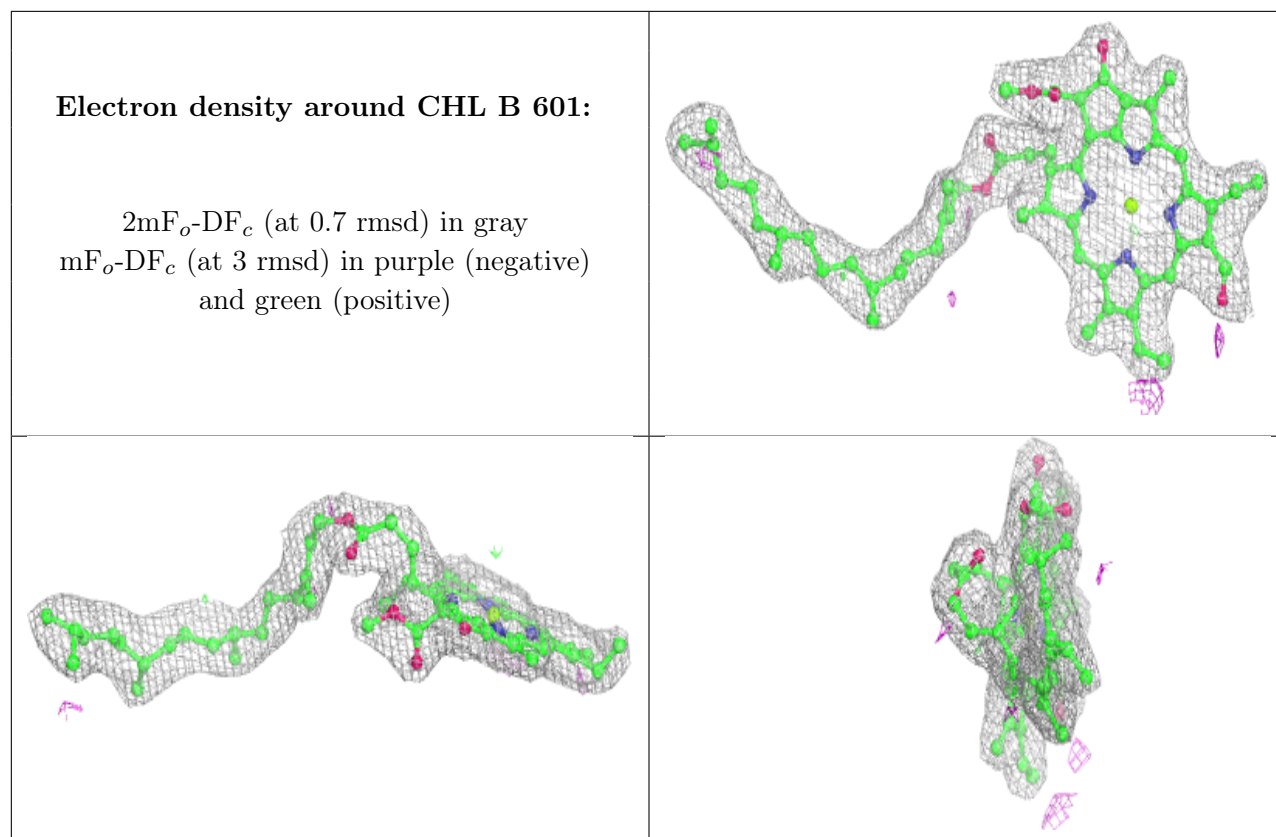




**Electron density around CHL E 605:**

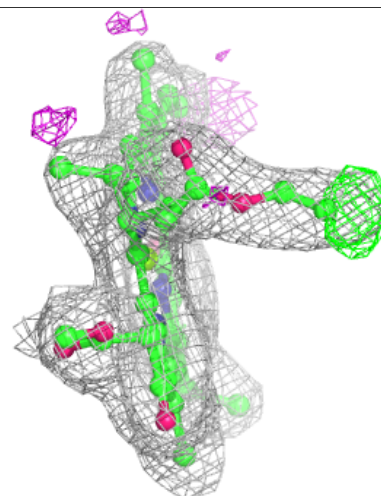
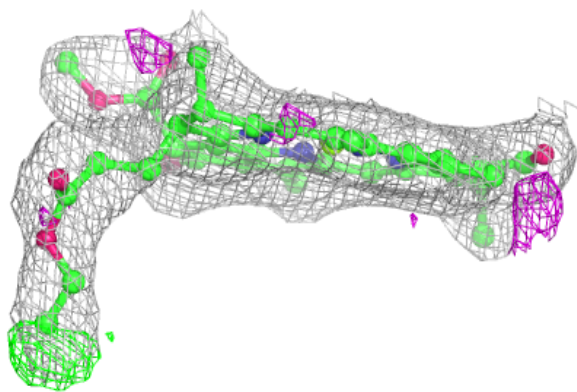
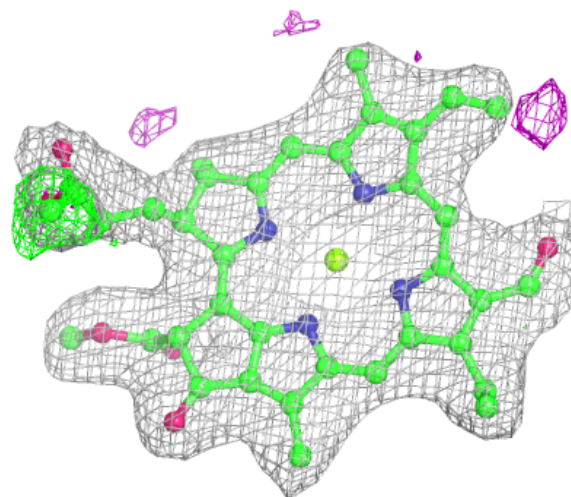
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





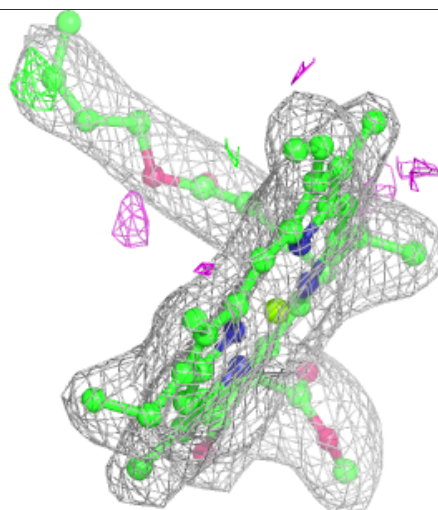
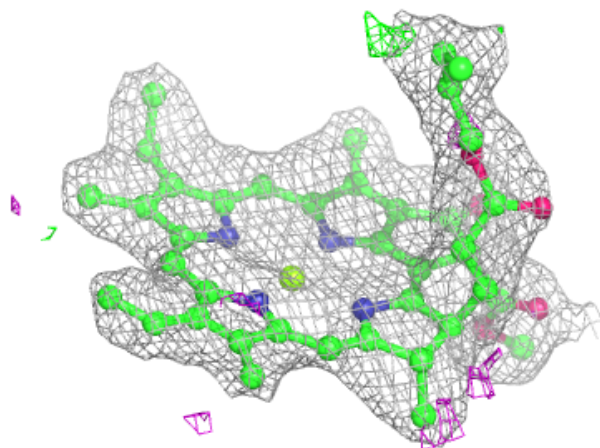
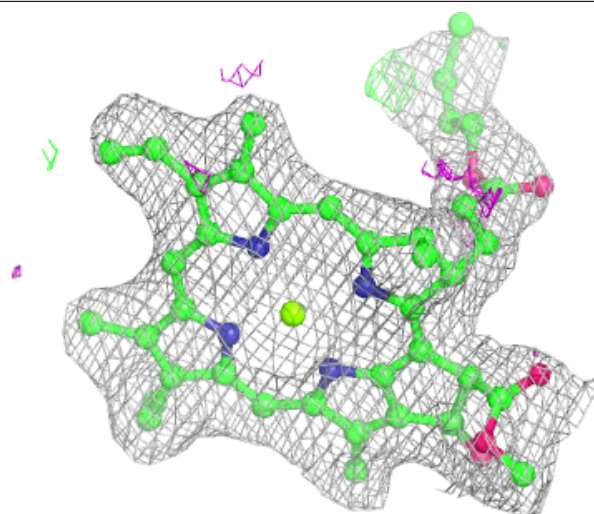
**Electron density around CHL A 605:**

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



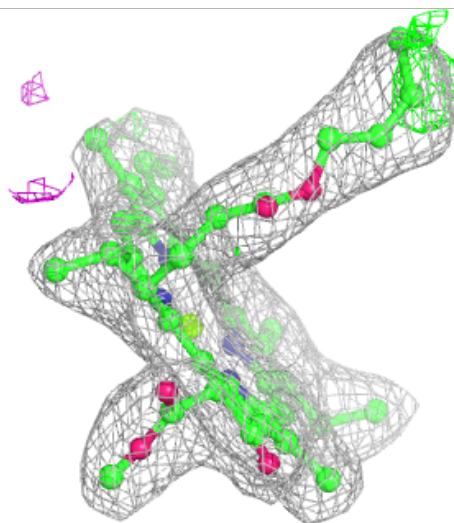
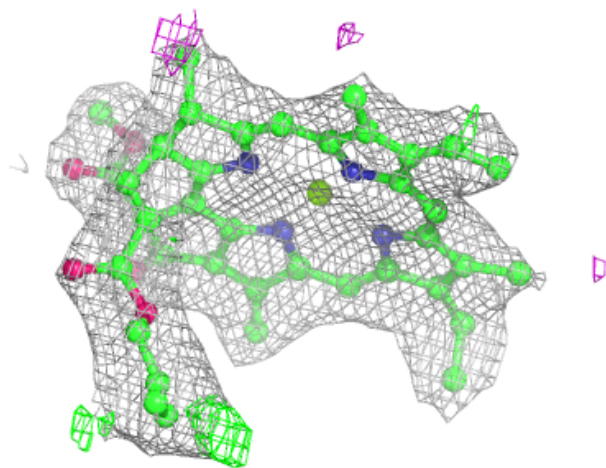
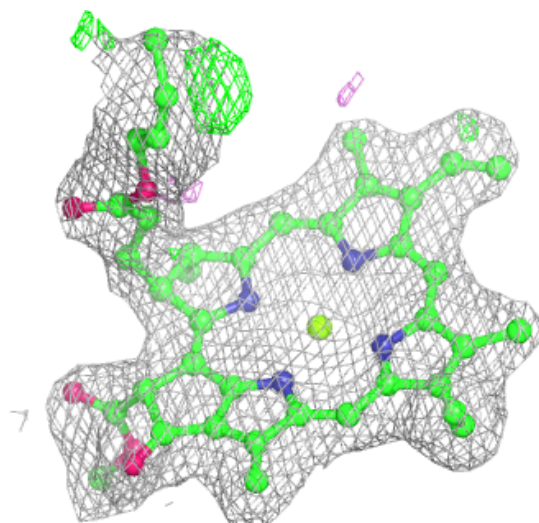
**Electron density around CLA I 614:**

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



**Electron density around CLA A 614:**

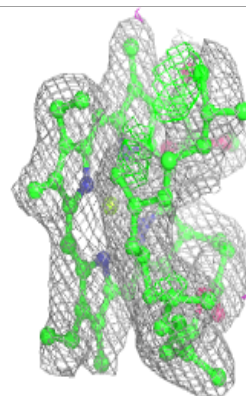
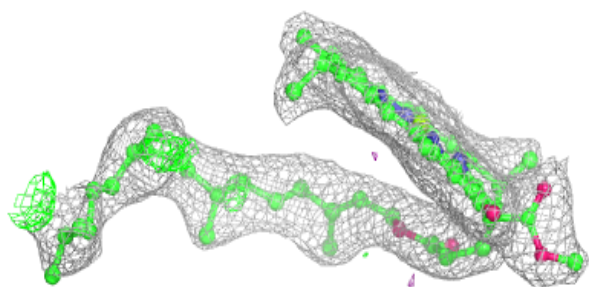
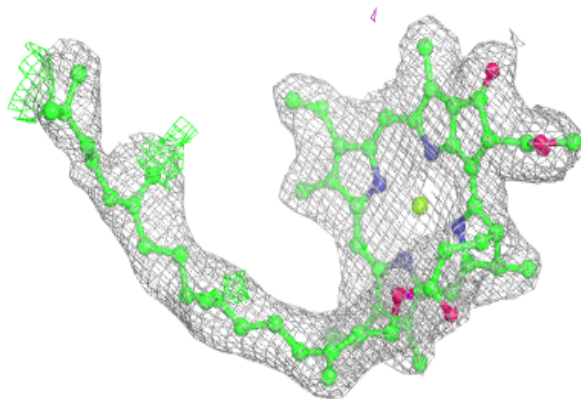
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



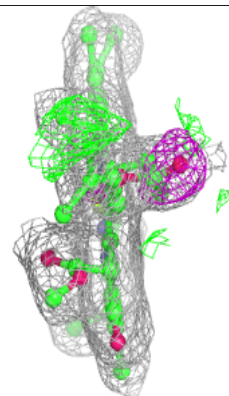
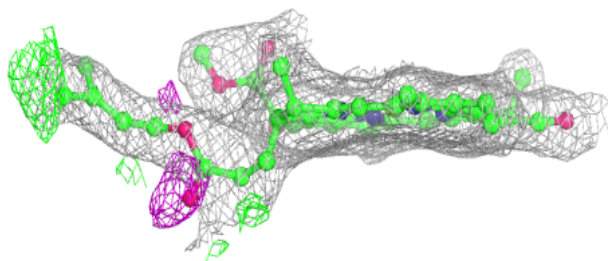
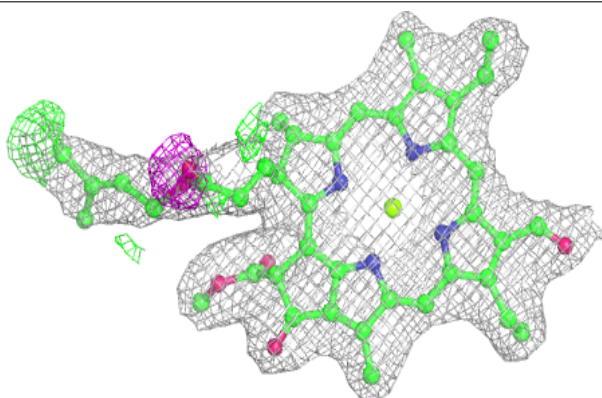


**Electron density around CLA J 610:**

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

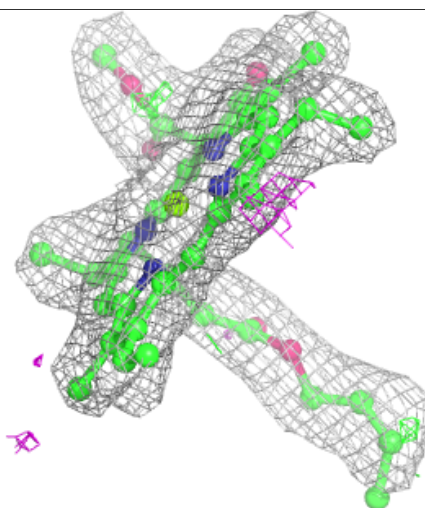
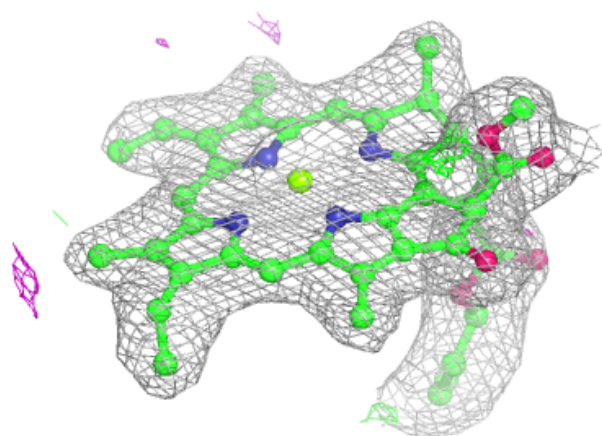
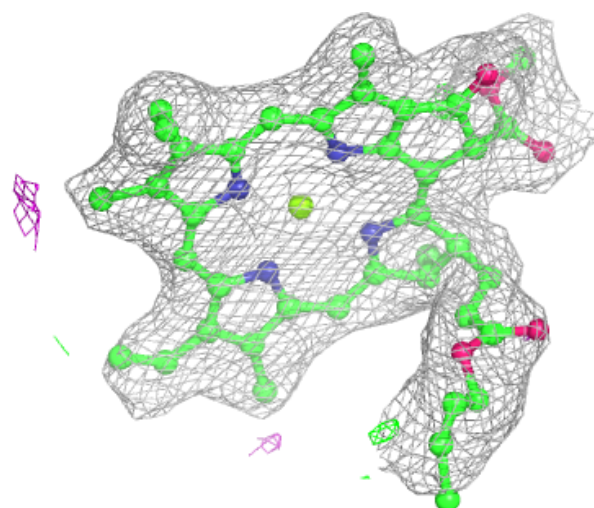
**Electron density around CHL B 606:**

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



**Electron density around CLA J 614:**

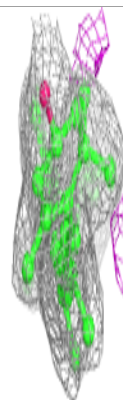
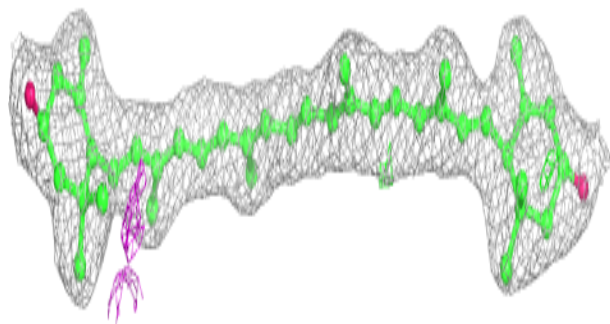
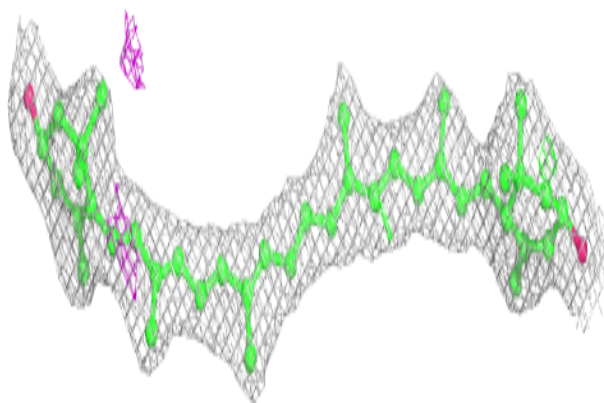
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



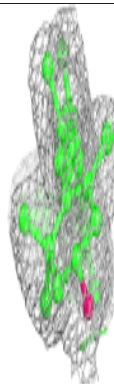
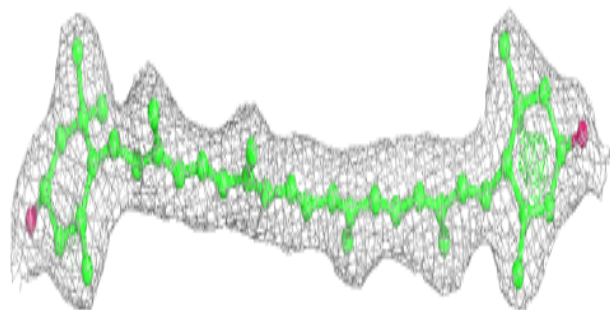
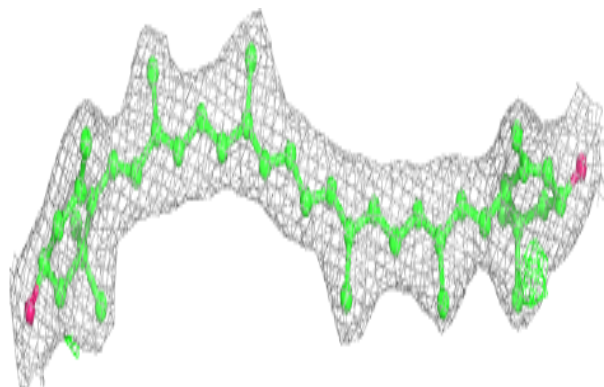


**Electron density around LUT A 620:**

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

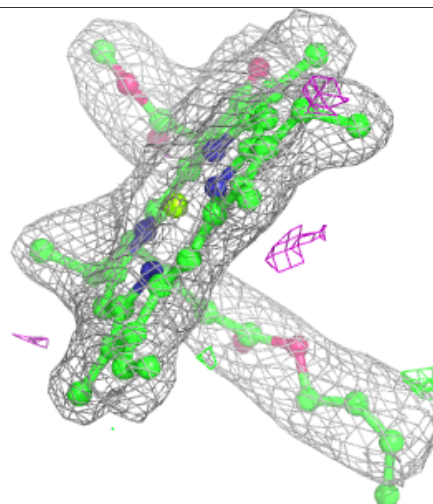
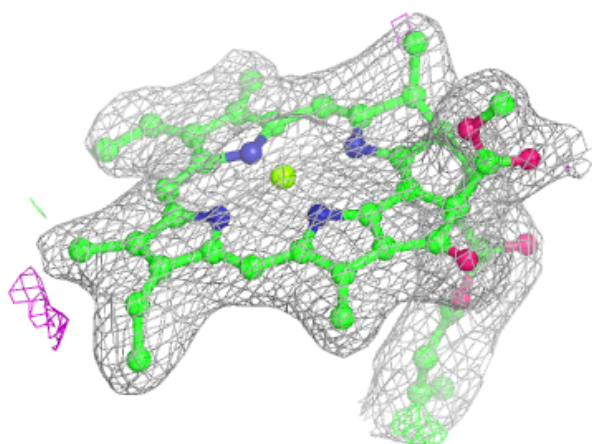
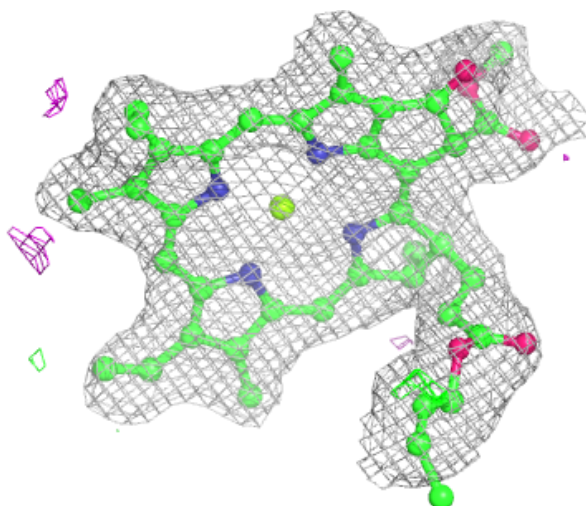
**Electron density around LUT H 7620:**

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



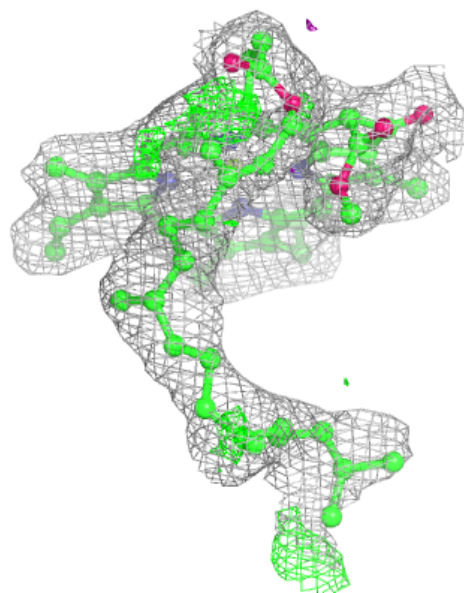
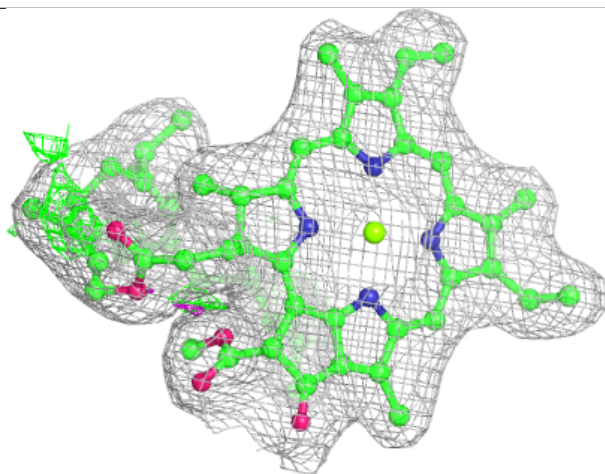
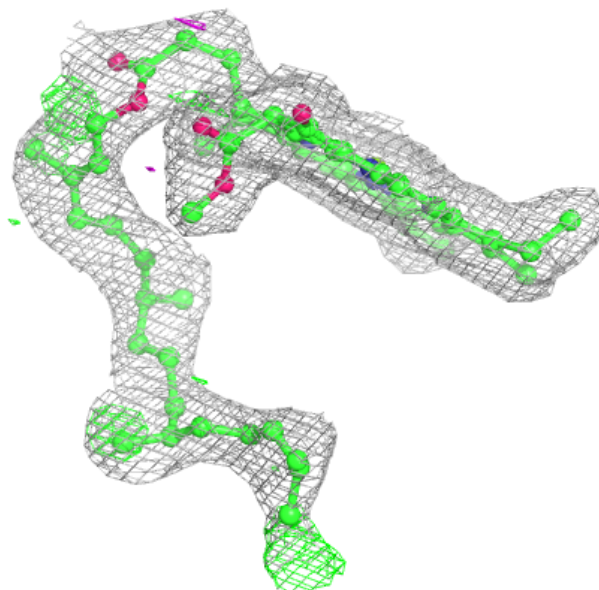
**Electron density around CLA E 614:**

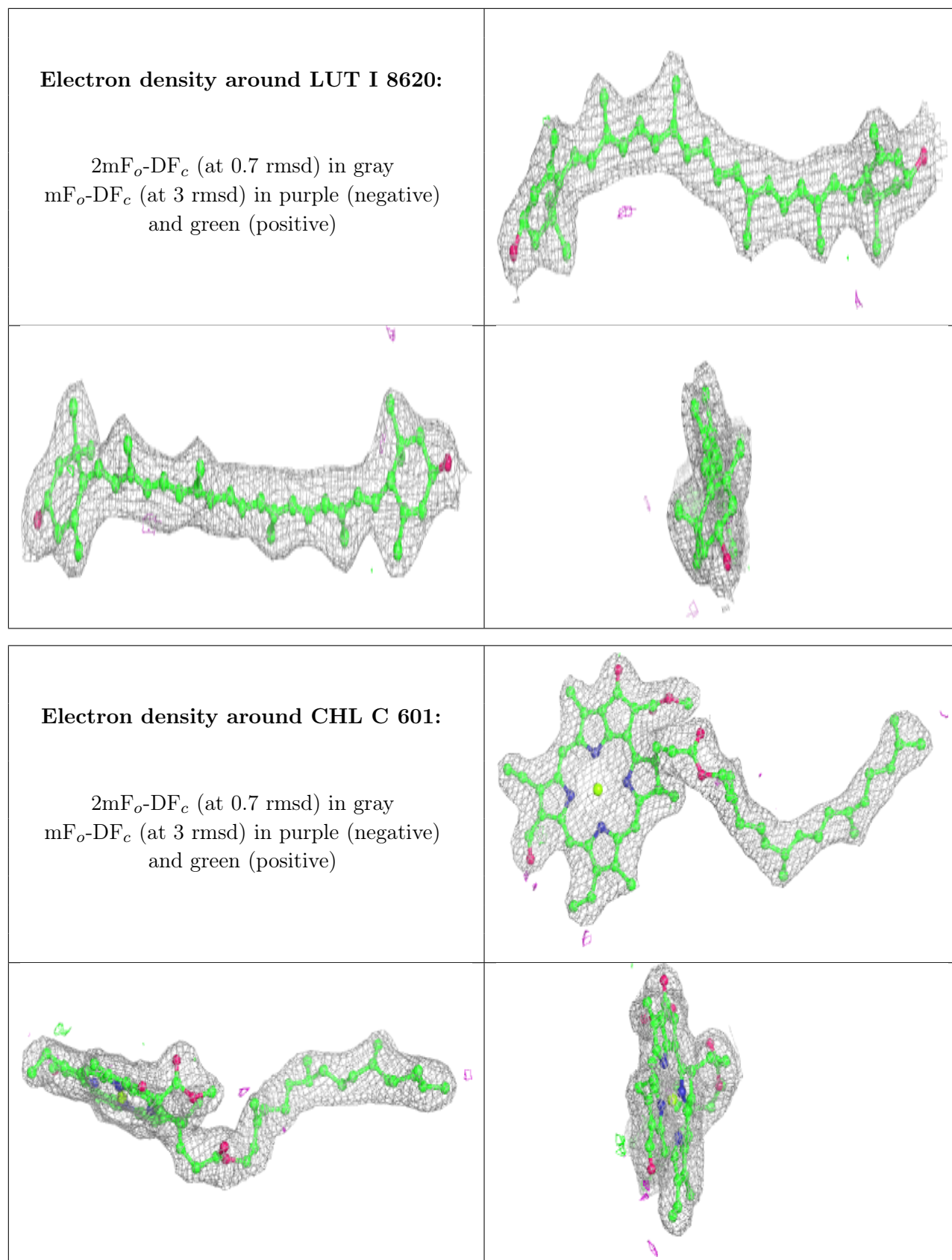
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)

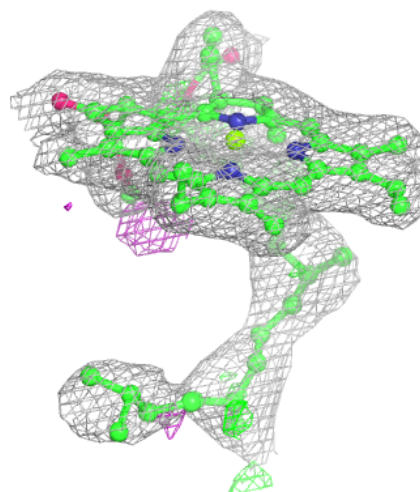
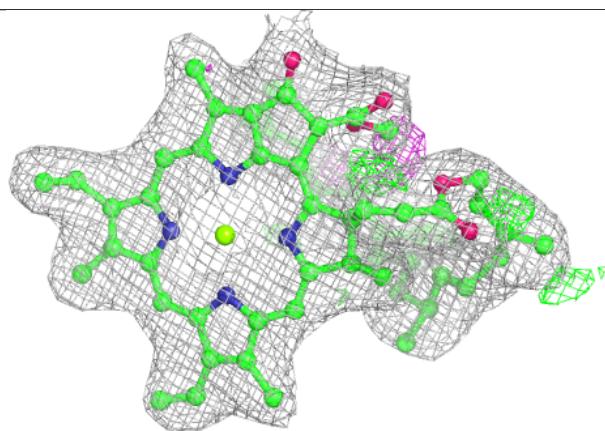
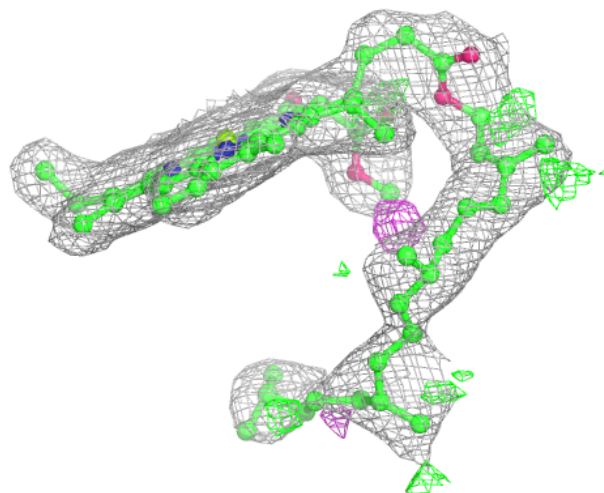






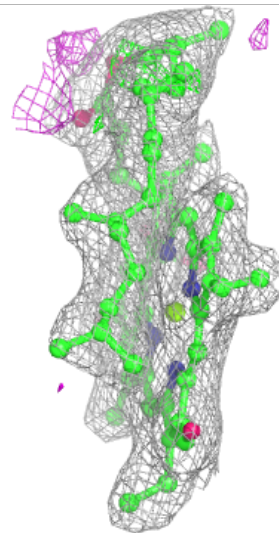
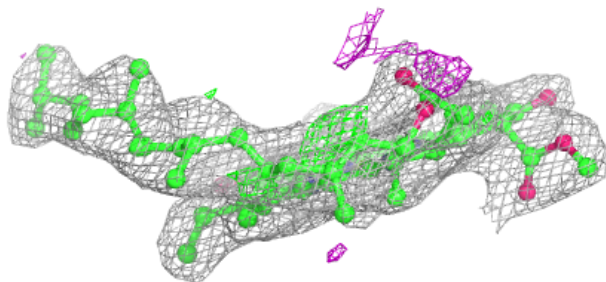
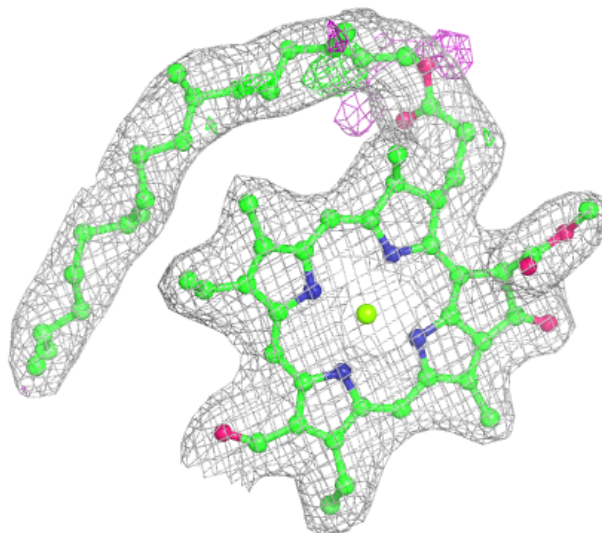
**Electron density around CLA B 603:**

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



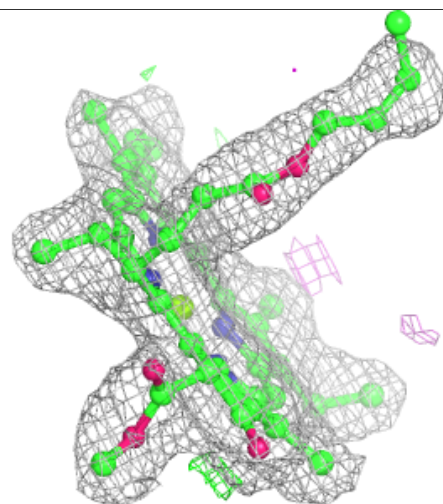
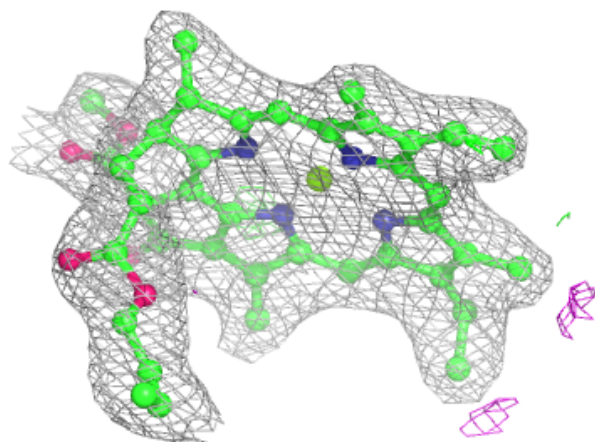
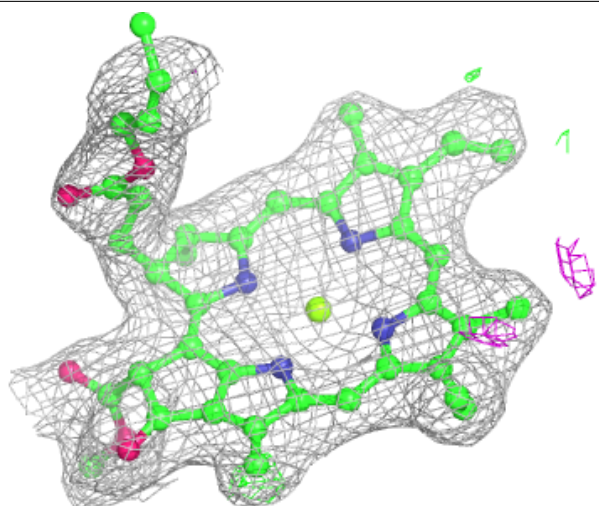
**Electron density around CHL E 607:**

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

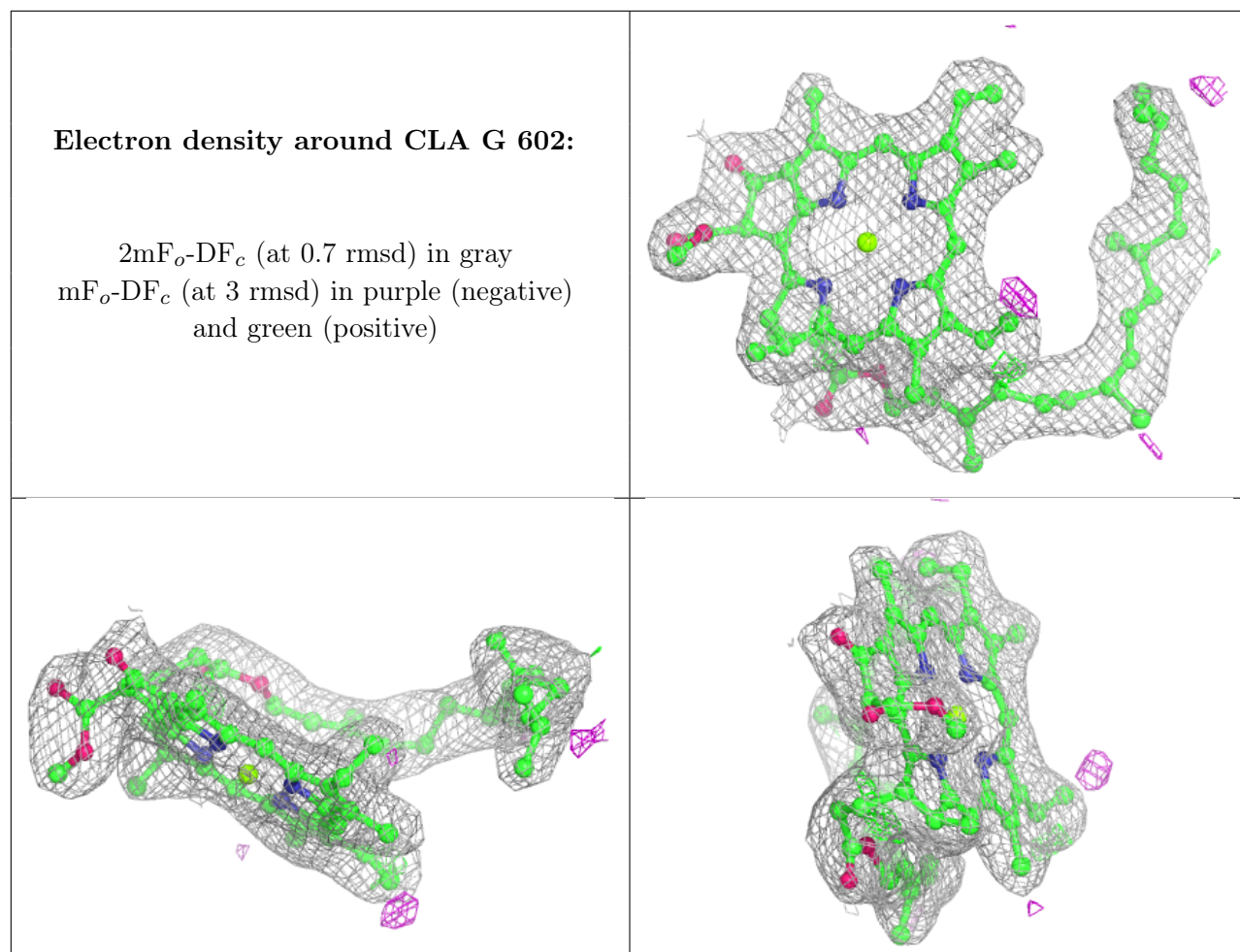


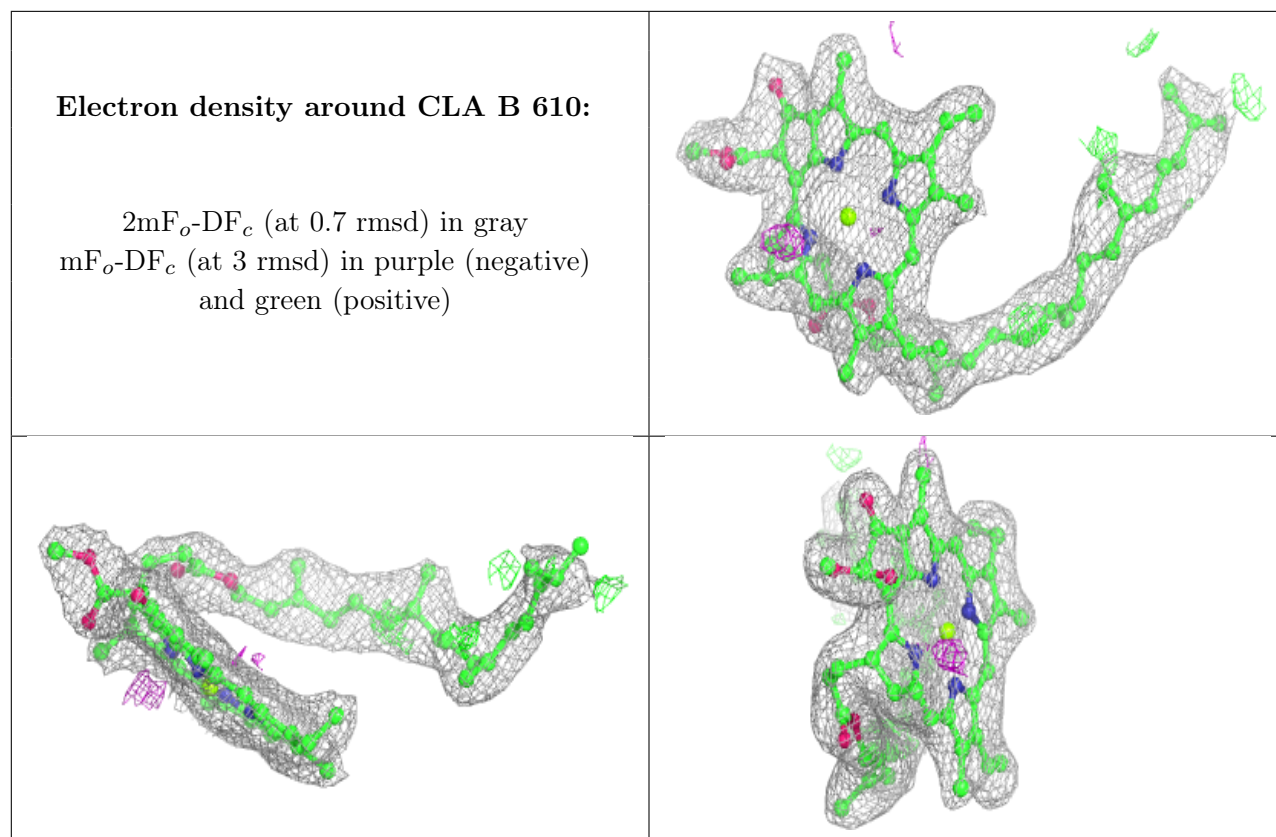
**Electron density around CLA F 614:**

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



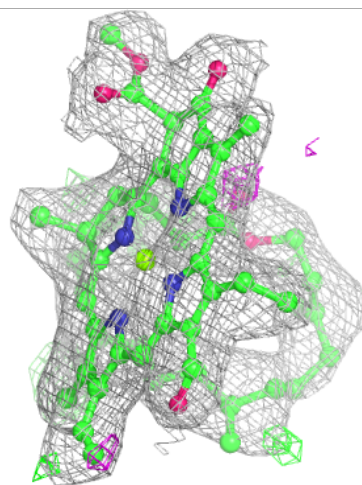
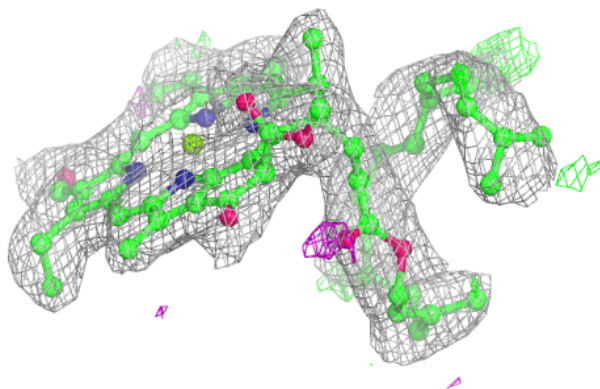
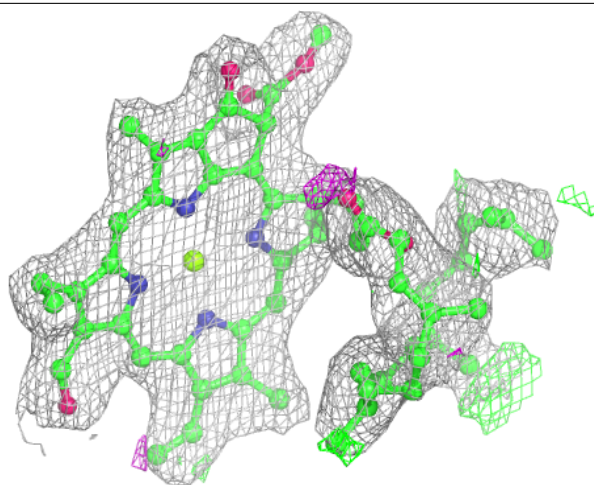






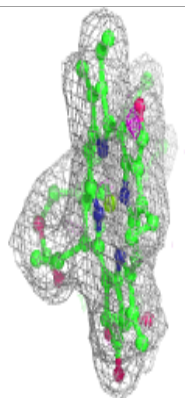
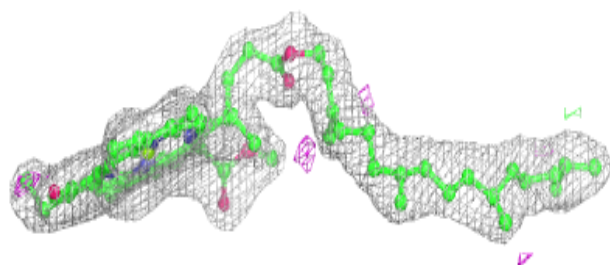
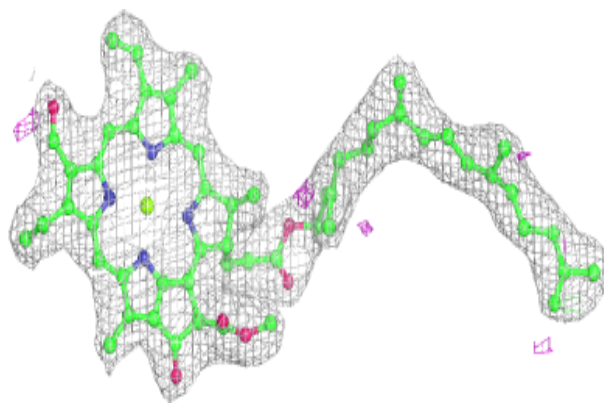
**Electron density around CHL E 608:**

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

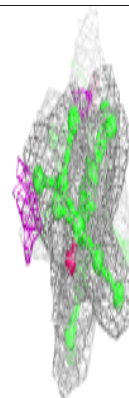
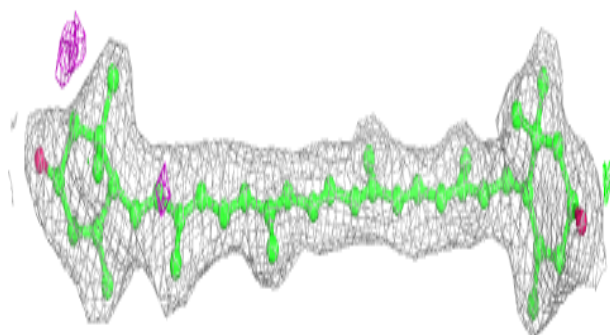
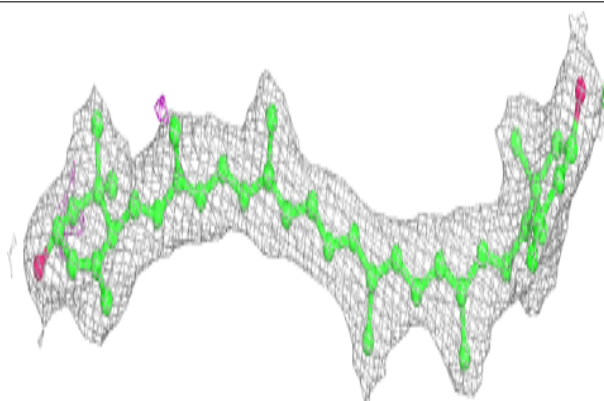


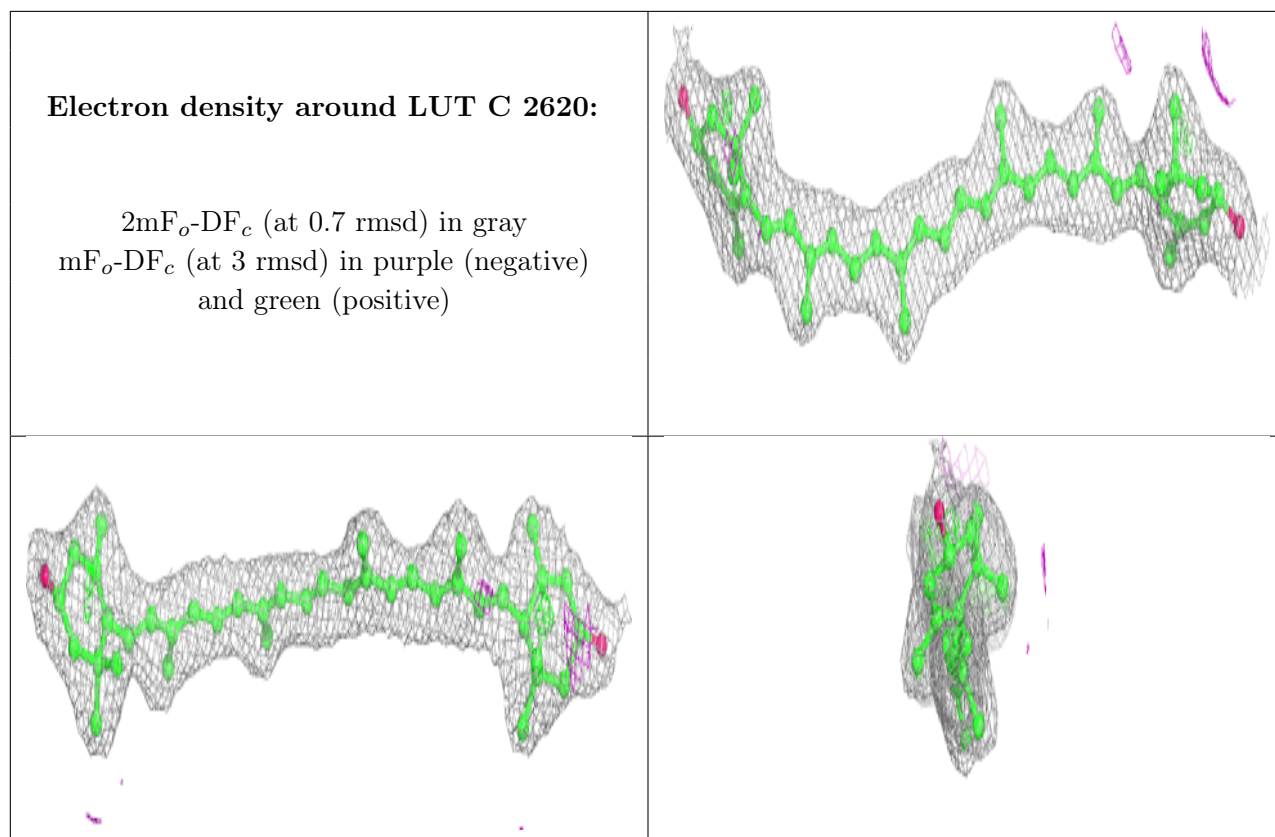
**Electron density around CHL F 601:**

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

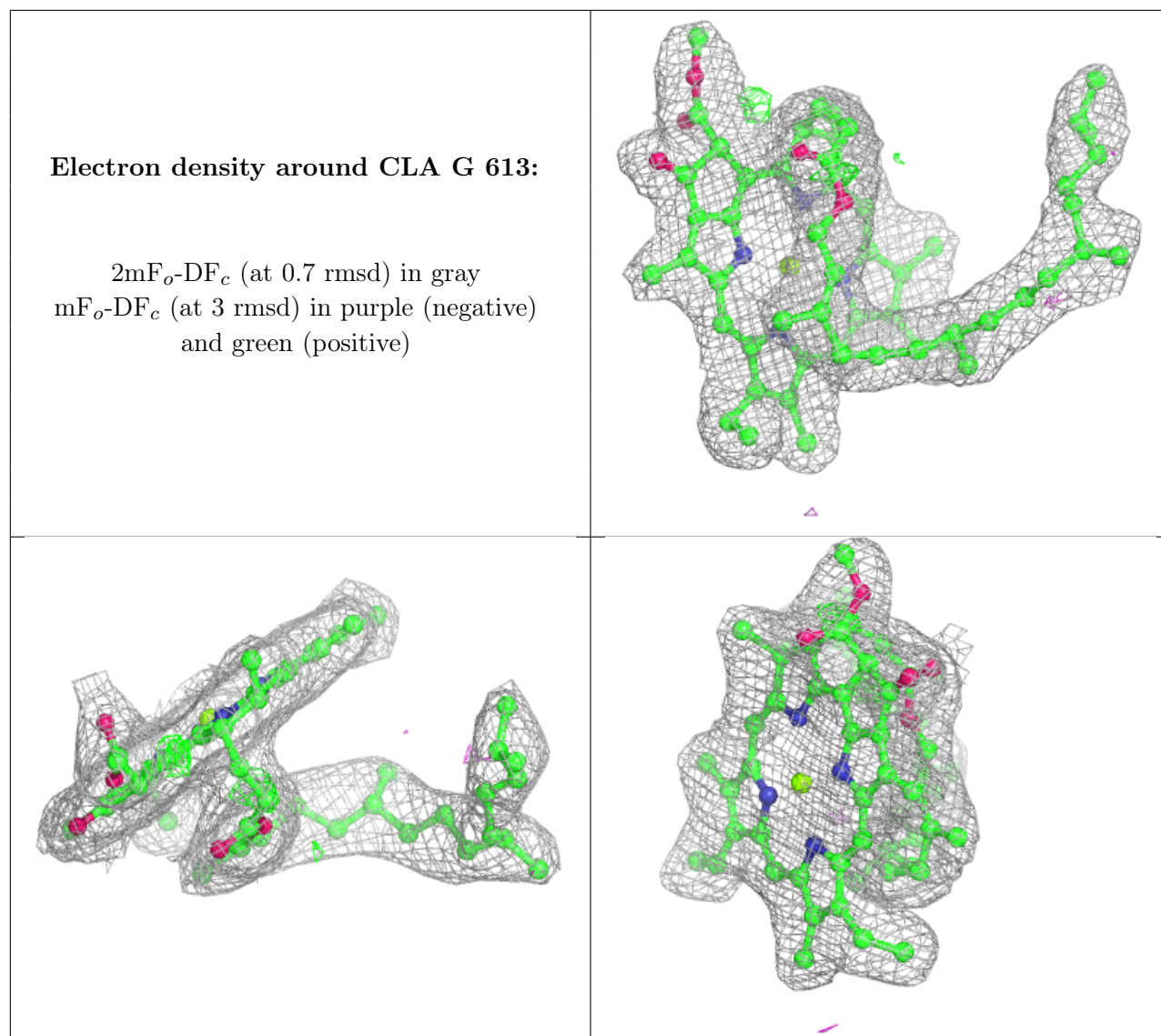
**Electron density around LUT B 1621:**

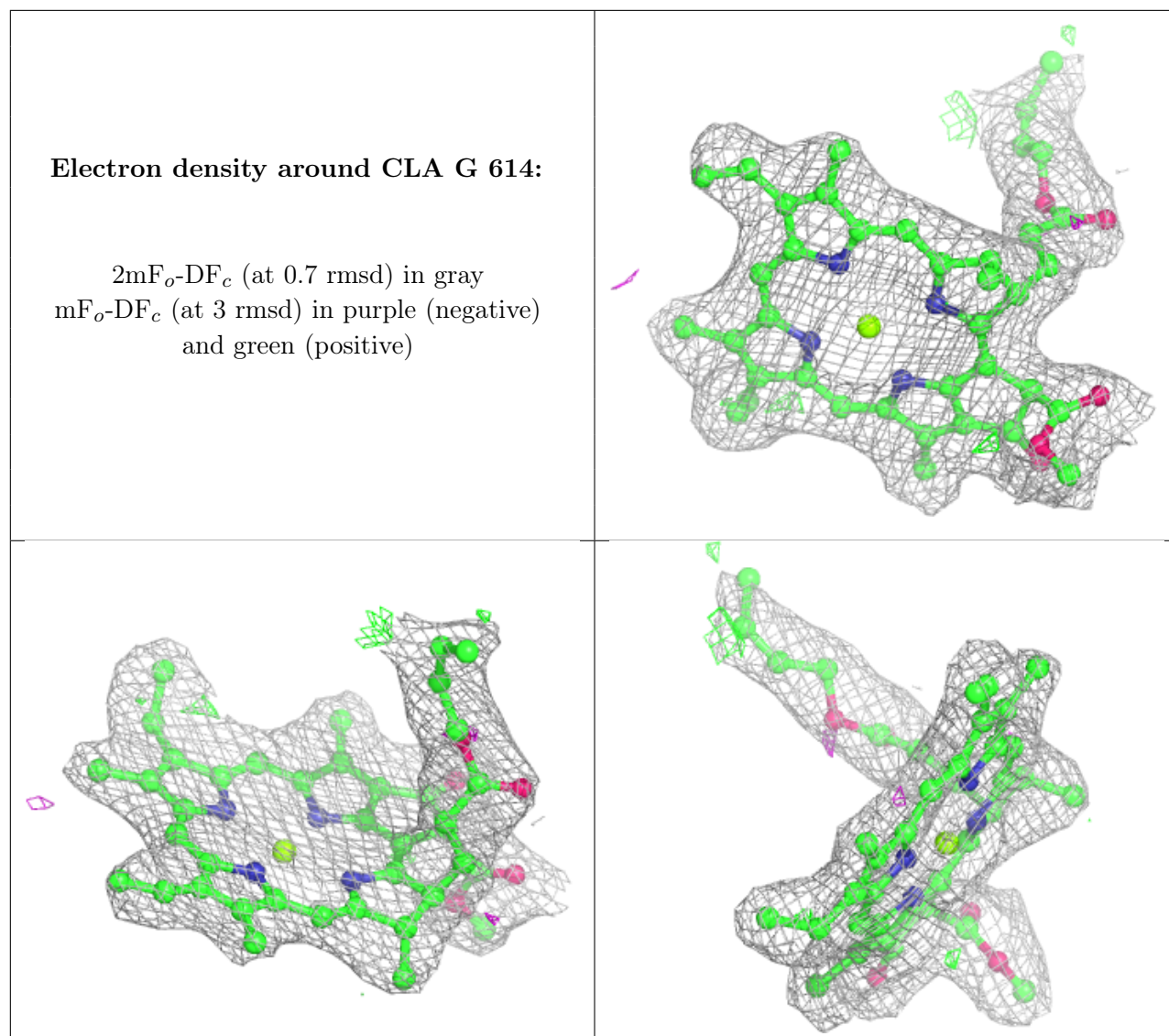
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



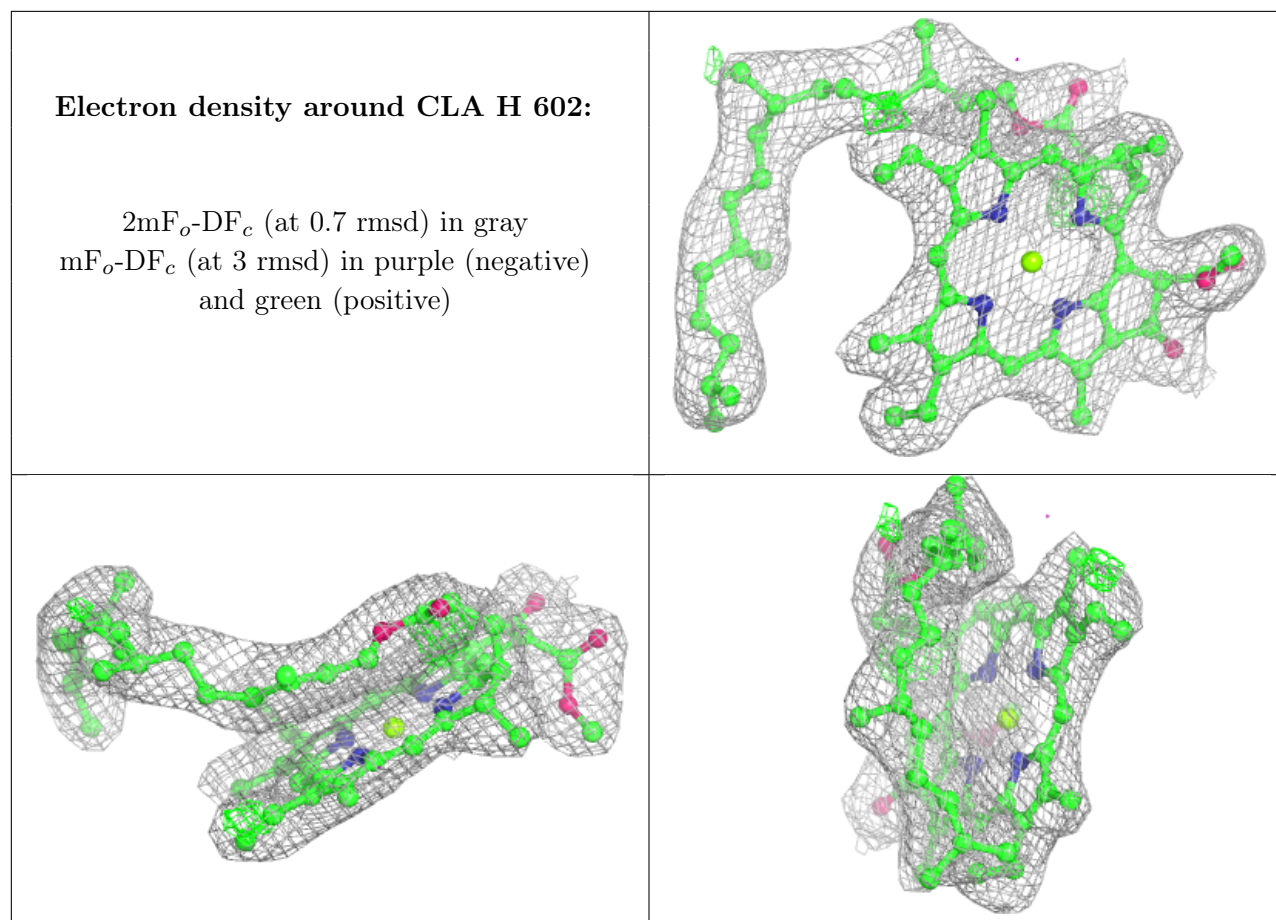


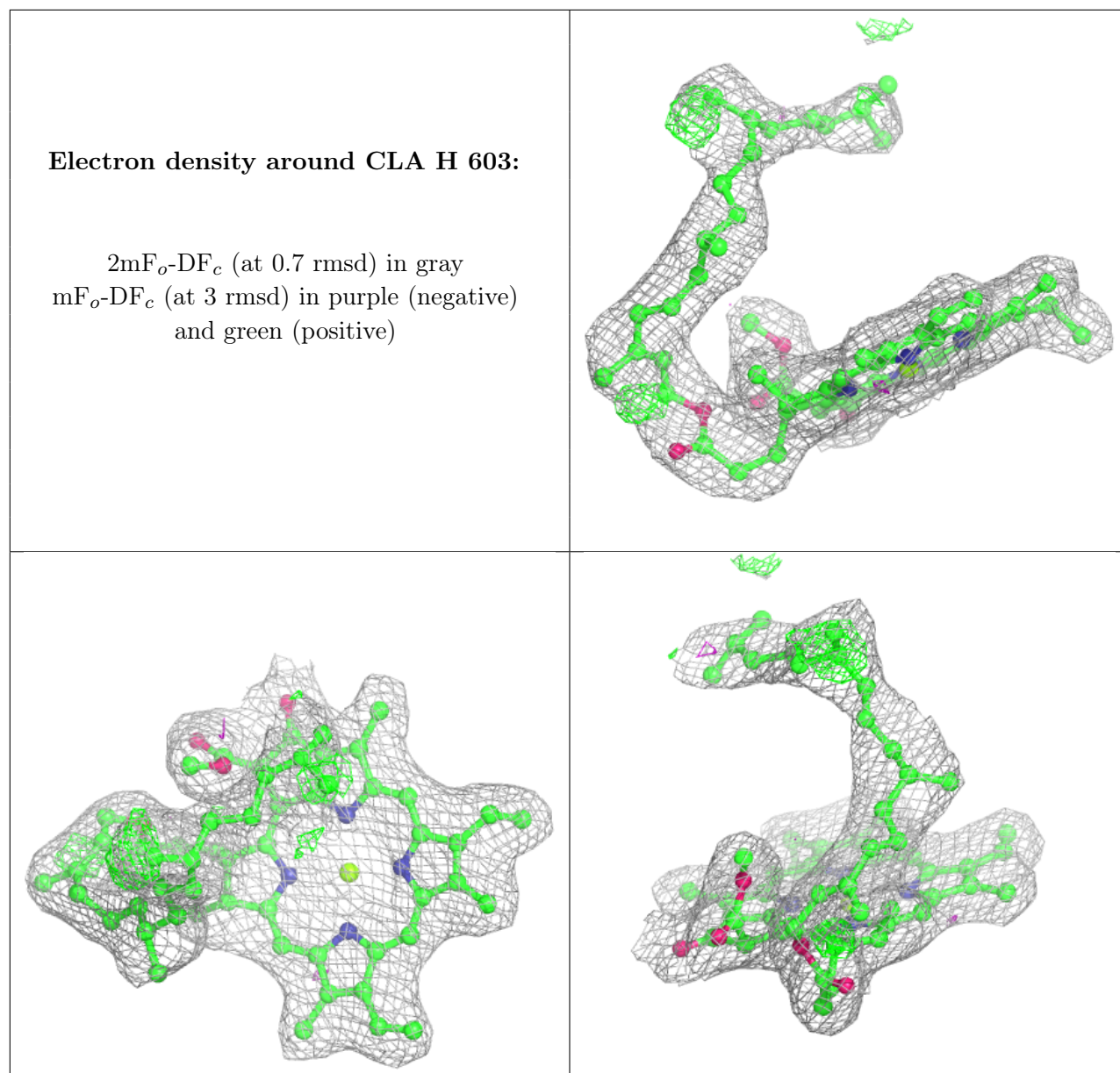






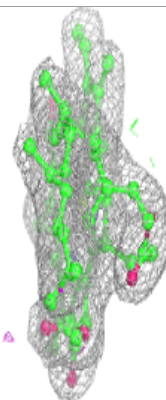
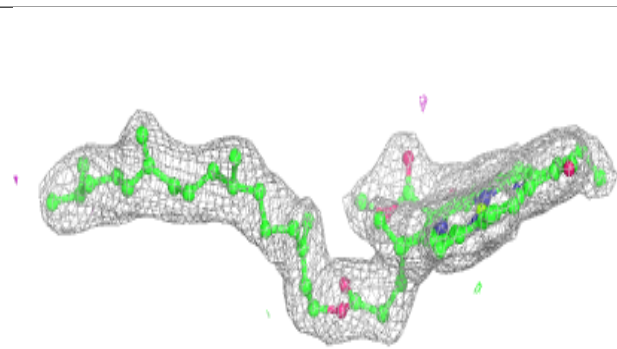
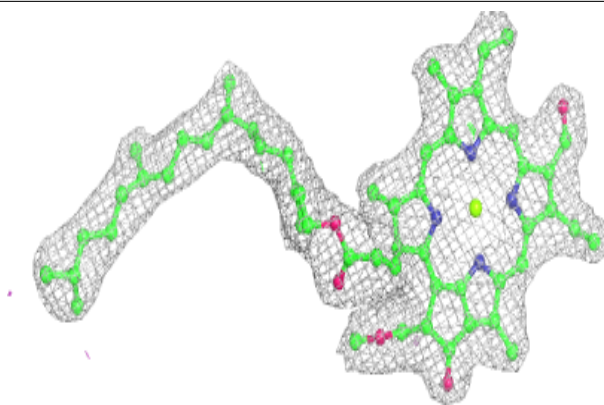






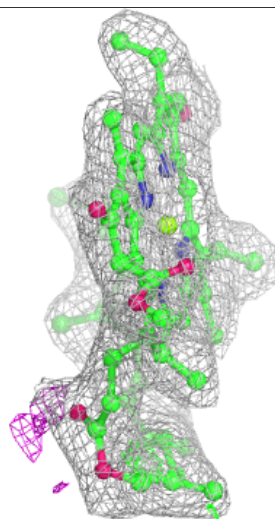
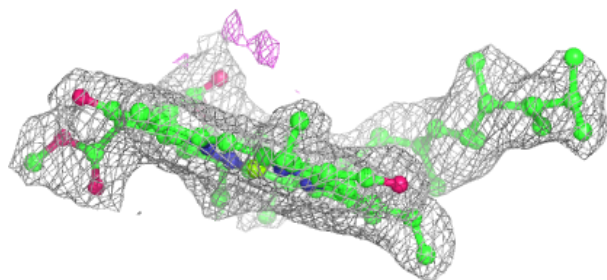
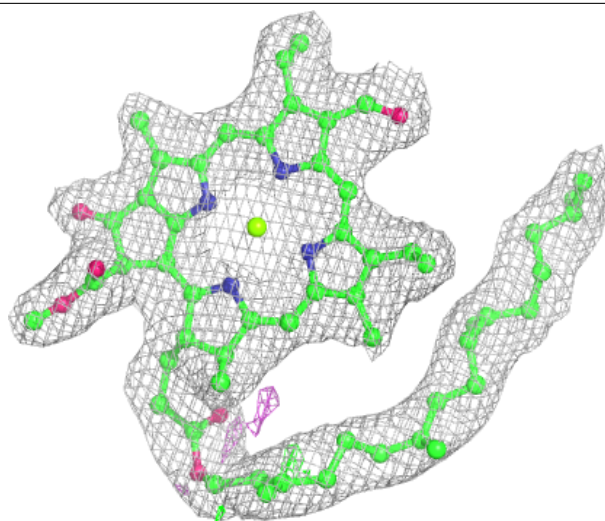
**Electron density around CHL J 601:**

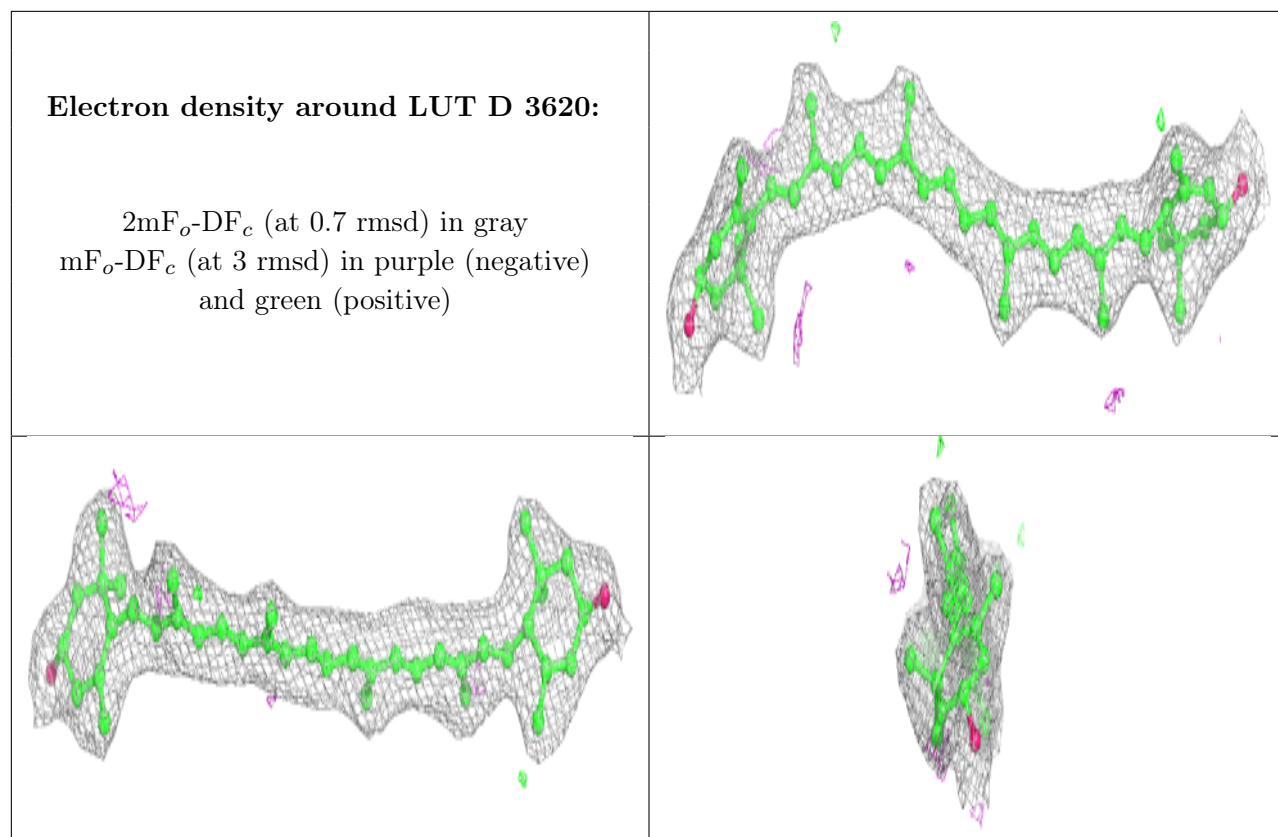
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CHL 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)

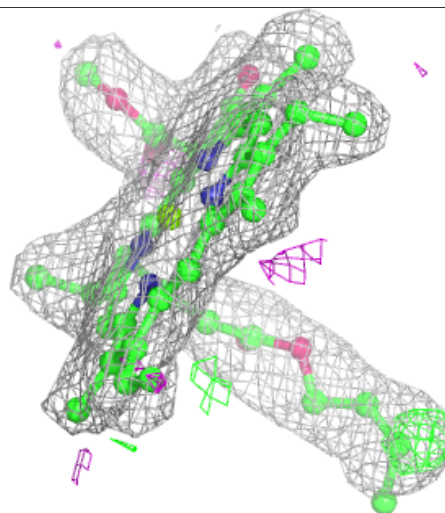
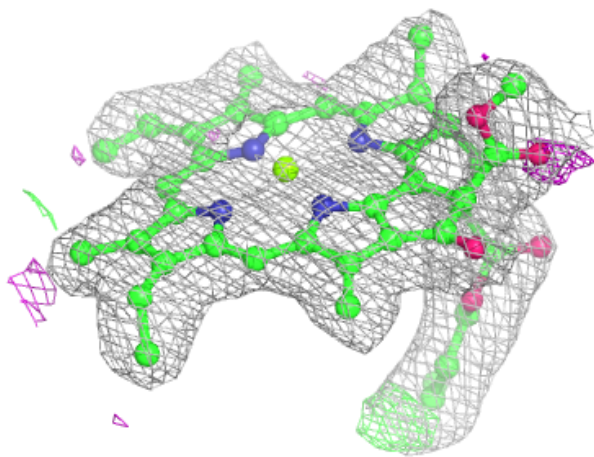
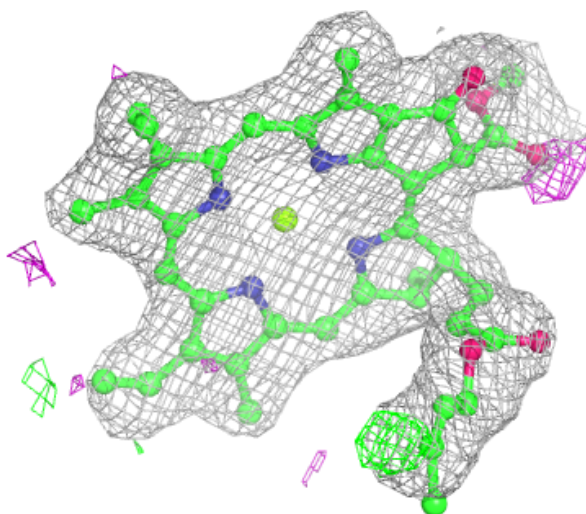






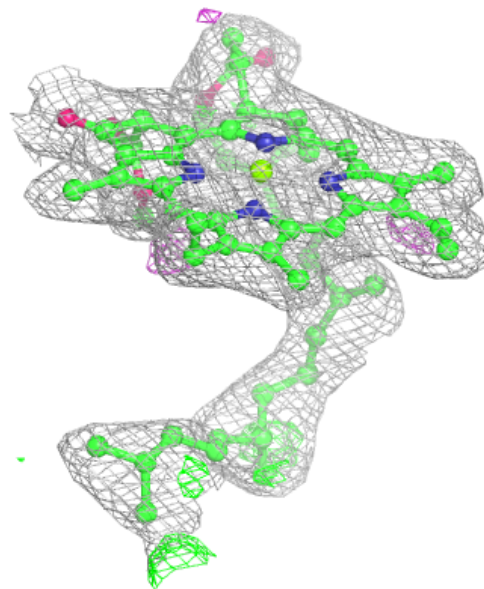
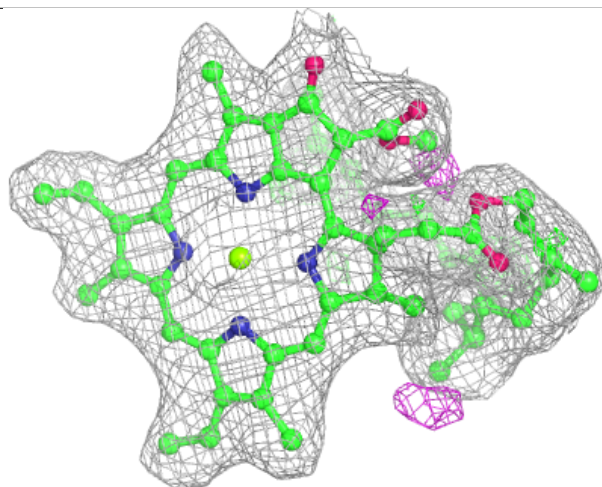
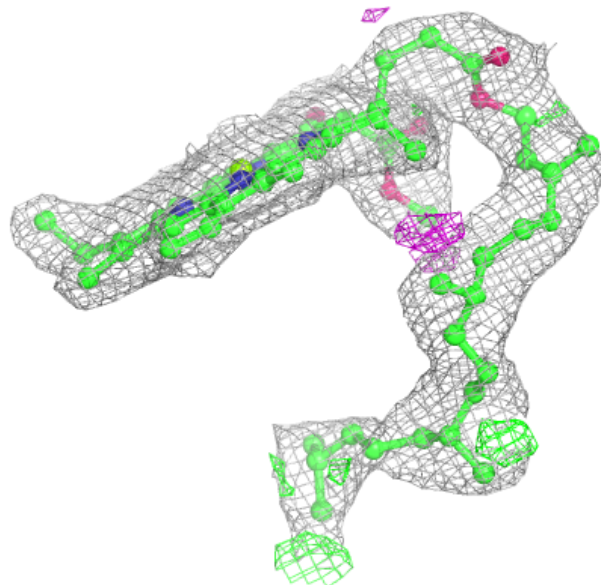
**Electron density around CLA C 614:**

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



**Electron density around CLA D 603:**

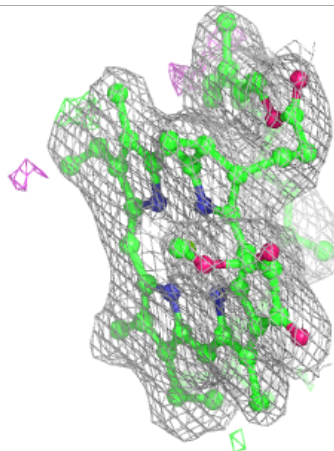
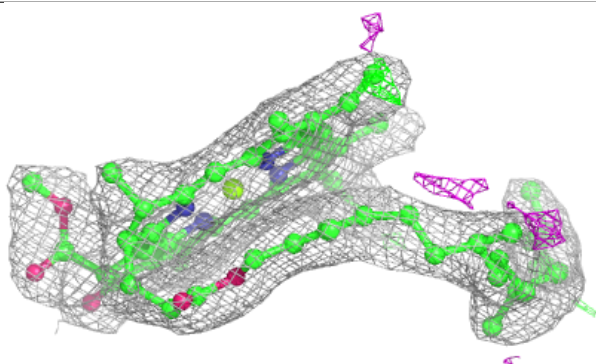
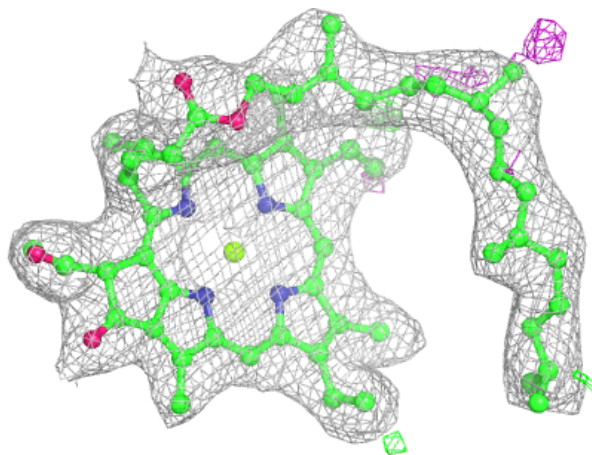
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





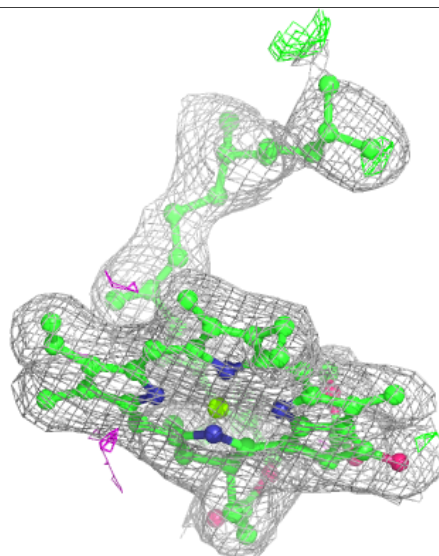
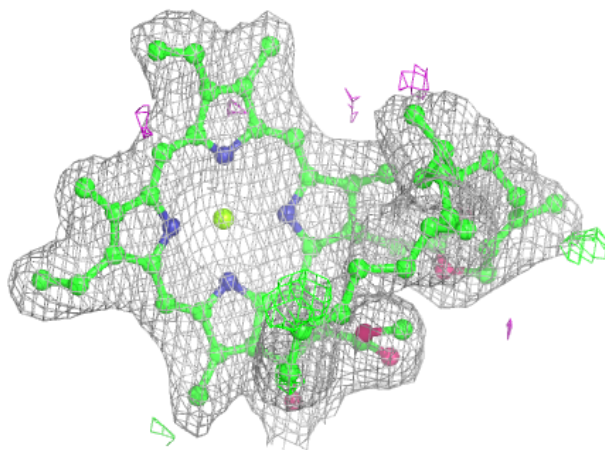
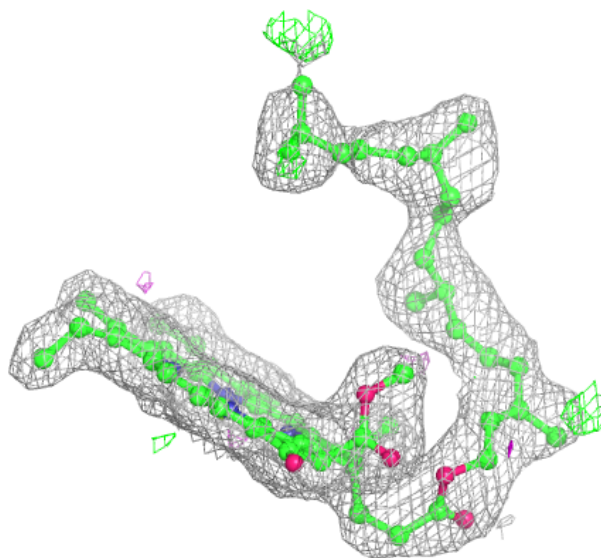
**Electron density around CLA I 602:**

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



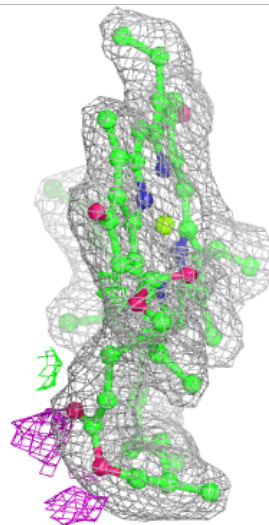
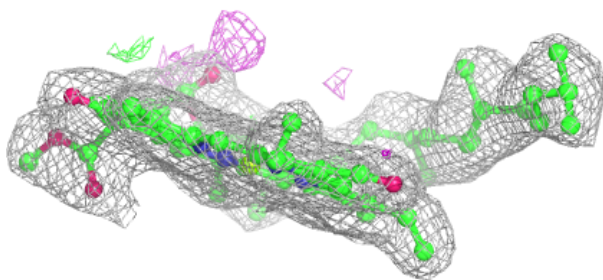
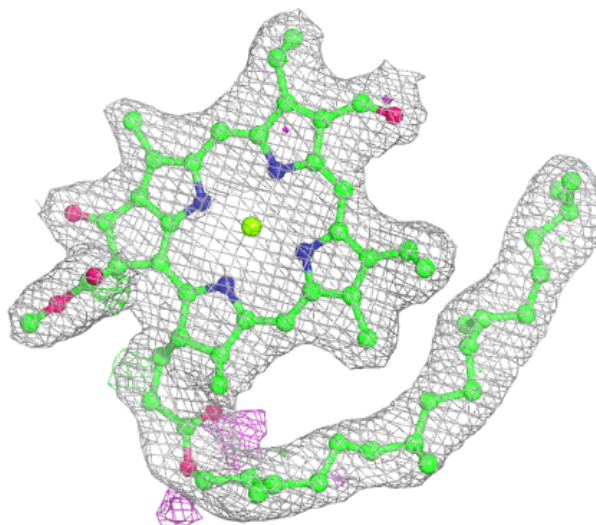
**Electron density around CLA I 603:**

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



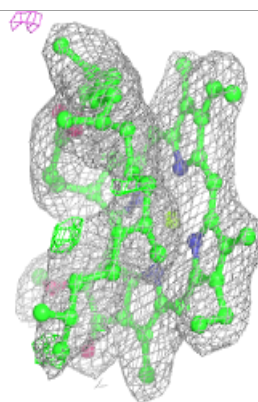
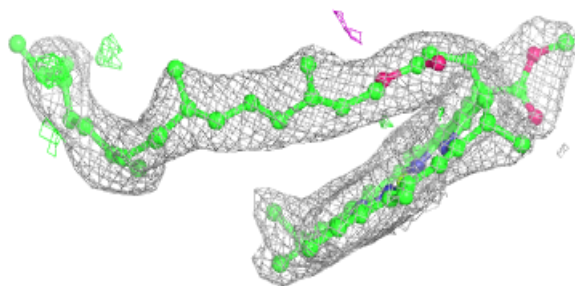
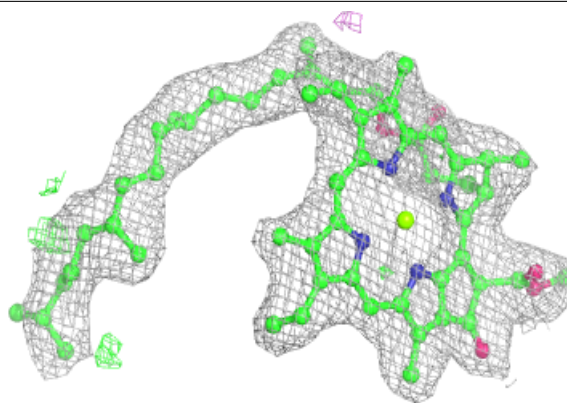
**Electron density around CHL J 607:**

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

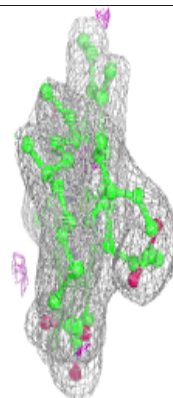
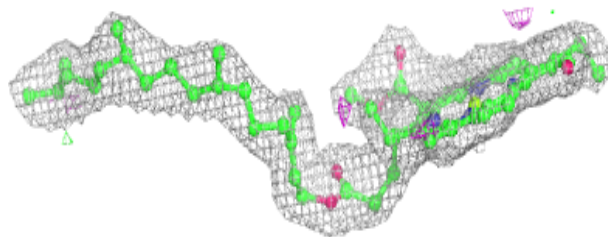
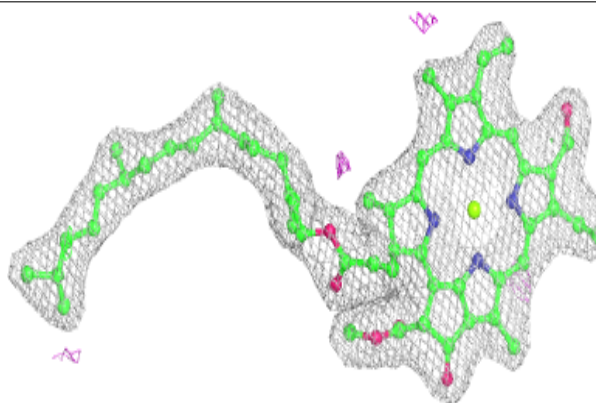


**Electron density around CLA D 610:**

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

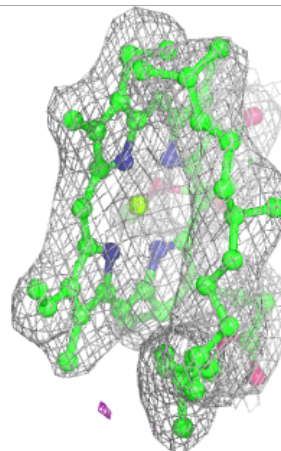
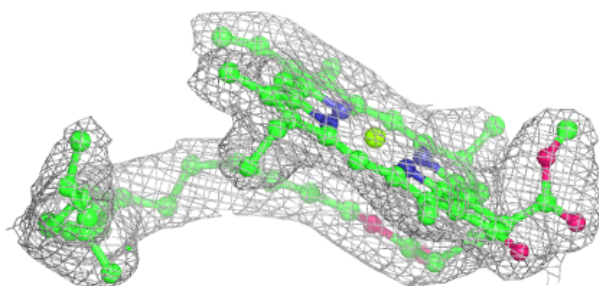
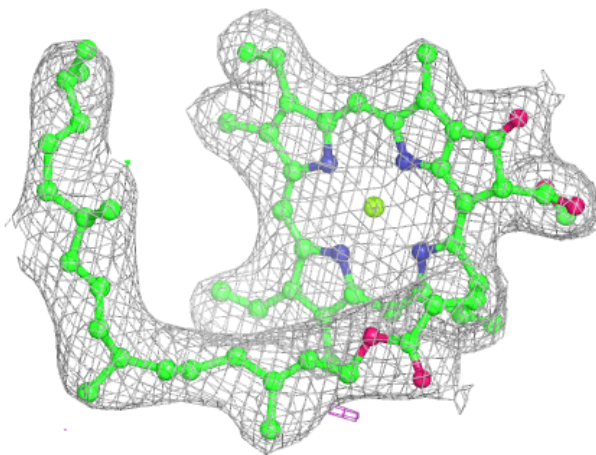
**Electron density around CHL D 601:**

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

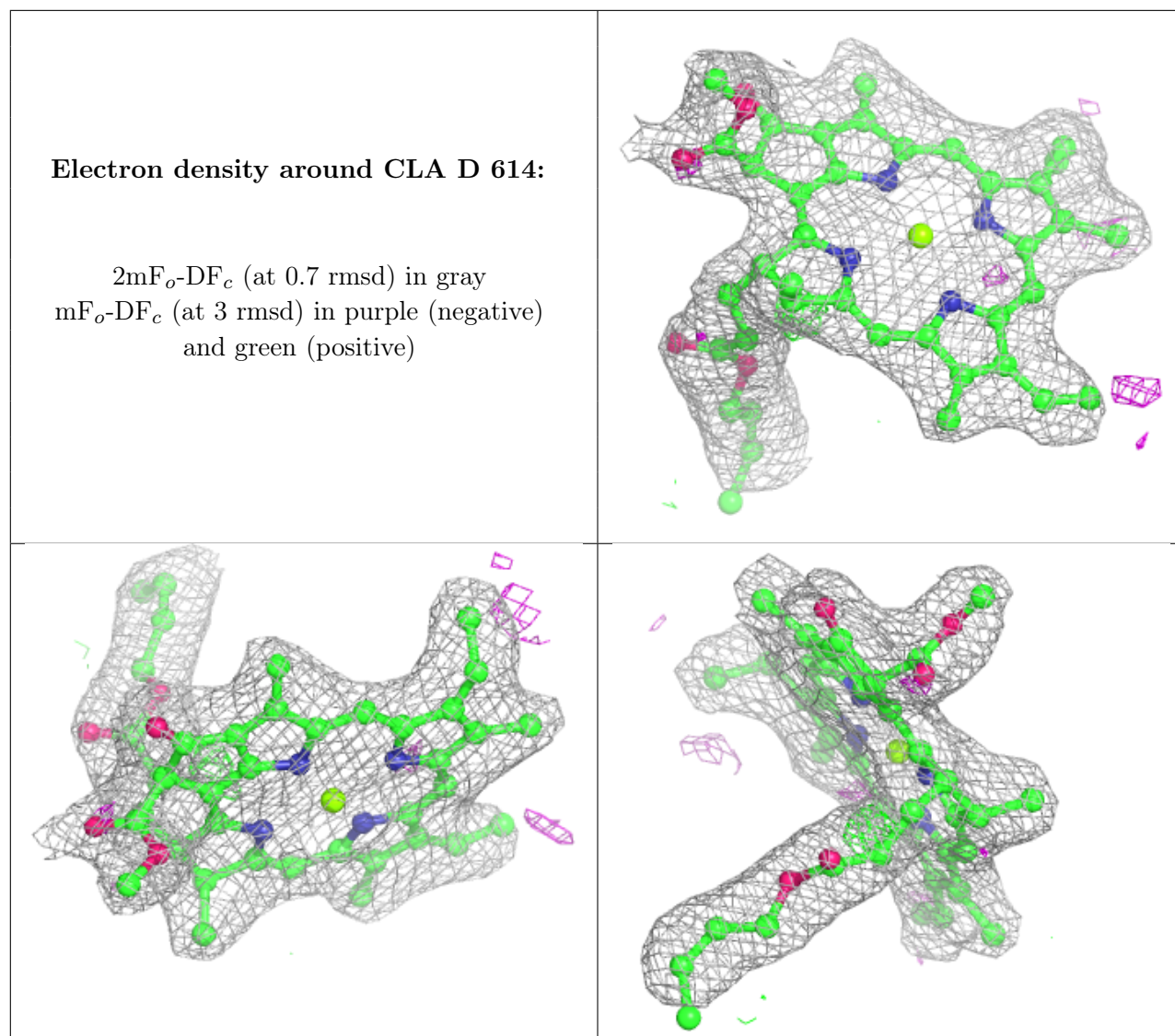


**Electron density around CLA A 602:**

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

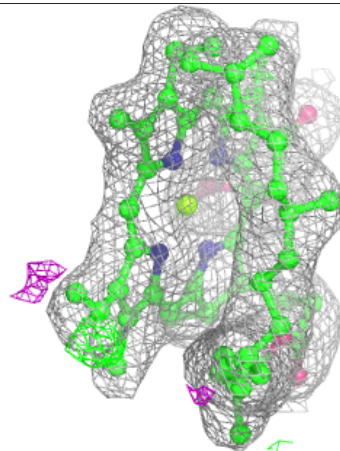
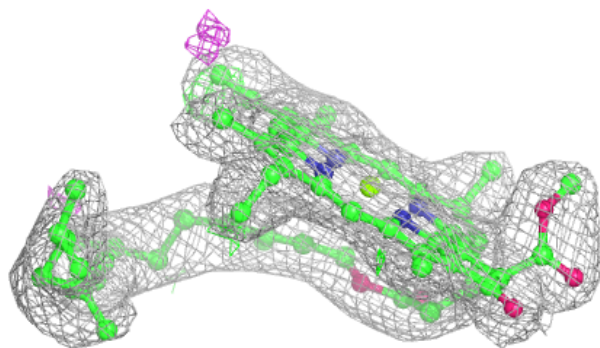
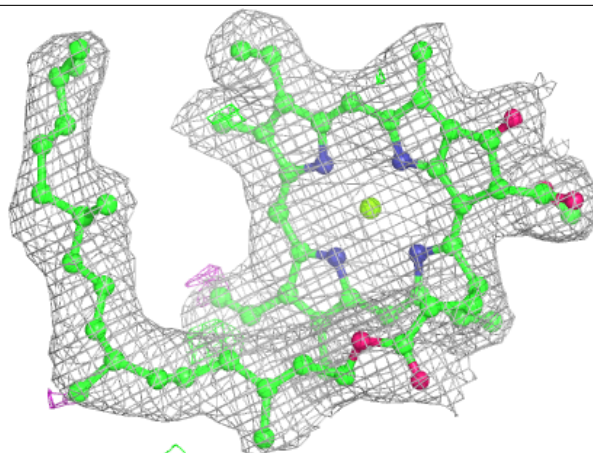






**Electron density around CLA J 602:**

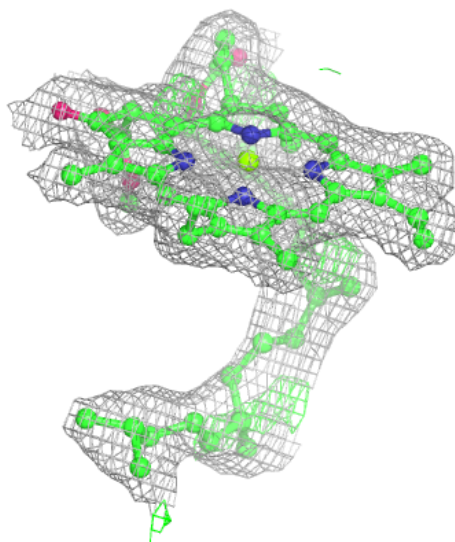
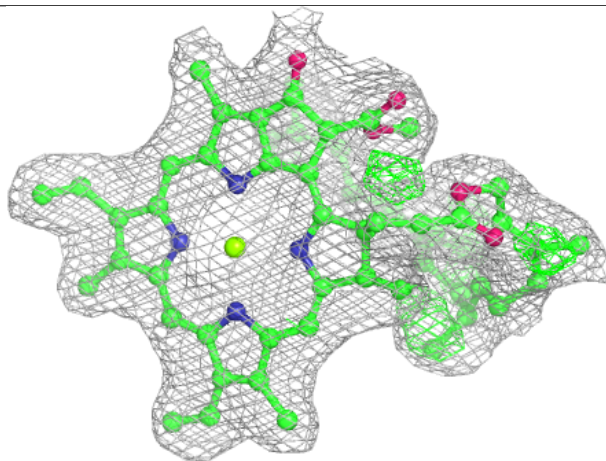
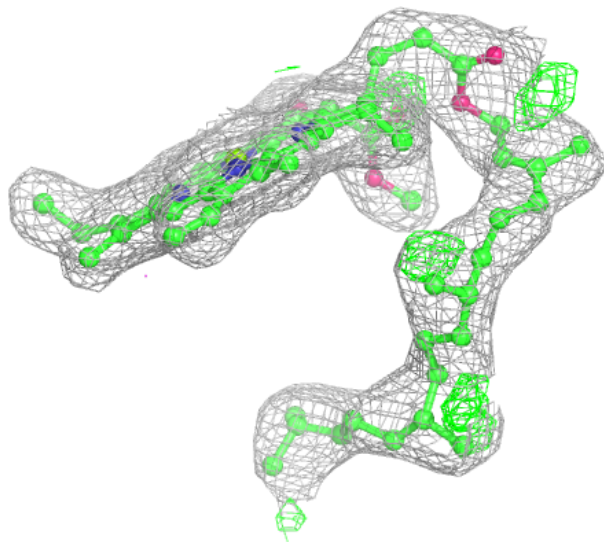
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





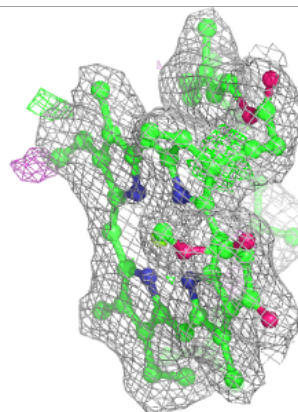
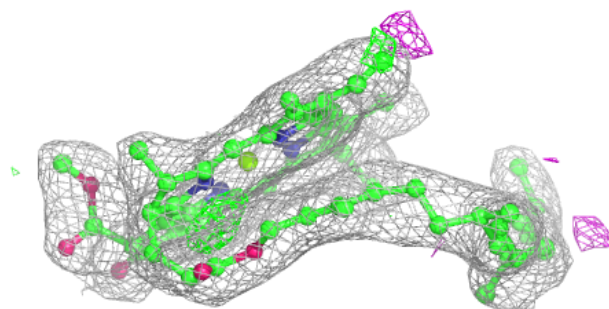
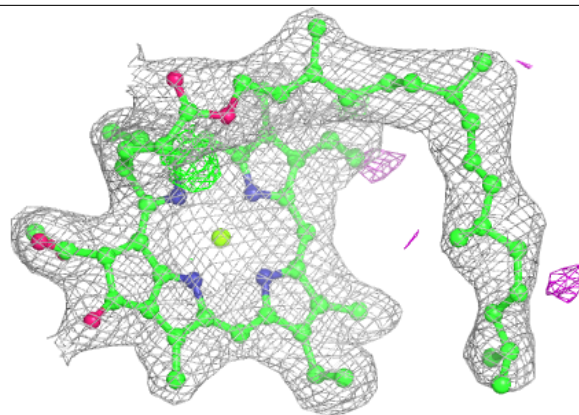
**Electron density around CLA J 603:**

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



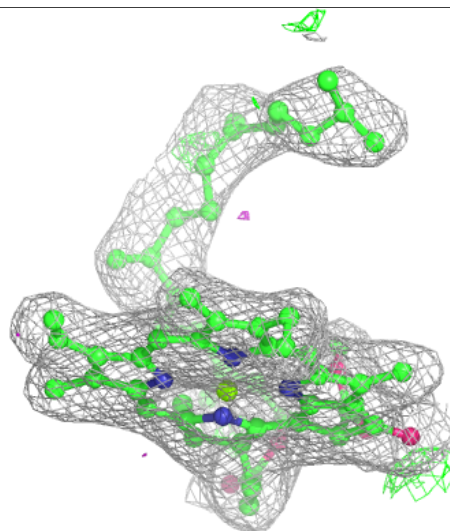
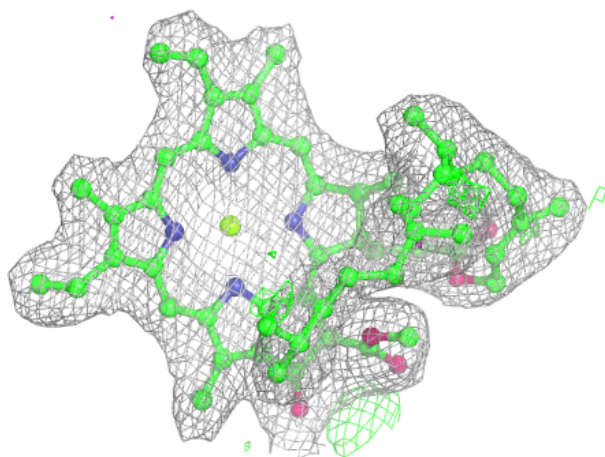
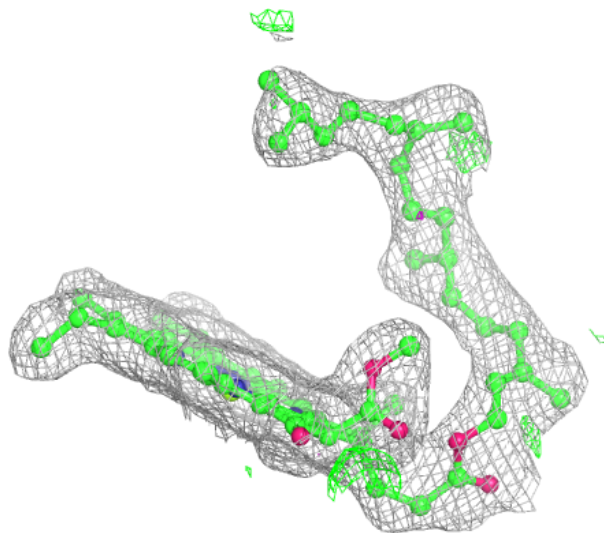
**Electron density around CLA E 602:**

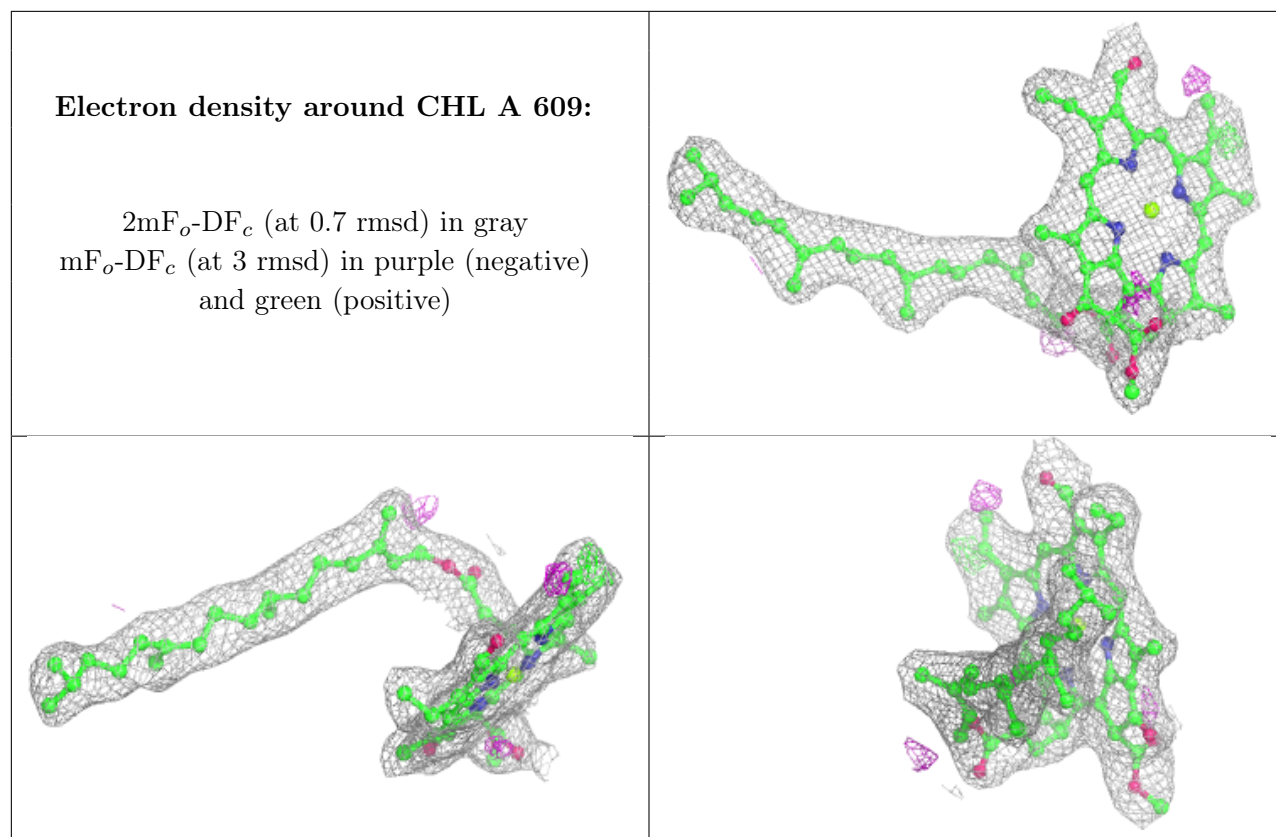
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA E 603:**

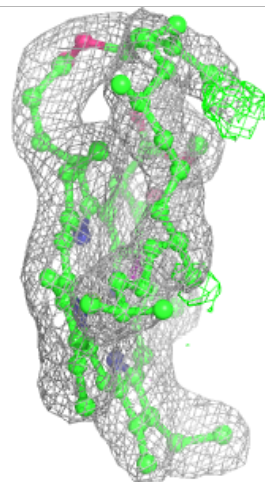
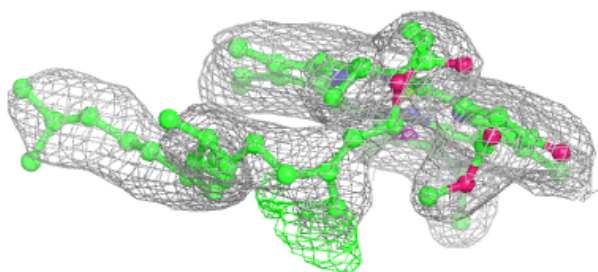
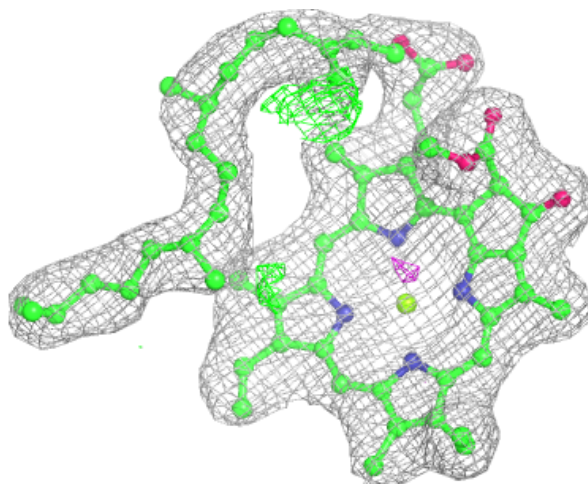
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

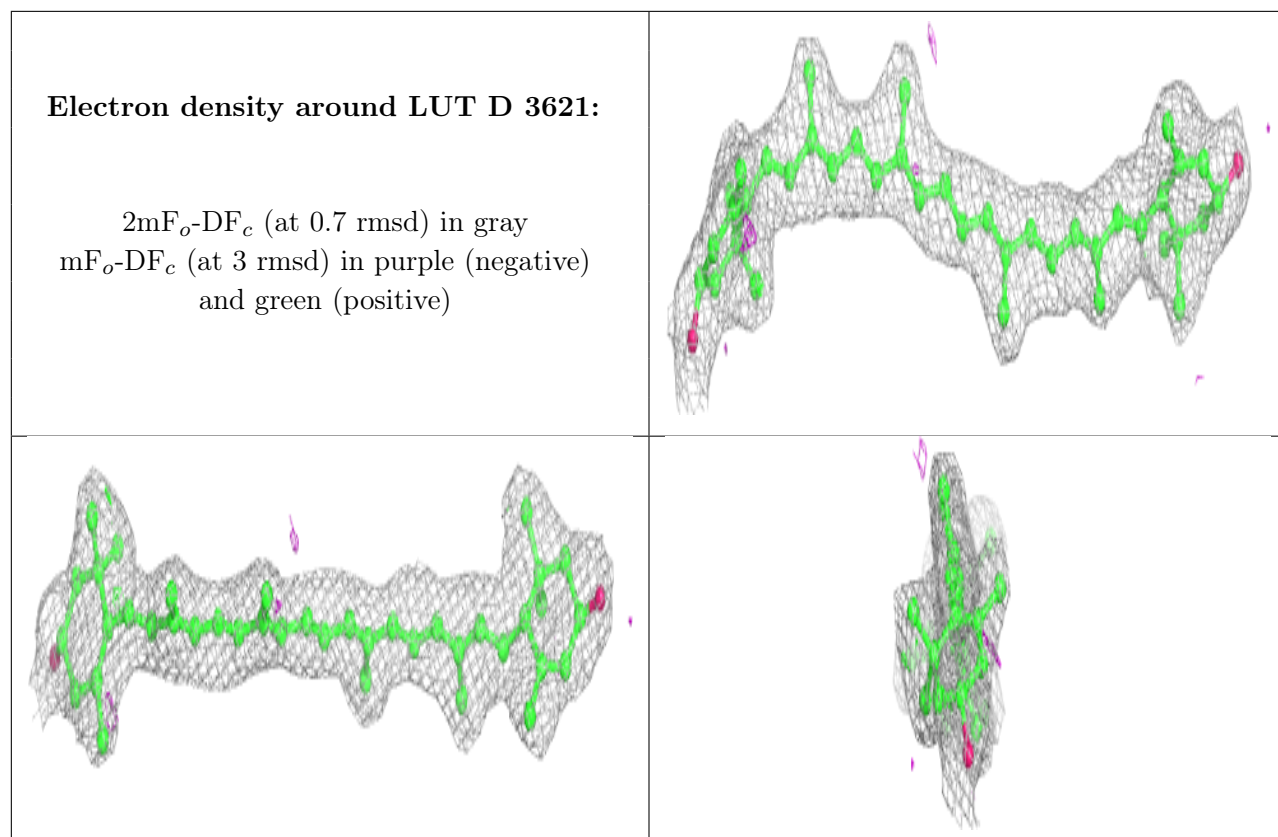




**Electron density around CLA J 612:**

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

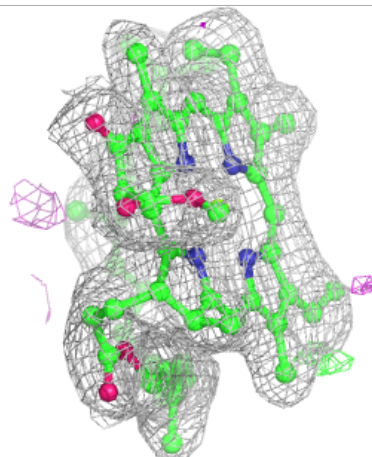
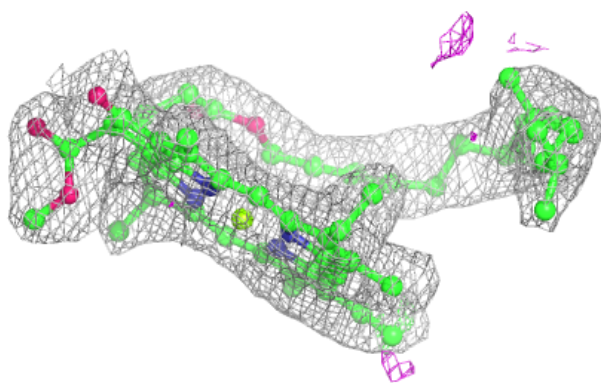
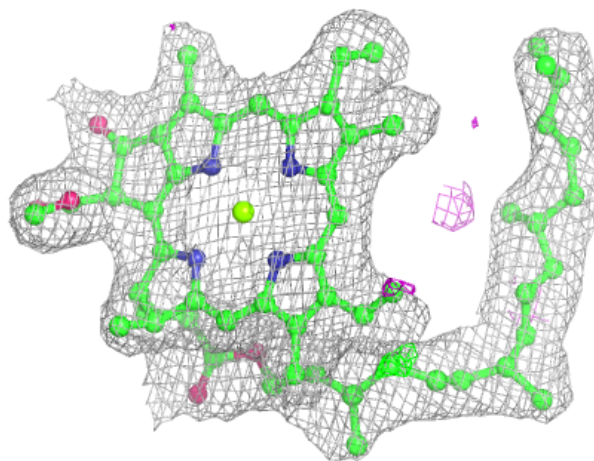






**Electron density around CLA F 602:**

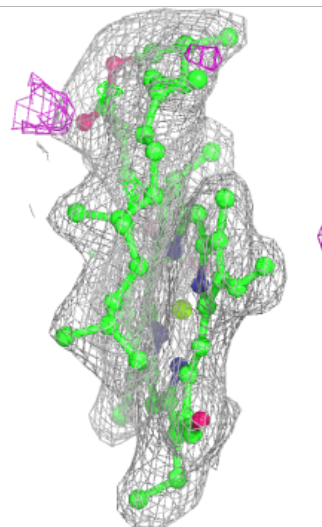
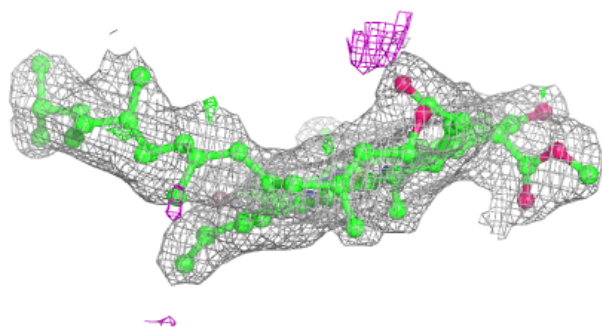
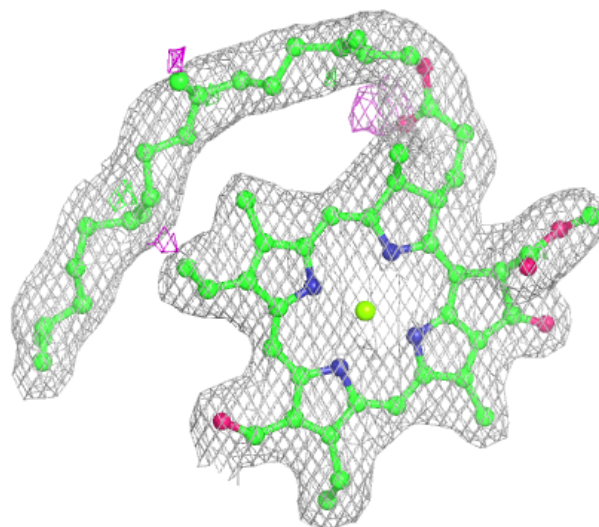
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





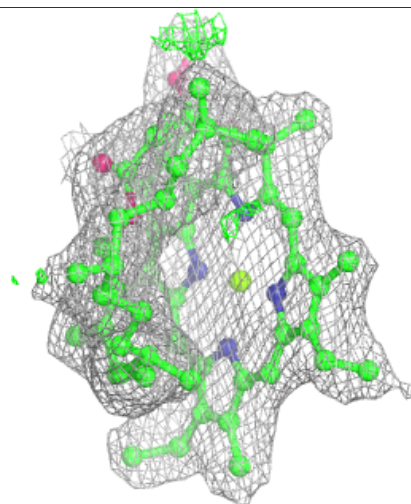
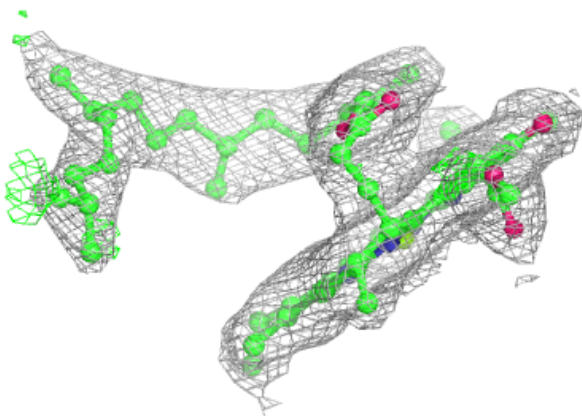
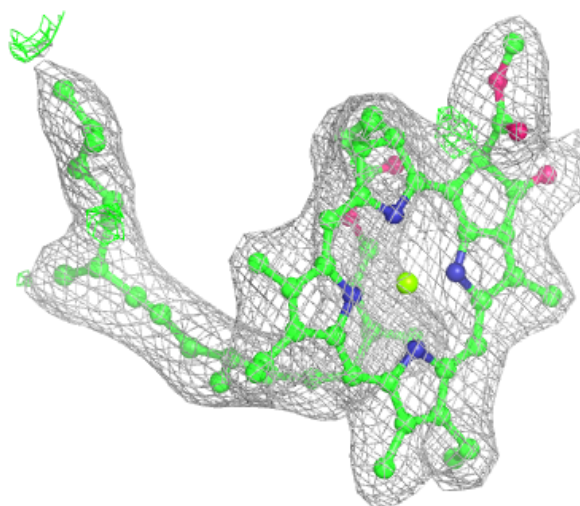
**Electron density around CHL G 607:**

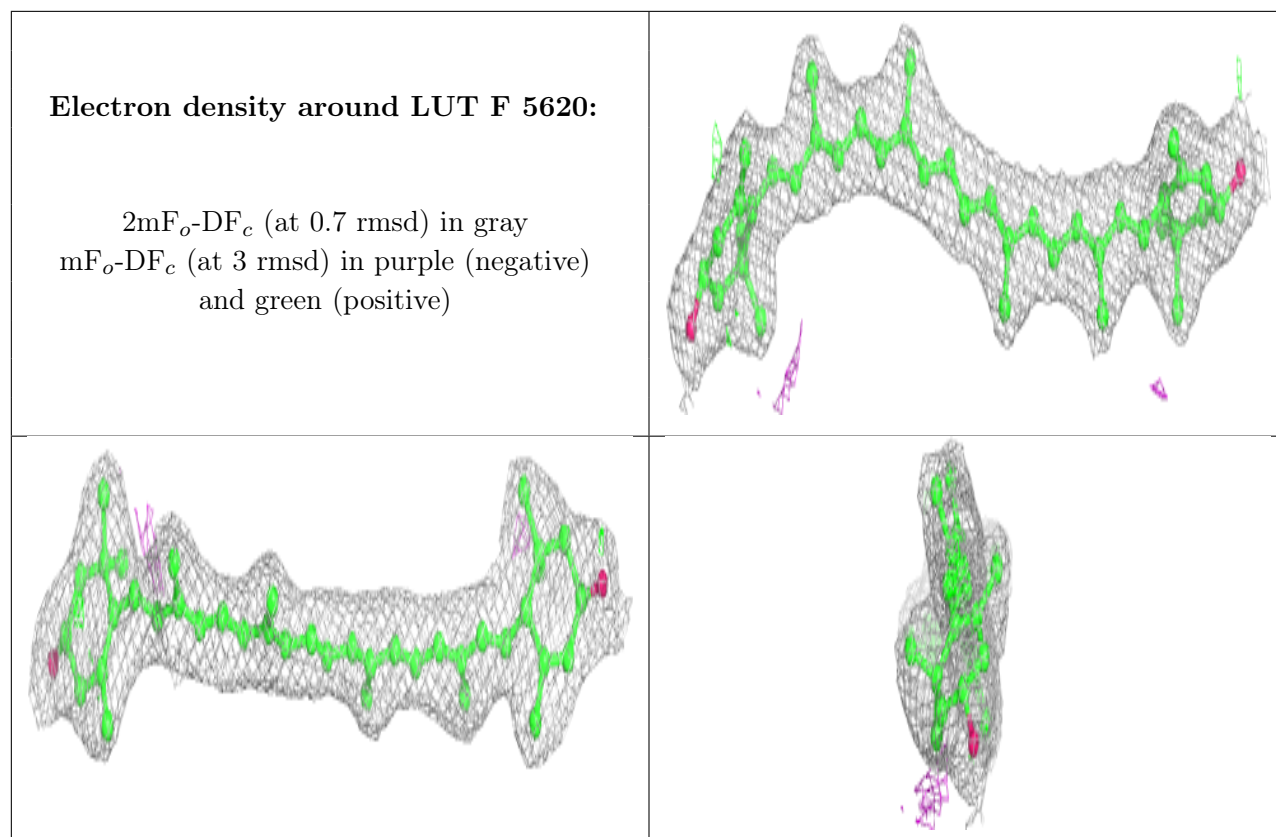
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 613:**

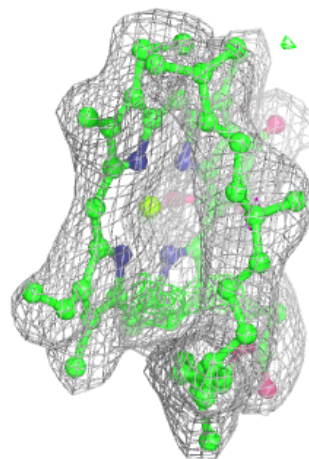
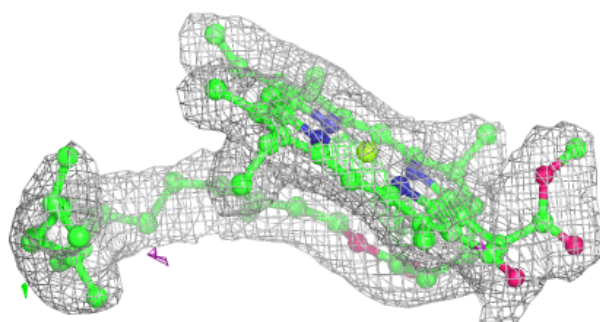
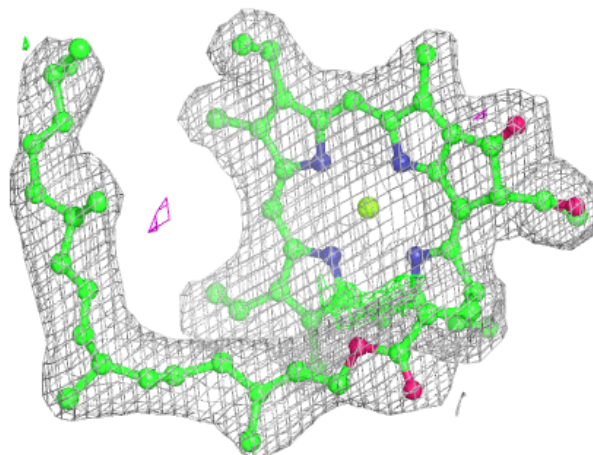
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

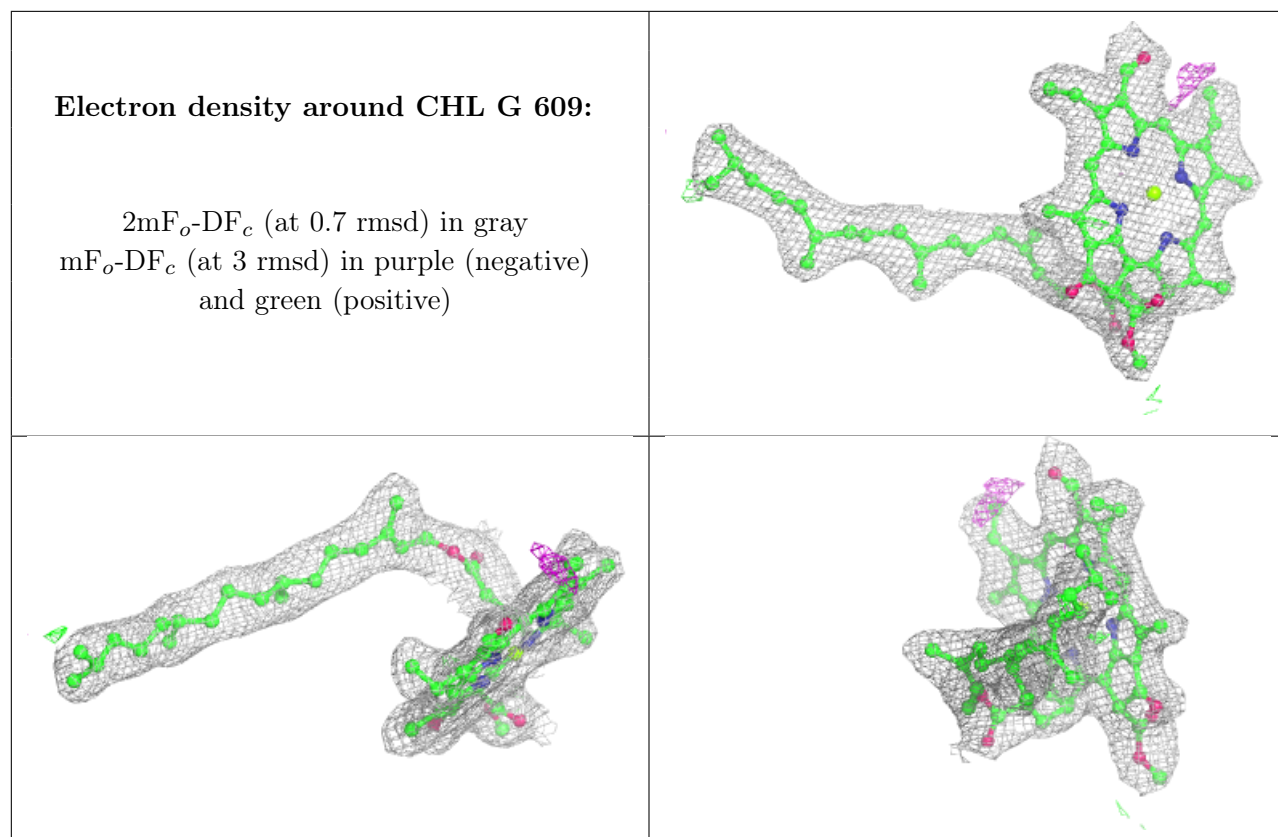




**Electron density around CLA B 602:**

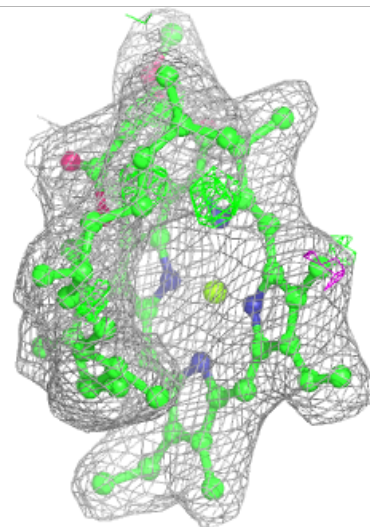
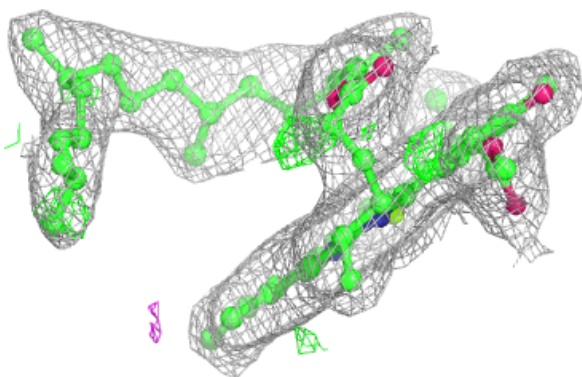
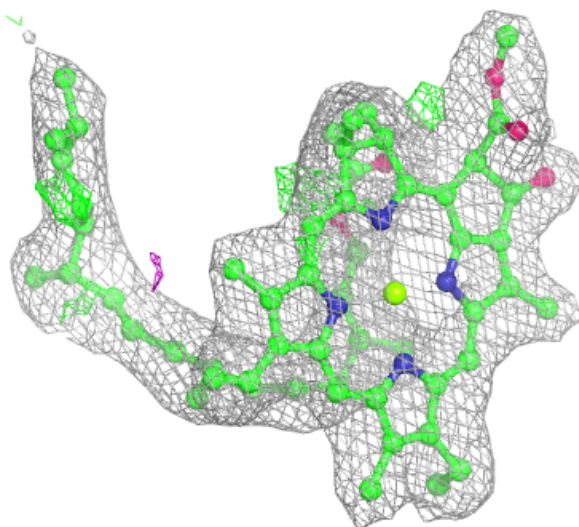
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA F 613:**

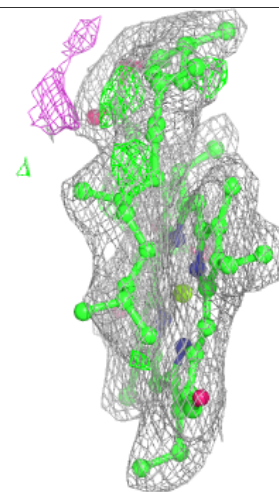
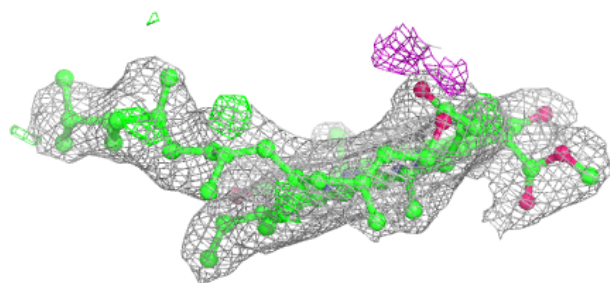
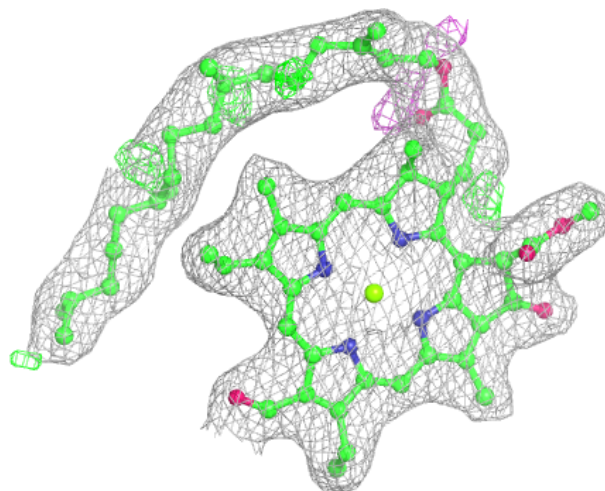
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



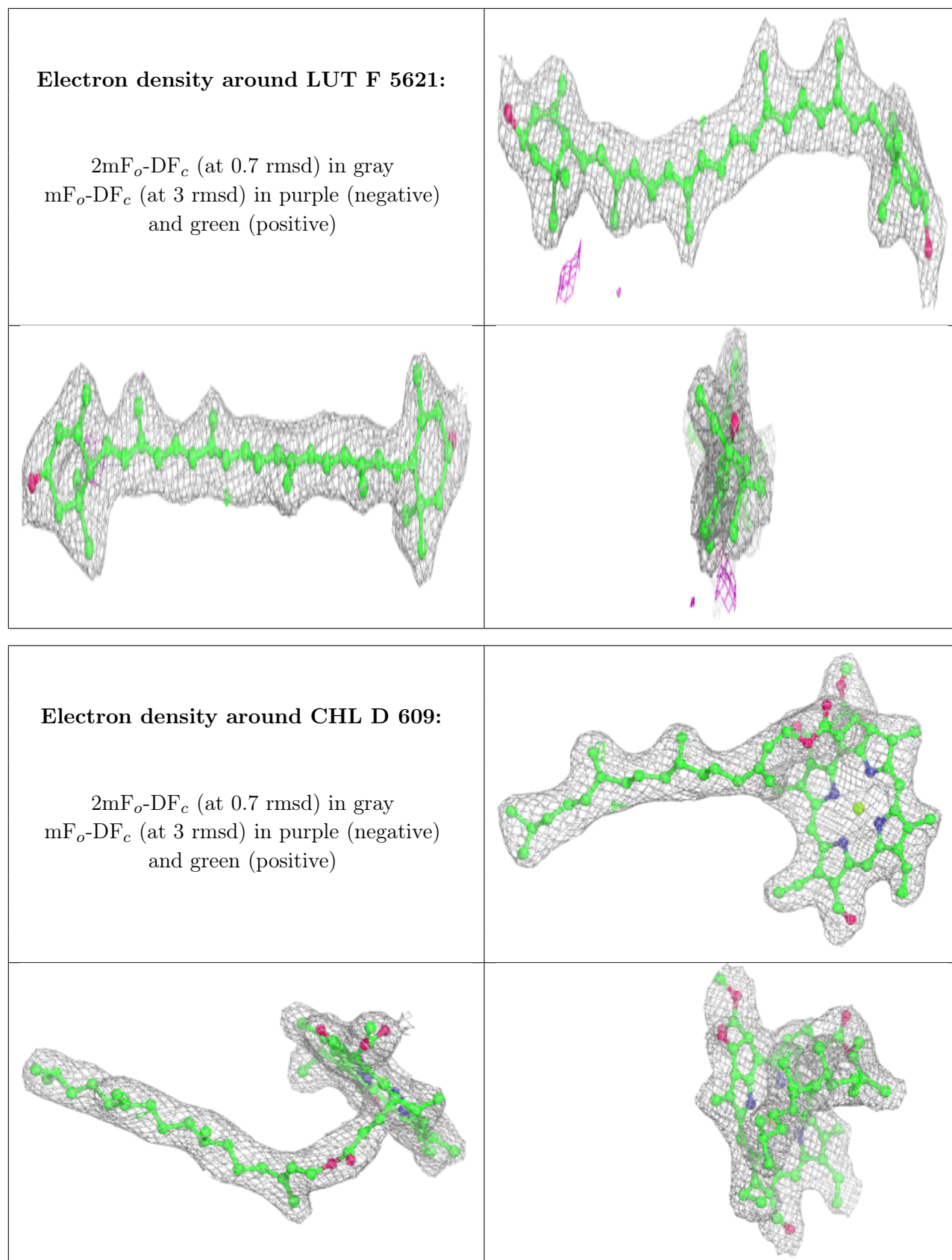


**Electron density around CHL D 607:**

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

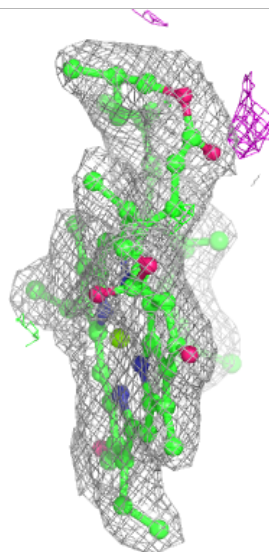
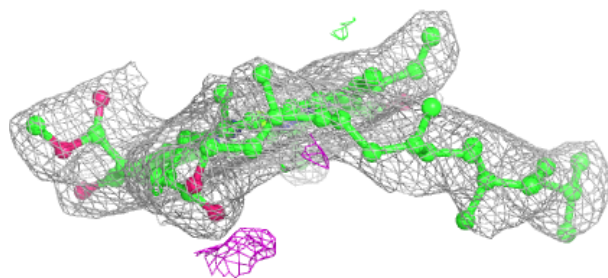
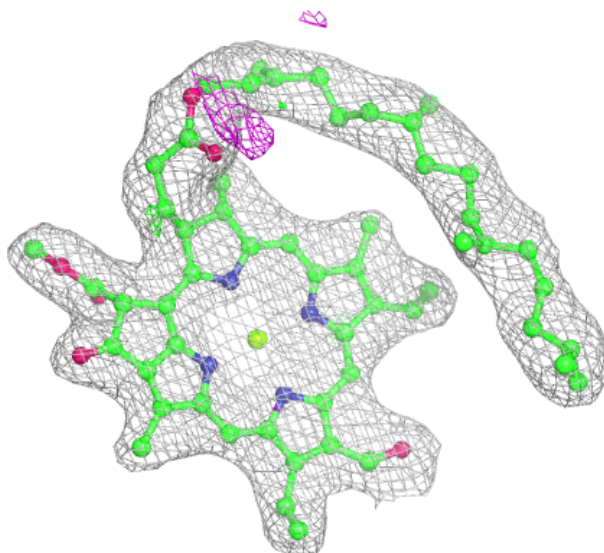






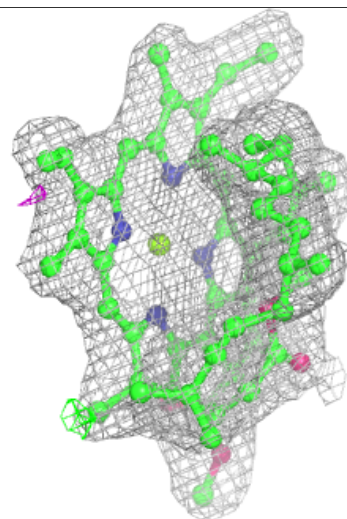
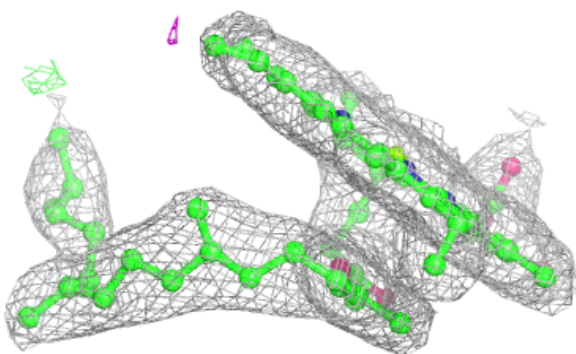
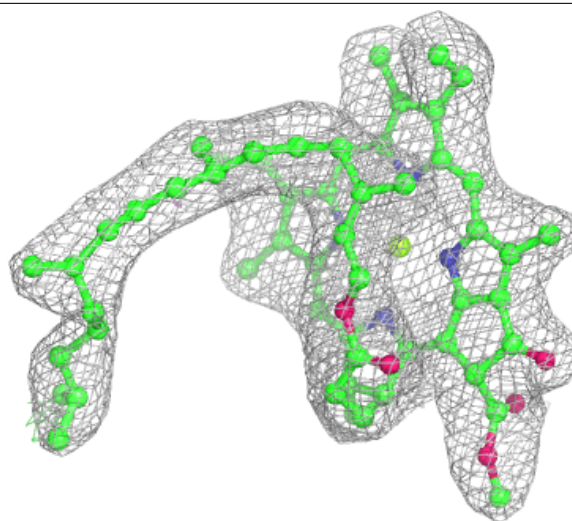
**Electron density around CHL H 607:**

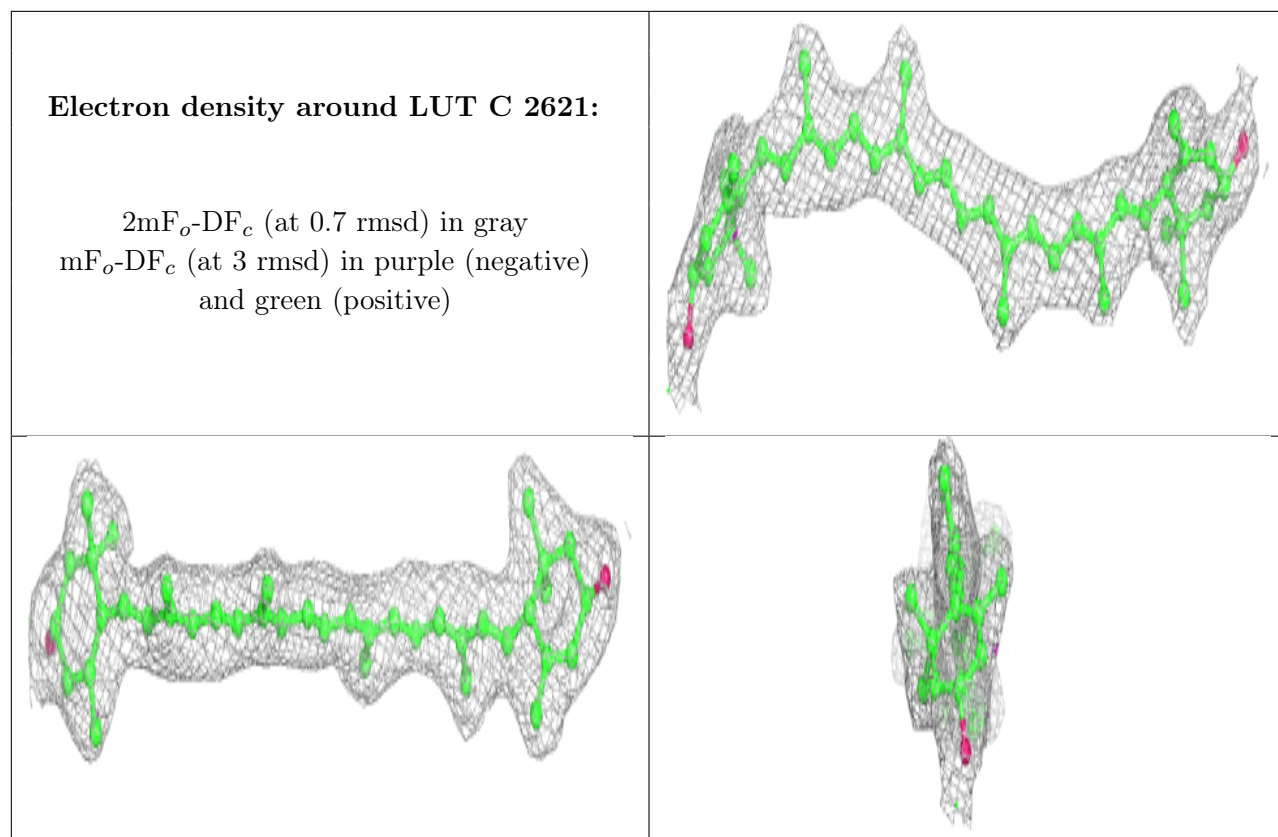
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 613:**

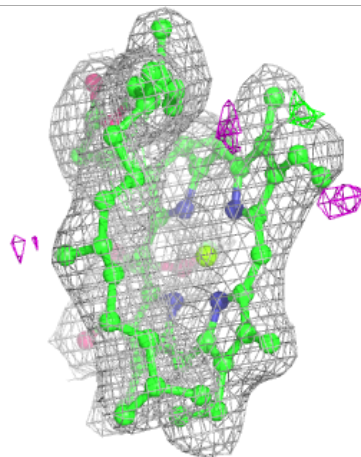
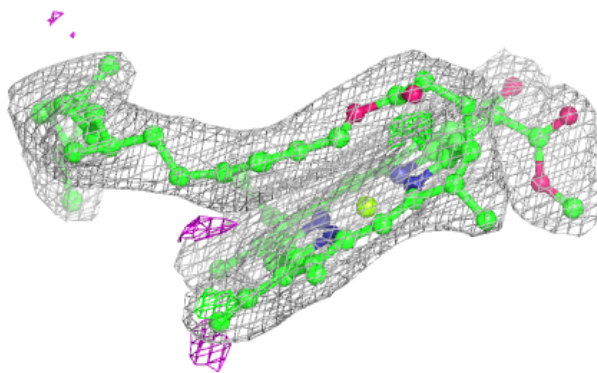
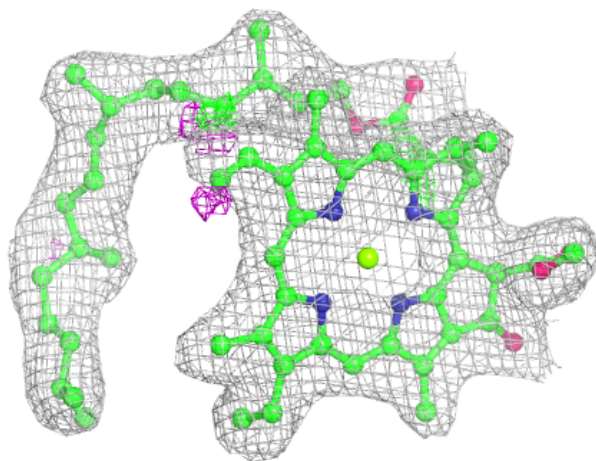
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA C 602:**

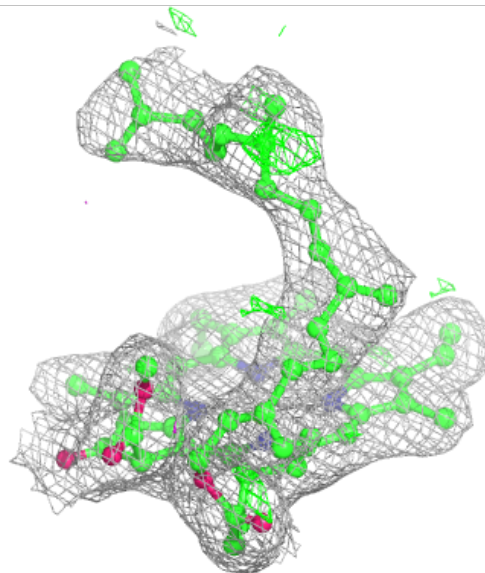
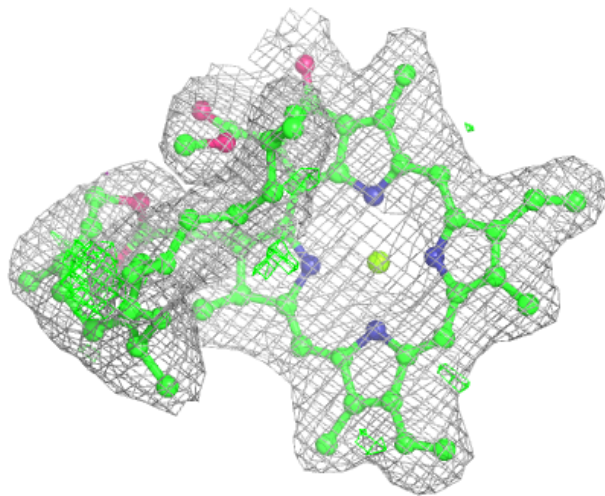
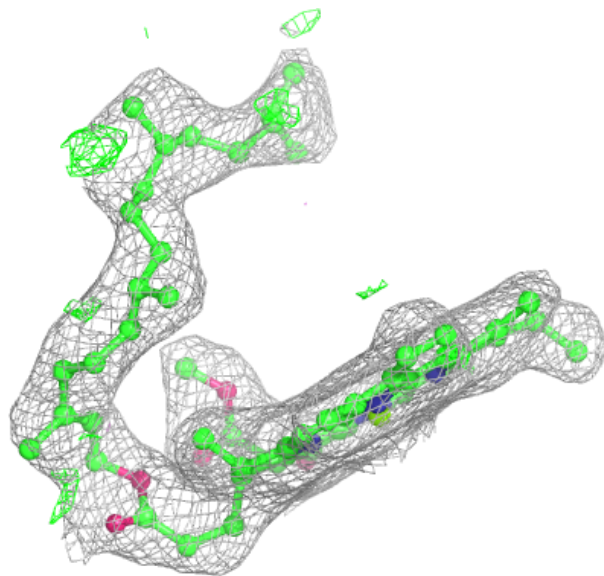
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

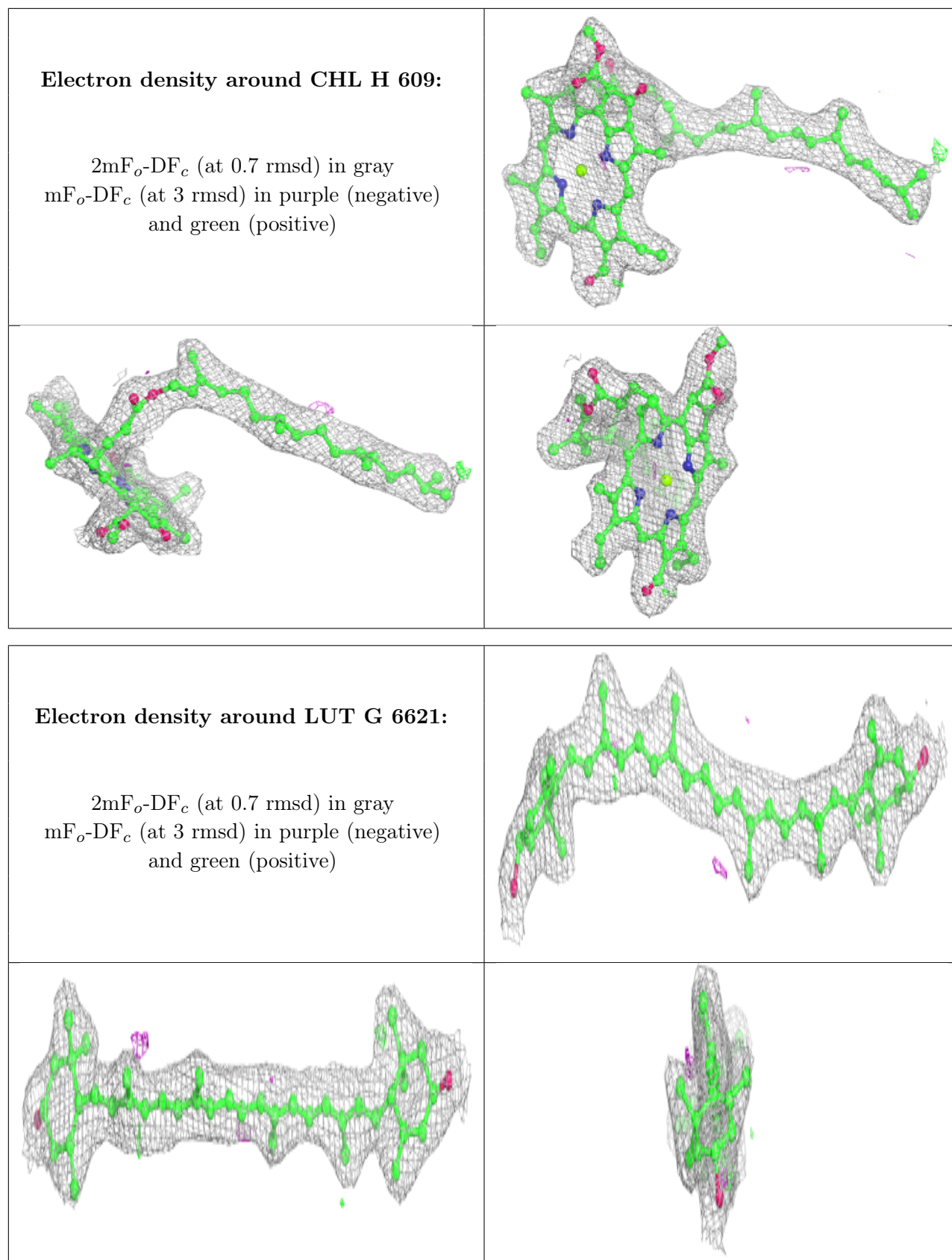




**Electron density around CLA C 603:**

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

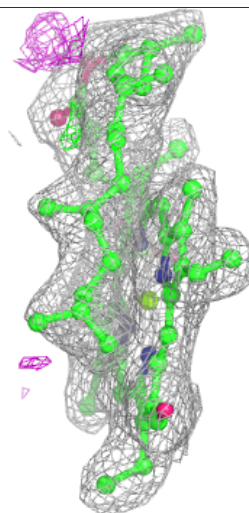
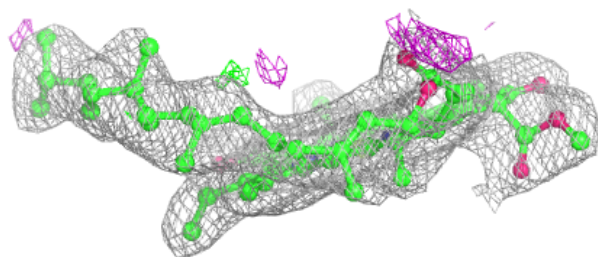
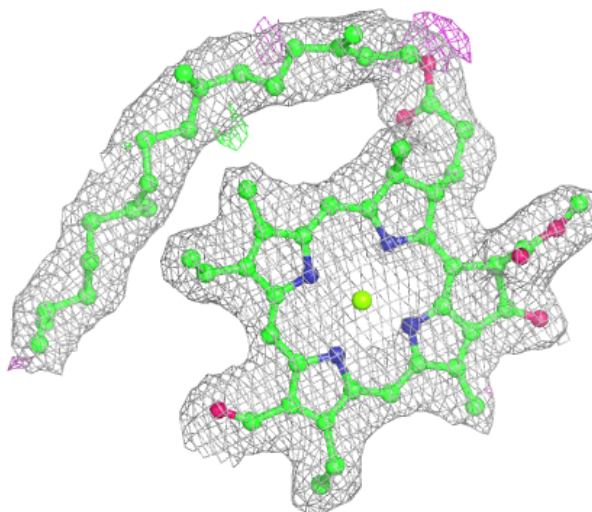


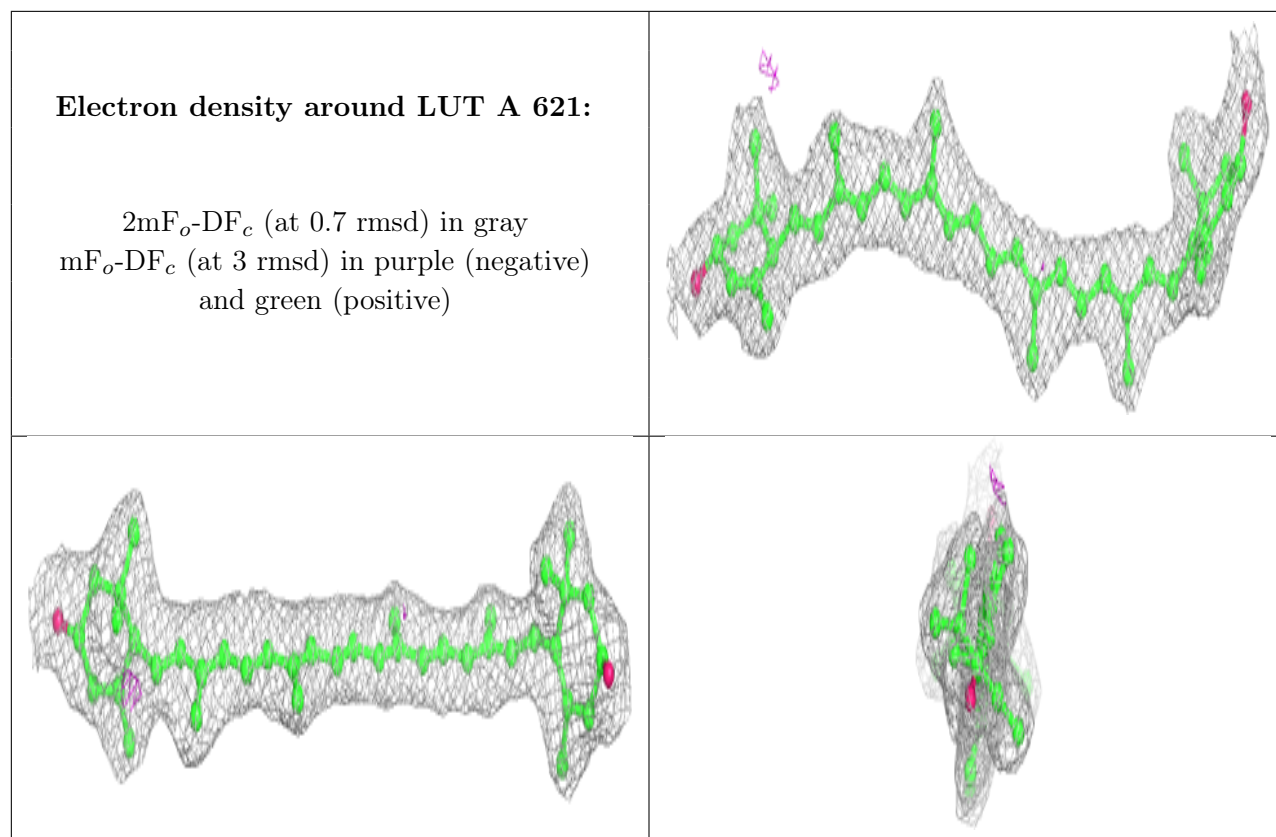




**Electron density around CHL B 607:**

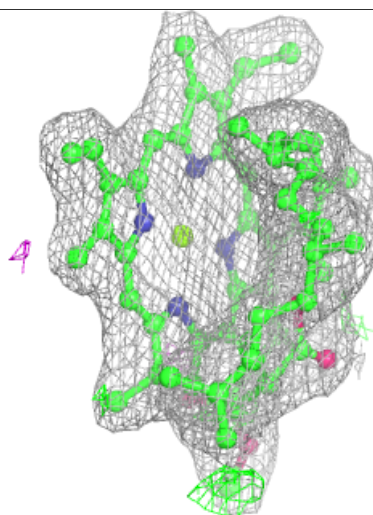
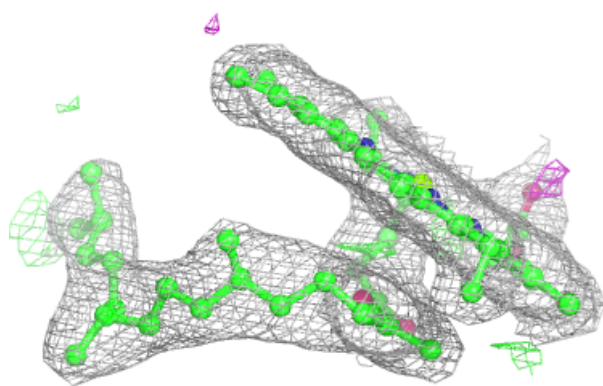
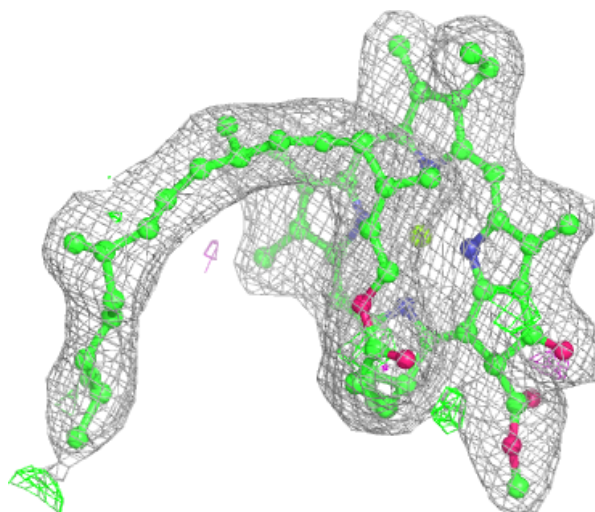
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





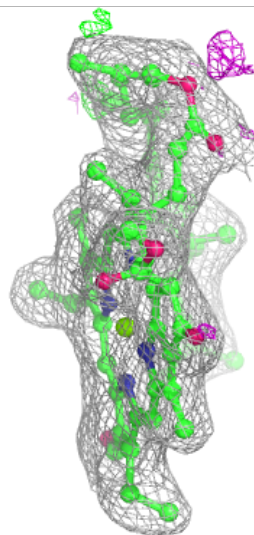
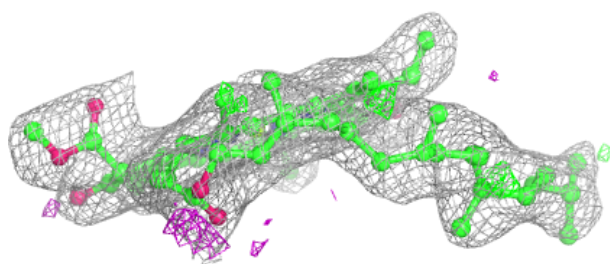
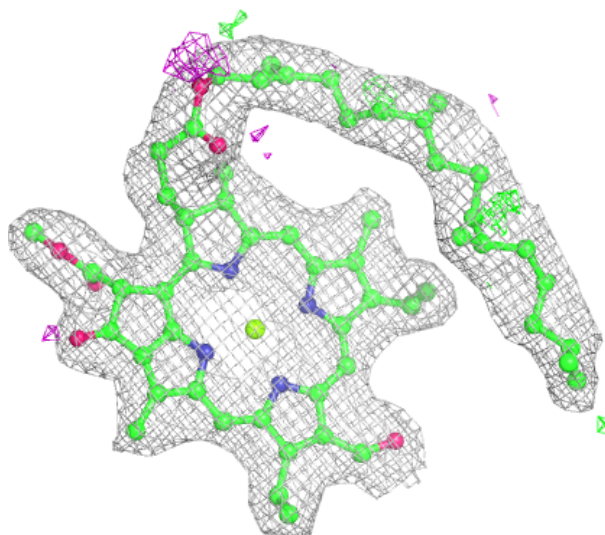
**Electron density around CLA C 613:**

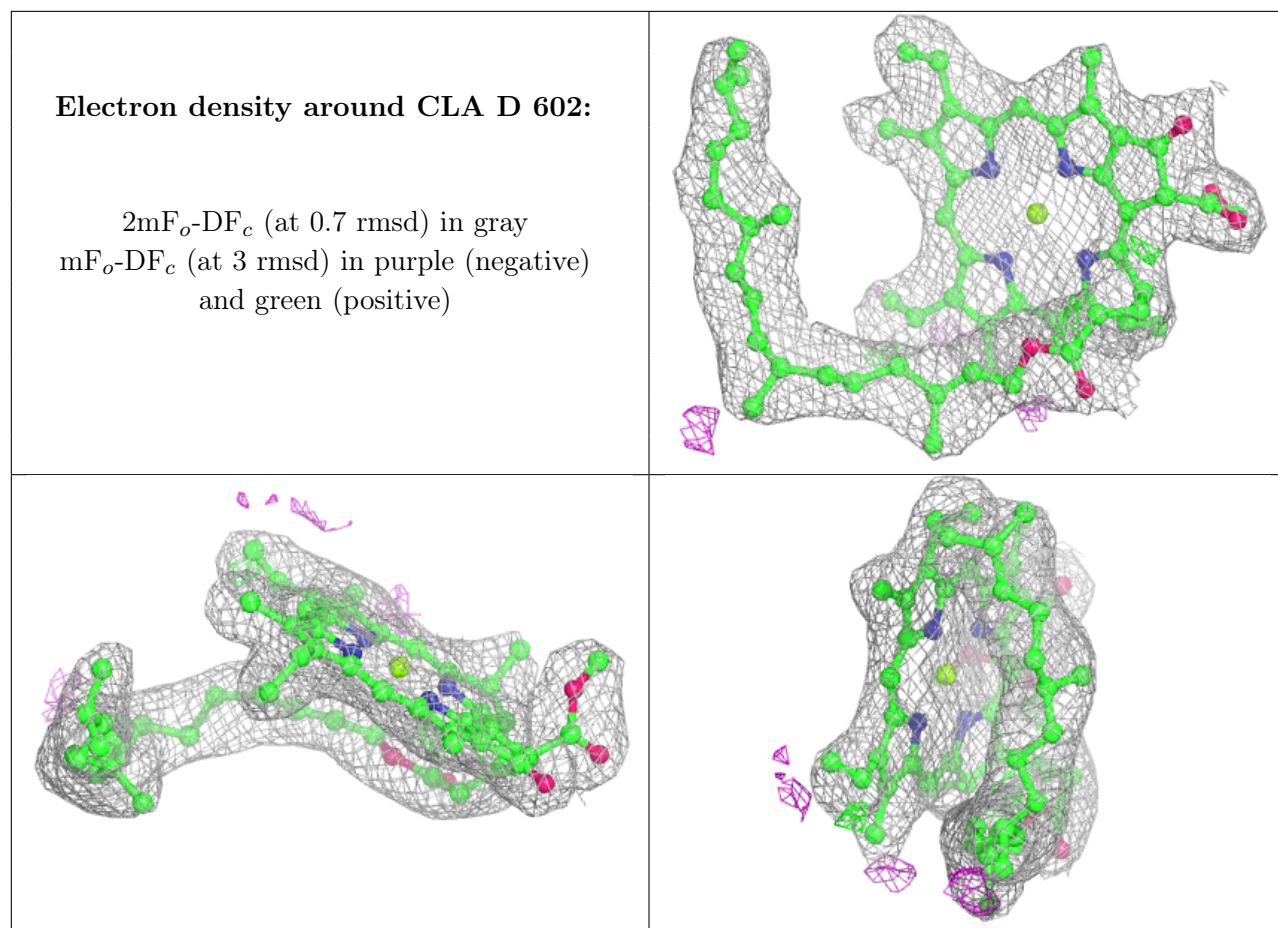
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 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)

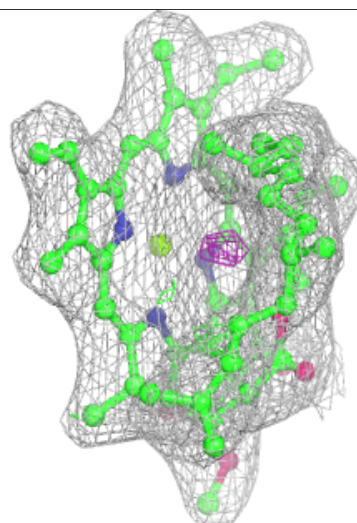
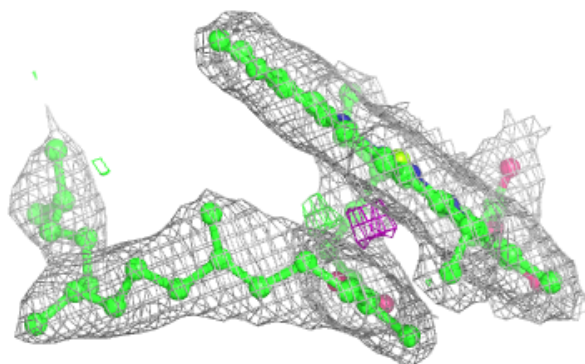
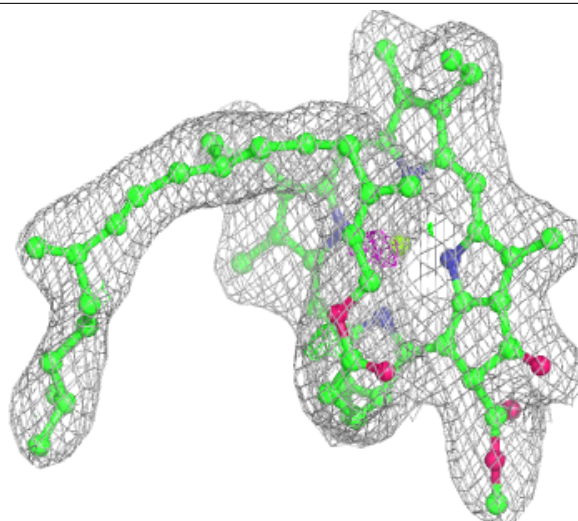






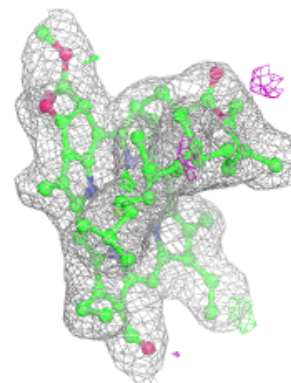
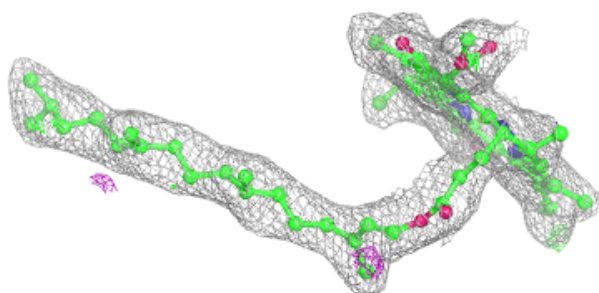
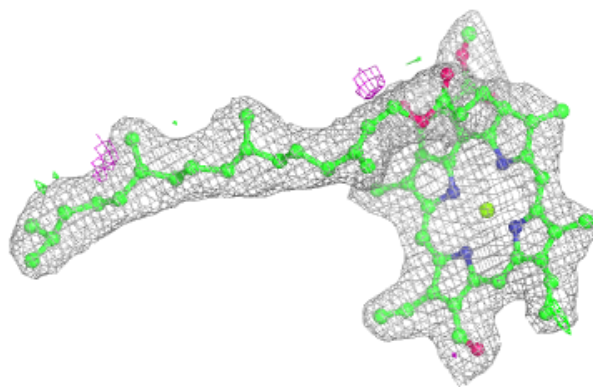
**Electron density around CLA H 613:**

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

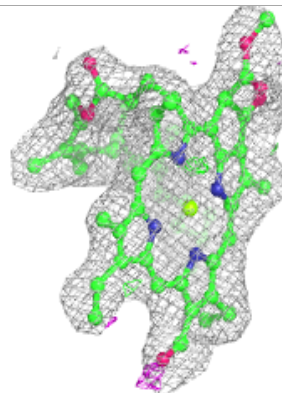
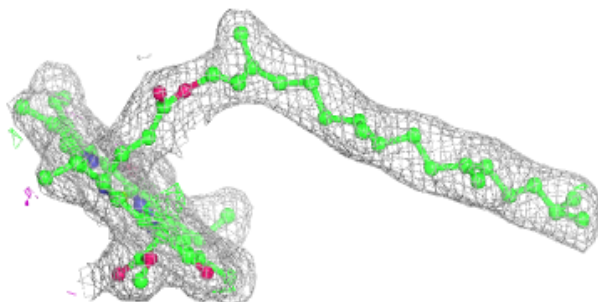
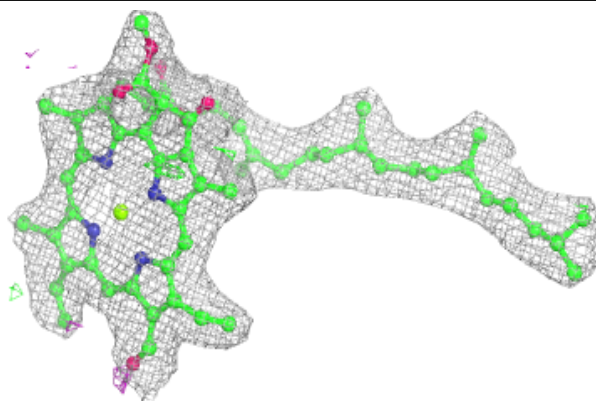


**Electron density around CHL B 609:**

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

**Electron density around CHL I 609:**

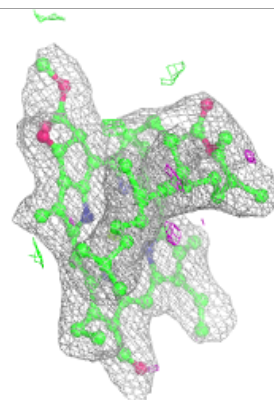
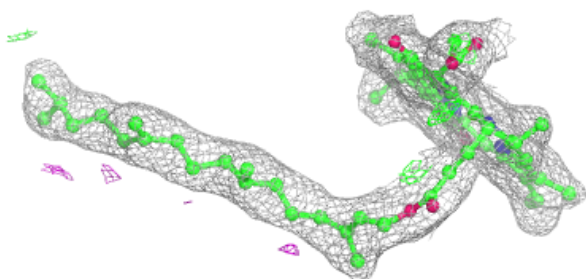
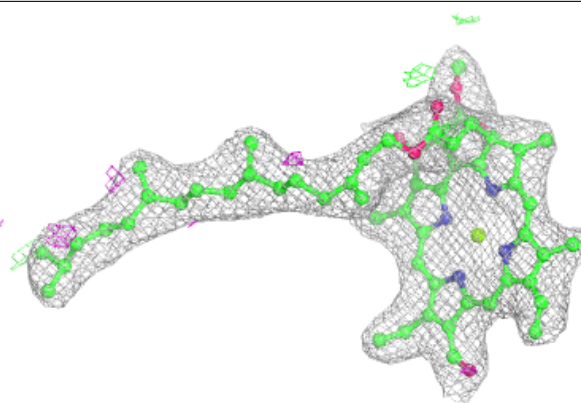
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



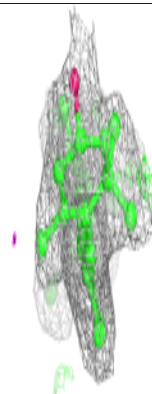
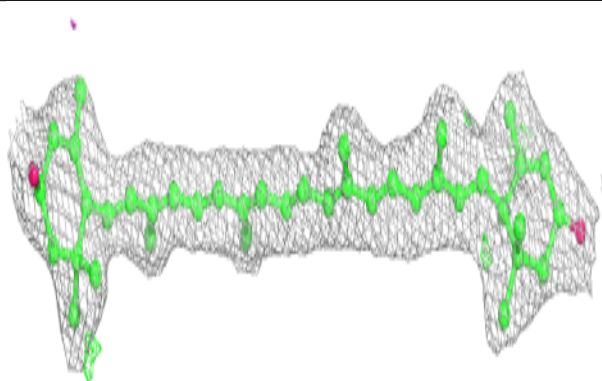
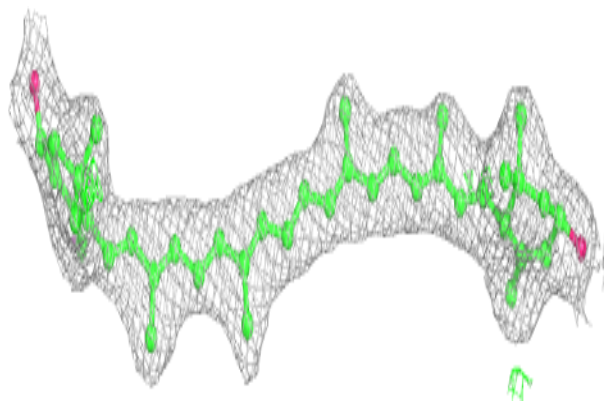


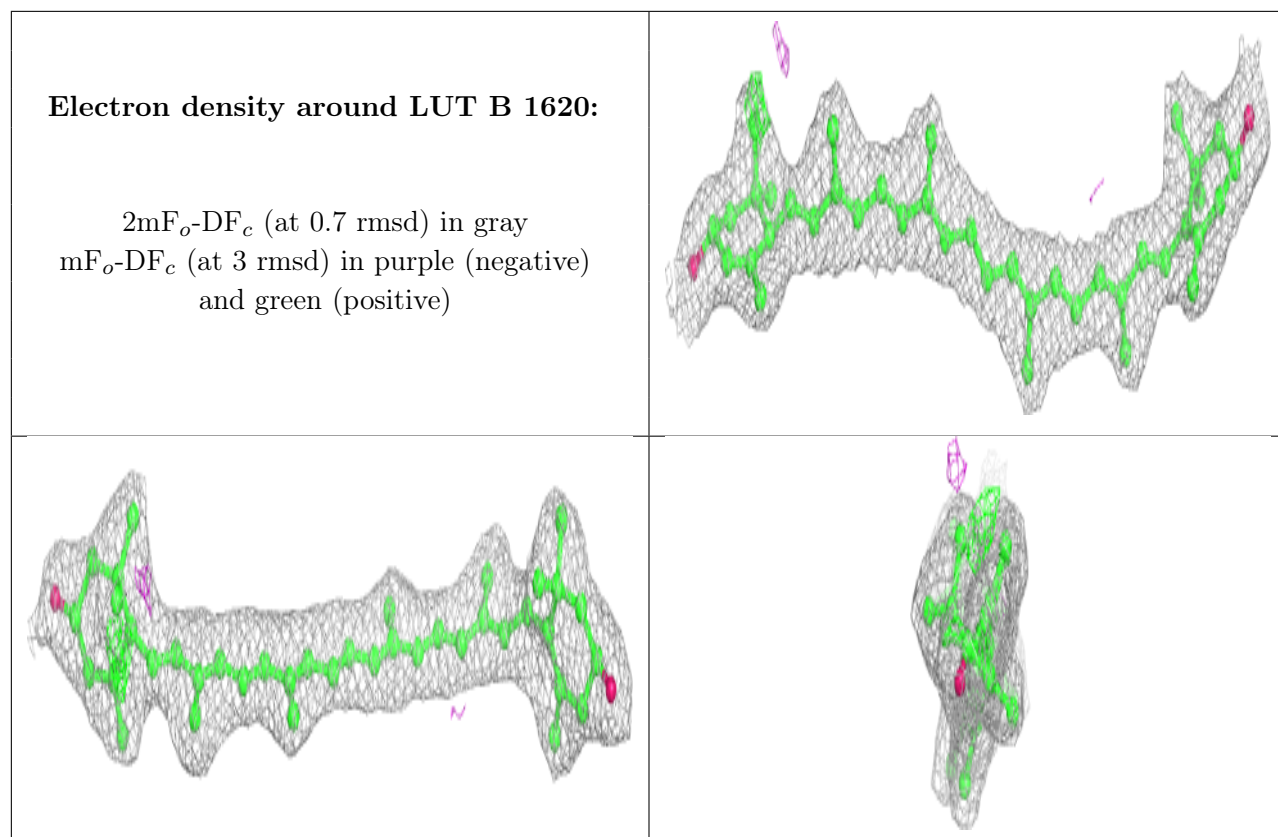
**Electron density around CHL E 609:**

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

**Electron density around LUT H 7621:**

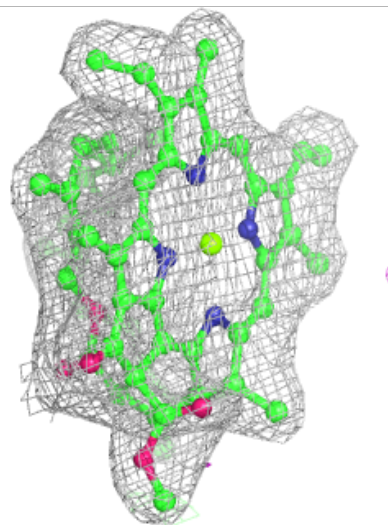
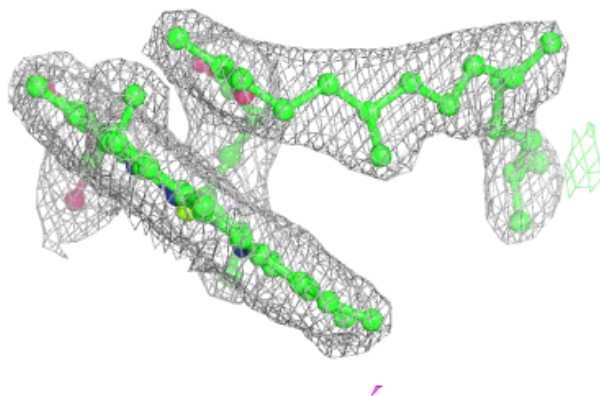
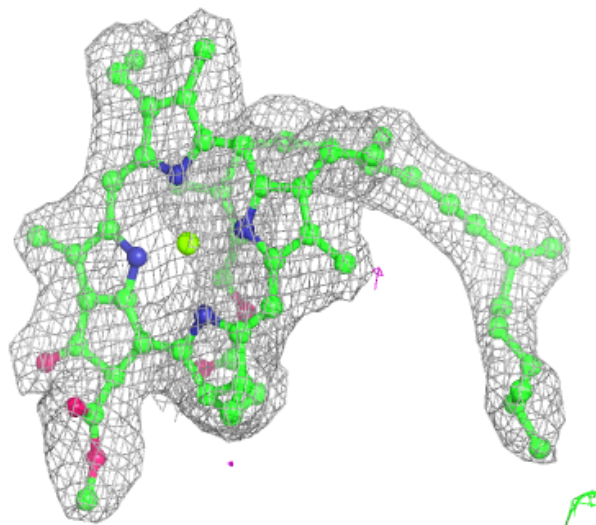
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

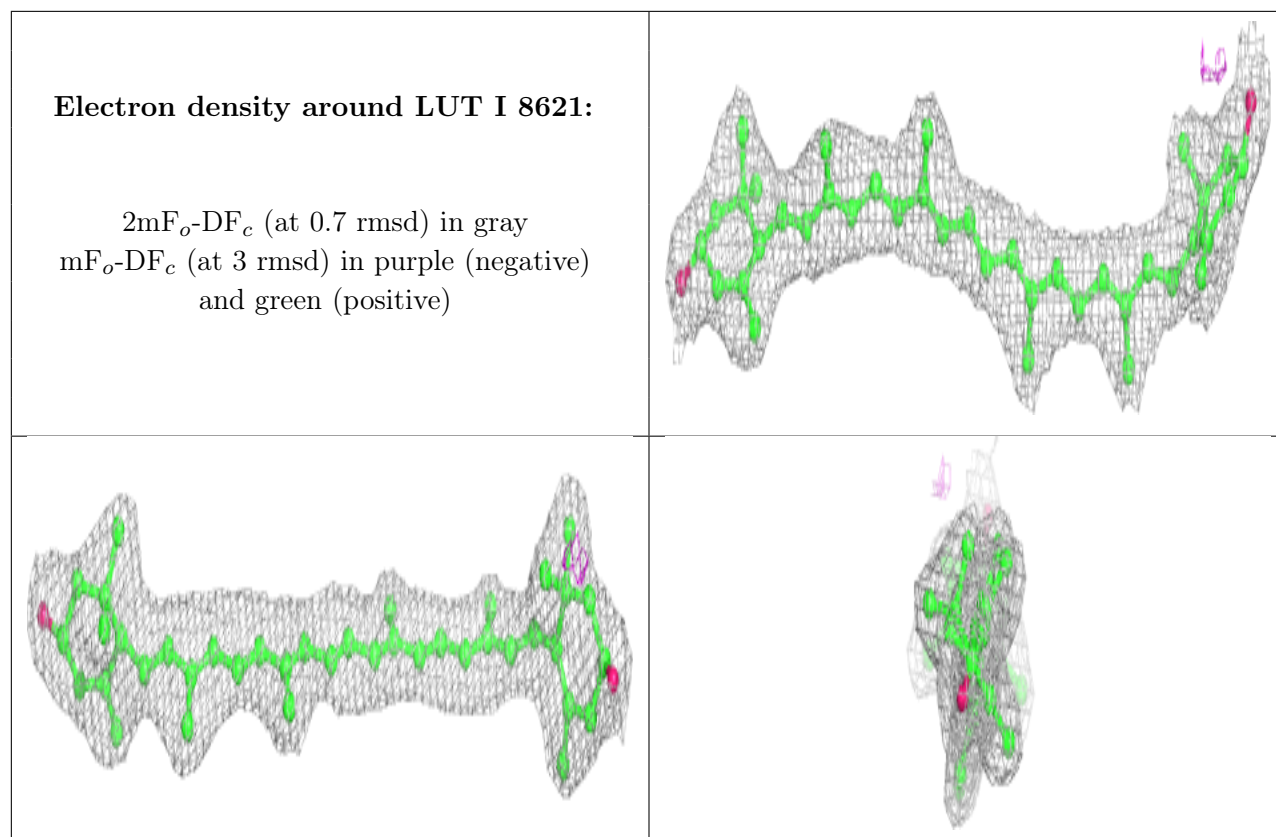




**Electron density around CLA D 613:**

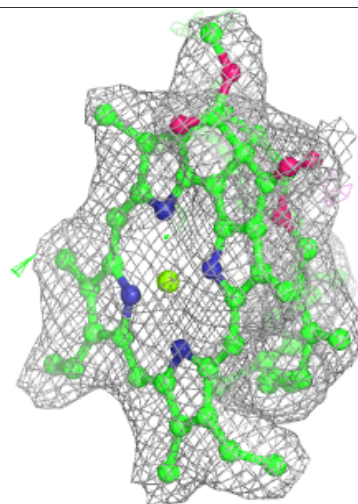
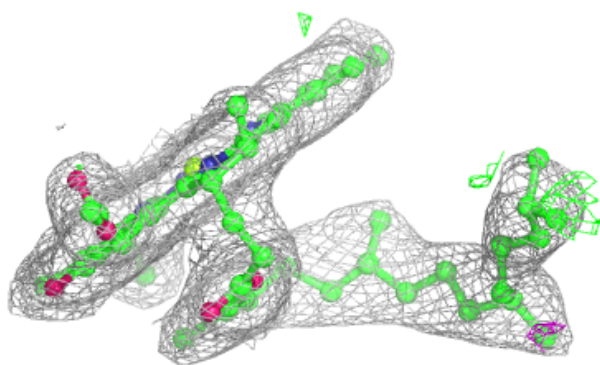
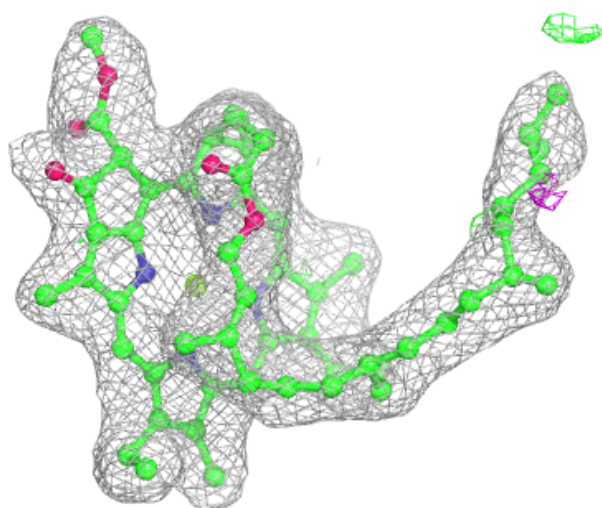
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA I 613:**

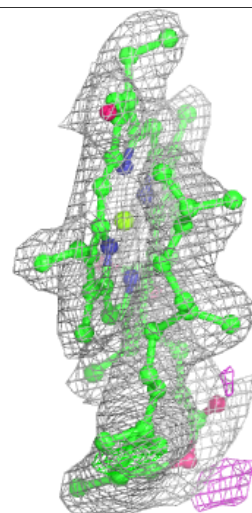
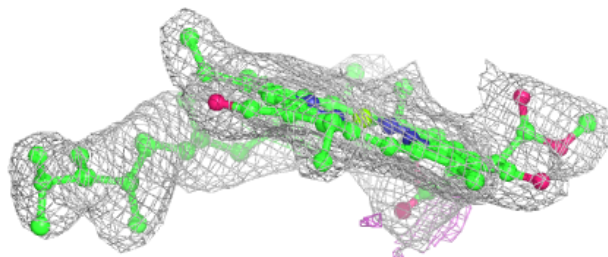
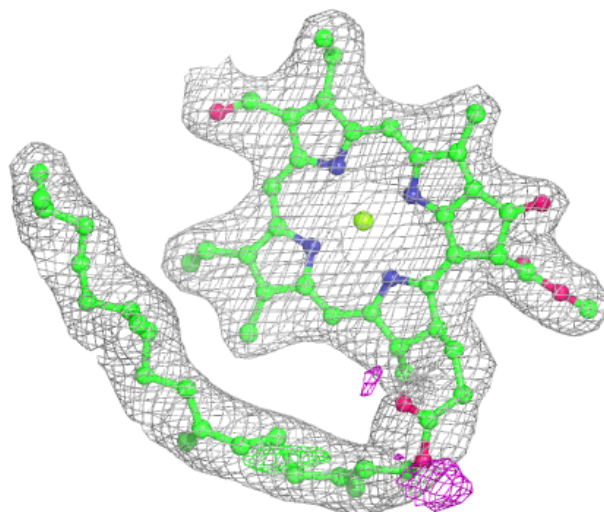
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





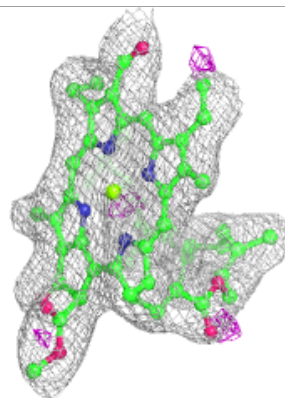
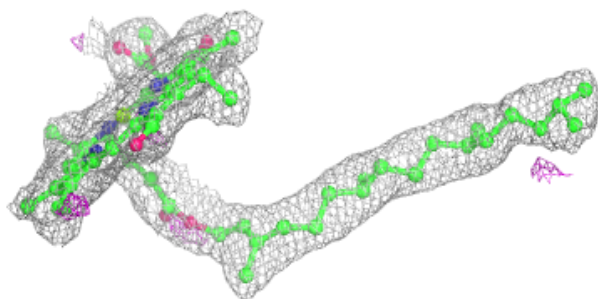
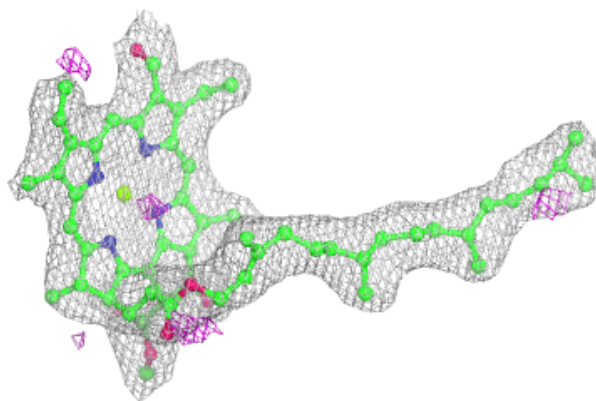
**Electron density around CHL C 607:**

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

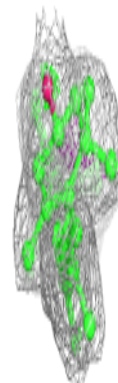
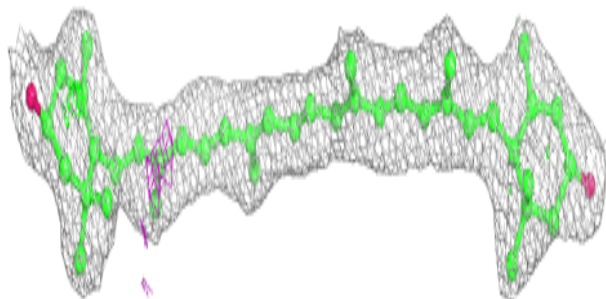
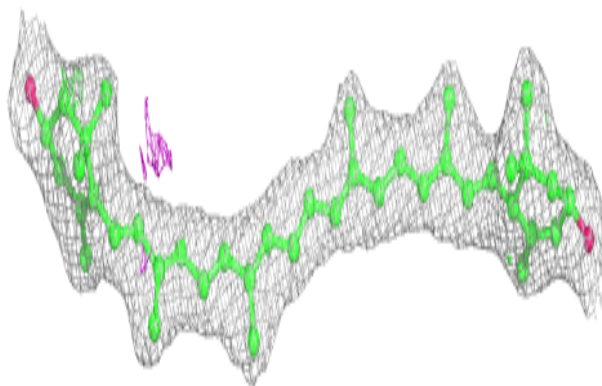


**Electron density around CHL J 609:**

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

**Electron density around LUT J 9620:**

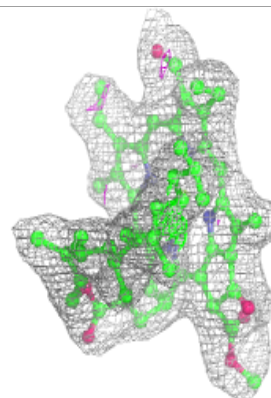
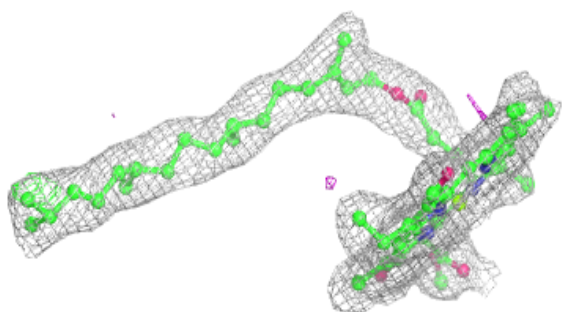
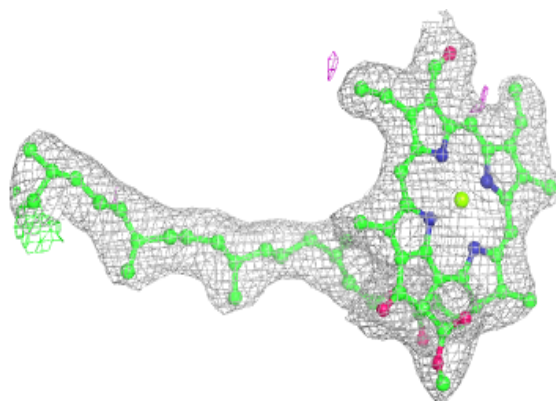
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



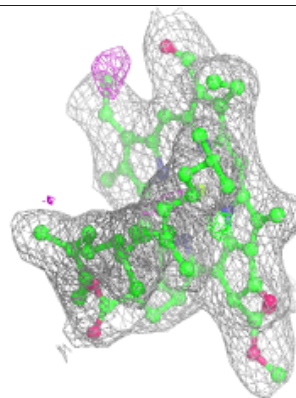
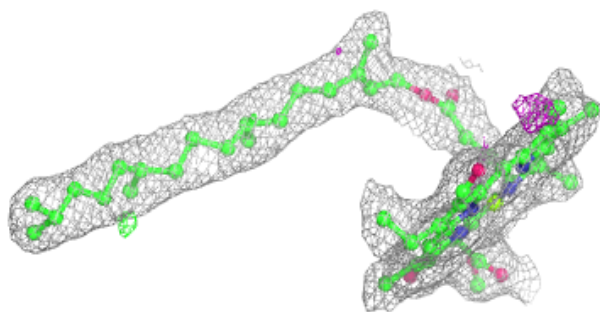
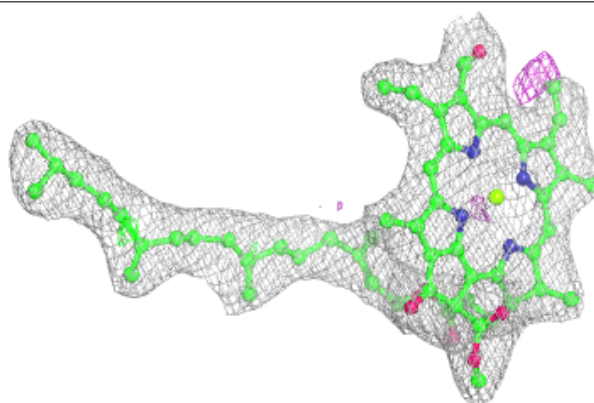


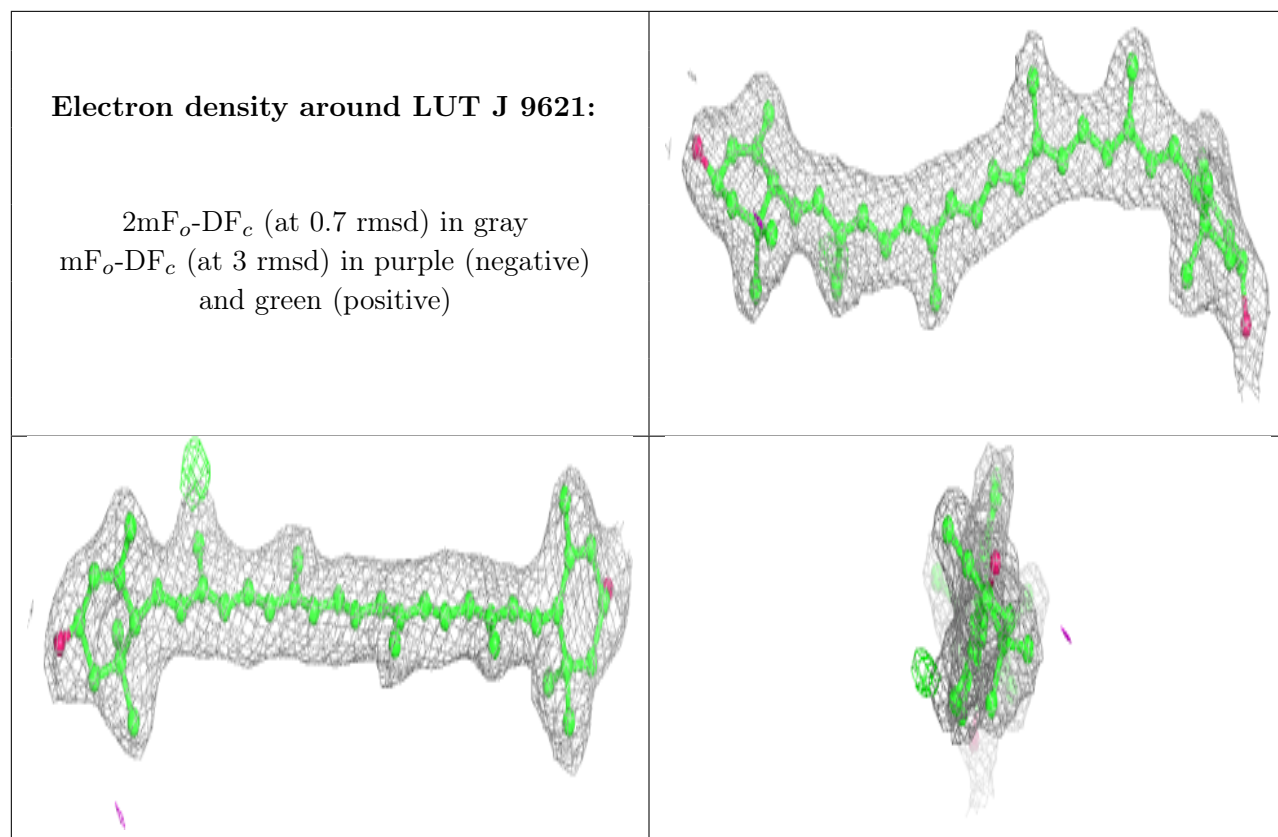
**Electron density around CHL F 609:**

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

**Electron density around CHL C 609:**

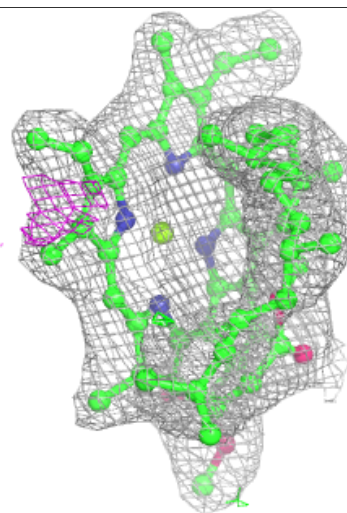
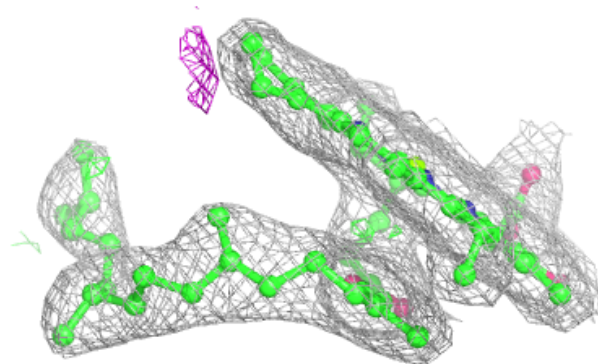
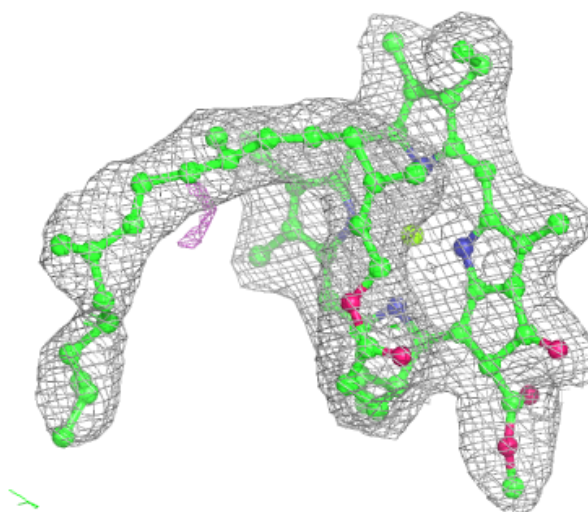
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





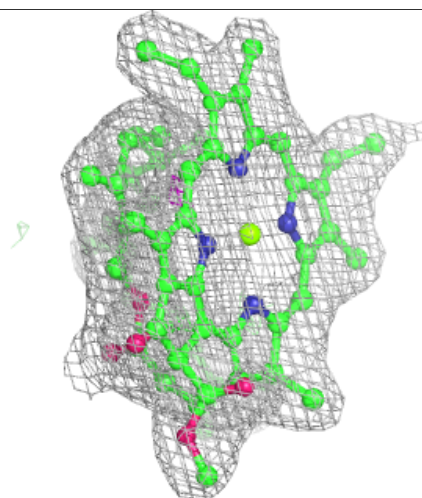
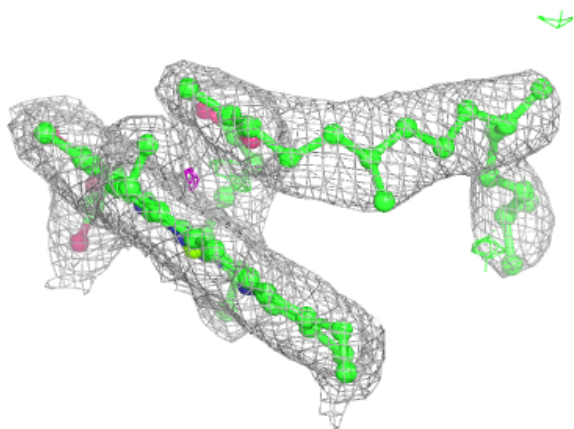
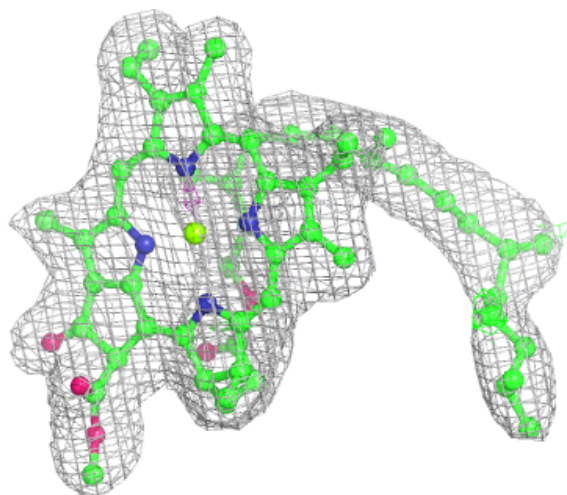
**Electron density around CLA E 613:**

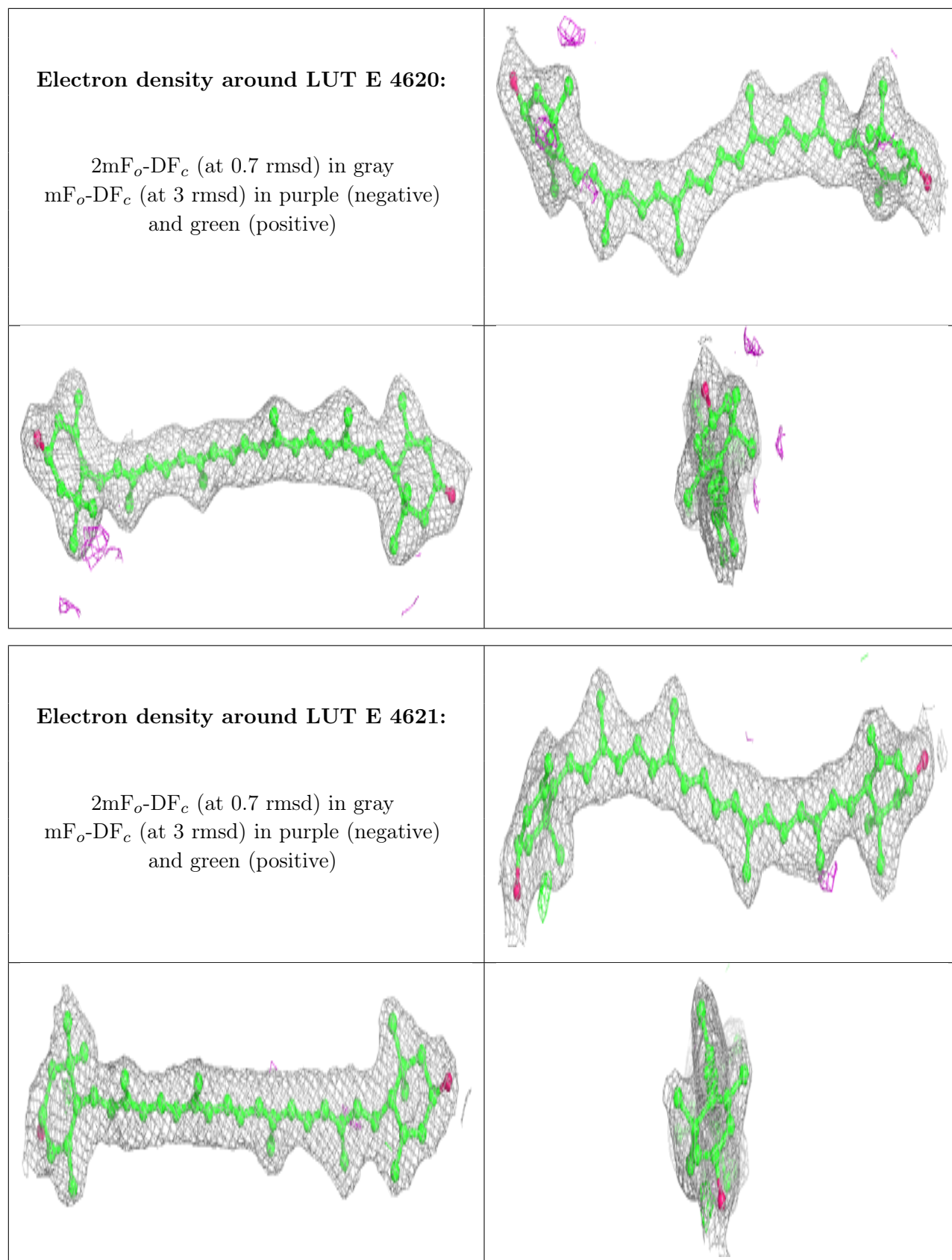
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.