



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2026 – 04:40 am BST

PDB ID : 2BHW / pdb_00002bhw
Title : PEA LIGHT-HARVESTING COMPLEX II AT 2.5 ANGSTROM RESOLUTION
Authors : Standfuss, J.; Terwisscha van Scheltinga, A.C.; Lamborghini, M.; Kuehlbrandt, W.
Deposited on : 2005-01-19
Resolution : 2.50 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

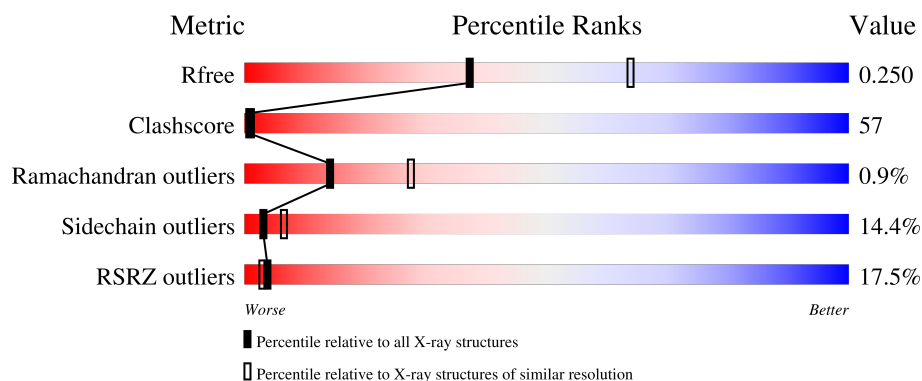
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	232	
1	C	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
2	LUX	A	501	X	-	X	-
2	LUX	A	502	X	-	-	-
2	LUX	B	501	X	-	X	-
2	LUX	B	502	X	-	-	-
2	LUX	C	501	X	-	X	-
2	LUX	C	502	X	-	-	-
4	XAT	A	504	X	-	-	-
4	XAT	B	504	X	-	-	-
4	XAT	C	504	X	-	-	-
5	CLA	A	601	X	-	-	-
5	CLA	A	603	X	-	-	-
5	CLA	A	604	X	-	-	-
5	CLA	A	605	X	-	-	-
5	CLA	A	606	X	-	-	-
5	CLA	B	601	X	-	X	-
5	CLA	B	603	X	-	X	-
5	CLA	B	604	X	-	X	-
5	CLA	B	605	X	-	X	-
5	CLA	B	606	X	-	-	-
5	CLA	B	608	-	-	X	-
5	CLA	C	601	X	-	X	-
5	CLA	C	603	X	-	-	-
5	CLA	C	604	X	-	-	-
5	CLA	C	605	X	-	-	-
5	CLA	C	606	X	-	-	-
6	CHL	A	609	X	-	X	-
6	CHL	A	610	X	-	X	-
6	CHL	A	611	X	-	-	-
6	CHL	B	609	X	-	X	-
6	CHL	B	610	X	-	X	-
6	CHL	B	611	X	-	X	-
6	CHL	B	612	-	-	X	-
6	CHL	C	609	X	-	X	-
6	CHL	C	610	X	-	X	-
6	CHL	C	611	X	-	X	-
6	CHL	C	612	-	-	X	-
8	DGD	A	802	X	-	-	-
8	DGD	B	802	X	-	-	-
8	DGD	C	802	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8373 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.

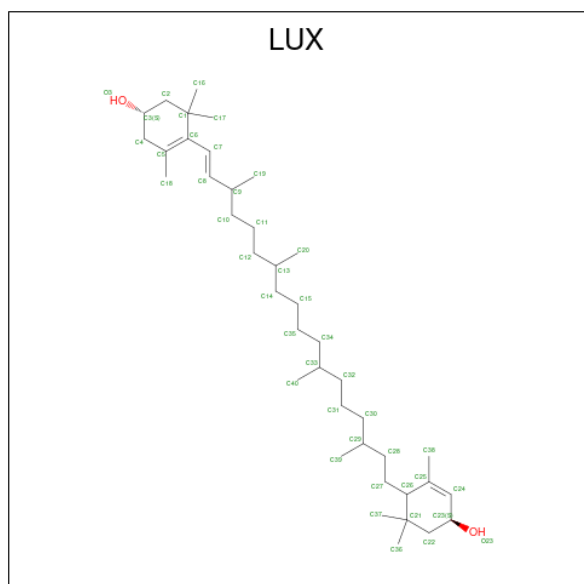
- Molecule 1 is a protein called CHLOROPHYLL A-B BINDING PROTEIN AB80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			
1	B	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			
1	C	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			

There are 3 discrepancies between the modelled and reference sequences:

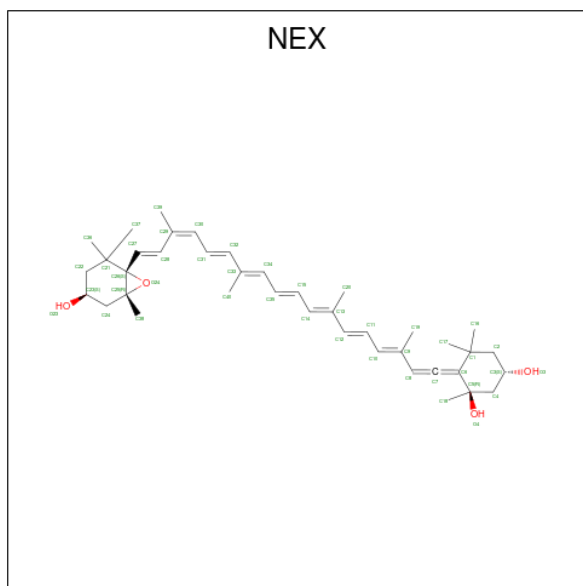
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	SER	CYS	conflict	UNP P07371
B	79	SER	CYS	conflict	UNP P07371
C	79	SER	CYS	conflict	UNP P07371

- Molecule 2 is (3R,3'R,6'S,9R,9'R,13R,13'S)-4',5'-DIDEHYDRO-5',6',7',8',9,9',10,10',11,11',12,12',13,13',14,14',15,15'-OCTADECALYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUX) (formula: C₄₀H₇₂O₂).



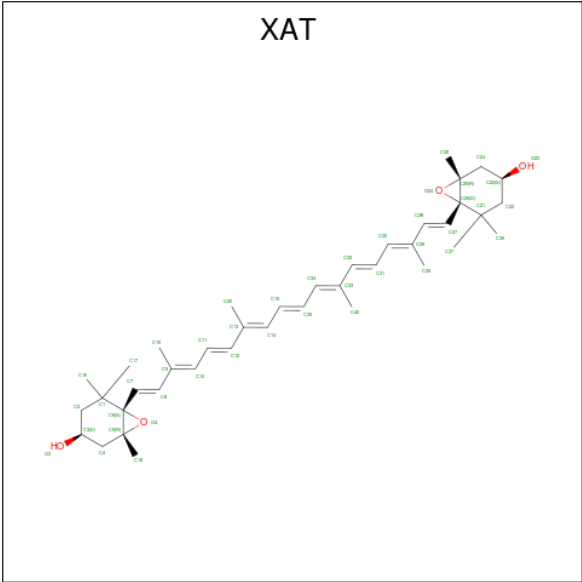
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			42	40	2		
2	A	1	Total	C	O	0	0
			42	40	2		
2	B	1	Total	C	O	0	0
			42	40	2		
2	B	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		

- Molecule 3 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 (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



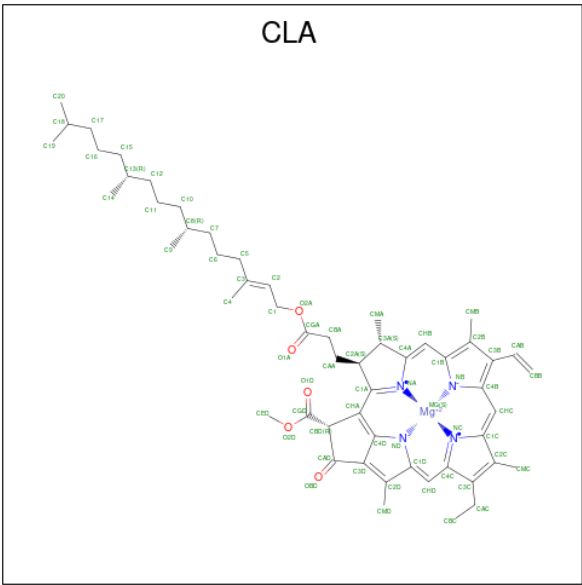
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			44	40	4		
3	B	1	Total	C	O	0	0
			44	40	4		
3	C	1	Total	C	O	0	0
			44	40	4		

- Molecule 4 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



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

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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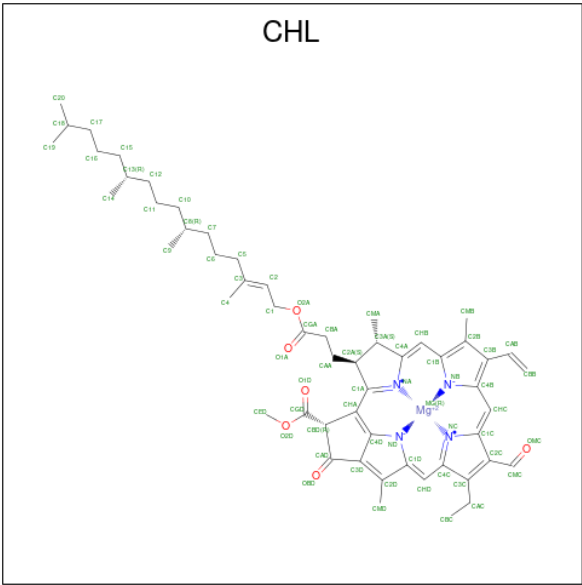
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		

- Molecule 6 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



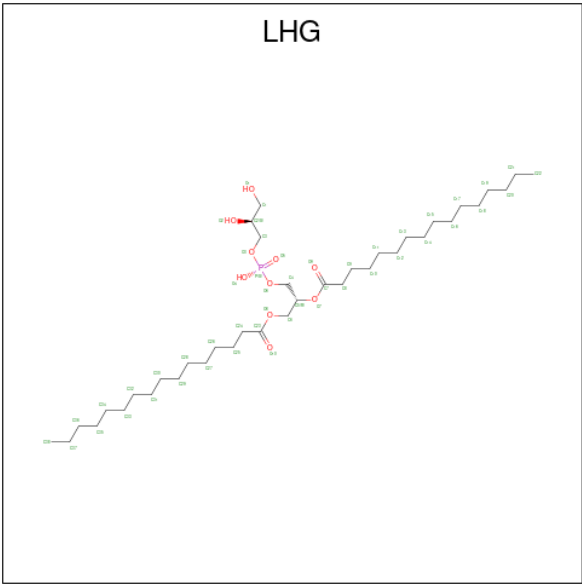
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



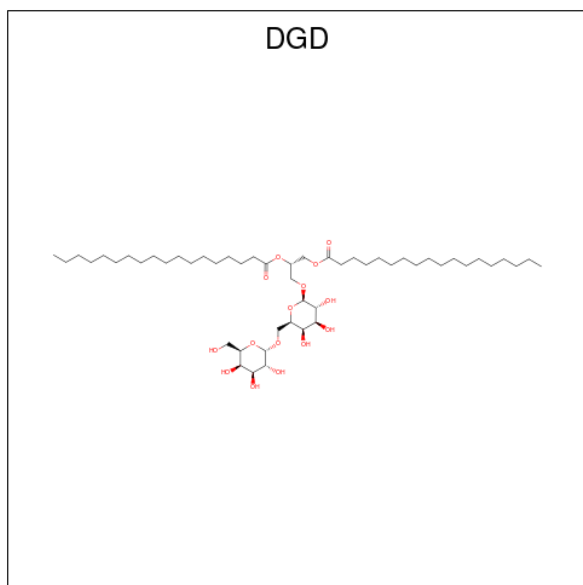
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			49	38	10	1		
7	B	1	Total	C	O	P	0	0
			49	38	10	1		

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			38	25	13		
8	B	1	Total	C	O	0	0
			38	25	13		
8	C	1	Total	C	O	0	0
			38	25	13		

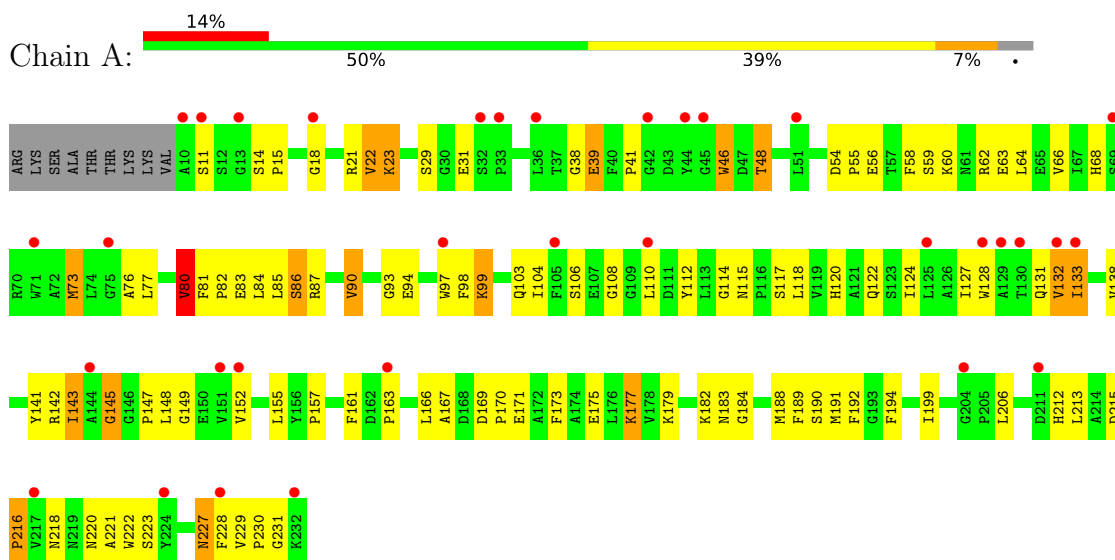
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	9	Total	O	0	0
			9	9		
9	B	7	Total	O	0	0
			7	7		
9	C	5	Total	O	0	0
			5	5		

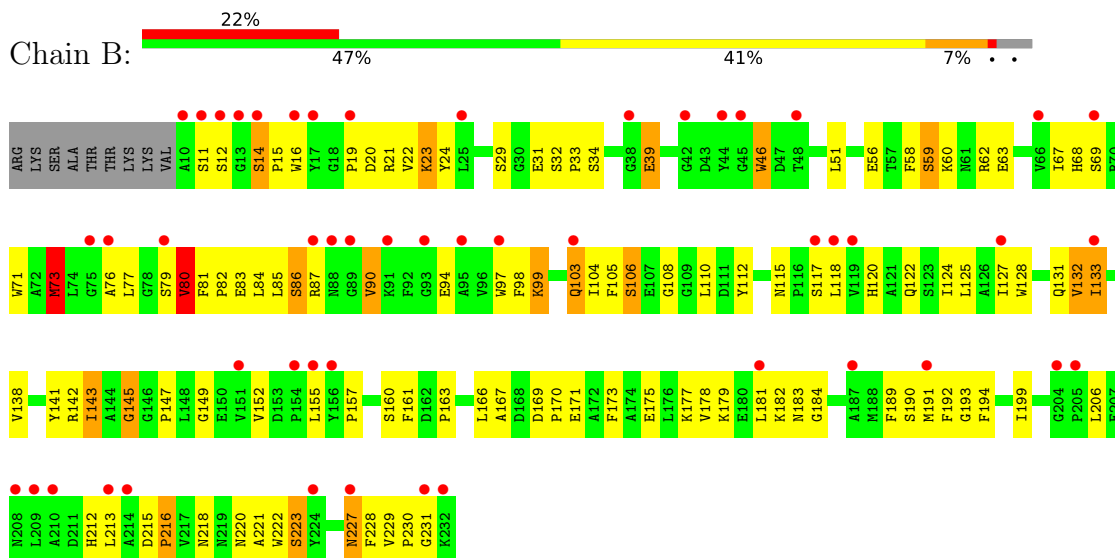
3 Residue-property plots

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 AB80

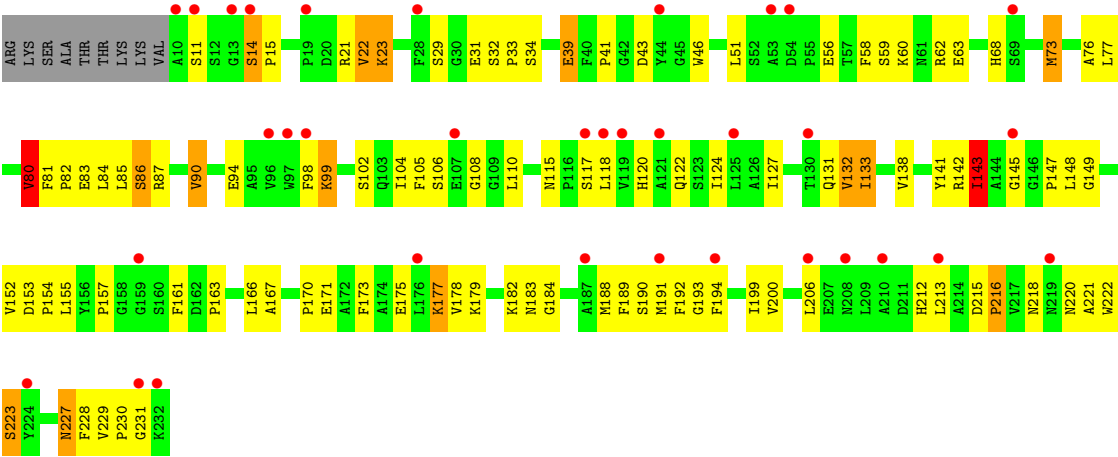


• Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80



• Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.40Å 128.00Å 62.00Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 85.7 (50.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.51Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.220 , 0.241 0.232 , 0.250	Depositor DCC
R_{free} test set	990 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 105.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8373	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.68	1/1735 (0.1%)	1.07	10/2363 (0.4%)
1	B	0.74	1/1735 (0.1%)	1.09	10/2363 (0.4%)
1	C	0.71	1/1735 (0.1%)	1.07	7/2363 (0.3%)
All	All	0.71	3/5205 (0.1%)	1.07	27/7089 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	MET	SD-CE	-8.90	1.57	1.79
1	B	73	MET	SD-CE	-7.88	1.59	1.79
1	A	73	MET	SD-CE	-6.99	1.62	1.79

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	GLY	N-CA-C	-9.39	102.08	111.56
1	A	80	VAL	N-CA-C	7.22	117.83	110.82
1	B	24	TYR	N-CA-C	6.71	120.56	112.38
1	A	145	GLY	N-CA-C	-6.63	103.89	111.85
1	B	145	GLY	N-CA-C	-6.62	103.90	111.85

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	1683	0	1601	128	0
1	B	1683	0	1601	145	0
1	C	1683	0	1601	137	0
2	A	84	0	134	44	0
2	B	84	0	134	45	0
2	C	84	0	134	46	0
3	A	44	0	56	3	0
3	B	44	0	56	3	0
3	C	44	0	56	3	0
4	A	44	0	56	18	0
4	B	44	0	56	16	0
4	C	44	0	56	16	0
5	A	490	0	508	119	0
5	B	490	0	508	139	0
5	C	490	0	508	124	0
6	A	352	0	338	109	0
6	B	352	0	338	109	0
6	C	352	0	338	112	0
7	A	49	0	74	12	0
7	B	49	0	74	13	0
7	C	49	0	74	13	0
8	A	38	0	40	4	0
8	B	38	0	40	2	0
8	C	38	0	40	4	0
9	A	9	0	0	1	0
9	B	7	0	0	1	0
9	C	5	0	0	1	0
All	All	8373	0	8421	964	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 57.

The worst 5 of 964 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:A:220:ASN:HB2	5:A:608:CLA:HED1	1.24	1.14
5:A:607:CLA:H121	5:A:607:CLA:H91	1.29	1.14
5:A:605:CLA:H41	5:C:605:CLA:H51	1.29	1.13
6:A:610:CHL:H92	6:A:612:CHL:H162	1.31	1.12
5:C:602:CLA:H121	5:C:602:CLA:H91	1.21	1.11

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	221/232 (95%)	210 (95%)	10 (4%)	1 (0%)	24	43
1	B	221/232 (95%)	210 (95%)	9 (4%)	2 (1%)	14	27
1	C	221/232 (95%)	208 (94%)	10 (4%)	3 (1%)	9	17
All	All	663/696 (95%)	628 (95%)	29 (4%)	6 (1%)	14	27

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	SER
1	C	14	SER
1	A	216	PRO
1	B	216	PRO
1	C	216	PRO

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	169/181 (93%)	145 (86%)	24 (14%)	3	7
1	B	169/181 (93%)	143 (85%)	26 (15%)	2	5
1	C	169/181 (93%)	146 (86%)	23 (14%)	3	8
All	All	507/543 (93%)	434 (86%)	73 (14%)	3	6

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	62	ARG
1	C	199	ILE
1	C	86	SER
1	C	133	ILE
1	B	11	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	208	ASN
1	C	197	GLN
1	B	197	GLN
1	C	131	GLN
1	B	131	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

60 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	LHG	B	801	5	48,48,48	1.66	6 (12%)	51,54,54	1.37	4 (7%)
6	CHL	A	612	1	70,74,74	1.35	8 (11%)	80,114,114	1.80	12 (15%)
4	XAT	A	504	-	39,47,47	2.21	15 (38%)	54,74,74	2.85	20 (37%)
7	LHG	C	801	5	48,48,48	1.68	6 (12%)	51,54,54	1.33	4 (7%)
5	CLA	B	604	1	69,73,73	1.28	6 (8%)	83,113,113	1.57	13 (15%)
3	NEX	A	503	-	38,46,46	2.32	11 (28%)	50,70,70	2.39	11 (22%)
2	LUX	B	501	-	43,43,43	4.71	25 (58%)	53,60,60	3.60	31 (58%)
5	CLA	B	608	1	52,56,73	1.37	7 (13%)	62,92,113	1.75	13 (20%)
6	CHL	A	610	9	70,74,74	1.42	9 (12%)	80,114,114	1.49	10 (12%)
5	CLA	A	603	1	69,73,73	1.14	7 (10%)	83,113,113	1.62	13 (15%)
5	CLA	B	601	1	69,73,73	1.20	11 (15%)	83,113,113	1.76	17 (20%)
5	CLA	A	608	1	52,56,73	1.52	9 (17%)	62,92,113	1.94	13 (20%)
6	CHL	C	613	-	50,54,74	1.55	8 (16%)	56,90,114	1.72	9 (16%)
5	CLA	B	607	7	69,73,73	1.40	8 (11%)	83,113,113	1.79	13 (15%)
5	CLA	C	601	1	69,73,73	1.34	9 (13%)	83,113,113	1.77	11 (13%)
5	CLA	B	606	-	61,65,73	1.24	8 (13%)	73,103,113	1.66	11 (15%)
5	CLA	A	602	1	64,68,73	1.26	7 (10%)	77,107,113	1.58	9 (11%)
6	CHL	B	609	1	70,74,74	1.40	8 (11%)	80,114,114	1.54	12 (15%)
5	CLA	A	601	1	69,73,73	1.28	8 (11%)	83,113,113	1.70	14 (16%)
2	LUX	B	502	-	43,43,43	4.65	25 (58%)	53,60,60	3.78	31 (58%)
6	CHL	C	609	1	70,74,74	1.38	8 (11%)	80,114,114	1.58	10 (12%)
6	CHL	A	611	9	70,74,74	1.32	9 (12%)	80,114,114	1.79	15 (18%)
5	CLA	B	605	1	69,73,73	1.22	7 (10%)	83,113,113	1.62	9 (10%)
8	DGD	C	802	-	39,39,67	1.41	5 (12%)	51,51,81	1.97	9 (17%)
3	NEX	B	503	-	38,46,46	2.40	10 (26%)	50,70,70	2.53	12 (24%)
5	CLA	A	606	-	61,65,73	1.19	5 (8%)	73,103,113	1.72	11 (15%)
5	CLA	A	605	1	69,73,73	1.17	5 (7%)	83,113,113	1.68	12 (14%)
5	CLA	C	603	1	69,73,73	1.14	7 (10%)	83,113,113	1.62	10 (12%)
5	CLA	C	608	1	52,56,73	1.31	5 (9%)	62,92,113	1.99	12 (19%)
3	NEX	C	503	-	38,46,46	2.25	8 (21%)	50,70,70	2.54	14 (28%)
8	DGD	A	802	-	39,39,67	1.32	4 (10%)	51,51,81	1.95	9 (17%)
6	CHL	B	610	9	70,74,74	1.41	10 (14%)	80,114,114	1.55	12 (15%)
5	CLA	C	604	1	69,73,73	1.11	6 (8%)	83,113,113	1.60	11 (13%)
7	LHG	A	801	5	48,48,48	1.71	6 (12%)	51,54,54	1.35	4 (7%)
6	CHL	B	613	-	50,54,74	1.53	9 (18%)	56,90,114	1.64	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CLA	C	602	1	64,68,73	1.32	7 (10%)	77,107,113	1.63	10 (12%)
5	CLA	C	607	7	69,73,73	1.28	8 (11%)	83,113,113	1.73	12 (14%)
6	CHL	C	611	9	70,74,74	1.33	8 (11%)	80,114,114	1.75	13 (16%)
5	CLA	A	604	1	69,73,73	1.22	7 (10%)	83,113,113	1.53	10 (12%)
2	LUX	A	501	-	43,43,43	4.65	26 (60%)	53,60,60	3.53	30 (56%)
5	CLA	B	603	1	69,73,73	1.17	9 (13%)	83,113,113	1.66	12 (14%)
6	CHL	B	614	1	46,50,74	1.61	7 (15%)	51,85,114	2.19	12 (23%)
6	CHL	A	614	1	46,50,74	1.58	7 (15%)	51,85,114	2.04	11 (21%)
2	LUX	C	502	-	43,43,43	4.52	26 (60%)	53,60,60	3.75	32 (60%)
5	CLA	A	607	7	69,73,73	1.38	9 (13%)	83,113,113	1.75	11 (13%)
5	CLA	B	602	1	64,68,73	1.33	8 (12%)	77,107,113	1.70	12 (15%)
4	XAT	B	504	-	39,47,47	2.20	14 (35%)	54,74,74	2.85	21 (38%)
6	CHL	A	609	1	70,74,74	1.31	7 (10%)	80,114,114	1.56	10 (12%)
6	CHL	A	613	-	50,54,74	1.62	7 (14%)	56,90,114	1.62	8 (14%)
2	LUX	A	502	-	43,43,43	4.59	26 (60%)	53,60,60	3.70	32 (60%)
5	CLA	C	605	1	69,73,73	1.19	8 (11%)	83,113,113	1.66	10 (12%)
2	LUX	C	501	-	43,43,43	4.65	25 (58%)	53,60,60	3.60	31 (58%)
6	CHL	B	612	1	70,74,74	1.34	8 (11%)	80,114,114	1.65	11 (13%)
6	CHL	B	611	9	70,74,74	1.37	7 (10%)	80,114,114	1.81	12 (15%)
6	CHL	C	612	1	70,74,74	1.44	10 (14%)	80,114,114	1.78	13 (16%)
6	CHL	C	614	1	46,50,74	1.60	7 (15%)	51,85,114	2.10	11 (21%)
6	CHL	C	610	9	70,74,74	1.39	10 (14%)	80,114,114	1.57	12 (15%)
8	DGD	B	802	-	39,39,67	1.32	4 (10%)	51,51,81	1.93	10 (19%)
5	CLA	C	606	-	61,65,73	1.24	6 (9%)	73,103,113	1.71	12 (16%)
4	XAT	C	504	-	39,47,47	2.20	13 (33%)	54,74,74	2.64	21 (38%)

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
7	LHG	B	801	5	-	22/53/53/53	-
6	CHL	A	612	1	-	16/41/117/117	-
4	XAT	A	504	-	2/2/12/26	0/31/93/93	0/4/4/4
7	LHG	C	801	5	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	B	604	1	1/1/15/20	12/39/115/115	-
3	NEX	A	503	-	-	2/27/83/83	0/3/3/3
2	LUX	B	501	-	5/5/12/15	11/29/67/67	0/2/2/2
5	CLA	B	608	1	-	7/19/95/115	-
6	CHL	A	610	9	1/1/15/21	15/41/117/117	-
5	CLA	A	603	1	1/1/15/20	13/39/115/115	-
5	CLA	B	601	1	1/1/15/20	12/39/115/115	-
5	CLA	A	608	1	-	6/19/95/115	-
6	CHL	C	613	-	-	0/17/93/117	-
5	CLA	B	607	7	-	16/39/115/115	-
5	CLA	C	601	1	1/1/15/20	14/39/115/115	-
5	CLA	B	606	-	1/1/13/20	11/30/106/115	-
5	CLA	A	602	1	-	13/33/109/115	-
6	CHL	B	609	1	1/1/15/21	16/41/117/117	-
5	CLA	A	601	1	1/1/15/20	13/39/115/115	-
2	LUX	B	502	-	5/5/12/15	11/29/67/67	0/2/2/2
6	CHL	C	609	1	1/1/15/21	15/41/117/117	-
6	CHL	A	611	9	1/1/15/21	16/41/117/117	-
5	CLA	B	605	1	1/1/15/20	11/39/115/115	-
8	DGD	C	802	-	1/1/11/13	16/24/64/95	0/2/2/2
3	NEX	B	503	-	-	2/27/83/83	0/3/3/3
5	CLA	A	606	-	1/1/13/20	10/30/106/115	-
5	CLA	A	605	1	1/1/15/20	11/39/115/115	-
5	CLA	C	603	1	1/1/15/20	13/39/115/115	-
5	CLA	C	608	1	-	6/19/95/115	-
3	NEX	C	503	-	-	2/27/83/83	0/3/3/3
8	DGD	A	802	-	1/1/11/13	16/24/64/95	0/2/2/2
6	CHL	B	610	9	1/1/15/21	14/41/117/117	-
5	CLA	C	604	1	1/1/15/20	15/39/115/115	-
7	LHG	A	801	5	-	22/53/53/53	-
6	CHL	C	611	9	1/1/15/21	16/41/117/117	-
5	CLA	C	602	1	-	13/33/109/115	-
5	CLA	C	607	7	-	15/39/115/115	-
6	CHL	B	613	-	-	1/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	A	604	1	1/1/15/20	12/39/115/115	-
2	LUX	A	501	-	5/5/12/15	11/29/67/67	0/2/2/2
5	CLA	B	603	1	1/1/15/20	12/39/115/115	-
6	CHL	B	614	1	-	0/12/88/117	-
6	CHL	A	614	1	-	0/12/88/117	-
2	LUX	C	502	-	5/5/12/15	10/29/67/67	0/2/2/2
5	CLA	A	607	7	-	17/39/115/115	-
5	CLA	B	602	1	-	13/33/109/115	-
4	XAT	B	504	-	2/2/12/26	2/31/93/93	0/4/4/4
6	CHL	A	609	1	1/1/15/21	18/41/117/117	-
6	CHL	A	613	-	-	0/17/93/117	-
2	LUX	A	502	-	5/5/12/15	10/29/67/67	0/2/2/2
5	CLA	C	605	1	1/1/15/20	11/39/115/115	-
2	LUX	C	501	-	5/5/12/15	11/29/67/67	0/2/2/2
6	CHL	B	612	1	-	14/41/117/117	-
6	CHL	B	611	9	1/1/15/21	17/41/117/117	-
6	CHL	C	612	1	-	16/41/117/117	-
6	CHL	C	614	1	-	1/12/88/117	-
6	CHL	C	610	9	1/1/15/21	14/41/117/117	-
8	DGD	B	802	-	1/1/11/13	17/24/64/95	0/2/2/2
5	CLA	C	606	-	1/1/13/20	11/30/106/115	-
4	XAT	C	504	-	2/2/12/26	2/31/93/93	0/4/4/4

The worst 5 of 579 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	LUX	C24-C25	19.56	1.57	1.33
2	B	502	LUX	C24-C25	18.51	1.56	1.33
2	A	501	LUX	C24-C25	18.34	1.56	1.33
2	B	501	LUX	C24-C25	18.20	1.55	1.33
2	A	502	LUX	C24-C25	18.19	1.55	1.33

The worst 5 of 808 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LUX	C27-C26-C25	12.98	136.38	111.96
2	C	501	LUX	C27-C26-C25	12.57	135.60	111.96
2	B	502	LUX	C27-C26-C25	12.25	135.00	111.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	LUX	C27-C26-C25	12.24	134.99	111.96
2	A	502	LUX	C27-C26-C25	12.02	134.56	111.96

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	LUX	C29
2	A	501	LUX	C26
2	A	501	LUX	C13
2	A	501	LUX	C9
2	A	501	LUX	C33

5 of 665 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LUX	C11-C10-C9-C19
2	A	501	LUX	C11-C12-C13-C20
2	A	501	LUX	C20-C13-C14-C15
2	A	501	LUX	C25-C26-C27-C28
2	A	501	LUX	C27-C28-C29-C39

There are no ring outliers.

60 monomers are involved in 769 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	801	LHG	13	0
6	A	612	CHL	17	0
4	A	504	XAT	18	0
7	C	801	LHG	13	0
5	B	604	CLA	22	0
3	A	503	NEX	3	0
2	B	501	LUX	29	0
5	B	608	CLA	21	0
6	A	610	CHL	30	0
5	A	603	CLA	13	0
5	B	601	CLA	24	0
5	A	608	CLA	13	0
6	C	613	CHL	5	0
5	B	607	CLA	17	0
5	C	601	CLA	23	0
5	B	606	CLA	18	0
5	A	602	CLA	12	0

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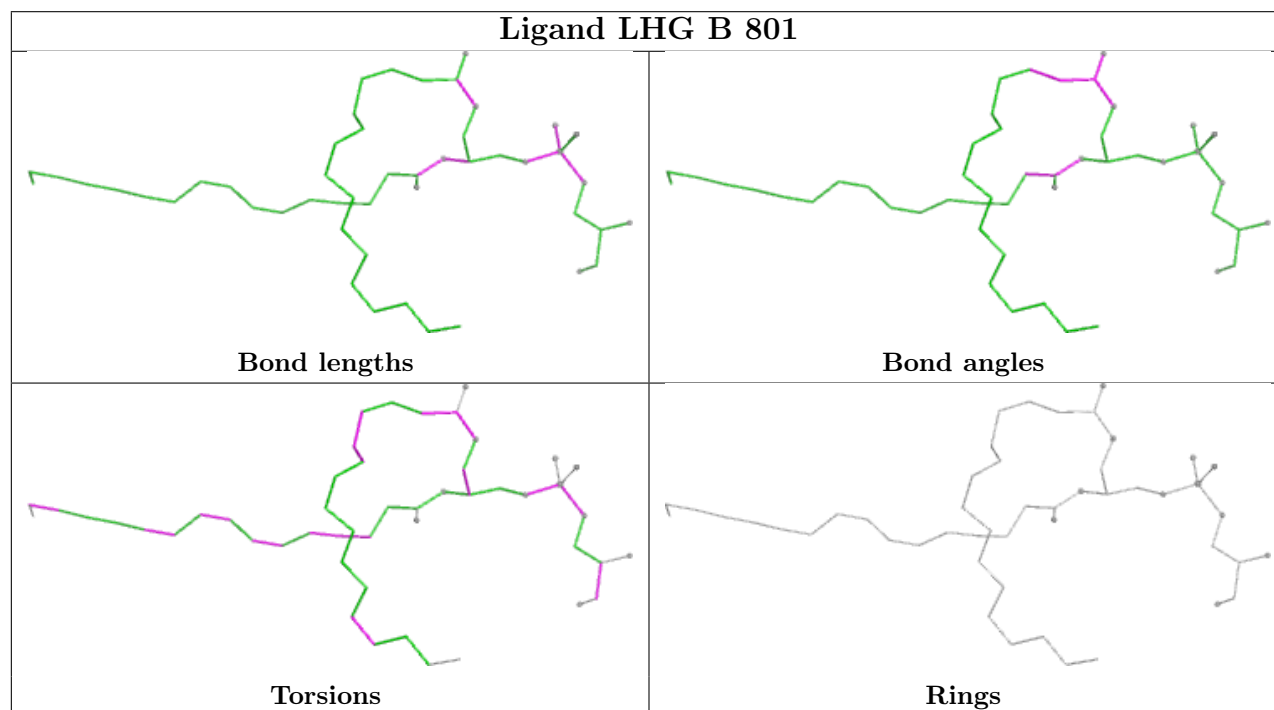
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	609	CHL	27	0
5	A	601	CLA	20	0
2	B	502	LUX	16	0
6	C	609	CHL	30	0
6	A	611	CHL	20	0
5	B	605	CLA	23	0
8	C	802	DGD	4	0
3	B	503	NEX	3	0
5	A	606	CLA	17	0
5	A	605	CLA	20	0
5	C	603	CLA	13	0
5	C	608	CLA	15	0
3	C	503	NEX	3	0
8	A	802	DGD	4	0
6	B	610	CHL	29	0
5	C	604	CLA	18	0
7	A	801	LHG	12	0
6	B	613	CHL	9	0
5	C	602	CLA	10	0
5	C	607	CLA	19	0
6	C	611	CHL	22	0
5	A	604	CLA	19	0
2	A	501	LUX	25	0
5	B	603	CLA	22	0
6	B	614	CHL	14	0
6	A	614	CHL	14	0
2	C	502	LUX	19	0
5	A	607	CLA	16	0
5	B	602	CLA	11	0
4	B	504	XAT	16	0
6	A	609	CHL	31	0
6	A	613	CHL	6	0
2	A	502	LUX	19	0
5	C	605	CLA	20	0
2	C	501	LUX	27	0
6	B	612	CHL	21	0
6	B	611	CHL	21	0
6	C	612	CHL	21	0
6	C	614	CHL	13	0
6	C	610	CHL	31	0
8	B	802	DGD	2	0
5	C	606	CLA	18	0

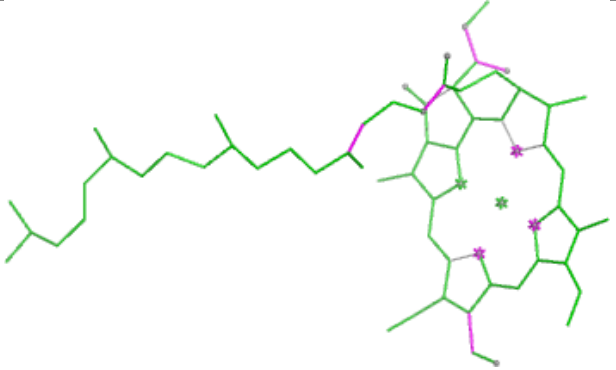
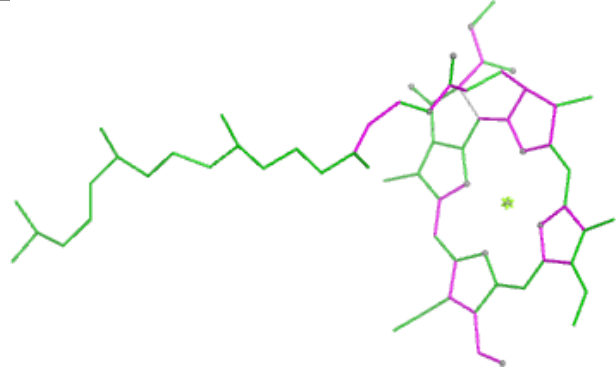
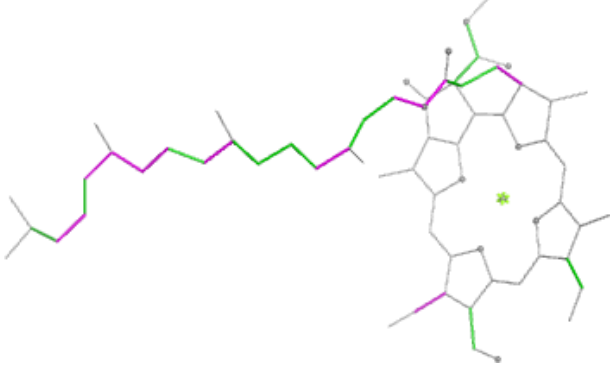
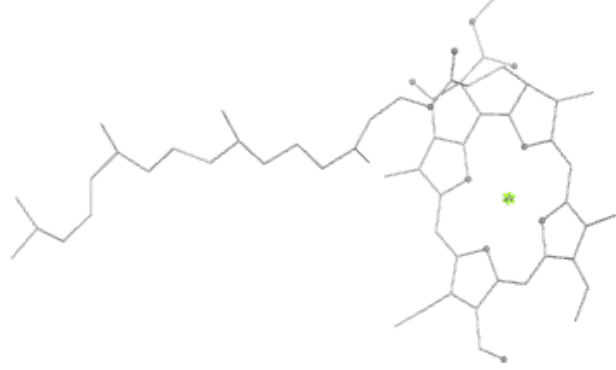
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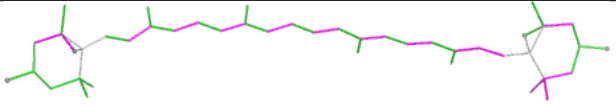
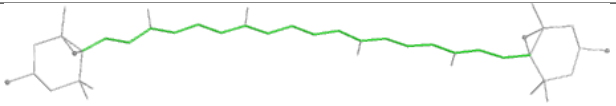
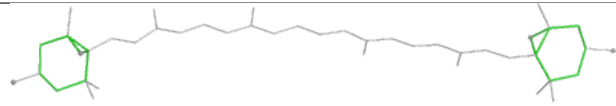
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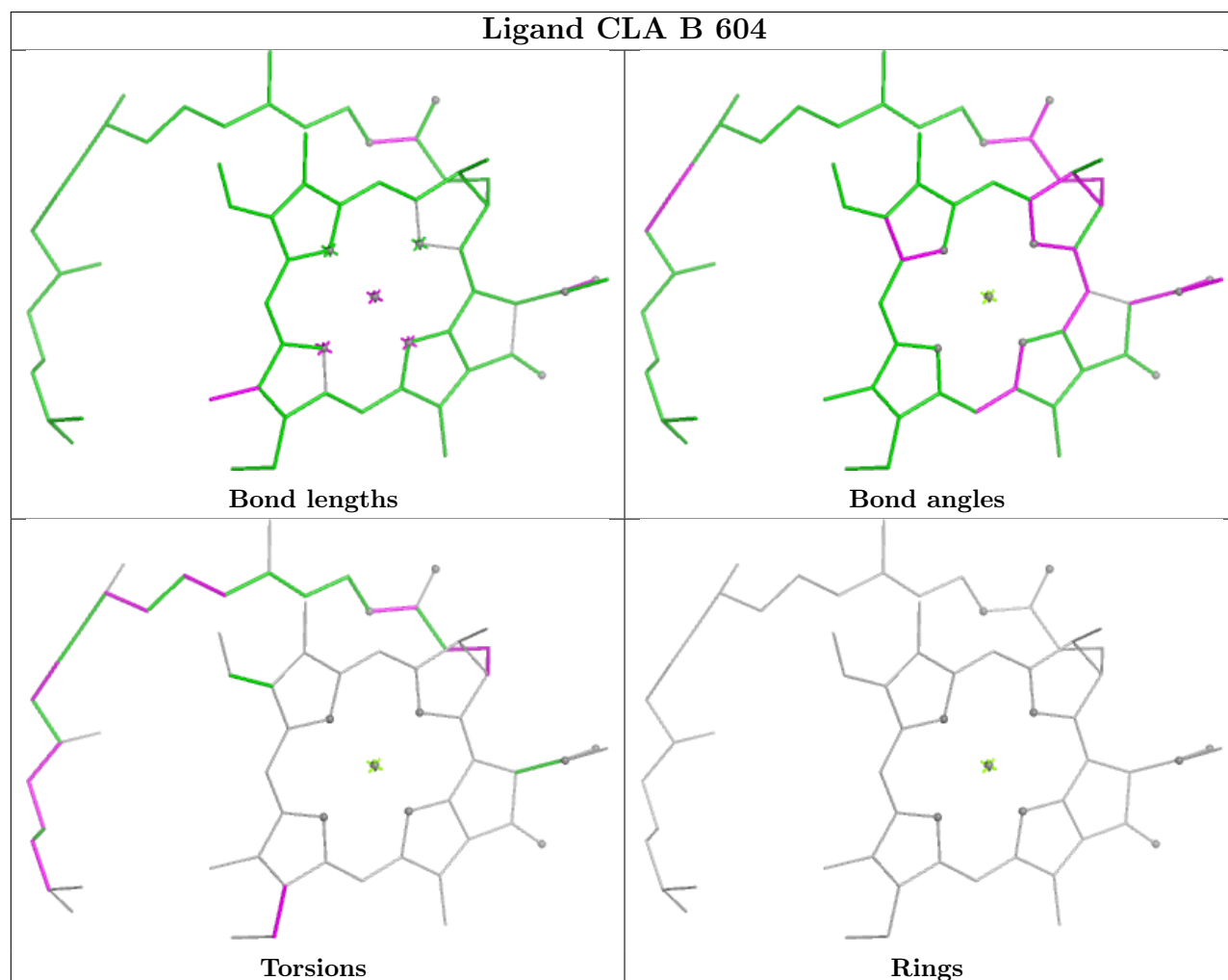
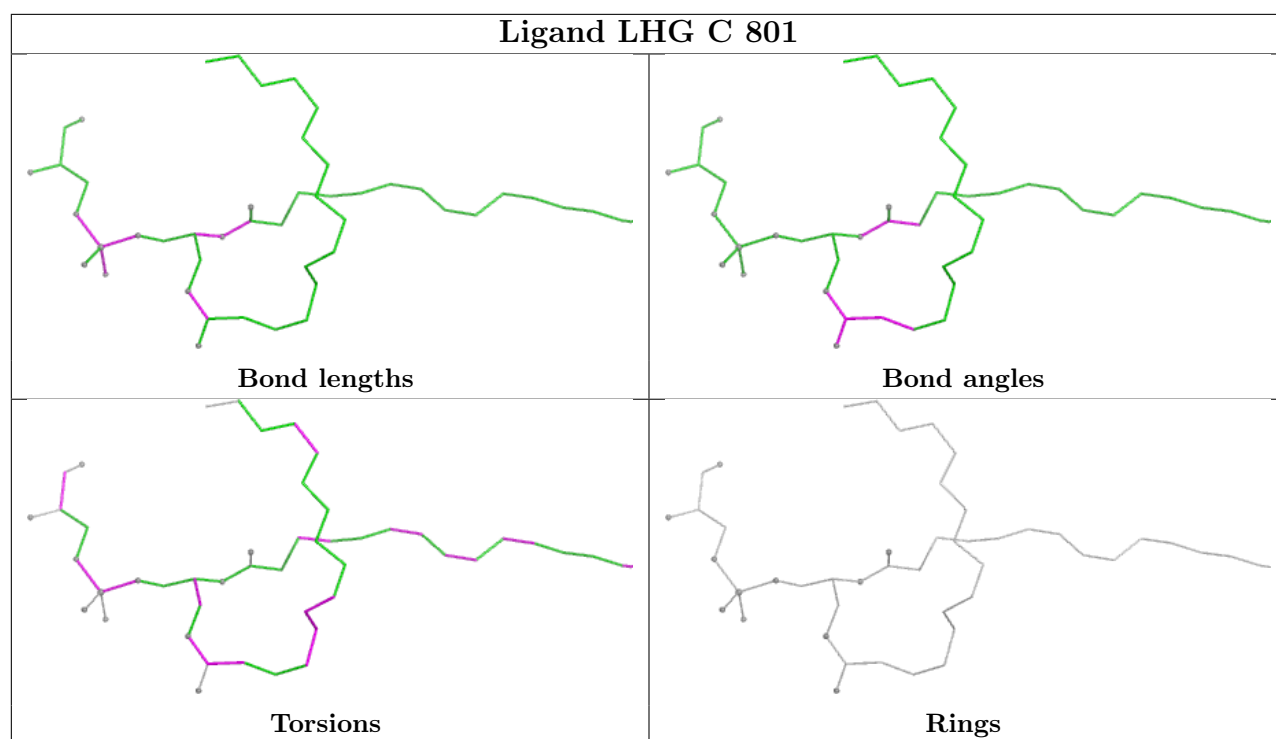
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	XAT	16	0

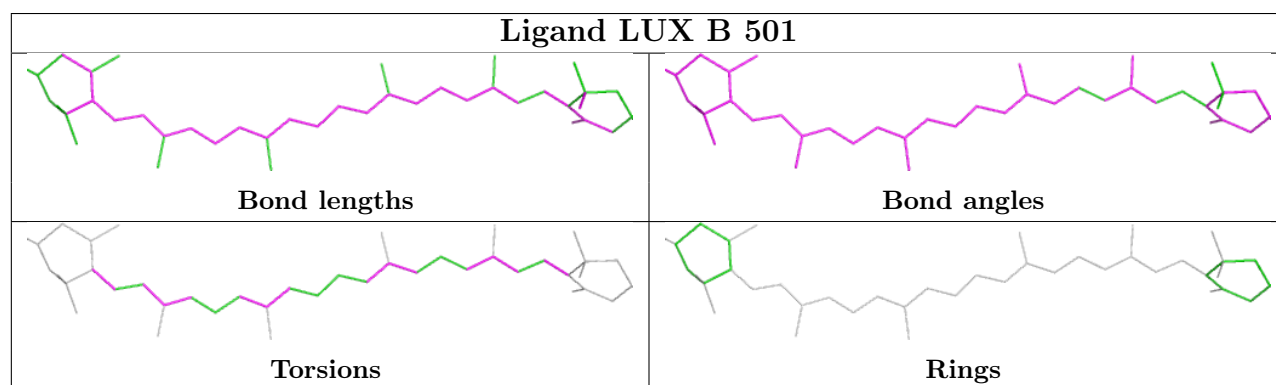
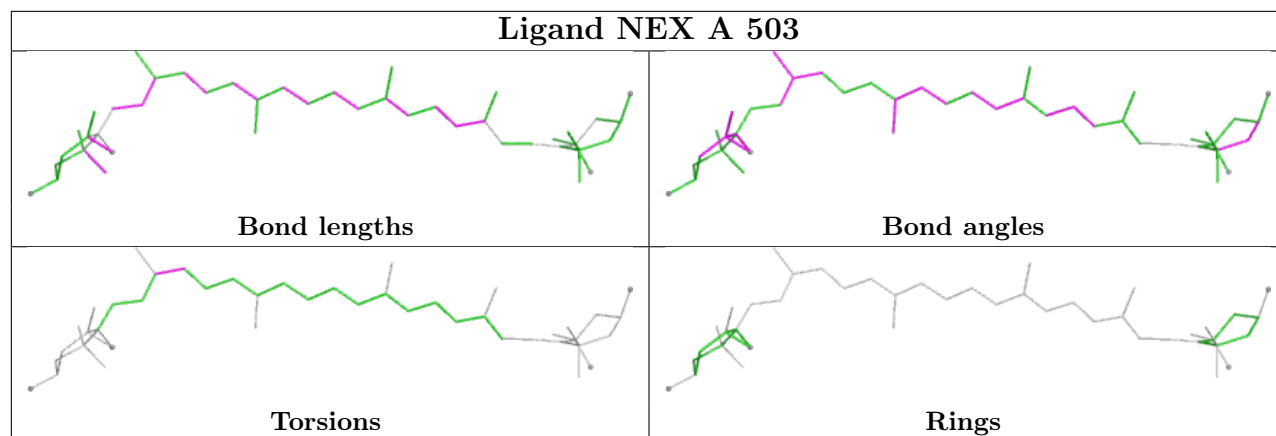
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



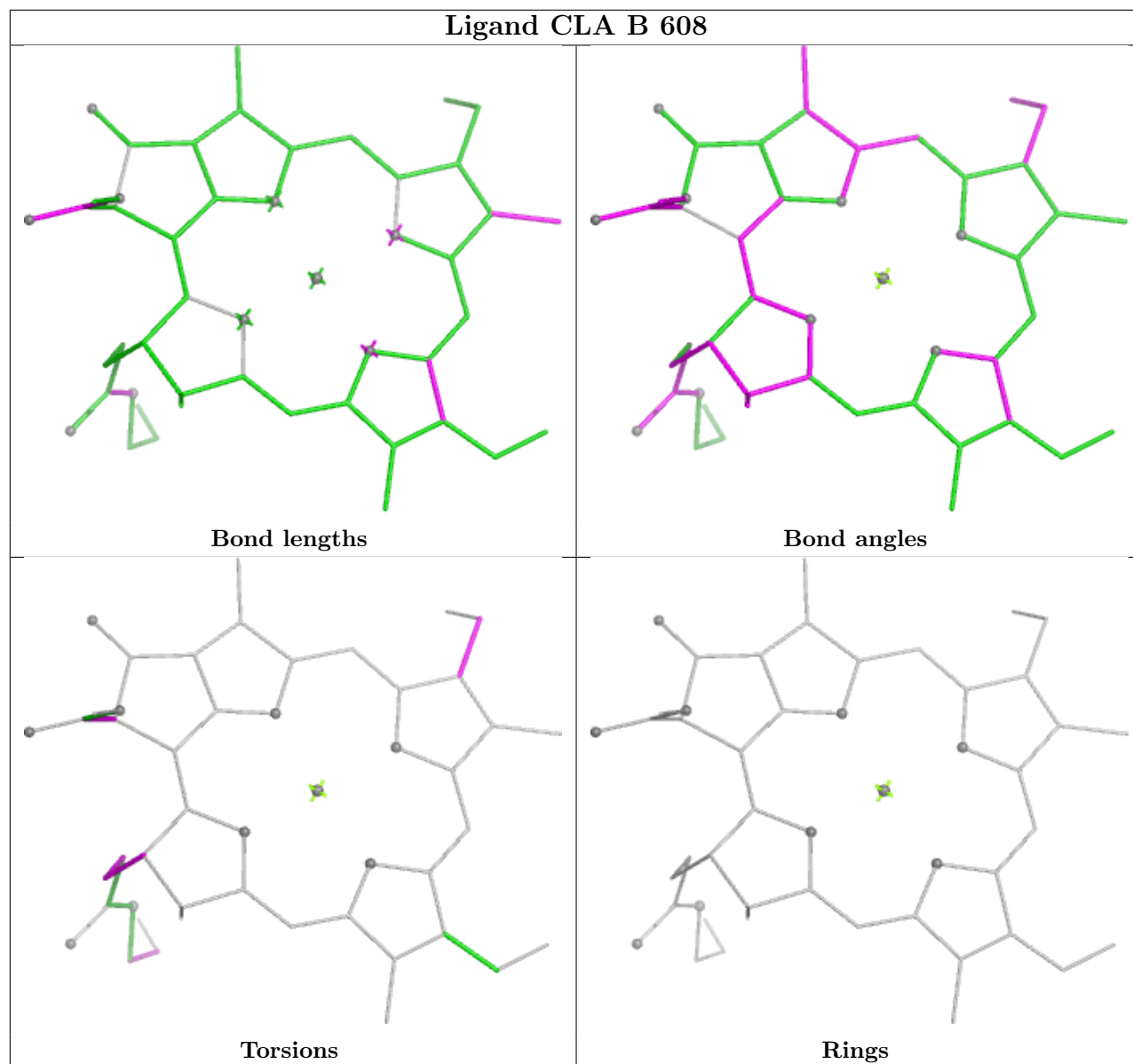
Ligand CHL A 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

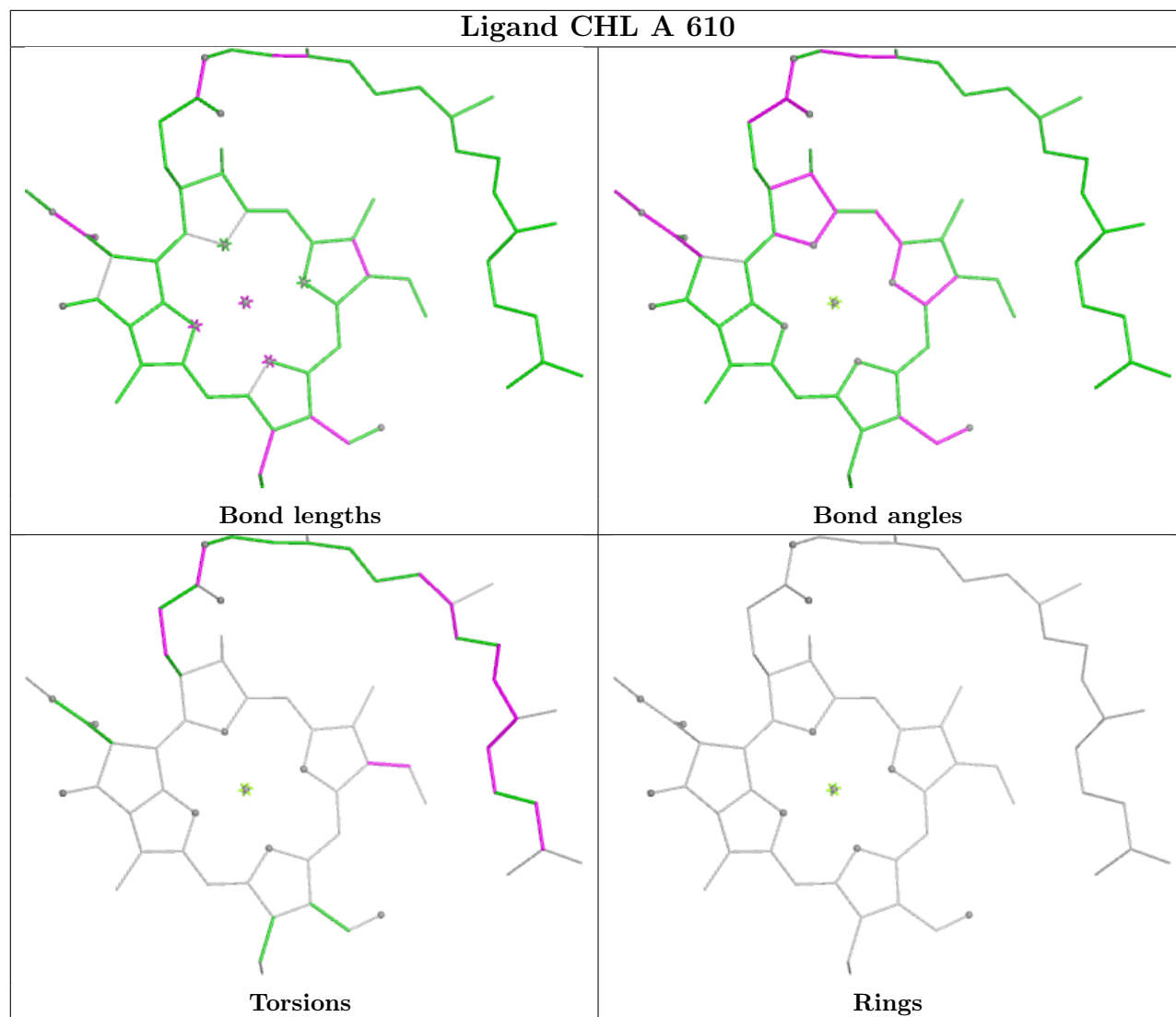
Ligand XAT A 504	
	
Bond lengths	Bond angles
	
Torsions	Rings



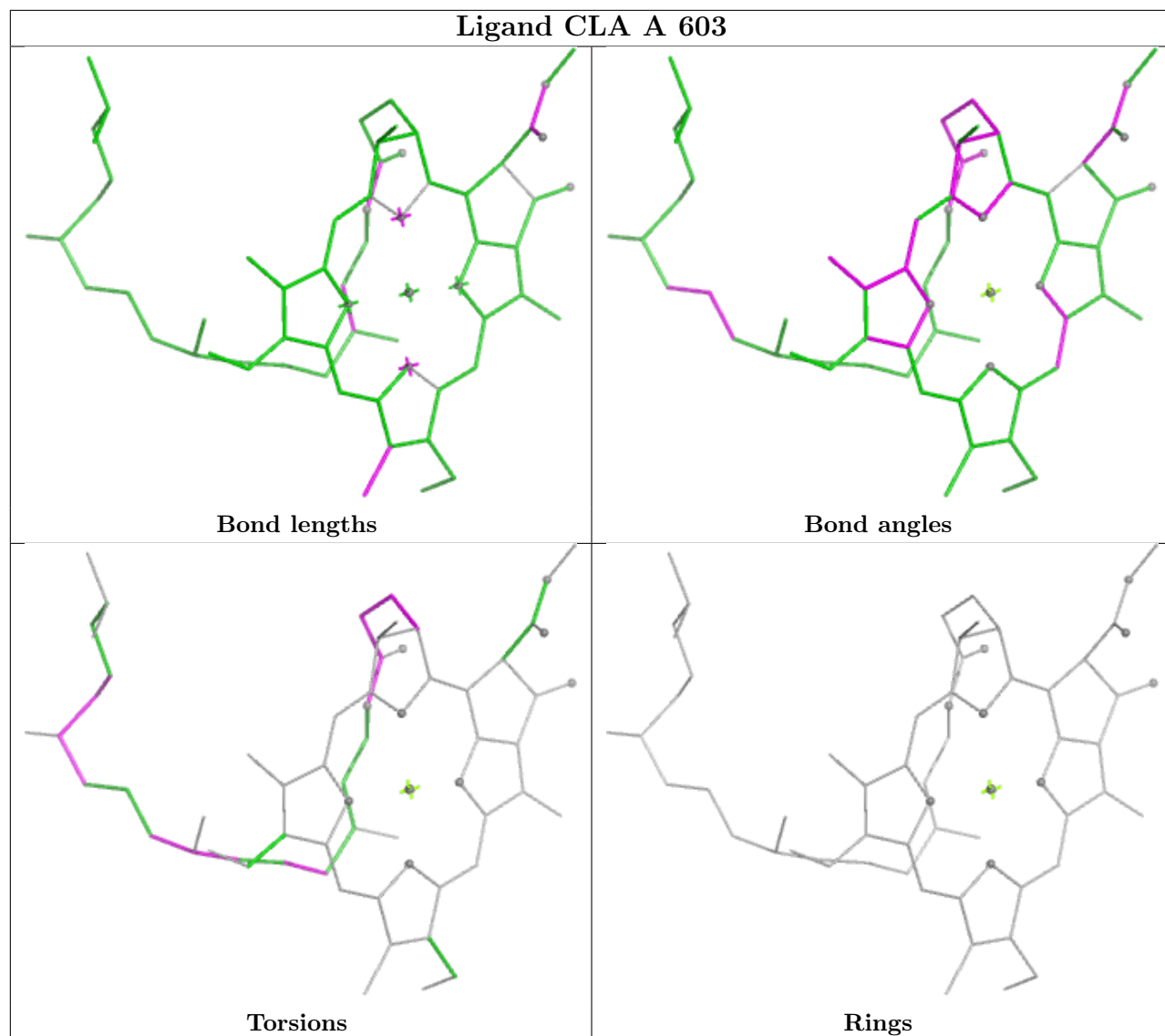


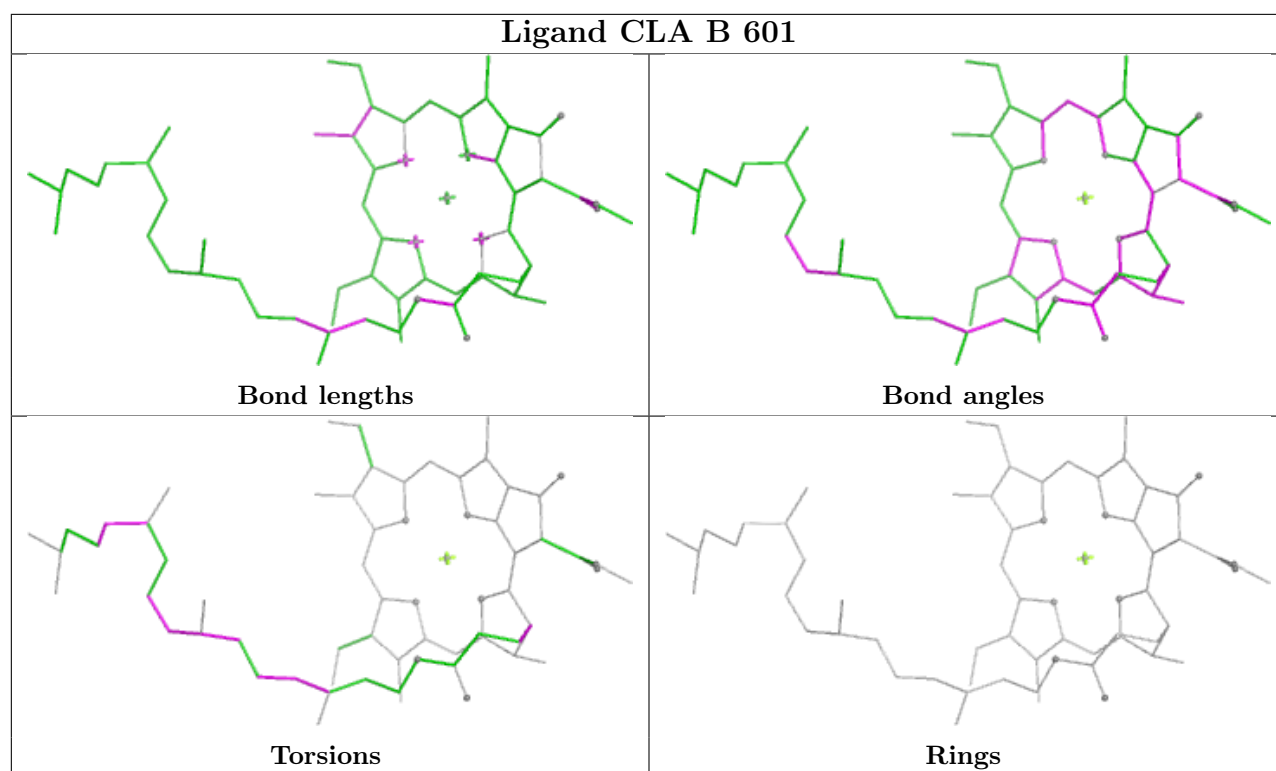
Ligand CLA B 608



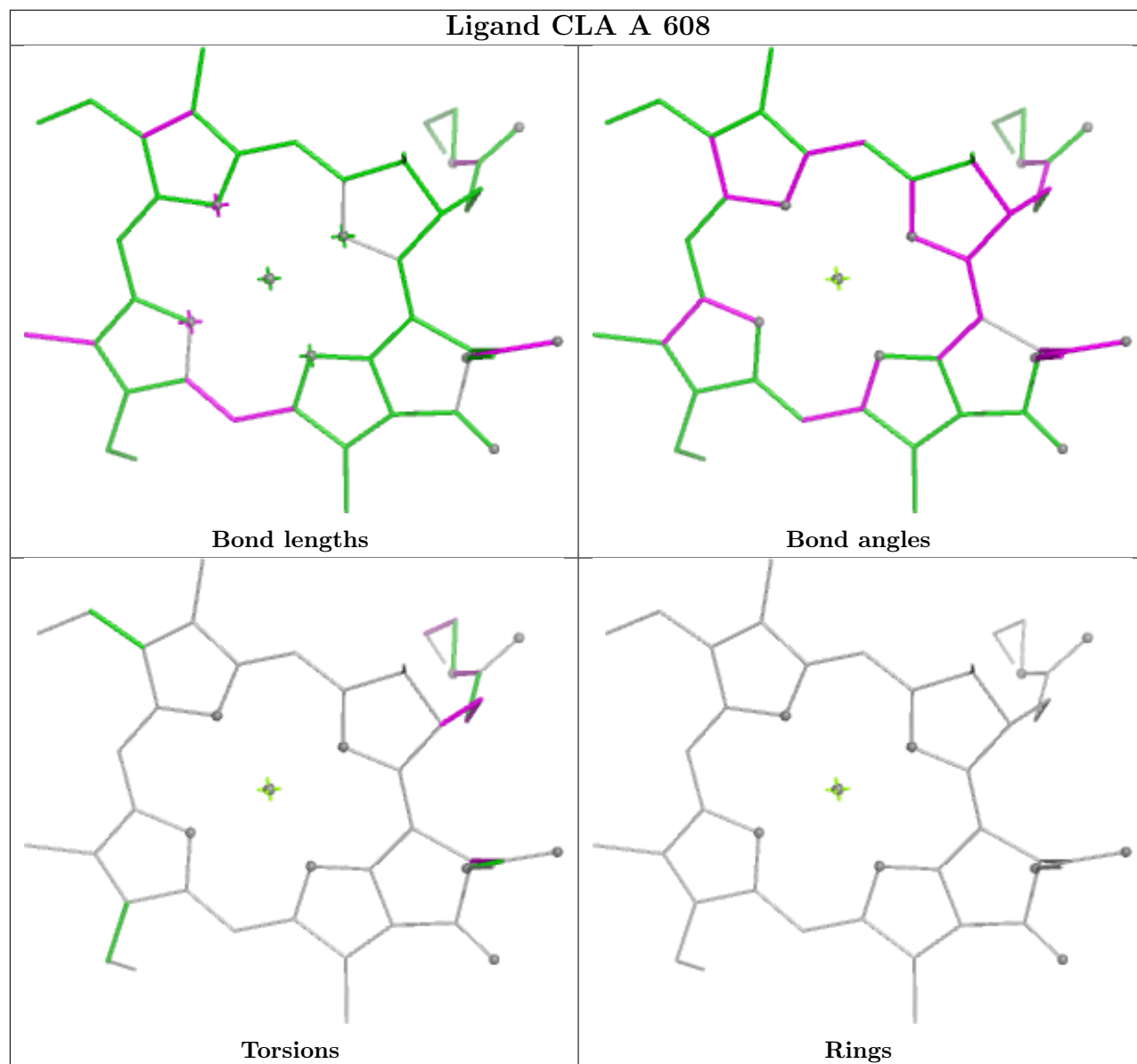


Ligand CLA A 603

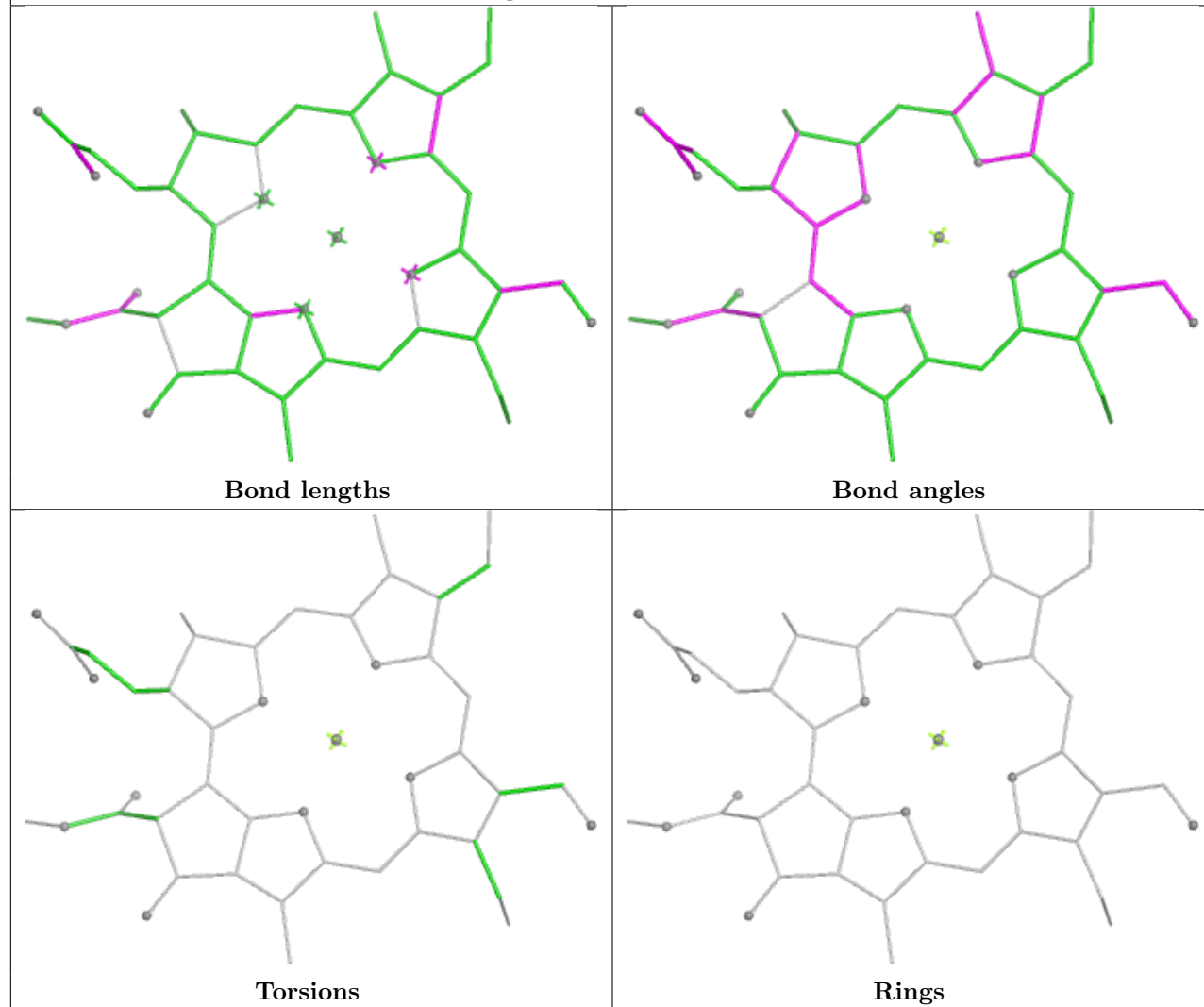


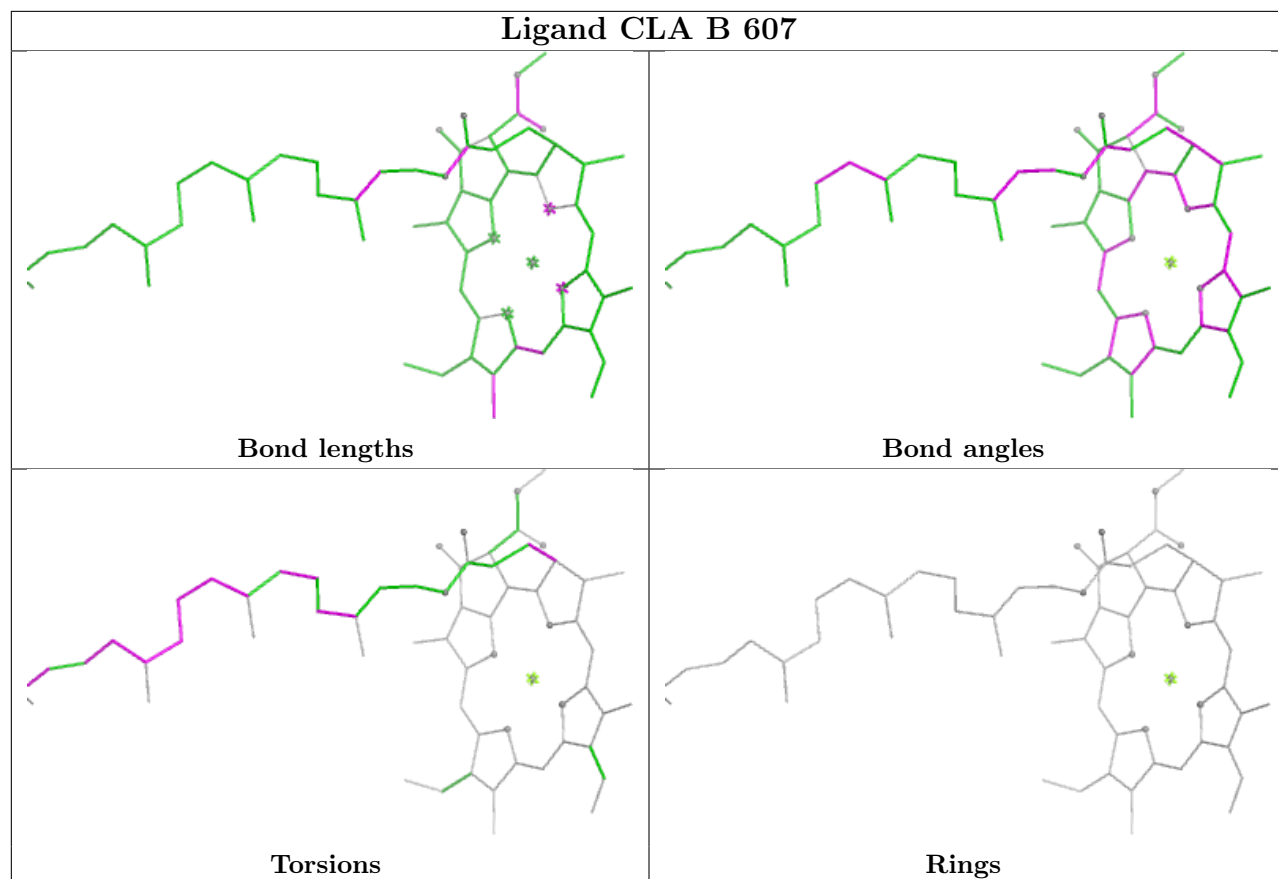
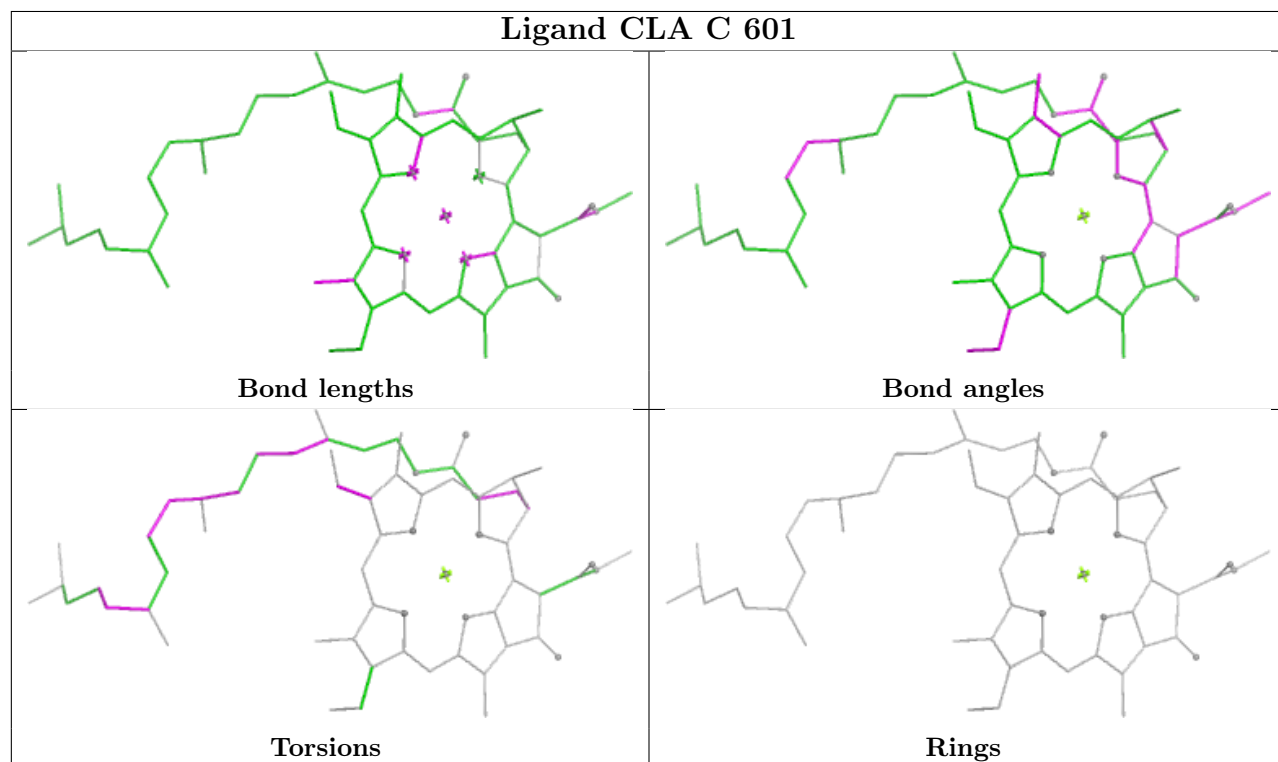


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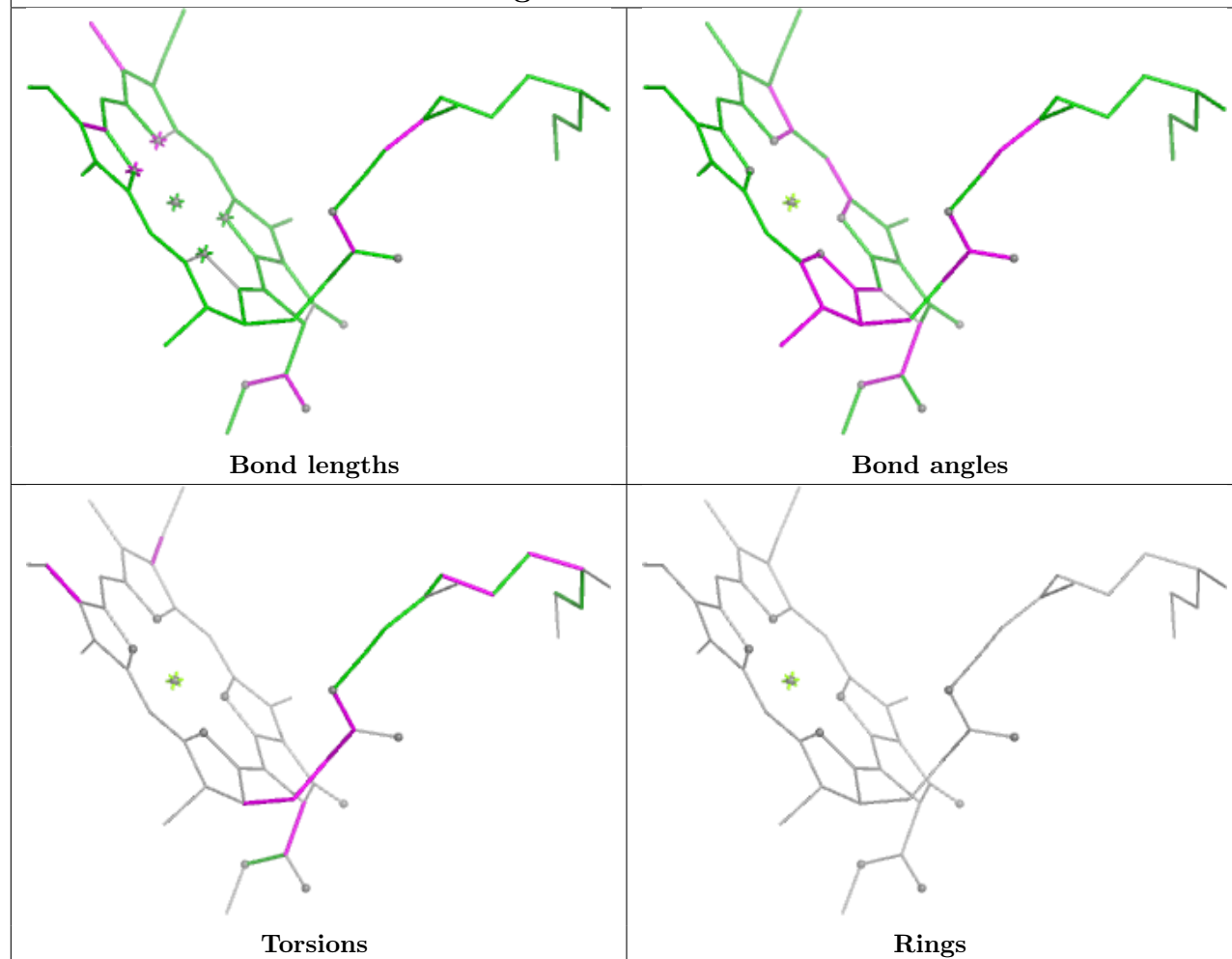


Ligand CHL C 613

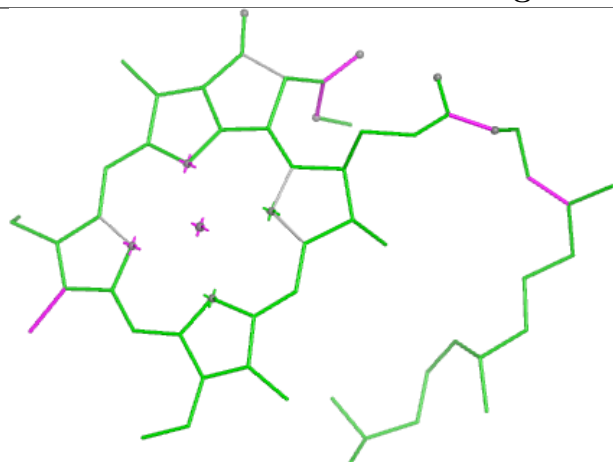


Ligand CLA B 607**Ligand CLA C 601**

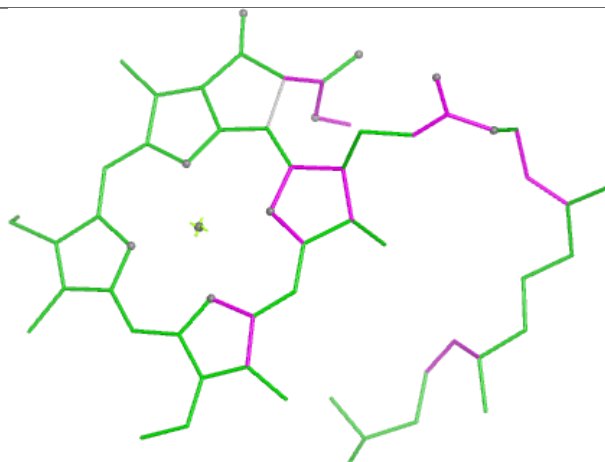
Ligand CLA B 606



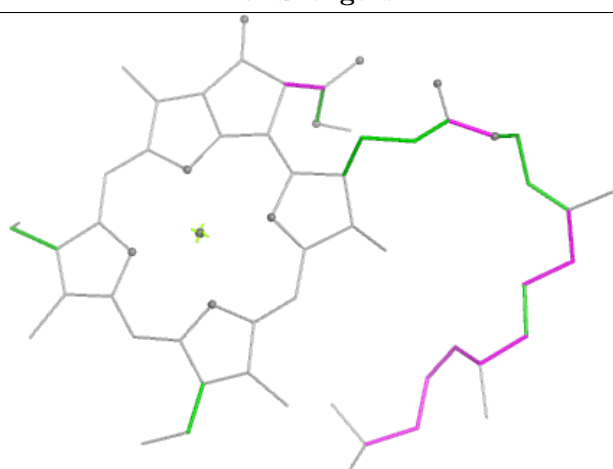
Ligand CLA A 602



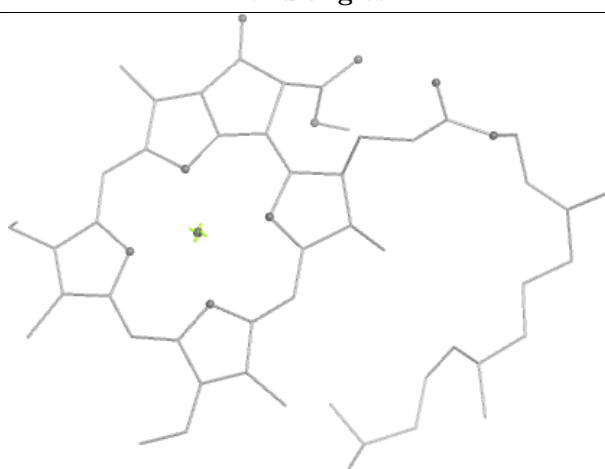
Bond lengths



Bond angles

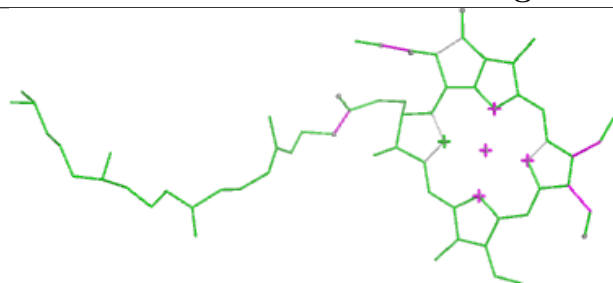


Torsions

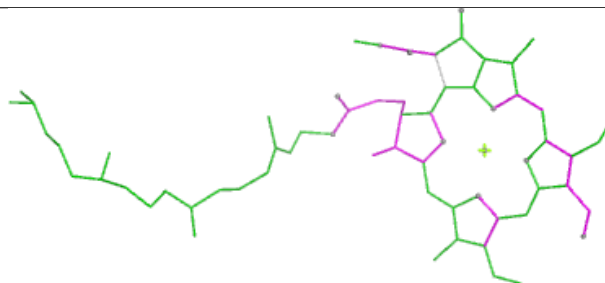


Rings

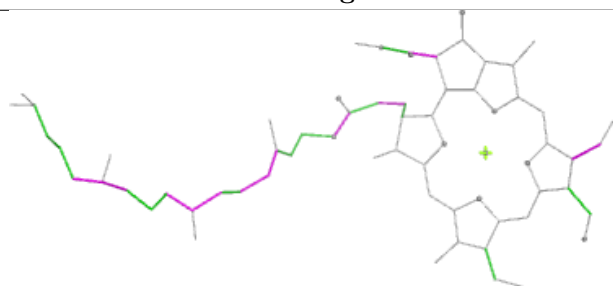
Ligand CHL B 609



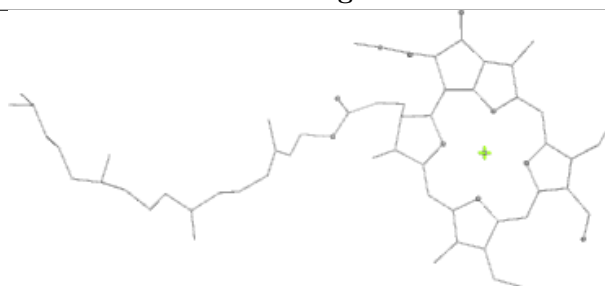
Bond lengths



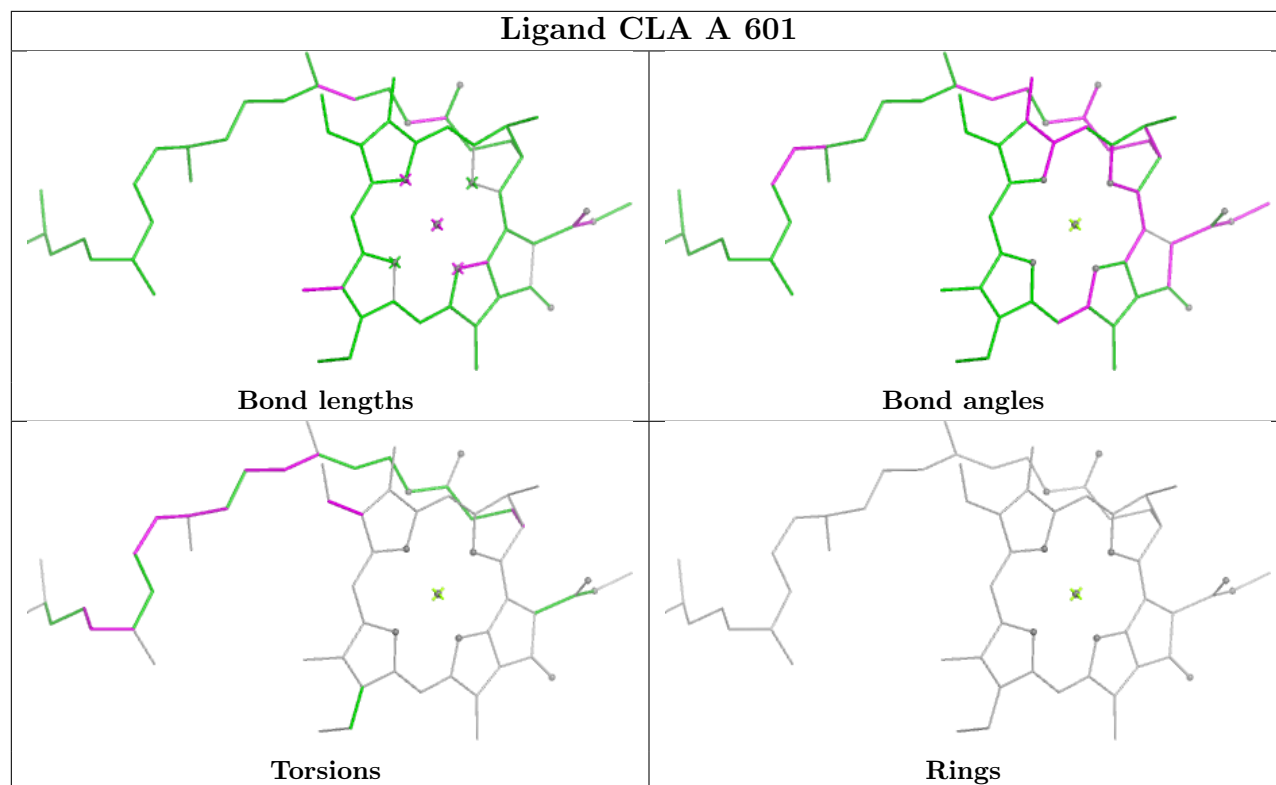
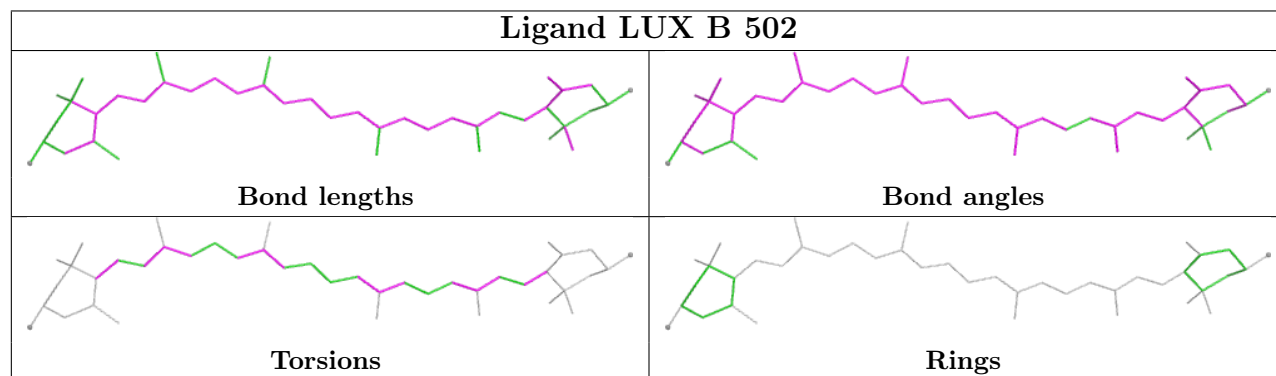
Bond angles

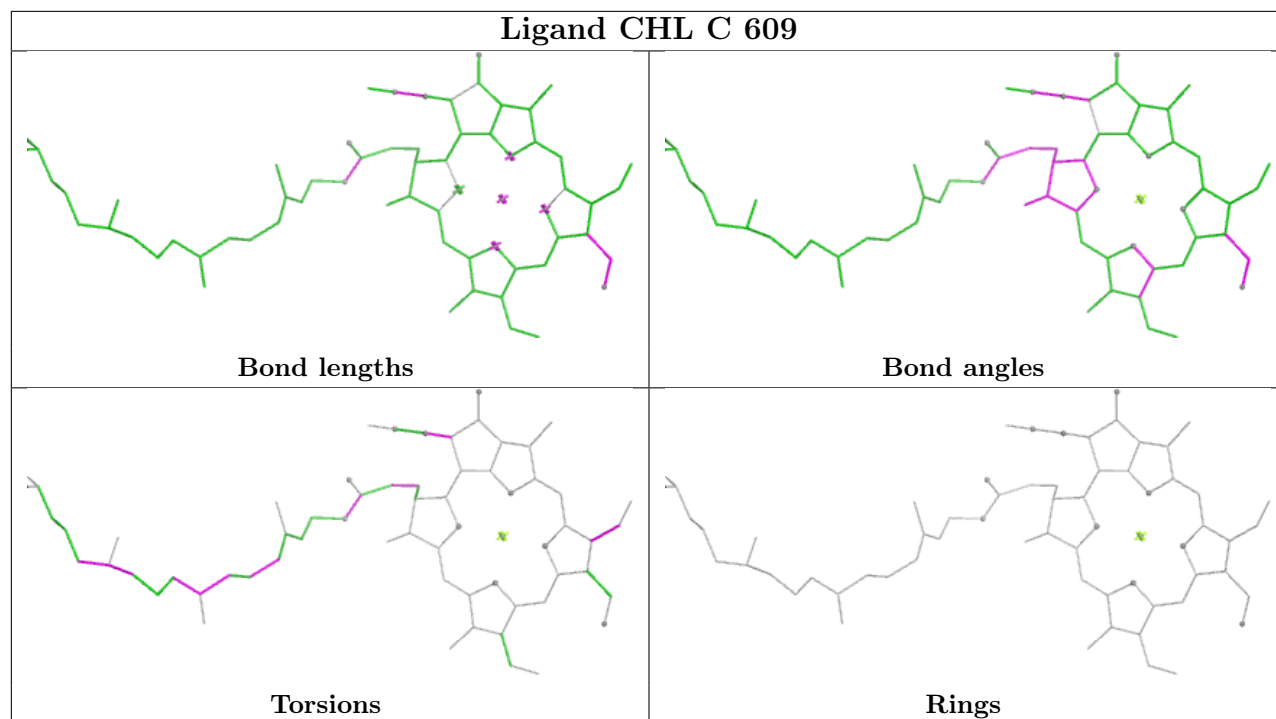


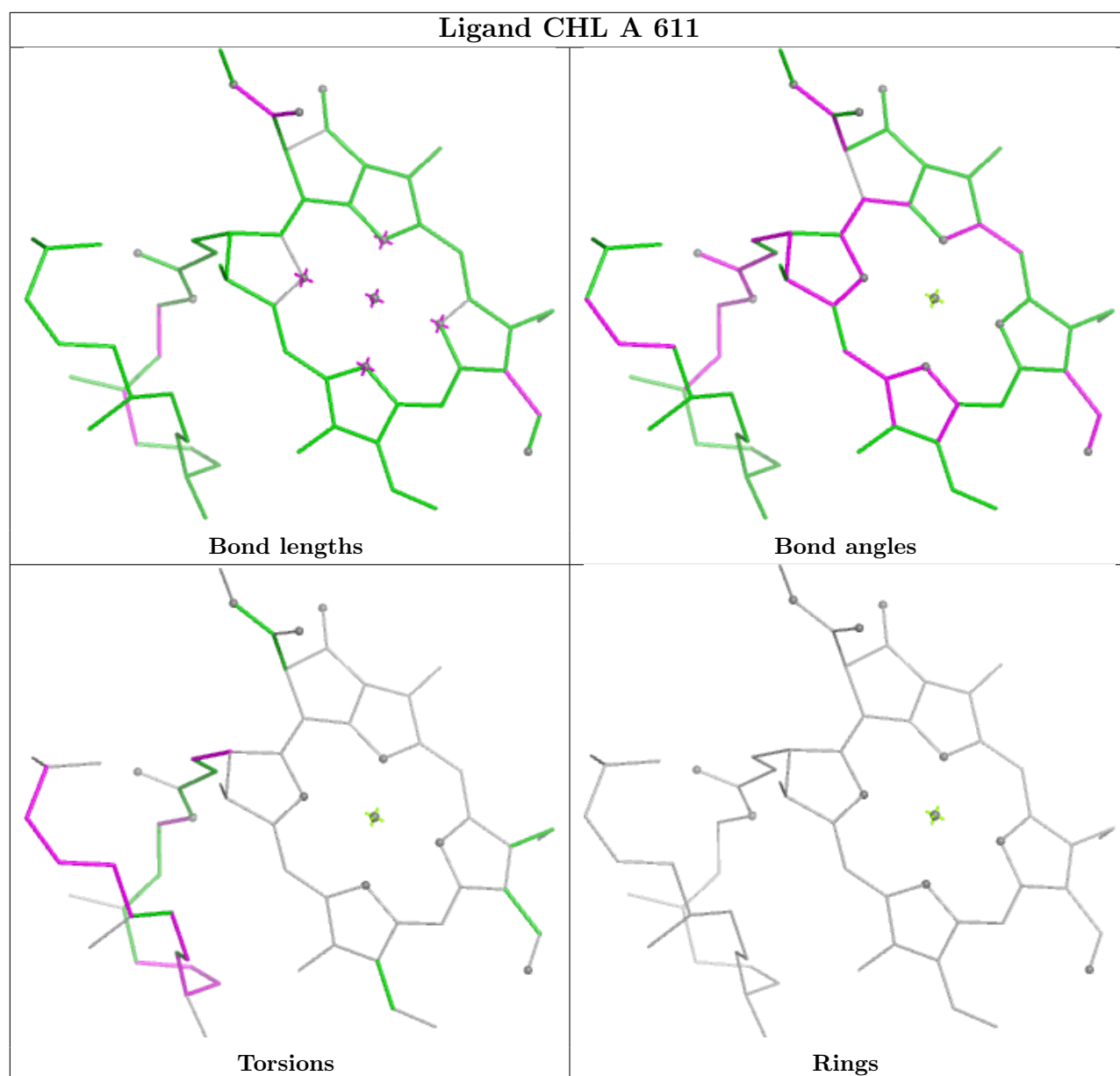
Torsions



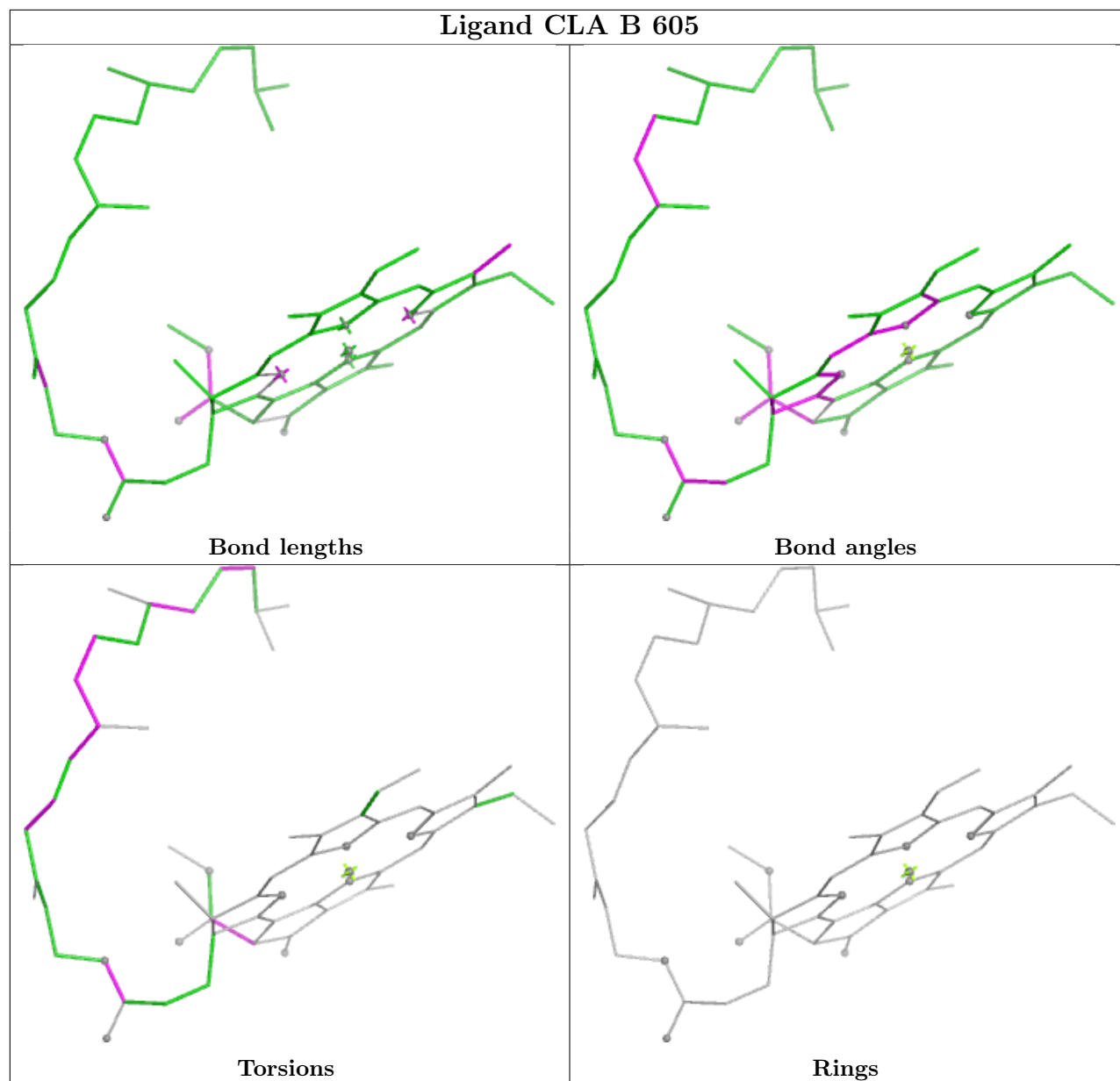
Rings

Ligand CLA A 601**Ligand LUX B 502**

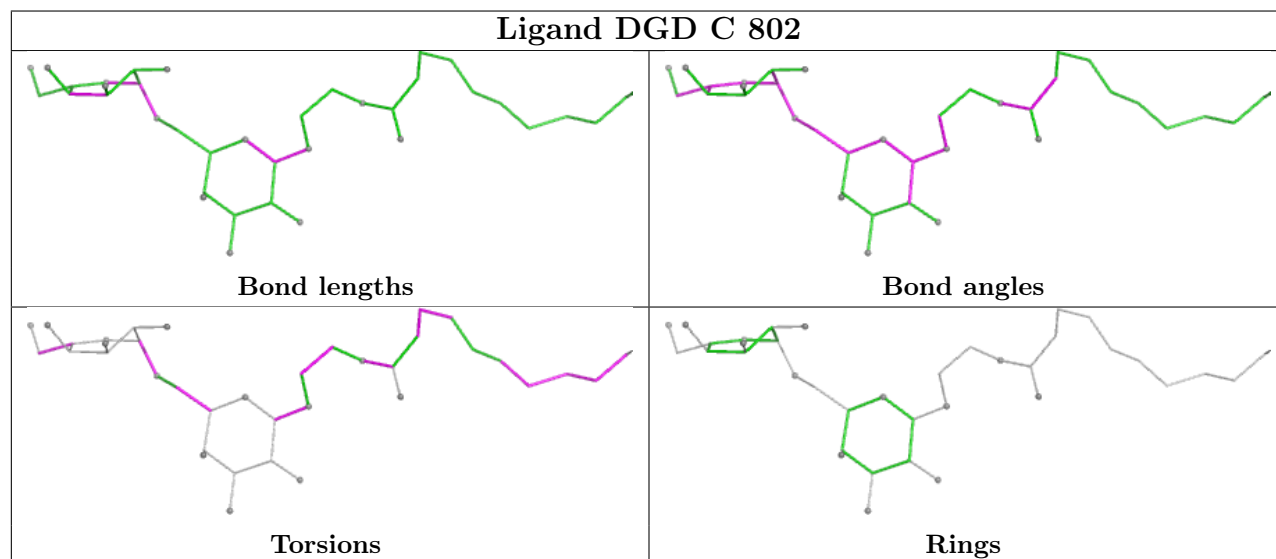


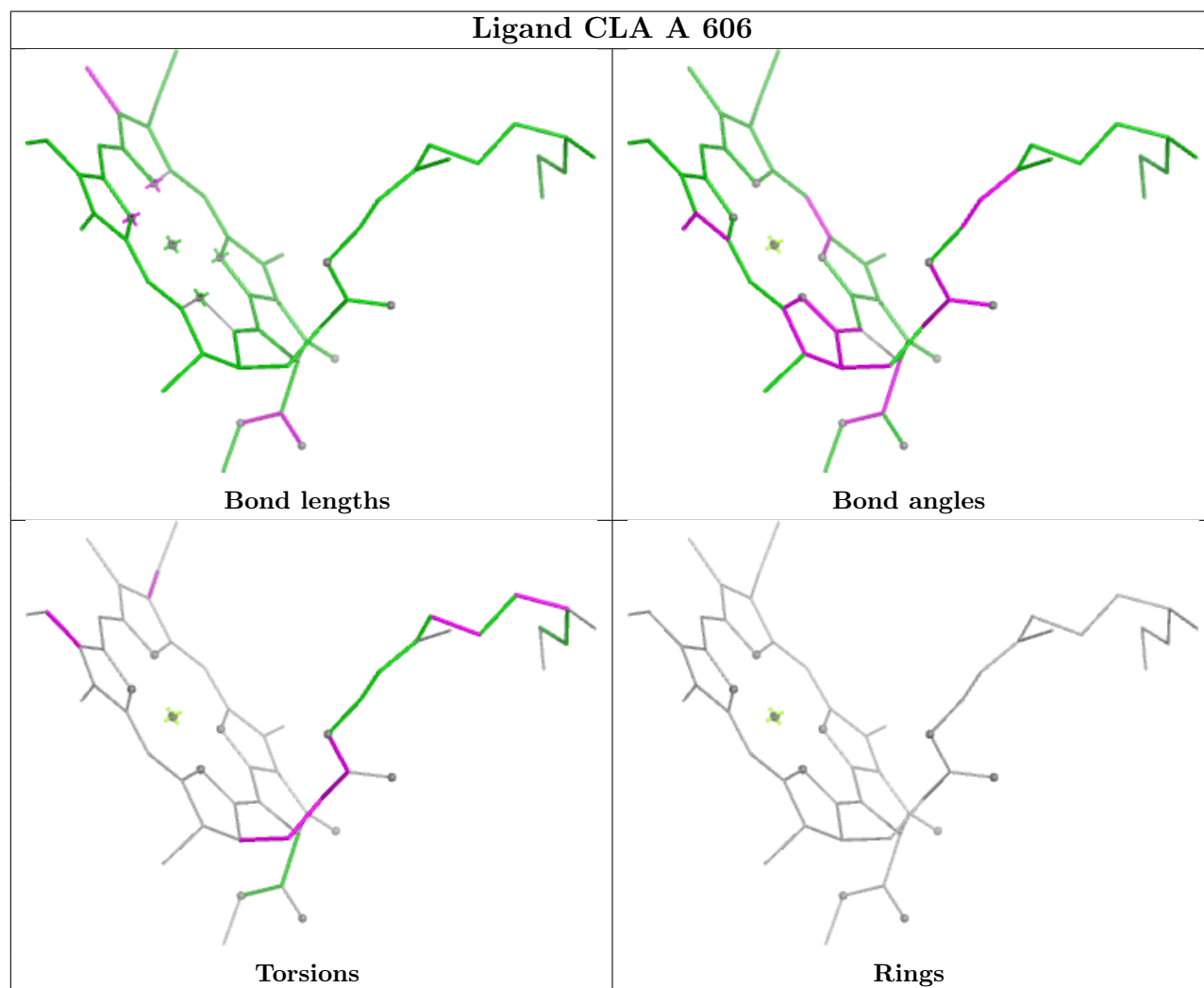
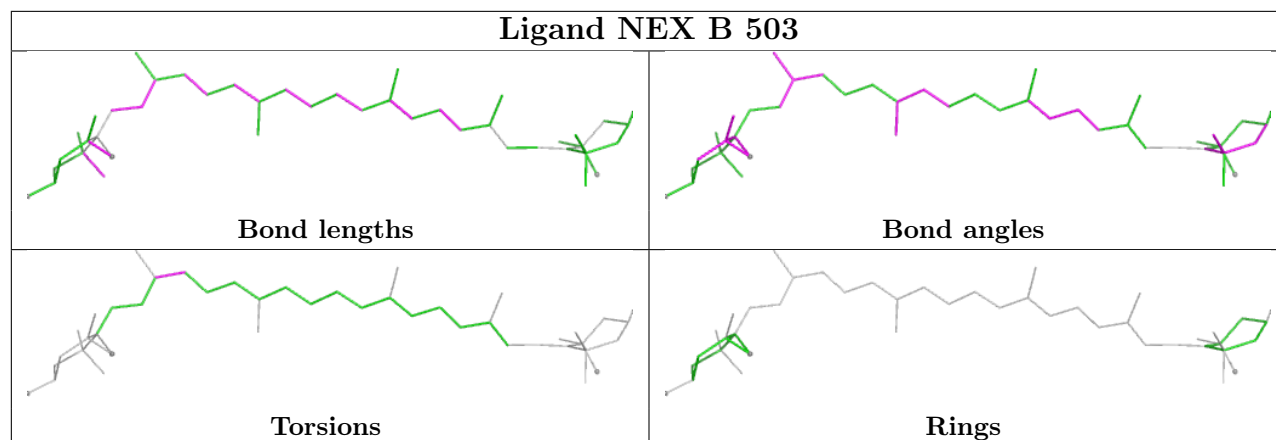


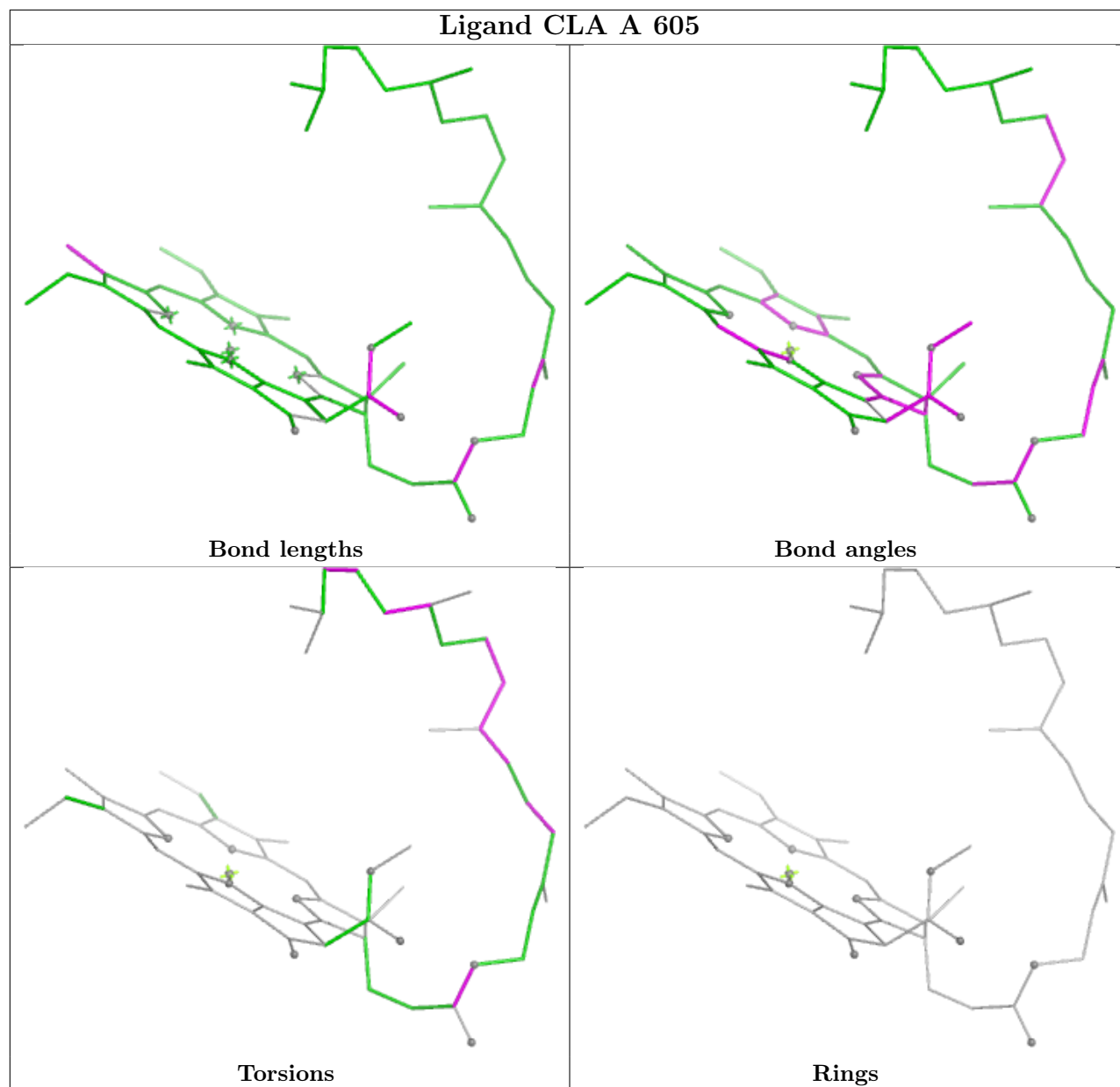
Ligand CLA B 605



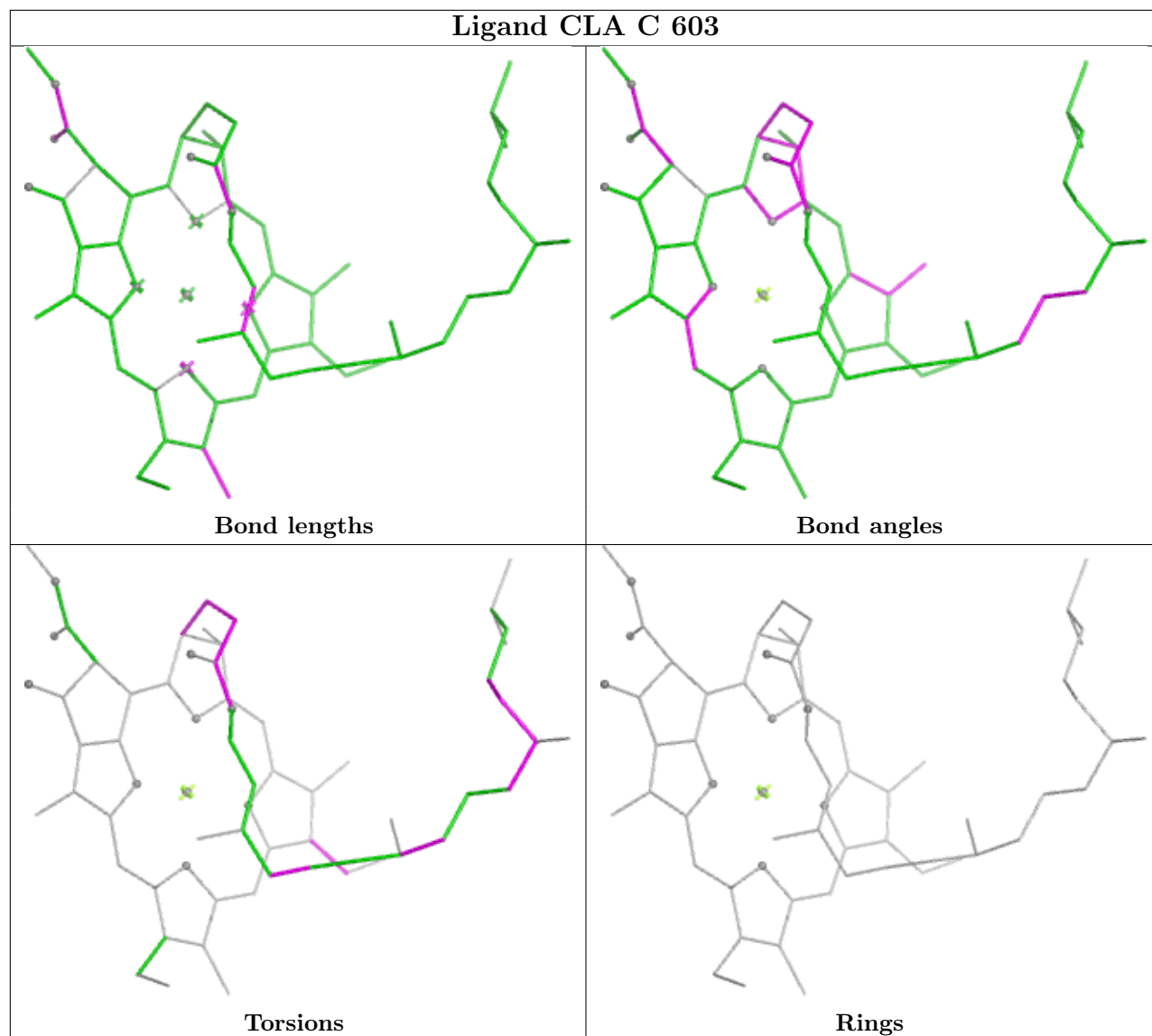
Ligand DGD C 802



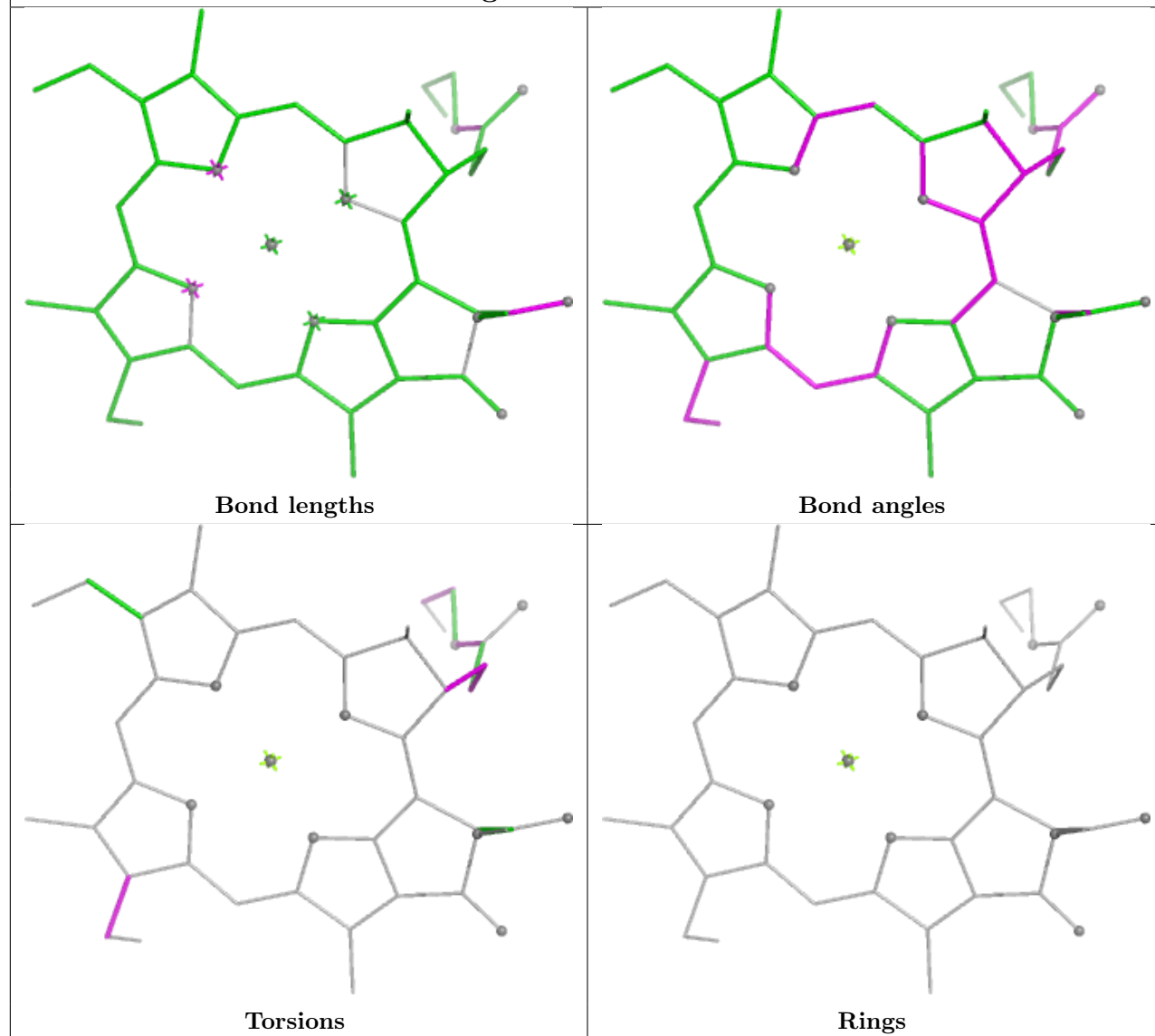




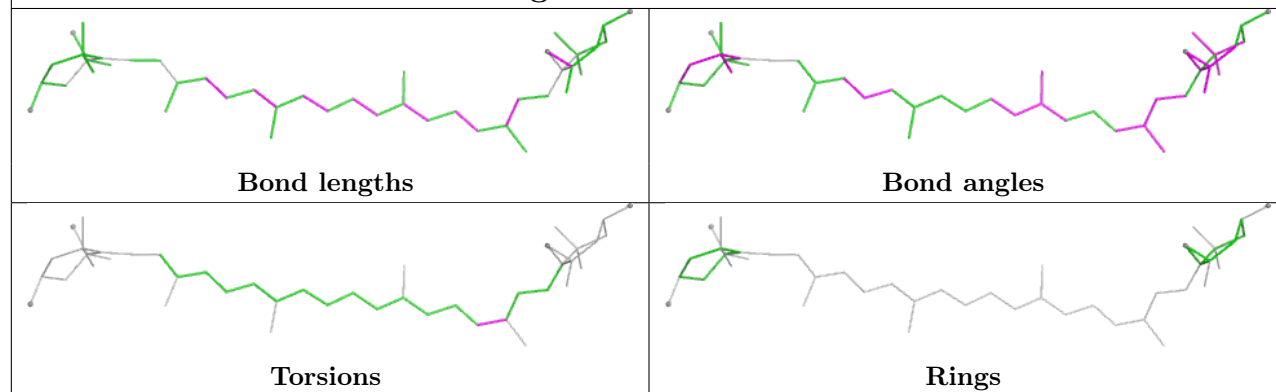
Ligand CLA C 603

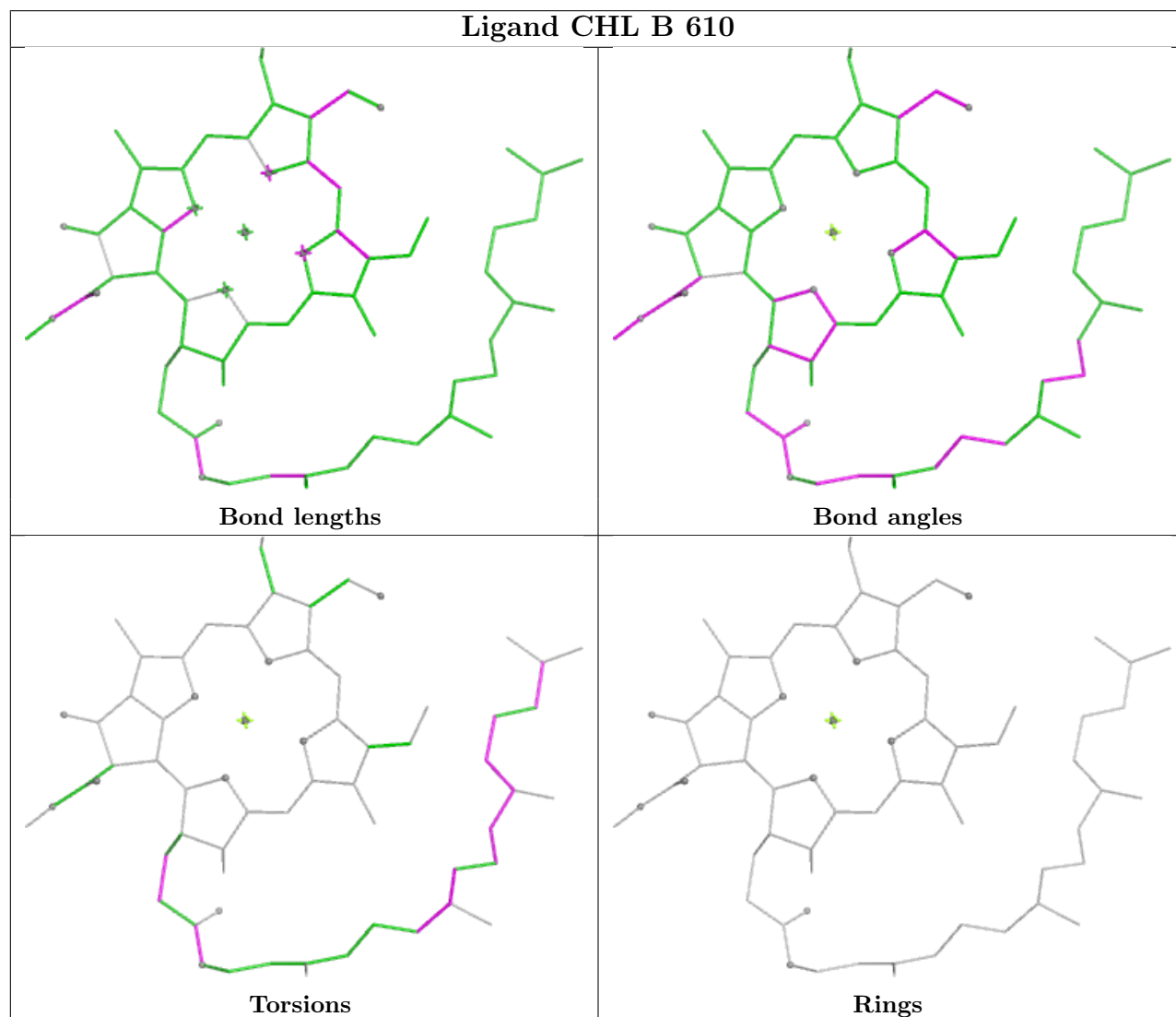
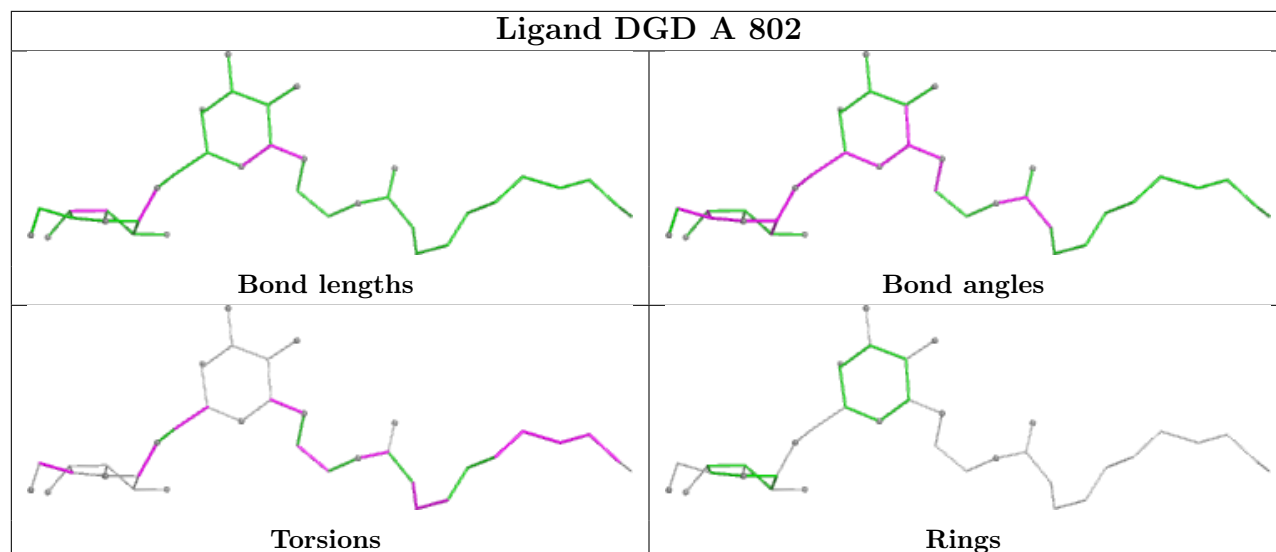


Ligand CLA C 608

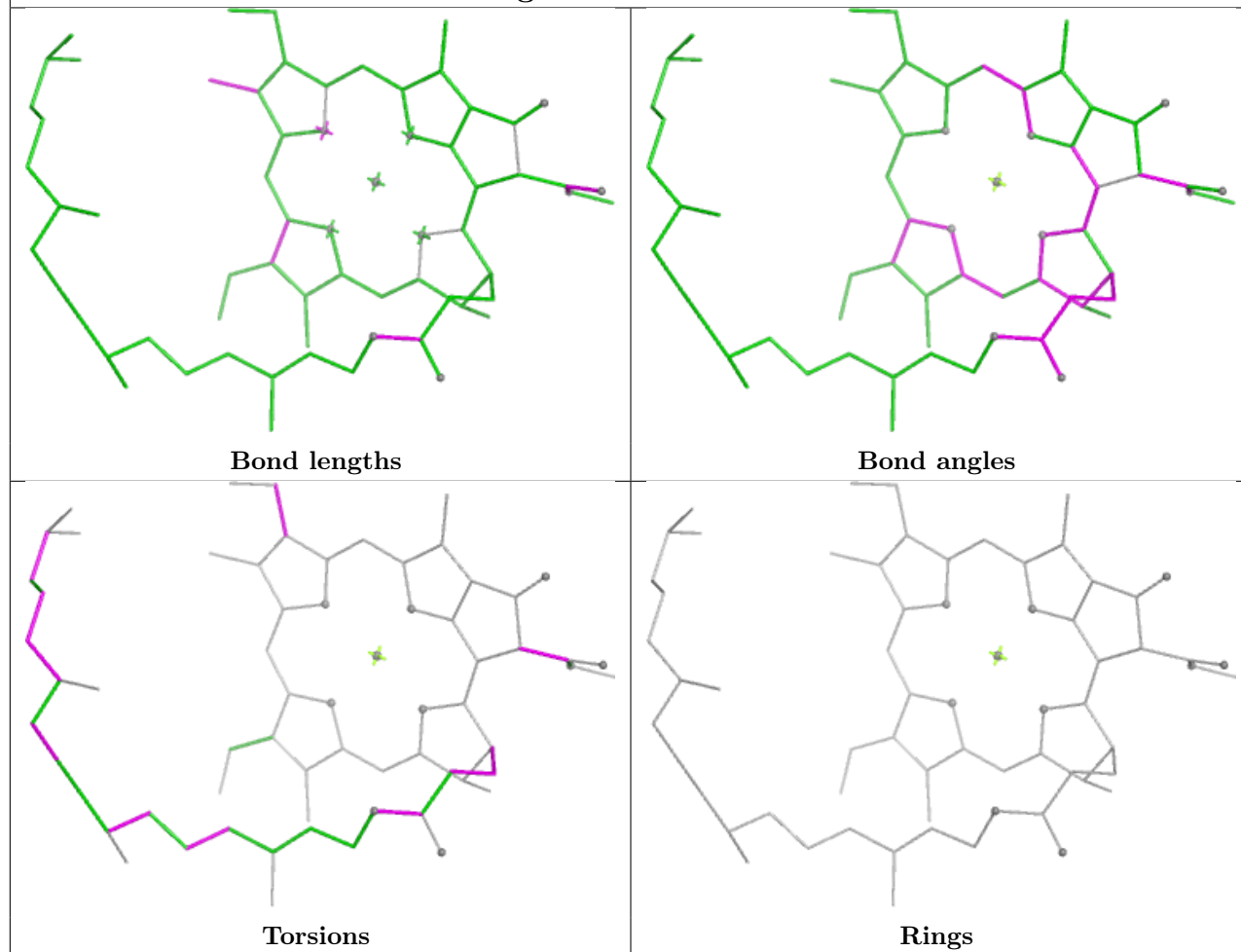


Ligand NEX C 503

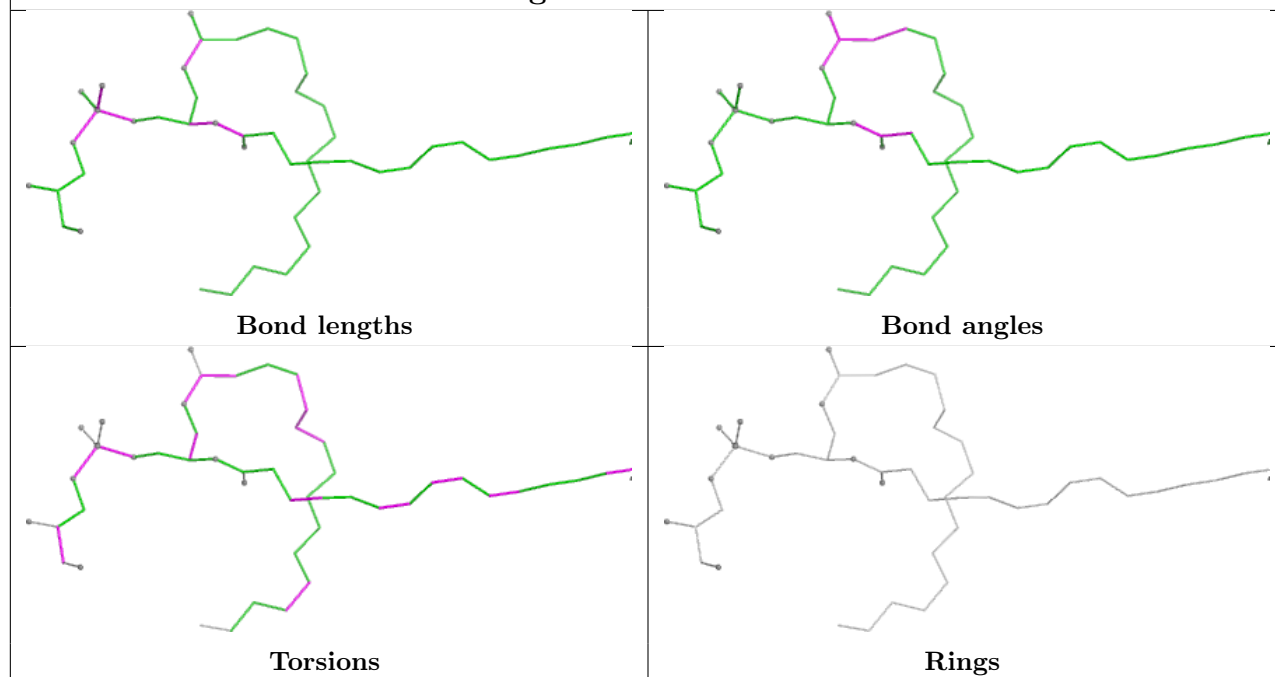




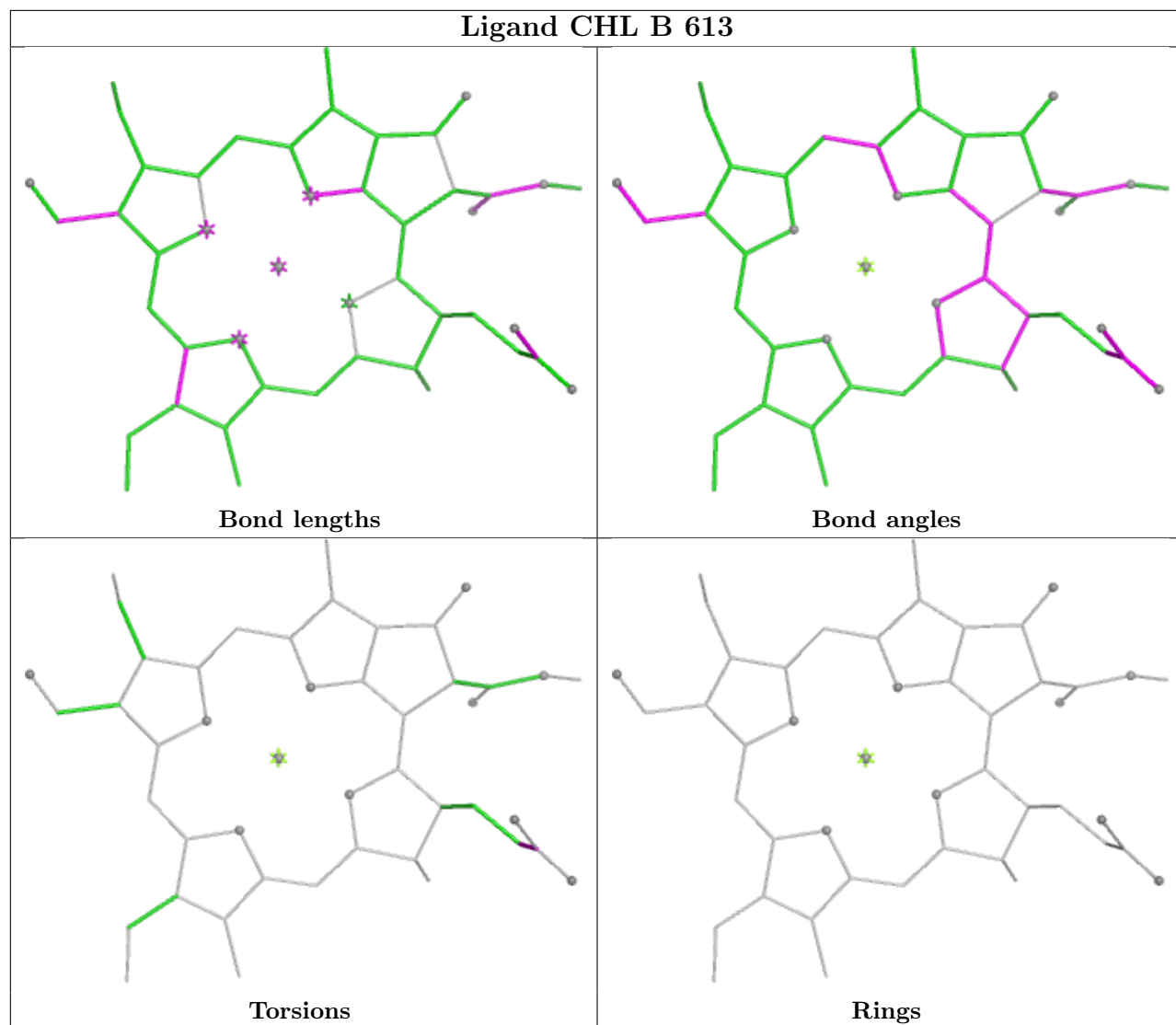
Ligand CLA C 604



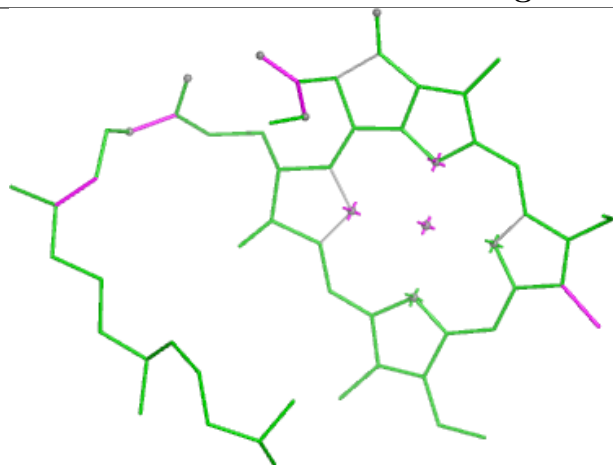
Ligand LHG A 801



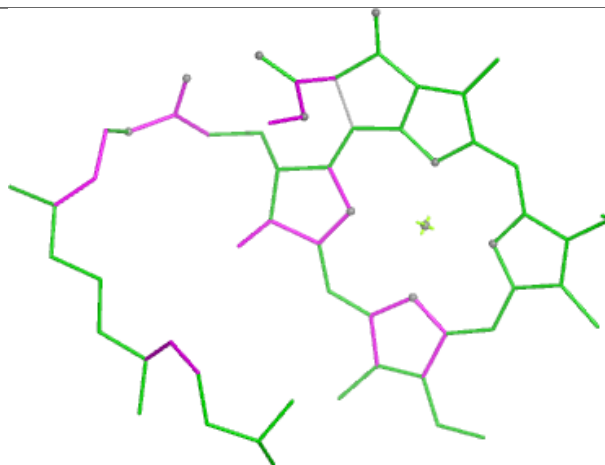
Ligand CHL B 613



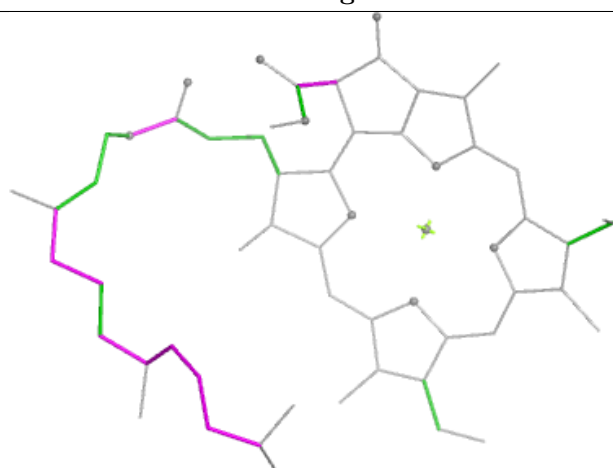
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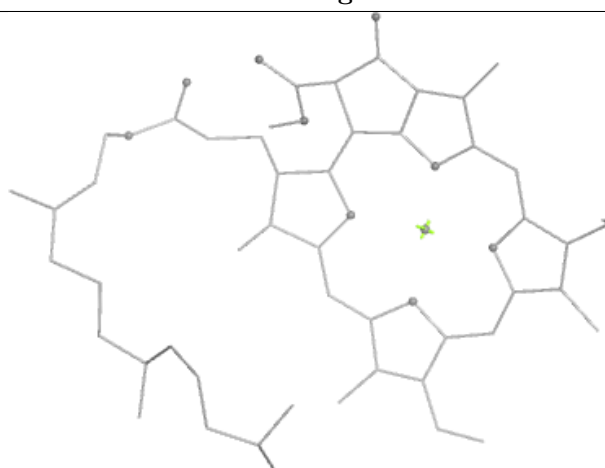
Bond lengths



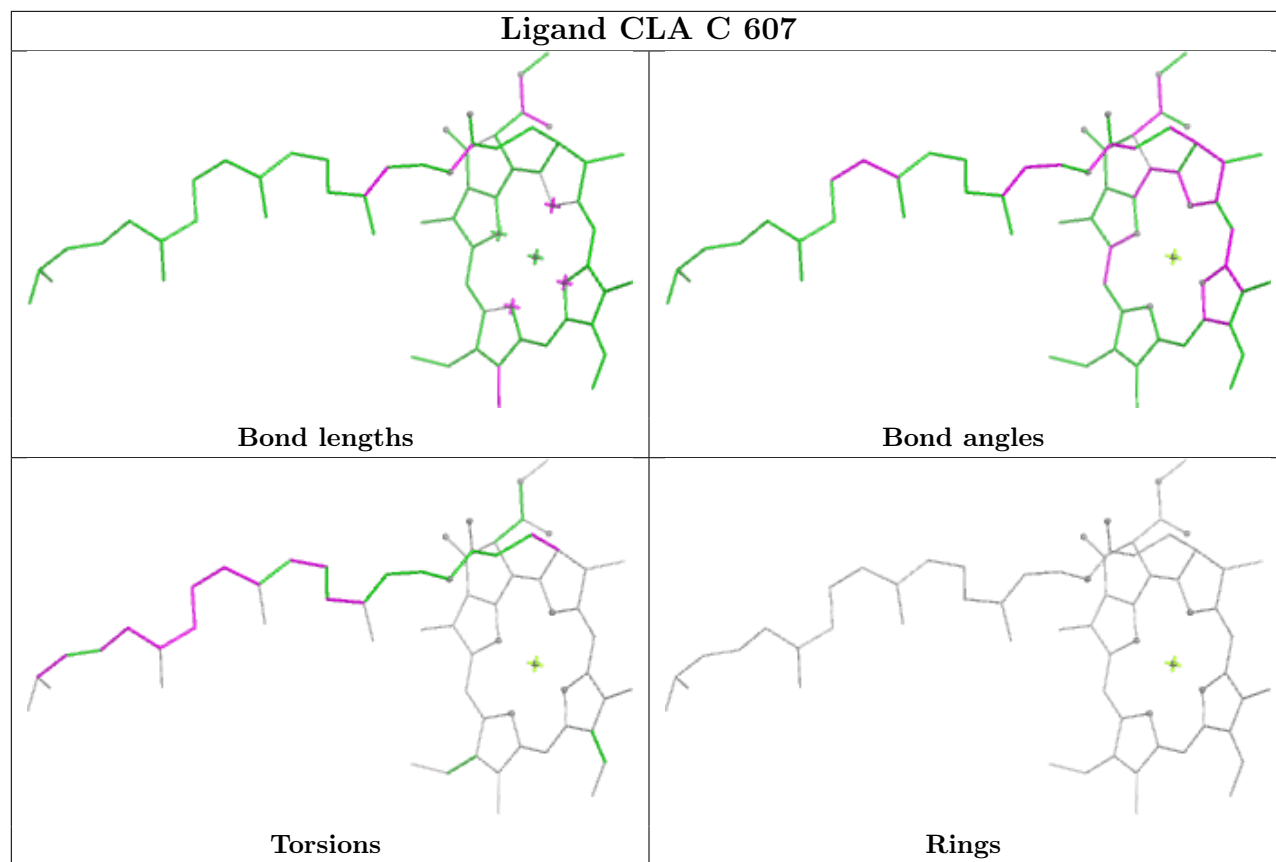
Bond angles



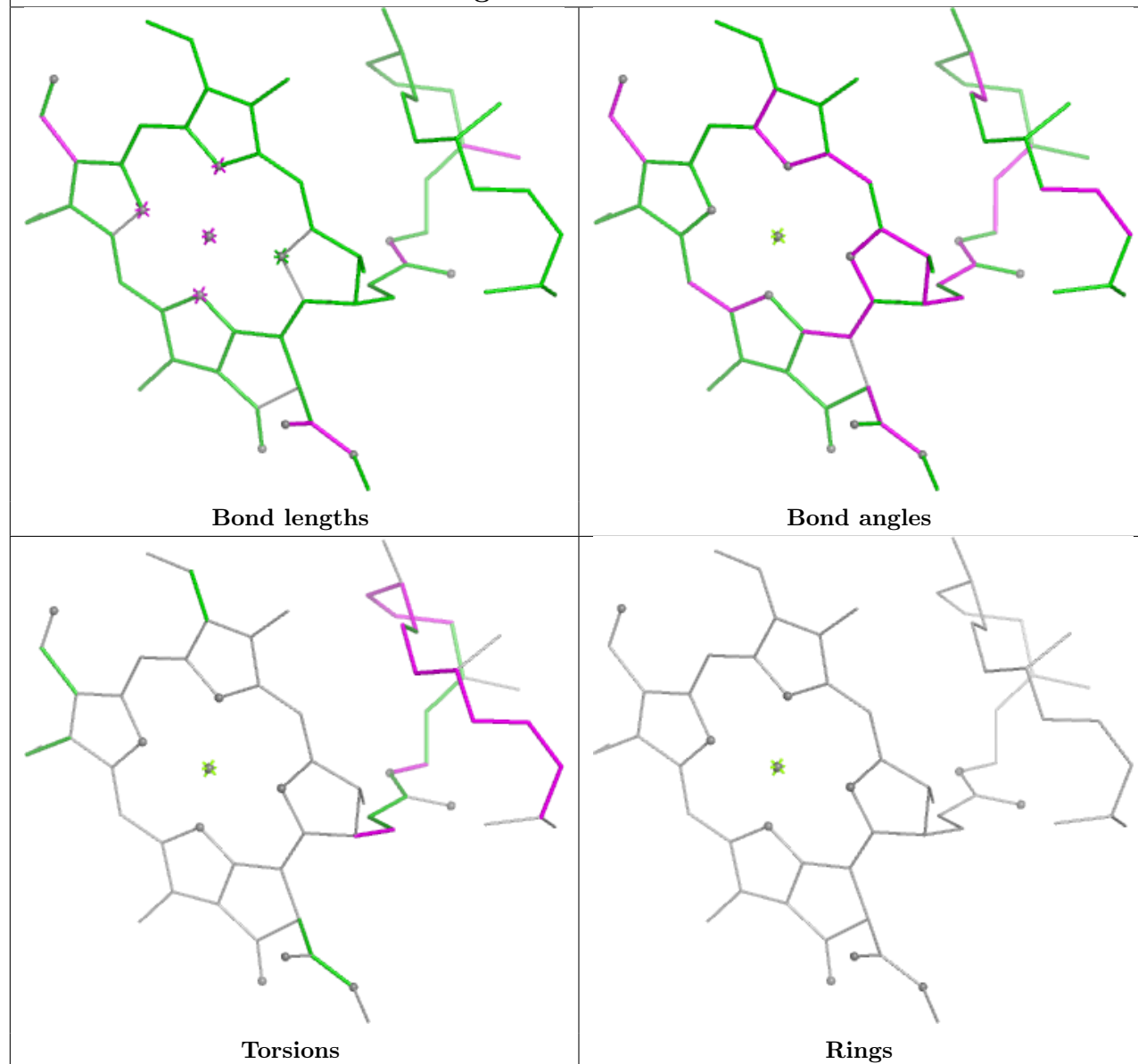
Torsions



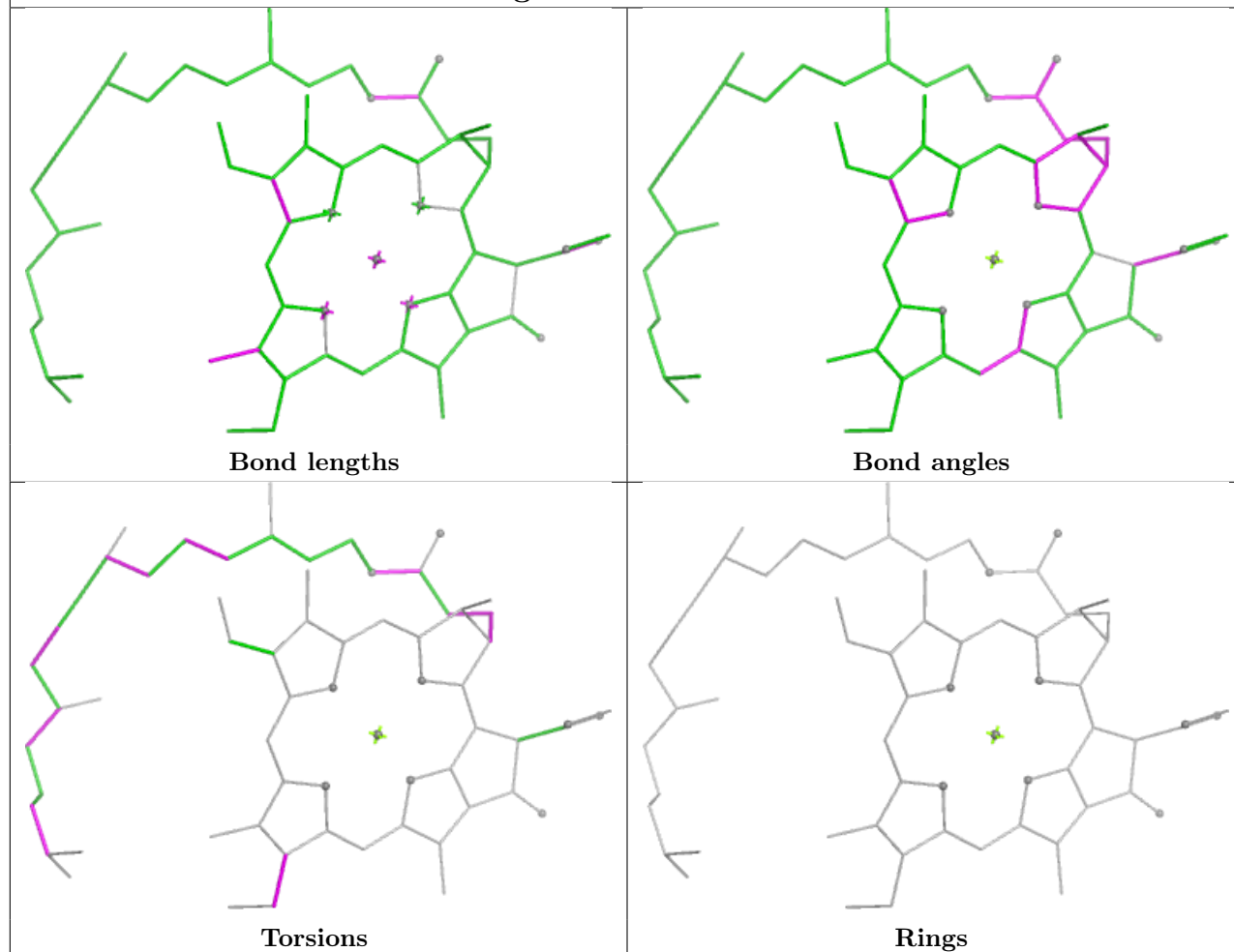
Rings



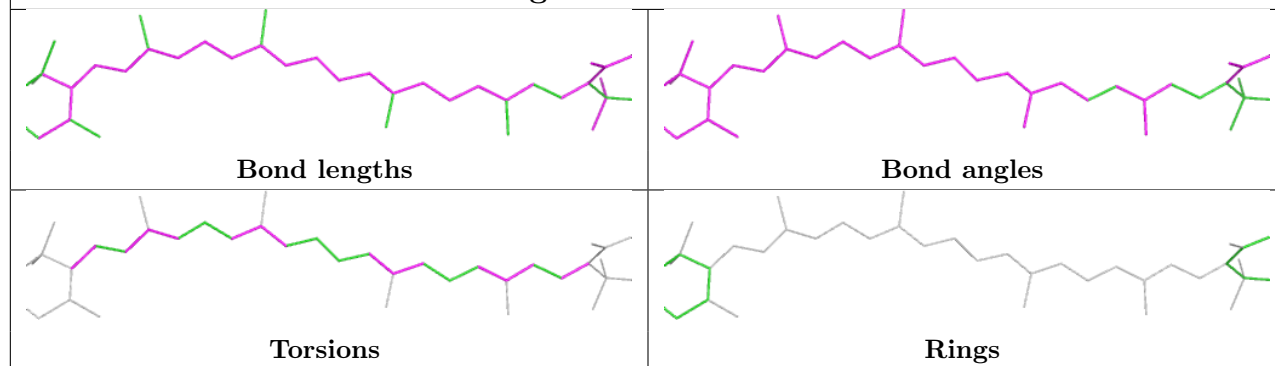
Ligand CHL C 611



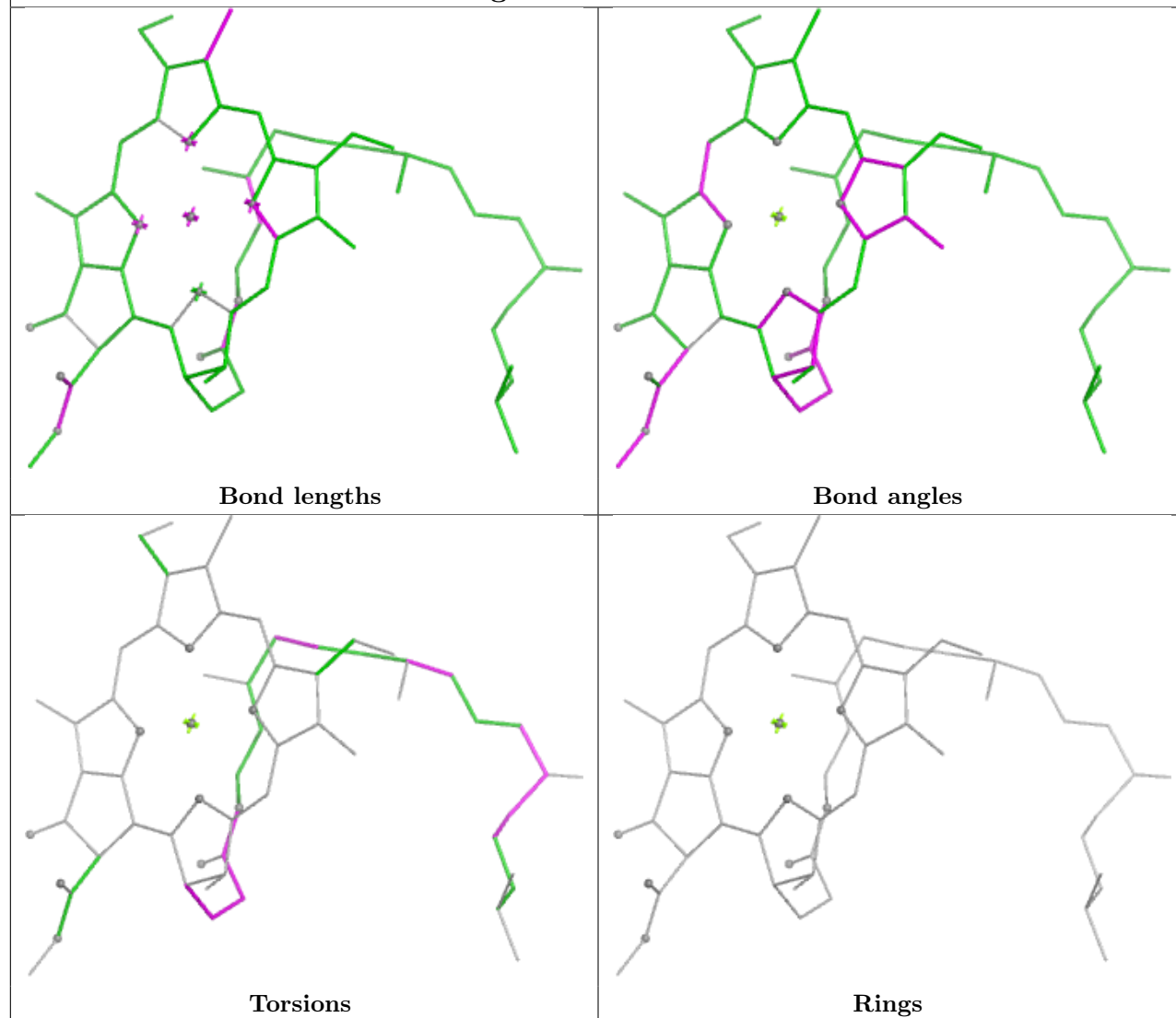
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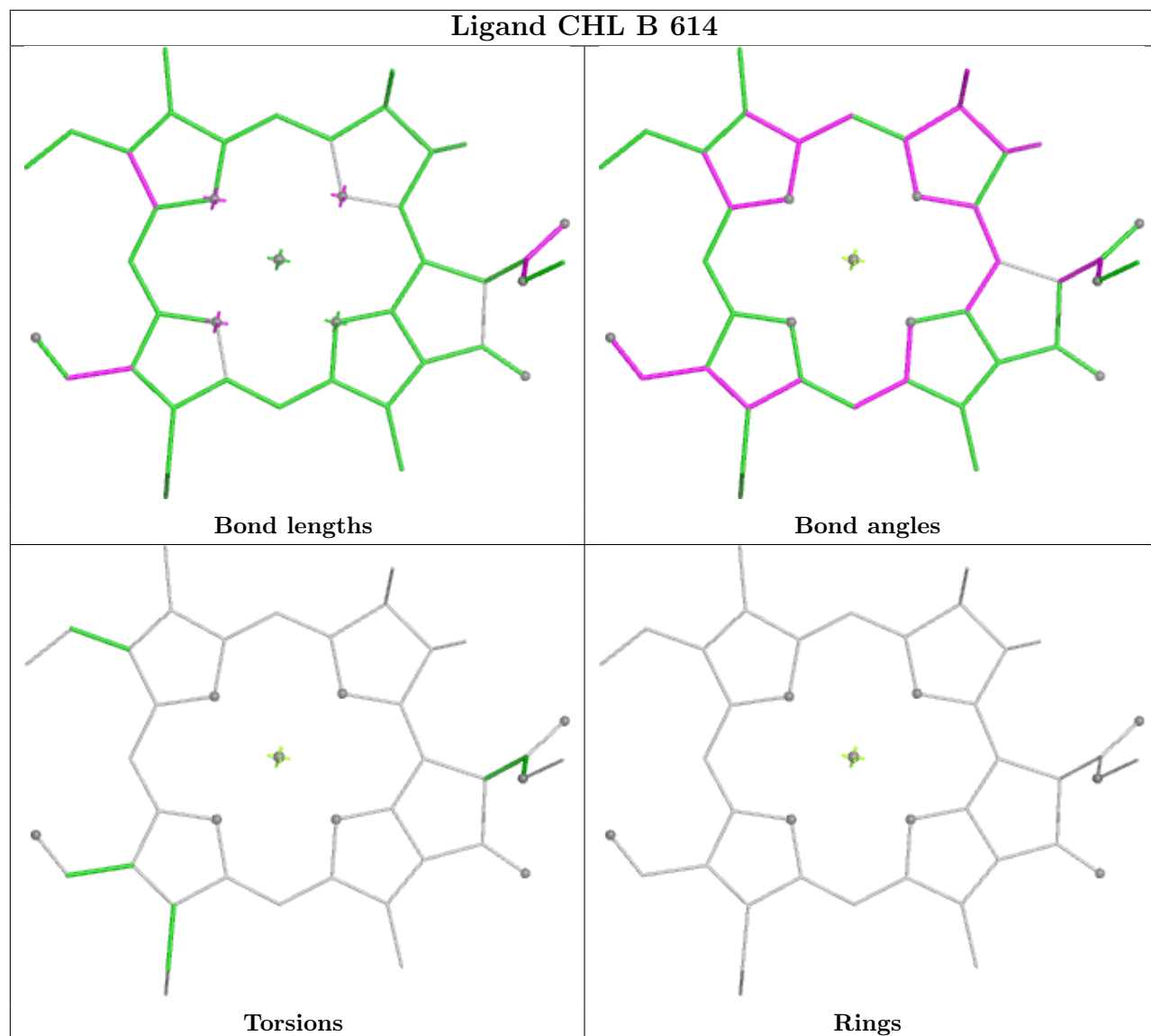
Ligand LUX A 501



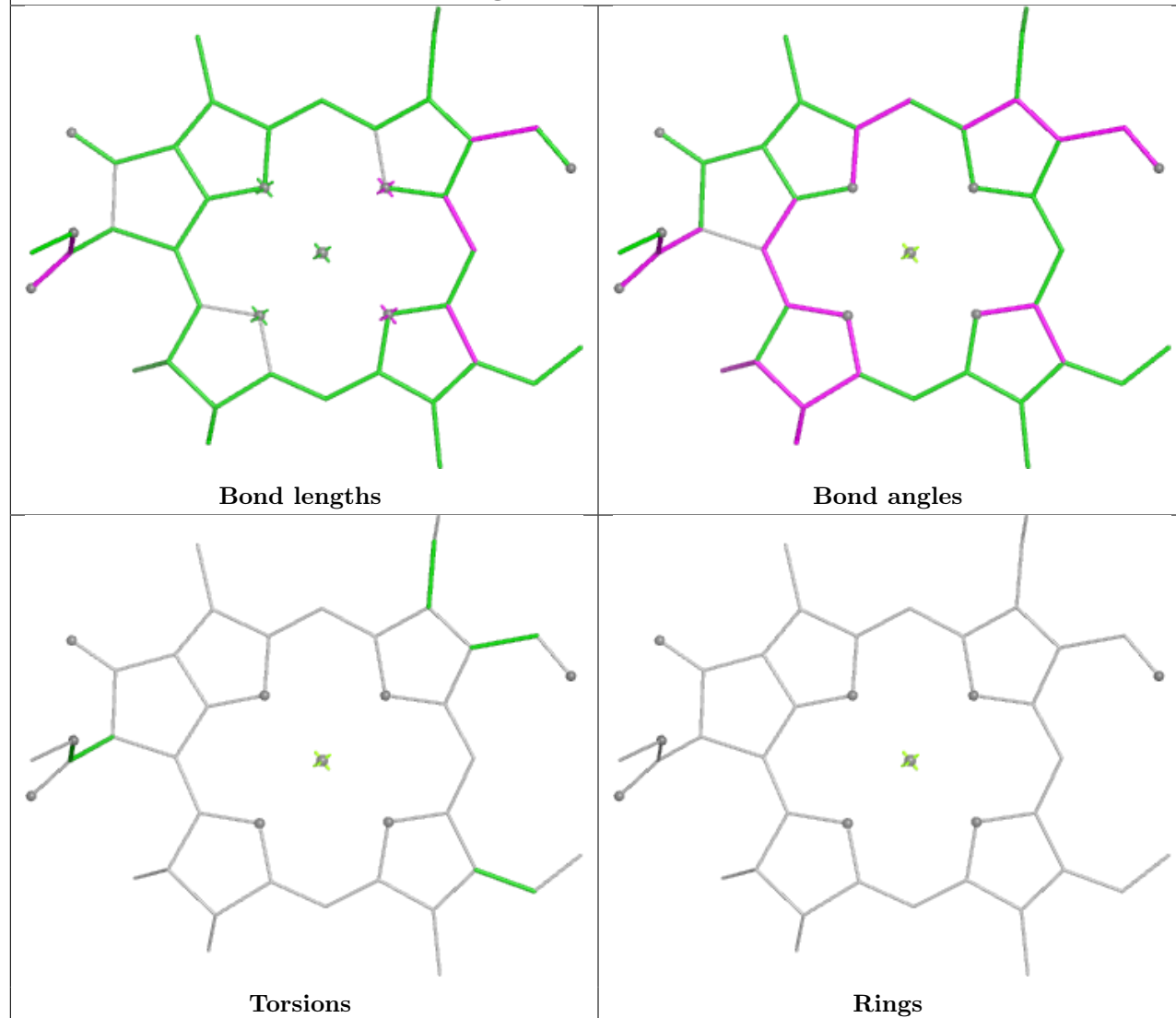
Ligand CLA B 603



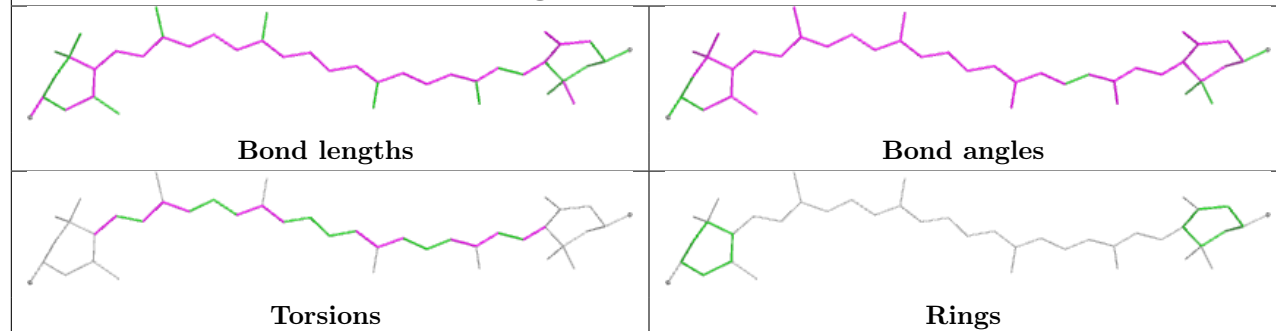
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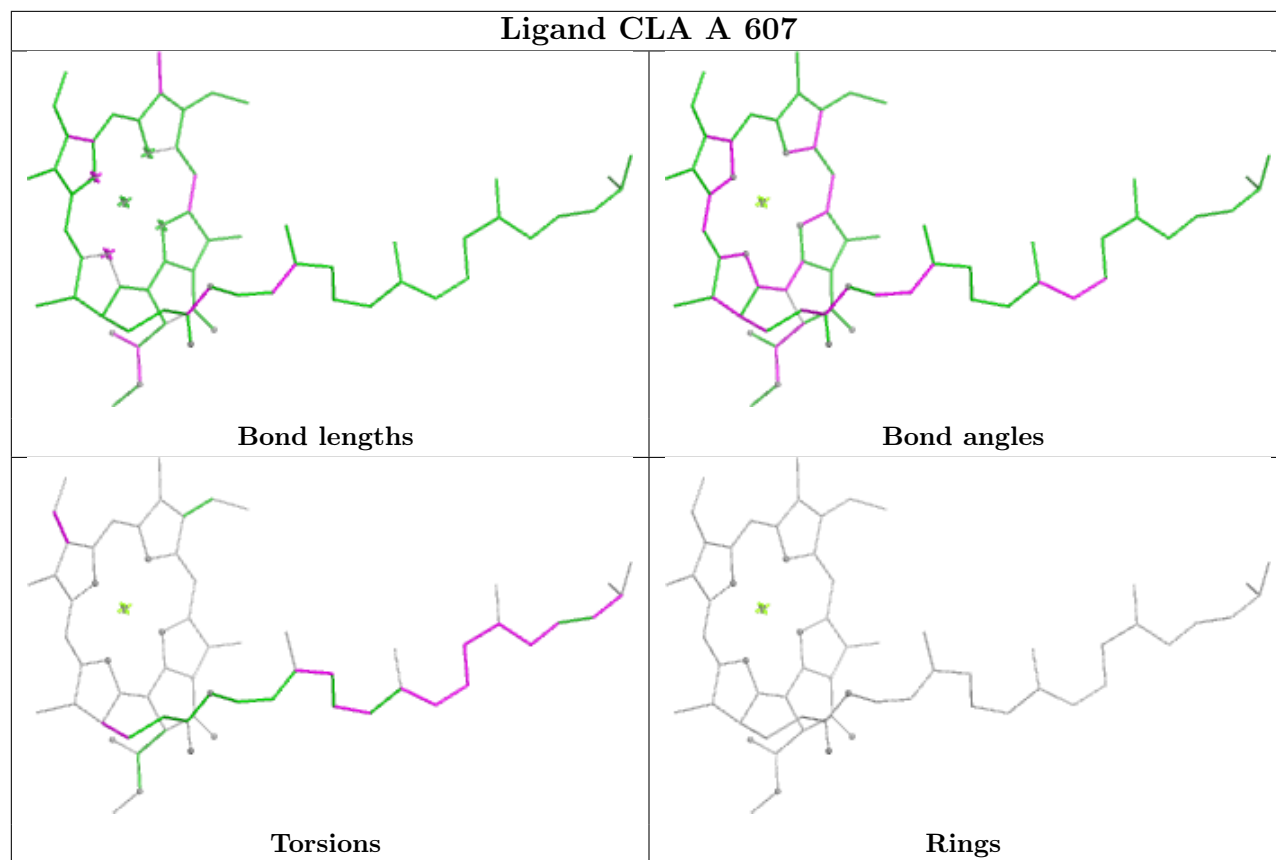


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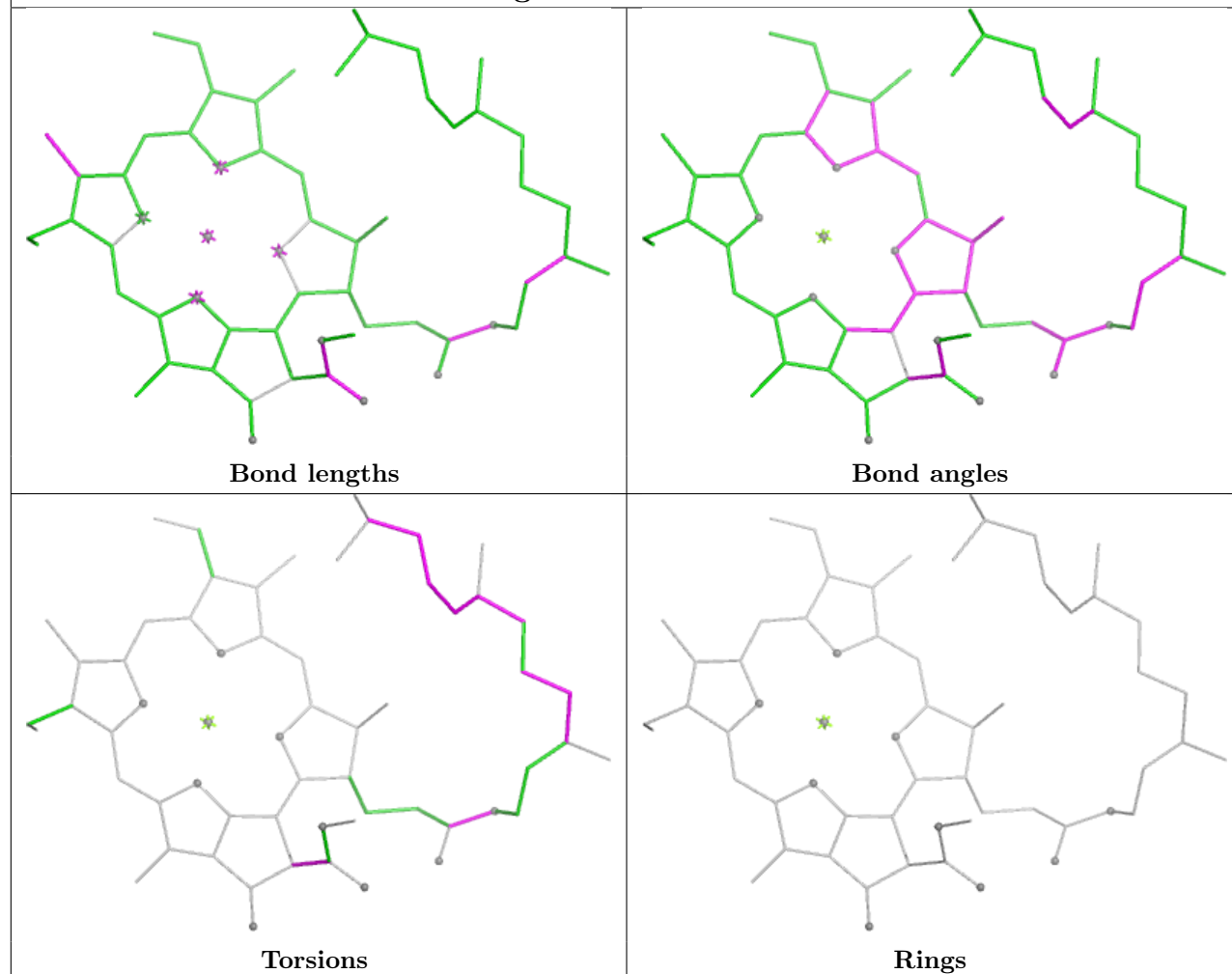


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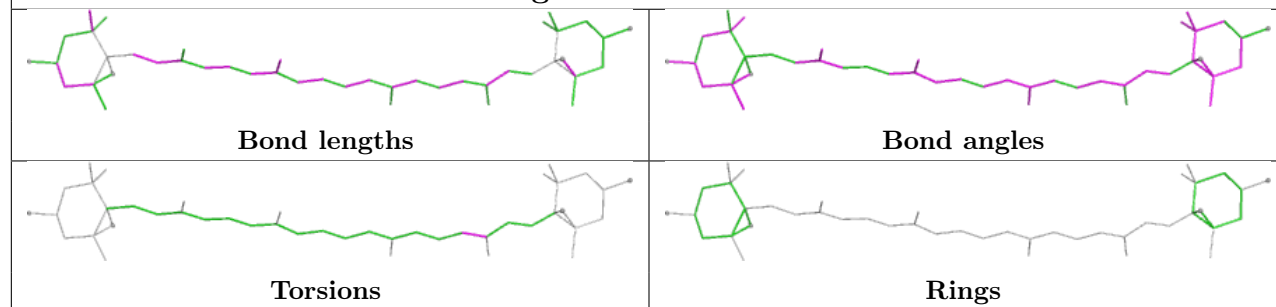


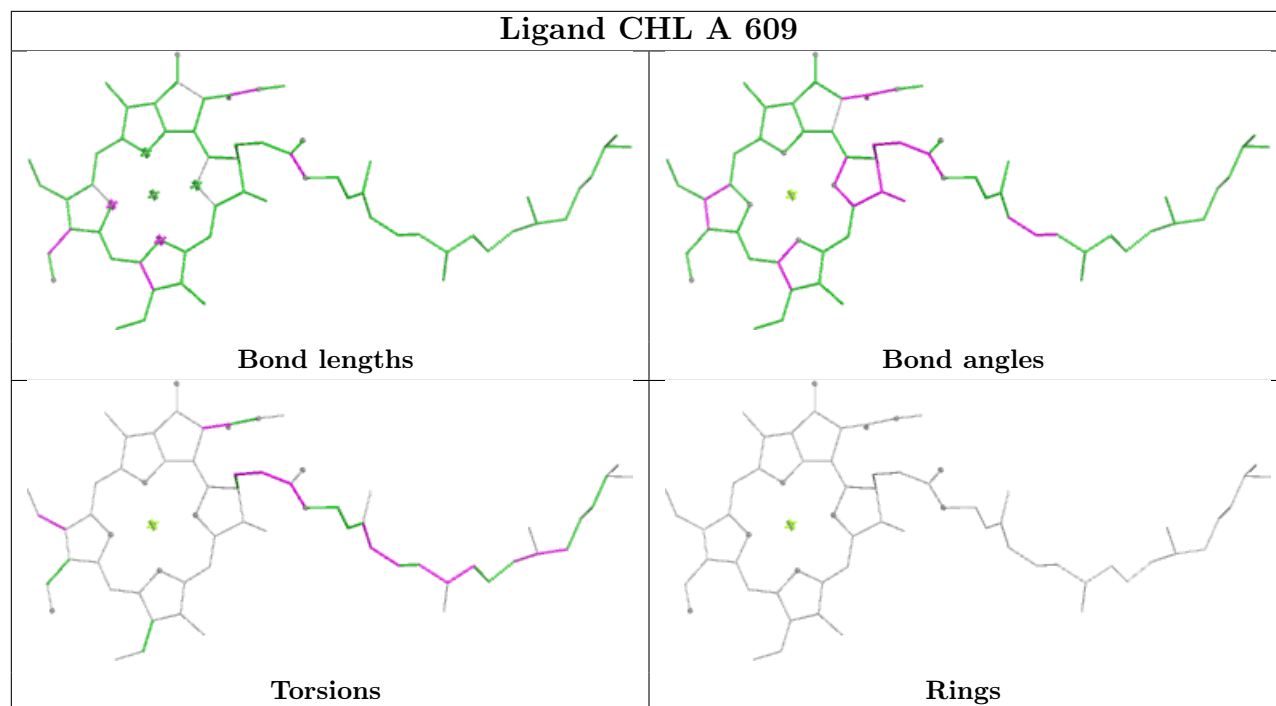


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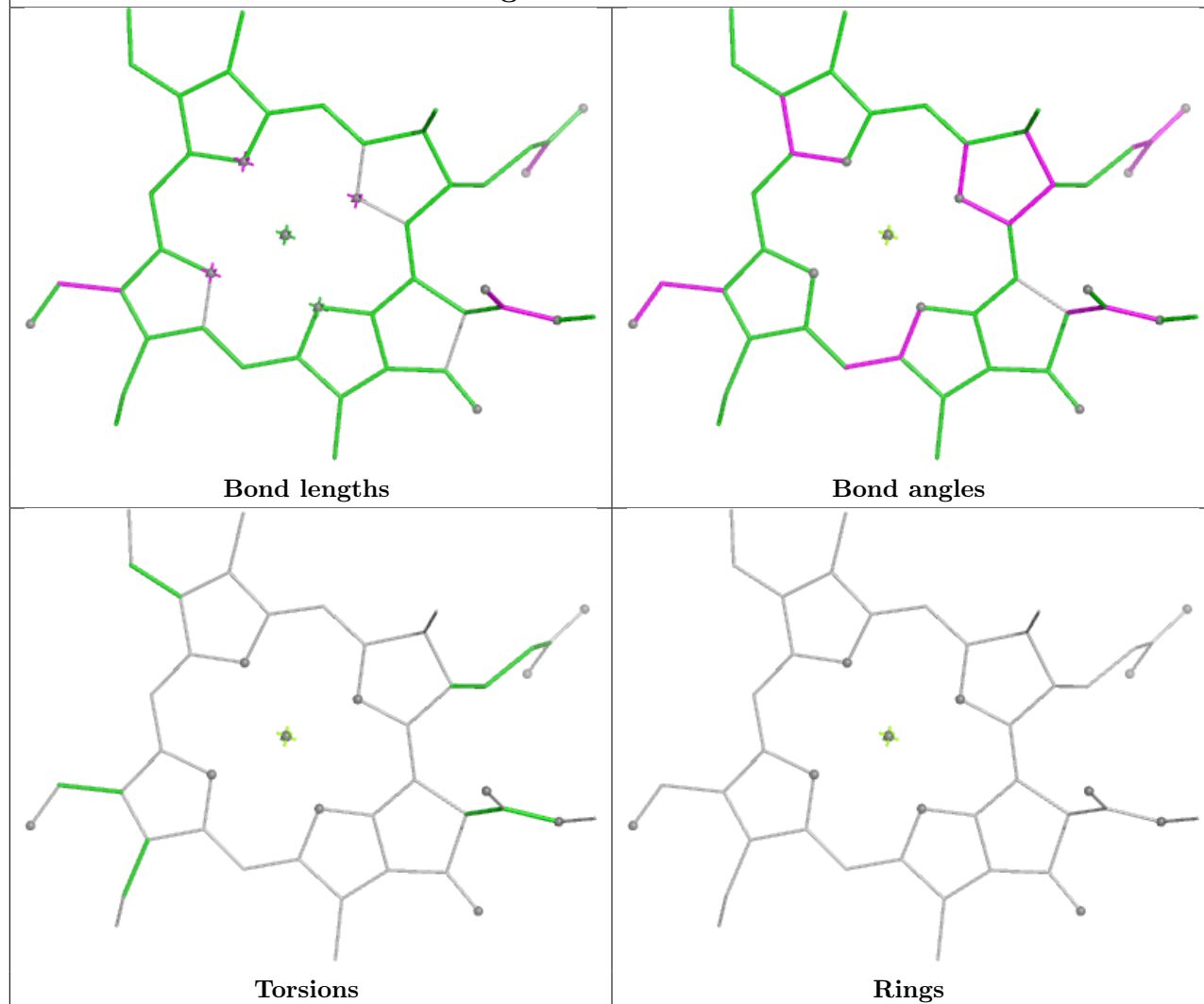


Ligand XAT B 504

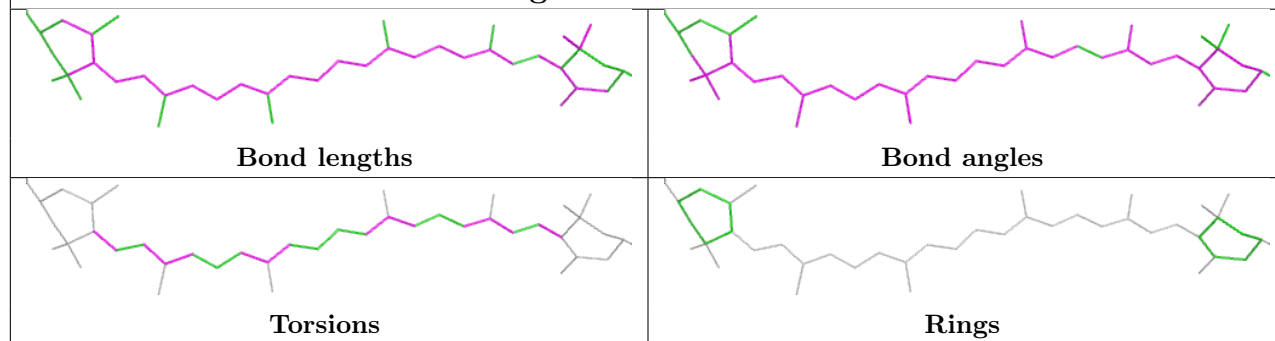


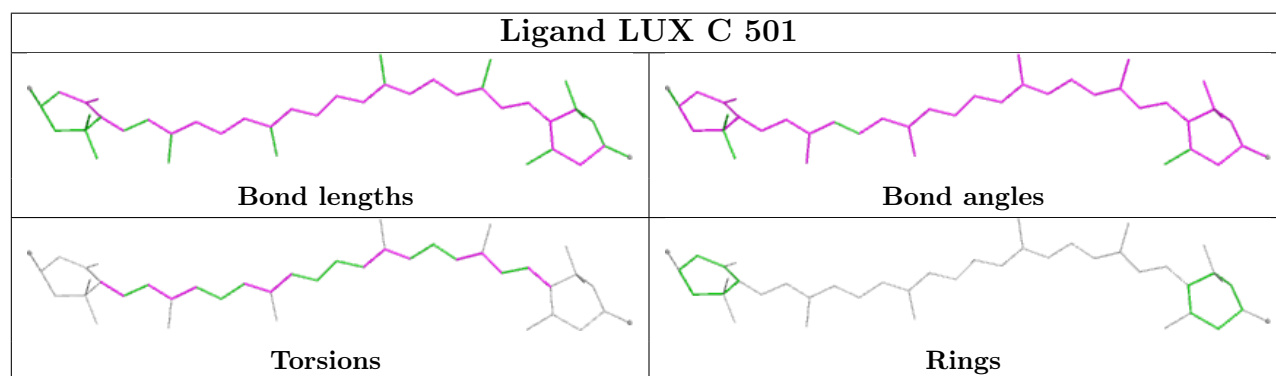
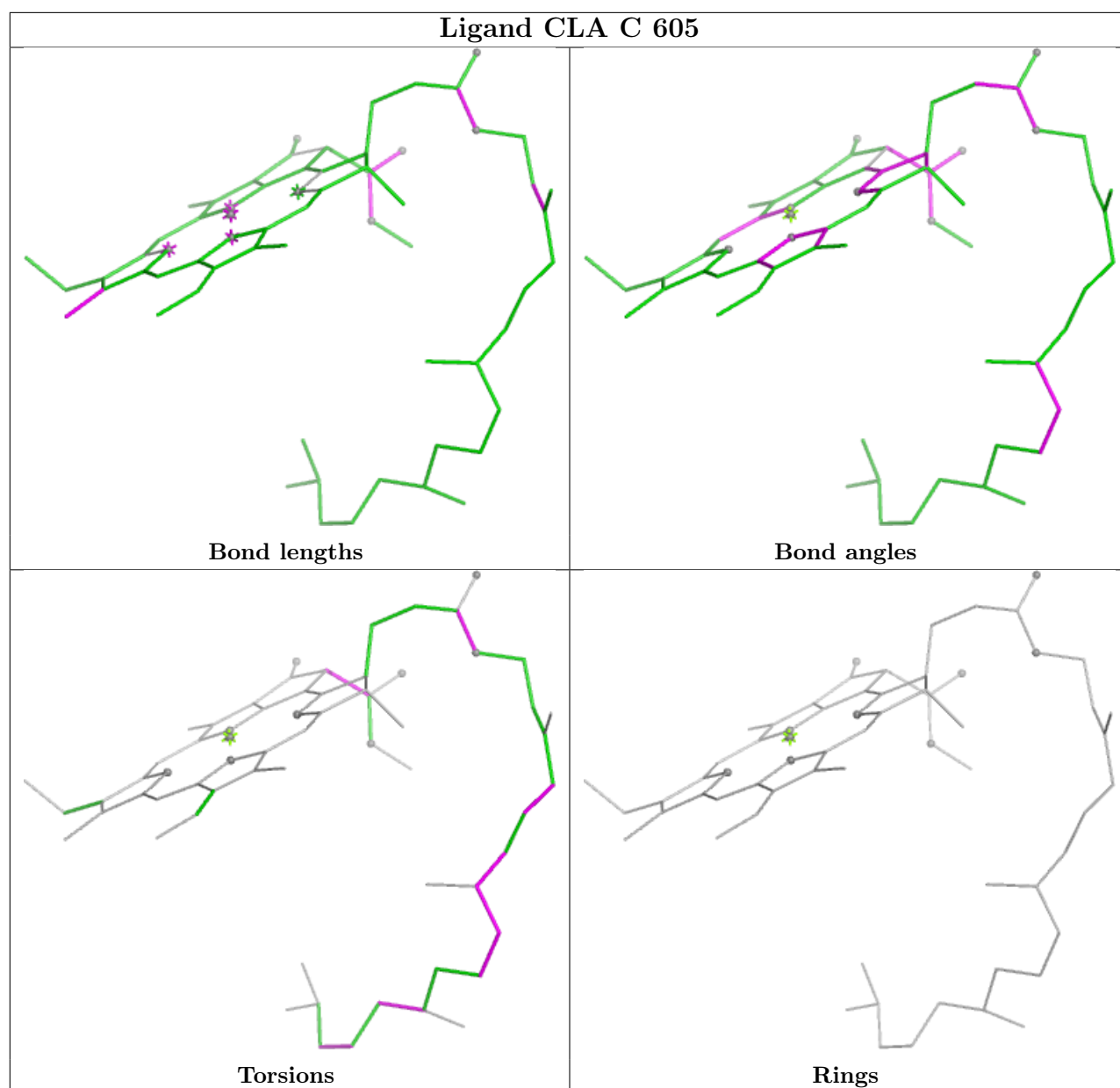


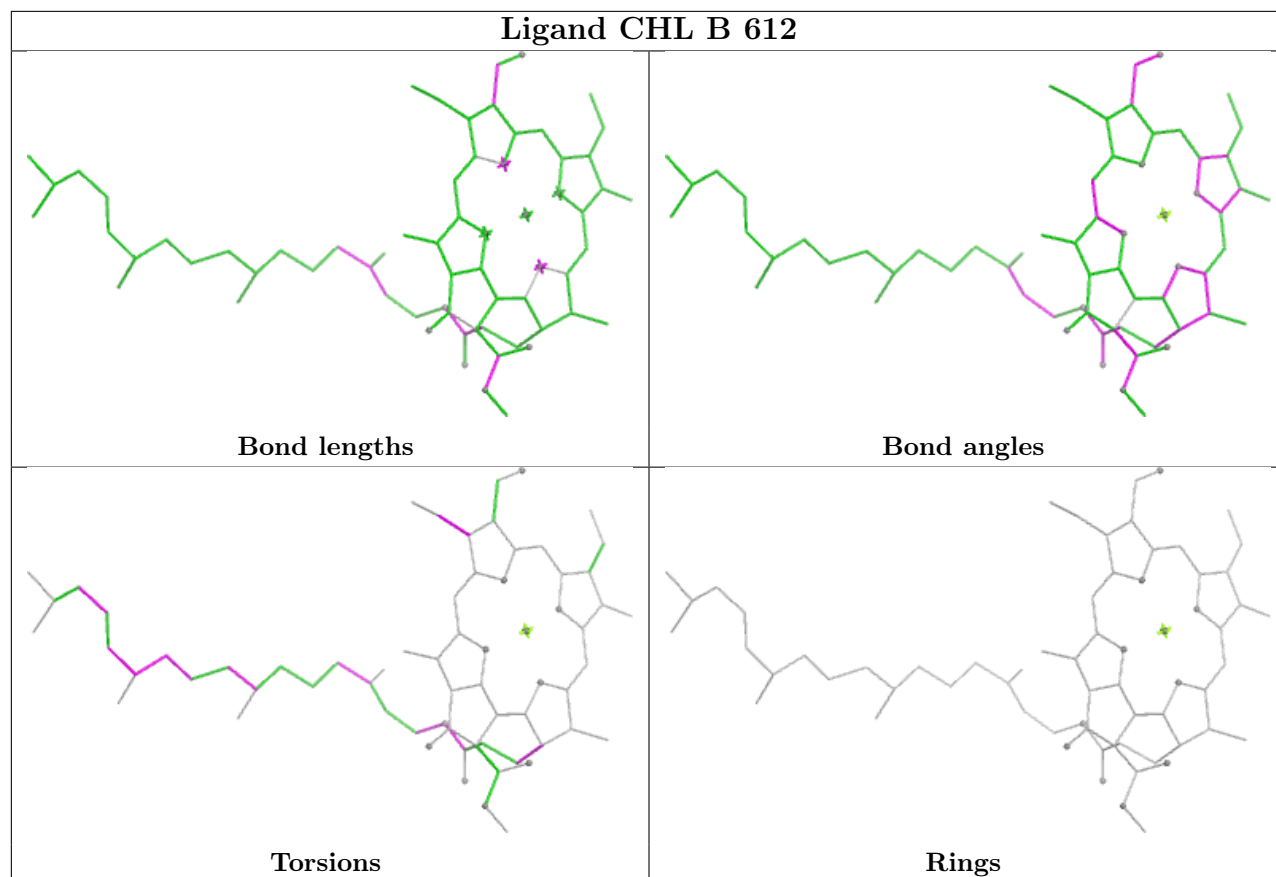
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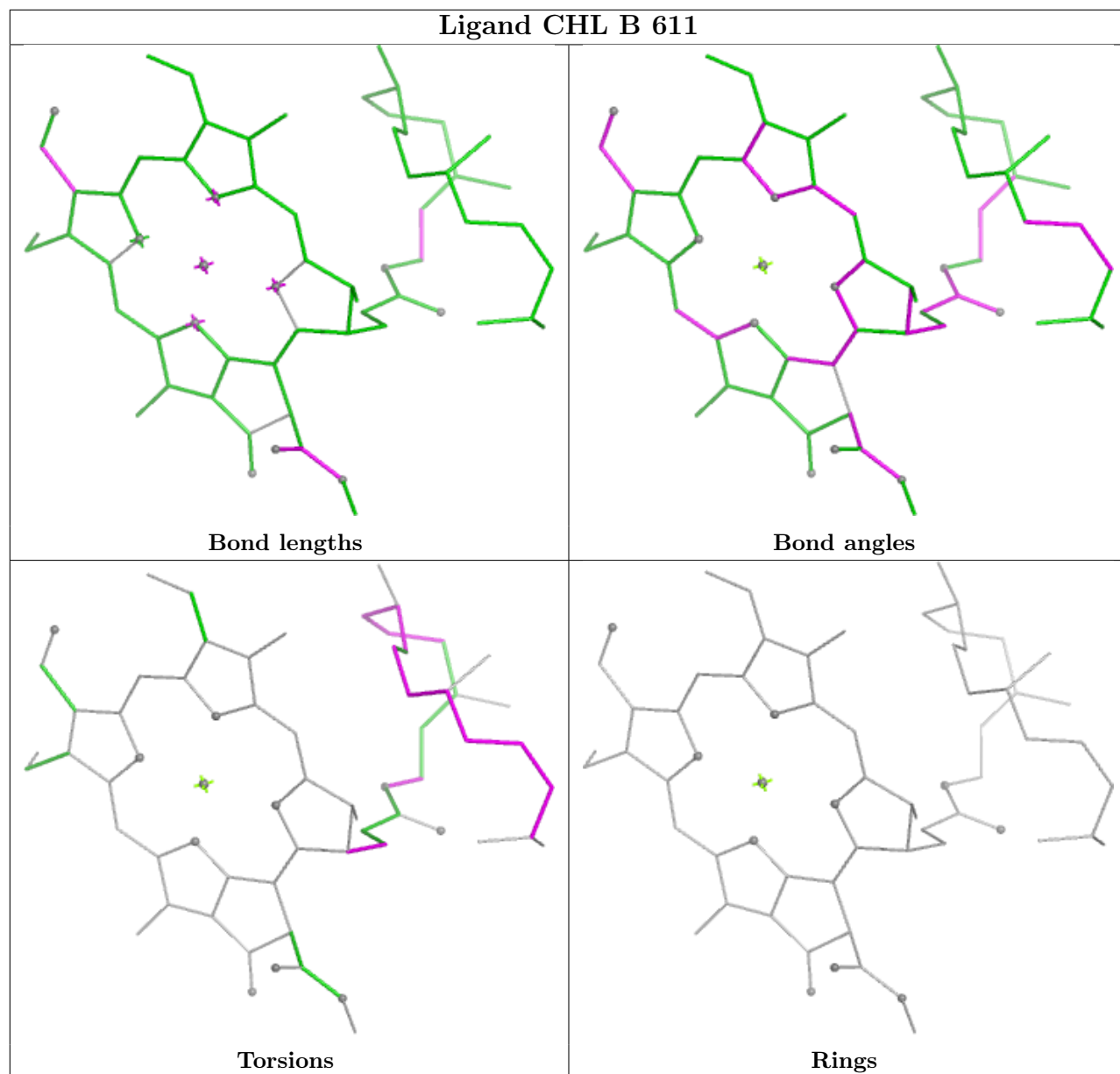
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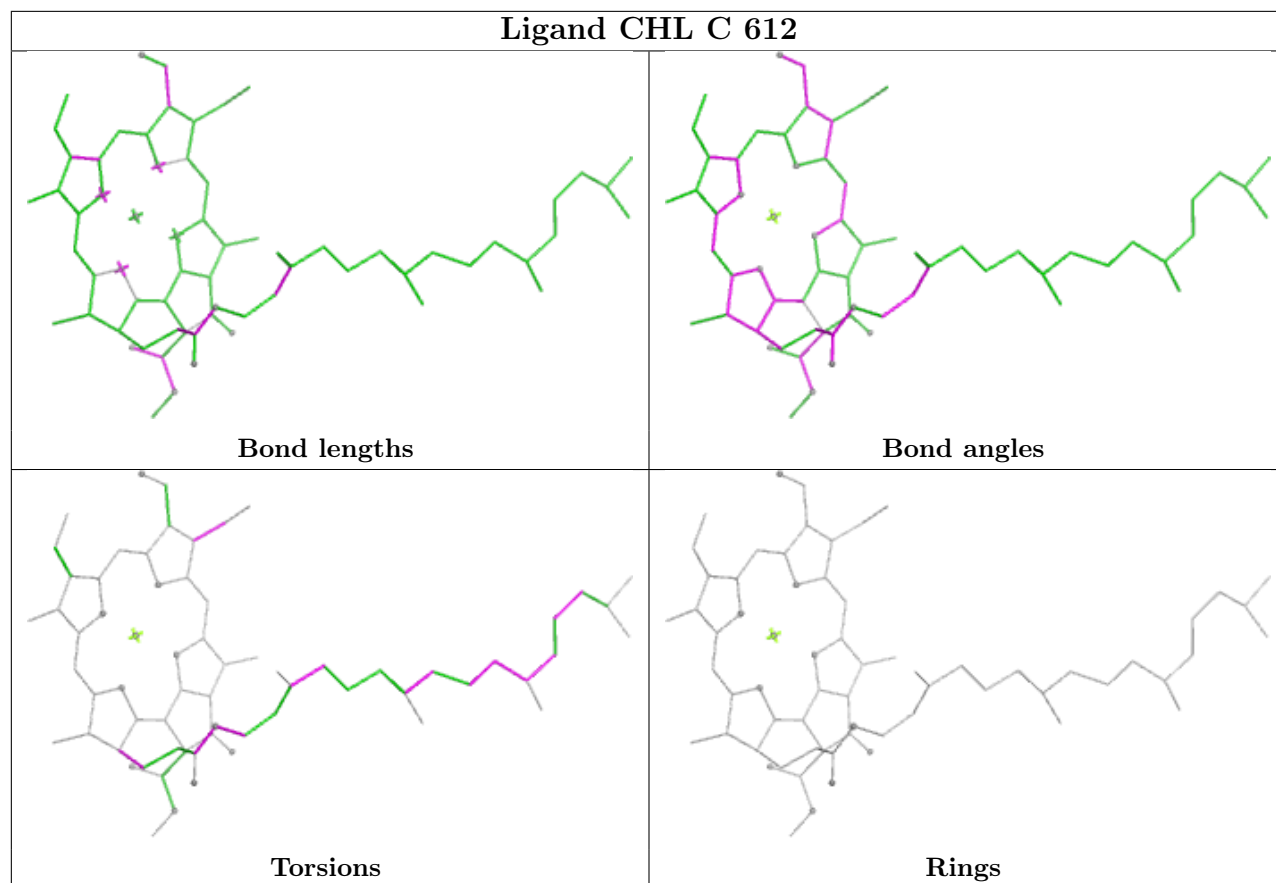




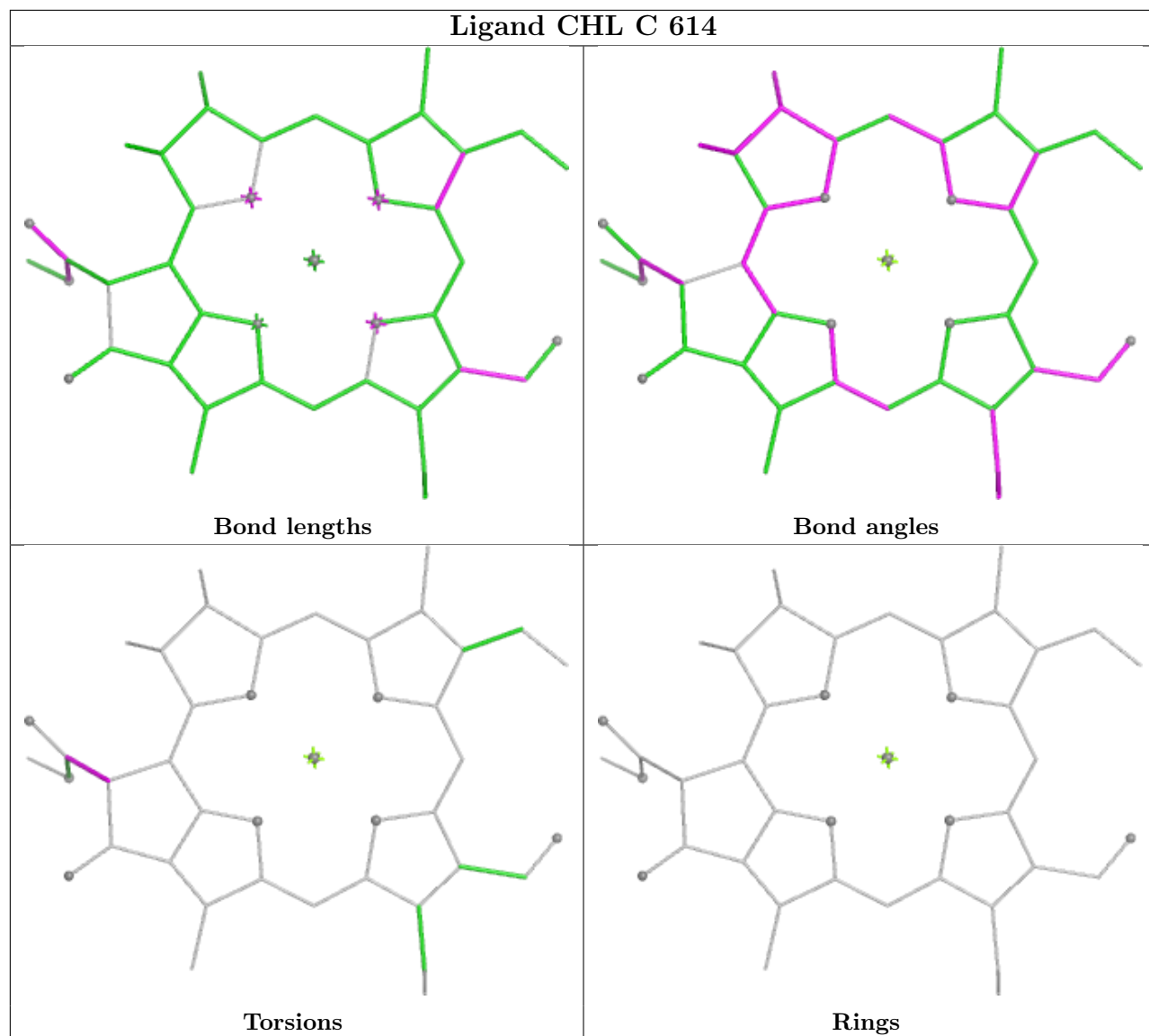


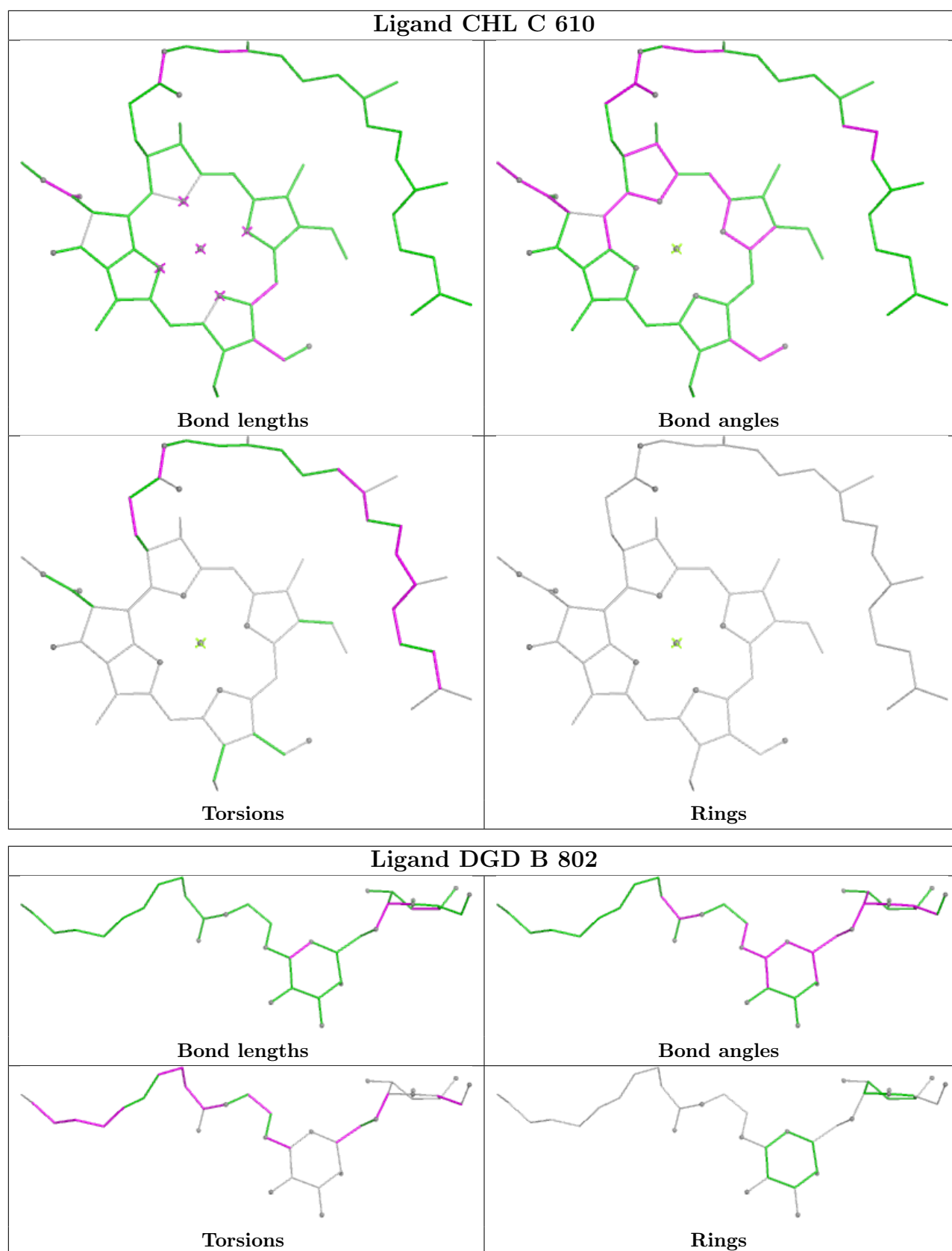
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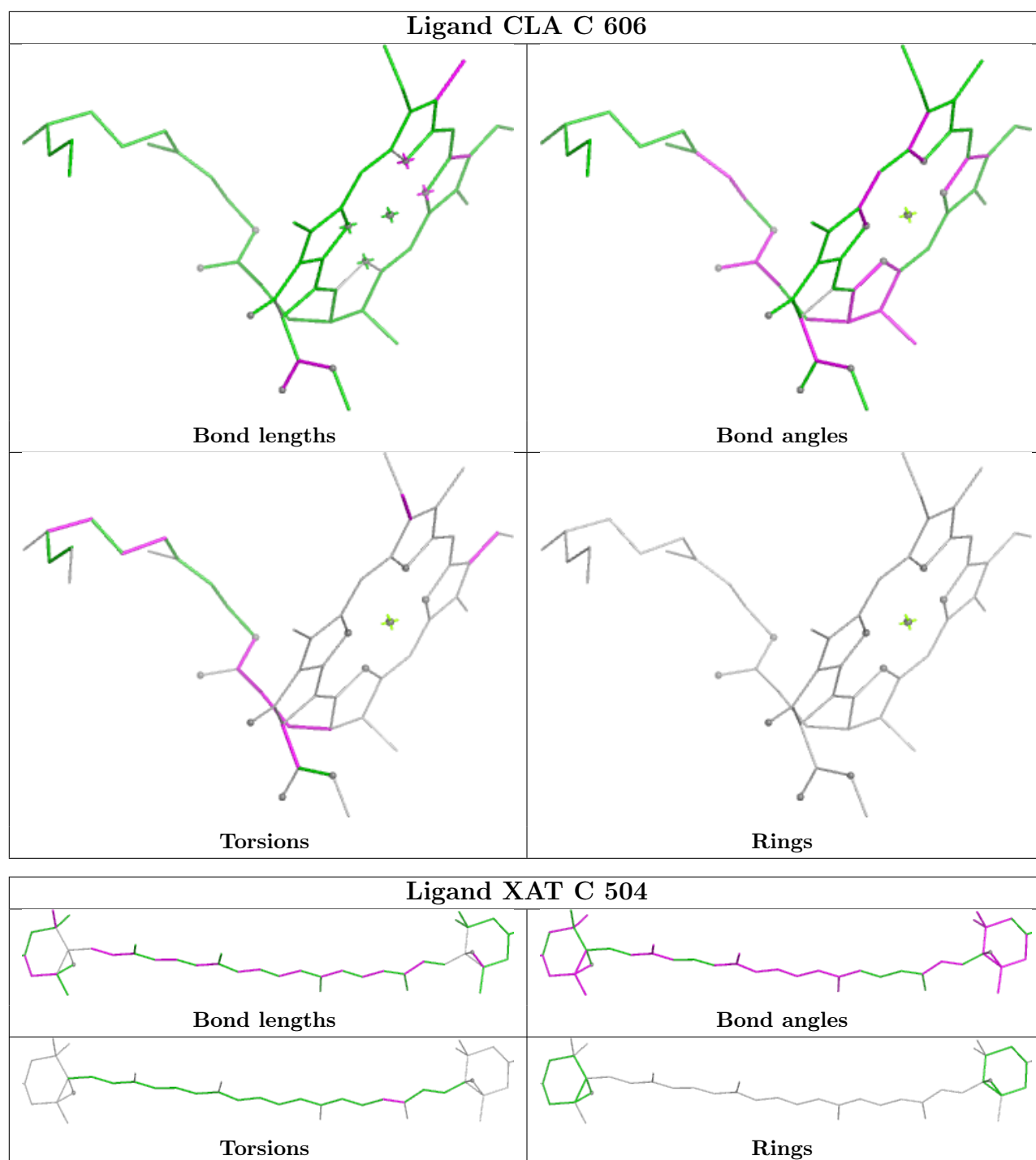




Ligand CHL C 614







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	223/232 (96%)	1.07	33 (14%) 5 4	72, 91, 109, 128	0
1	B	223/232 (96%)	1.38	50 (22%) 2 2	70, 89, 107, 126	0
1	C	223/232 (96%)	1.17	34 (15%) 5 4	73, 91, 109, 129	0
All	All	669/696 (96%)	1.21	117 (17%) 4 3	70, 90, 109, 129	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	GLY	7.5
1	B	205	PRO	4.9
1	B	12	SER	4.7
1	A	13	GLY	4.6
1	B	10	ALA	4.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

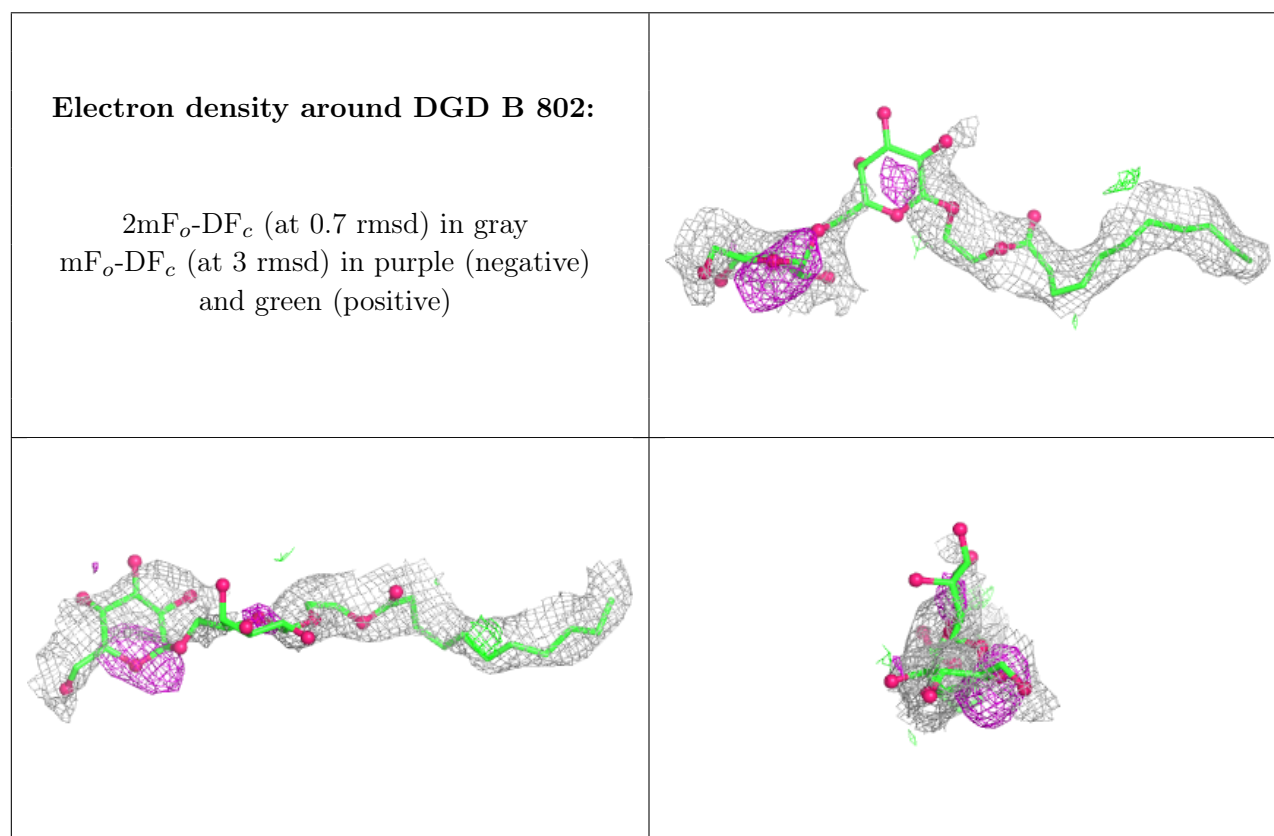
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	DGD	B	802	38/66	0.61	0.19	104,118,139,140	0
8	DGD	C	802	38/66	0.73	0.18	106,119,141,141	0
8	DGD	A	802	38/66	0.78	0.17	106,119,140,140	0
5	CLA	B	601	65/65	0.82	0.19	68,77,111,113	0
2	LUX	B	501	42/42	0.85	0.22	59,86,118,134	0
5	CLA	B	608	48/65	0.86	0.17	88,97,115,117	0
2	LUX	C	501	42/42	0.86	0.20	62,88,120,136	0
6	CHL	C	614	42/66	0.87	0.16	99,107,113,137	0
6	CHL	B	611	66/66	0.87	0.17	68,82,115,121	0
5	CLA	B	607	65/65	0.88	0.19	75,88,101,104	0
6	CHL	C	611	66/66	0.88	0.17	69,85,118,124	0
3	NEX	C	503	44/44	0.89	0.16	67,98,128,133	0
2	LUX	A	501	42/42	0.89	0.19	61,87,120,136	0
2	LUX	B	502	42/42	0.89	0.18	53,76,113,126	0
2	LUX	A	502	42/42	0.89	0.18	57,78,115,128	0
6	CHL	A	611	66/66	0.89	0.17	70,85,117,123	0
6	CHL	A	612	66/66	0.89	0.14	76,85,102,104	0
3	NEX	A	503	44/44	0.90	0.14	66,97,128,132	0
5	CLA	B	602	60/65	0.90	0.15	77,85,114,114	0
4	XAT	A	504	44/44	0.90	0.15	65,91,117,148	0
5	CLA	A	602	60/65	0.90	0.16	79,87,115,116	0
7	LHG	B	801	49/49	0.90	0.18	72,88,109,115	0
5	CLA	C	605	65/65	0.90	0.13	77,86,108,110	0
5	CLA	C	607	65/65	0.90	0.16	77,91,104,106	0
5	CLA	A	605	65/65	0.90	0.15	77,86,107,110	0
5	CLA	B	605	65/65	0.91	0.14	75,84,105,108	0
5	CLA	A	601	65/65	0.91	0.15	69,79,112,115	0
5	CLA	A	606	57/65	0.91	0.16	79,90,107,110	0
6	CHL	C	612	66/66	0.91	0.14	77,85,102,104	0
5	CLA	C	602	60/65	0.91	0.13	80,87,116,117	0
7	LHG	A	801	49/49	0.91	0.18	74,90,110,116	0
5	CLA	A	608	48/65	0.91	0.16	90,99,116,118	0
2	LUX	C	502	42/42	0.91	0.17	58,79,115,128	0
5	CLA	C	608	48/65	0.91	0.14	90,99,117,119	0
5	CLA	A	603	65/65	0.91	0.15	75,85,102,105	0
5	CLA	B	603	65/65	0.92	0.13	74,83,100,103	0
6	CHL	C	613	46/66	0.92	0.13	73,82,107,121	0
5	CLA	C	601	65/65	0.92	0.16	70,79,113,115	0
5	CLA	A	607	65/65	0.92	0.16	77,90,103,106	0
6	CHL	A	614	42/66	0.92	0.13	99,106,113,136	0
7	LHG	C	801	49/49	0.92	0.17	74,90,111,117	0
5	CLA	B	606	57/65	0.92	0.16	78,89,105,109	0
6	CHL	B	614	42/66	0.92	0.14	97,105,111,134	0

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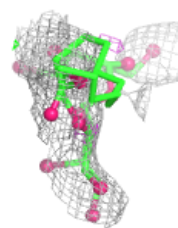
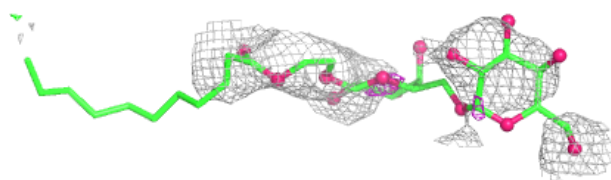
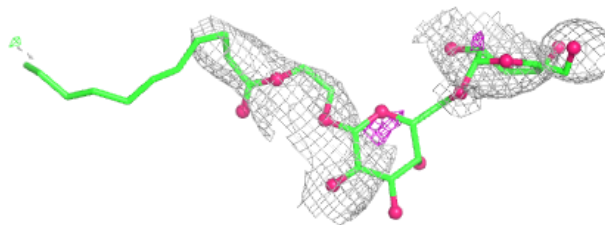
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NEX	B	503	44/44	0.92	0.15	64,96,126,131	0
5	CLA	B	604	65/65	0.93	0.14	56,69,95,100	0
6	CHL	B	610	66/66	0.93	0.13	65,79,106,108	0
6	CHL	A	609	66/66	0.93	0.13	75,85,97,100	0
5	CLA	C	606	57/65	0.93	0.14	80,91,107,111	0
6	CHL	C	609	66/66	0.93	0.14	77,85,98,101	0
6	CHL	C	610	66/66	0.93	0.13	67,81,108,110	0
5	CLA	C	603	65/65	0.93	0.14	75,85,102,105	0
6	CHL	A	613	46/66	0.93	0.11	73,81,107,120	0
5	CLA	C	604	65/65	0.94	0.14	60,72,97,102	0
4	XAT	C	504	44/44	0.94	0.15	65,91,117,149	0
6	CHL	A	610	66/66	0.94	0.14	65,80,108,110	0
4	XAT	B	504	44/44	0.94	0.13	63,89,115,147	0
6	CHL	B	612	66/66	0.94	0.12	74,83,100,102	0
5	CLA	A	604	65/65	0.94	0.12	59,71,96,101	0
6	CHL	B	613	46/66	0.95	0.10	71,80,106,119	0
6	CHL	B	609	66/66	0.95	0.12	75,83,95,99	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.

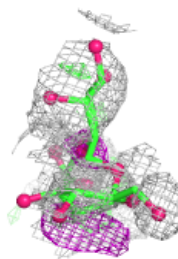
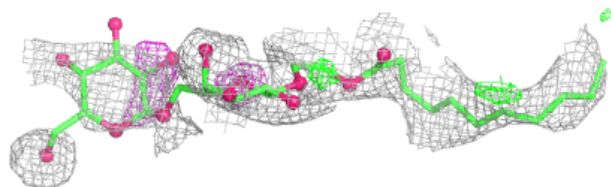
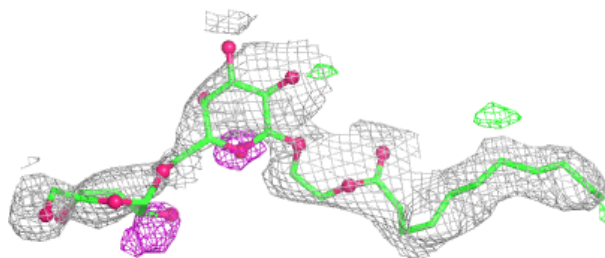


Electron density around DGD C 802:

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

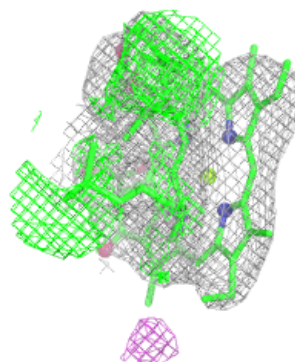
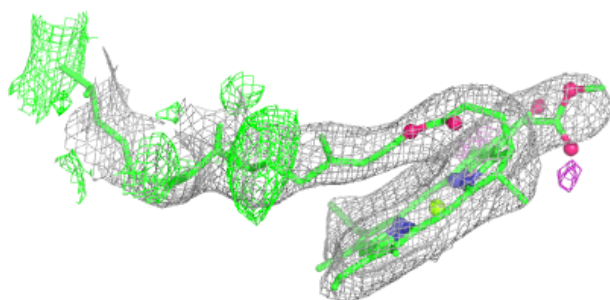
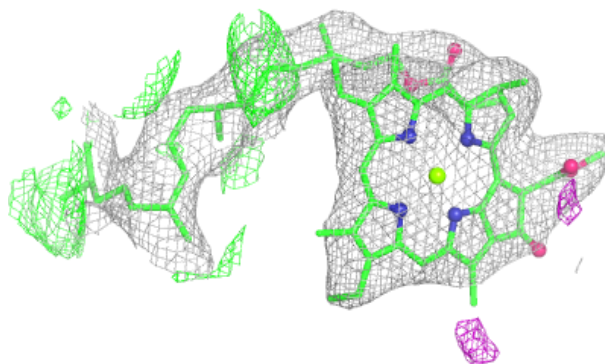
**Electron density around DGD A 802:**

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

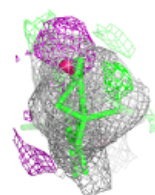
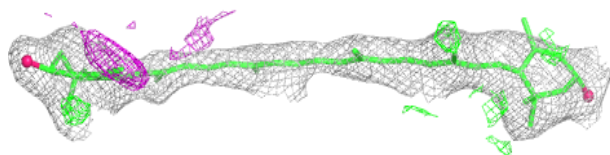
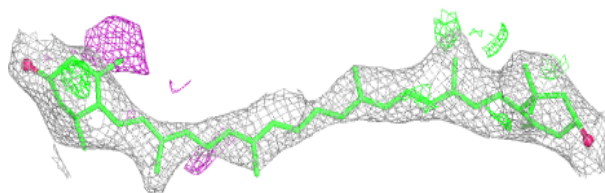


Electron density around CLA B 601:

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

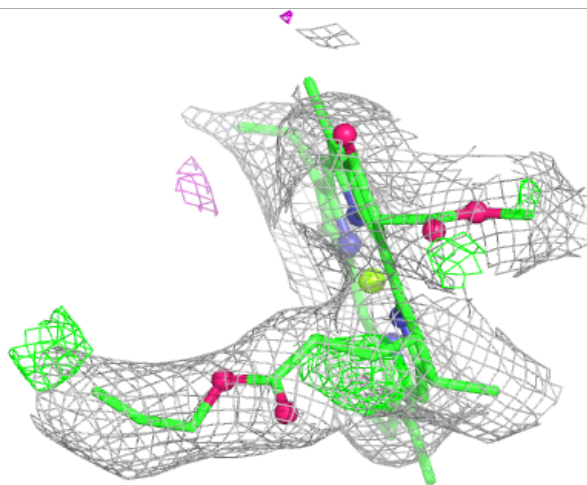
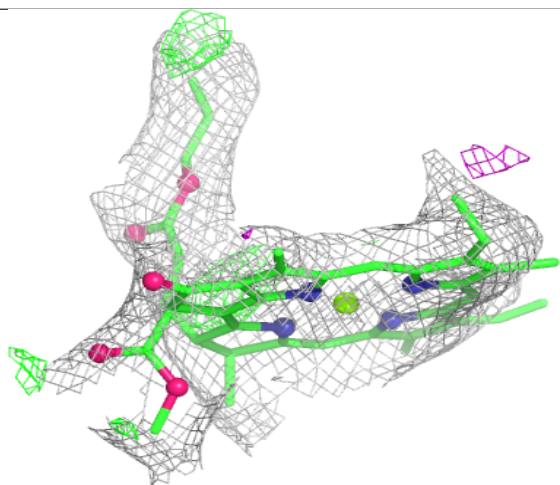
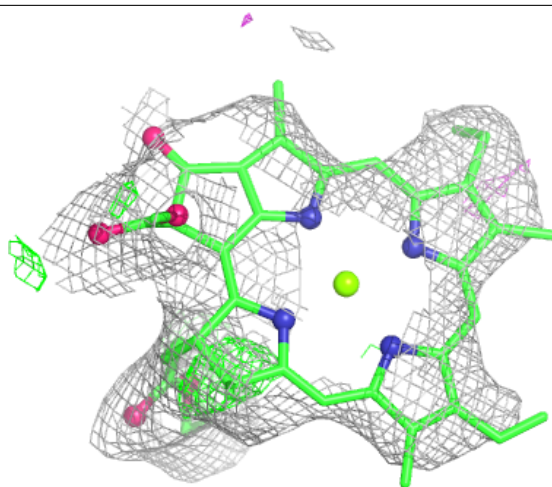
**Electron density around LUX B 501:**

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



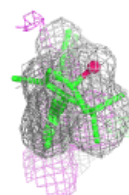
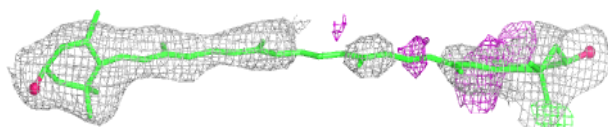
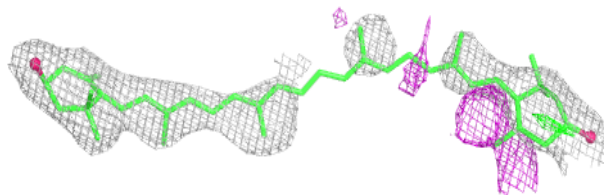
Electron density around CLA B 608:

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

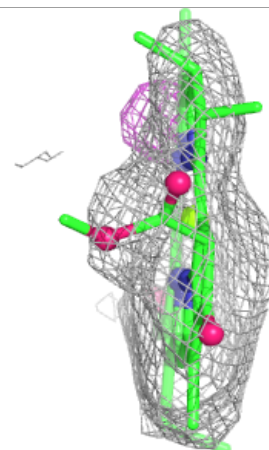
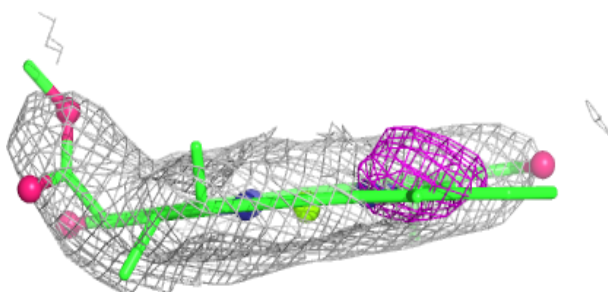
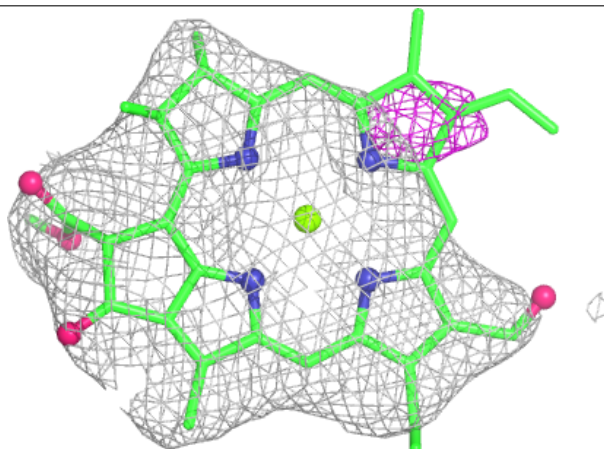


Electron density around LUX C 501:

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

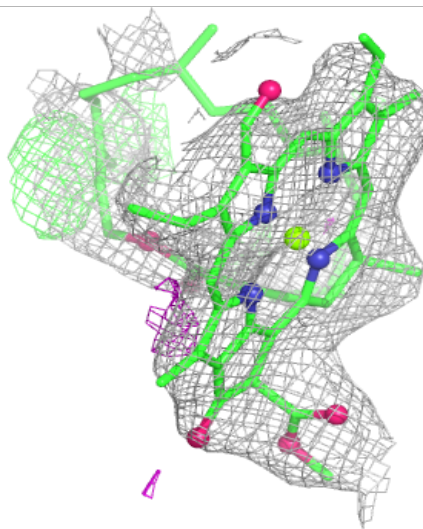
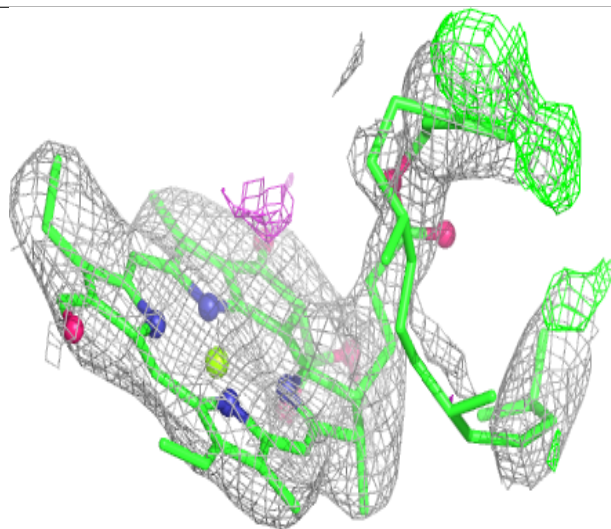
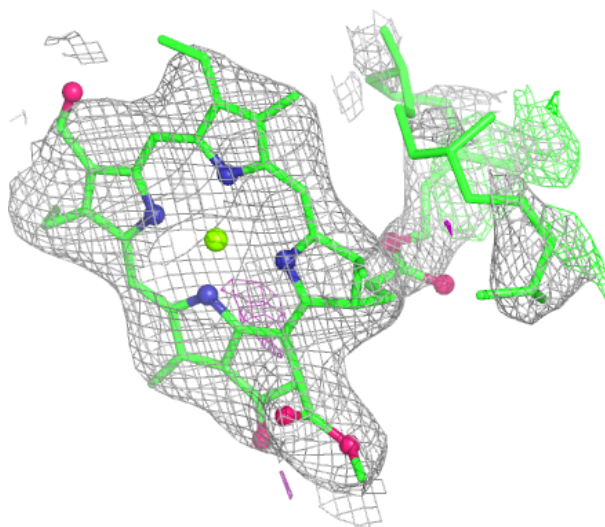
**Electron density around CHL C 614:**

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



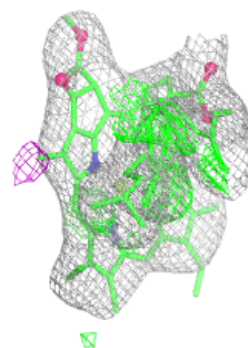
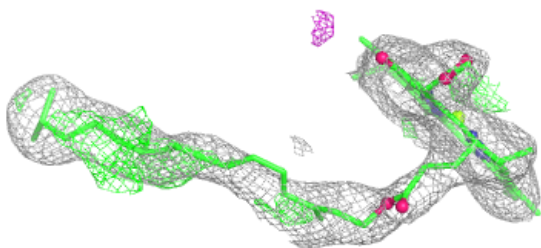
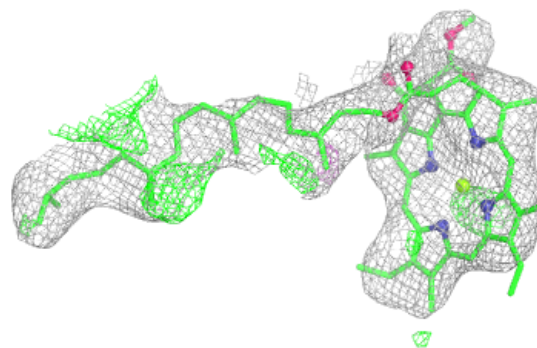
Electron density around CHL B 611:

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



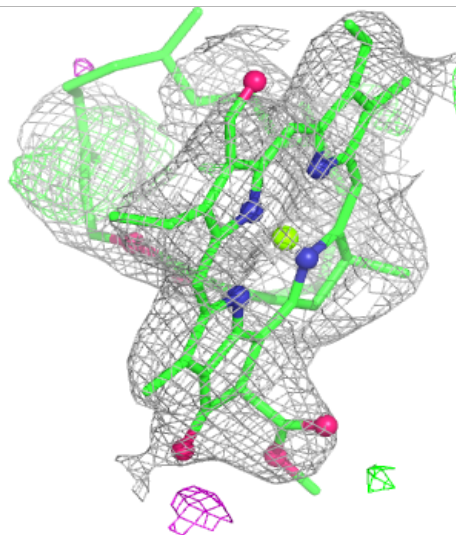
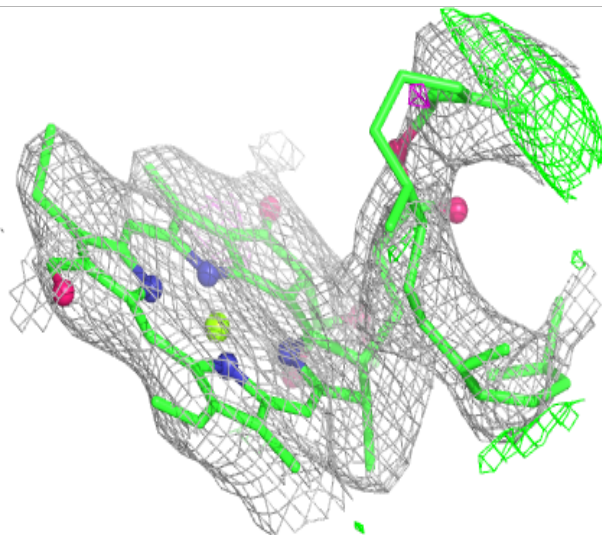
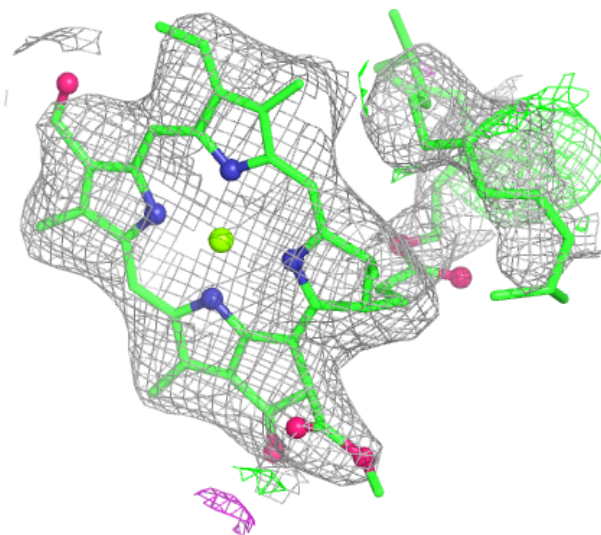
Electron density around CLA B 607:

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



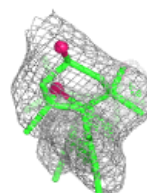
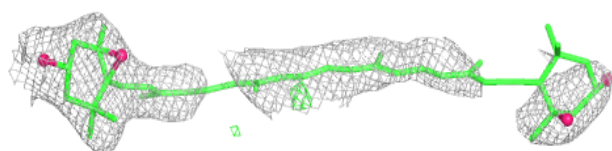
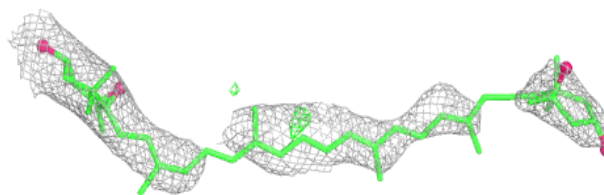
Electron density around CHL C 611:

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

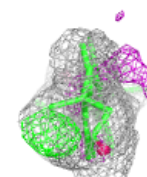
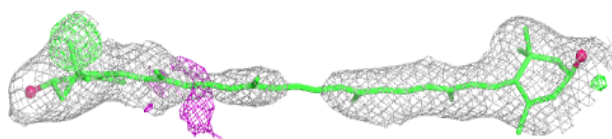
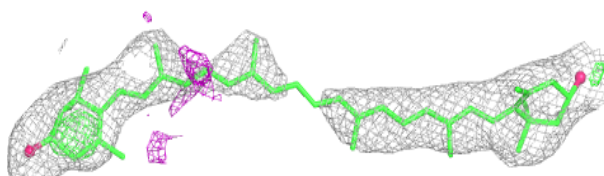


Electron density around NEX C 503:

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

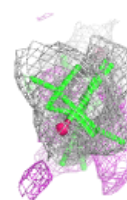
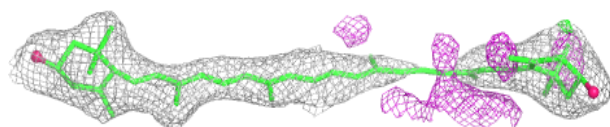
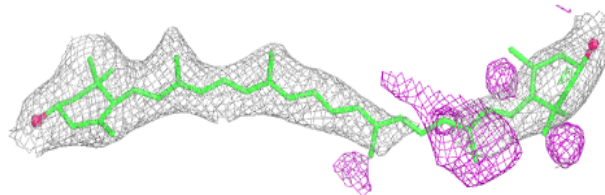
**Electron density around LUX A 501:**

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

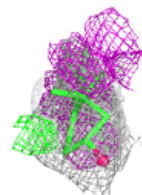
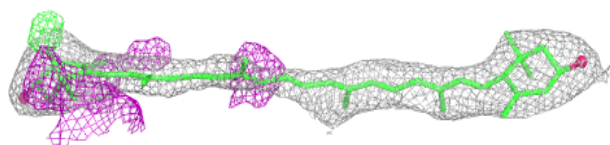
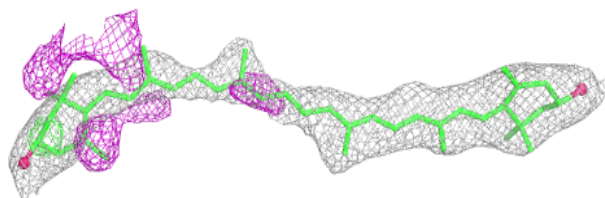


Electron density around LUX B 502:

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

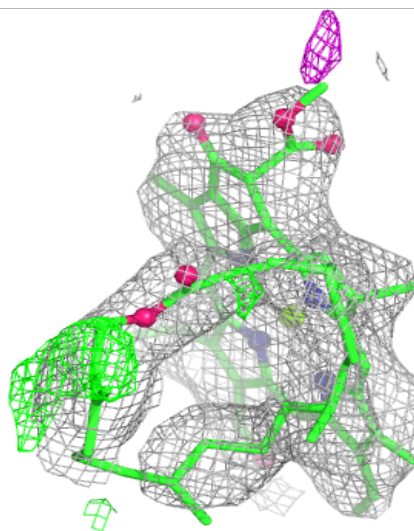
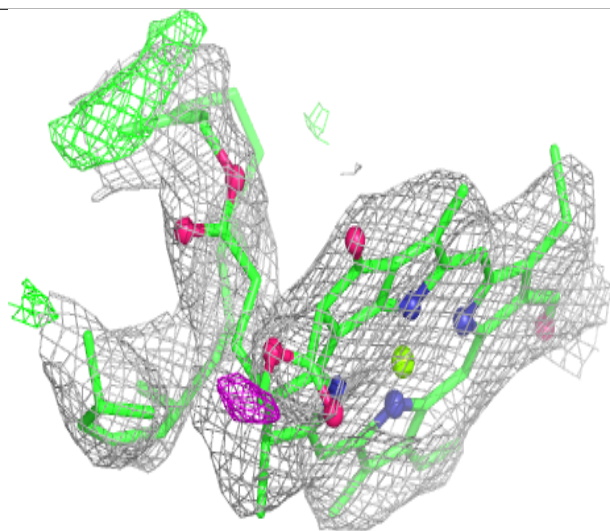
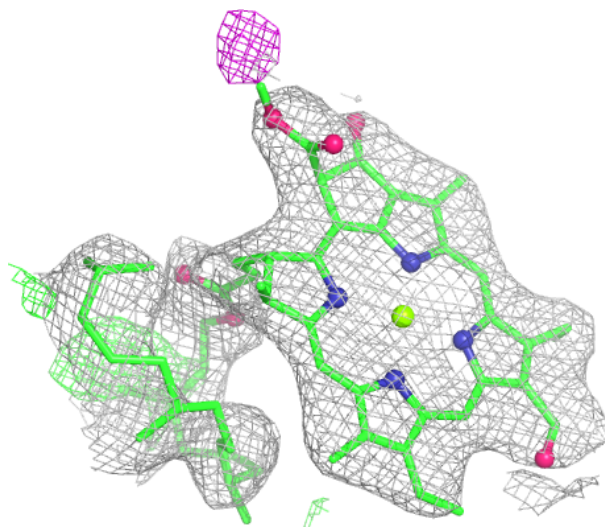
**Electron density around LUX A 502:**

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



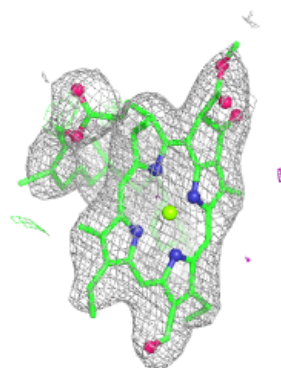
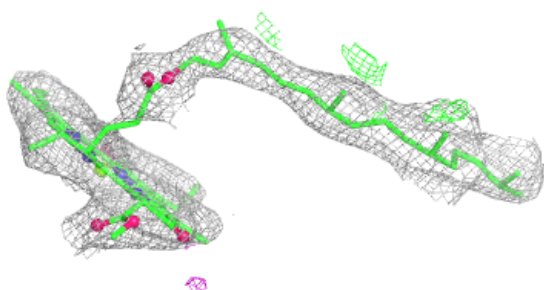
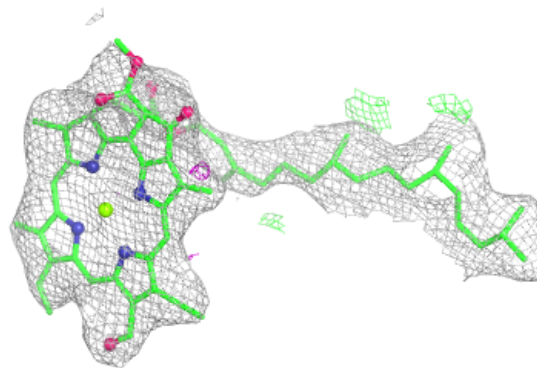
Electron density around CHL A 611:

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

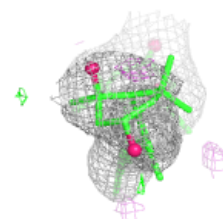
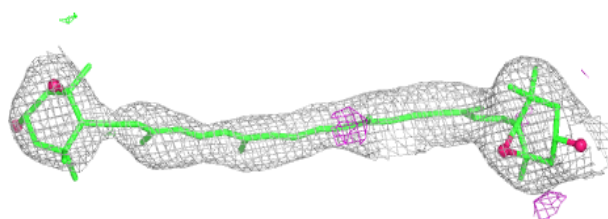
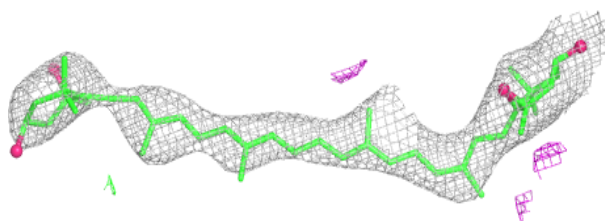


Electron density around CHL A 612:

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

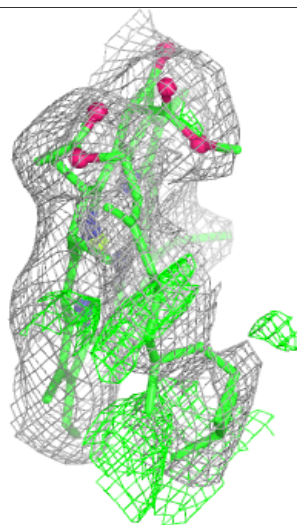
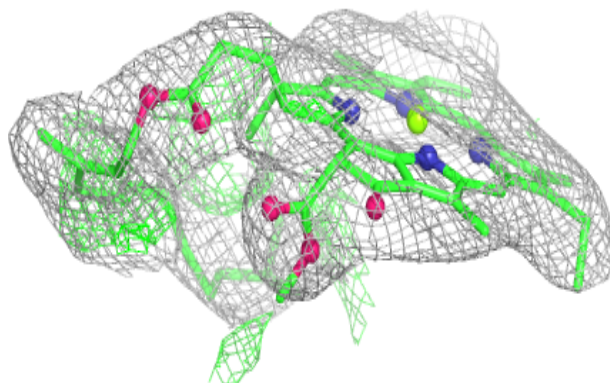
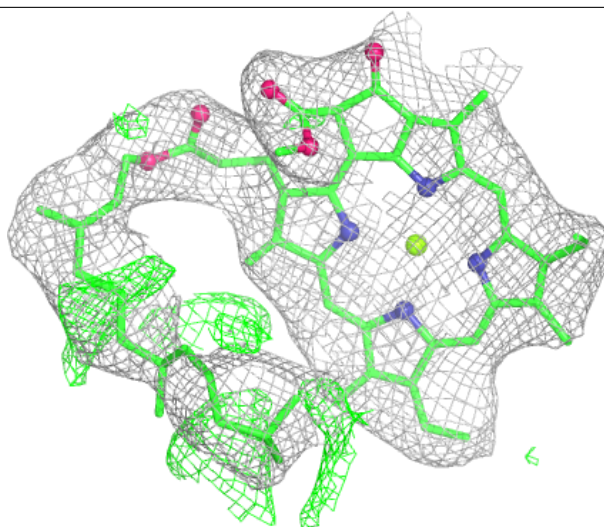
**Electron density around NEX A 503:**

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



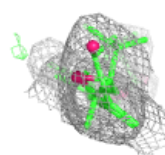
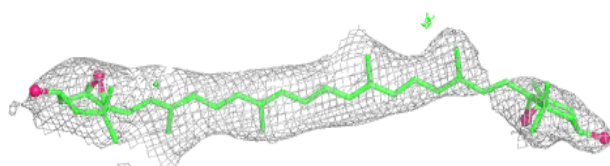
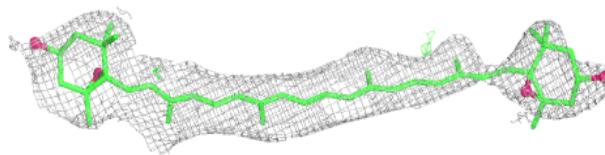
Electron density around CLA B 602:

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



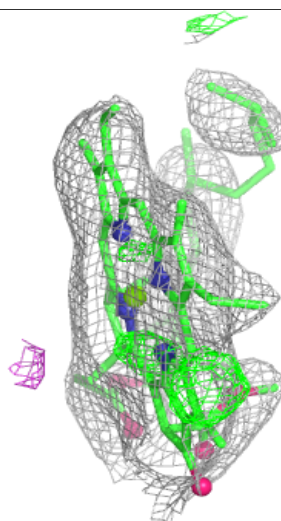
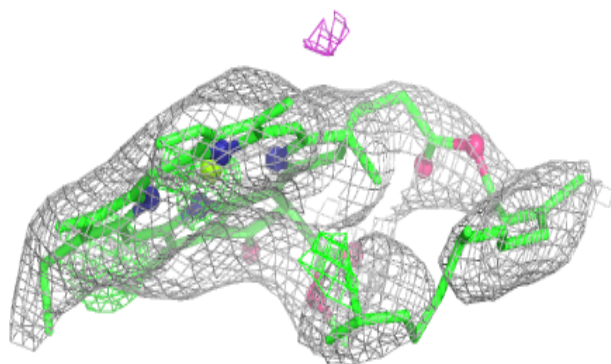
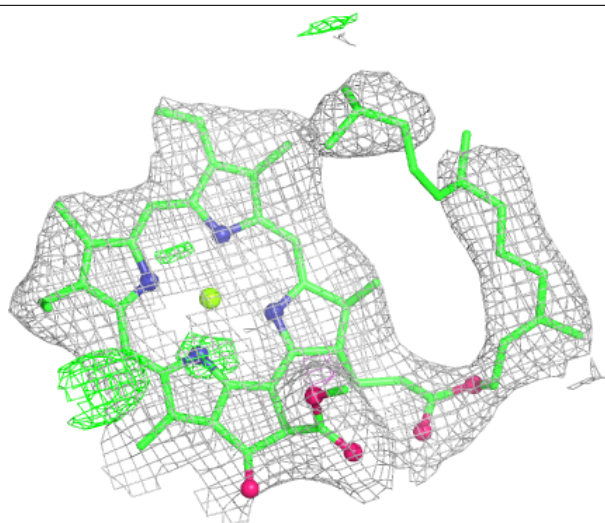
Electron density around XAT A 504:

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



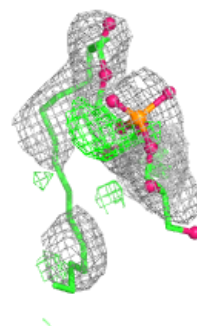
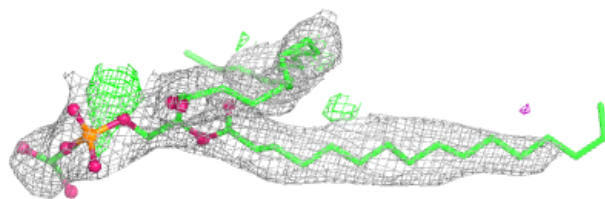
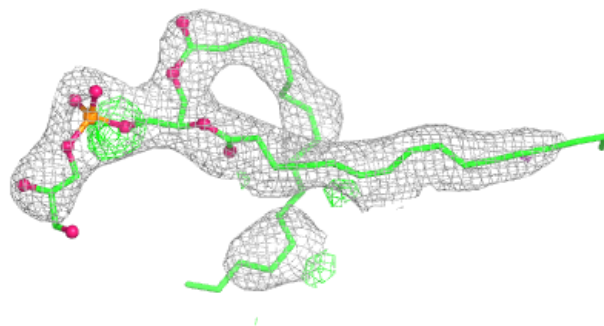
Electron density around CLA A 602:

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and green (positive)



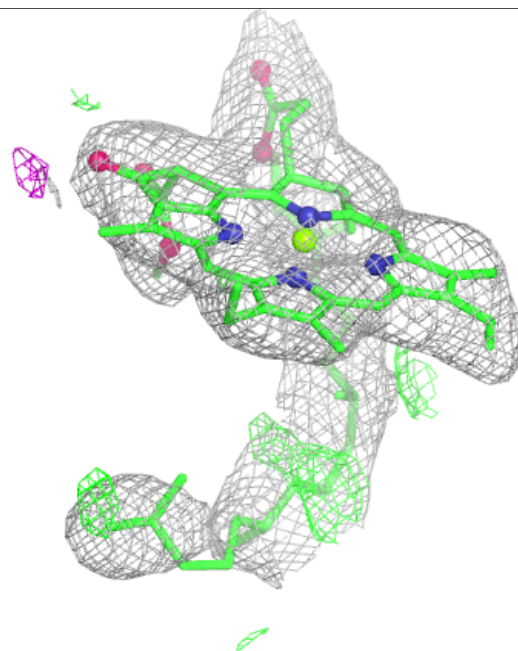
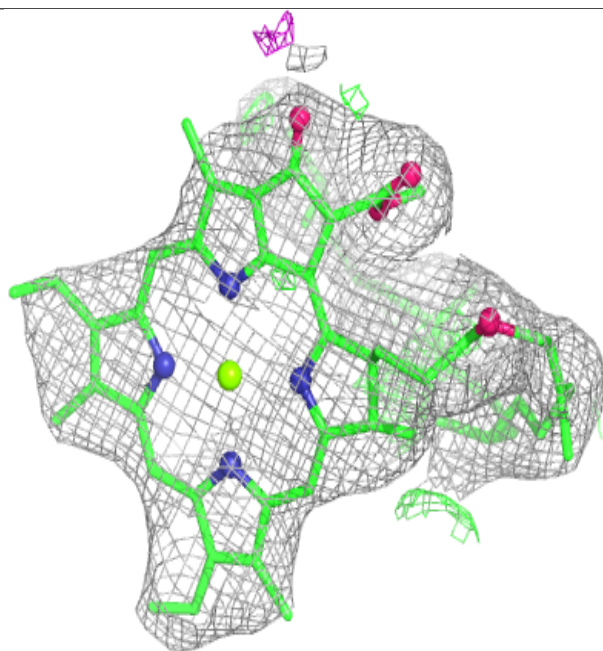
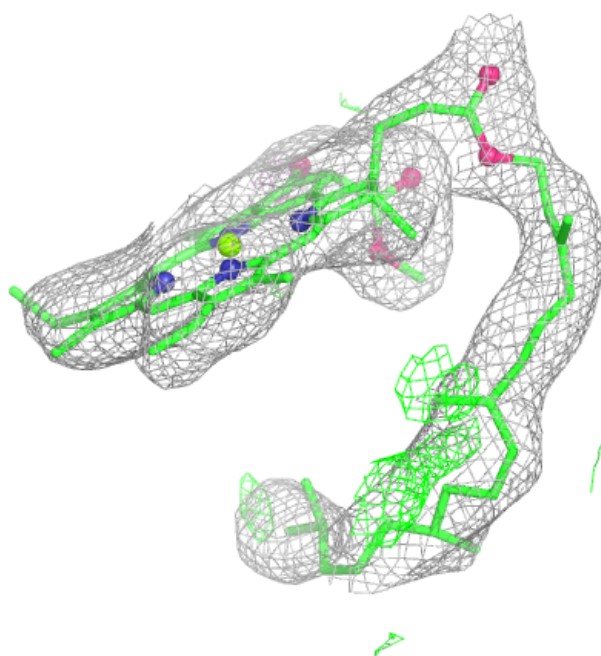
Electron density around LHG B 801:

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



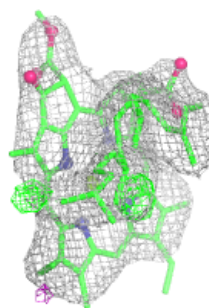
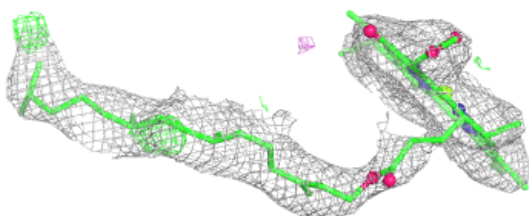
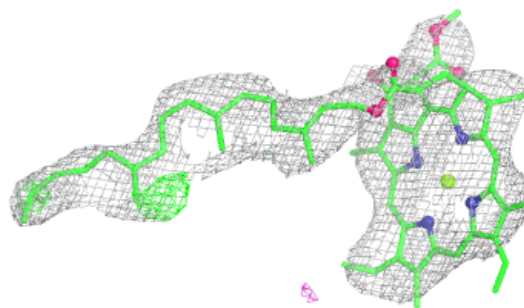
Electron density around CLA C 605:

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



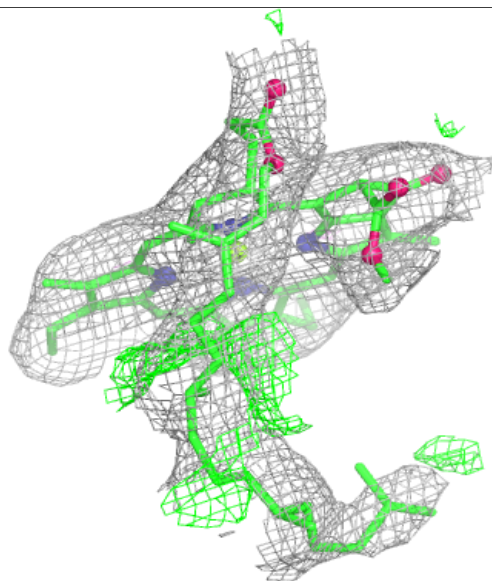
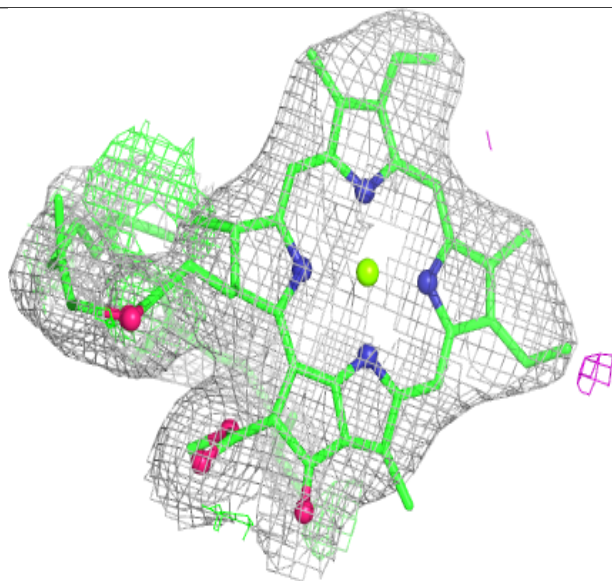
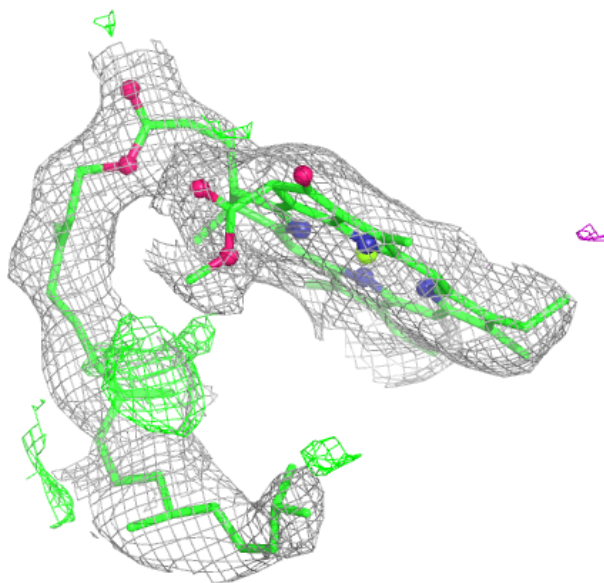
Electron density around CLA C 607:

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



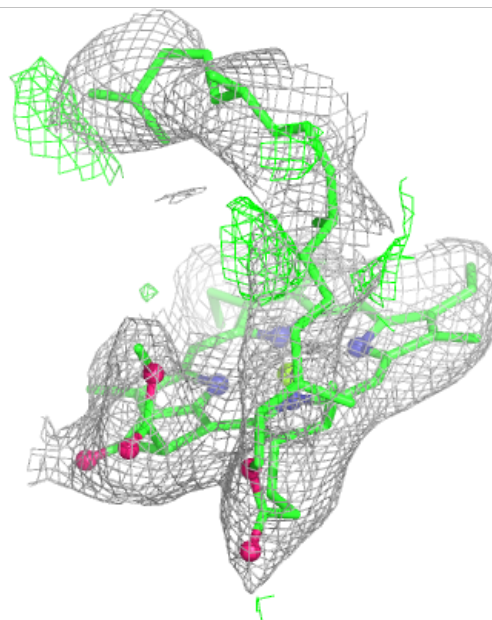
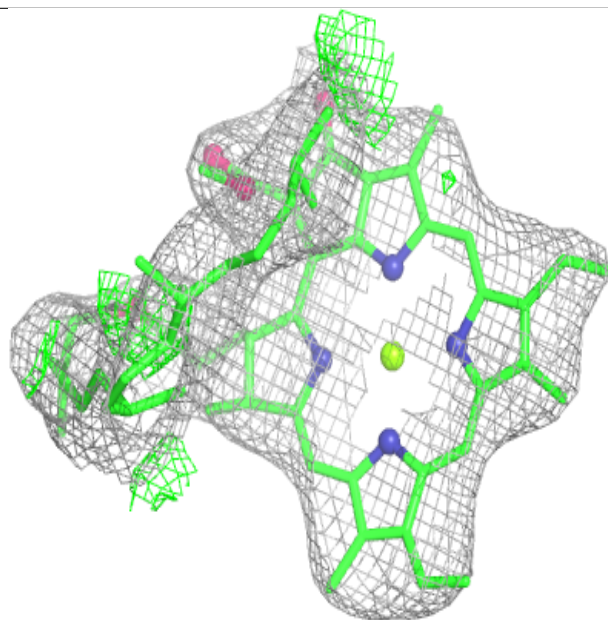
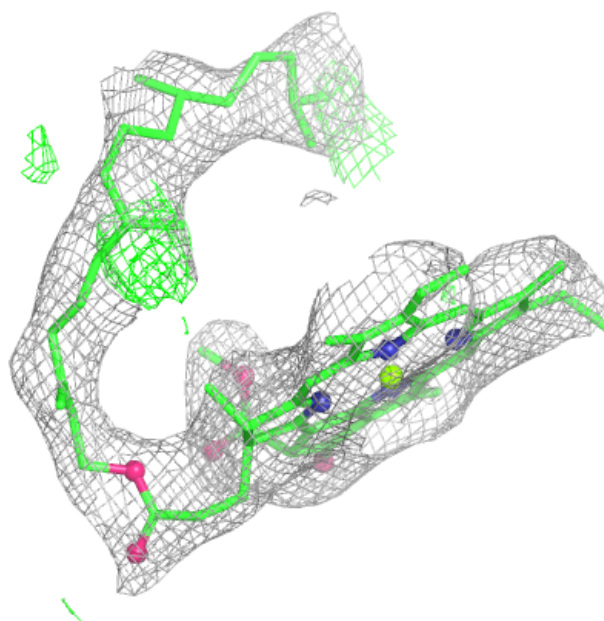
Electron density around CLA A 605:

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



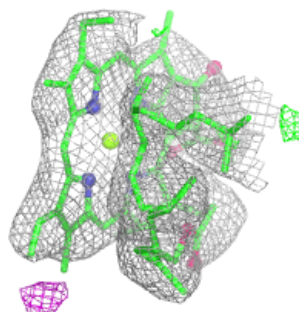
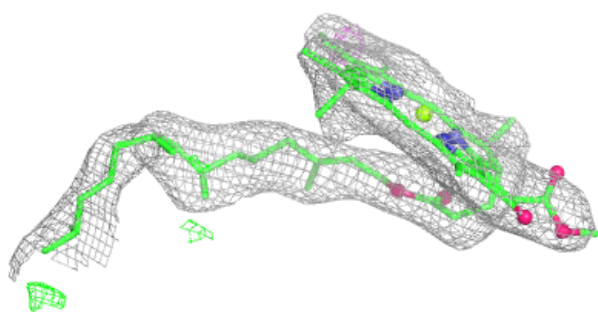
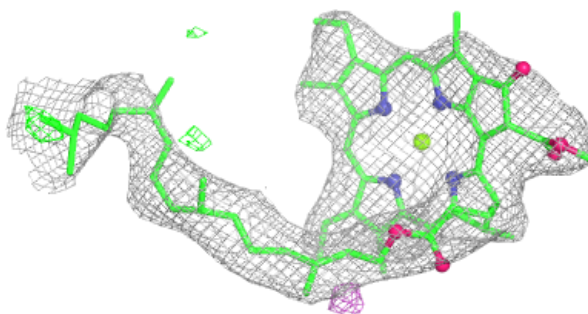
Electron density around CLA B 605:

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

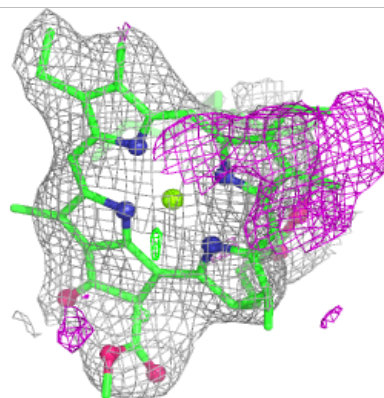
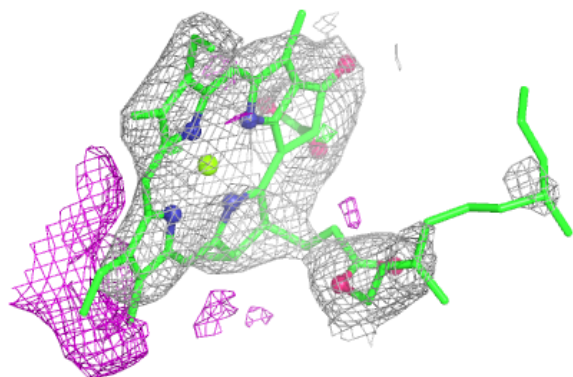
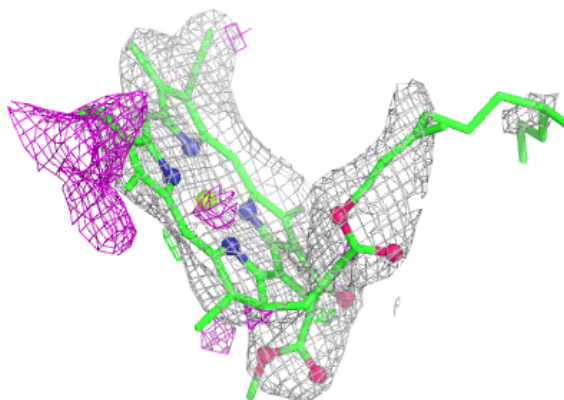


Electron density around CLA A 601:

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

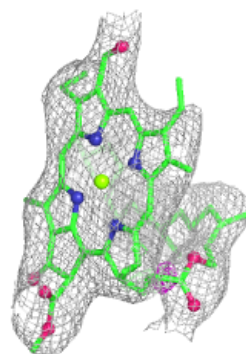
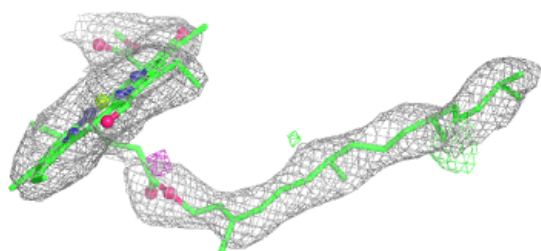
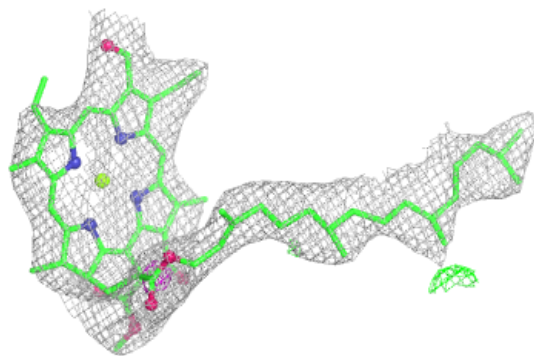
**Electron density around CLA A 606:**

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



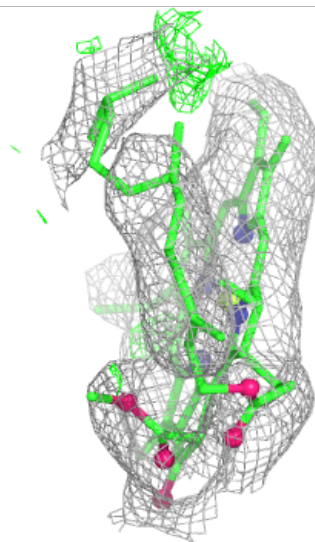
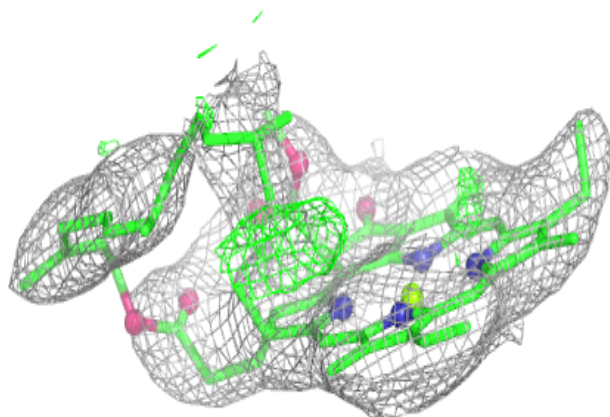
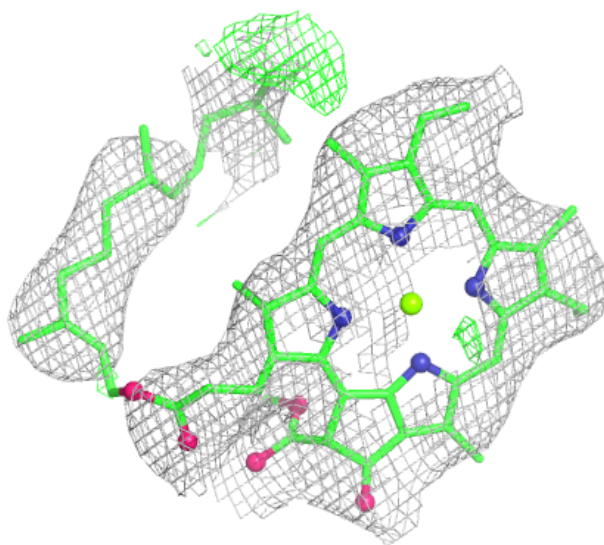
Electron density around CHL C 612:

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



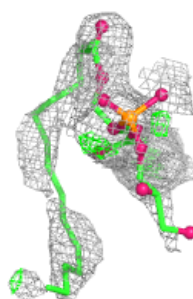
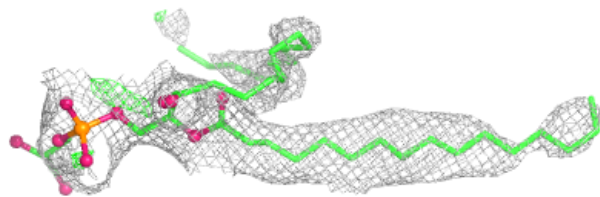
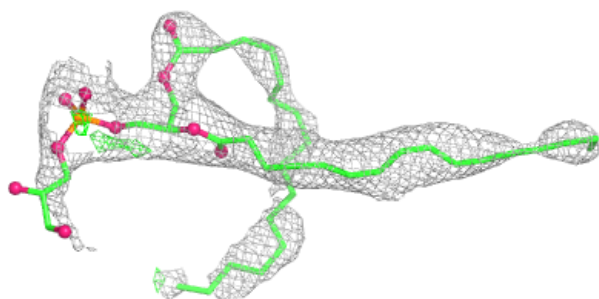
Electron density around CLA C 602:

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



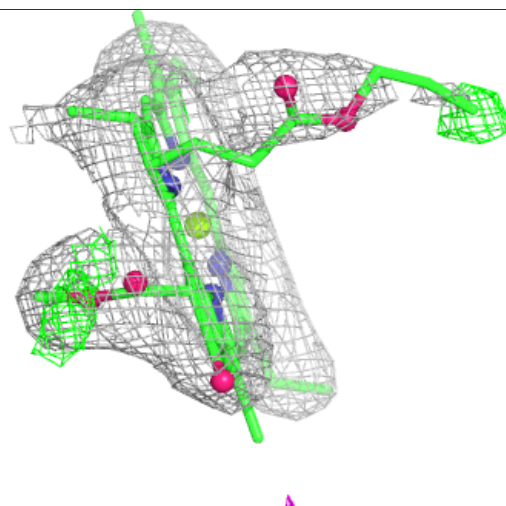
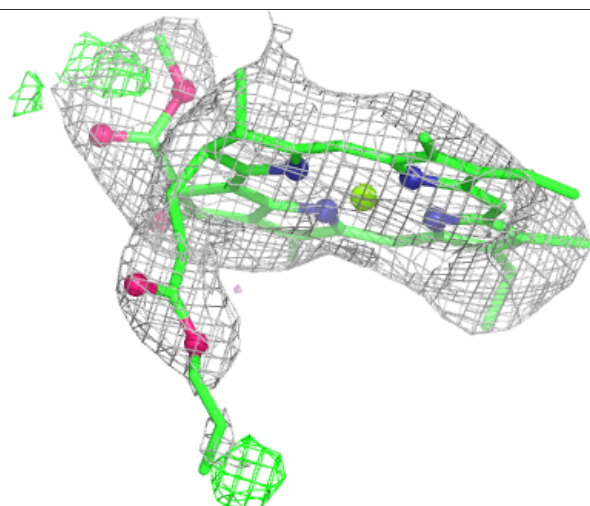
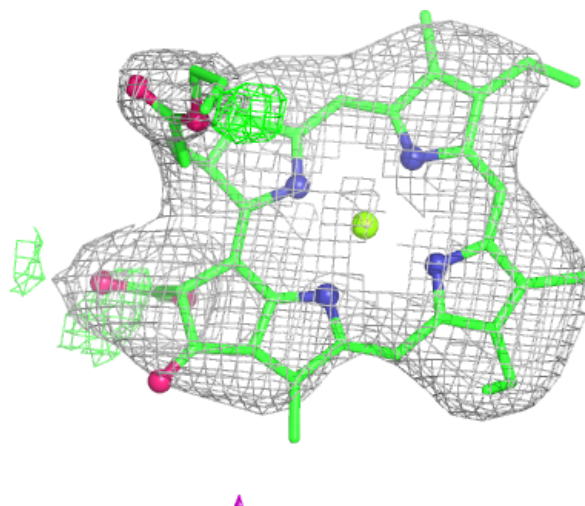
Electron density around LHG A 801:

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



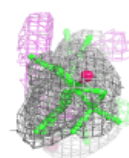
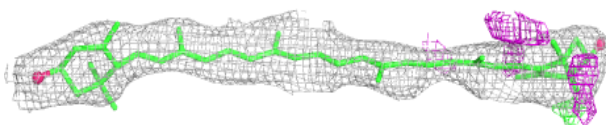
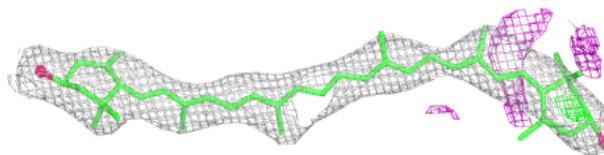
Electron density around CLA A 608:

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

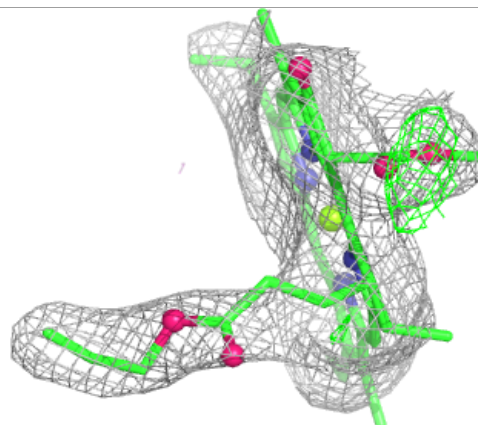
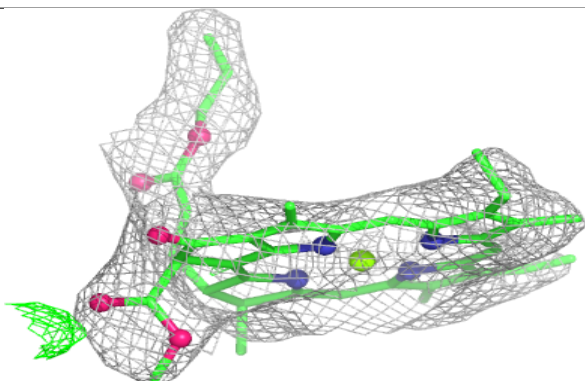
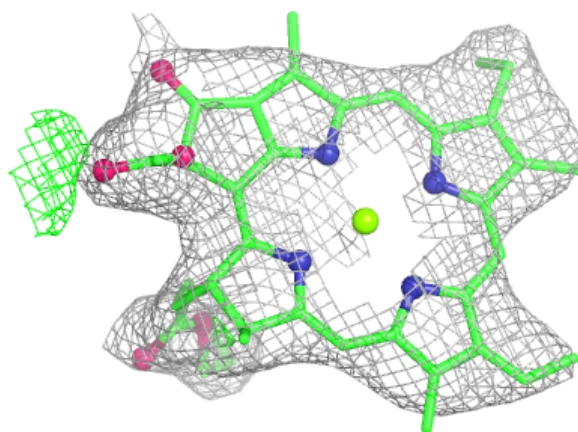


Electron density around LUX C 502:

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

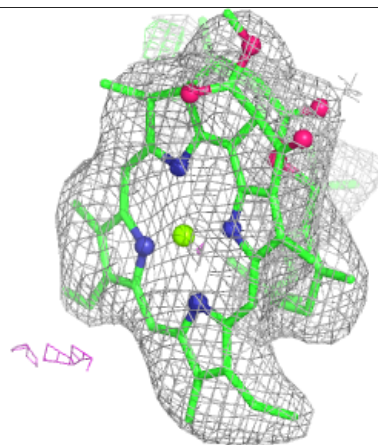
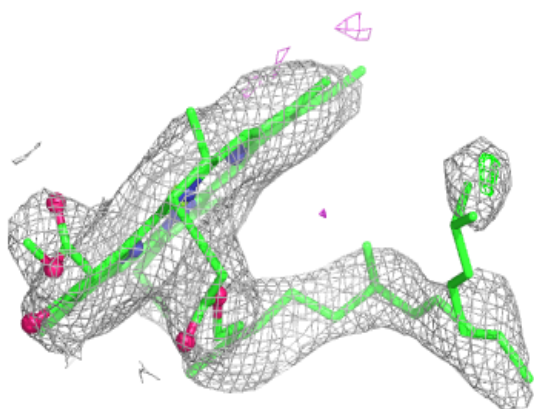
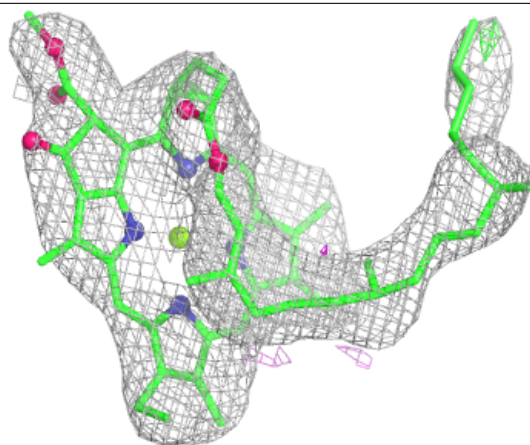
**Electron density around CLA C 608:**

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



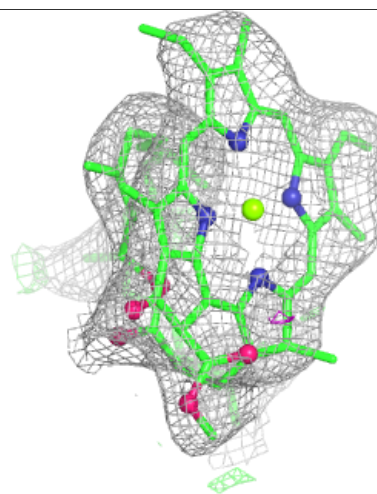
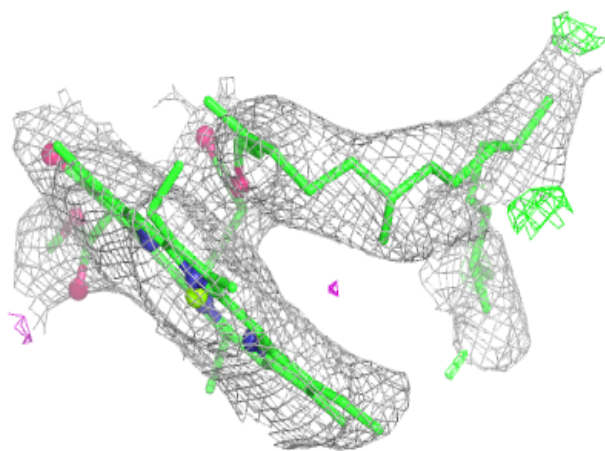
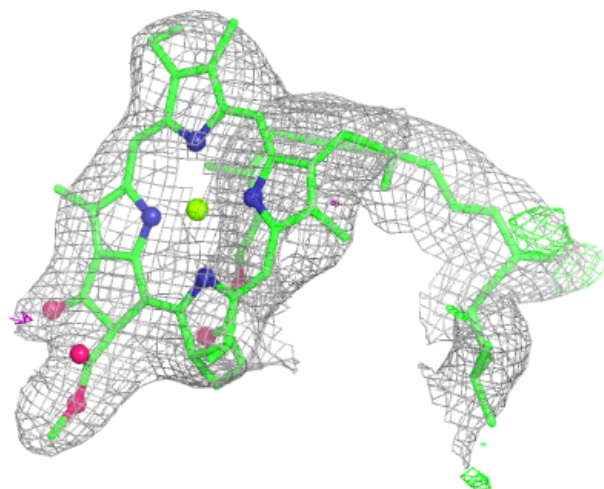
Electron density around CLA A 603:

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



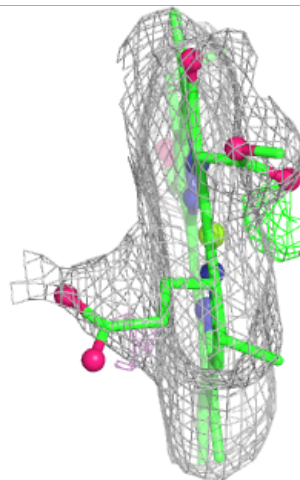
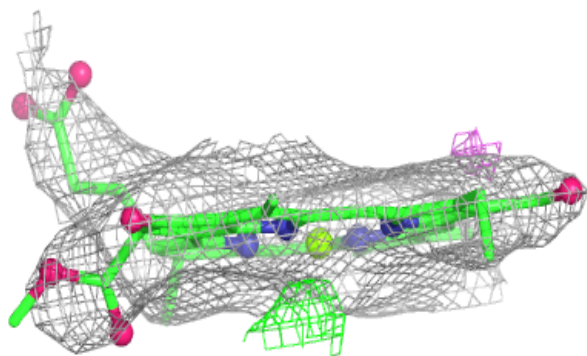
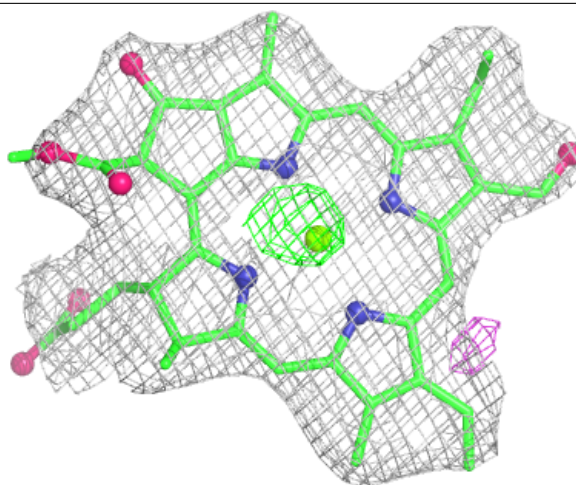
Electron density around CLA B 603:

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



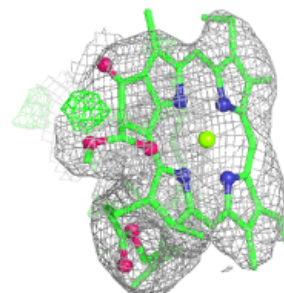
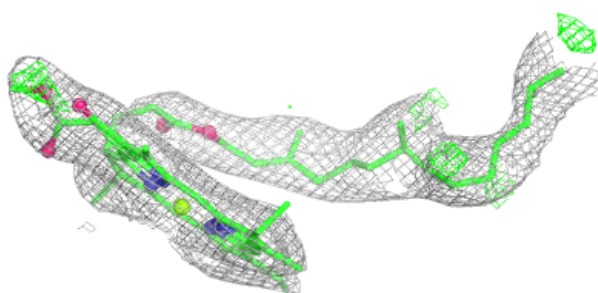
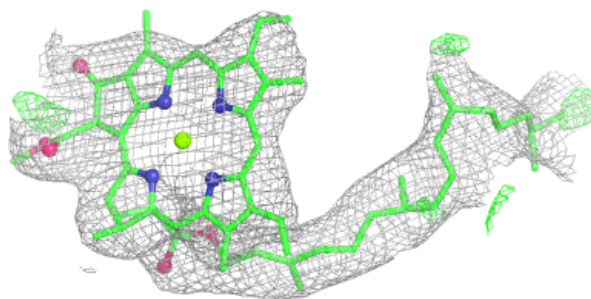
Electron density around CHL C 613:

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

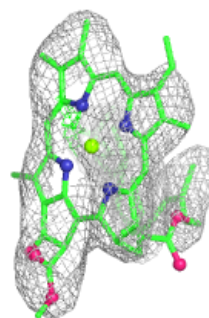
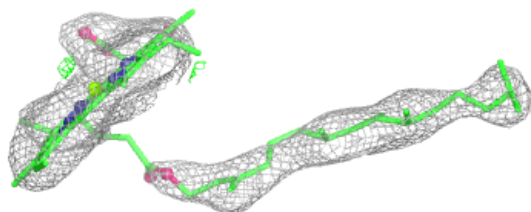
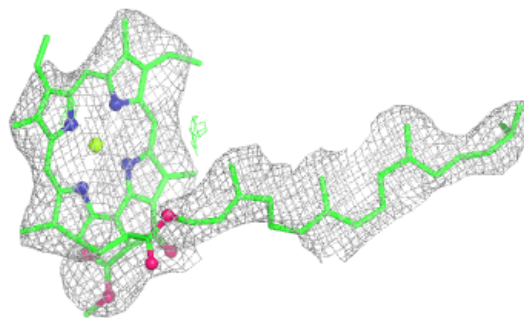


Electron density around CLA C 601:

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

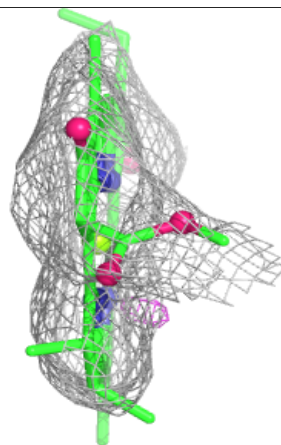
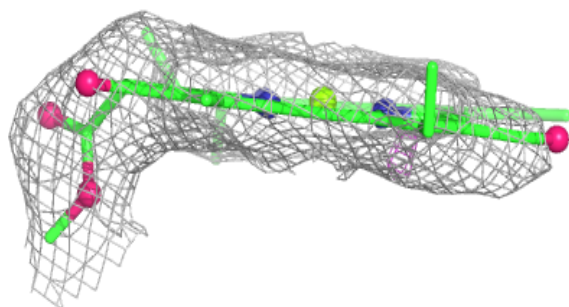
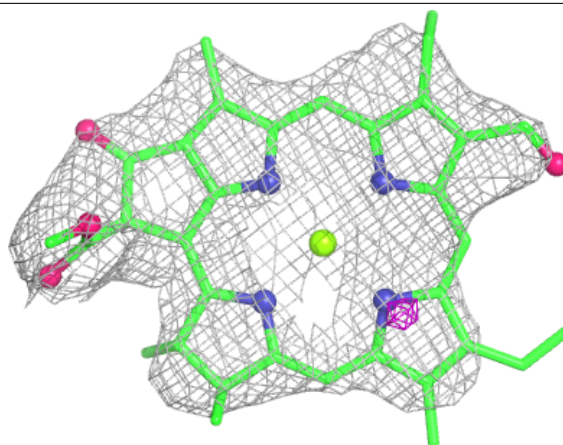
**Electron density around CLA A 607:**

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



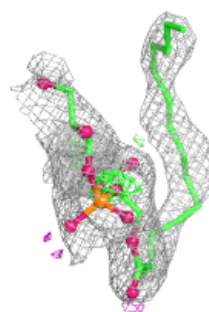
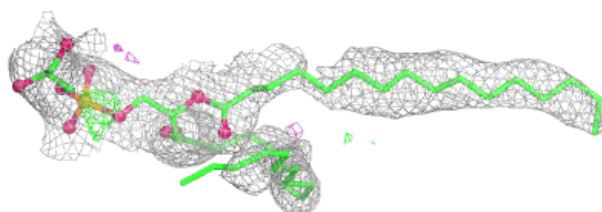
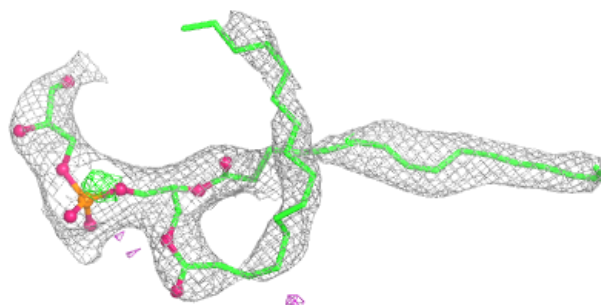
Electron density around CHL A 614:

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



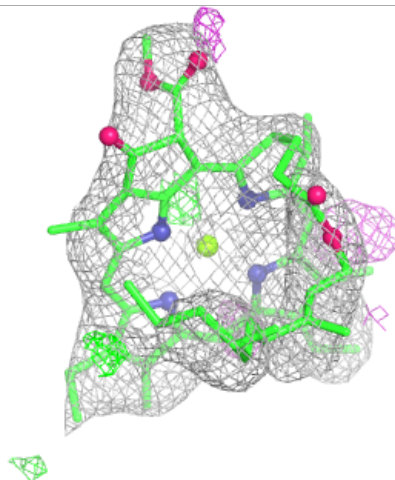
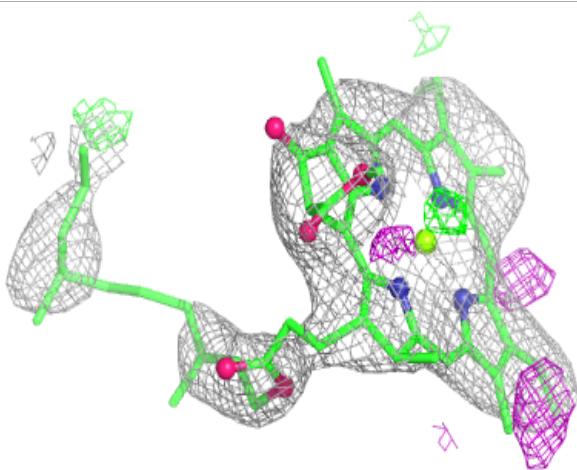
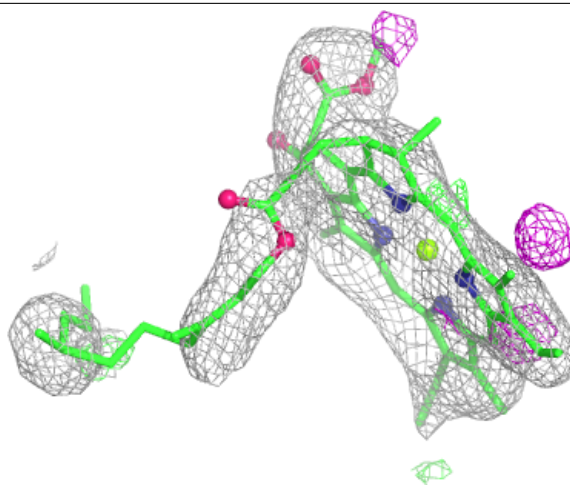
Electron density around LHG C 801:

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



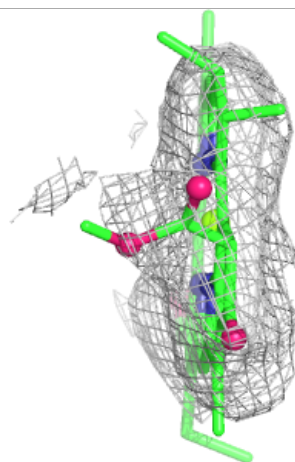
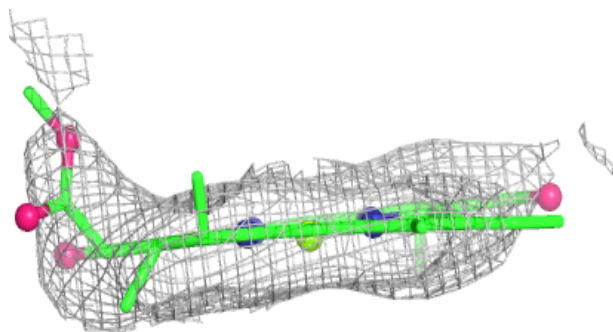
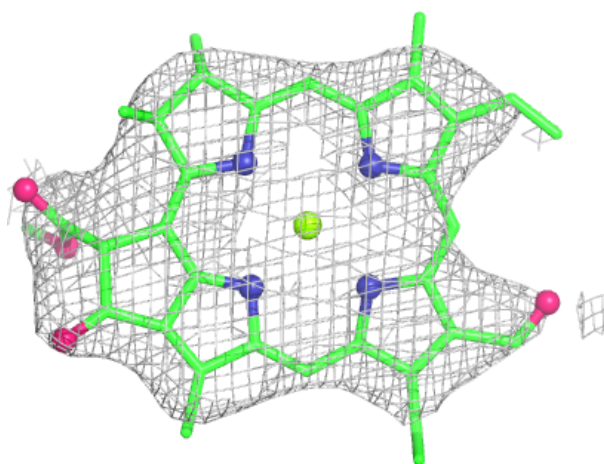
Electron density around CLA B 606:

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



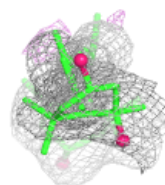
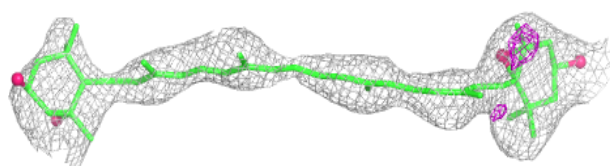
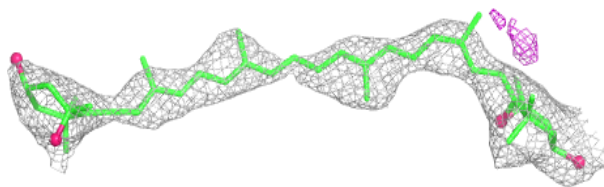
Electron density around CHL B 614:

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

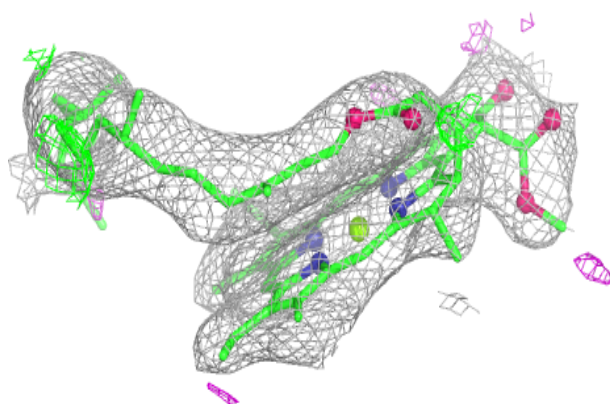
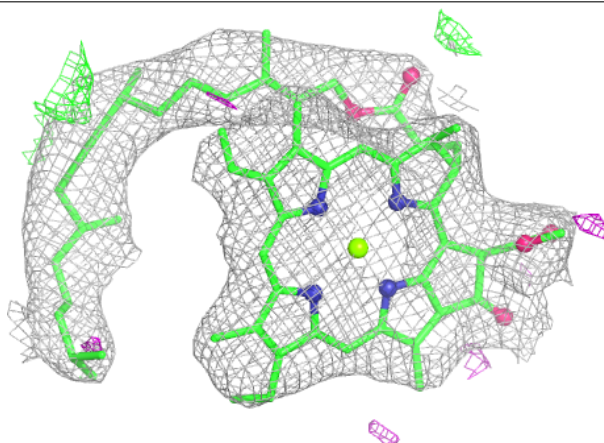


Electron density around NEX B 503:

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

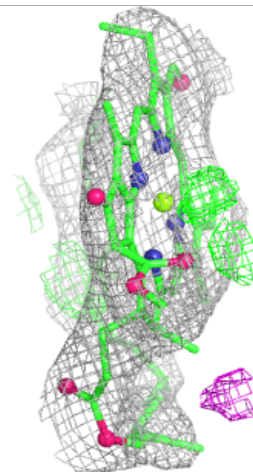
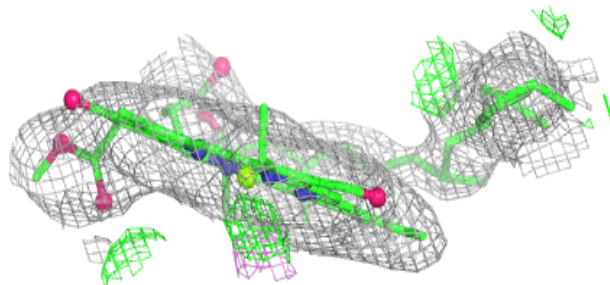
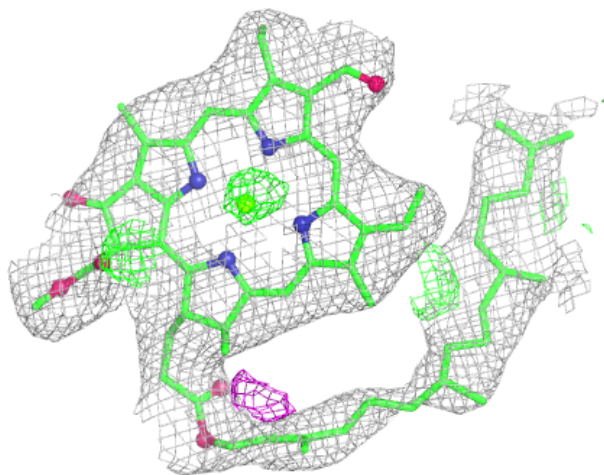
**Electron density around CLA B 604:**

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



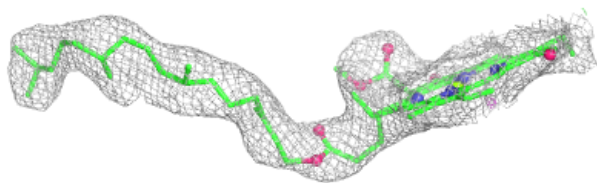
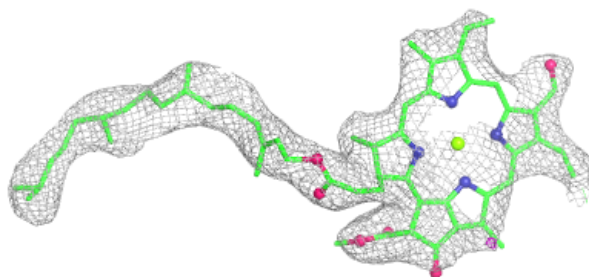
Electron density around CHL B 610:

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

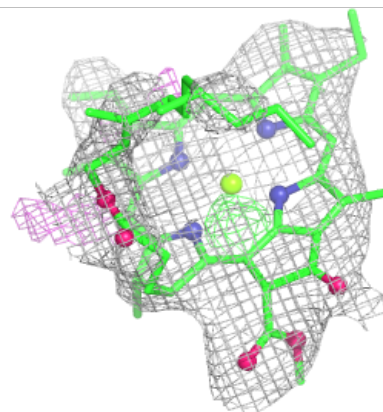
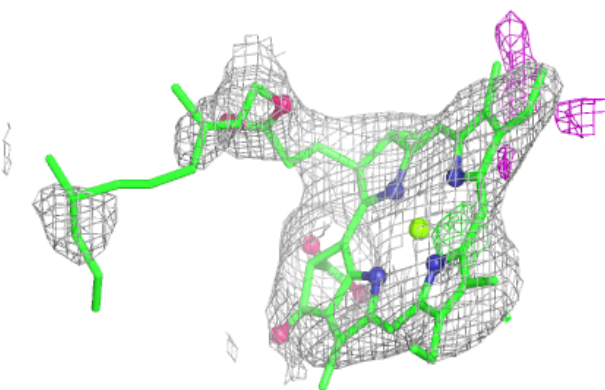
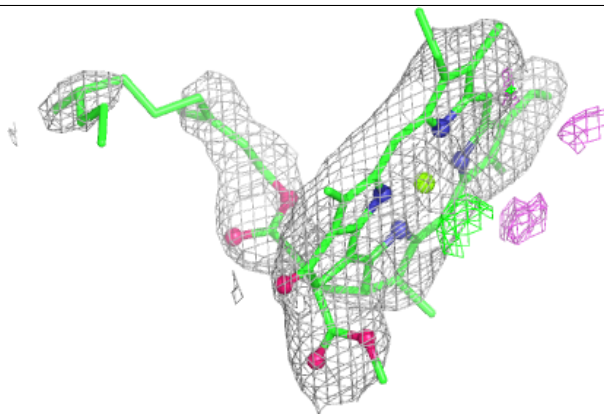


Electron density around CHL A 609:

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

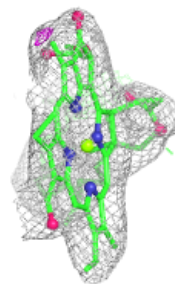
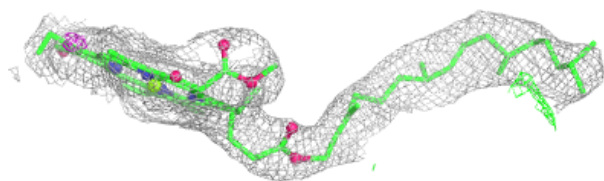
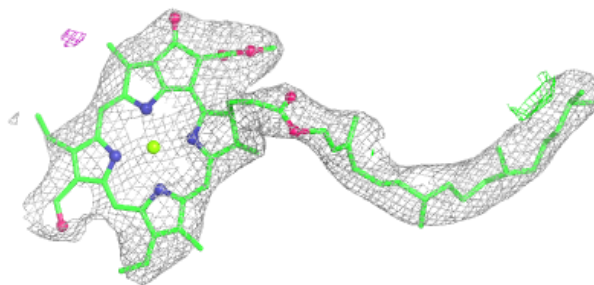
**Electron density around CLA C 606:**

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



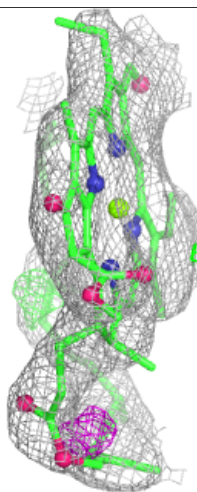
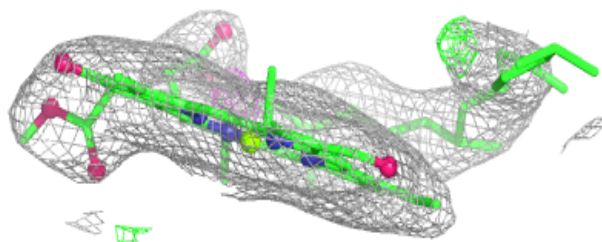
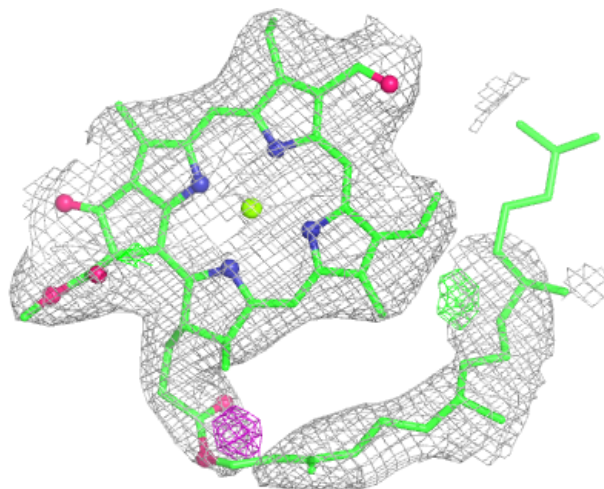
Electron density around CHL C 609:

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



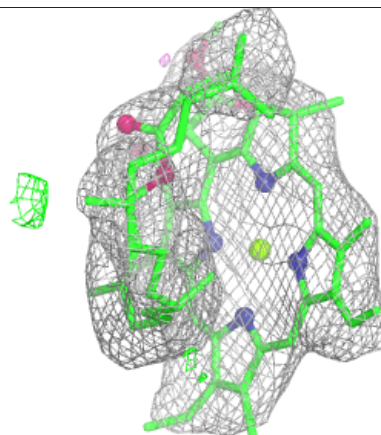
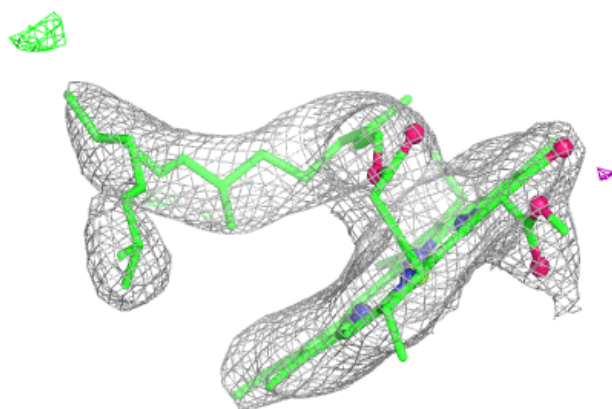
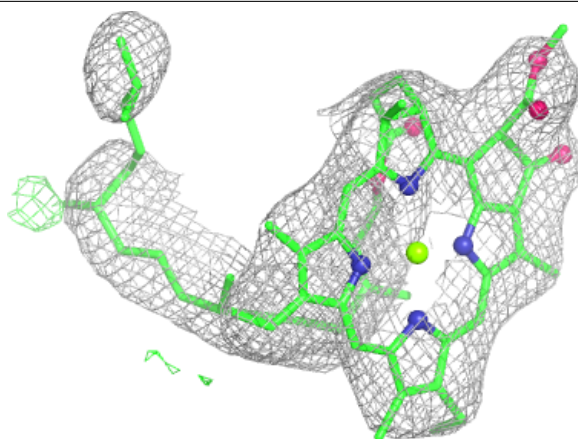
Electron density around CHL C 610:

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

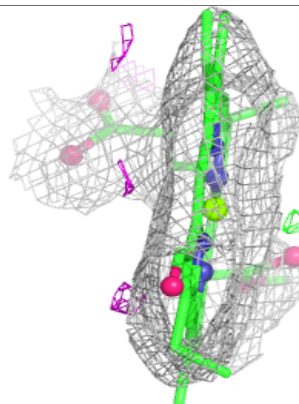
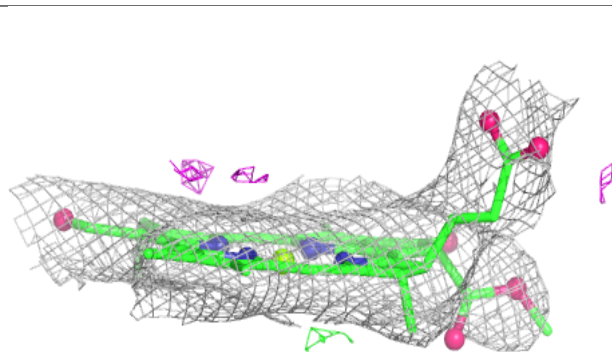
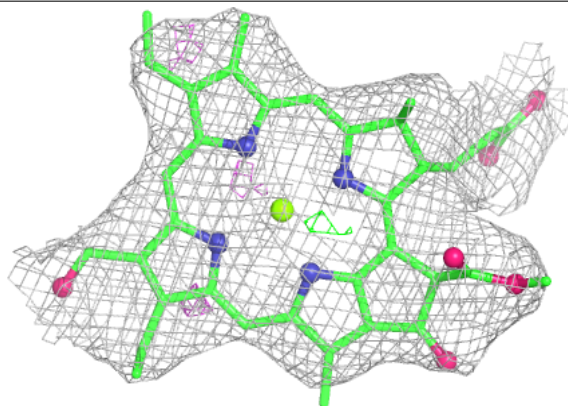


Electron density around CLA C 603:

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

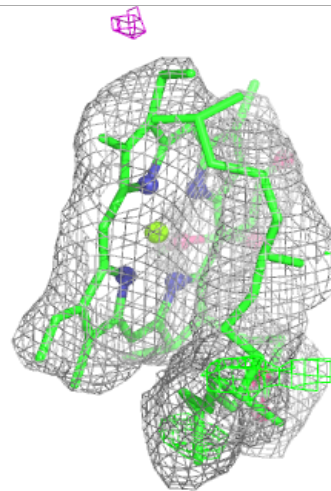
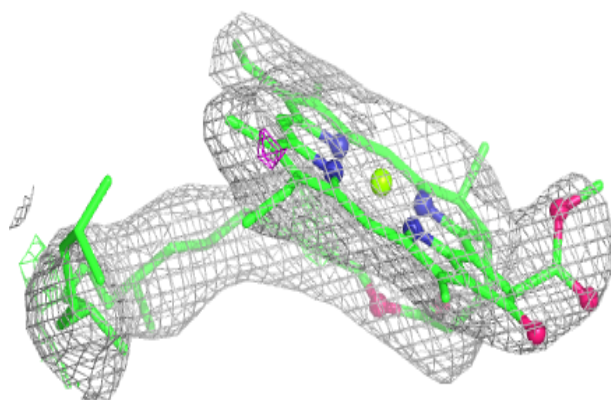
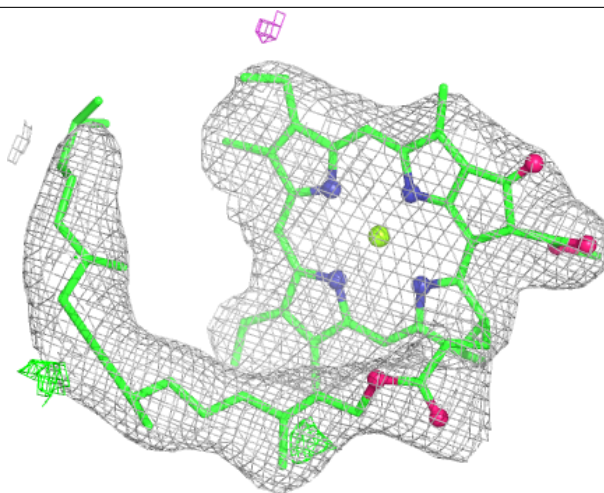
**Electron density around CHL A 613:**

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



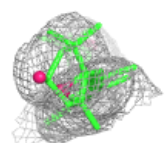
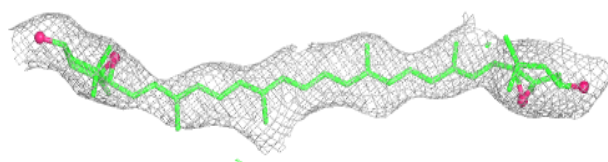
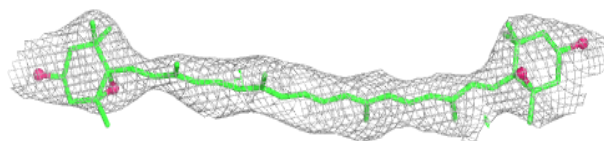
Electron density around CLA C 604:

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



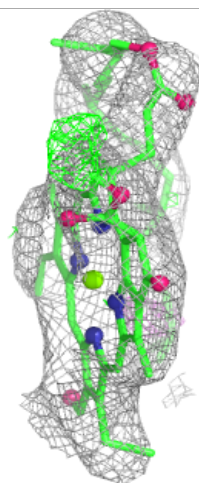
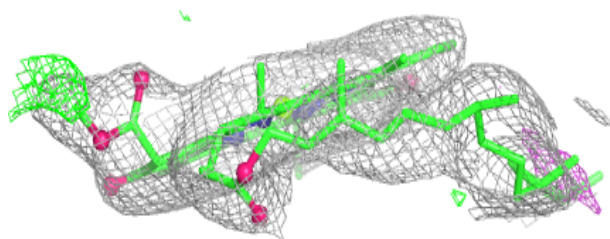
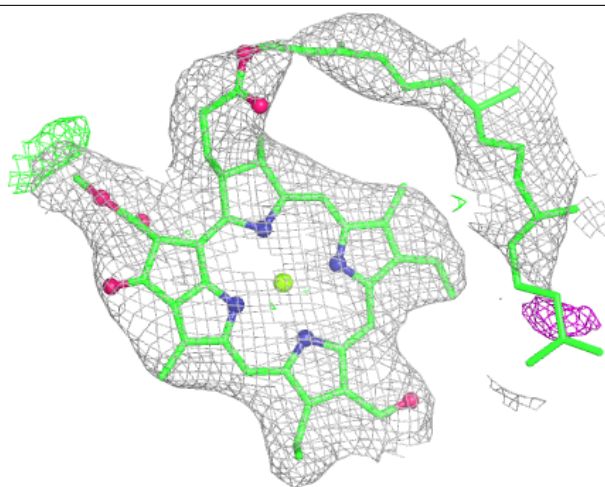
Electron density around XAT C 504:

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



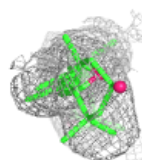
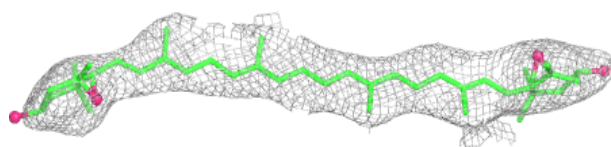
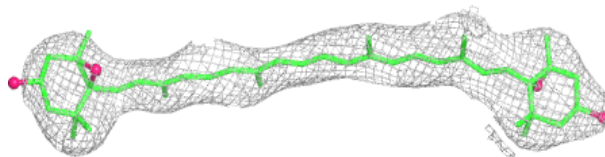
Electron density around CHL A 610:

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

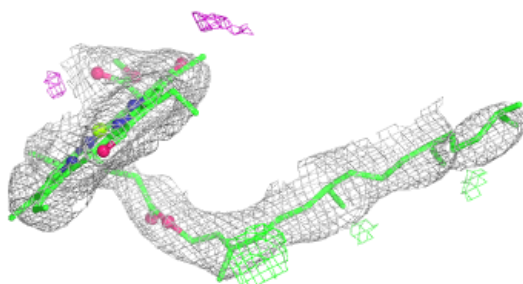
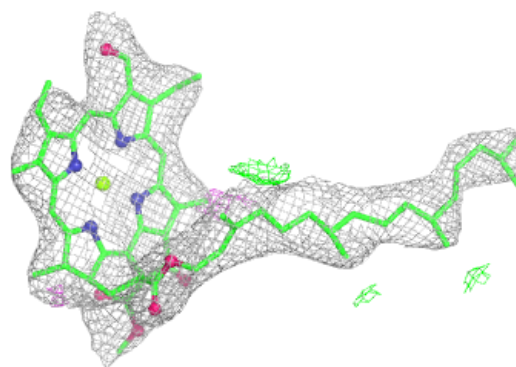


Electron density around XAT B 504:

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

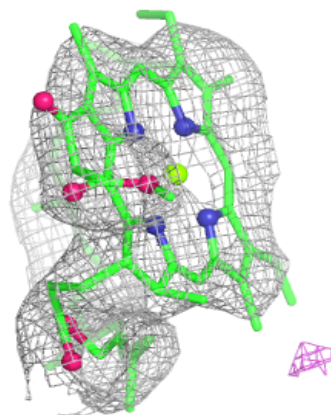
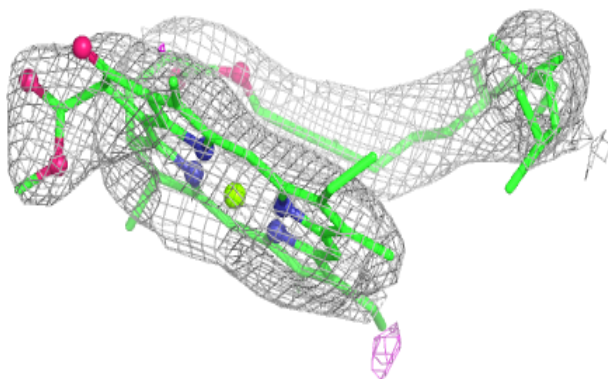
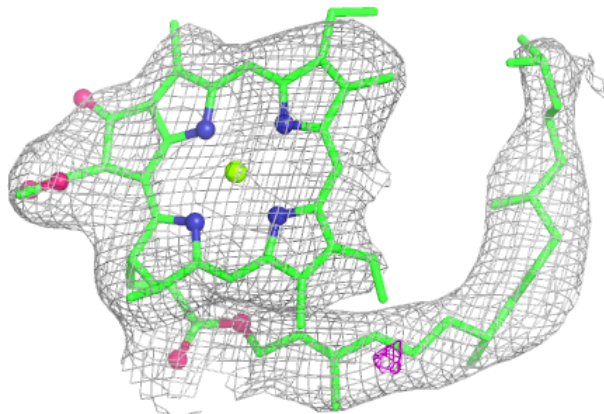
**Electron density around CHL B 612:**

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



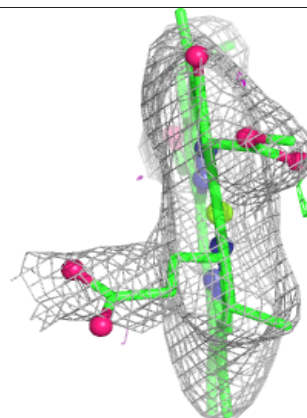
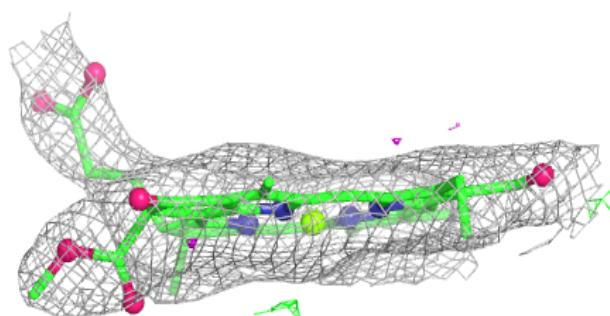
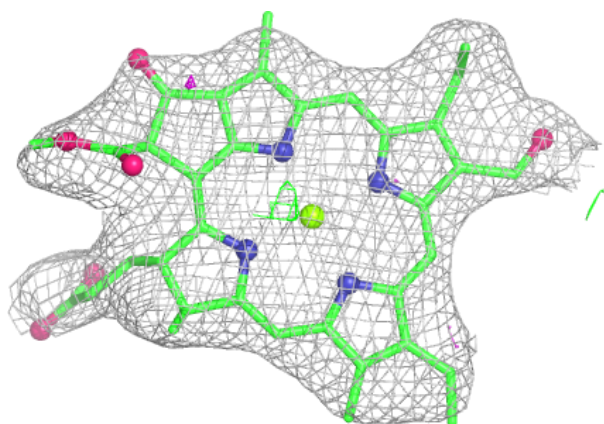
Electron density around CLA A 604:

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

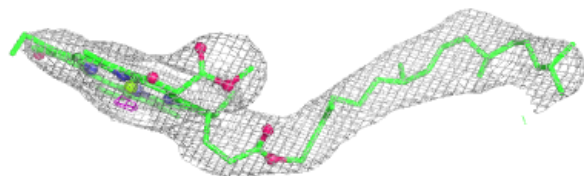
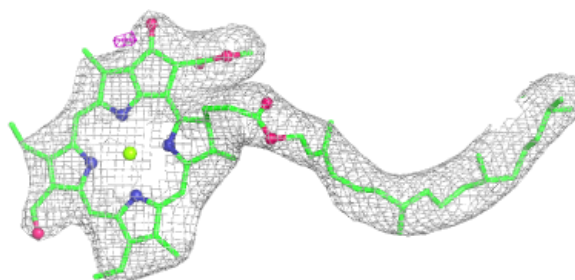


Electron density around CHL B 613:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.