



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 05:16 PM BST

PDB ID : 6RF3  
Title : Crystal structure of the potassium-pumping G263F mutant of the light-driven sodium pump KR2 in the pentameric form, pH 8.0  
Authors : Kovalev, K.; Polovinkin, V.; Gushchin, I.; Borshchevskiy, V.; Gordeliy, V.  
Deposited on : 2019-04-12  
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

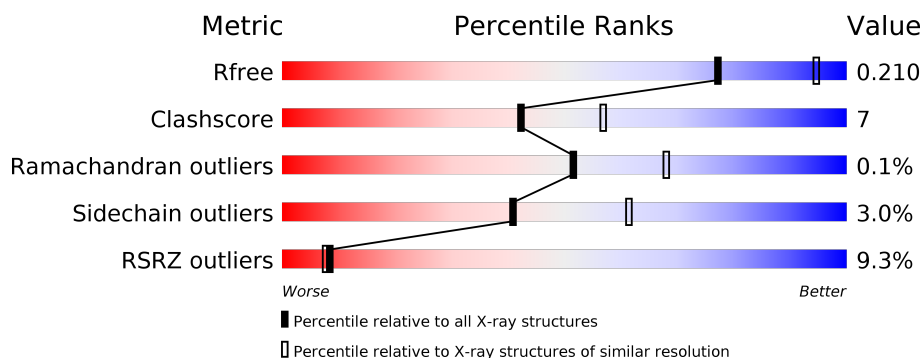
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	288	<div> <div>9%</div> <div>81% 14% • 5%</div> </div>
1	B	288	<div> <div>8%</div> <div>80% 14% • 5%</div> </div>
1	C	288	<div> <div>8%</div> <div>80% 14% • 5%</div> </div>
1	D	288	<div> <div>11%</div> <div>82% 12% 5%</div> </div>
1	E	288	<div> <div>8%</div> <div>82% 11% • 5%</div> </div>

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	OLC	A	301	-	-	-	X
2	OLC	A	304	-	-	-	X
2	OLC	A	306	-	-	-	X
2	OLC	A	307	-	-	-	X
2	OLC	A	308	-	-	-	X
2	OLC	A	310	-	-	-	X
2	OLC	B	303	-	-	-	X
2	OLC	B	307	-	-	-	X
2	OLC	B	309	-	-	-	X
2	OLC	B	311	-	-	-	X
2	OLC	C	303	-	-	-	X
2	OLC	C	308	-	-	-	X
2	OLC	C	309	-	-	-	X
2	OLC	C	310	-	-	-	X
2	OLC	D	302	-	-	-	X
2	OLC	D	305	-	-	-	X
2	OLC	D	306	-	-	-	X
2	OLC	E	303	-	-	-	X
2	OLC	E	306	-	-	-	X
2	OLC	E	308	-	-	-	X
2	OLC	E	312	-	-	-	X
2	OLC	E	313	-	-	-	X
2	OLC	E	314	-	-	-	X
3	LFA	B	302	-	-	-	X
3	LFA	C	302	-	-	-	X
3	LFA	C	319	-	-	-	X
3	LFA	E	302	-	-	-	X
3	LFA	E	319	-	-	-	X
3	LFA	E	323	-	-	-	X
5	BOG	A	320	-	-	-	X
5	BOG	B	321	-	-	-	X
5	BOG	C	321	-	-	-	X
5	BOG	D	317	-	-	-	X
5	BOG	E	321	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13092 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 Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2200	1475	329	387	9			
1	B	273	Total	C	N	O	S	0	0	0
			2194	1470	330	385	9			
1	C	273	Total	C	N	O	S	0	0	0
			2199	1474	329	387	9			
1	D	273	Total	C	N	O	S	0	0	0
			2191	1469	329	384	9			
1	E	273	Total	C	N	O	S	0	0	0
			2193	1471	329	384	9			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	PHE	GLY	engineered mutation	UNP N0DKS8
A	281	LEU	-	expression tag	UNP N0DKS8
A	282	GLU	-	expression tag	UNP N0DKS8
A	283	HIS	-	expression tag	UNP N0DKS8
A	284	HIS	-	expression tag	UNP N0DKS8
A	285	HIS	-	expression tag	UNP N0DKS8
A	286	HIS	-	expression tag	UNP N0DKS8
A	287	HIS	-	expression tag	UNP N0DKS8
A	288	HIS	-	expression tag	UNP N0DKS8
B	263	PHE	GLY	engineered mutation	UNP N0DKS8
B	281	LEU	-	expression tag	UNP N0DKS8
B	282	GLU	-	expression tag	UNP N0DKS8
B	283	HIS	-	expression tag	UNP N0DKS8
B	284	HIS	-	expression tag	UNP N0DKS8
B	285	HIS	-	expression tag	UNP N0DKS8
B	286	HIS	-	expression tag	UNP N0DKS8
B	287	HIS	-	expression tag	UNP N0DKS8
B	288	HIS	-	expression tag	UNP N0DKS8
C	263	PHE	GLY	engineered mutation	UNP N0DKS8

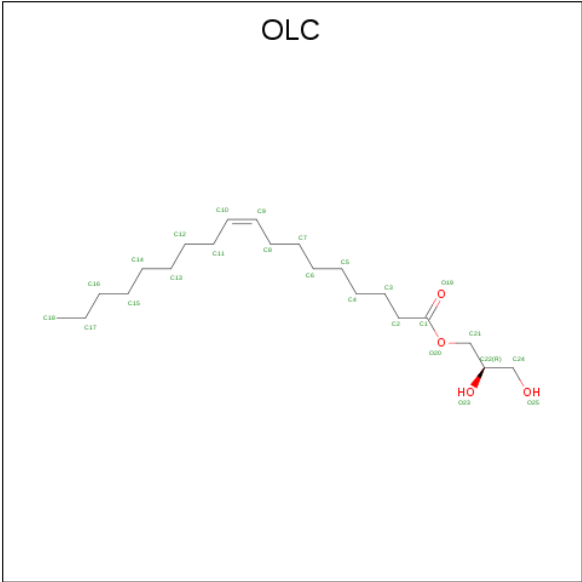
*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	281	LEU	-	expression tag	UNP N0DKS8
C	282	GLU	-	expression tag	UNP N0DKS8
C	283	HIS	-	expression tag	UNP N0DKS8
C	284	HIS	-	expression tag	UNP N0DKS8
C	285	HIS	-	expression tag	UNP N0DKS8
C	286	HIS	-	expression tag	UNP N0DKS8
C	287	HIS	-	expression tag	UNP N0DKS8
C	288	HIS	-	expression tag	UNP N0DKS8
D	263	PHE	GLY	engineered mutation	UNP N0DKS8
D	281	LEU	-	expression tag	UNP N0DKS8
D	282	GLU	-	expression tag	UNP N0DKS8
D	283	HIS	-	expression tag	UNP N0DKS8
D	284	HIS	-	expression tag	UNP N0DKS8
D	285	HIS	-	expression tag	UNP N0DKS8
D	286	HIS	-	expression tag	UNP N0DKS8
D	287	HIS	-	expression tag	UNP N0DKS8
D	288	HIS	-	expression tag	UNP N0DKS8
E	263	PHE	GLY	engineered mutation	UNP N0DKS8
E	281	LEU	-	expression tag	UNP N0DKS8
E	282	GLU	-	expression tag	UNP N0DKS8
E	283	HIS	-	expression tag	UNP N0DKS8
E	284	HIS	-	expression tag	UNP N0DKS8
E	285	HIS	-	expression tag	UNP N0DKS8
E	286	HIS	-	expression tag	UNP N0DKS8
E	287	HIS	-	expression tag	UNP N0DKS8
E	288	HIS	-	expression tag	UNP N0DKS8

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			15	11	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			22	18	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			13	9	4		
2	A	1	Total	C	O	0	0
			15	11	4		
2	A	1	Total	C	O	0	0
			16	12	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			15	11	4		
2	A	1	Total	C	O	0	0
			16	12	4		
2	A	1	Total	C	O	0	0
			16	12	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			14	10	4		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			15	11	4		
2	B	1	Total	C	O	0	0
			20	16	4		
2	B	1	Total	C	O	0	0
			24	20	4		
2	B	1	Total	C	O	0	0
			20	16	4		
2	B	1	Total	C	O	0	0
			21	17	4		
2	B	1	Total	C	O	0	0
			16	12	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			16	12	4		
2	B	1	Total	C	O	0	0
			17	13	4		
2	B	1	Total	C	O	0	0
			15	11	4		
2	B	1	Total	C	O	0	0
			16	12	4		
2	C	1	Total	C	O	0	0
			21	17	4		
2	C	1	Total	C	O	0	0
			14	10	4		
2	C	1	Total	C	O	0	0
			21	17	4		
2	C	1	Total	C	O	0	0
			23	19	4		
2	C	1	Total	C	O	0	0
			25	21	4		
2	C	1	Total	C	O	0	0
			25	21	4		
2	C	1	Total	C	O	0	0
			22	18	4		
2	C	1	Total	C	O	0	0
			16	12	4		
2	C	1	Total	C	O	0	0
			25	21	4		

*Continued on next page...*

*Continued from previous page...*

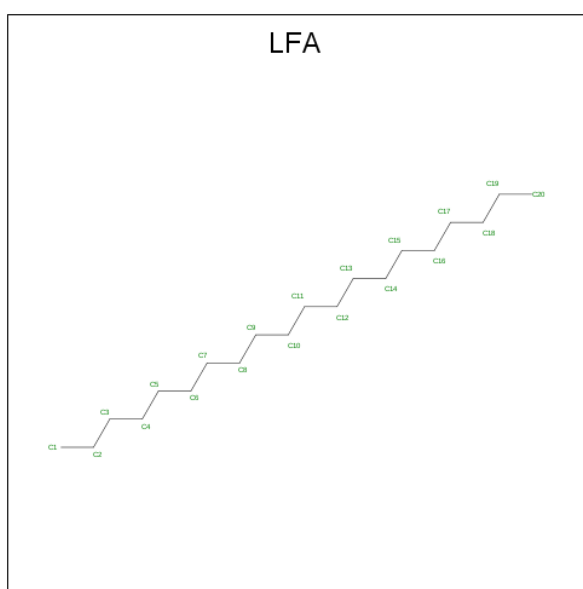
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			16	12	4		
2	C	1	Total	C	O	0	0
			16	12	4		
2	C	1	Total	C	O	0	0
			16	12	4		
2	D	1	Total	C	O	0	0
			18	14	4		
2	D	1	Total	C	O	0	0
			13	9	4		
2	D	1	Total	C	O	0	0
			25	21	4		
2	D	1	Total	C	O	0	0
			18	14	4		
2	D	1	Total	C	O	0	0
			23	19	4		
2	D	1	Total	C	O	0	0
			25	21	4		
2	D	1	Total	C	O	0	0
			14	10	4		
2	D	1	Total	C	O	0	0
			15	11	4		
2	D	1	Total	C	O	0	0
			25	21	4		
2	E	1	Total	C	O	0	0
			25	21	4		
2	E	1	Total	C	O	0	0
			14	10	4		
2	E	1	Total	C	O	0	0
			16	12	4		
2	E	1	Total	C	O	0	0
			24	20	4		
2	E	1	Total	C	O	0	0
			24	20	4		
2	E	1	Total	C	O	0	0
			20	16	4		
2	E	1	Total	C	O	0	0
			15	11	4		
2	E	1	Total	C	O	0	0
			25	21	4		
2	E	1	Total	C	O	0	0
			15	11	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			11	7	4		
2	E	1	Total	C	O	0	0
			25	21	4		
2	E	1	Total	C	O	0	0
			20	16	4		
2	E	1	Total	C	O	0	0
			25	21	4		

- Molecule 3 is EICOSANE (three-letter code: LFA) (formula:  $C_{20}H_{42}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			7	7		
3	A	1	Total	C	0	0
			8	8		
3	A	1	Total	C	0	0
			8	8		
3	A	1	Total	C	0	0
			12	12		
3	A	1	Total	C	0	0
			4	4		
3	A	1	Total	C	0	0
			6	6		
3	A	1	Total	C	0	0
			20	20		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 20 20	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 7 7	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 11 11	0	0
3	C	1	Total C 4 4	0	0
3	C	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 17 17	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 6 6	0	0
3	E	1	Total C 20 20	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 14 14	0	0

*Continued on next page...*

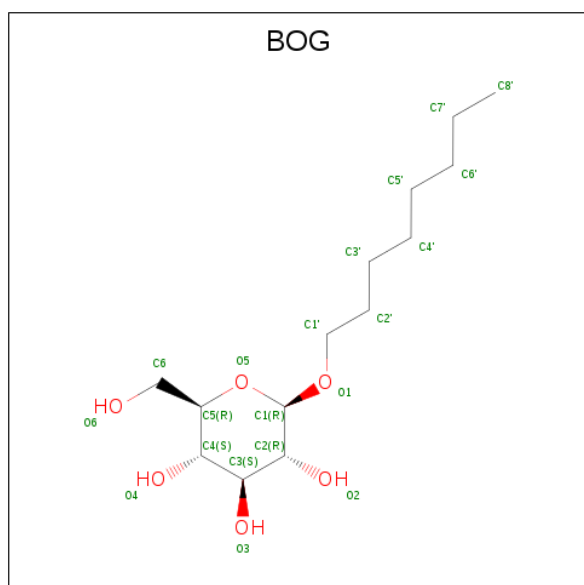
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C 4 4	0	0
3	E	1	Total C 5 5	0	0
3	E	1	Total C 20 20	0	0
3	E	1	Total C 4 4	0	0
3	E	1	Total C 14 14	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			20	14	6		
5	B	1	Total	C	O	0	0
			20	14	6		
5	C	1	Total	C	O	0	0
			20	14	6		
5	D	1	Total	C	O	0	0
			20	14	6		
5	E	1	Total	C	O	0	0
			20	14	6		

- Molecule 6 is water.

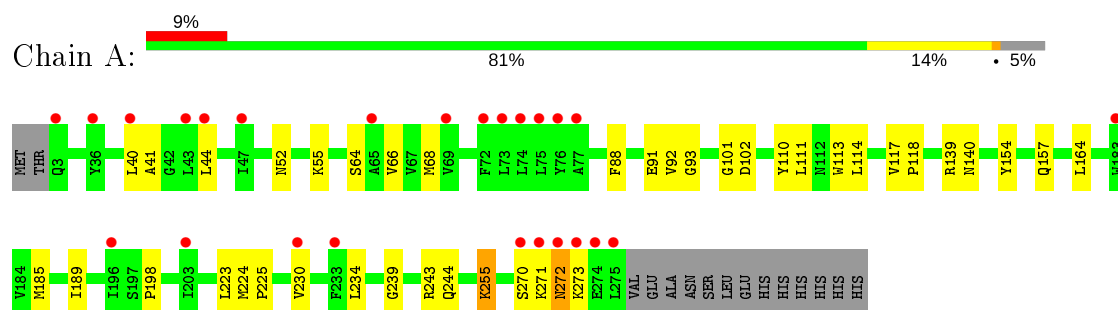
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total	O	0	0
			97	97		
6	B	86	Total	O	0	0
			86	86		
6	C	94	Total	O	0	0
			94	94		
6	D	89	Total	O	0	0
			89	89		
6	E	96	Total	O	0	0
			96	96		



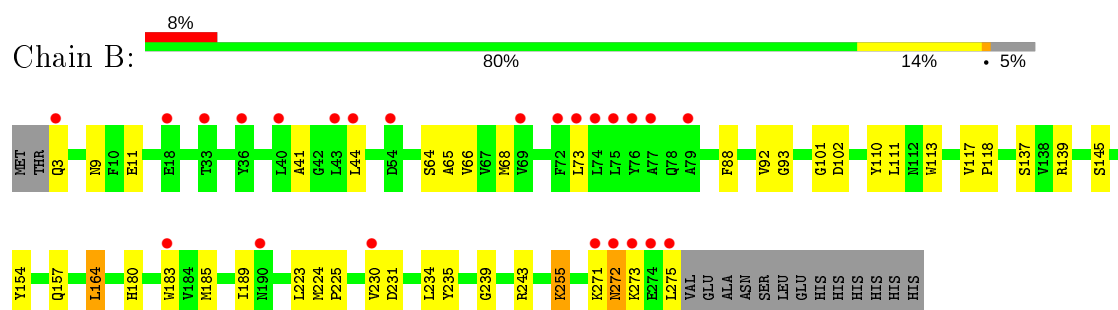
### 3 Residue-property plots [i](#)

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.

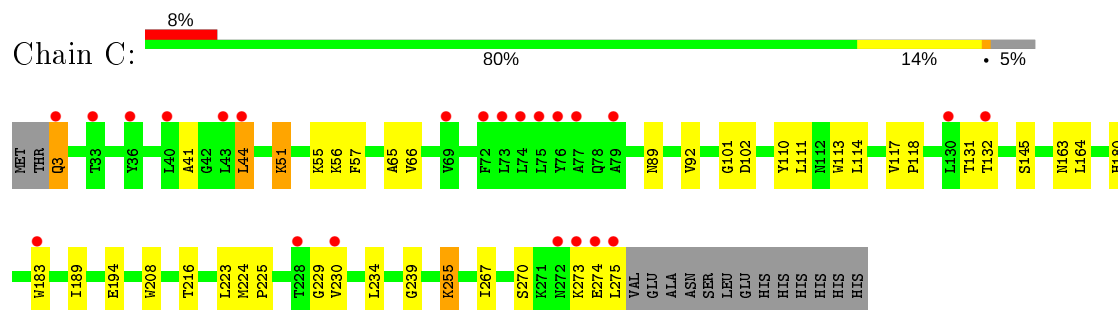
#### • Molecule 1: Sodium pumping rhodopsin



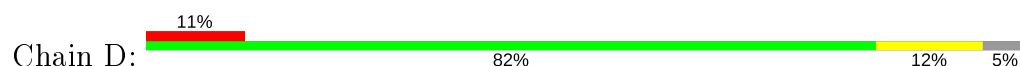
#### • Molecule 1: Sodium pumping rhodopsin

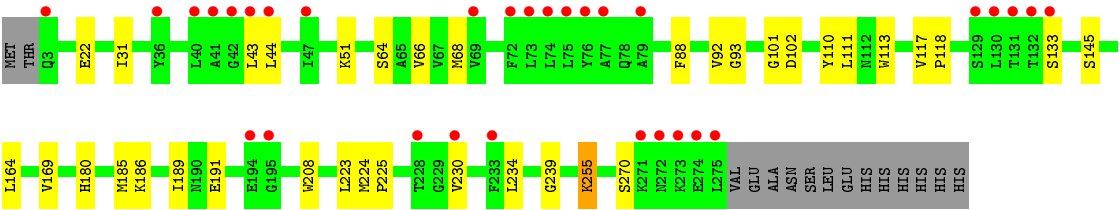


#### • Molecule 1: Sodium pumping rhodopsin

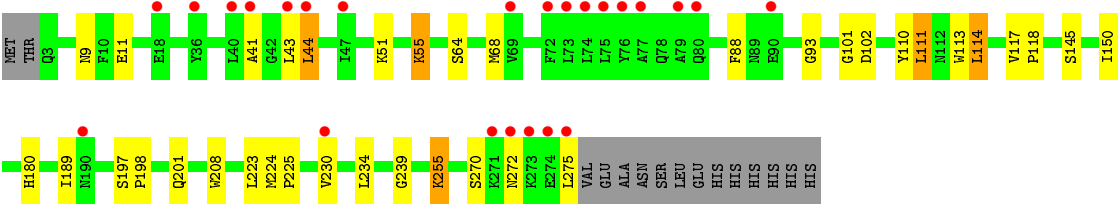
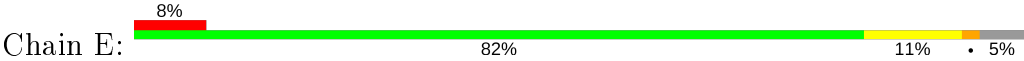


#### • Molecule 1: Sodium pumping rhodopsin





● Molecule 1: Sodium pumping rhodopsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.68Å 239.69Å 134.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.97 – 2.40 47.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.97-2.40) 99.9 (47.94-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.172 , 0.205 0.184 , 0.210	Depositor DCC
$R_{free}$ test set	4195 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, OLC, LFA, LYR, BOG

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	0.29	0/2229	0.42	0/3030
1	B	0.29	0/2223	0.42	0/3023
1	C	0.28	0/2228	0.42	0/3029
1	D	0.28	0/2220	0.43	0/3018
1	E	0.29	0/2222	0.42	0/3021
All	All	0.28	0/11122	0.42	0/15121

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Sidechain
1	B	243	ARG	Sidechain
1	B	273	LYS	Peptide
1	C	270	SER	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2200	0	2184	33	0
1	B	2194	0	2179	36	0
1	C	2199	0	2182	39	0
1	D	2191	0	2172	28	0
1	E	2193	0	2179	27	0
2	A	228	0	326	7	0
2	B	269	0	378	7	0
2	C	240	0	343	5	0
2	D	176	0	250	2	0
2	E	259	0	371	13	0
3	A	65	0	126	1	0
3	B	54	0	106	1	0
3	C	90	0	182	6	0
3	D	78	0	153	3	0
3	E	89	0	176	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	20	0	28	3	0
5	B	20	0	28	4	0
5	C	20	0	28	1	0
5	D	20	0	28	1	0
5	E	20	0	28	0	0
6	A	97	0	0	4	0
6	B	86	0	0	1	0
6	C	94	0	0	3	0
6	D	89	0	0	2	0
6	E	96	0	0	4	0
All	All	13092	0	13447	179	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 179 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)
3:E:316:LFA:H141	3:E:317:LFA:H201	1.51	0.89
1:C:267:ILE:HG21	1:C:275:LEU:HB3	1.57	0.85
3:E:316:LFA:C14	3:E:317:LFA:H201	2.05	0.84
1:B:255:LYR:H9	1:B:255:LYR:H183	1.60	0.82
1:A:164:LEU:HD21	5:A:320:BOG:H2'1	1.61	0.80

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	270/288 (94%)	265 (98%)	5 (2%)	0	100	100
1	B	270/288 (94%)	264 (98%)	6 (2%)	0	100	100
1	C	270/288 (94%)	265 (98%)	5 (2%)	0	100	100
1	D	270/288 (94%)	265 (98%)	5 (2%)	0	100	100
1	E	270/288 (94%)	265 (98%)	4 (2%)	1 (0%)	34	48
All	All	1350/1440 (94%)	1324 (98%)	25 (2%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	272	ASN

### 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	230/248 (93%)	222 (96%)	8 (4%)	36	55
1	B	230/248 (93%)	223 (97%)	7 (3%)	41	61
1	C	230/248 (93%)	222 (96%)	8 (4%)	36	55
1	D	228/248 (92%)	224 (98%)	4 (2%)	59	76
1	E	229/248 (92%)	222 (97%)	7 (3%)	40	60
All	All	1147/1240 (92%)	1113 (97%)	34 (3%)	41	61

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	GLN
1	C	132	THR
1	E	230	VAL
1	C	51	LYS
1	A	272	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	GLN
1	E	180	HIS
1	D	3	GLN
1	B	272	ASN
1	C	180	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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
1	LYR	E	255	1	27,29,30	0.66	0	30,37,39	1.87	8 (26%)
1	LYR	B	255	1	27,29,30	0.62	0	30,37,39	1.85	8 (26%)
1	LYR	D	255	1	27,29,30	0.62	0	30,37,39	1.86	8 (26%)
1	LYR	A	255	1	27,29,30	0.63	0	30,37,39	1.82	8 (26%)
1	LYR	C	255	1	27,29,30	0.61	0	30,37,39	1.84	8 (26%)

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
1	LYR	E	255	1	-	3/22/40/42	0/1/1/1
1	LYR	B	255	1	-	4/22/40/42	0/1/1/1
1	LYR	D	255	1	-	4/22/40/42	0/1/1/1
1	LYR	A	255	1	-	4/22/40/42	0/1/1/1
1	LYR	C	255	1	-	3/22/40/42	0/1/1/1

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	255	LYR	C1-NZ-CE	5.37	121.84	113.33
1	D	255	LYR	C1-NZ-CE	5.33	121.78	113.33
1	C	255	LYR	C1-NZ-CE	5.31	121.75	113.33
1	B	255	LYR	C1-NZ-CE	5.02	121.28	113.33
1	A	255	LYR	C1-NZ-CE	4.54	120.52	113.33

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	255	LYR	C2-C1-NZ-CE
1	A	255	LYR	C2-C1-NZ-CE
1	C	255	LYR	C2-C1-NZ-CE
1	B	255	LYR	C2-C1-NZ-CE
1	D	255	LYR	C2-C1-NZ-CE

There are no ring outliers.



5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	255	LYR	4	0
1	B	255	LYR	5	0
1	D	255	LYR	5	0
1	A	255	LYR	4	0
1	C	255	LYR	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 103 ligands modelled in this entry, 5 are monoatomic - leaving 98 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	$\# Z  > 2$
2	OLC	B	312	-	15,15,24	1.13	1 (6%)	16,16,25	0.92	1 (6%)
2	OLC	C	312	-	15,15,24	1.21	1 (6%)	16,16,25	1.01	1 (6%)
3	LFA	D	310	-	19,19,19	0.29	0	18,18,18	0.53	0
2	OLC	A	306	-	14,14,24	1.22	1 (7%)	15,15,25	0.99	1 (6%)
5	BOG	B	321	-	20,20,20	0.60	1 (5%)	25,25,25	0.61	0
3	LFA	D	312	-	7,7,19	0.29	0	6,6,18	0.41	0
2	OLC	B	315	-	15,15,24	1.26	1 (6%)	16,16,25	0.96	1 (6%)
3	LFA	B	318	-	9,9,19	0.31	0	8,8,18	0.49	0
3	LFA	E	322	-	3,3,19	0.37	0	2,2,18	0.60	0
2	OLC	E	311	-	10,10,24	1.47	1 (10%)	11,11,25	1.19	2 (18%)
5	BOG	D	317	-	20,20,20	0.54	0	25,25,25	0.70	0
2	OLC	B	301	-	24,24,24	0.95	1 (4%)	25,25,25	0.89	1 (4%)
2	OLC	D	308	-	14,14,24	1.24	1 (7%)	15,15,25	0.91	1 (6%)
3	LFA	B	302	-	19,19,19	0.36	0	18,18,18	0.39	0
2	OLC	E	306	-	23,23,24	0.99	1 (4%)	24,24,25	0.84	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	D	304	-	17,17,24	1.13	1 (5%)	18,18,25	1.05	1 (5%)
2	OLC	B	314	-	14,14,24	1.26	1 (7%)	15,15,25	0.99	1 (6%)
2	OLC	E	313	-	19,19,24	1.09	1 (5%)	20,20,25	0.98	1 (5%)
3	LFA	D	315	-	5,5,19	0.33	0	4,4,18	0.28	0
2	OLC	A	308	-	24,24,24	0.97	1 (4%)	25,25,25	0.87	1 (4%)
3	LFA	D	311	-	19,19,19	0.26	0	18,18,18	0.55	0
2	OLC	C	309	-	15,15,24	1.23	1 (6%)	16,16,25	1.08	1 (6%)
3	LFA	C	316	-	19,19,19	0.28	0	18,18,18	0.50	0
2	OLC	E	314	-	24,24,24	0.95	1 (4%)	25,25,25	0.85	1 (4%)
3	LFA	A	318	-	19,19,19	0.28	0	18,18,18	0.51	0
3	LFA	E	302	-	19,19,19	0.38	0	18,18,18	0.36	0
2	OLC	E	312	-	24,24,24	0.98	1 (4%)	25,25,25	0.84	1 (4%)
3	LFA	C	318	-	3,3,19	0.34	0	2,2,18	0.66	0
5	BOG	A	320	-	20,20,20	0.55	0	25,25,25	0.64	0
5	BOG	E	321	-	20,20,20	0.54	0	25,25,25	0.53	0
2	OLC	A	310	-	15,15,24	1.17	1 (6%)	16,16,25	0.92	1 (6%)
2	OLC	B	309	-	20,20,24	1.05	1 (5%)	21,21,25	0.99	1 (4%)
2	OLC	B	311	-	24,24,24	0.97	1 (4%)	25,25,25	0.84	2 (8%)
2	OLC	A	307	-	15,15,24	1.20	1 (6%)	16,16,25	1.27	2 (12%)
2	OLC	D	306	-	24,24,24	1.00	1 (4%)	25,25,25	0.91	1 (4%)
2	OLC	B	313	-	16,16,24	1.17	1 (6%)	17,17,25	0.97	1 (5%)
2	OLC	D	303	-	24,24,24	0.97	1 (4%)	25,25,25	0.91	1 (4%)
2	OLC	E	310	-	14,14,24	1.22	1 (7%)	15,15,25	0.93	1 (6%)
3	LFA	A	314	-	7,7,19	0.27	0	6,6,18	0.44	0
2	OLC	B	303	-	13,13,24	1.26	1 (7%)	14,14,25	1.08	1 (7%)
2	OLC	C	313	-	15,15,24	1.25	1 (6%)	16,16,25	1.07	1 (6%)
3	LFA	C	302	-	19,19,19	0.39	0	18,18,18	0.29	0
3	LFA	A	316	-	3,3,19	0.38	0	2,2,18	0.60	0
2	OLC	E	303	-	13,13,24	1.29	1 (7%)	14,14,25	1.05	1 (7%)
3	LFA	C	315	-	7,7,19	0.28	0	6,6,18	0.36	0
2	OLC	B	305	-	14,14,24	1.24	1 (7%)	15,15,25	0.97	1 (6%)
3	LFA	E	315	-	7,7,19	0.27	0	6,6,18	0.48	0
2	OLC	E	309	-	24,24,24	0.92	1 (4%)	25,25,25	0.87	2 (8%)
2	OLC	A	321	-	24,24,24	0.95	1 (4%)	25,25,25	0.86	1 (4%)
3	LFA	C	317	-	10,10,19	0.31	0	9,9,18	0.48	0
2	OLC	C	307	-	24,24,24	0.97	1 (4%)	25,25,25	0.89	1 (4%)
3	LFA	C	314	-	6,6,19	0.33	0	5,5,18	0.34	0
2	OLC	D	309	-	24,24,24	0.96	1 (4%)	25,25,25	0.77	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	E	305	-	23,23,24	0.95	1 (4%)	24,24,25	0.95	2 (8%)
2	OLC	A	311	-	15,15,24	1.24	1 (6%)	16,16,25	1.00	1 (6%)
2	OLC	D	307	-	13,13,24	1.24	1 (7%)	14,14,25	1.05	2 (14%)
2	OLC	B	304	-	24,24,24	0.98	1 (4%)	25,25,25	0.86	1 (4%)
2	OLC	C	304	-	20,20,24	1.06	1 (5%)	21,21,25	0.89	1 (4%)
2	OLC	A	304	-	24,24,24	0.97	1 (4%)	25,25,25	0.83	1 (4%)
2	OLC	E	308	-	14,14,24	1.24	1 (7%)	15,15,25	1.05	1 (6%)
2	OLC	C	301	-	20,20,24	0.97	1 (5%)	21,21,25	0.95	1 (4%)
2	OLC	C	305	-	22,22,24	0.98	1 (4%)	23,23,25	0.89	2 (8%)
3	LFA	E	316	-	13,13,19	0.28	0	12,12,18	0.50	0
3	LFA	A	317	-	5,5,19	0.27	0	4,4,18	0.35	0
3	LFA	E	317	-	3,3,19	0.34	0	2,2,18	0.65	0
3	LFA	B	316	-	8,8,19	0.30	0	7,7,18	0.44	0
3	LFA	B	317	-	7,7,19	0.27	0	6,6,18	0.46	0
2	OLC	B	306	-	19,19,24	1.07	1 (5%)	20,20,25	0.88	1 (5%)
3	LFA	B	319	-	6,6,19	0.31	0	5,5,18	0.35	0
3	LFA	A	315	-	11,11,19	0.30	0	10,10,18	0.46	0
2	OLC	A	302	-	24,24,24	0.97	1 (4%)	25,25,25	0.82	1 (4%)
2	OLC	A	305	-	12,12,24	1.31	1 (8%)	13,13,25	1.17	2 (15%)
3	LFA	E	323	-	13,13,19	0.30	0	12,12,18	0.48	0
3	LFA	E	319	-	19,19,19	0.40	0	18,18,18	0.31	0
3	LFA	E	318	-	4,4,19	0.29	0	3,3,18	0.37	0
2	OLC	B	310	-	15,15,24	1.21	1 (6%)	16,16,25	1.01	1 (6%)
2	OLC	B	307	-	23,23,24	0.98	1 (4%)	24,24,25	0.85	1 (4%)
2	OLC	C	306	-	24,24,24	0.97	1 (4%)	25,25,25	0.89	1 (4%)
3	LFA	D	314	-	6,6,19	0.31	0	5,5,18	0.37	0
2	OLC	C	310	-	24,24,24	0.96	1 (4%)	25,25,25	0.82	1 (4%)
5	BOG	C	321	-	20,20,20	0.56	0	25,25,25	0.60	0
2	OLC	E	307	-	19,19,24	1.05	1 (5%)	20,20,25	0.94	1 (5%)
2	OLC	C	308	-	21,21,24	1.01	1 (4%)	22,22,25	0.94	2 (9%)
2	OLC	A	301	-	14,14,24	1.22	1 (7%)	15,15,25	1.00	1 (6%)
2	OLC	D	305	-	22,22,24	0.99	1 (4%)	23,23,25	0.82	1 (4%)
2	OLC	E	301	-	24,24,24	0.95	1 (4%)	25,25,25	0.87	1 (4%)
2	OLC	D	301	-	17,17,24	1.13	1 (5%)	18,18,25	1.00	1 (5%)
2	OLC	B	308	-	19,19,24	1.07	1 (5%)	20,20,25	0.95	2 (10%)
2	OLC	A	303	-	21,21,24	0.99	1 (4%)	22,22,25	0.86	2 (9%)
2	OLC	E	304	-	15,15,24	1.18	1 (6%)	16,16,25	1.03	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	D	302	-	12,12,24	1.34	1 (8%)	13,13,25	1.10	1 (7%)
2	OLC	A	309	-	14,14,24	1.23	1 (7%)	15,15,25	1.12	2 (13%)
2	OLC	C	311	-	15,15,24	1.18	1 (6%)	16,16,25	0.97	2 (12%)
3	LFA	C	319	-	19,19,19	0.36	0	18,18,18	0.41	0
3	LFA	A	312	-	6,6,19	0.29	0	5,5,18	0.38	0
2	OLC	C	303	-	13,13,24	1.27	1 (7%)	14,14,25	1.03	1 (7%)
3	LFA	D	313	-	16,16,19	0.31	0	15,15,18	0.48	0
3	LFA	A	313	-	7,7,19	0.29	0	6,6,18	0.44	0

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
2	OLC	B	312	-	-	5/15/15/24	-
2	OLC	C	312	-	-	11/15/15/24	-
3	LFA	D	310	-	-	11/17/17/17	-
2	OLC	A	306	-	-	5/14/14/24	-
5	BOG	B	321	-	-	5/11/31/31	0/1/1/1
3	LFA	D	312	-	-	4/5/5/17	-
2	OLC	B	315	-	-	7/15/15/24	-
3	LFA	B	318	-	-	5/7/7/17	-
3	LFA	E	322	-	-	0/1/1/17	-
2	OLC	E	311	-	-	6/10/10/24	-
5	BOG	D	317	-	-	2/11/31/31	0/1/1/1
2	OLC	B	301	-	-	10/24/24/24	-
2	OLC	D	308	-	-	11/14/14/24	-
3	LFA	B	302	-	-	6/17/17/17	-
2	OLC	E	306	-	-	14/23/23/24	-
2	OLC	D	304	-	-	5/17/17/24	-
2	OLC	B	314	-	-	8/14/14/24	-
2	OLC	E	313	-	-	12/19/19/24	-
3	LFA	D	315	-	-	0/3/3/17	-
2	OLC	A	308	-	-	15/24/24/24	-
3	LFA	D	311	-	-	8/17/17/17	-
2	OLC	C	309	-	-	8/15/15/24	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	C	316	-	-	11/17/17/17	-
2	OLC	E	314	-	-	10/24/24/24	-
3	LFA	A	318	-	-	8/17/17/17	-
3	LFA	E	302	-	-	8/17/17/17	-
2	OLC	E	312	-	-	10/24/24/24	-
3	LFA	C	318	-	-	1/1/1/17	-
5	BOG	A	320	-	-	5/11/31/31	0/1/1/1
5	BOG	E	321	-	-	9/11/31/31	0/1/1/1
2	OLC	A	310	-	-	8/15/15/24	-
2	OLC	B	309	-	-	9/20/20/24	-
2	OLC	B	311	-	-	15/24/24/24	-
2	OLC	A	307	-	-	4/15/15/24	-
2	OLC	D	306	-	-	12/24/24/24	-
2	OLC	B	313	-	-	10/16/16/24	-
2	OLC	D	303	-	-	10/24/24/24	-
2	OLC	E	310	-	-	8/14/14/24	-
3	LFA	A	314	-	-	3/5/5/17	-
2	OLC	B	303	-	-	8/13/13/24	-
2	OLC	C	313	-	-	9/15/15/24	-
3	LFA	C	302	-	-	12/17/17/17	-
3	LFA	A	316	-	-	0/1/1/17	-
2	OLC	E	303	-	-	5/13/13/24	-
3	LFA	C	315	-	-	4/5/5/17	-
2	OLC	B	305	-	-	4/14/14/24	-
3	LFA	E	315	-	-	1/5/5/17	-
2	OLC	E	309	-	-	17/24/24/24	-
2	OLC	A	321	-	-	10/24/24/24	-
3	LFA	C	317	-	-	3/8/8/17	-
2	OLC	C	307	-	-	6/24/24/24	-
3	LFA	C	314	-	-	3/4/4/17	-
2	OLC	D	309	-	-	13/24/24/24	-
2	OLC	E	305	-	-	12/23/23/24	-
2	OLC	A	311	-	-	7/15/15/24	-
2	OLC	D	307	-	-	7/13/13/24	-
2	OLC	B	304	-	-	9/24/24/24	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	304	-	-	9/20/20/24	-
2	OLC	A	304	-	-	14/24/24/24	-
2	OLC	E	308	-	-	9/14/14/24	-
2	OLC	C	301	-	-	12/20/20/24	-
2	OLC	C	305	-	-	11/22/22/24	-
3	LFA	E	316	-	-	5/11/11/17	-
3	LFA	A	317	-	-	1/3/3/17	-
3	LFA	E	317	-	-	1/1/1/17	-
3	LFA	B	316	-	-	3/6/6/17	-
3	LFA	B	317	-	-	4/5/5/17	-
2	OLC	B	306	-	-	10/19/19/24	-
3	LFA	B	319	-	-	2/4/4/17	-
3	LFA	A	315	-	-	5/9/9/17	-
2	OLC	A	302	-	-	15/24/24/24	-
2	OLC	A	305	-	-	1/12/12/24	-
3	LFA	E	323	-	-	4/11/11/17	-
3	LFA	E	319	-	-	10/17/17/17	-
3	LFA	E	318	-	-	1/2/2/17	-
2	OLC	B	310	-	-	9/15/15/24	-
2	OLC	B	307	-	-	8/23/23/24	-
2	OLC	C	306	-	-	10/24/24/24	-
3	LFA	D	314	-	-	3/4/4/17	-
2	OLC	C	310	-	-	13/24/24/24	-
5	BOG	C	321	-	-	3/11/31/31	0/1/1/1
2	OLC	E	307	-	-	7/19/19/24	-
2	OLC	C	308	-	-	8/21/21/24	-
2	OLC	A	301	-	-	6/14/14/24	-
2	OLC	D	305	-	-	7/22/22/24	-
2	OLC	E	301	-	-	13/24/24/24	-
2	OLC	D	301	-	-	9/17/17/24	-
2	OLC	B	308	-	-	6/19/19/24	-
2	OLC	A	303	-	-	7/21/21/24	-
2	OLC	E	304	-	-	6/15/15/24	-
2	OLC	D	302	-	-	7/12/12/24	-
2	OLC	A	309	-	-	8/14/14/24	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	311	-	-	7/15/15/24	-
3	LFA	C	319	-	-	9/17/17/17	-
3	LFA	A	312	-	-	3/4/4/17	-
2	OLC	C	303	-	-	9/13/13/24	-
3	LFA	D	313	-	-	9/14/14/17	-
3	LFA	A	313	-	-	1/5/5/17	-

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	OLC	O20-C1	4.66	1.47	1.33
2	A	311	OLC	O20-C1	4.62	1.46	1.33
2	D	306	OLC	O20-C1	4.62	1.46	1.33
2	C	313	OLC	O20-C1	4.60	1.46	1.33
2	C	309	OLC	O20-C1	4.57	1.46	1.33

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	307	OLC	O20-C1-C2	3.46	122.77	111.91
2	A	305	OLC	O20-C1-C2	3.08	121.58	111.91
2	E	313	OLC	O20-C1-C2	3.07	121.54	111.91
2	A	309	OLC	O20-C1-C2	3.06	121.51	111.91
2	C	307	OLC	O20-C1-C2	3.04	121.45	111.91

There are no chirality outliers.

5 of 714 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	312	OLC	C21-C22-C24-O25
2	C	312	OLC	O23-C22-C24-O25
2	C	312	OLC	O20-C21-C22-C24
2	C	312	OLC	C2-C1-O20-C21
2	C	312	OLC	O19-C1-O20-C21

There are no ring outliers.

42 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	306	OLC	1	0

*Continued on next page...*

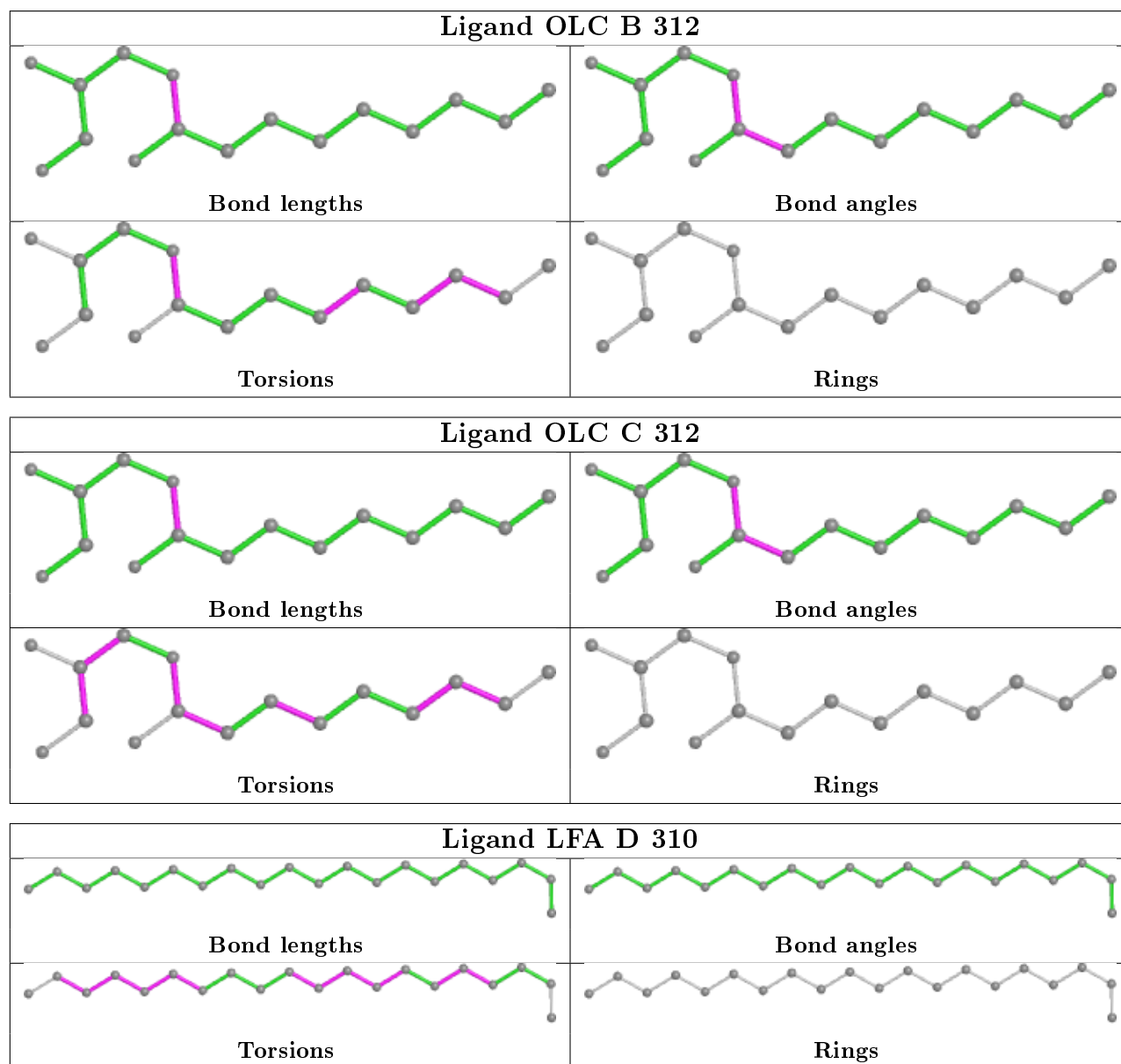
*Continued from previous page...*

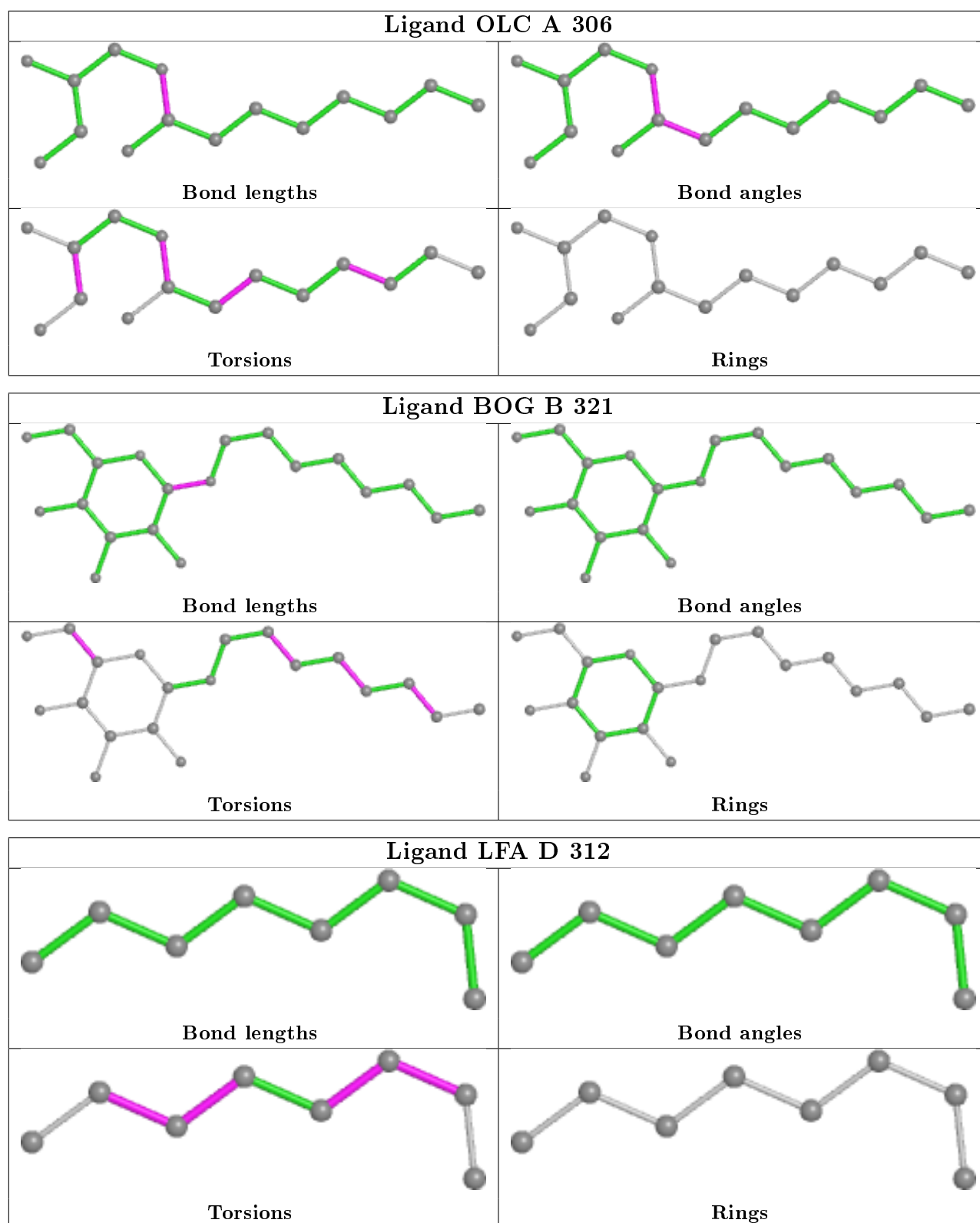
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	321	BOG	4	0
2	B	315	OLC	1	0
5	D	317	BOG	1	0
2	B	301	OLC	4	0
2	E	306	OLC	1	0
2	D	304	OLC	1	0
2	A	308	OLC	1	0
3	D	311	LFA	1	0
2	C	309	OLC	1	0
2	E	312	OLC	4	0
3	C	318	LFA	3	0
5	A	320	BOG	3	0
2	A	310	OLC	1	0
2	A	307	OLC	1	0
2	B	313	OLC	1	0
2	E	310	OLC	1	0
3	C	302	LFA	1	0
2	E	303	OLC	3	0
3	E	315	LFA	3	0
2	E	309	OLC	1	0
3	C	314	LFA	2	0
2	E	305	OLC	3	0
2	A	311	OLC	2	0
2	B	304	OLC	1	0
2	C	304	OLC	2	0
2	A	304	OLC	1	0
2	C	305	OLC	1	0
3	E	316	LFA	2	0
3	E	317	LFA	2	0
3	B	316	LFA	1	0
2	B	306	OLC	1	0
3	A	315	LFA	1	0
2	A	302	OLC	1	0
3	E	323	LFA	1	0
5	C	321	BOG	1	0
2	A	301	OLC	1	0
2	E	301	OLC	2	0
2	E	304	OLC	2	0
2	D	302	OLC	1	0
2	C	311	OLC	1	0
3	D	313	LFA	2	0

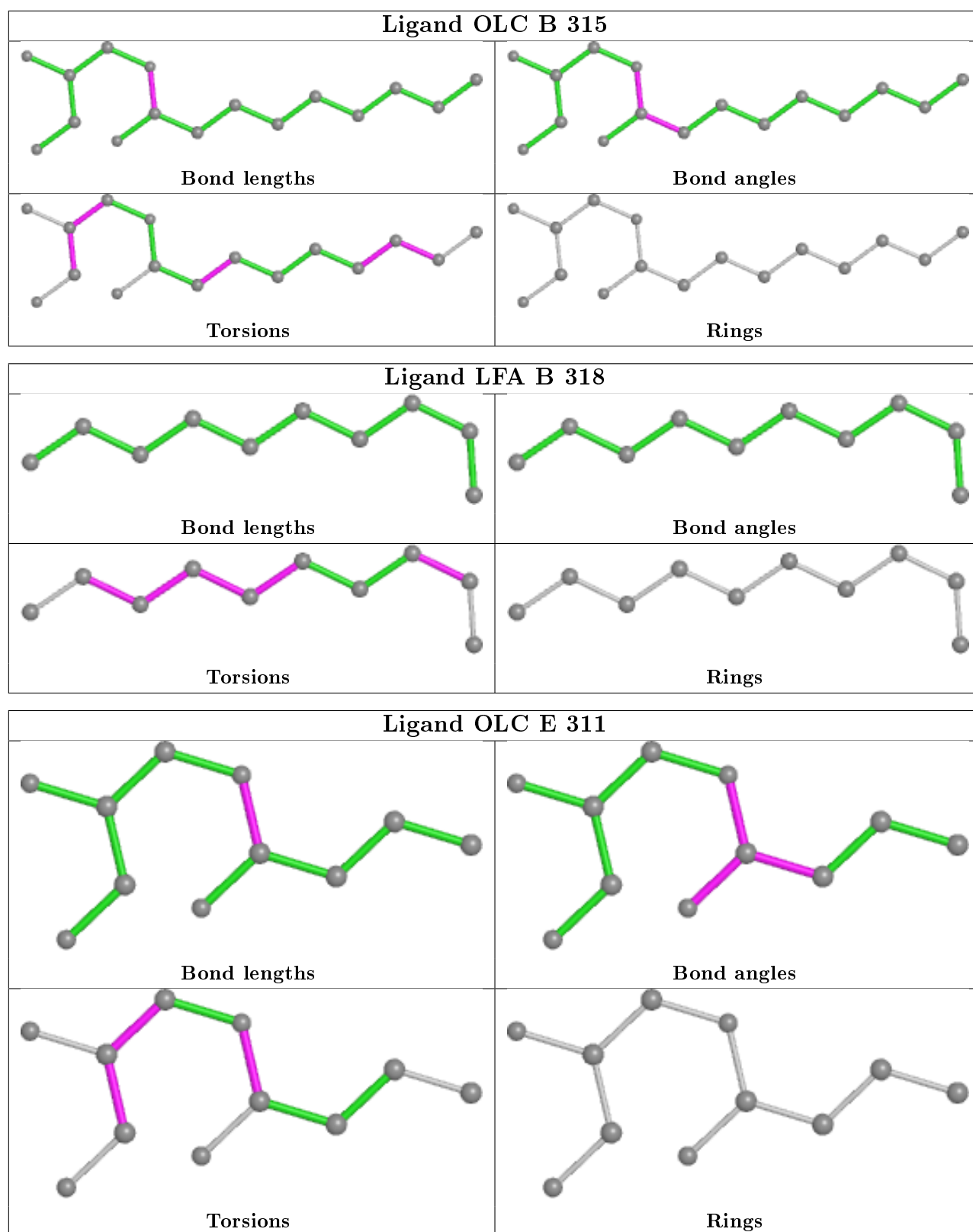
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

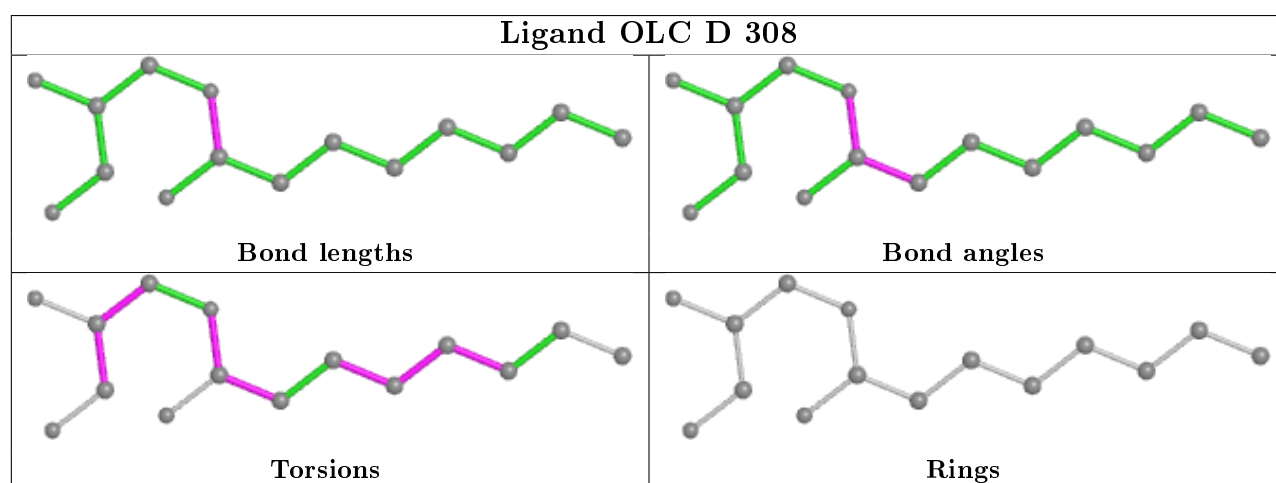
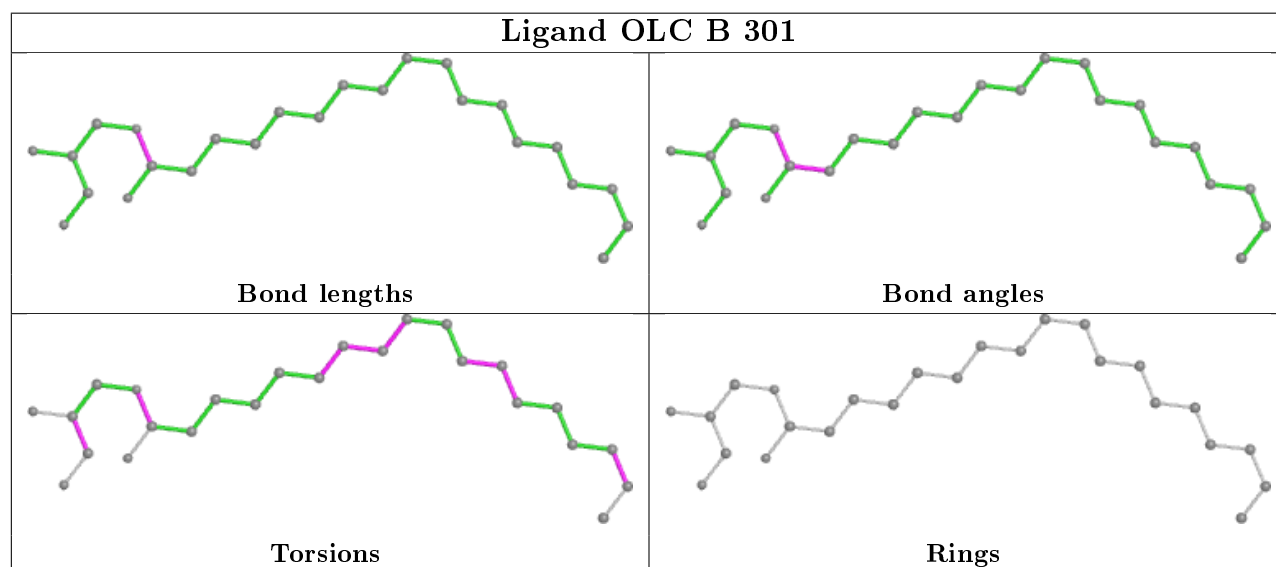
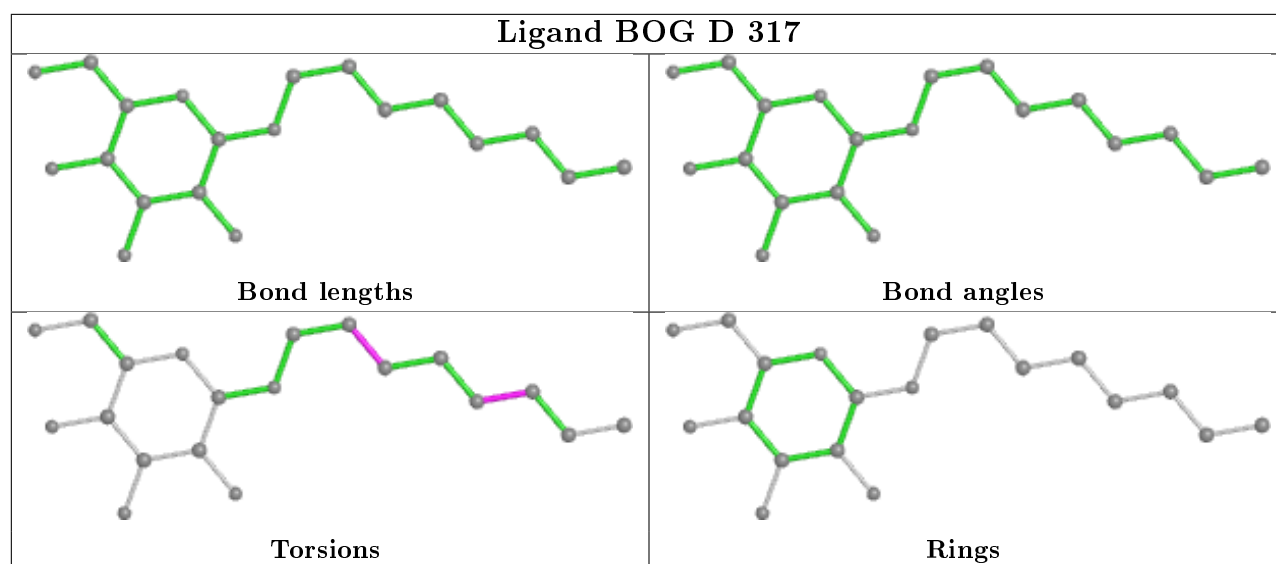


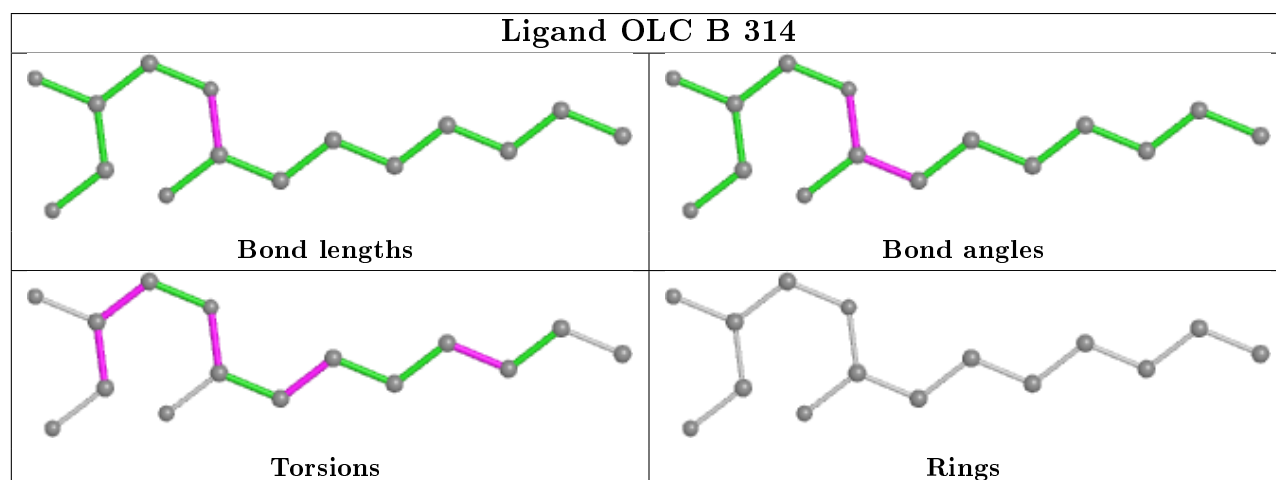
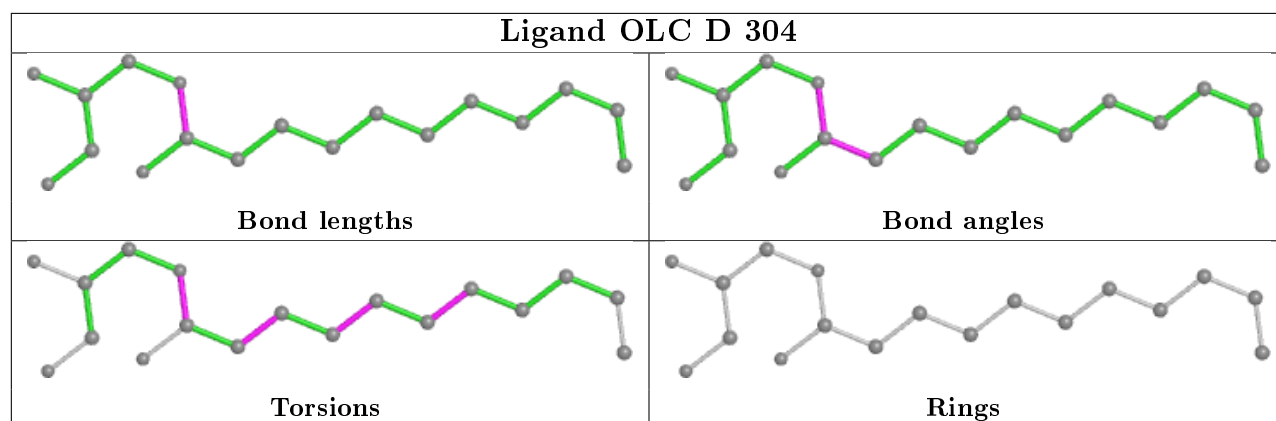
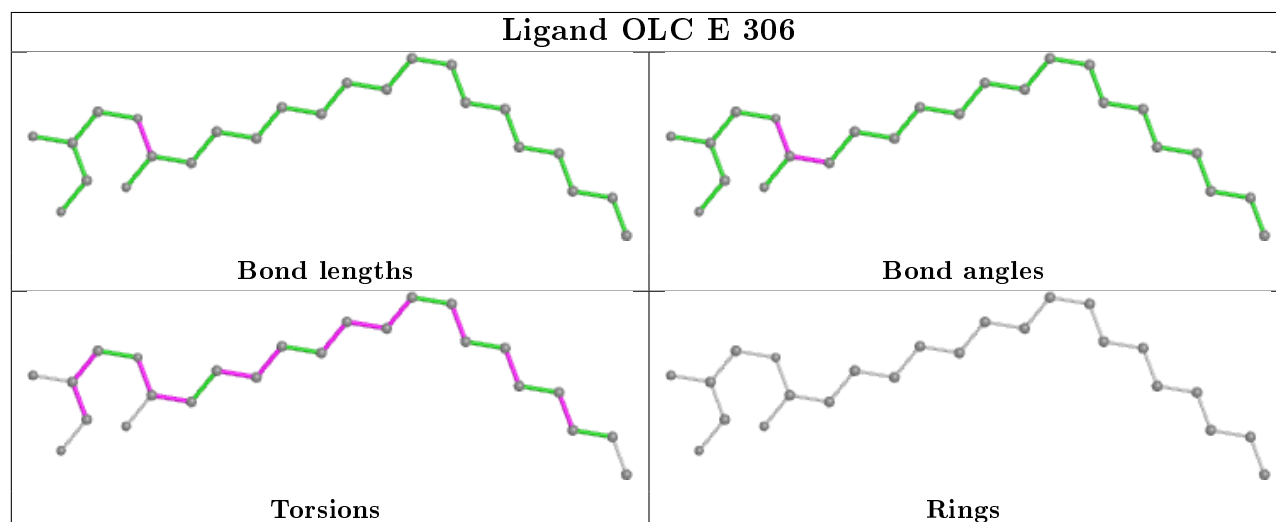
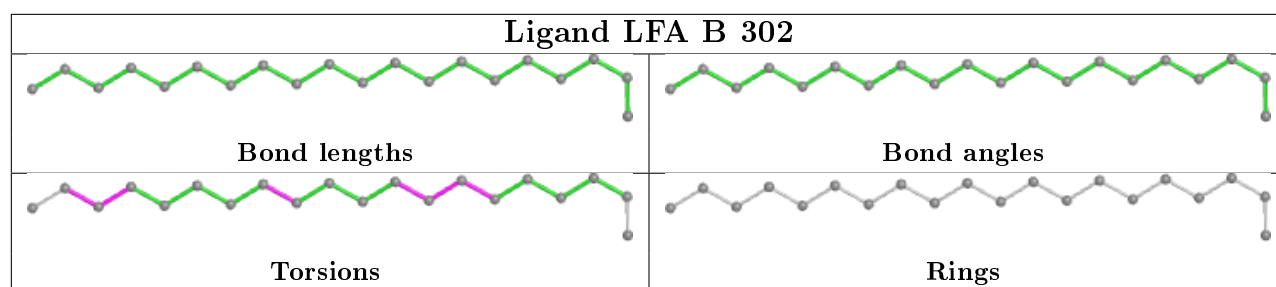
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

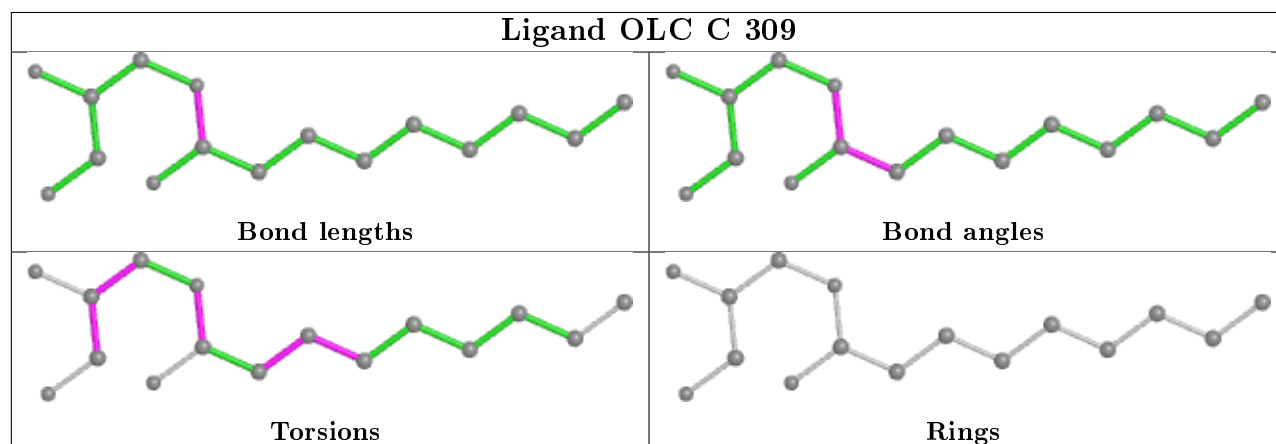
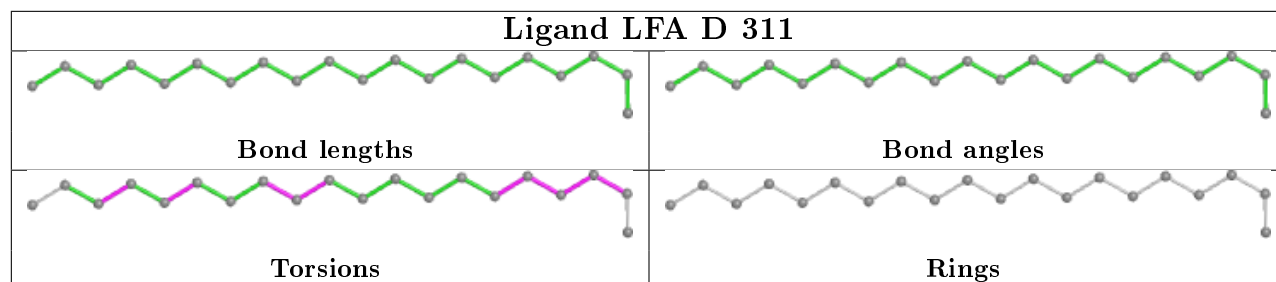
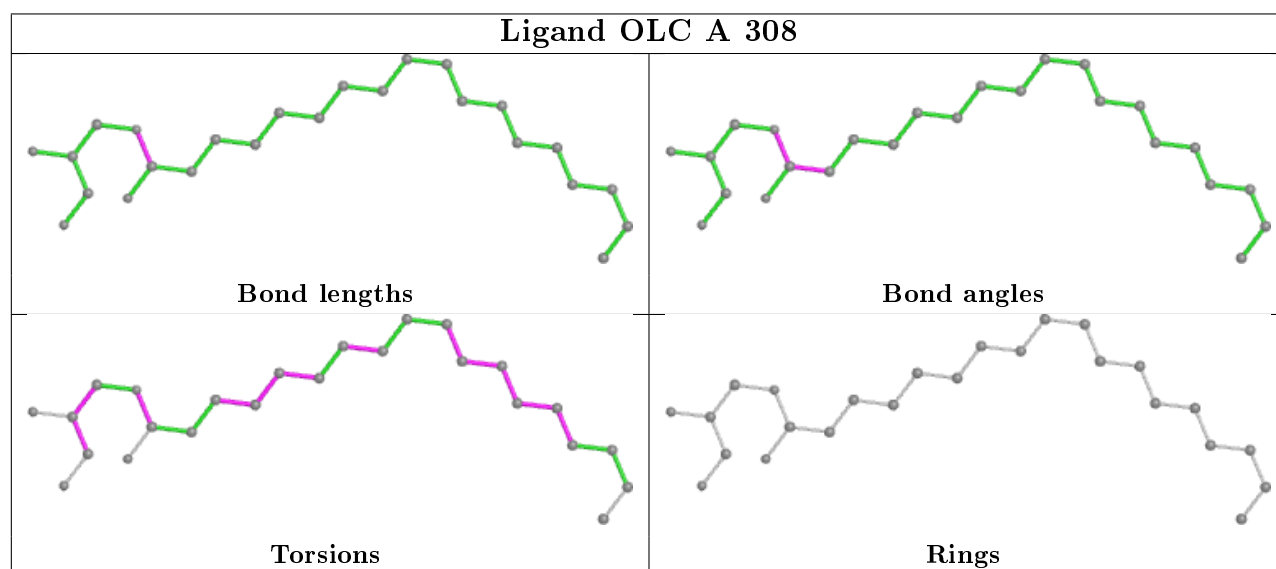
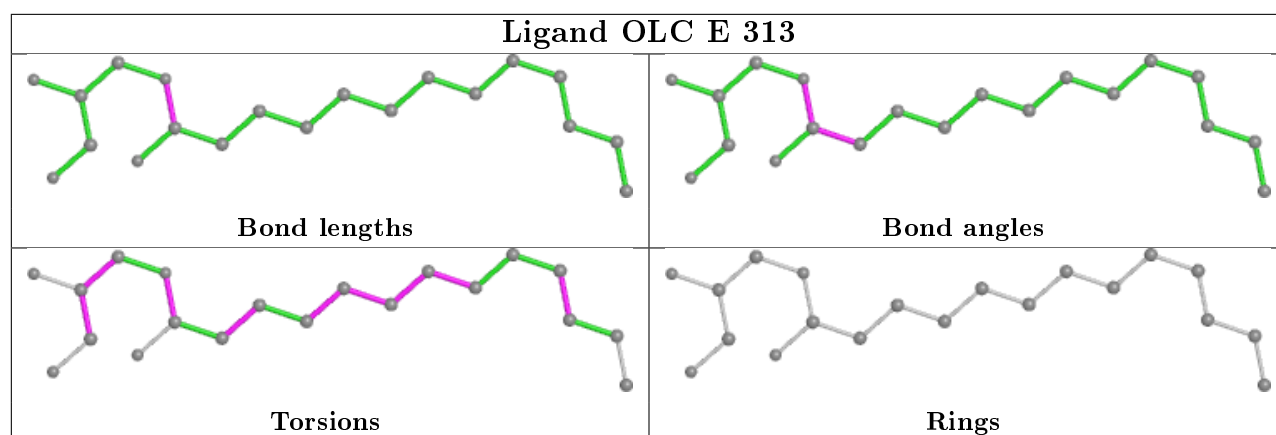


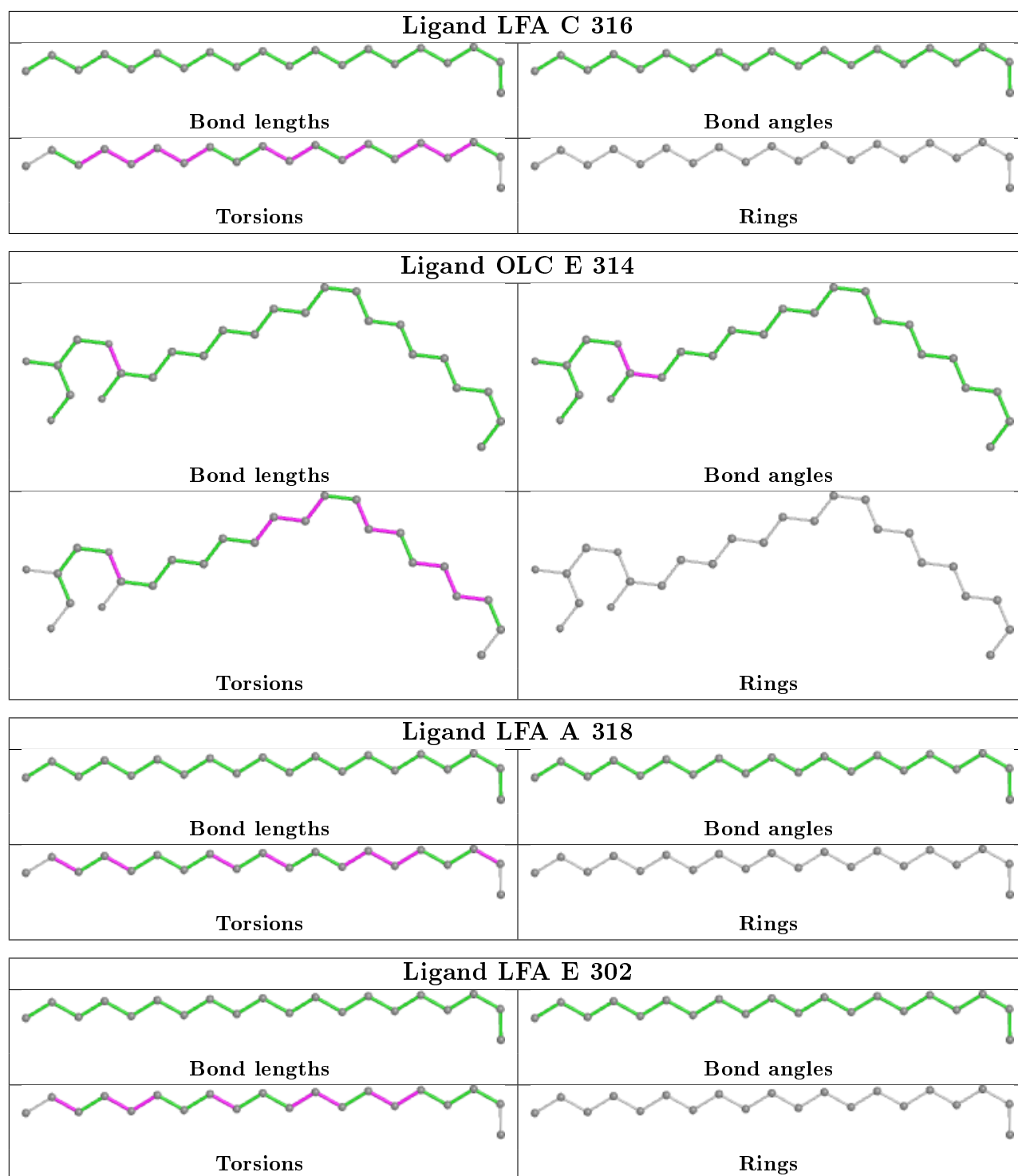




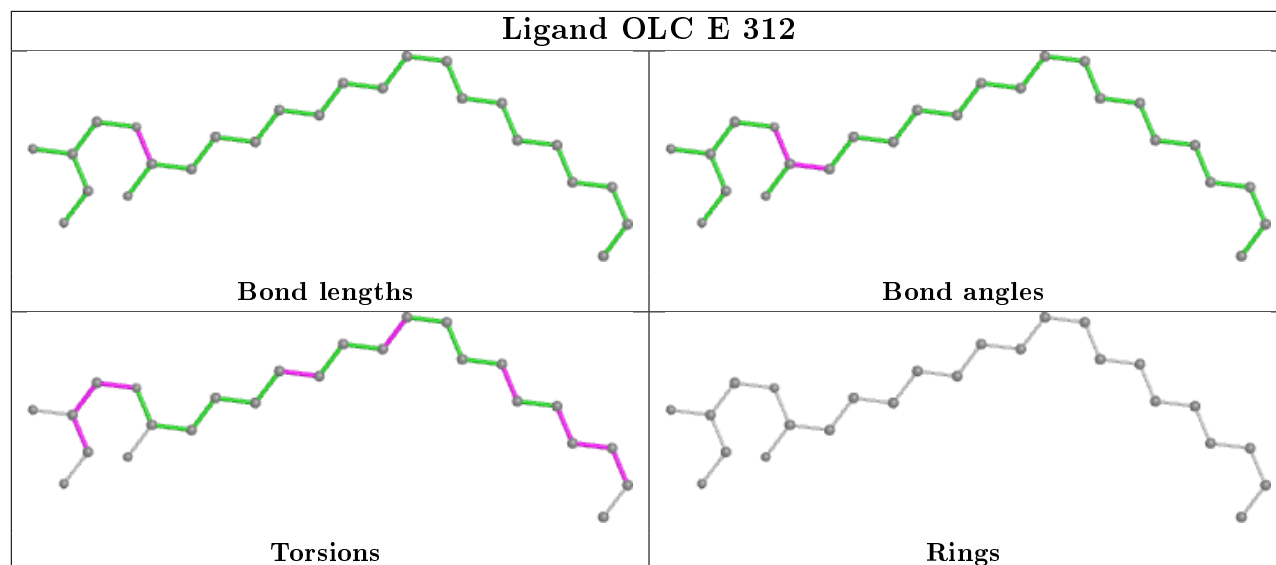




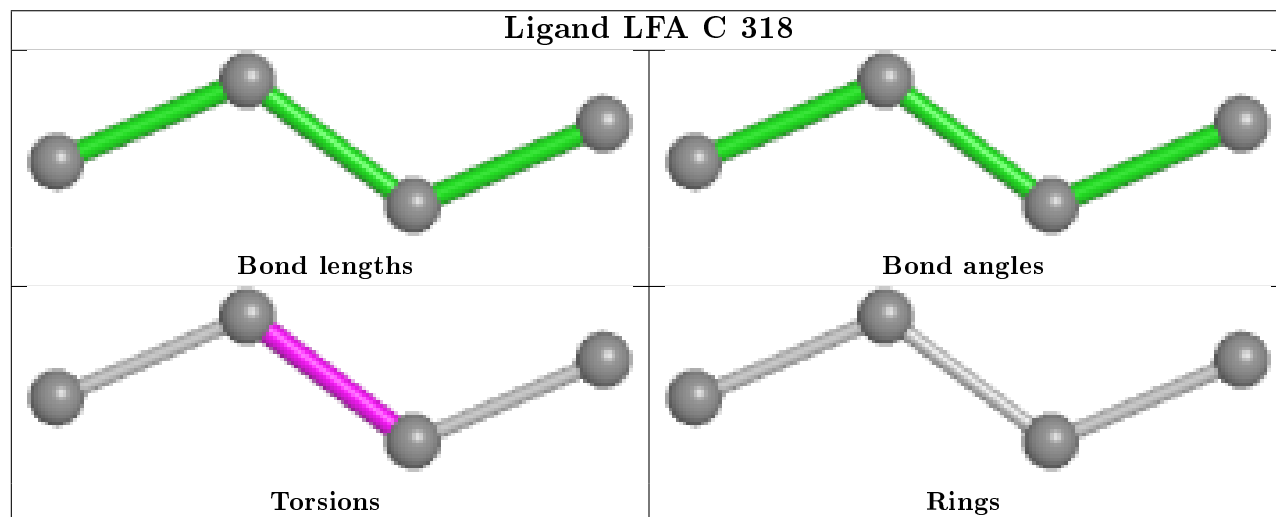




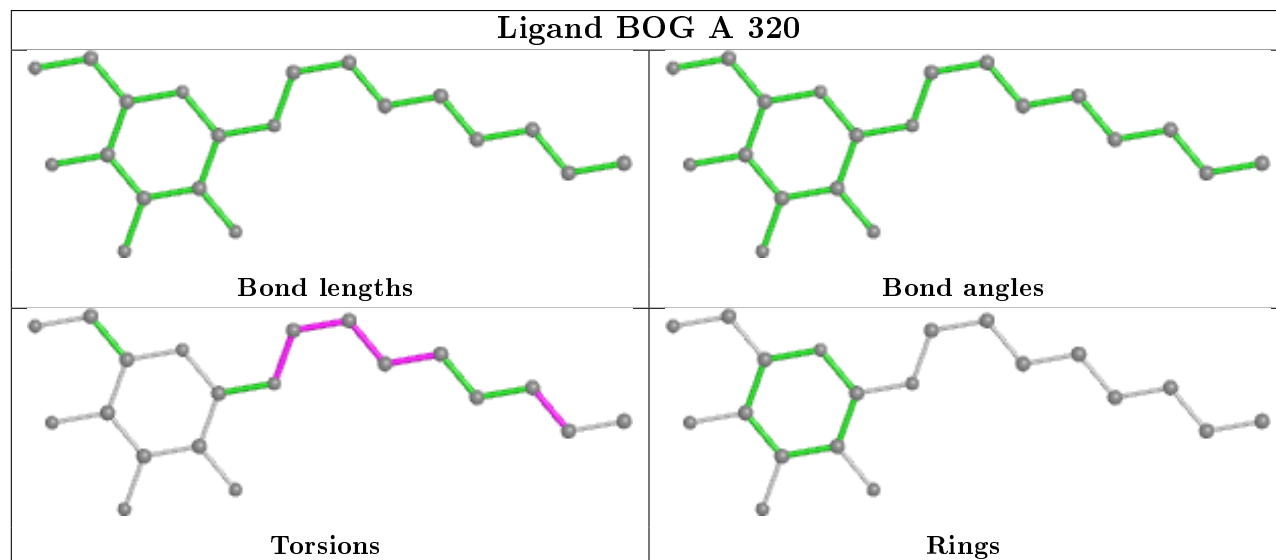
## Ligand OLC E 312



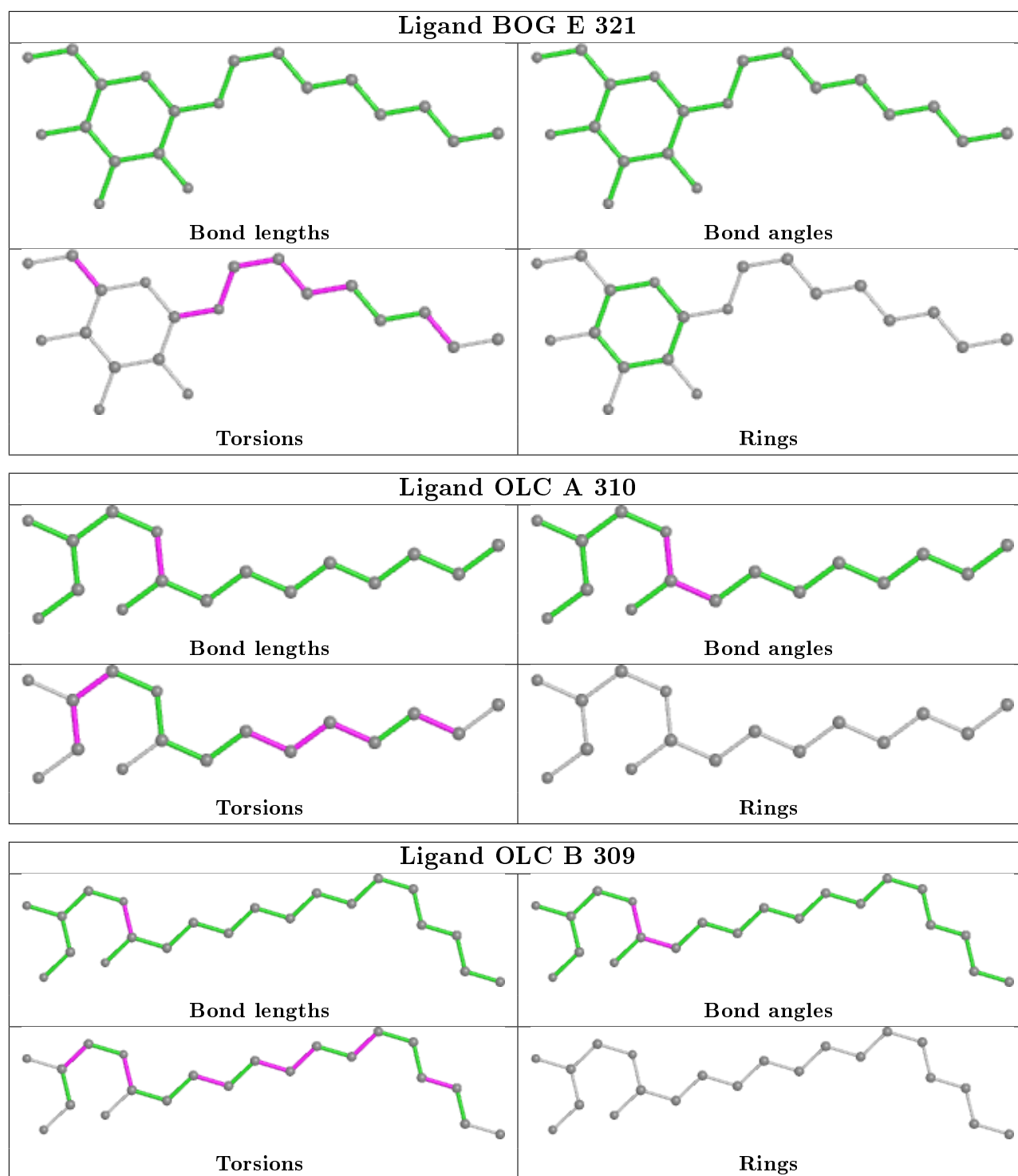
## Ligand LFA C 318

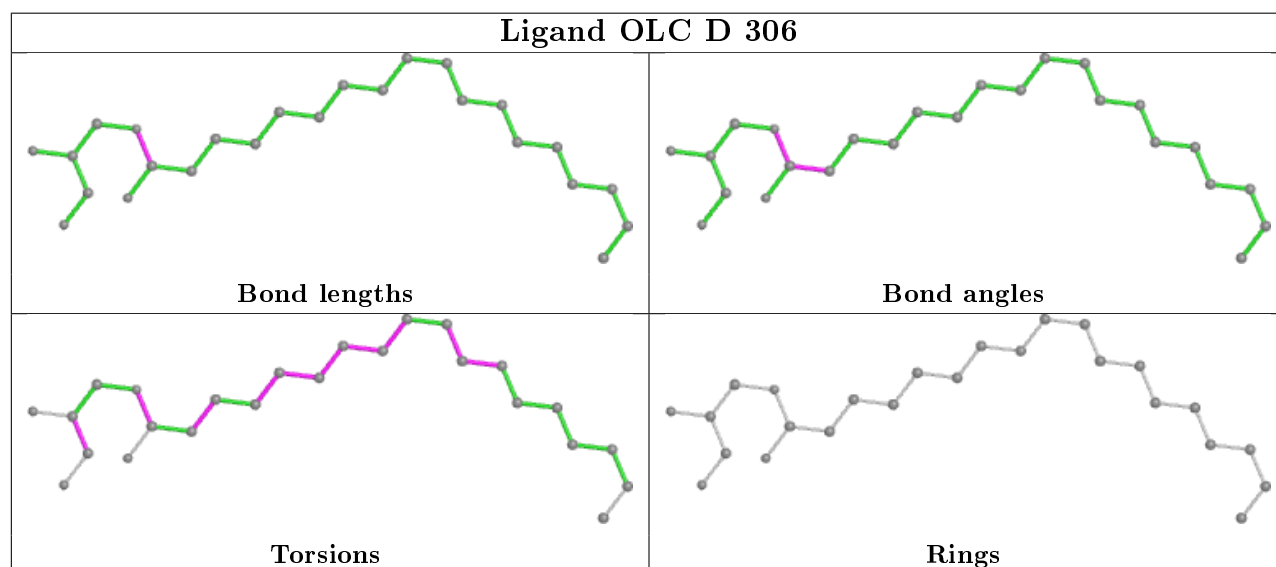
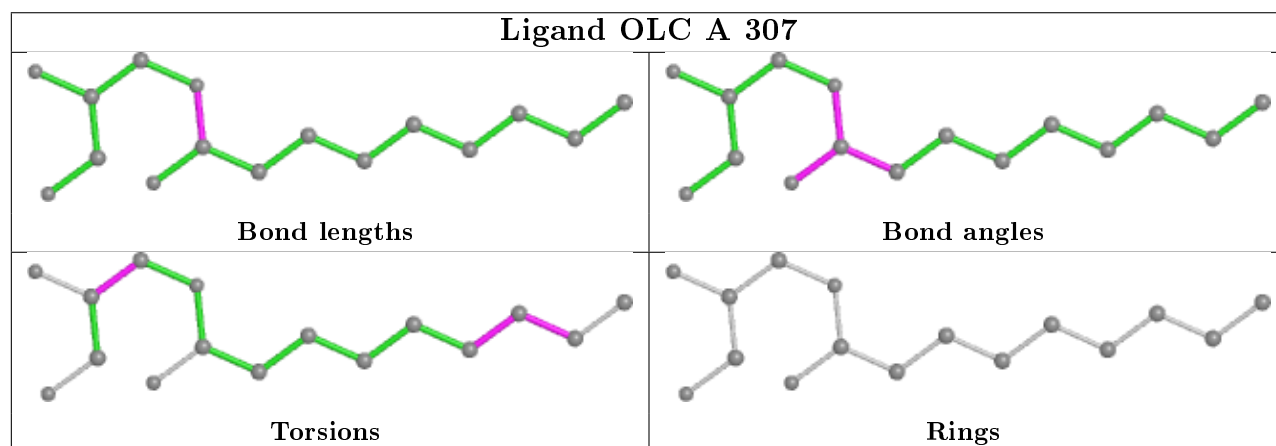
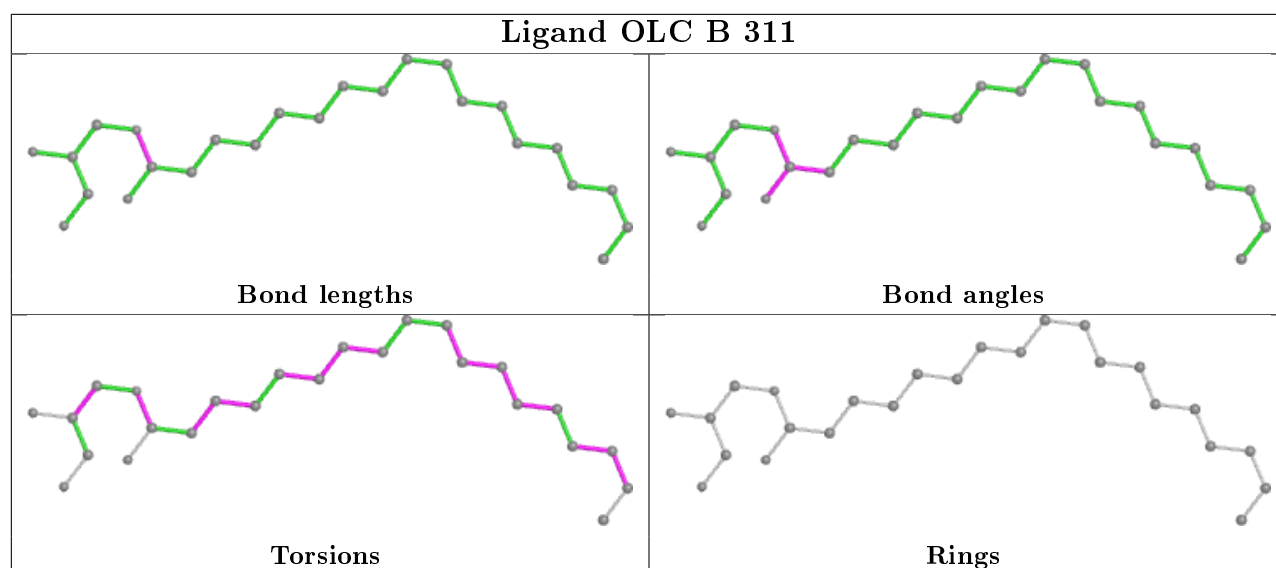


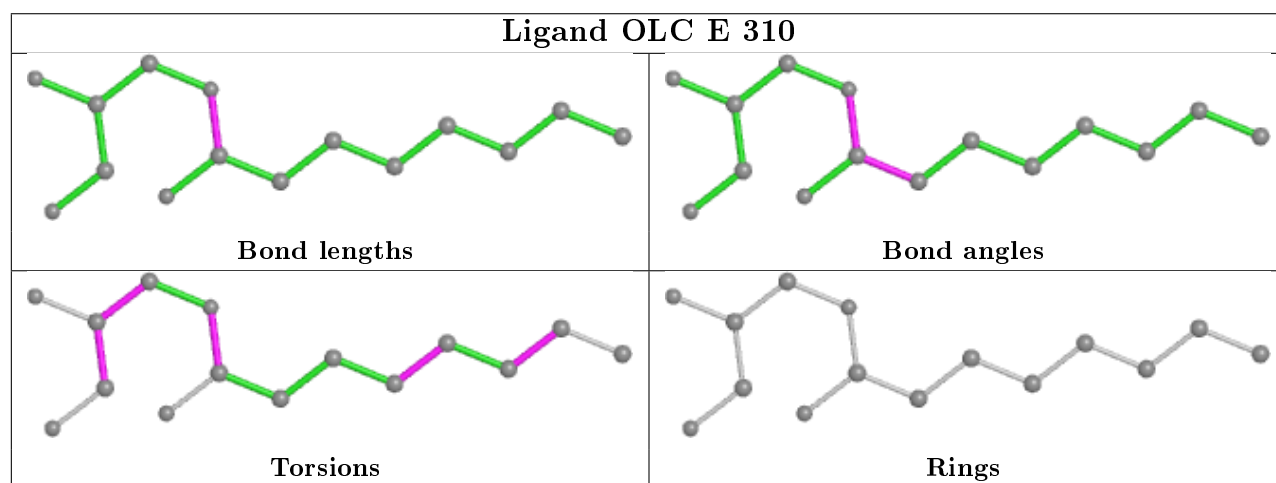
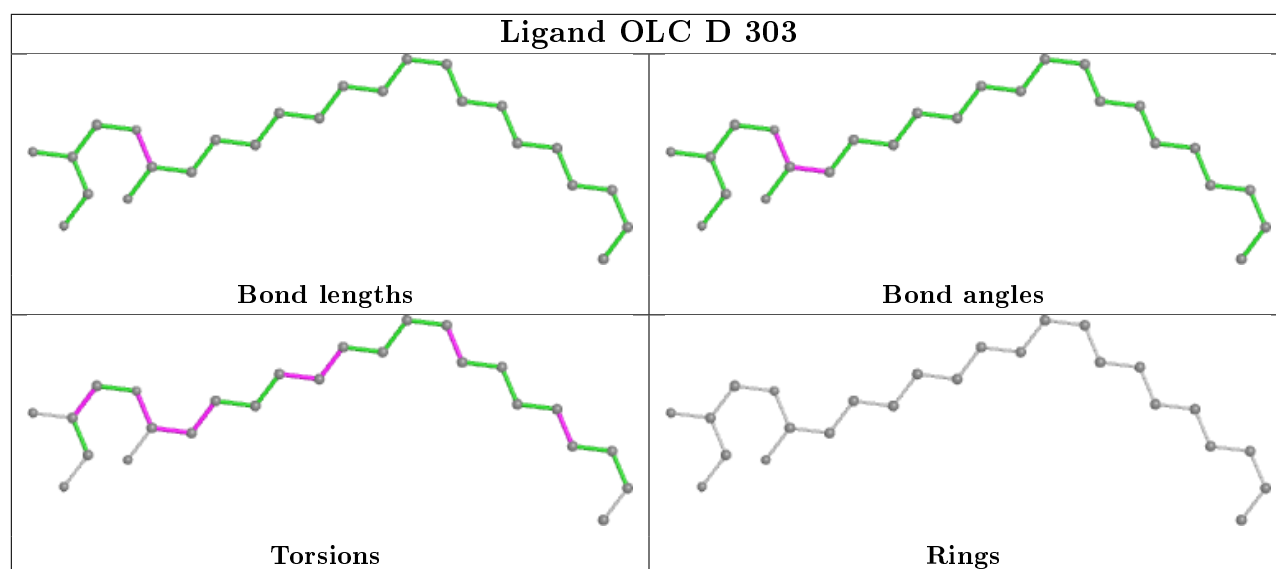
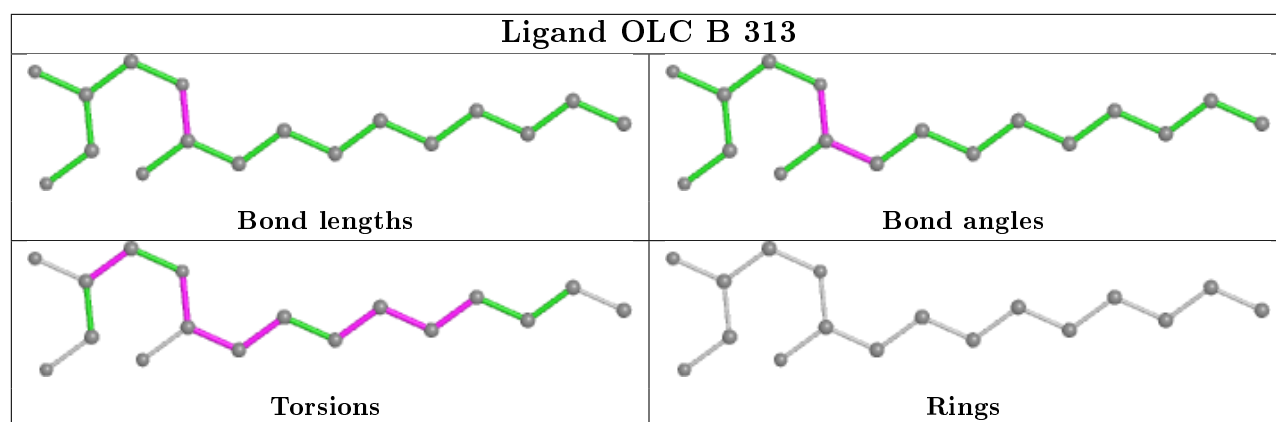
## Ligand BOG A 320

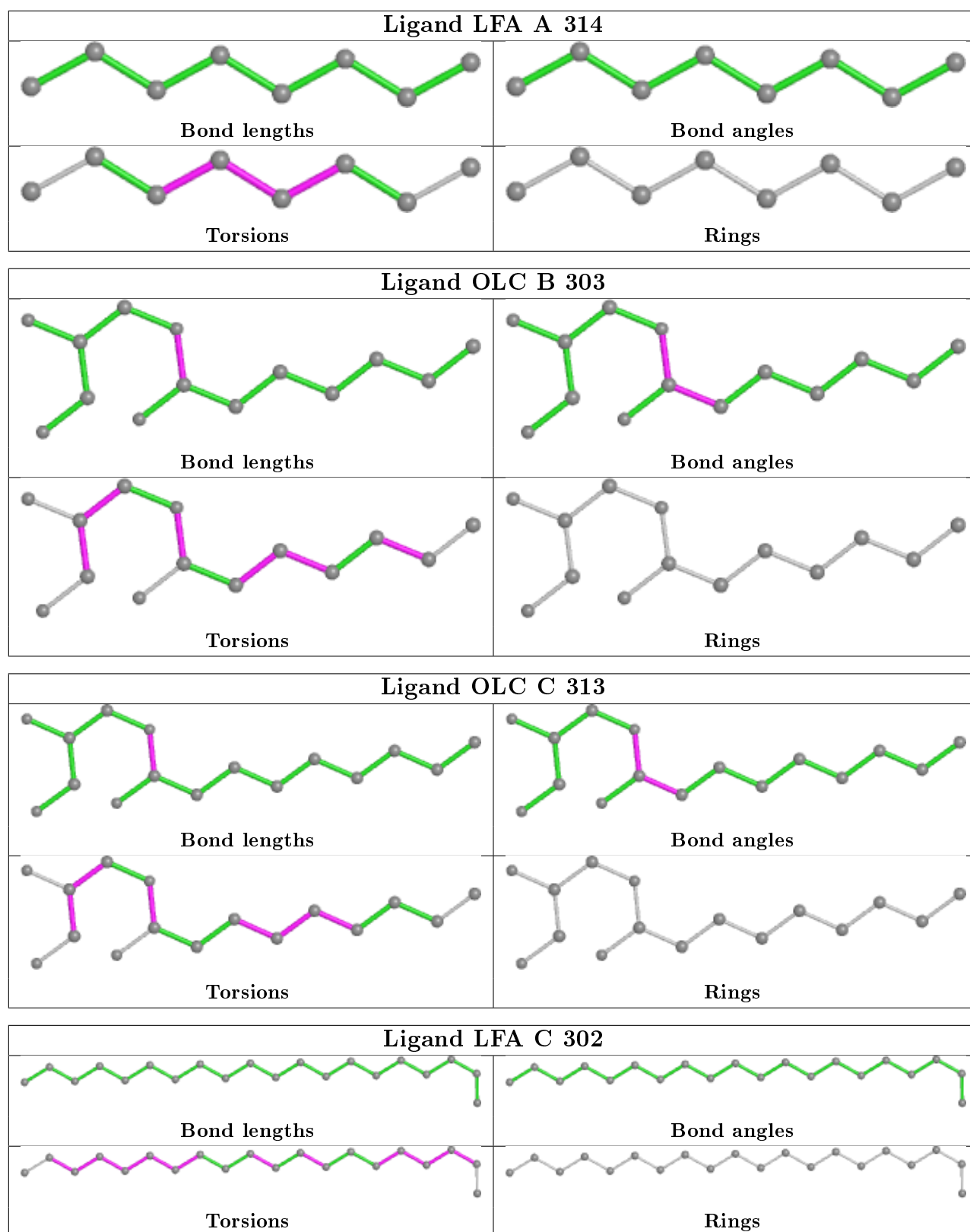


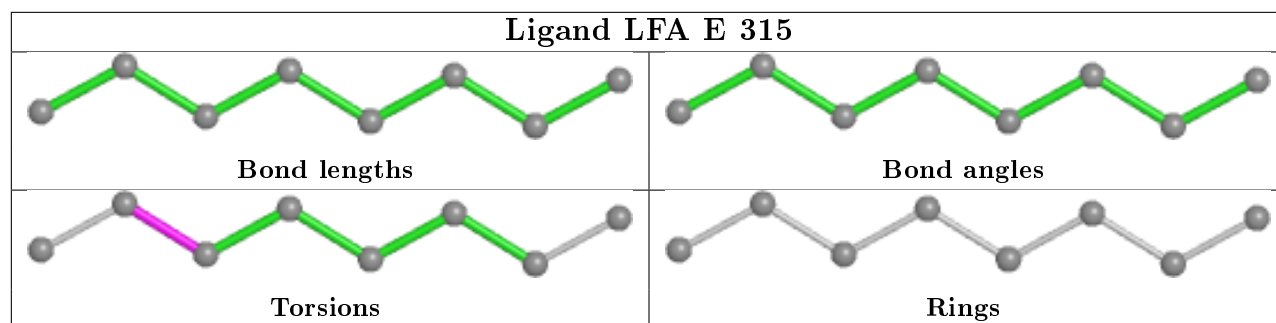
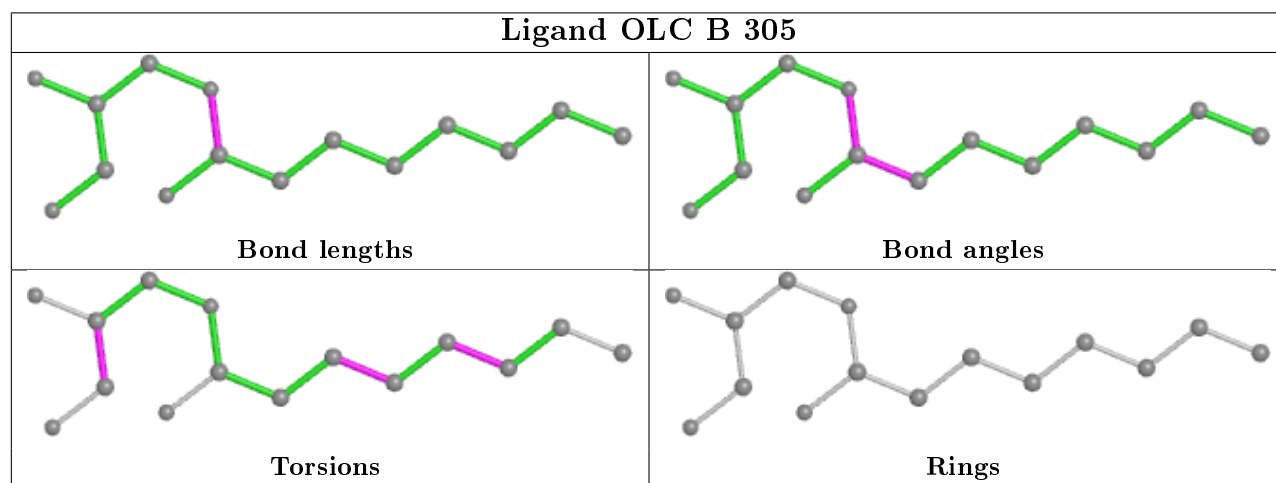
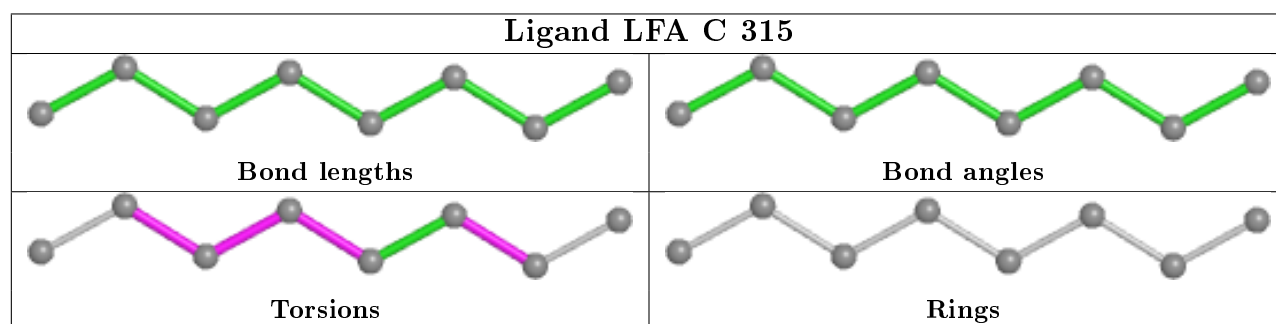
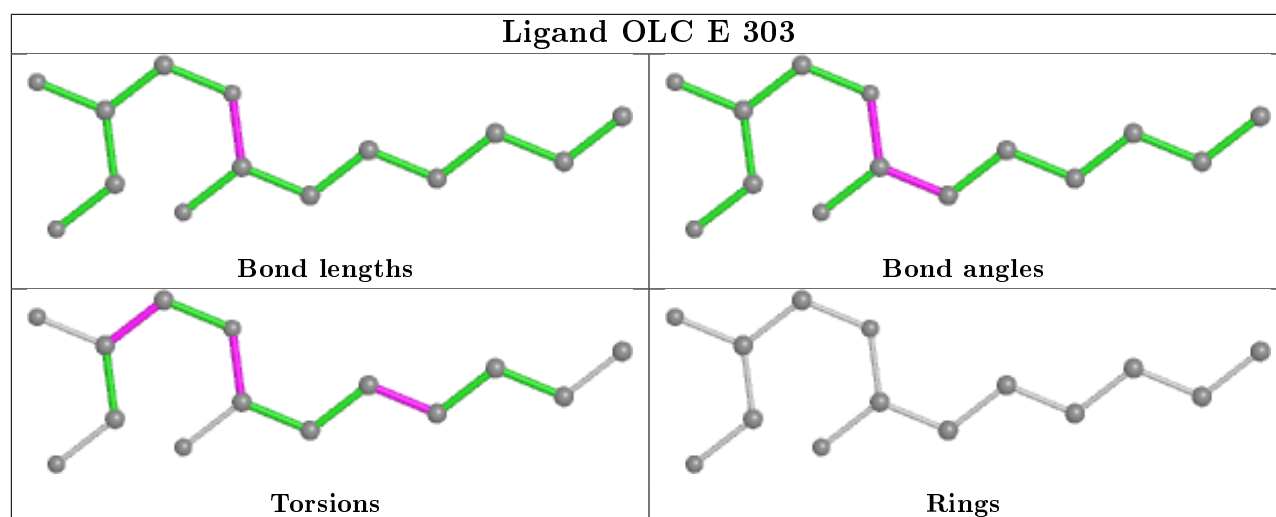


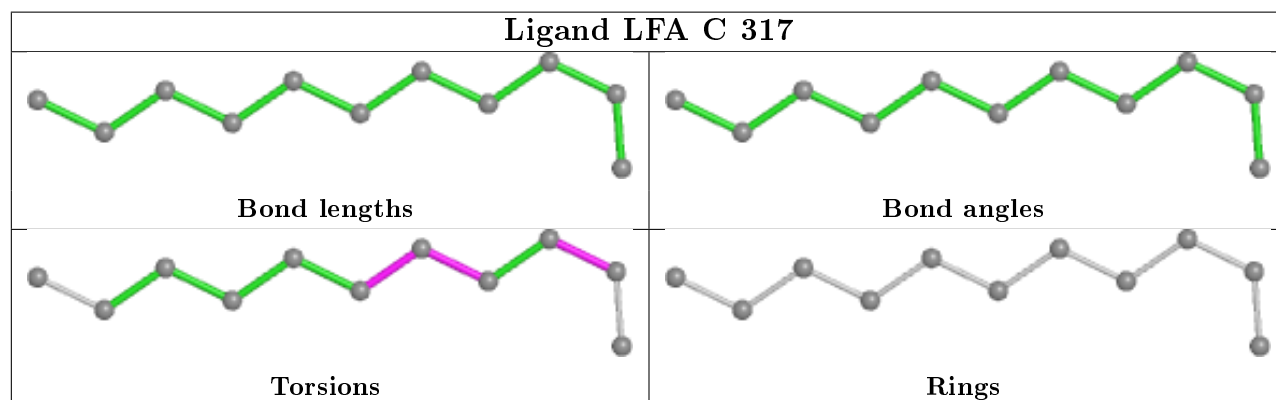
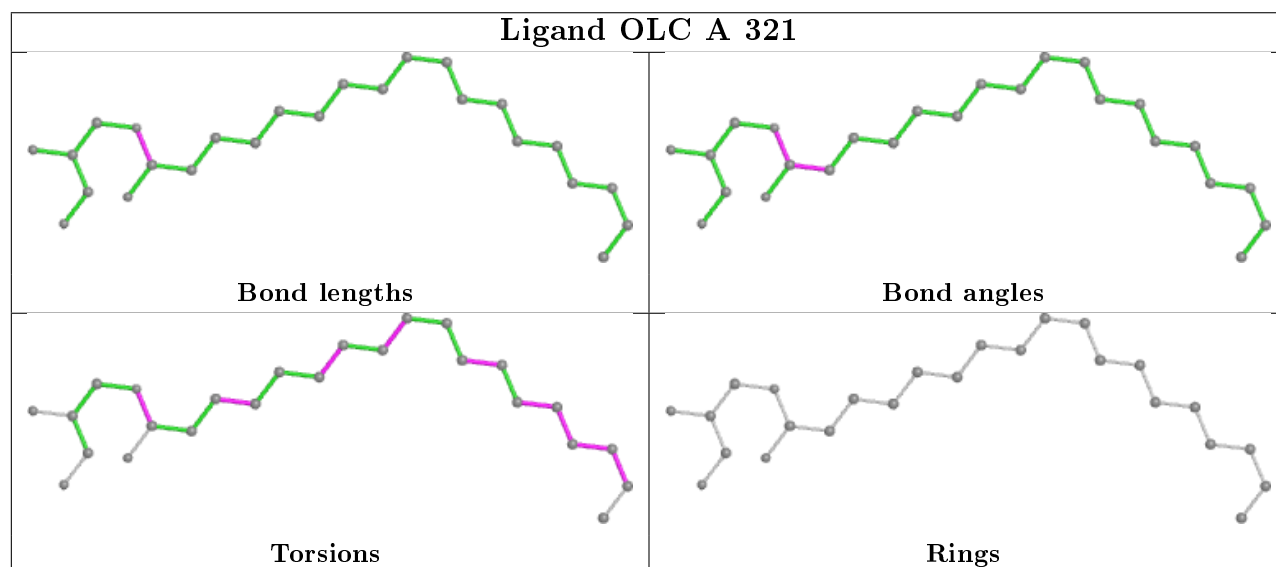
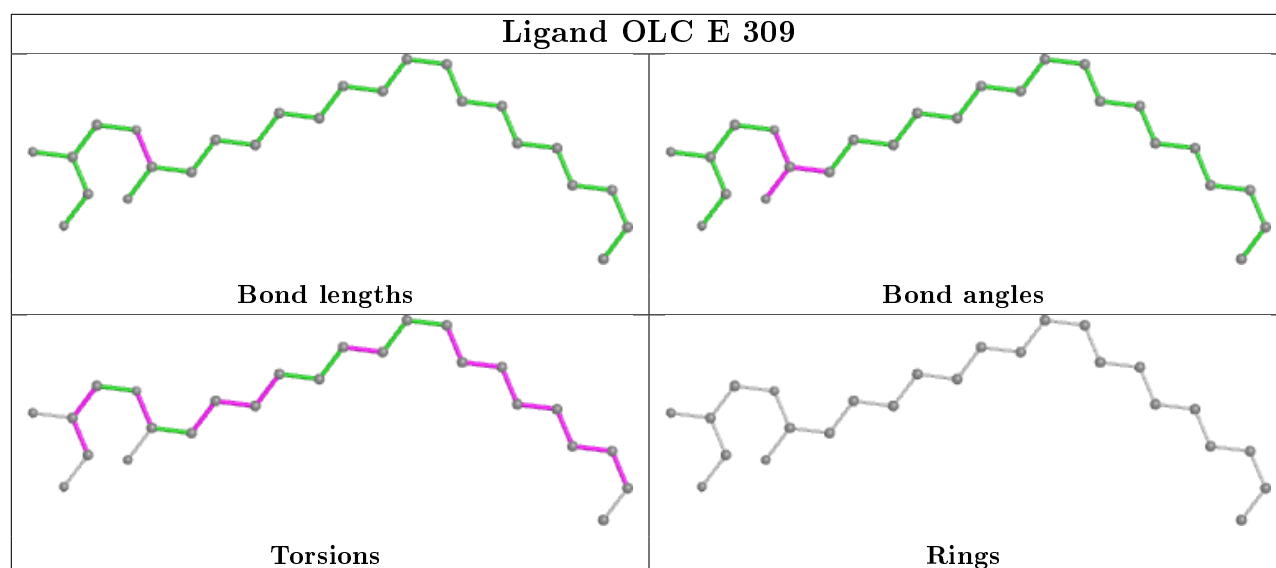


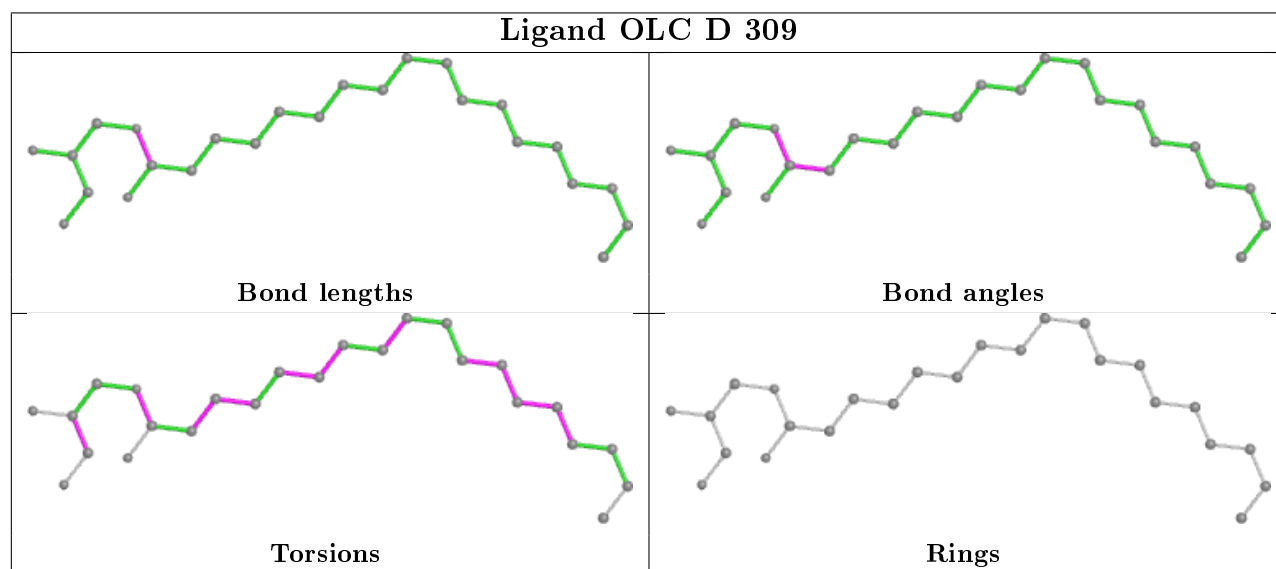
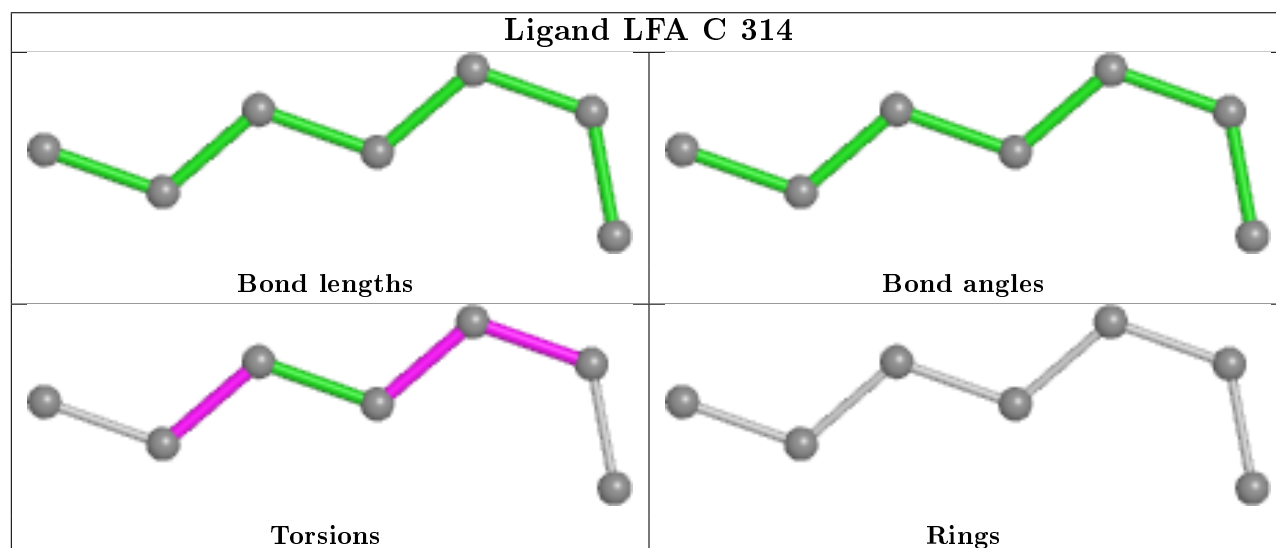
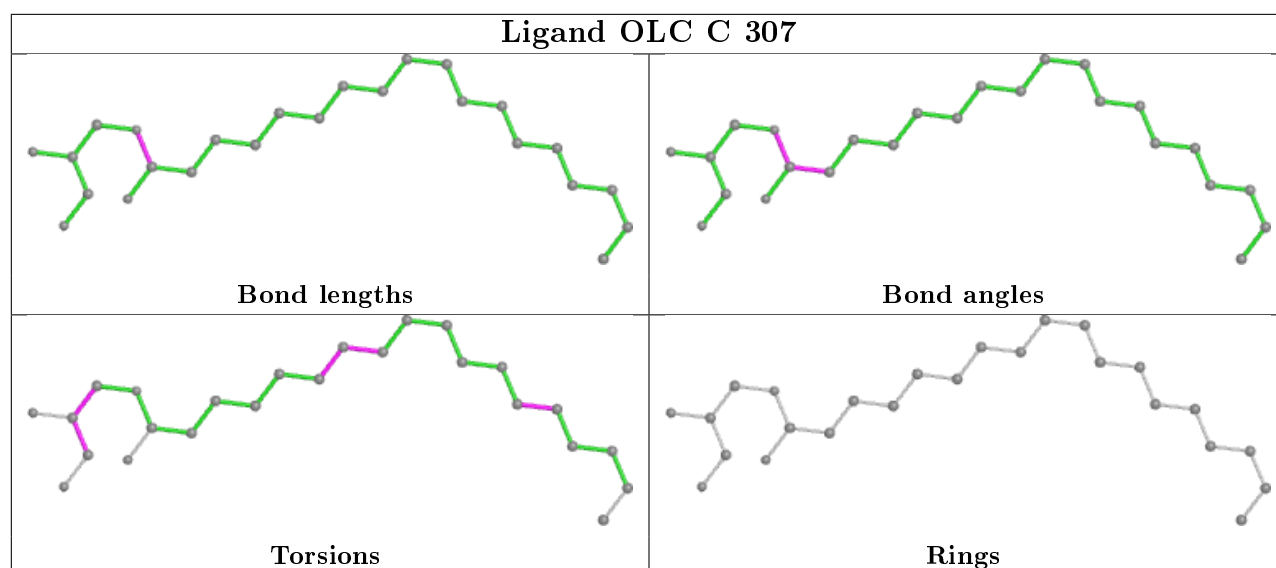


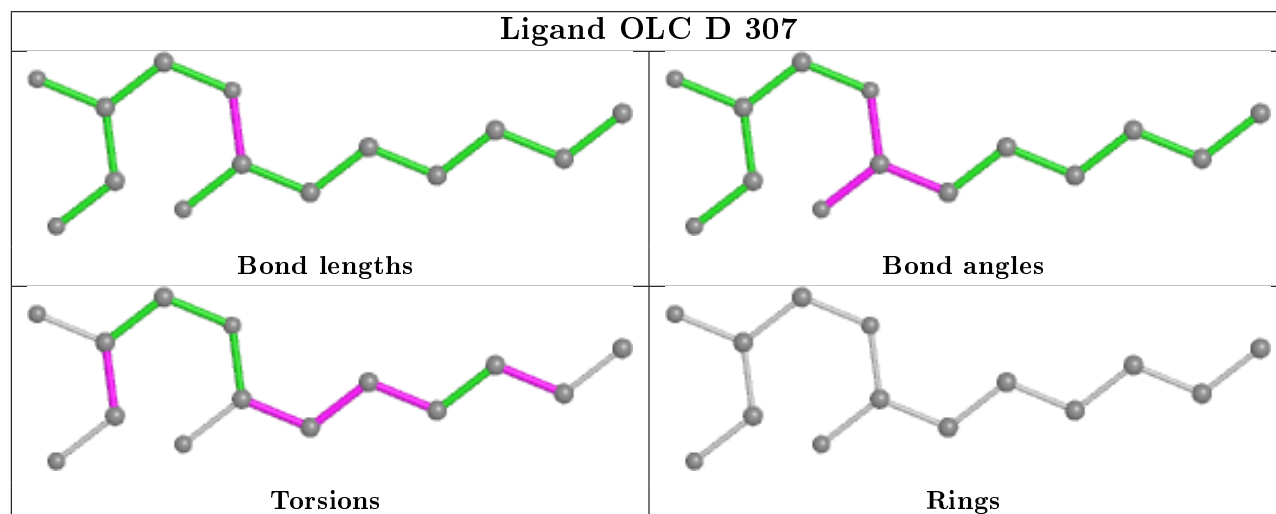
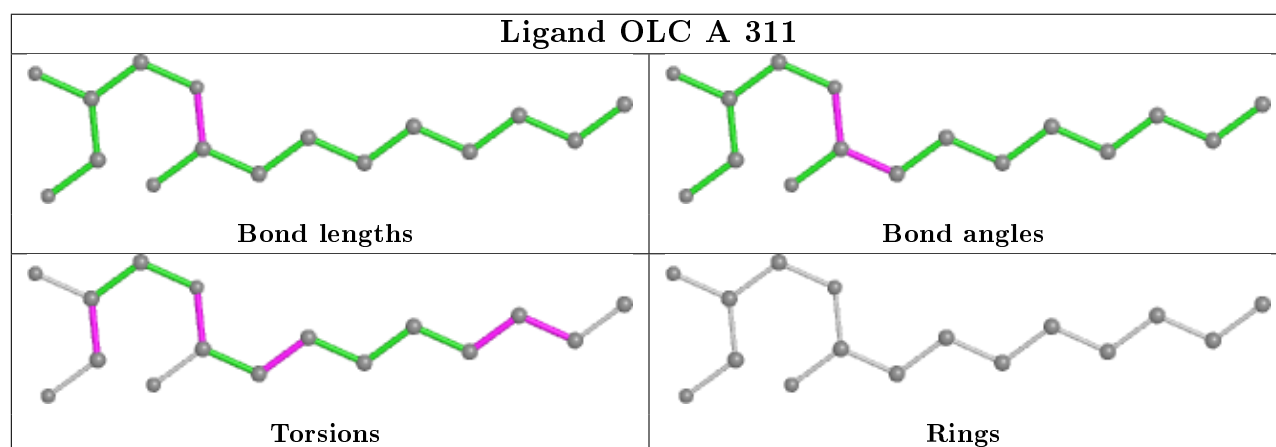
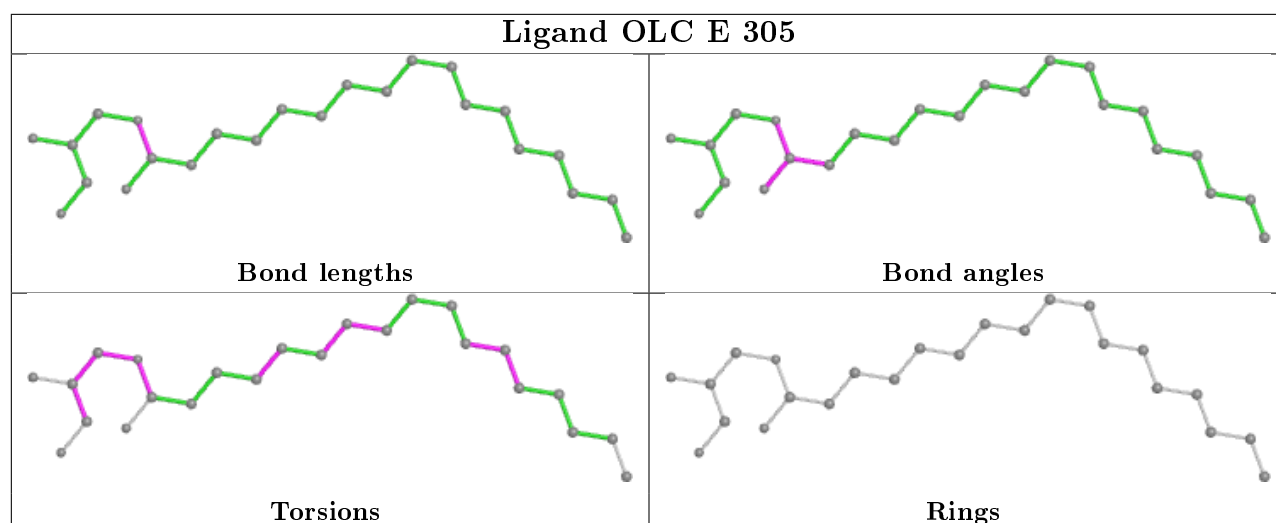




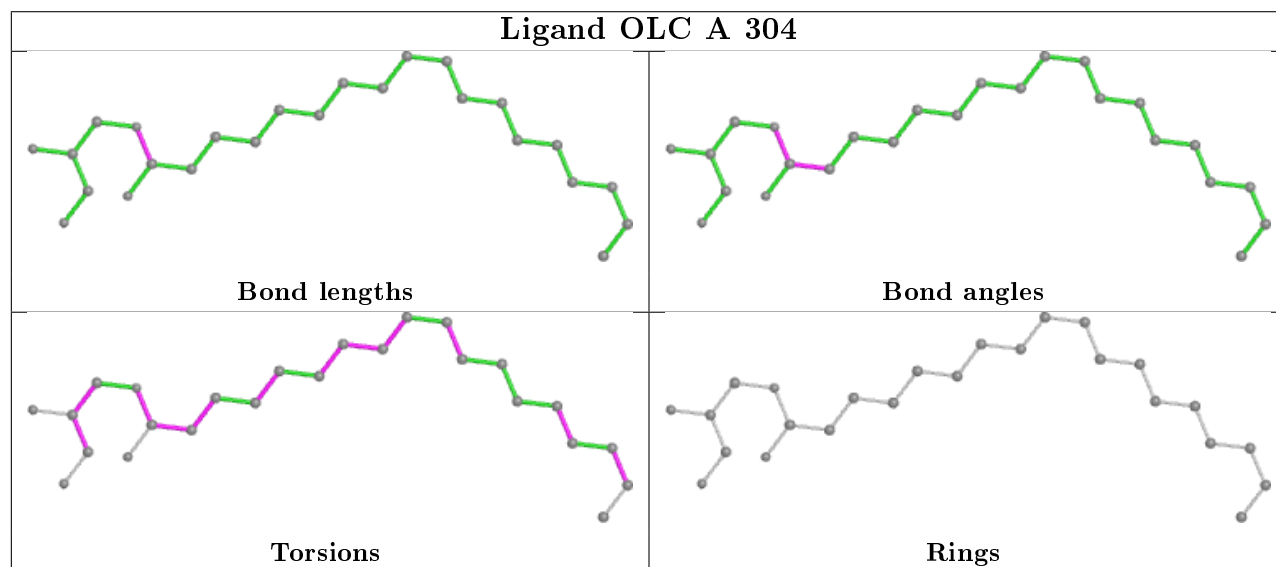
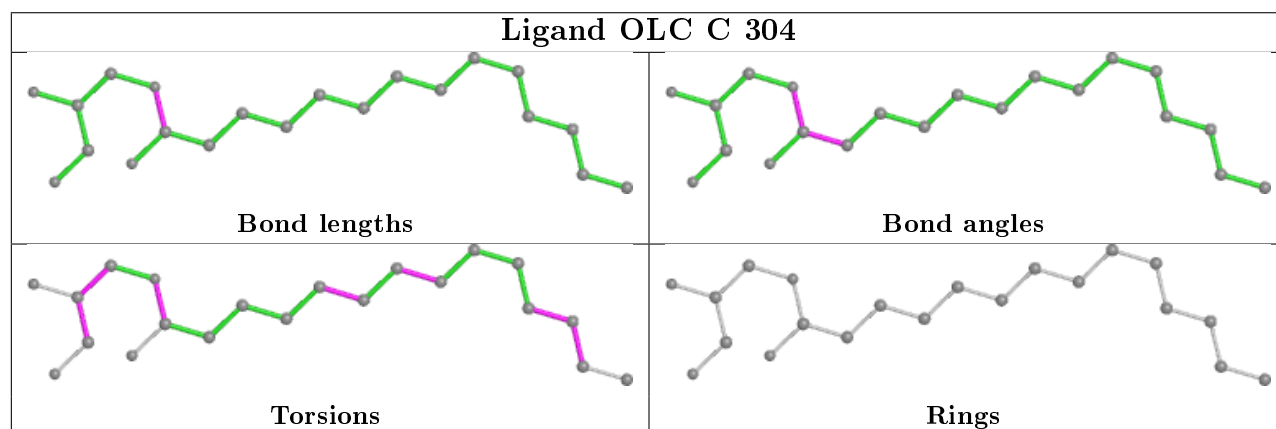
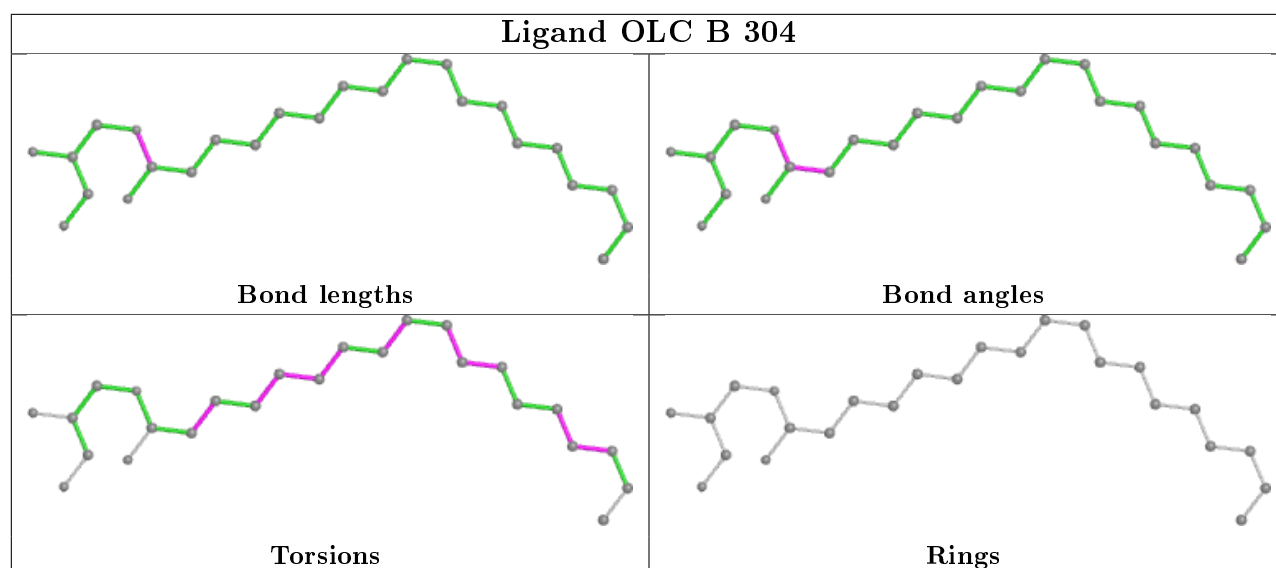


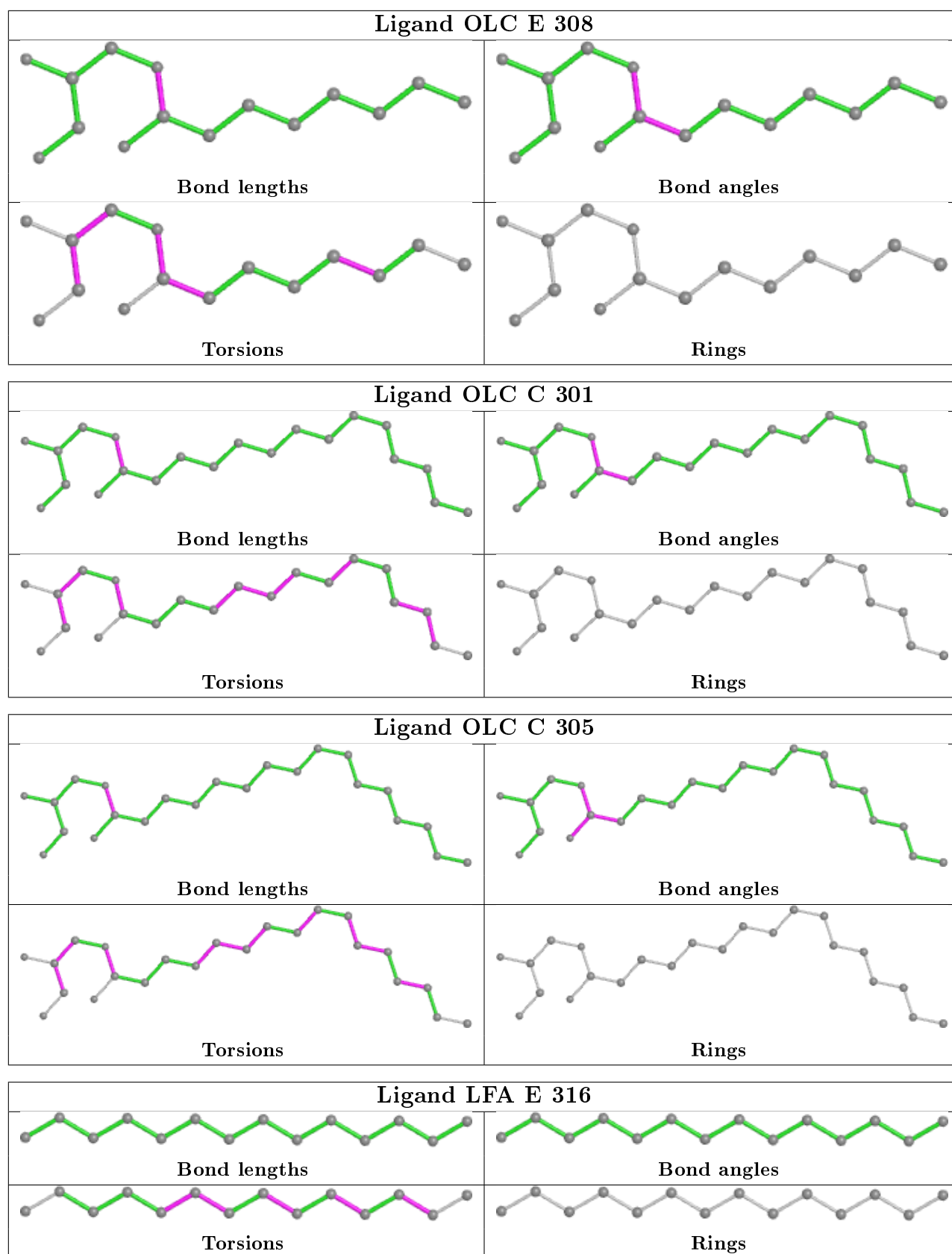


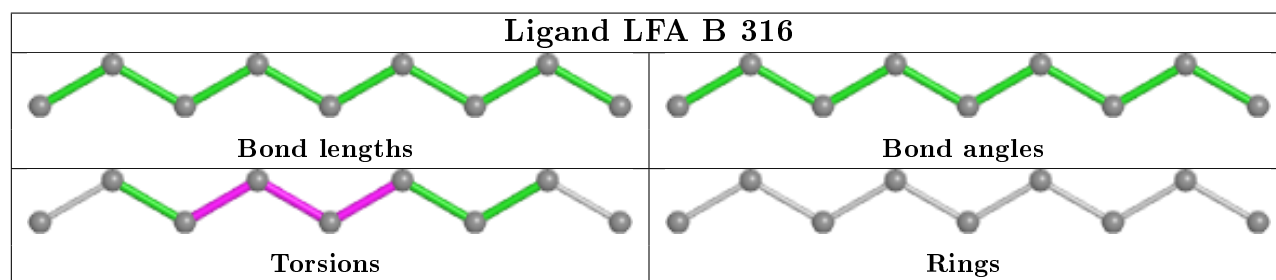
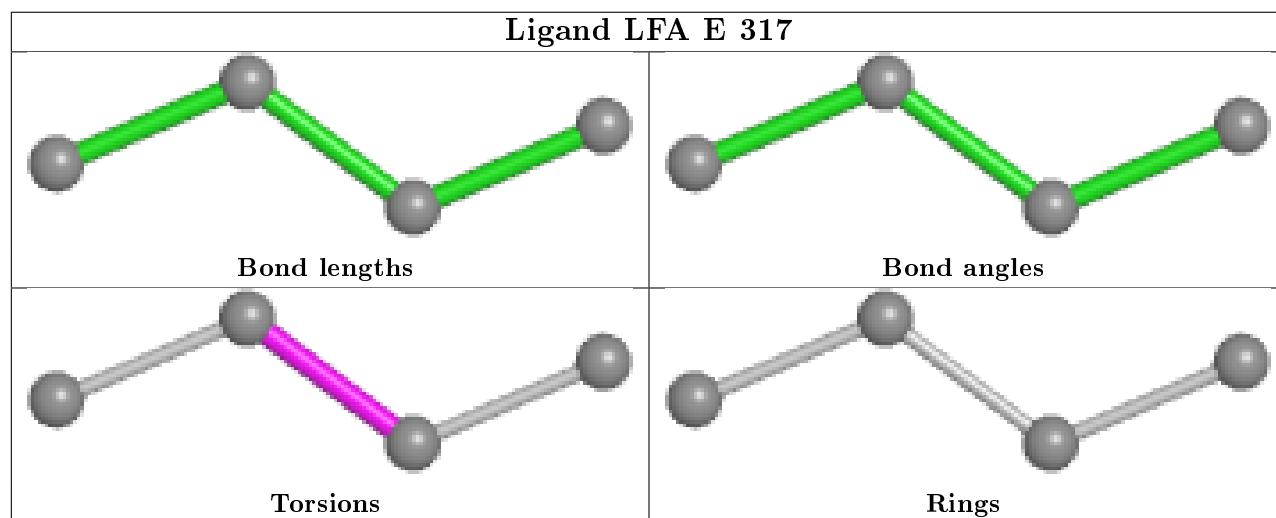
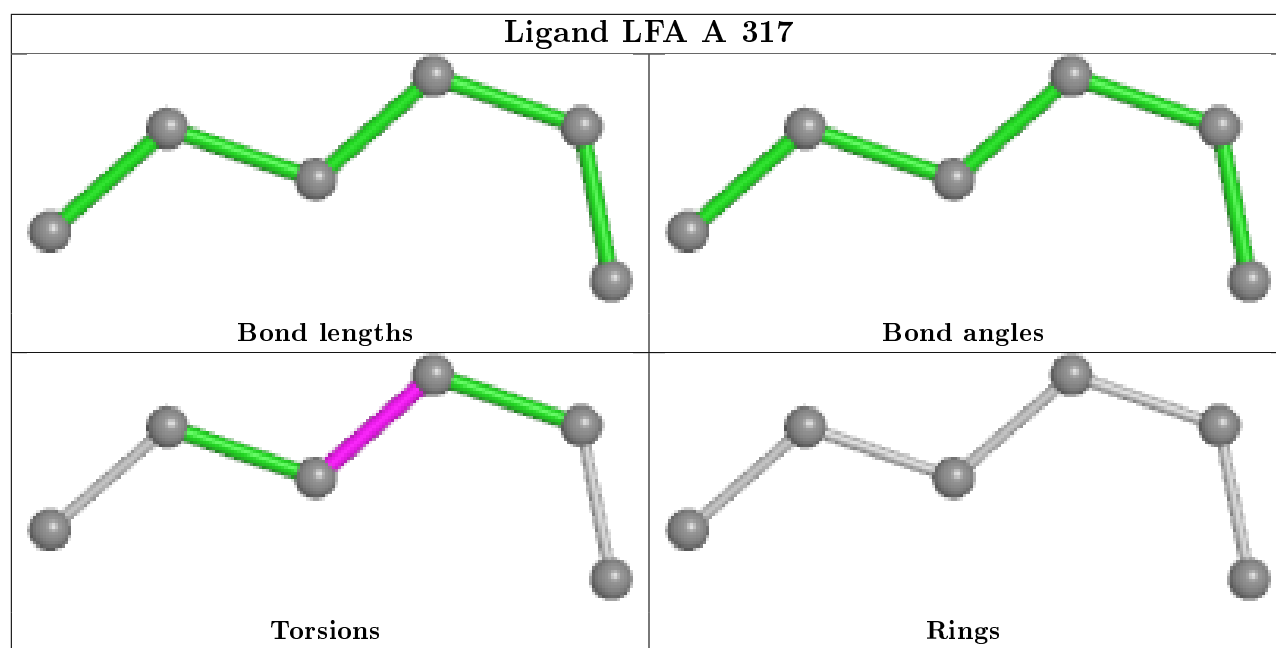


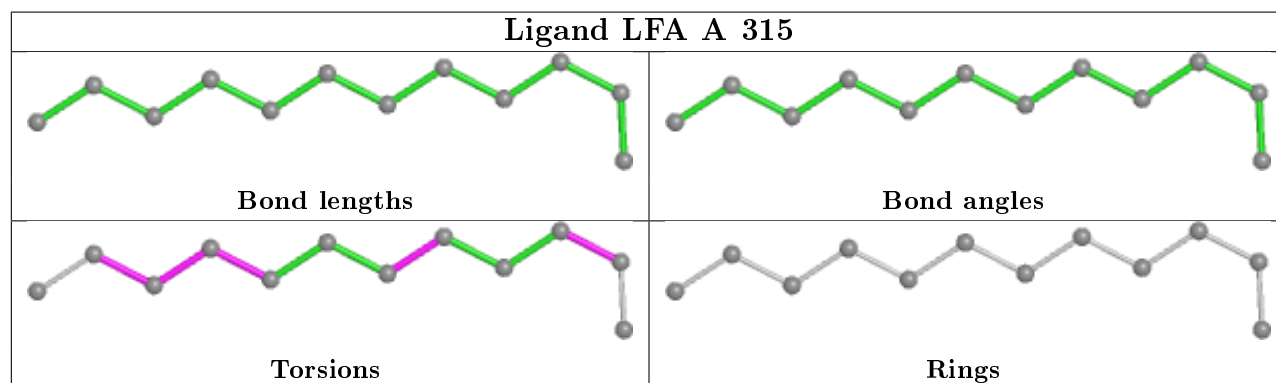
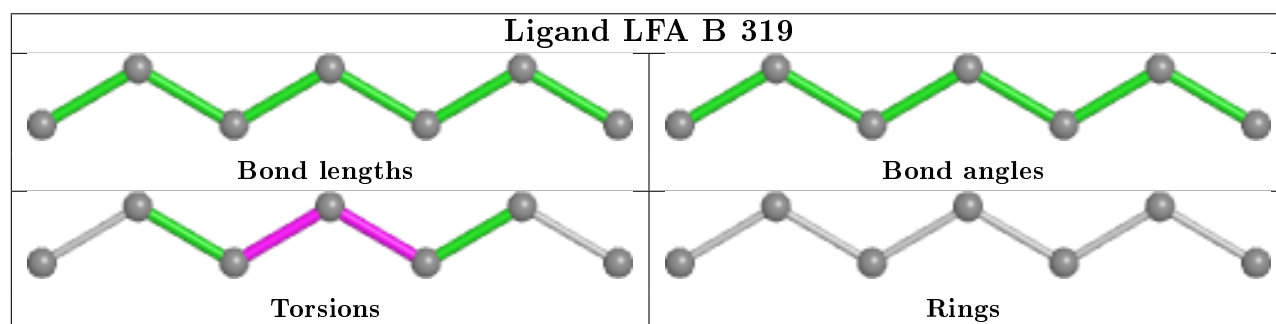
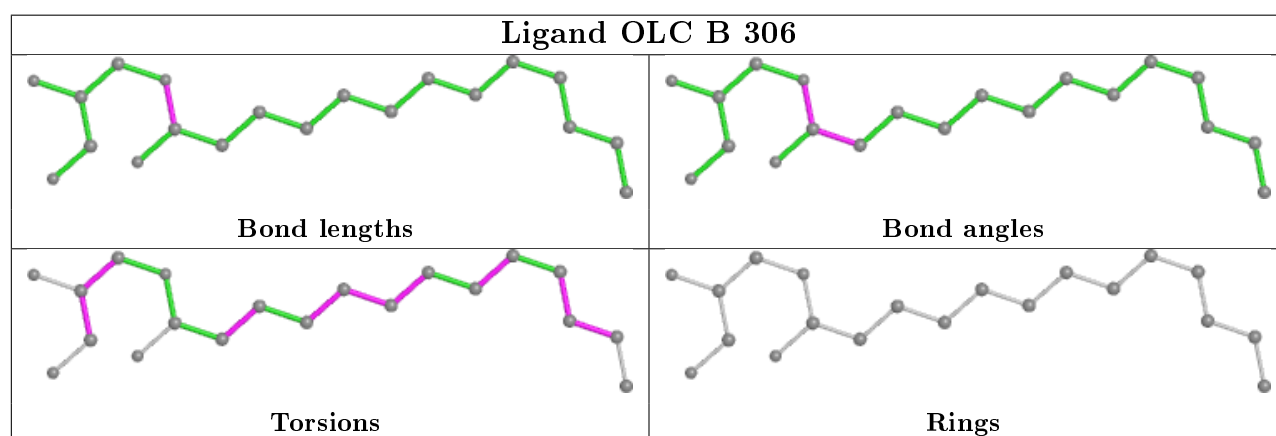
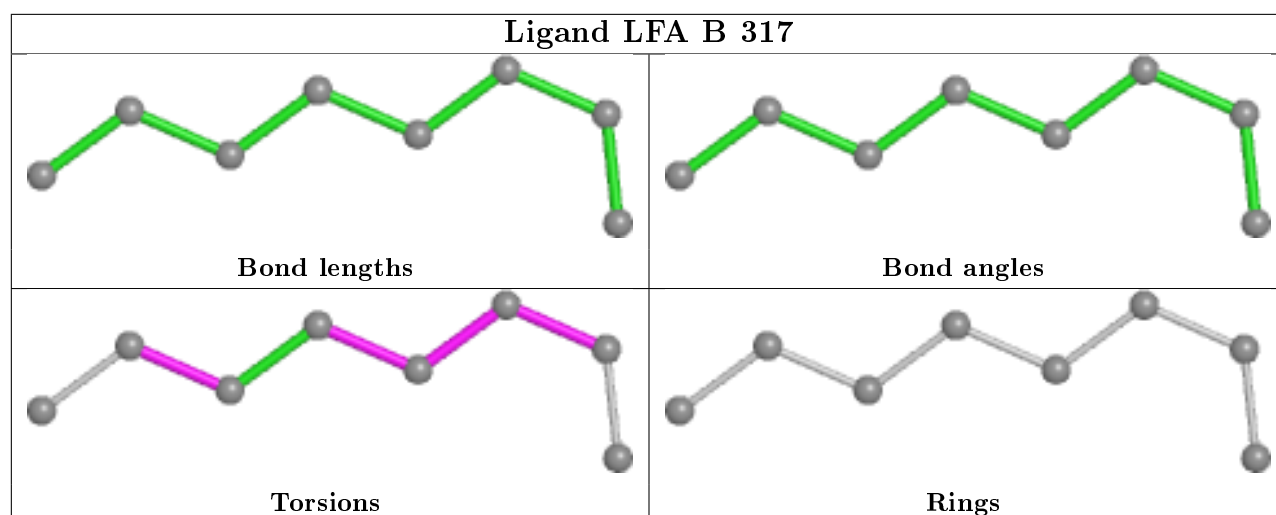


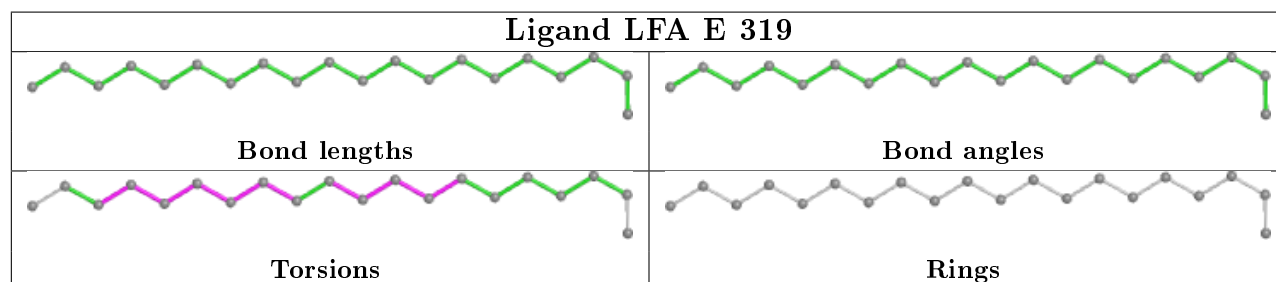
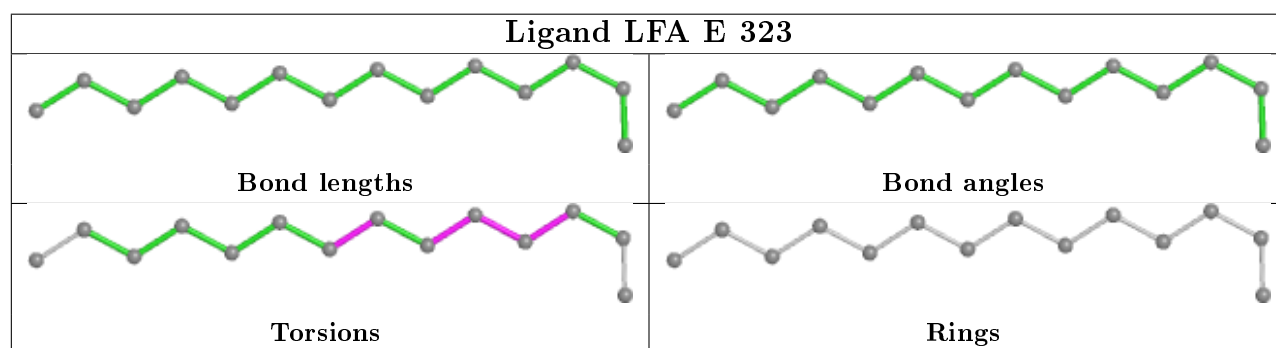
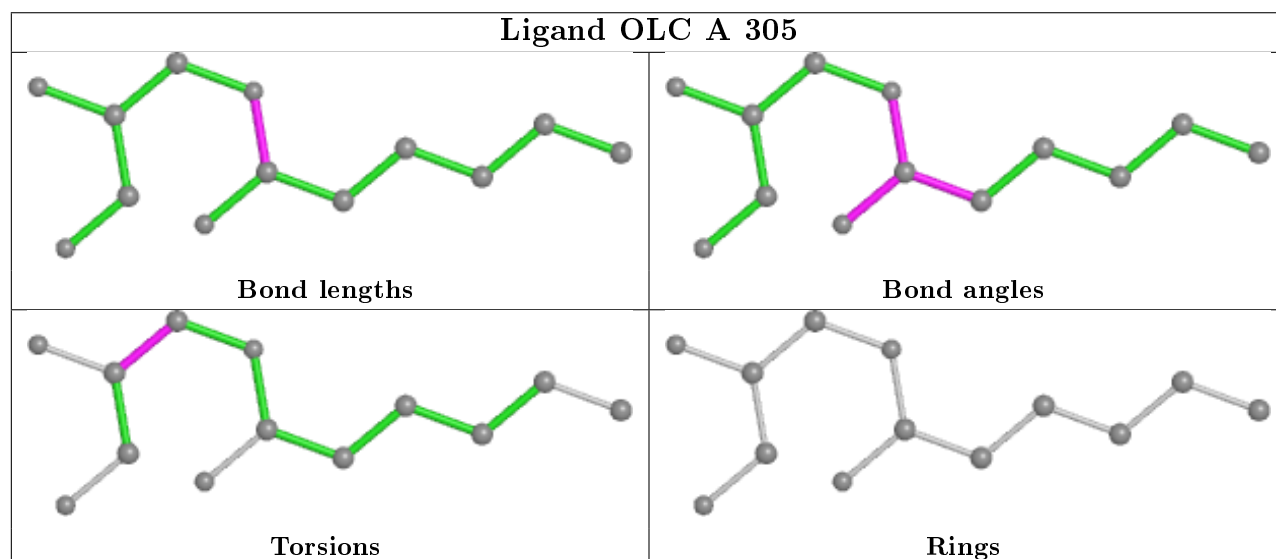
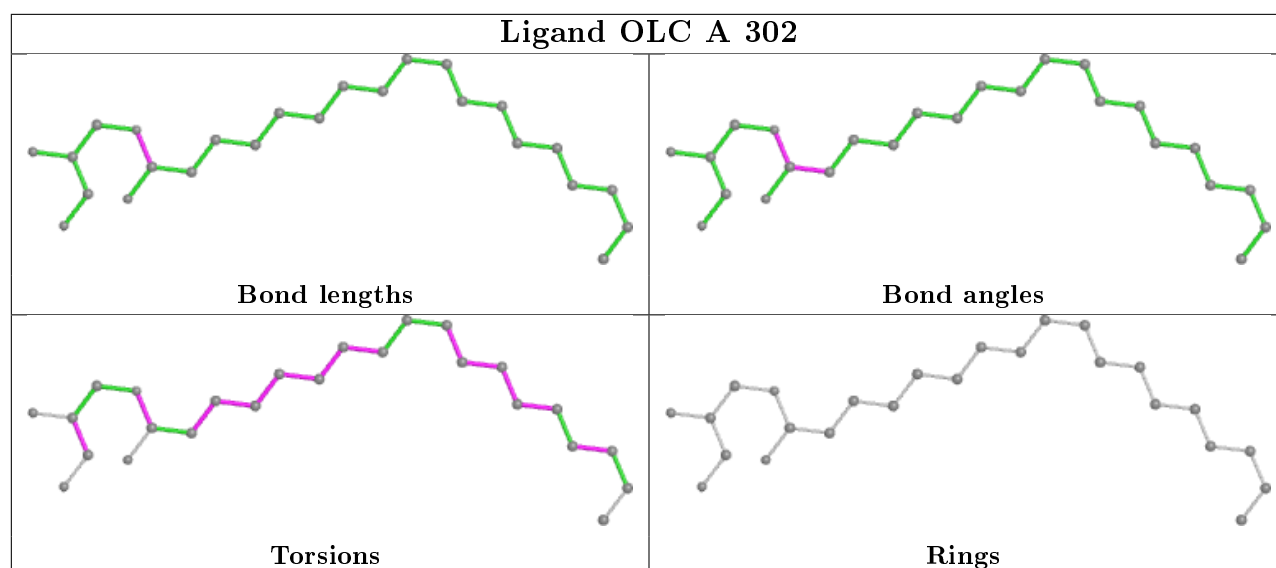


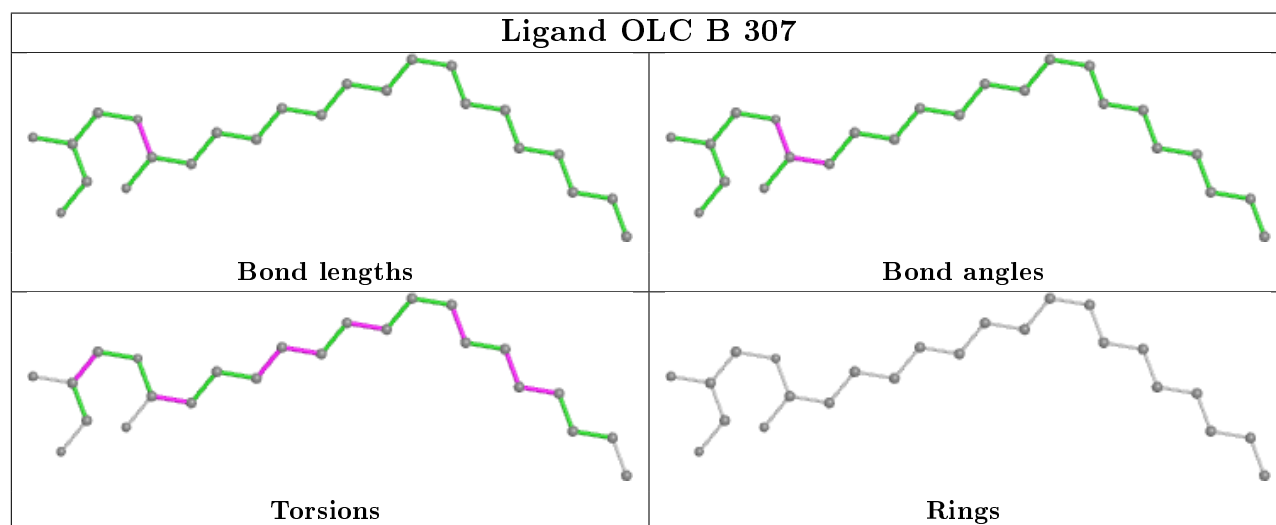
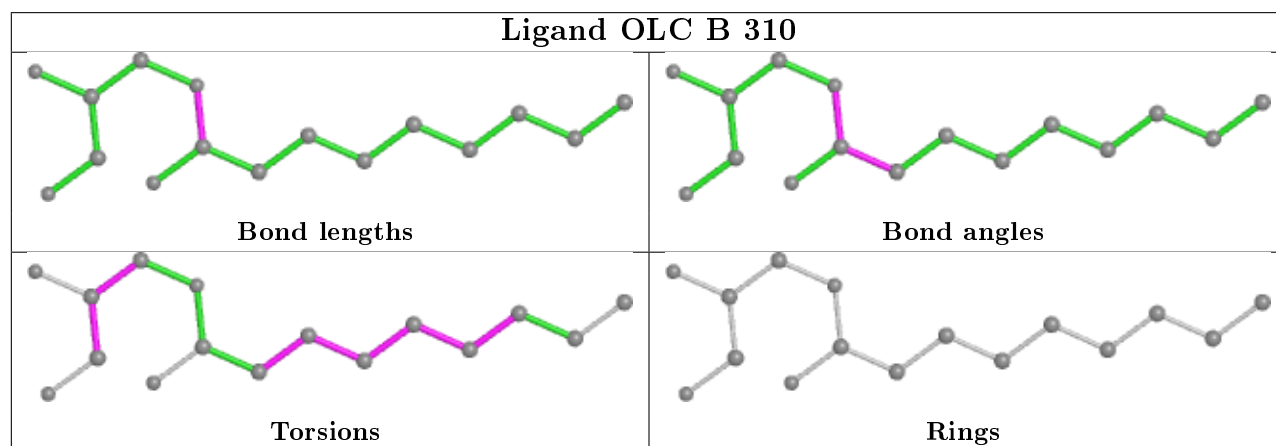
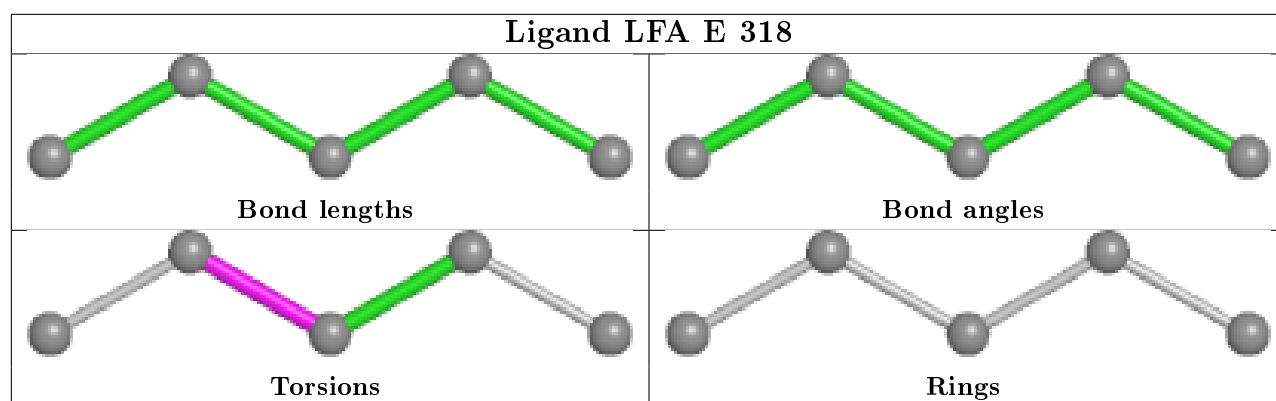


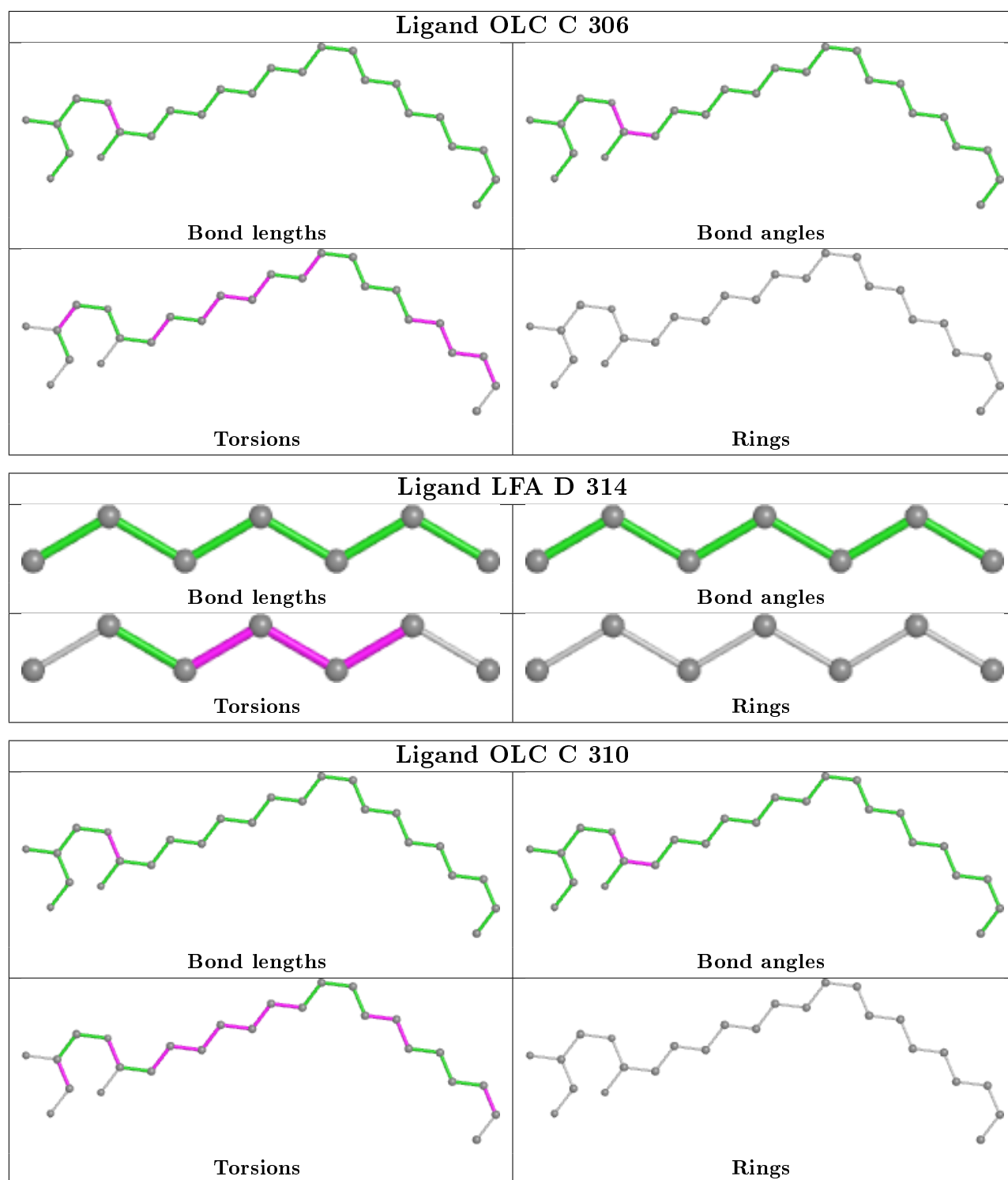


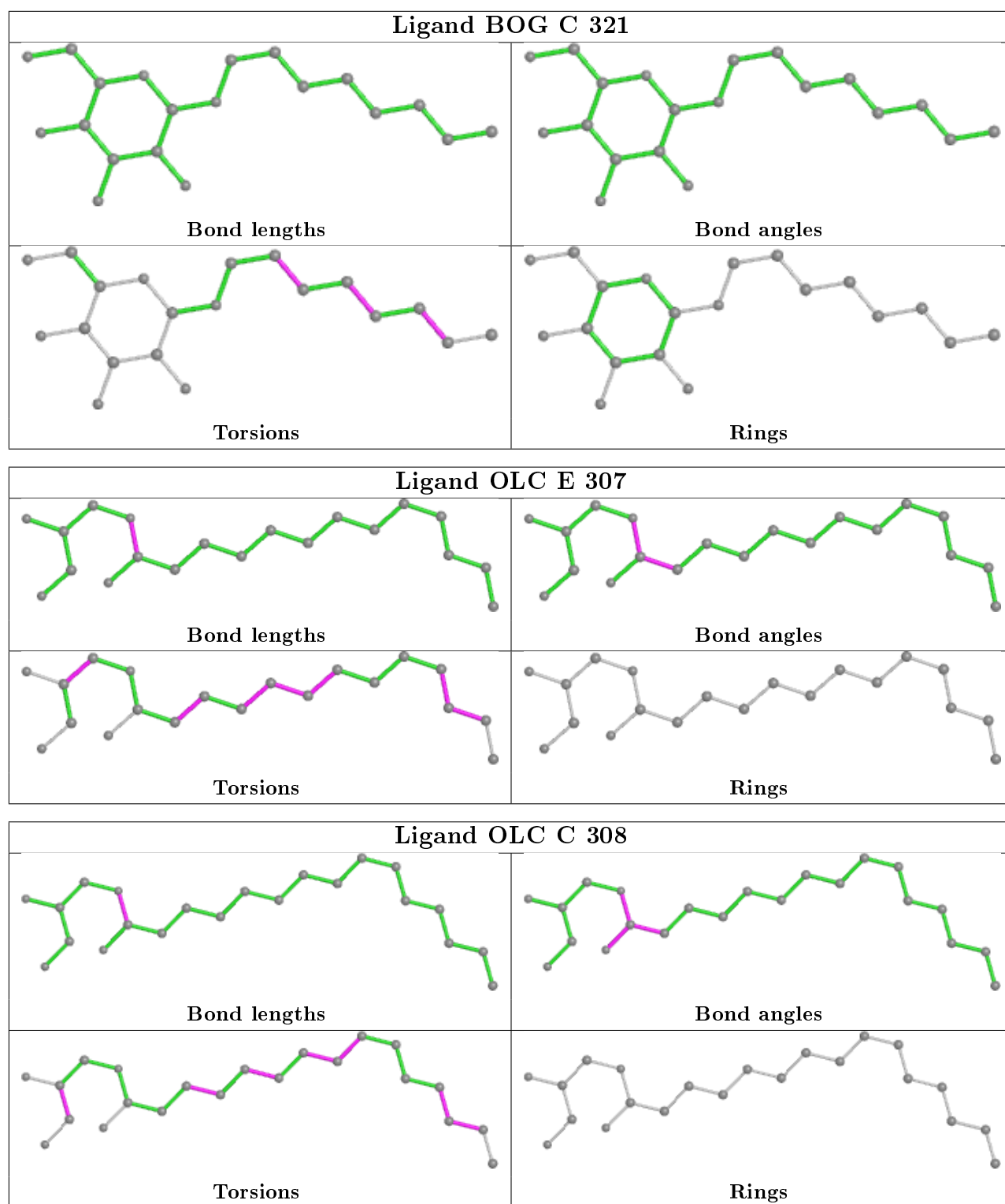




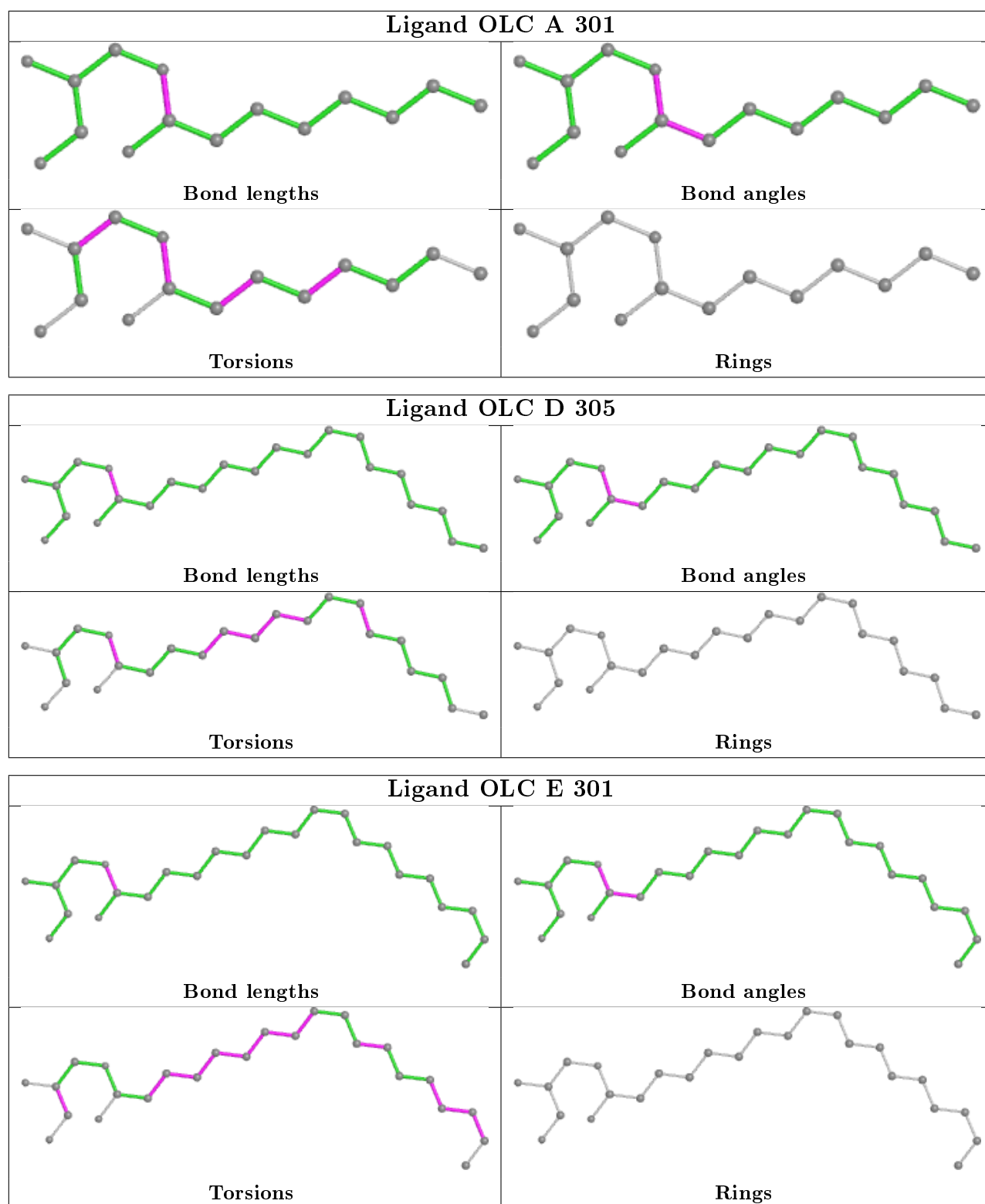


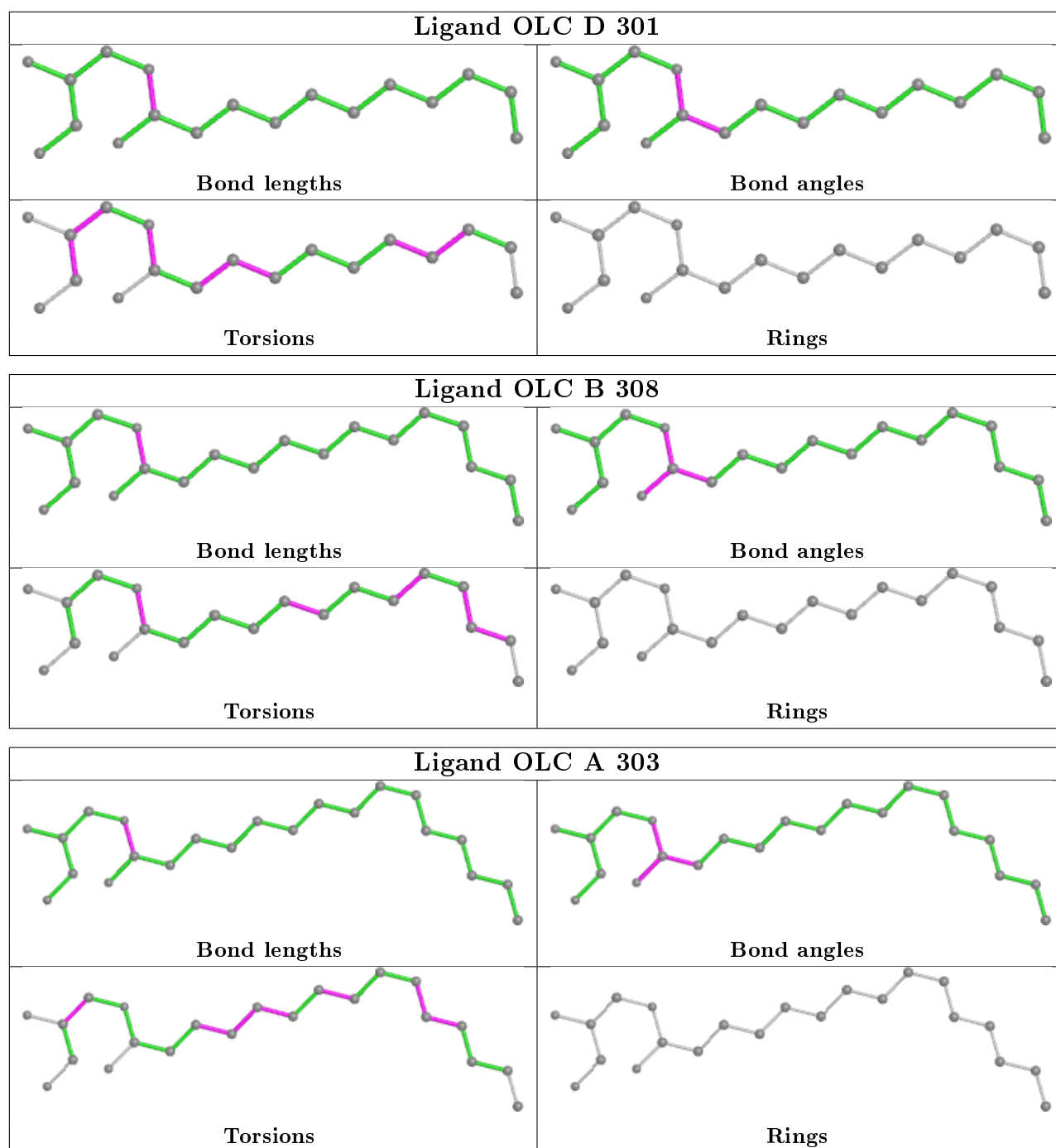


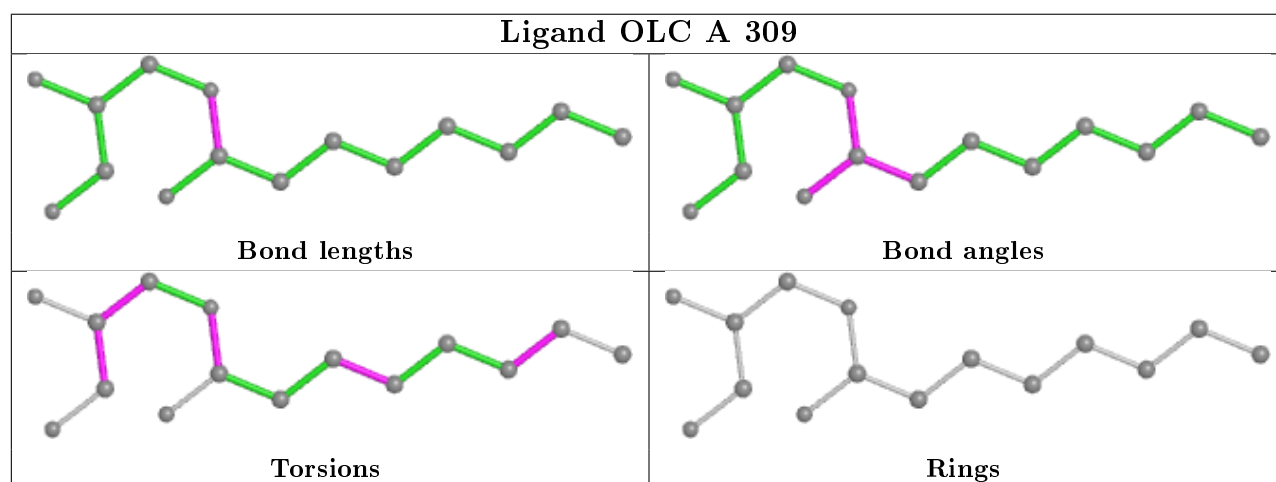
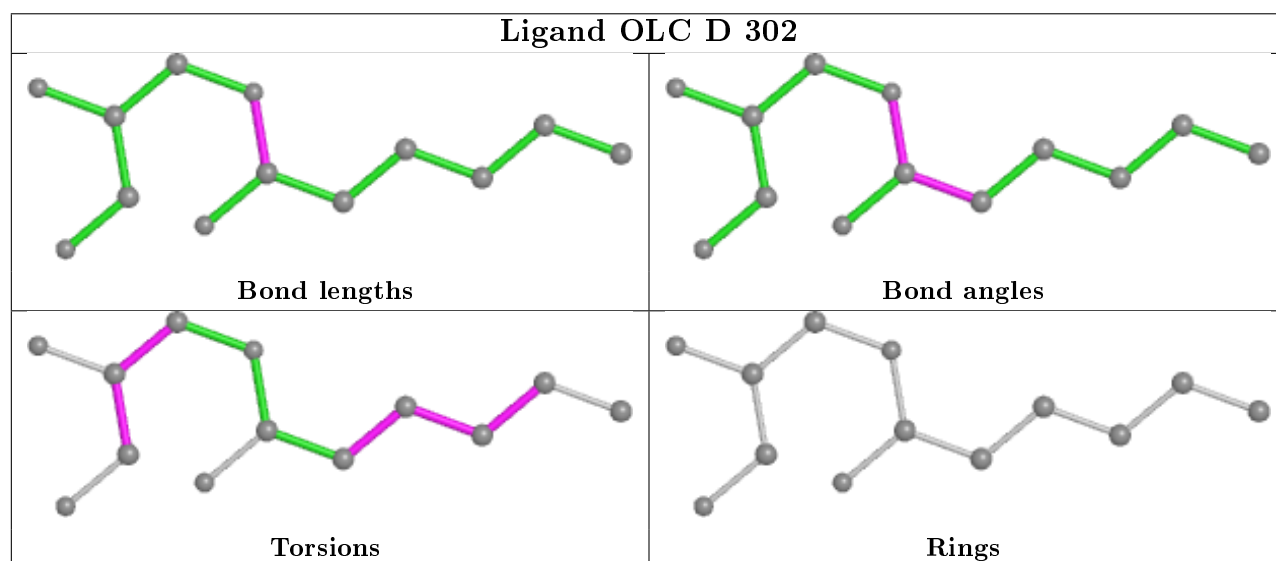
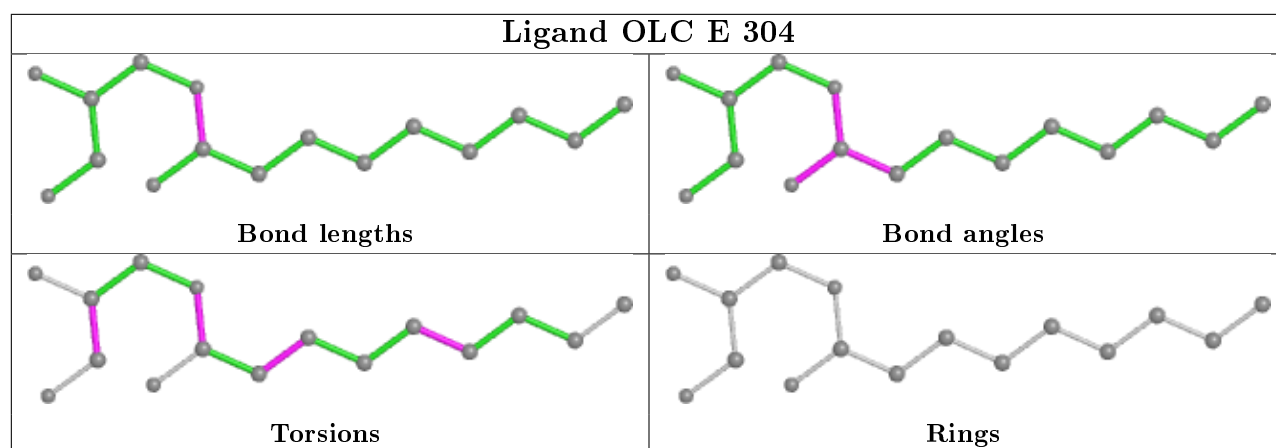


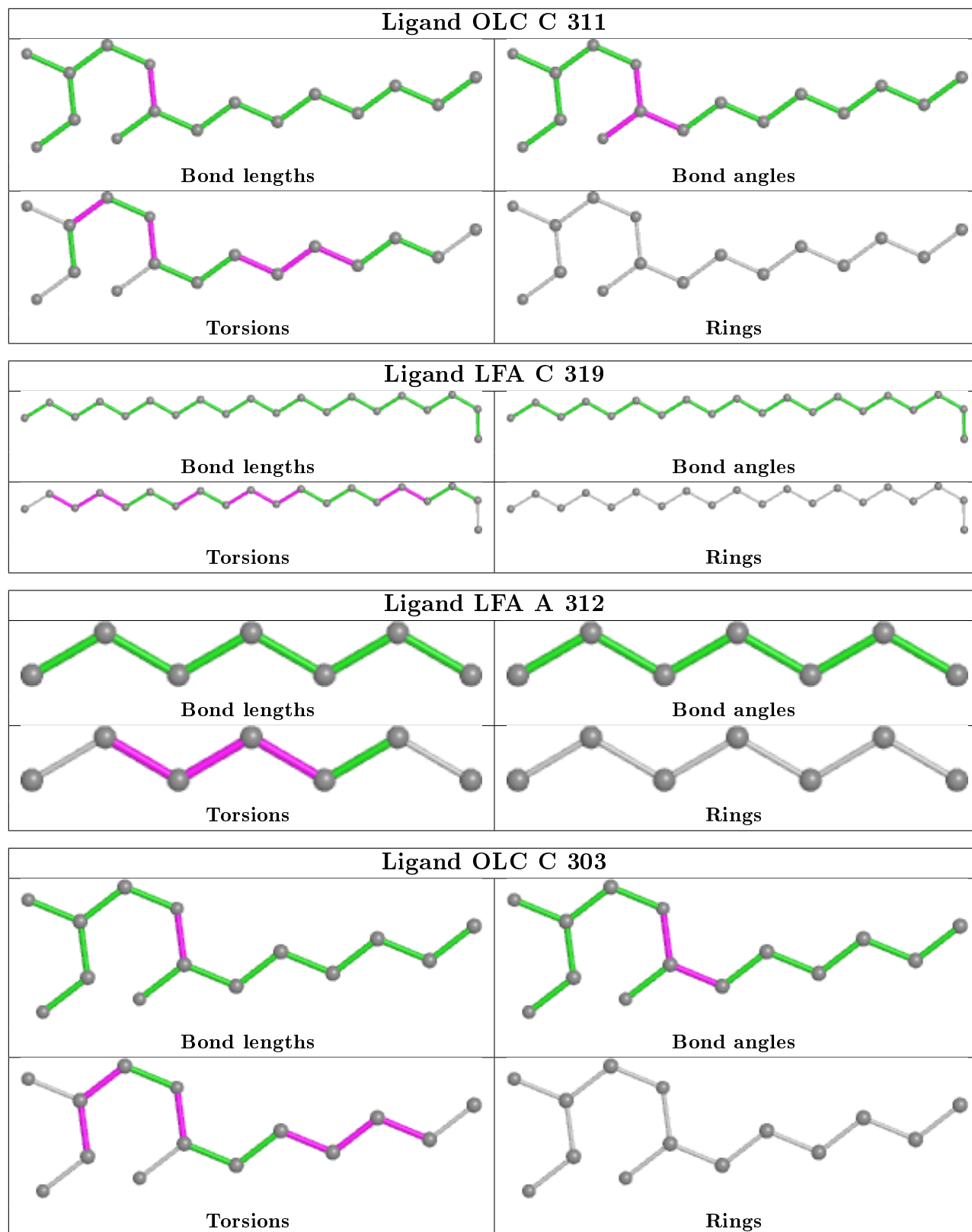


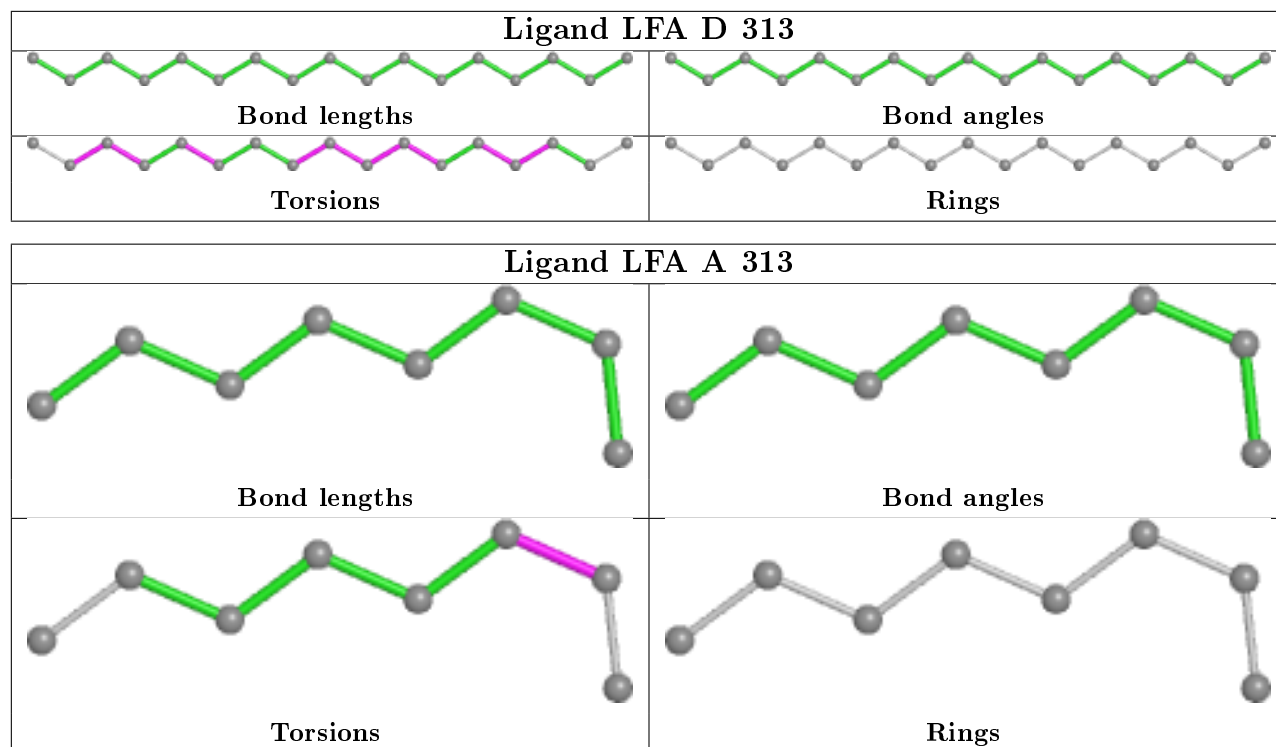












## 5.7 Other polymers [i](#)

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	272/288 (94%)	0.33	25 (9%) 9 8	34, 45, 68, 152	0
1	B	272/288 (94%)	0.27	24 (8%) 10 9	36, 45, 69, 148	0
1	C	272/288 (94%)	0.28	23 (8%) 10 10	35, 45, 68, 179	0
1	D	272/288 (94%)	0.48	31 (11%) 5 4	35, 47, 74, 176	0
1	E	272/288 (94%)	0.34	24 (8%) 10 9	33, 45, 69, 179	0
All	All	1360/1440 (94%)	0.34	127 (9%) 8 8	33, 45, 70, 179	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	274	GLU	11.3
1	A	275	LEU	10.7
1	E	274	GLU	9.5
1	A	272	ASN	9.1
1	C	275	LEU	8.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	LYR	A	255	29/30	0.91	0.16	34,40,48,51	0
1	LYR	B	255	29/30	0.93	0.17	33,39,53,57	0
1	LYR	D	255	29/30	0.94	0.17	35,42,49,49	0
1	LYR	E	255	29/30	0.94	0.16	34,39,44,47	0
1	LYR	C	255	29/30	0.95	0.15	34,42,48,52	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
2	OLC	D	306	25/25	0.29	0.45	80,101,115,122	0
2	OLC	C	309	16/25	0.34	0.52	82,110,137,140	0
2	OLC	E	303	14/25	0.44	0.41	104,126,146,183	0
2	OLC	A	301	15/25	0.45	0.51	95,124,172,178	0
2	OLC	A	308	25/25	0.46	0.42	78,103,127,132	0
2	OLC	B	303	14/25	0.47	0.42	101,136,164,188	0
2	OLC	A	310	16/25	0.51	0.43	76,105,138,148	0
2	OLC	A	307	16/25	0.54	0.48	90,107,122,128	0
5	BOG	C	321	20/20	0.57	0.54	76,93,115,115	0
2	OLC	E	312	25/25	0.58	0.43	80,98,116,135	0
2	OLC	B	313	17/25	0.58	0.29	73,99,129,136	0
3	LFA	E	302	20/20	0.59	1.39	57,76,93,105	0
2	OLC	B	311	25/25	0.59	0.43	82,102,121,127	0
5	BOG	A	320	20/20	0.59	0.61	76,107,122,122	0
3	LFA	C	314	7/20	0.60	0.26	67,79,104,106	0
2	OLC	B	310	16/25	0.60	0.37	71,96,130,131	0
2	OLC	D	303	25/25	0.60	0.38	75,101,114,115	0
2	OLC	B	305	15/25	0.60	0.32	87,114,139,139	0
2	OLC	E	310	15/25	0.61	0.31	58,97,131,132	0
5	BOG	E	321	20/20	0.61	0.46	73,106,121,123	0
2	OLC	E	304	16/25	0.61	0.39	67,116,151,155	0
3	LFA	E	323	14/20	0.62	1.50	101,125,159,162	0
2	OLC	E	313	20/25	0.62	0.56	65,112,127,135	0
2	OLC	A	306	15/25	0.62	0.56	69,96,128,137	0
2	OLC	B	314	15/25	0.62	0.28	90,107,125,126	0
2	OLC	E	308	15/25	0.62	0.53	84,107,142,147	0
2	OLC	C	308	22/25	0.63	0.45	58,98,127,148	0
2	OLC	C	303	14/25	0.63	0.44	93,115,149,167	0
2	OLC	D	305	23/25	0.64	0.45	60,112,160,166	0
5	BOG	B	321	20/20	0.65	0.54	75,102,116,129	0
3	LFA	B	318	10/20	0.65	0.28	75,92,103,104	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLC	E	314	25/25	0.65	0.46	86,115,149,161	0
2	OLC	C	304	21/25	0.66	0.33	74,115,144,153	0
2	OLC	B	307	24/25	0.66	0.41	83,112,130,134	0
3	LFA	B	302	20/20	0.66	1.25	59,75,86,93	0
2	OLC	B	304	25/25	0.66	0.34	78,107,124,133	0
2	OLC	D	308	15/25	0.67	0.32	66,90,129,139	0
3	LFA	C	317	11/20	0.67	0.30	72,88,105,107	0
2	OLC	C	307	25/25	0.67	0.24	69,93,114,123	0
3	LFA	C	319	20/20	0.67	1.18	55,68,79,80	0
3	LFA	D	312	8/20	0.67	0.30	74,83,108,109	0
2	OLC	A	321	25/25	0.68	0.31	65,91,126,134	0
2	OLC	D	302	13/25	0.68	0.47	116,129,142,171	0
3	LFA	E	319	20/20	0.69	1.24	52,75,89,95	0
2	OLC	B	308	20/25	0.70	0.22	64,86,109,114	0
3	LFA	B	316	9/20	0.70	0.33	75,92,99,101	0
2	OLC	B	306	20/25	0.70	0.31	75,90,119,120	0
2	OLC	E	306	24/25	0.70	0.45	85,103,140,162	0
2	OLC	C	306	25/25	0.70	0.29	72,95,117,128	0
2	OLC	C	312	16/25	0.71	0.27	65,90,118,120	0
2	OLC	B	315	16/25	0.71	0.35	75,88,123,145	0
2	OLC	C	313	16/25	0.72	0.37	64,85,112,122	0
2	OLC	E	311	11/25	0.72	0.28	94,110,127,133	0
2	OLC	A	304	25/25	0.73	0.44	70,98,119,137	0
3	LFA	A	312	7/20	0.73	0.24	86,90,92,101	0
2	OLC	A	311	16/25	0.73	0.36	73,91,128,145	0
3	LFA	B	319	7/20	0.74	0.26	65,76,100,111	0
2	OLC	D	309	25/25	0.74	0.38	79,95,116,131	0
3	LFA	C	315	8/20	0.74	0.24	79,90,98,101	0
3	LFA	A	314	8/20	0.74	0.24	66,91,111,123	0
3	LFA	D	315	6/20	0.74	0.26	73,87,99,104	0
2	OLC	E	301	25/25	0.74	0.32	63,92,133,149	0
2	OLC	A	303	22/25	0.75	0.33	48,65,121,170	0
3	LFA	E	316	14/20	0.75	0.27	69,91,104,110	0
3	LFA	D	310	20/20	0.75	0.26	81,94,105,115	0
3	LFA	C	302	20/20	0.75	1.12	61,71,77,81	0
5	BOG	D	317	20/20	0.75	0.60	89,102,112,114	0
2	OLC	C	305	23/25	0.75	0.34	49,66,121,135	0
2	OLC	A	302	25/25	0.76	0.26	74,111,124,141	0
3	LFA	E	315	8/20	0.76	0.31	72,99,104,104	0
3	LFA	A	315	12/20	0.76	0.19	92,99,111,112	0
2	OLC	C	310	25/25	0.76	0.47	89,100,121,127	0
3	LFA	A	313	8/20	0.76	0.28	74,83,90,91	0

*Continued on next page...*



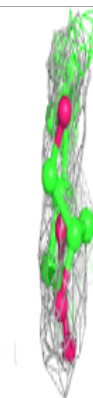
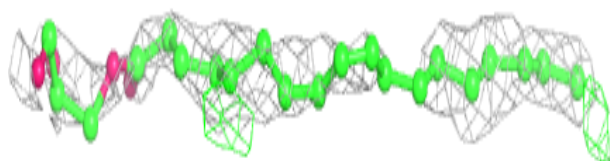
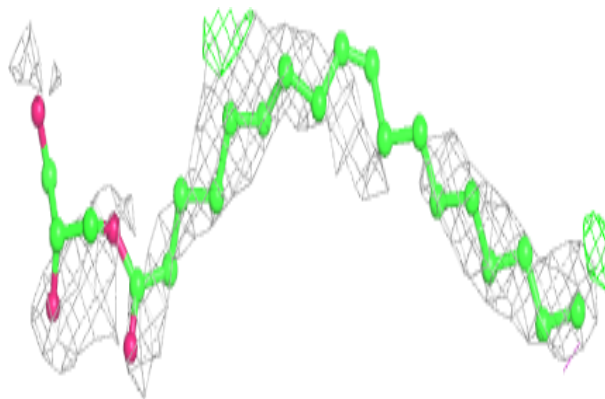
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LFA	D	314	7/20	0.78	0.19	71,82,99,105	0
3	LFA	A	318	20/20	0.79	0.32	80,107,126,131	0
3	LFA	E	318	5/20	0.79	0.24	83,83,92,101	0
3	LFA	E	317	4/20	0.79	0.28	68,71,76,85	0
2	OLC	D	301	18/25	0.79	0.30	77,96,118,128	0
2	OLC	E	305	24/25	0.80	0.34	51,66,129,145	0
2	OLC	B	309	21/25	0.80	0.42	58,87,118,143	0
2	OLC	B	301	25/25	0.80	0.25	74,90,122,124	0
3	LFA	D	311	20/20	0.82	0.28	70,98,113,113	0
2	OLC	A	305	13/25	0.82	0.25	64,73,86,86	0
3	LFA	C	316	20/20	0.82	0.25	63,92,121,125	0
2	OLC	D	304	18/25	0.83	0.30	74,96,115,118	0
2	OLC	C	301	21/25	0.83	0.29	48,62,101,113	0
3	LFA	A	316	4/20	0.83	0.27	81,85,93,95	0
2	OLC	E	307	20/25	0.84	0.29	75,96,108,113	0
3	LFA	C	318	4/20	0.84	0.42	87,93,94,97	0
3	LFA	B	317	8/20	0.85	0.31	75,103,106,107	0
3	LFA	D	313	17/20	0.88	0.47	49,57,84,85	0
2	OLC	C	311	16/25	0.88	0.20	60,86,99,103	0
2	OLC	B	312	16/25	0.89	0.23	65,83,97,111	0
2	OLC	E	309	25/25	0.90	0.26	56,98,132,140	0
2	OLC	A	309	15/25	0.90	0.15	60,76,101,104	0
2	OLC	D	307	14/25	0.92	0.12	56,82,98,102	0
3	LFA	A	317	6/20	0.92	0.24	64,73,82,82	0
3	LFA	E	322	4/20	0.95	2.40	73,79,81,83	0
4	NA	E	320	1/1	0.95	0.07	38,38,38,38	0
4	NA	A	319	1/1	0.96	0.11	45,45,45,45	0
4	NA	B	320	1/1	0.97	0.08	39,39,39,39	0
4	NA	D	316	1/1	0.98	0.08	41,41,41,41	0
4	NA	C	320	1/1	0.99	0.10	42,42,42,42	0

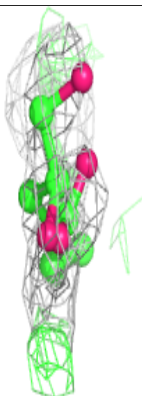
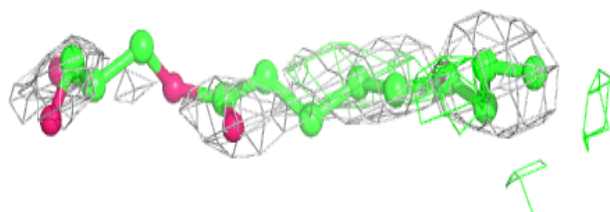
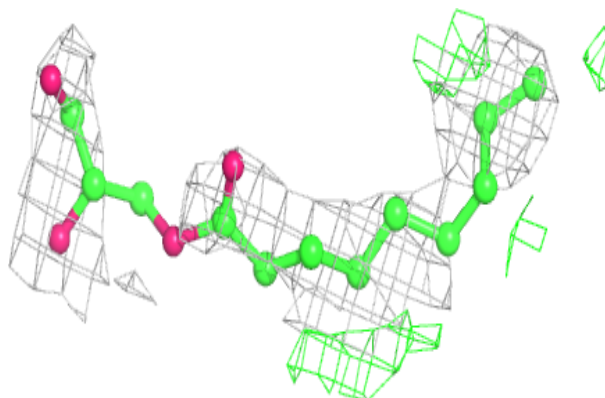
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLC D 306:**

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

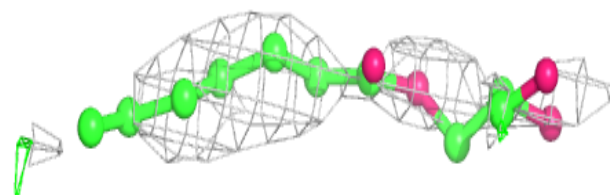
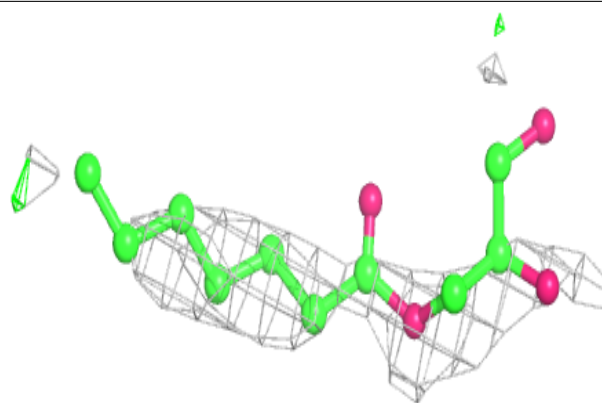
**Electron density around OLC C 309:**

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

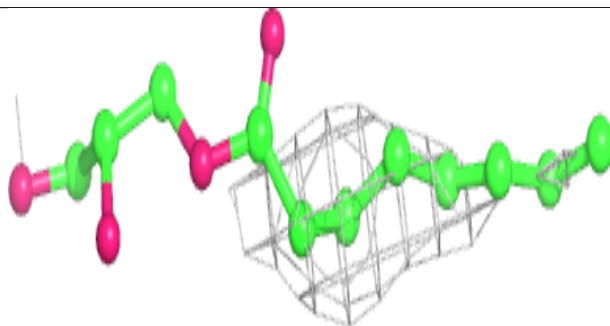
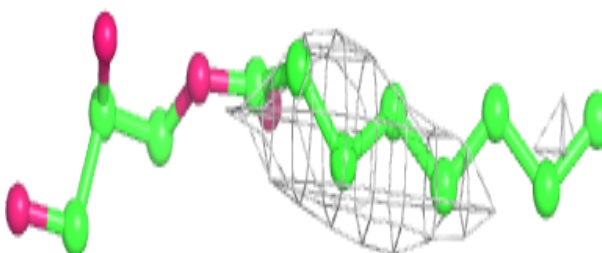


**Electron density around OLC E 303:**

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

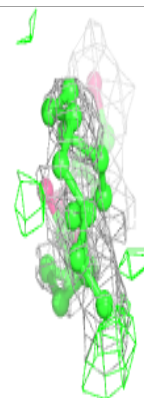
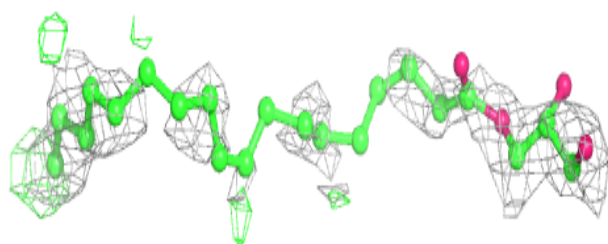
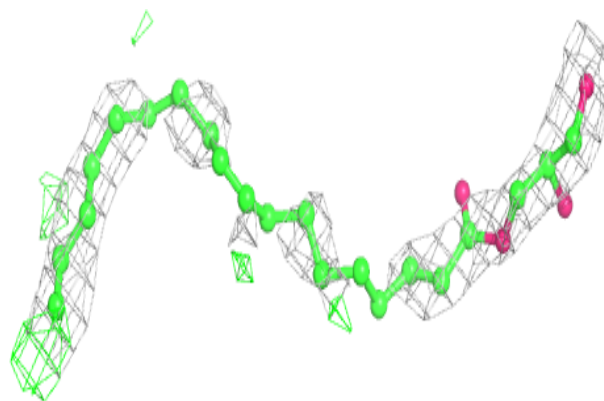
**Electron density around OLC A 301:**

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

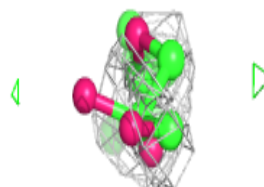
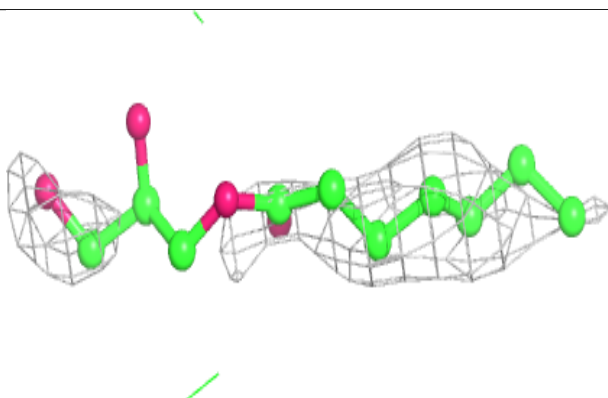
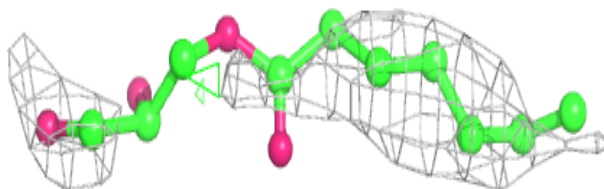


**Electron density around OLC A 308:**

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

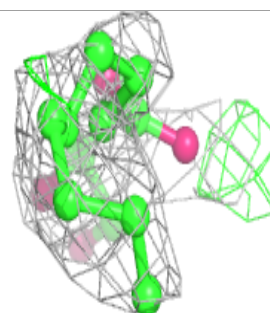
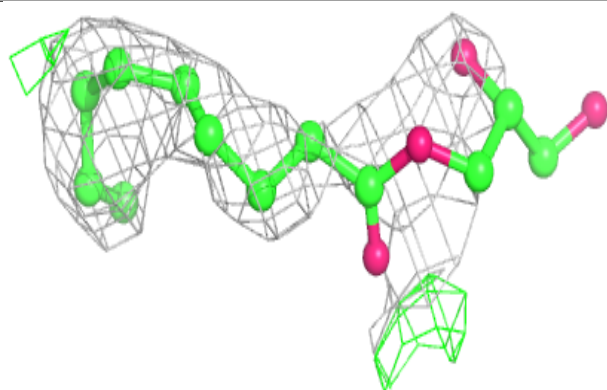
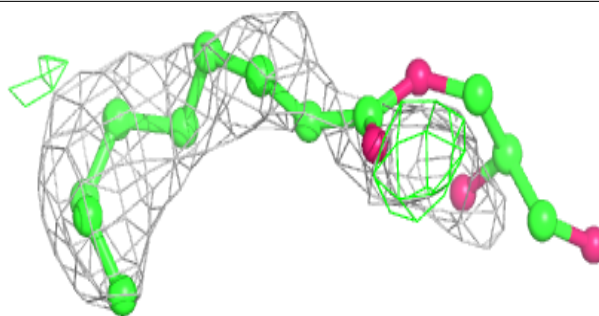
**Electron density around OLC B 303:**

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

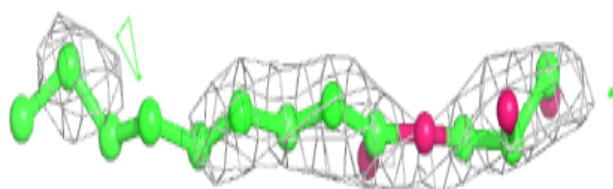
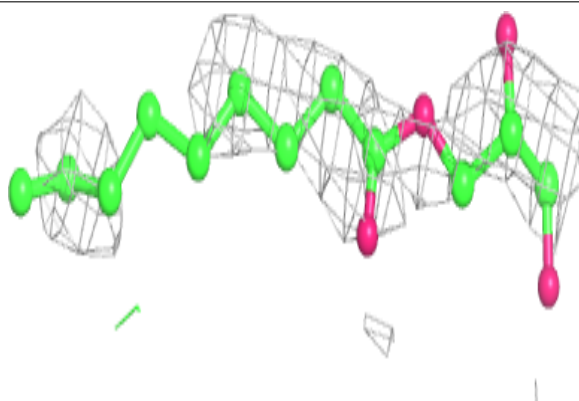


**Electron density around OLC A 310:**

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

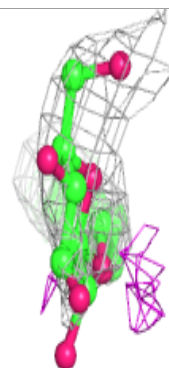
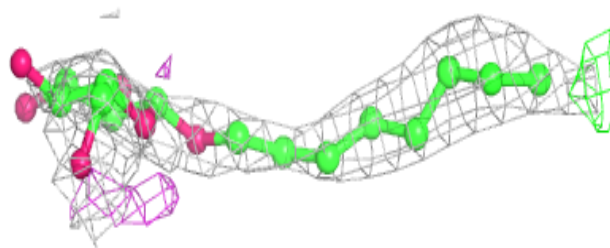
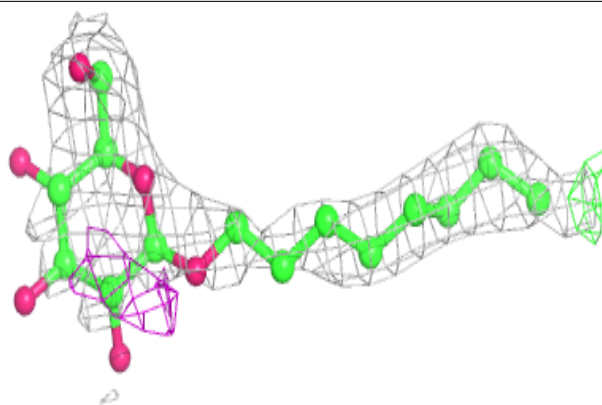
**Electron density around OLC A 307:**

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

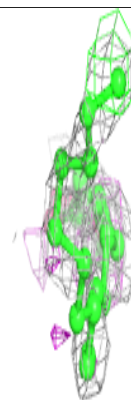
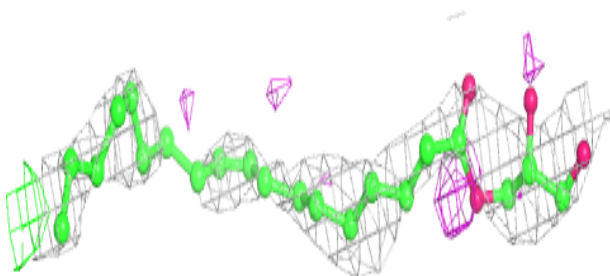
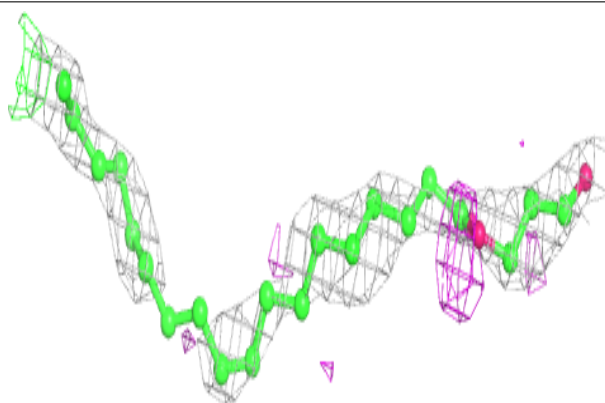


**Electron density around BOG C 321:**

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

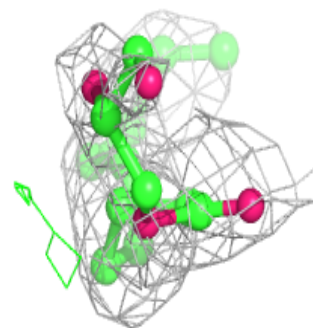
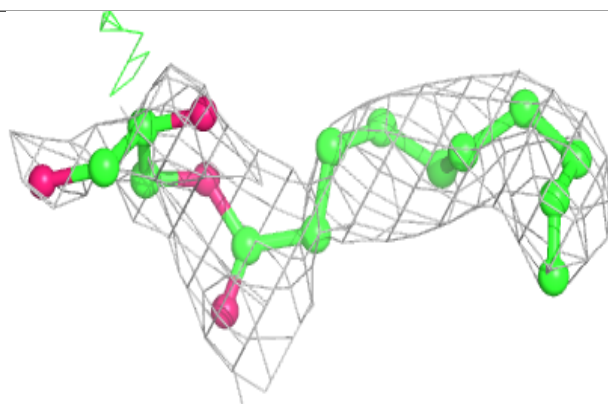
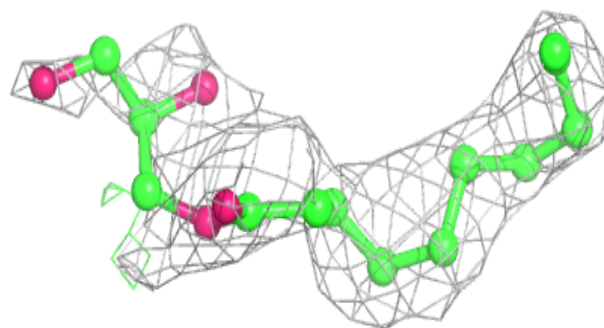
**Electron density around OLC E 312:**

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

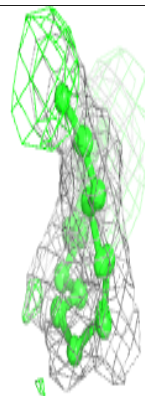
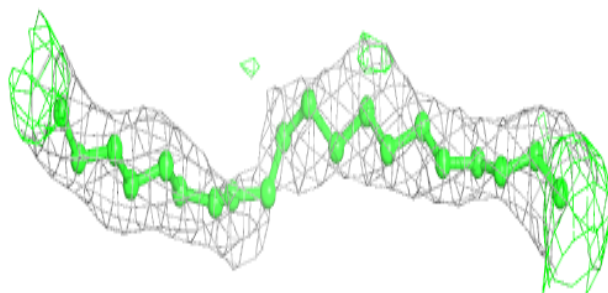
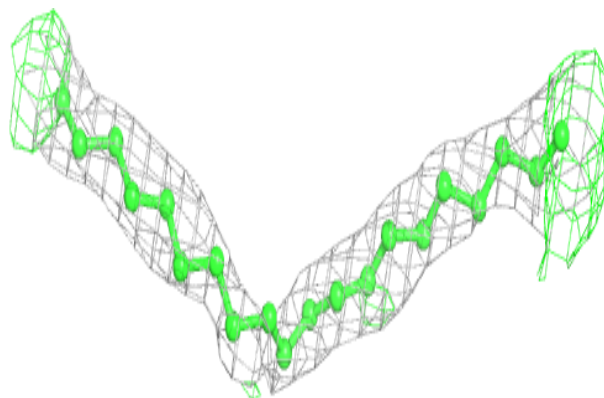


**Electron density around OLC B 313:**

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

**Electron density around LFA E 302:**

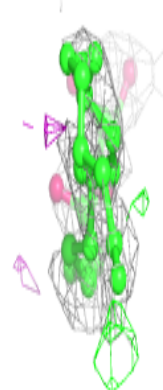
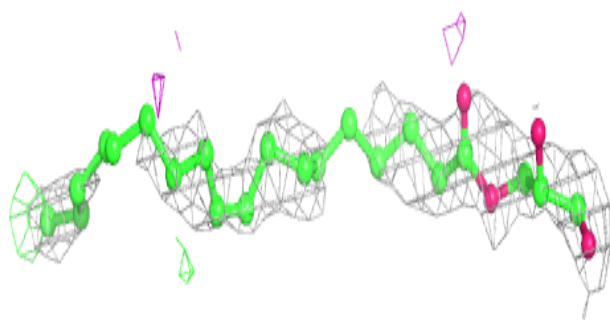
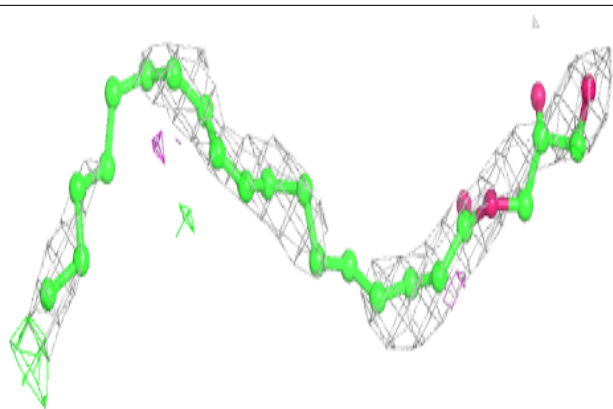
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



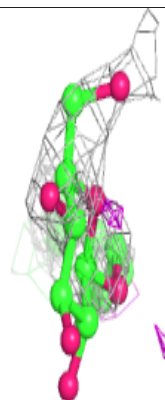
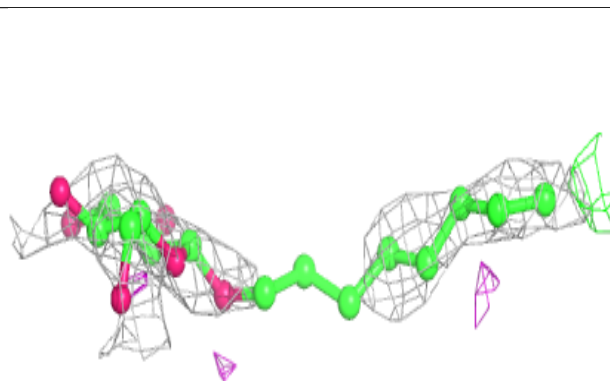
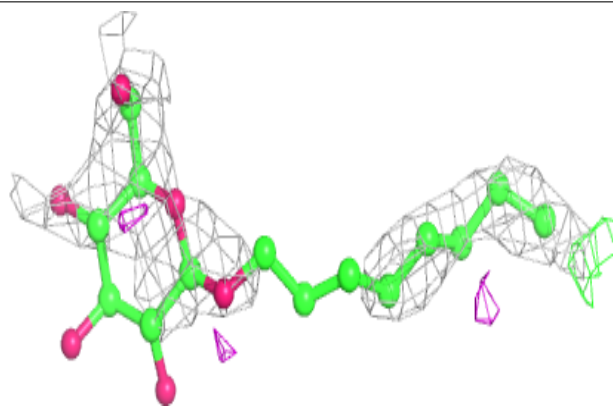


**Electron density around OLC B 311:**

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

**Electron density around BOG A 320:**

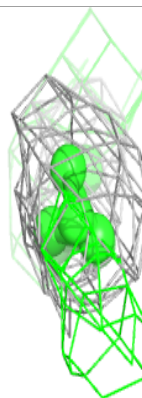
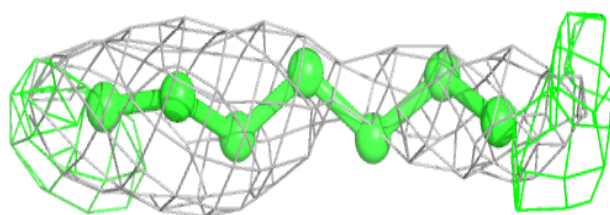
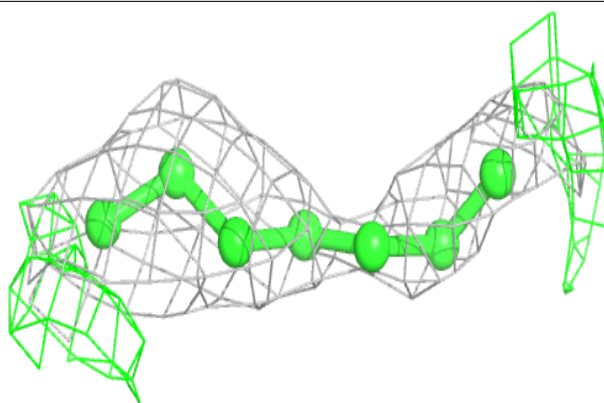
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



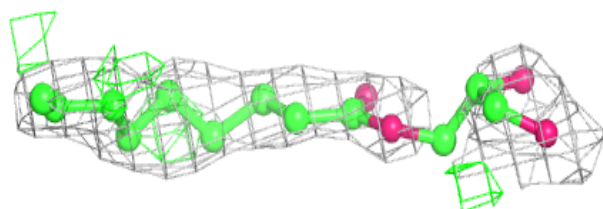
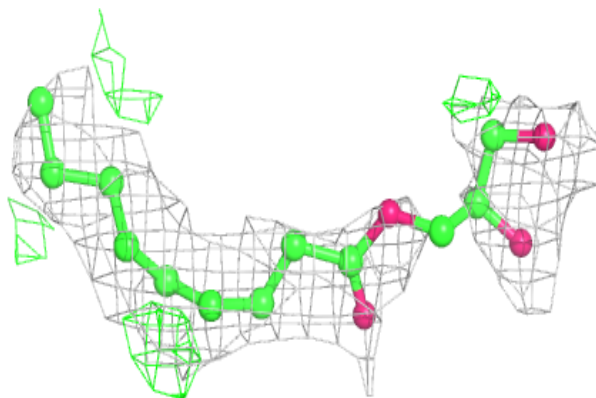


**Electron density around LFA C 314:**

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

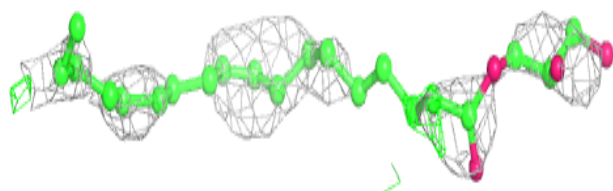
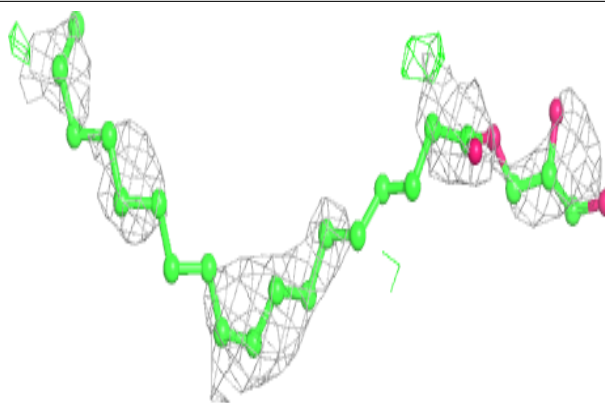
**Electron density around OLC B 310:**

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

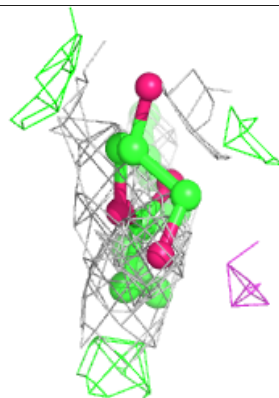
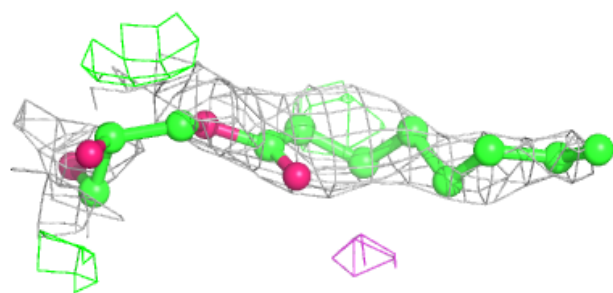
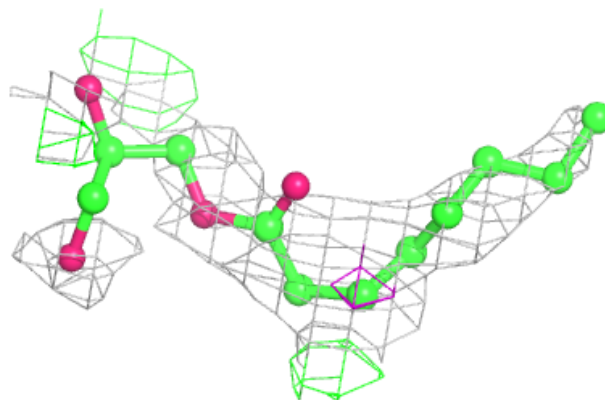


**Electron density around OLC D 303:**

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

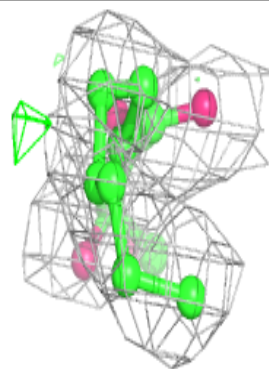
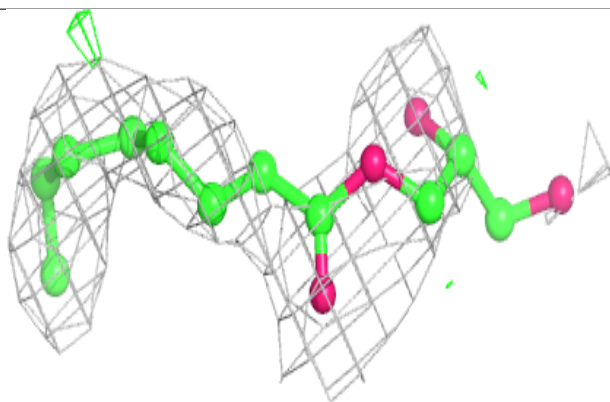
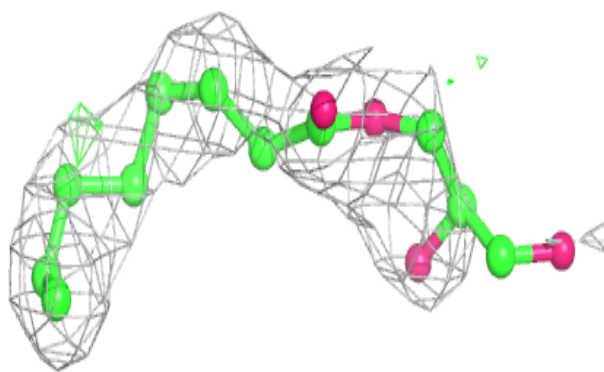
**Electron density around OLC B 305:**

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

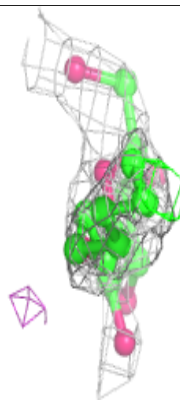
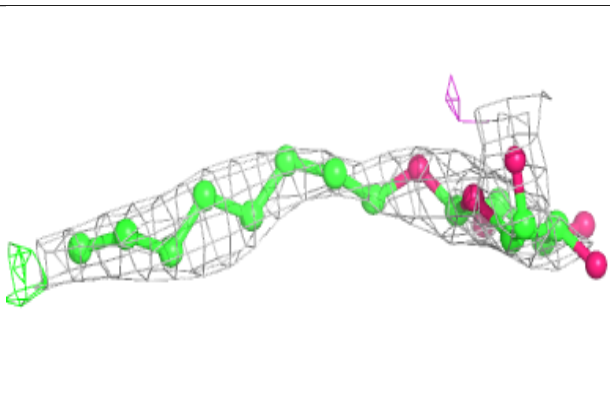
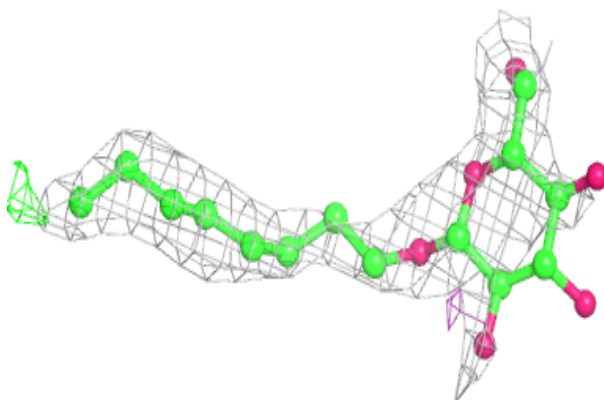


**Electron density around OLC E 310:**

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

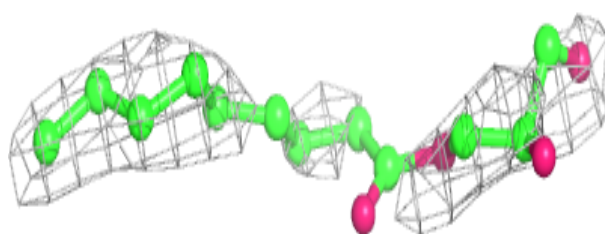
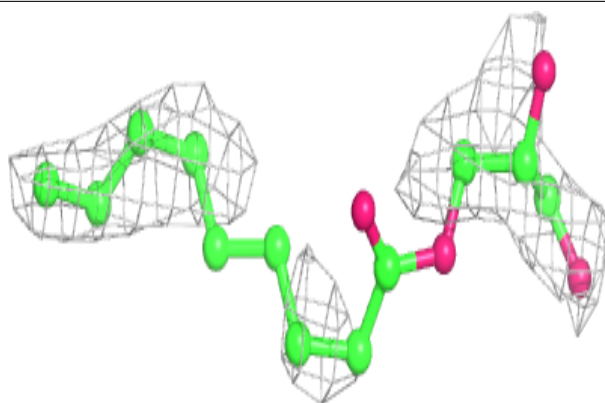
**Electron density around BOG E 321:**

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

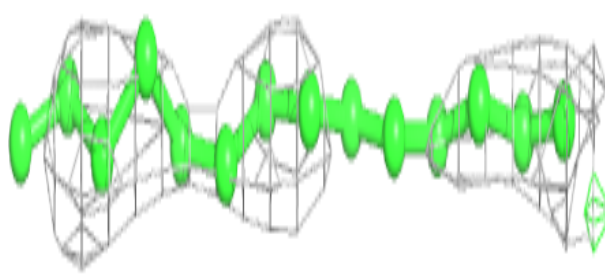
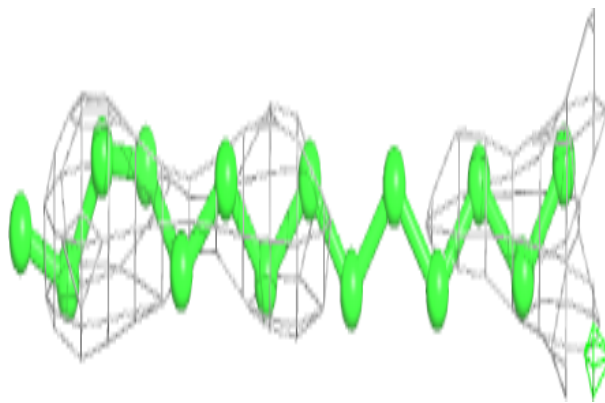


**Electron density around OLC E 304:**

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

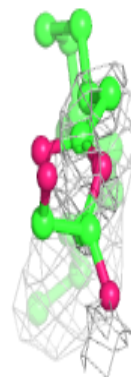
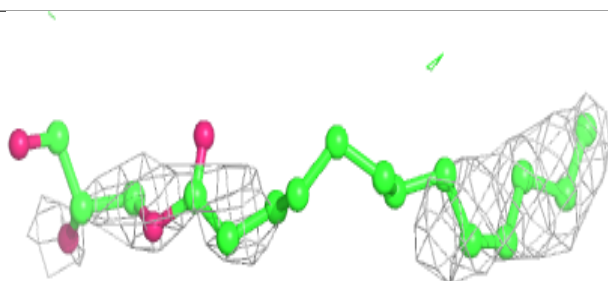
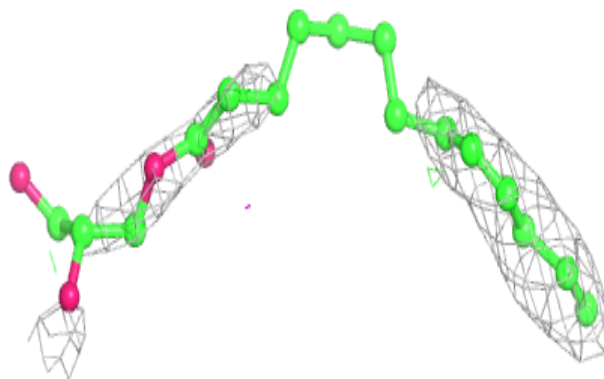
**Electron density around LFA E 323:**

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

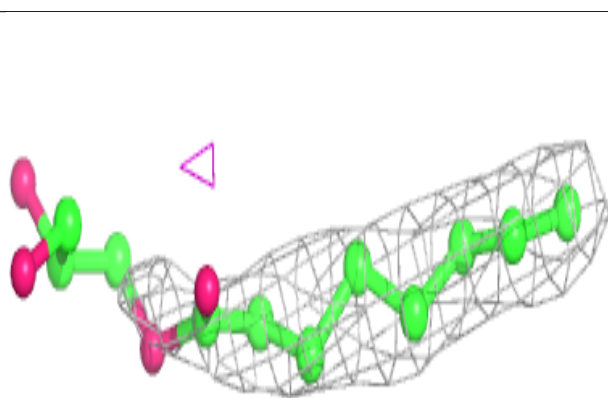
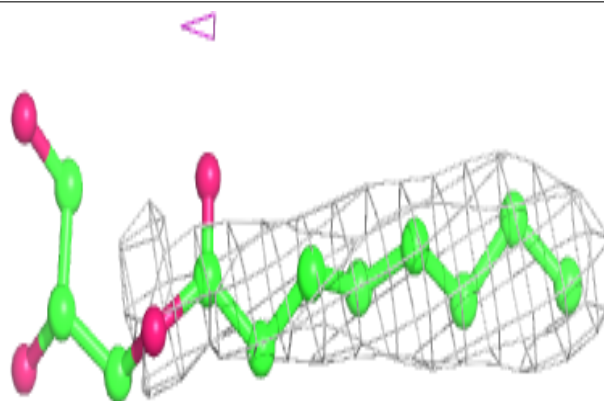


**Electron density around OLC E 313:**

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

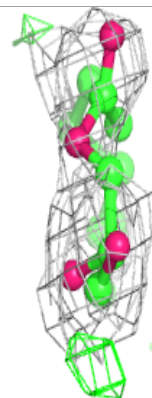
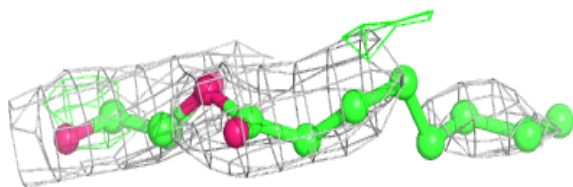
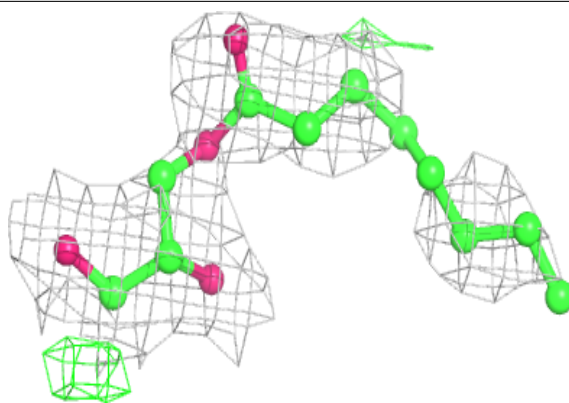
**Electron density around OLC A 306:**

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

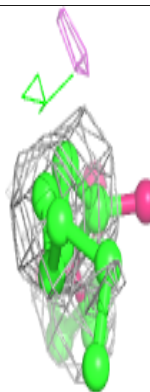
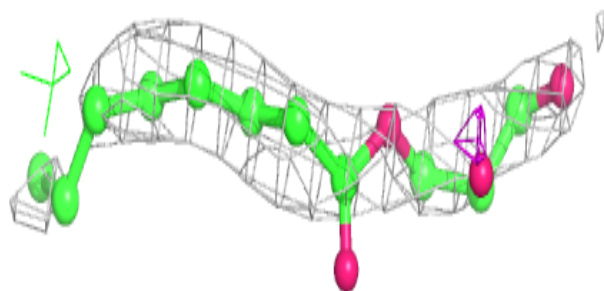
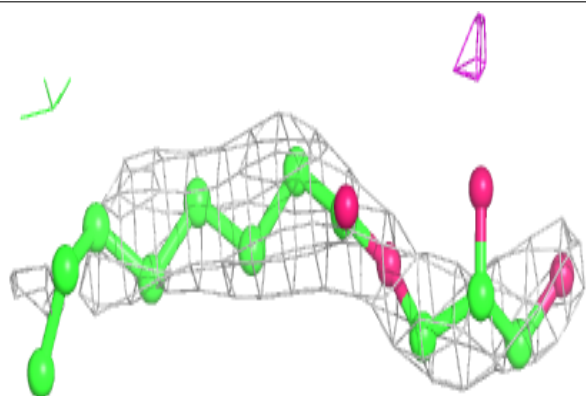


**Electron density around OLC B 314:**

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

**Electron density around OLC E 308:**

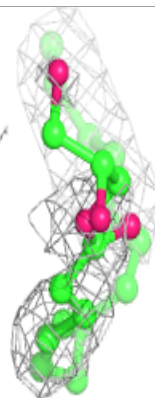
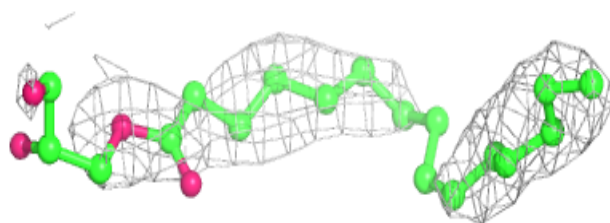
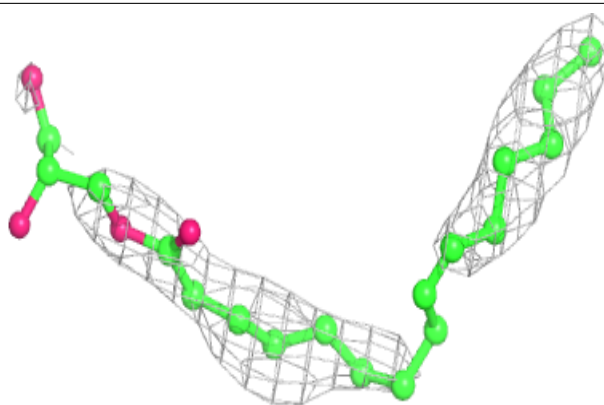
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



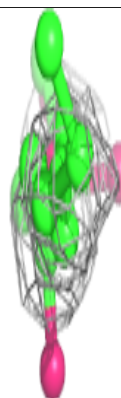
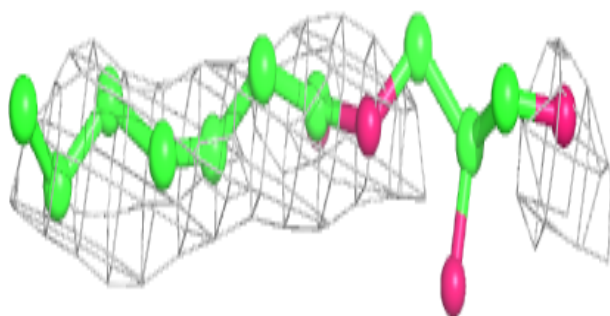
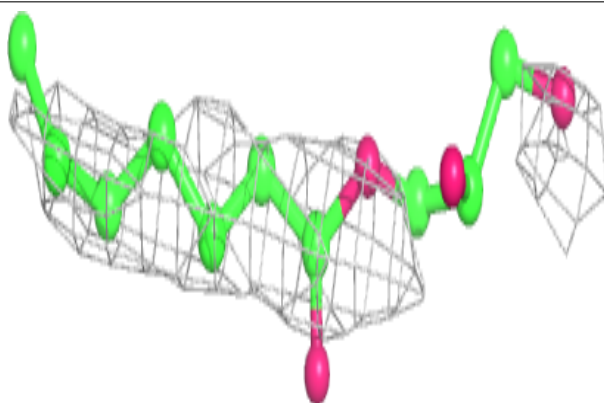


**Electron density around OLC C 308:**

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

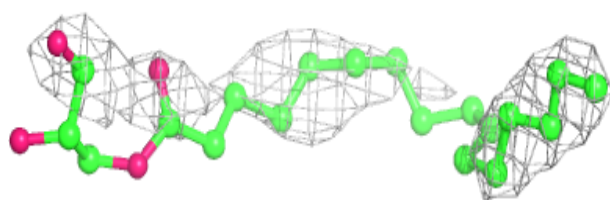
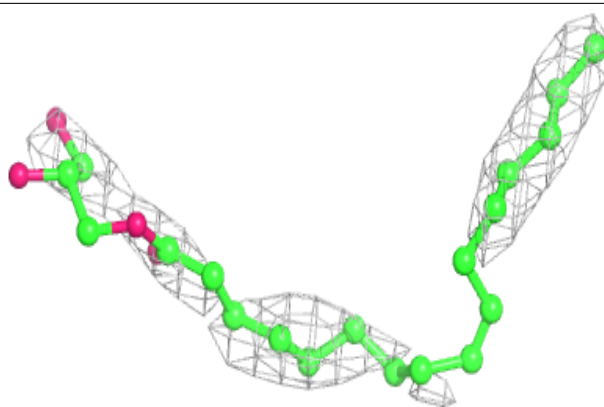
**Electron density around OLC C 303:**

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

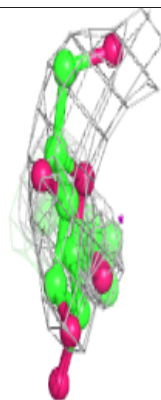
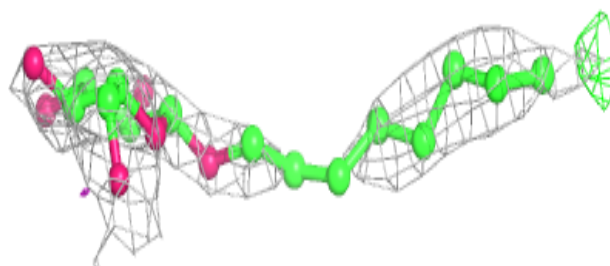
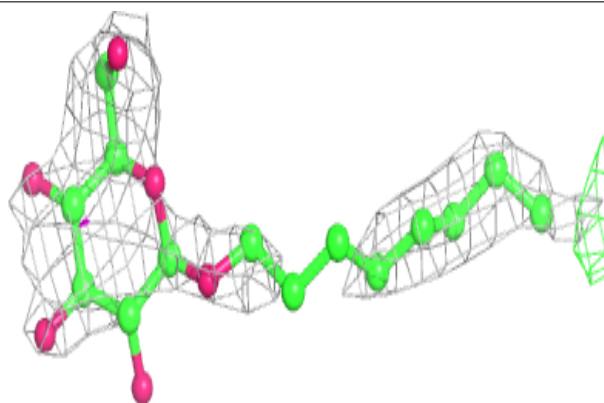


**Electron density around OLC D 305:**

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

**Electron density around BOG B 321:**

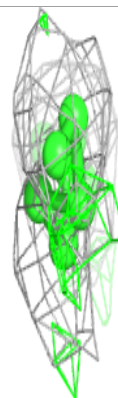
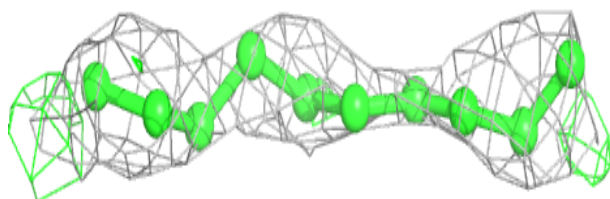
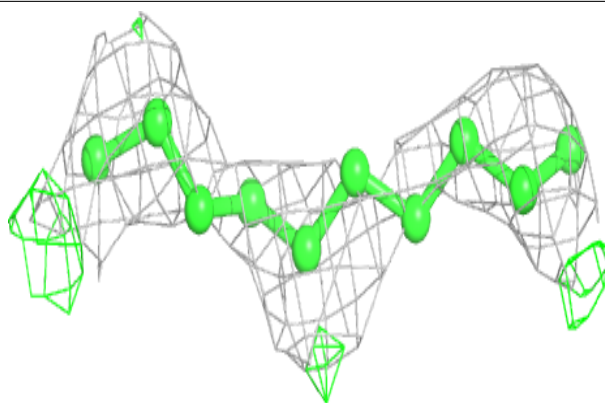
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



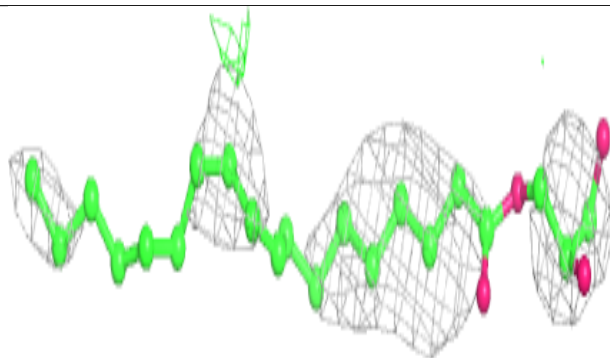
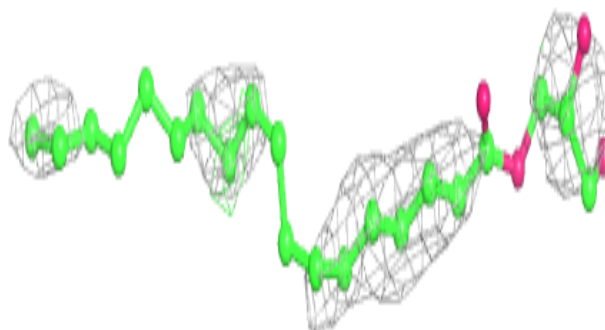


**Electron density around LFA B 318:**

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

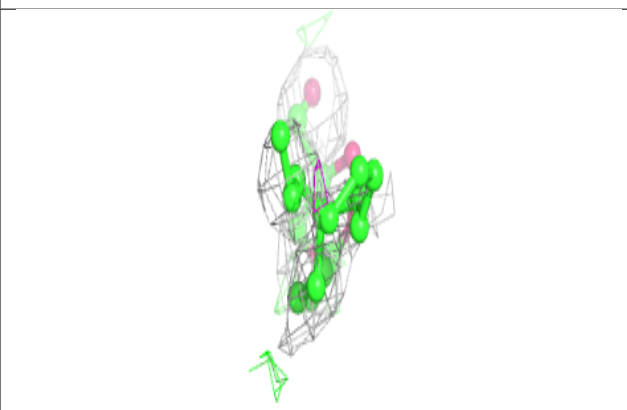
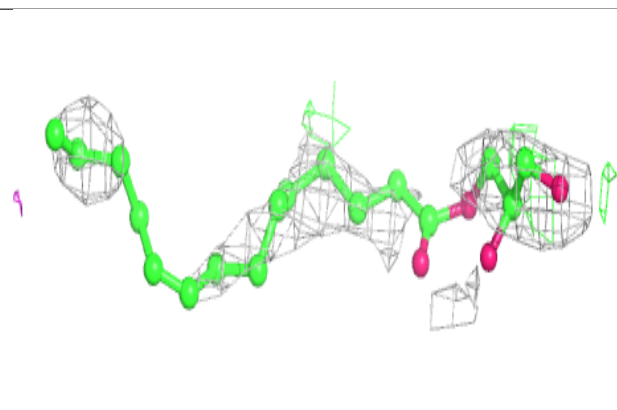
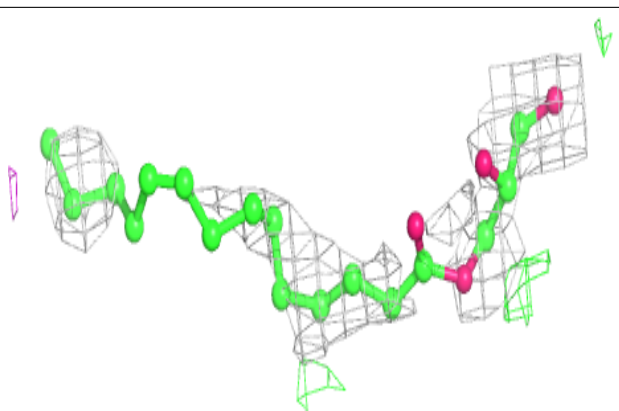
**Electron density around OLC E 314:**

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

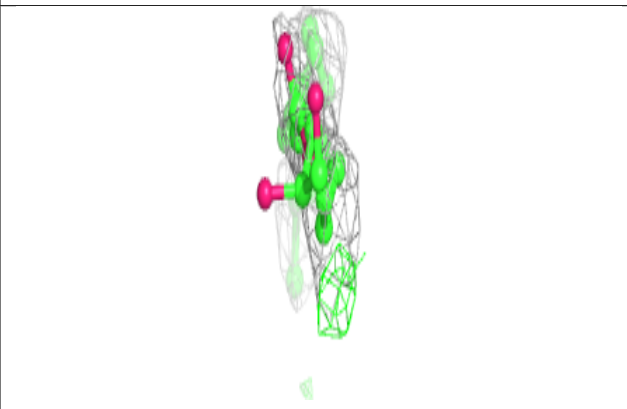
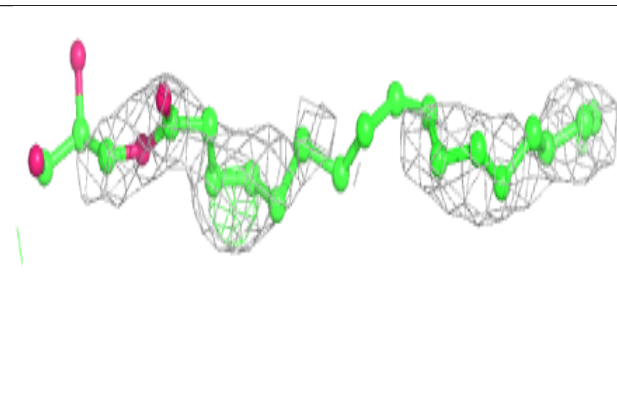
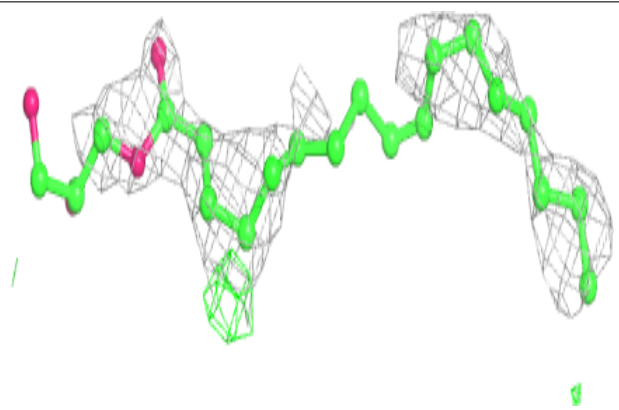


**Electron density around OLC C 304:**

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

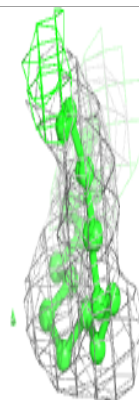
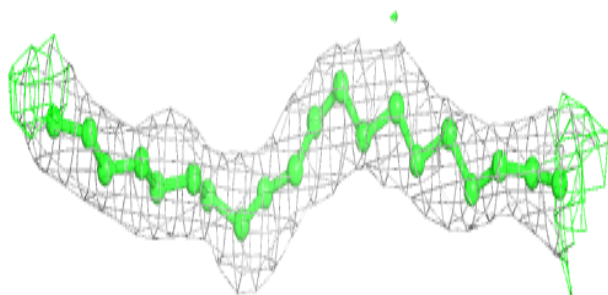
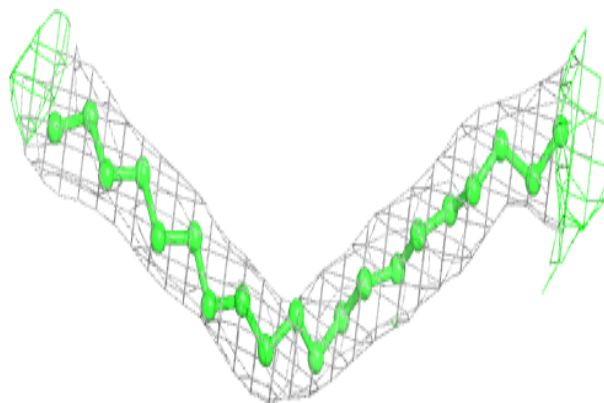
**Electron density around OLC B 307:**

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

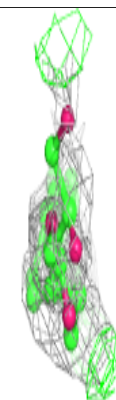
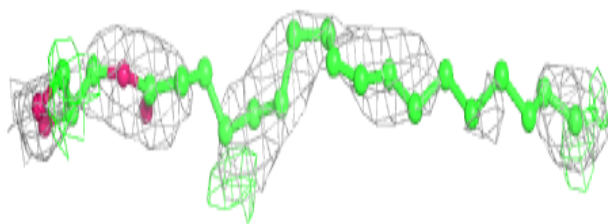
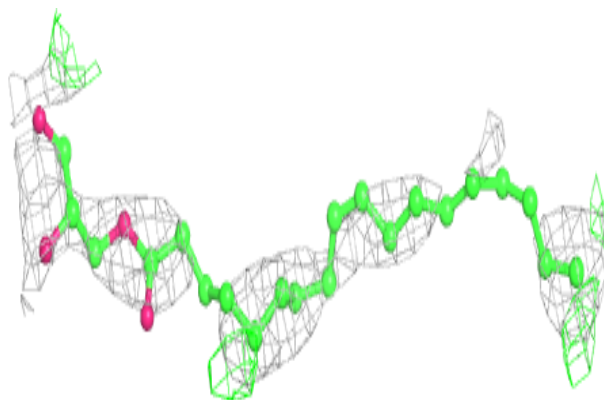


**Electron density around LFA B 302:**

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

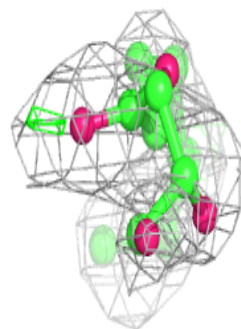
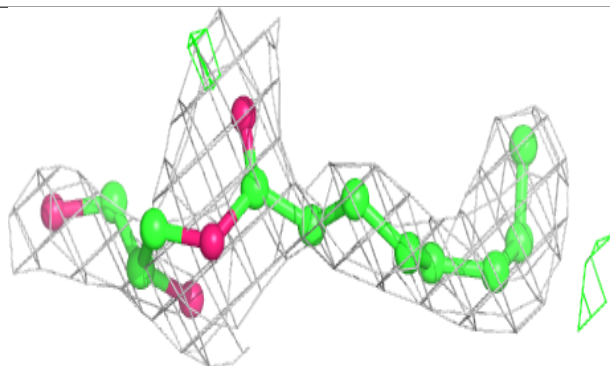
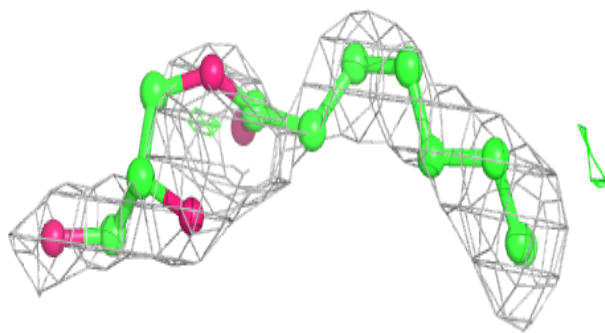
**Electron density around OLC B 304:**

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

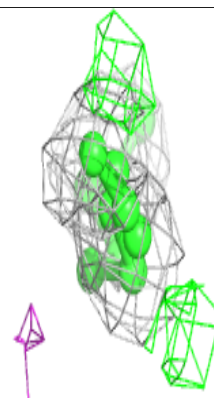
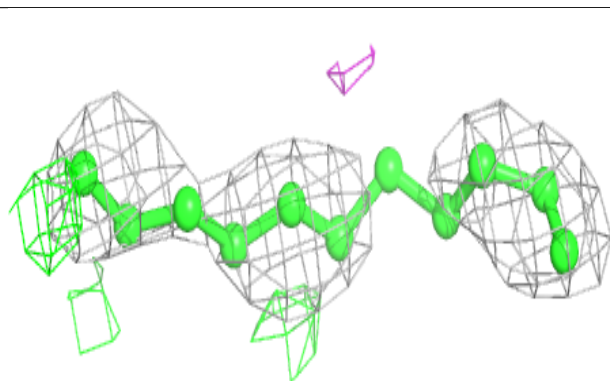
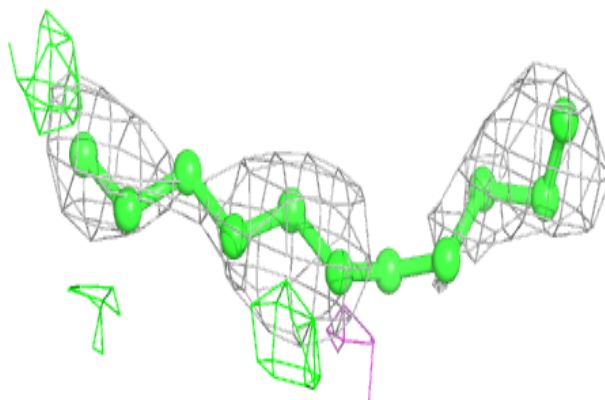


**Electron density around OLC D 308:**

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

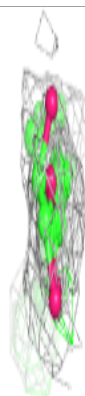
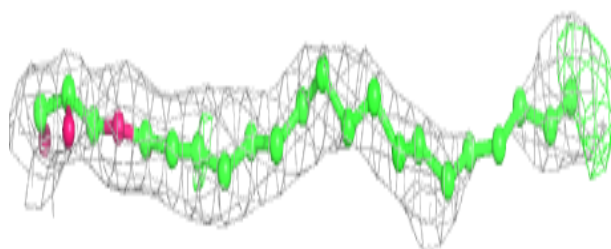
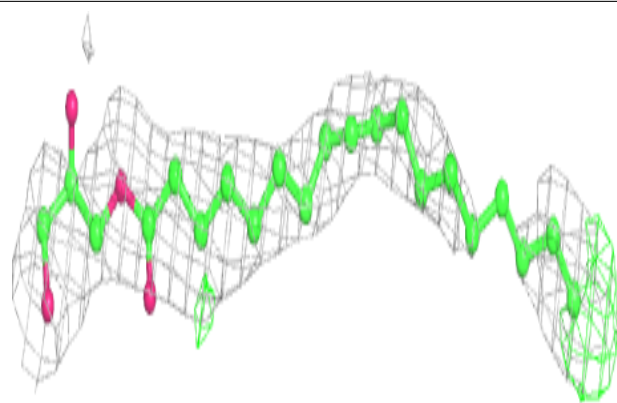
**Electron density around LFA C 317:**

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

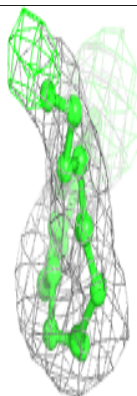
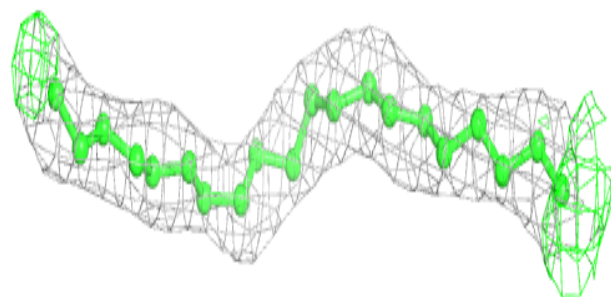
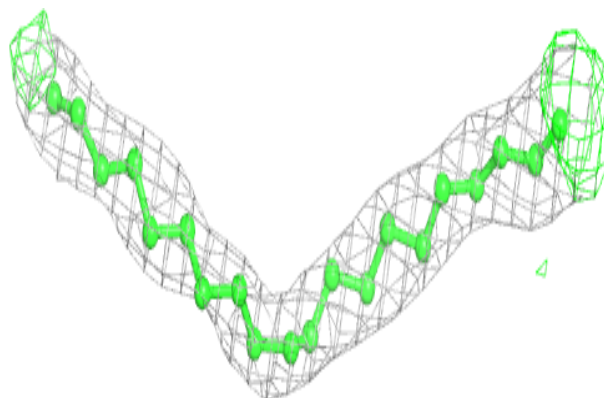


**Electron density around OLC C 307:**

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

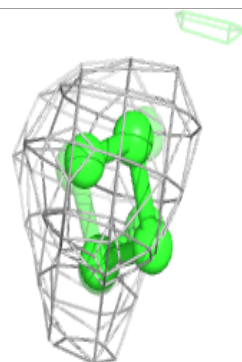
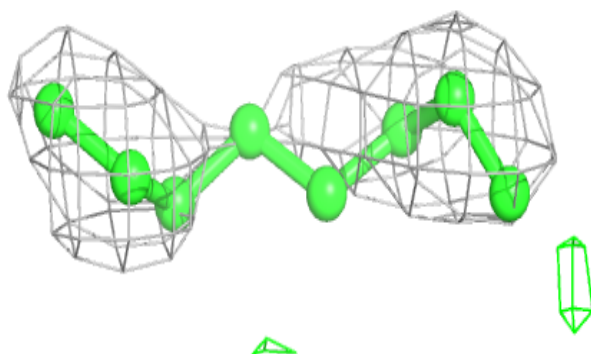
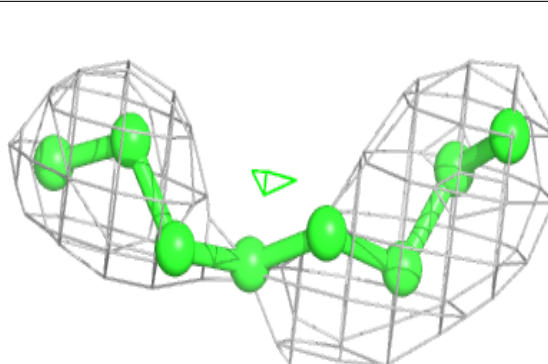
**Electron density around LFA C 319:**

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

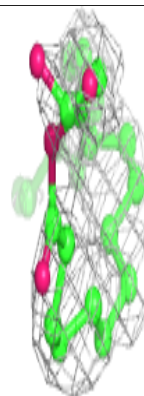
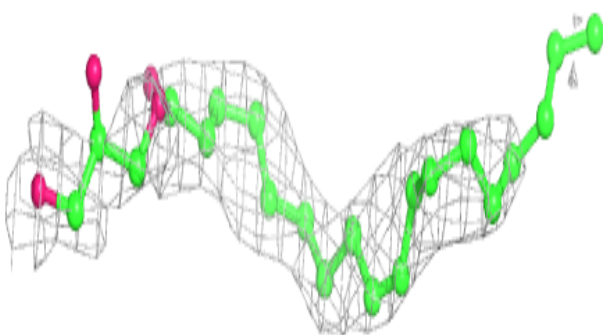
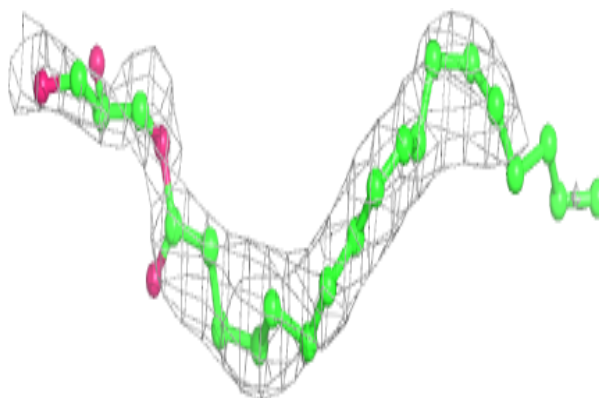


**Electron density around LFA D 312:**

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

**Electron density around OLC A 321:**

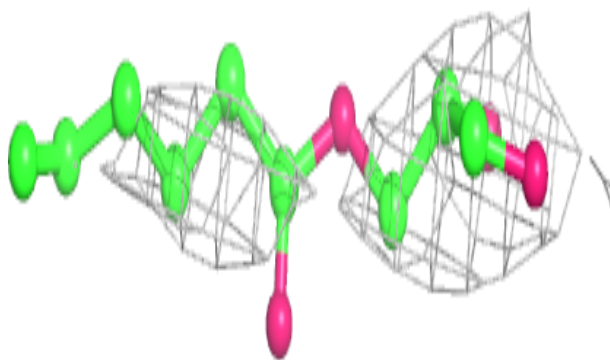
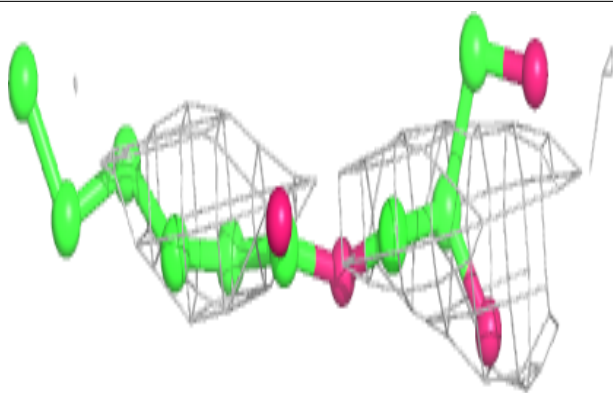
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



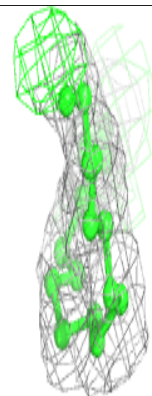
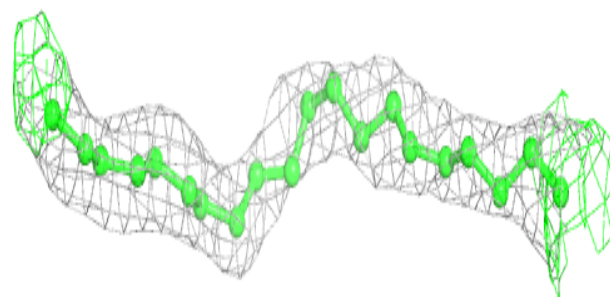
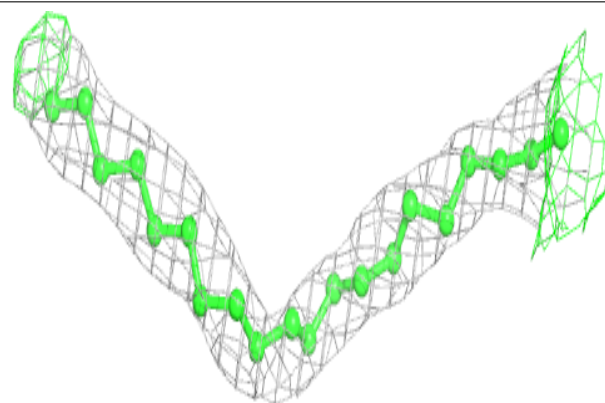


**Electron density around OLC D 302:**

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

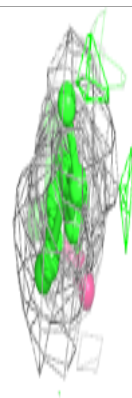
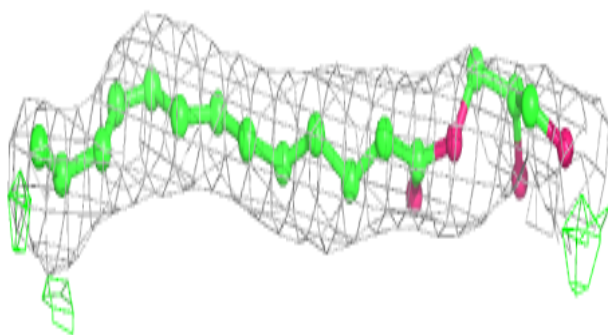
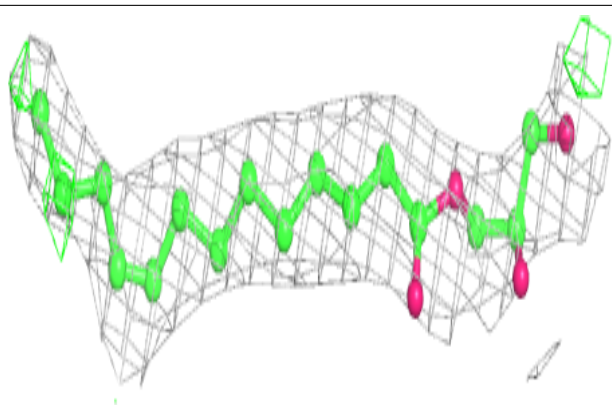
**Electron density around LFA E 319:**

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

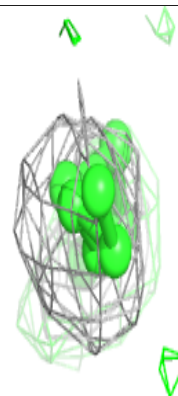
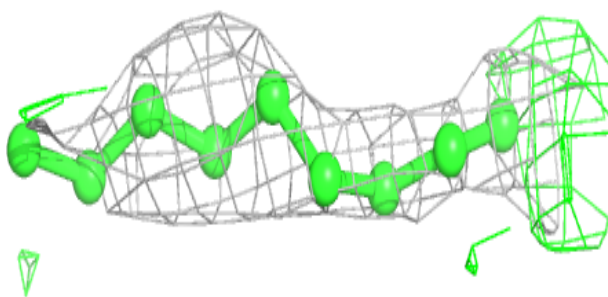
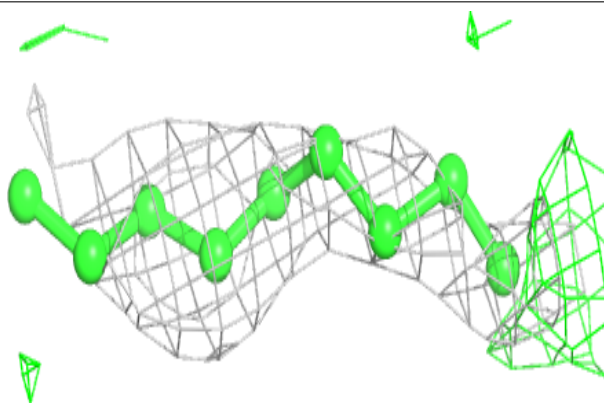


**Electron density around OLC B 308:**

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

**Electron density around LFA B 316:**

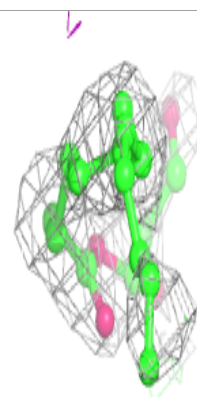
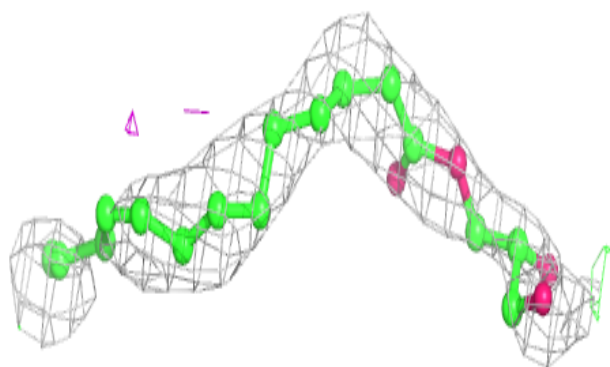
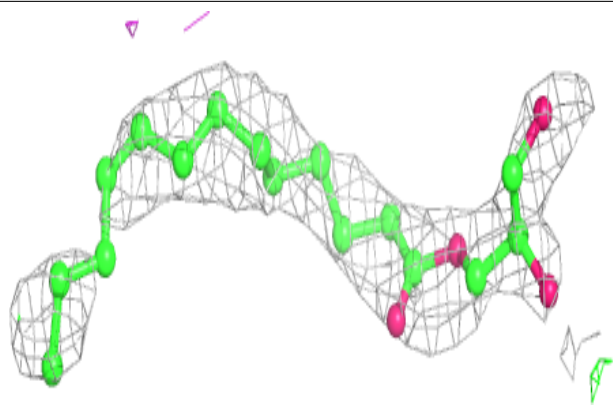
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



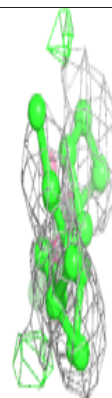
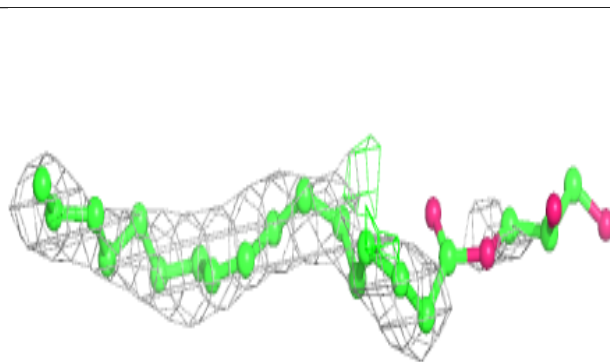
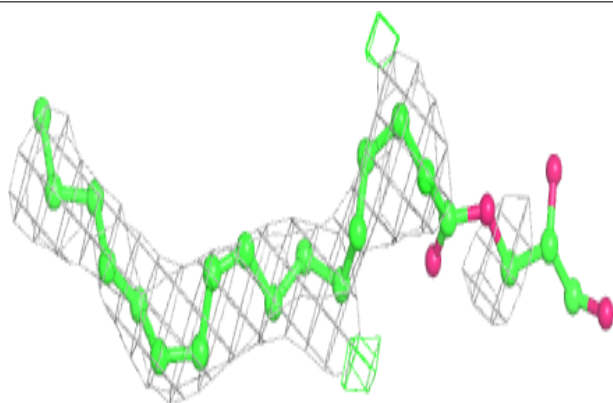


**Electron density around OLC B 306:**

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

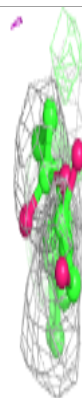
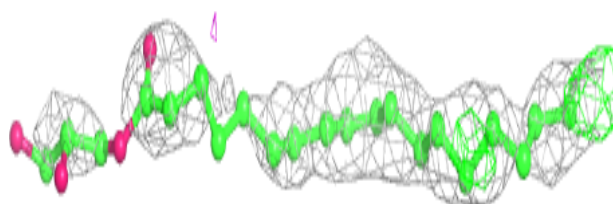
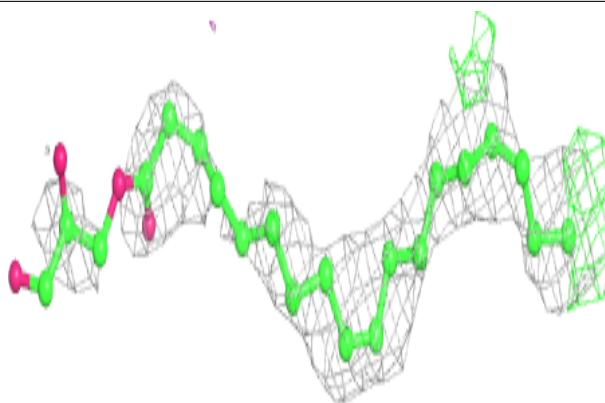
**Electron density around OLC E 306:**

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

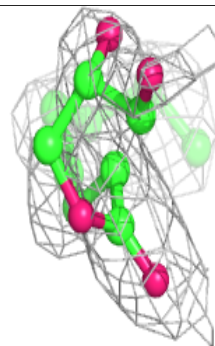
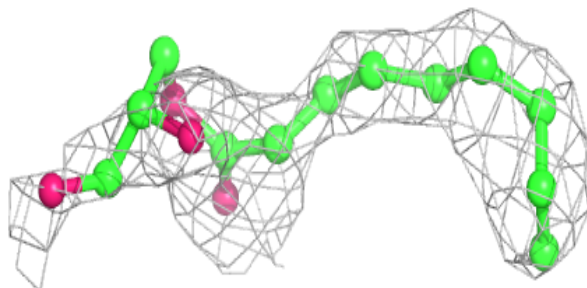
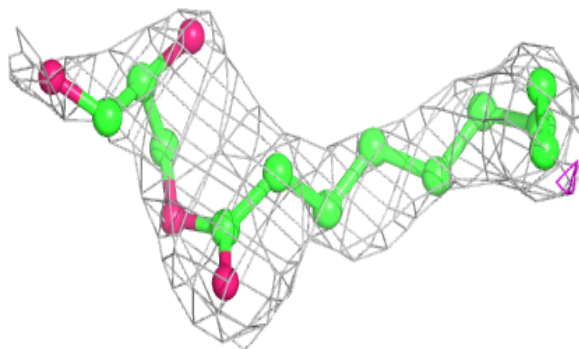


**Electron density around OLC C 306:**

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

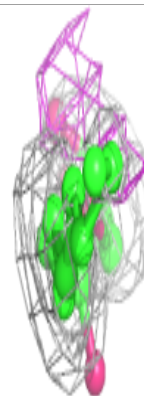
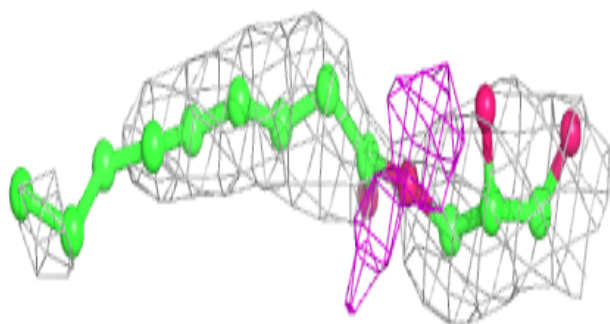
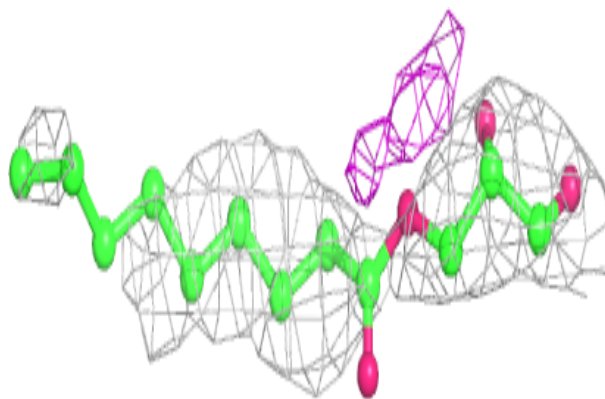
**Electron density around OLC C 312:**

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

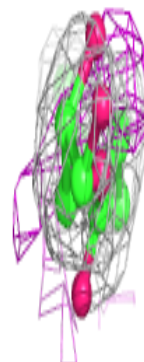
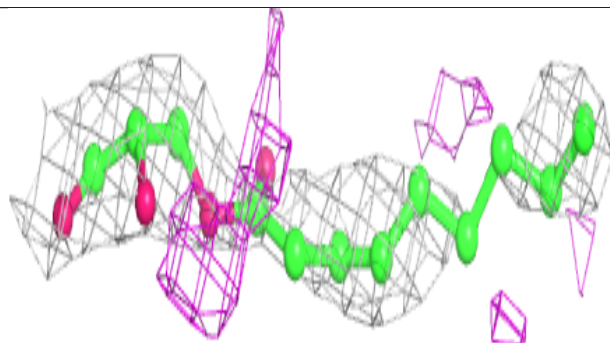
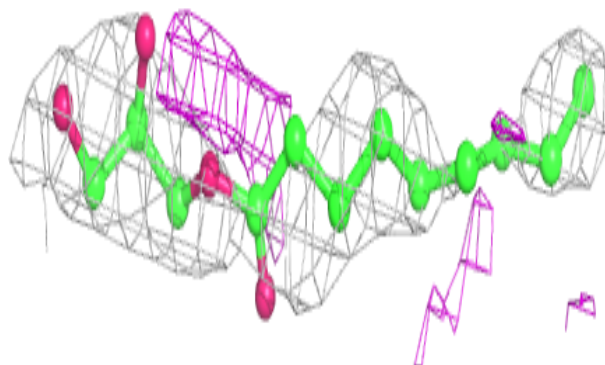


**Electron density around OLC B 315:**

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

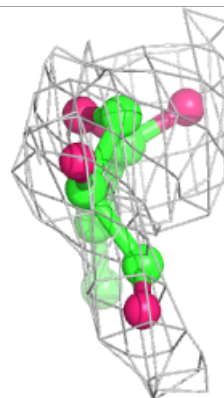
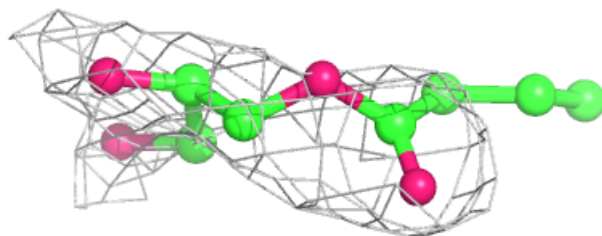
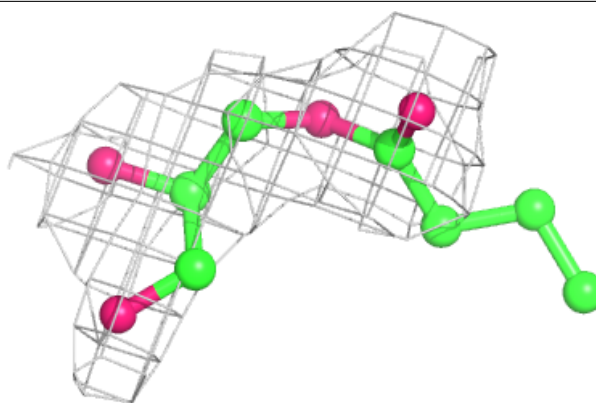
**Electron density around OLC C 313:**

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

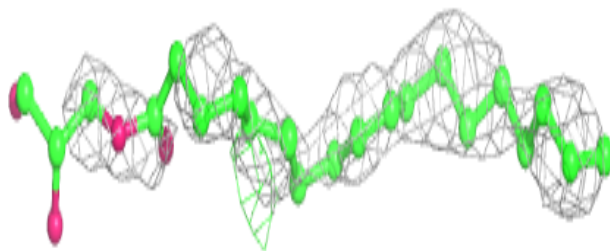
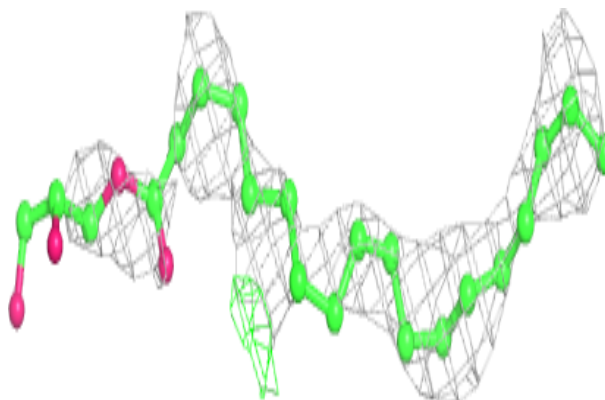


**Electron density around OLC E 311:**

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

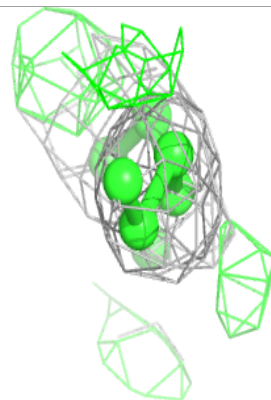
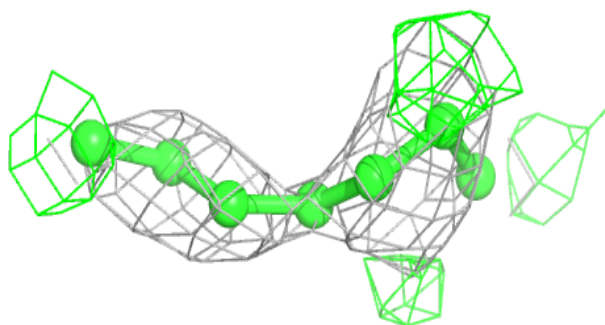
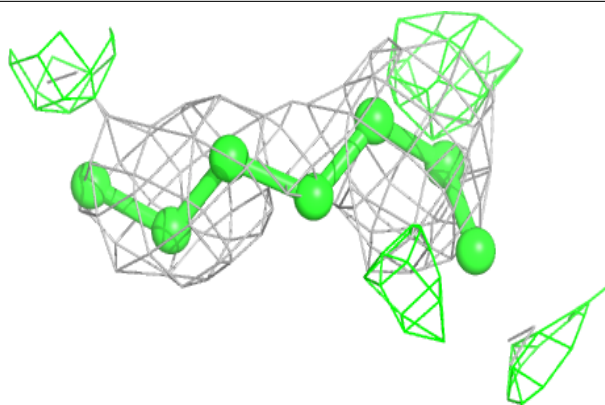
**Electron density around OLC A 304:**

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

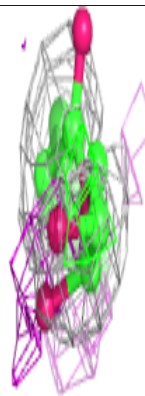
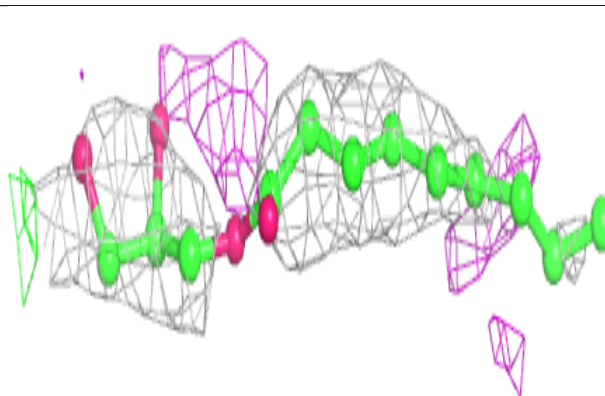
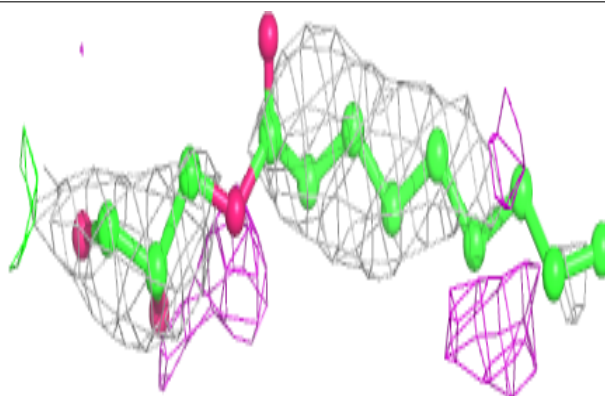


**Electron density around LFA A 312:**

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

**Electron density around OLC A 311:**

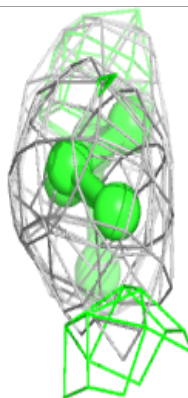
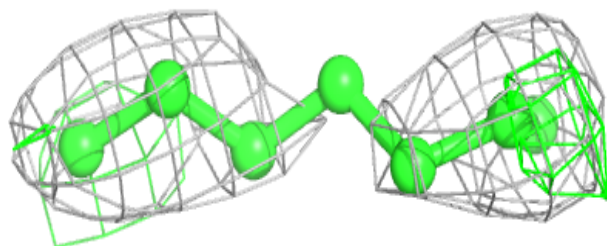
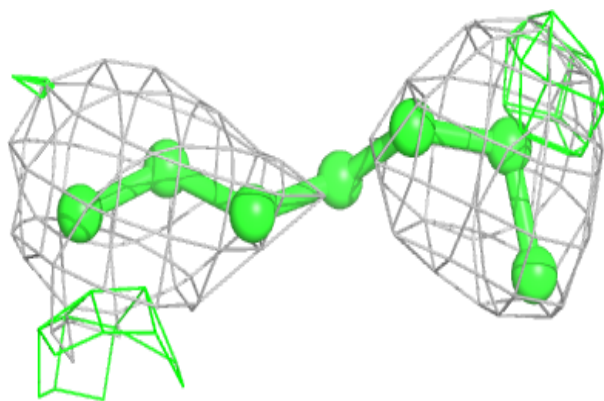
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



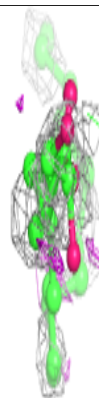
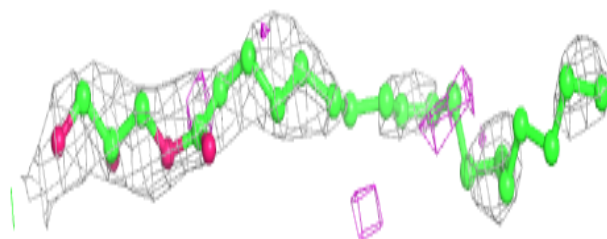
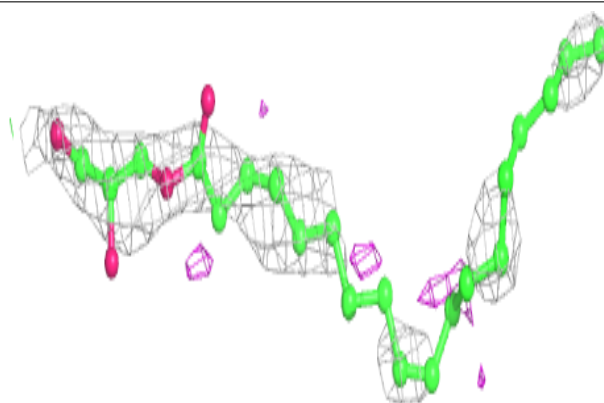


**Electron density around LFA B 319:**

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

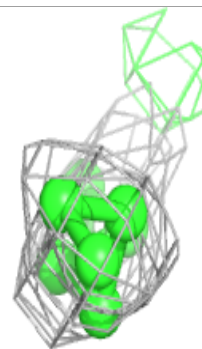
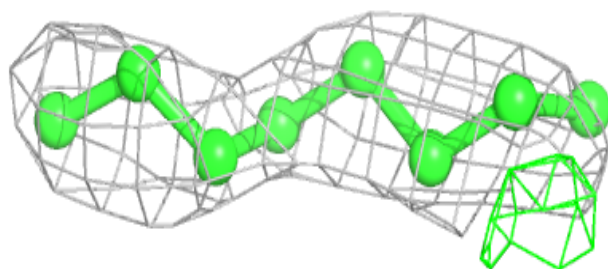
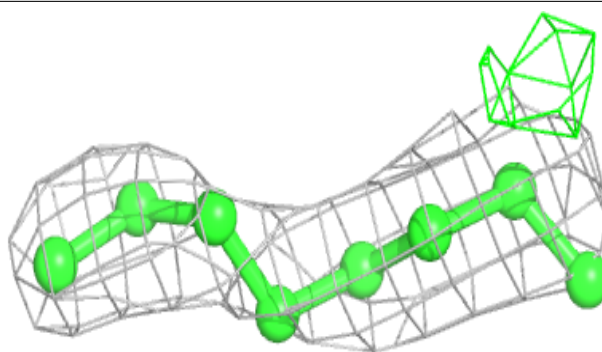
**Electron density around OLC D 309:**

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

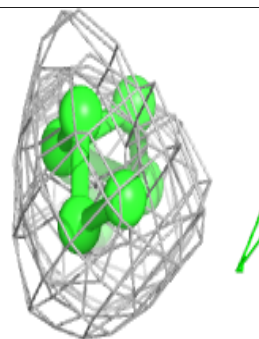
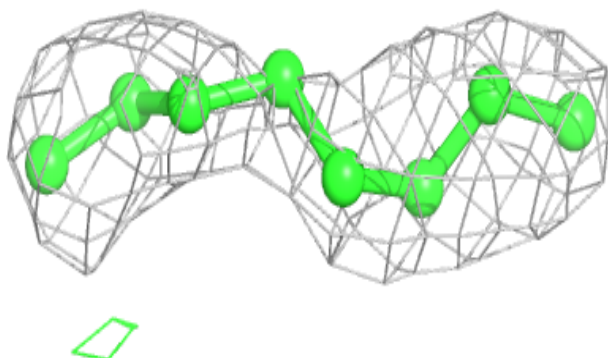
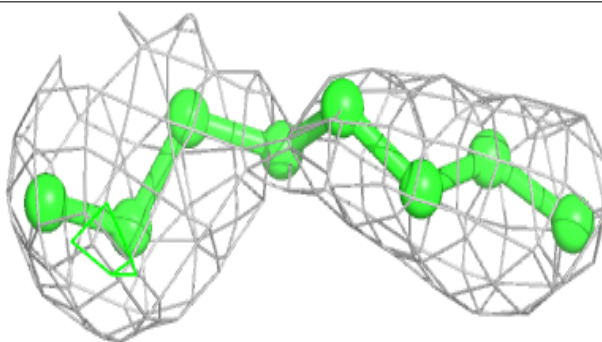


**Electron density around LFA C 315:**

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

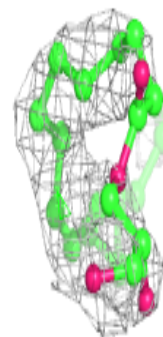
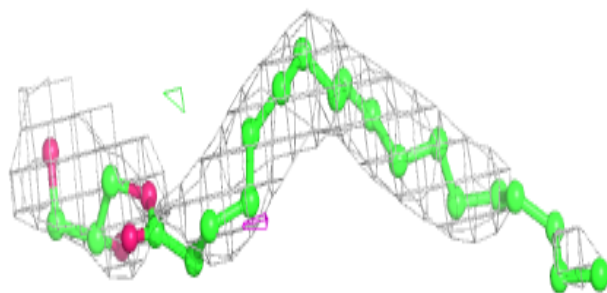
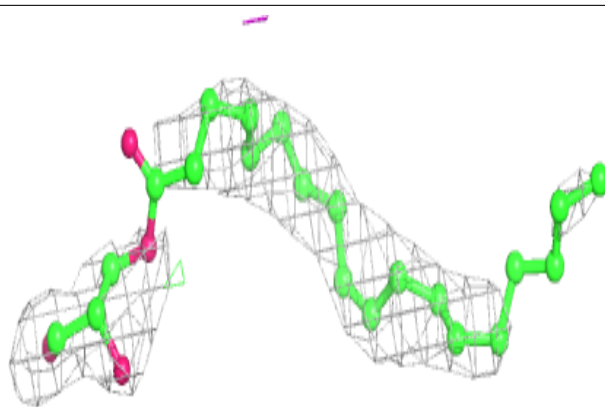
**Electron density around LFA A 314:**

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

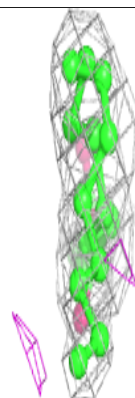
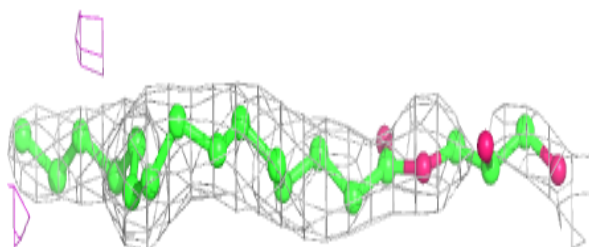
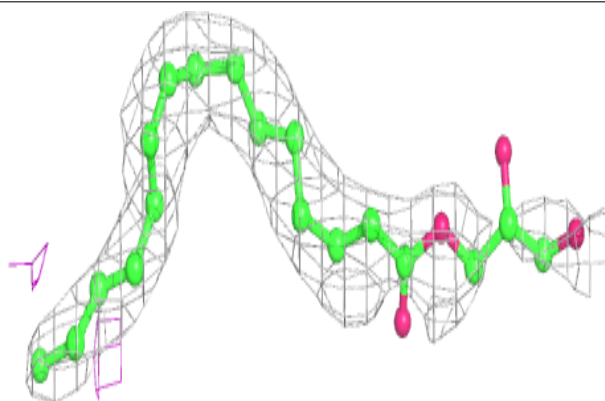


**Electron density around OLC E 301:**

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

**Electron density around OLC A 303:**

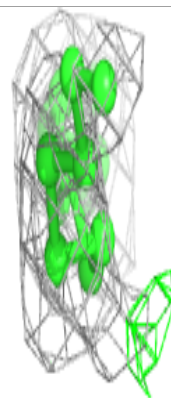
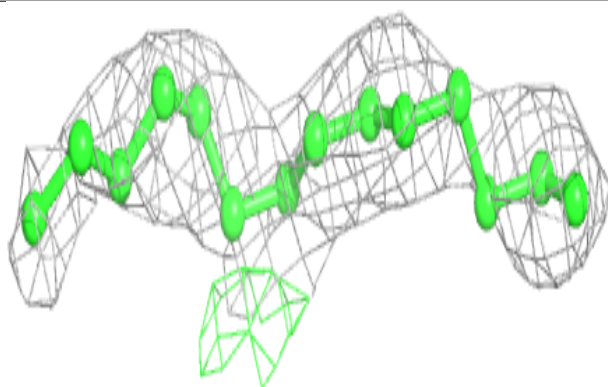
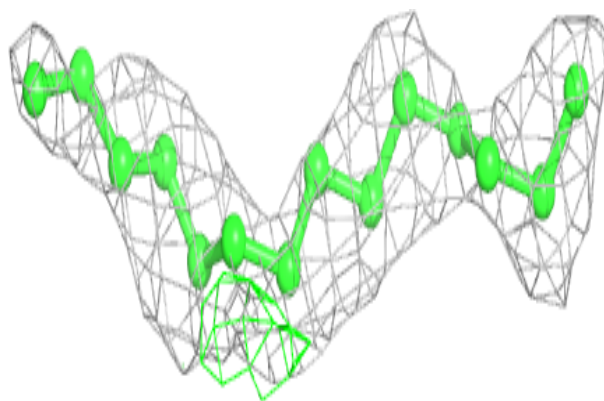
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



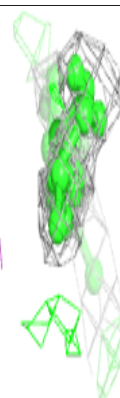
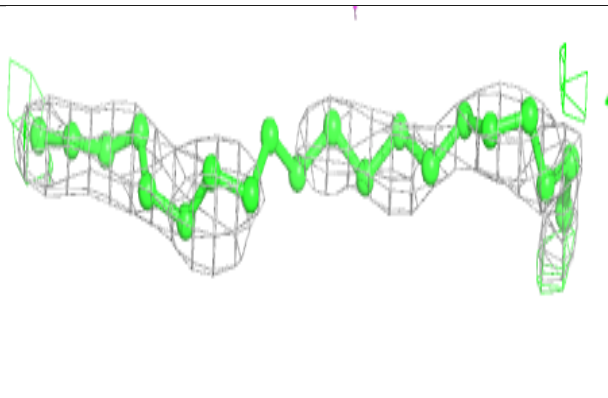
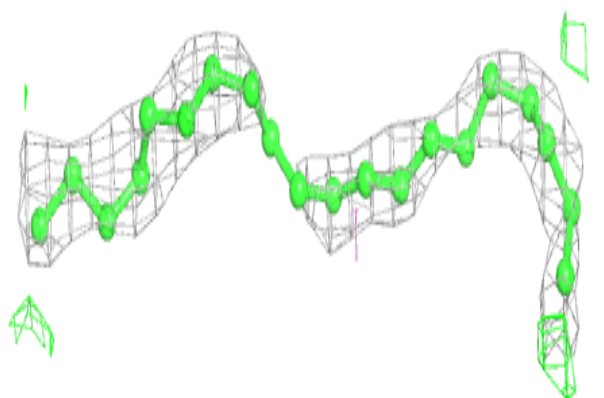


**Electron density around LFA E 316:**

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

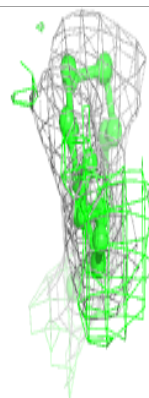
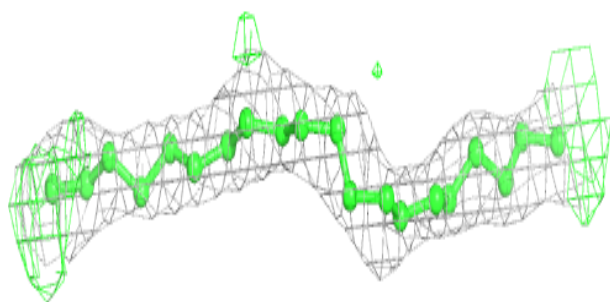
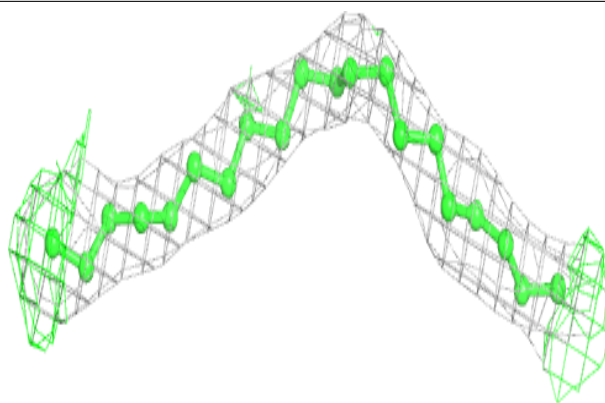
**Electron density around LFA D 310:**

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

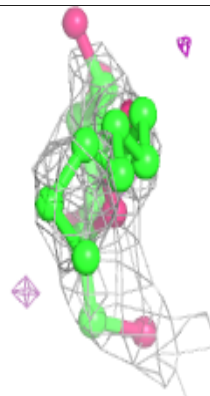
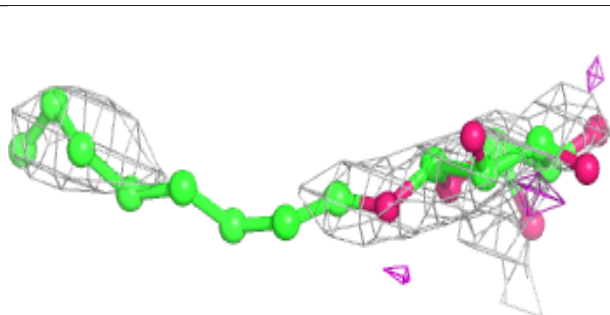
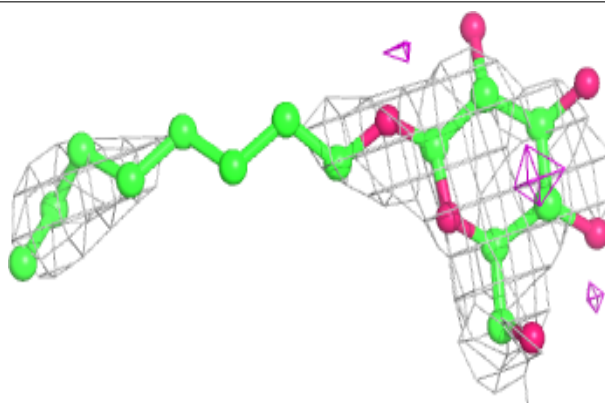


**Electron density around LFA C 302:**

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

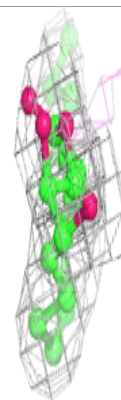
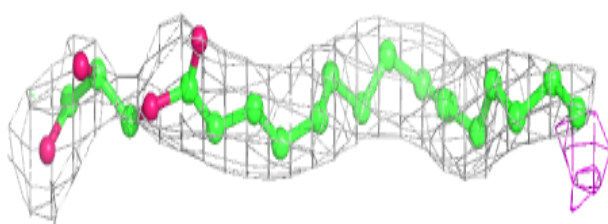
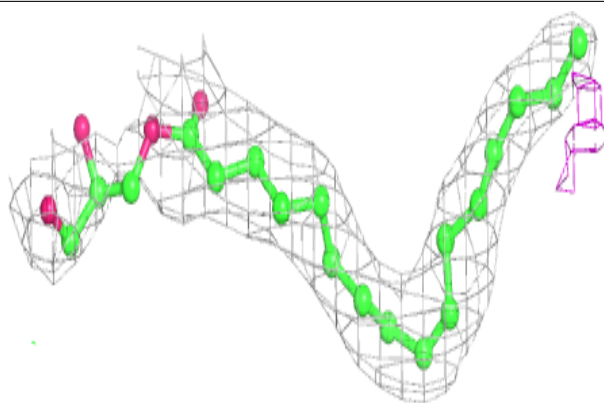
**Electron density around BOG D 317:**

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

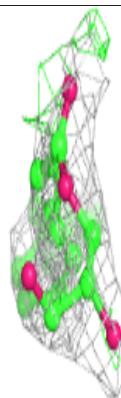
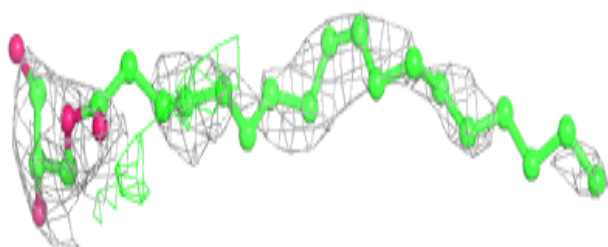
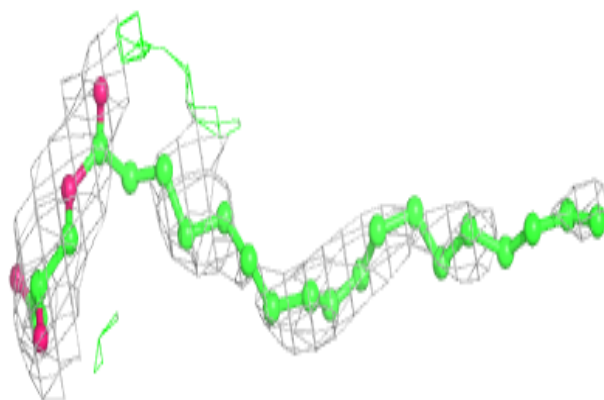


**Electron density around OLC C 305:**

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

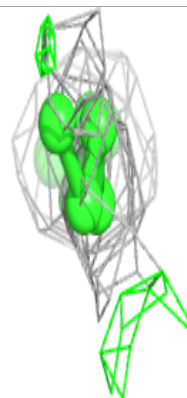
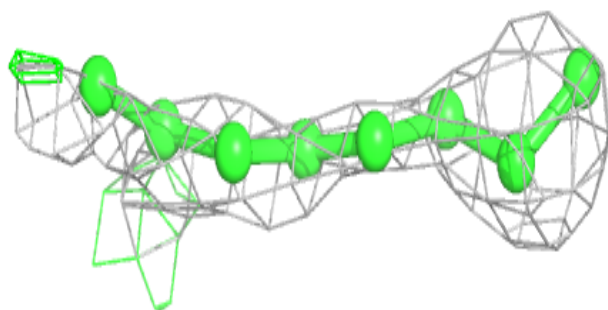
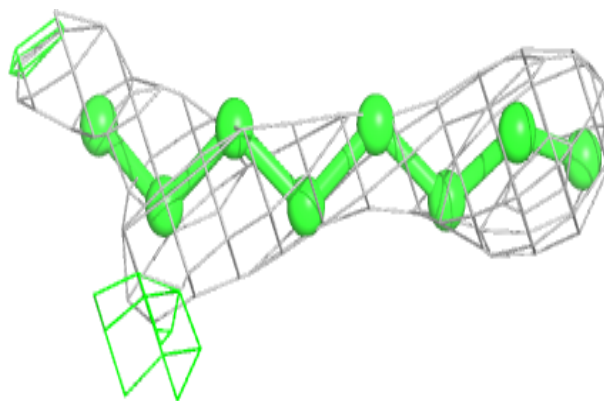
**Electron density around OLC A 302:**

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

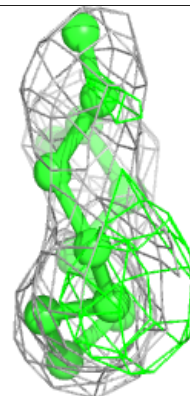
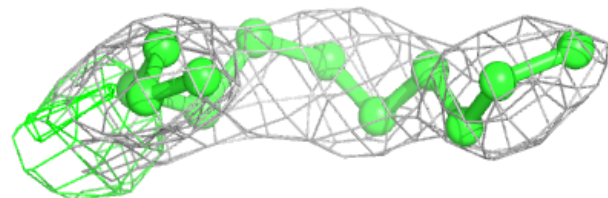
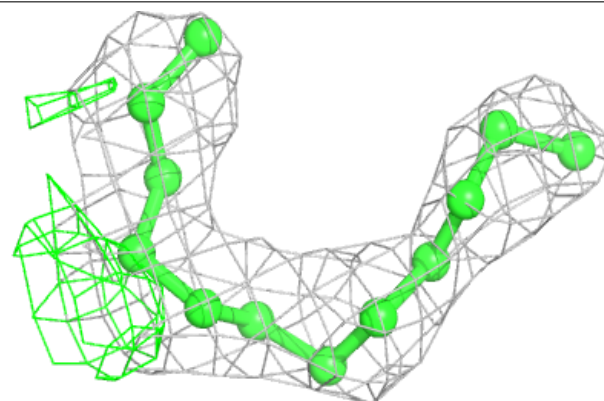


**Electron density around LFA E 315:**

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

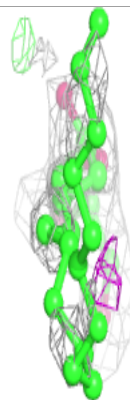
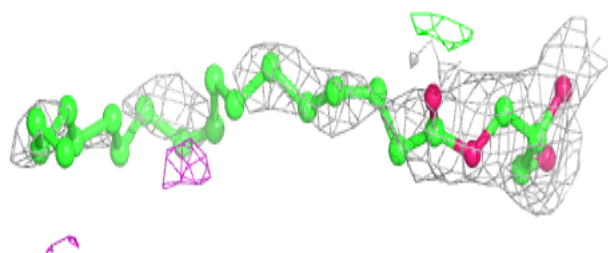
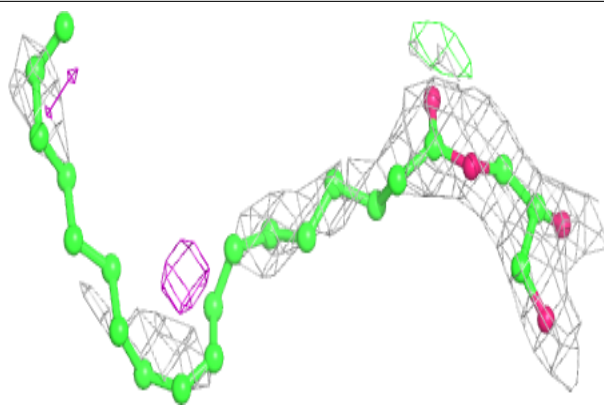
**Electron density around LFA A 315:**

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

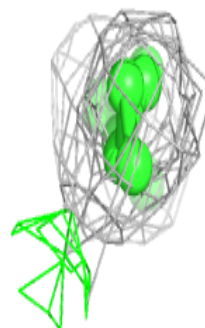
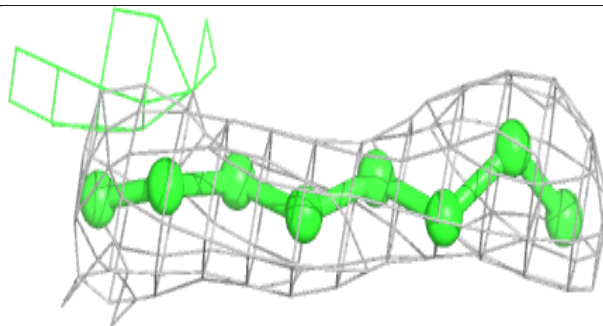
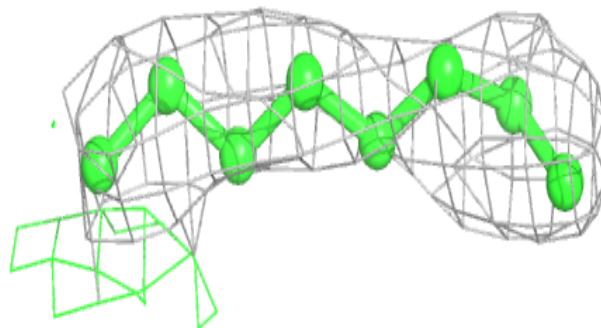


**Electron density around OLC C 310:**

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

**Electron density around LFA A 313:**

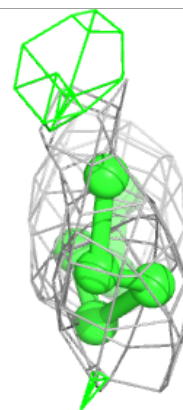
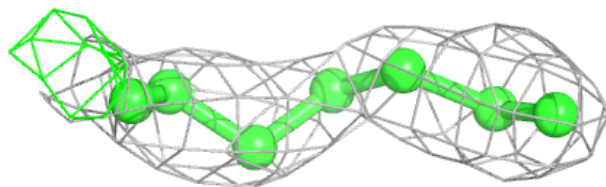
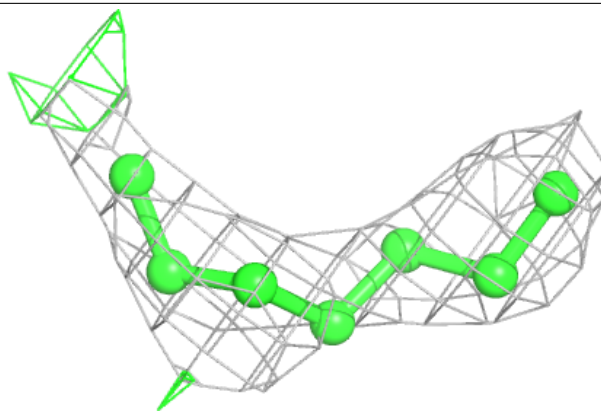
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



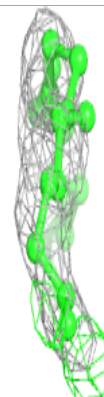
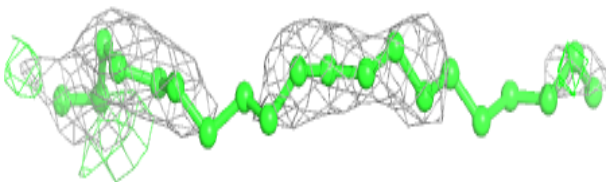
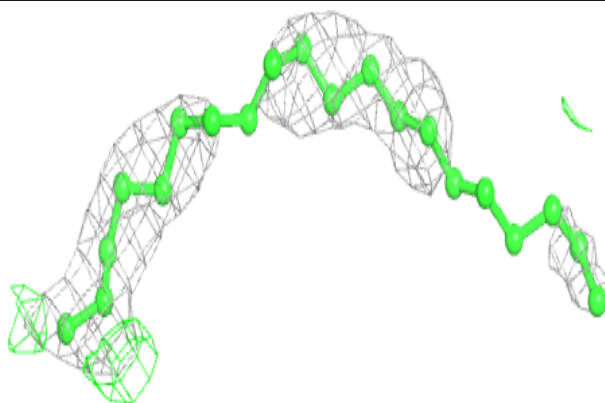


**Electron density around LFA D 314:**

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

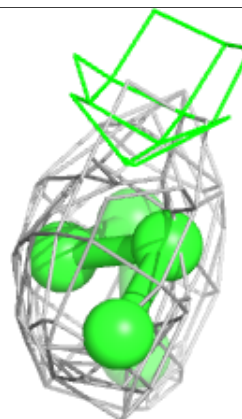
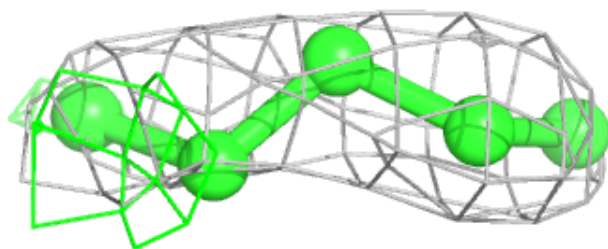
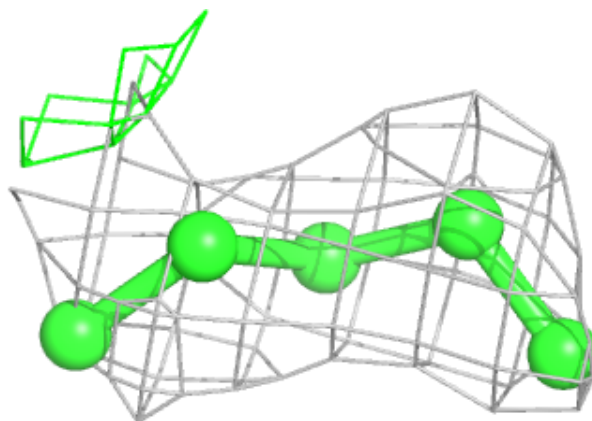
**Electron density around LFA A 318:**

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



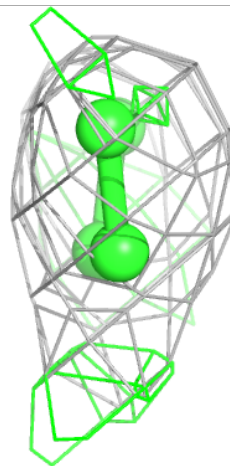
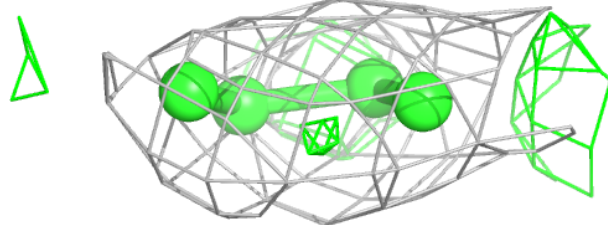
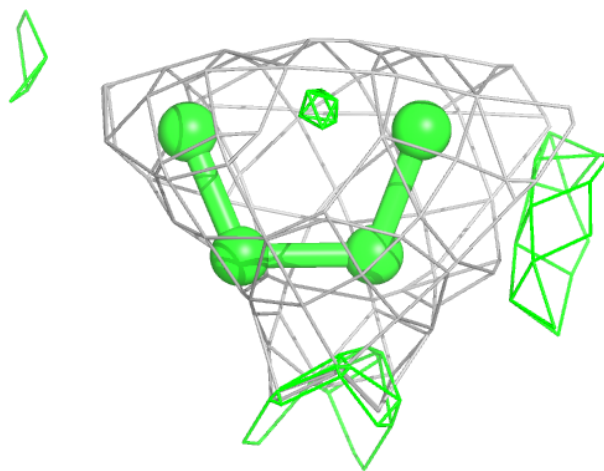
**Electron density around LFA E 318:**

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



**Electron density around LFA E 317:**

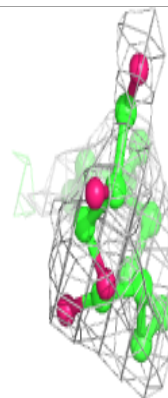
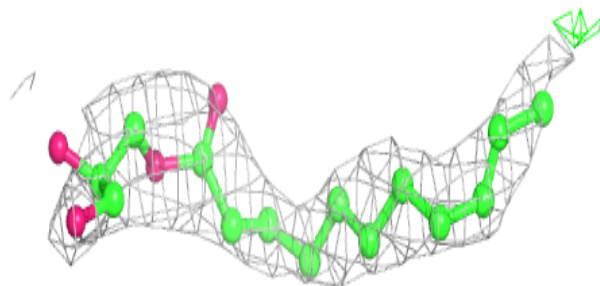
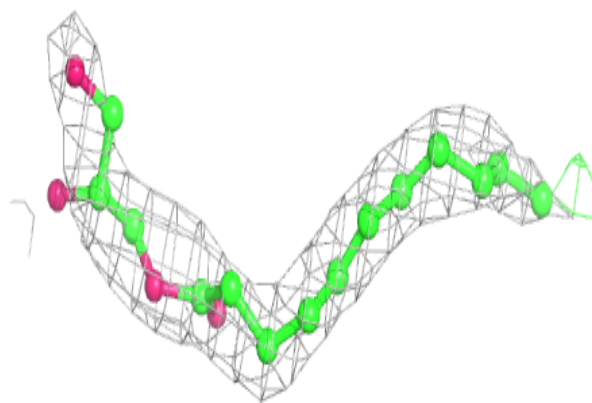
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



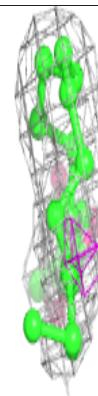
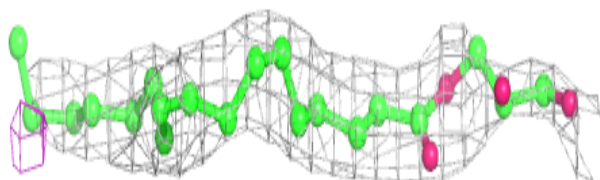
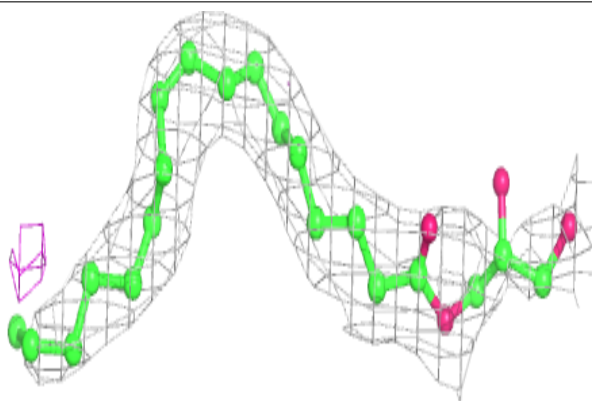


**Electron density around OLC D 301:**

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

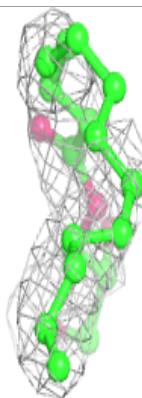
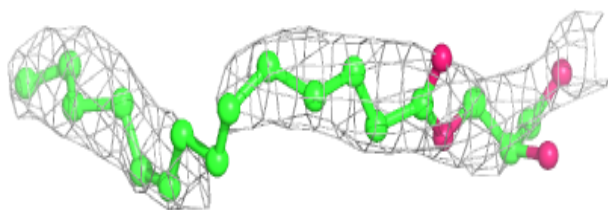
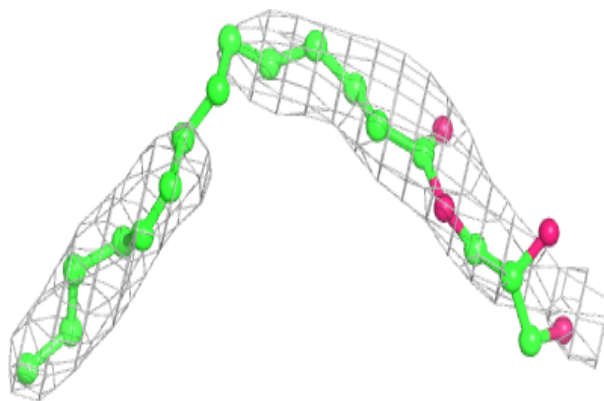
**Electron density around OLC E 305:**

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

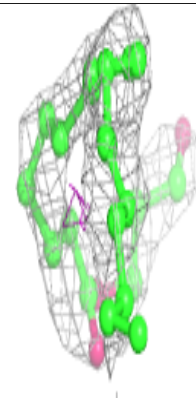
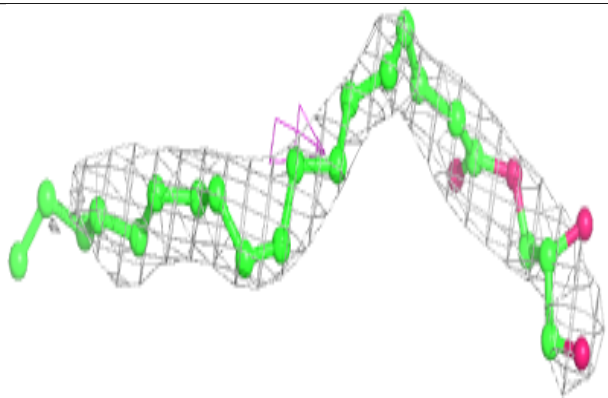
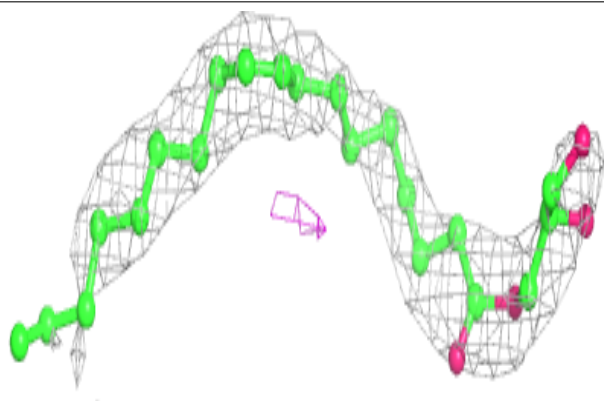


**Electron density around OLC B 309:**

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

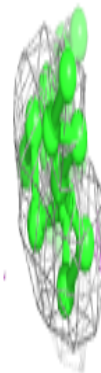
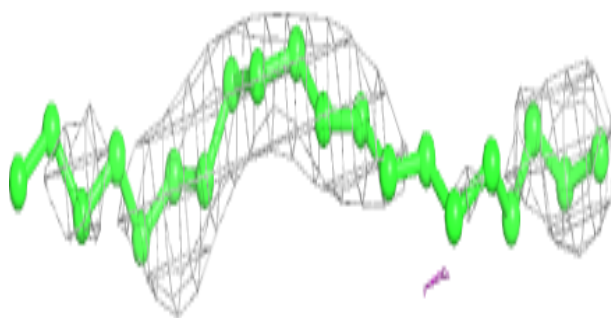
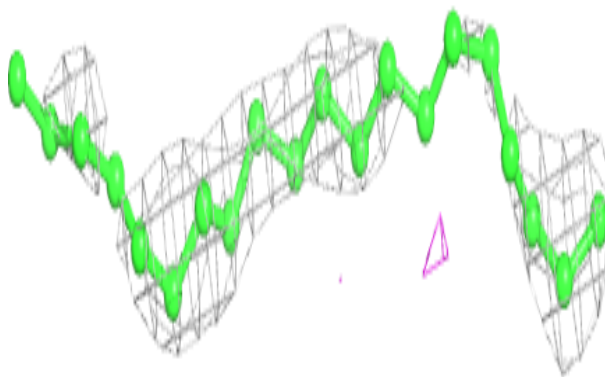
**Electron density around OLC B 301:**

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

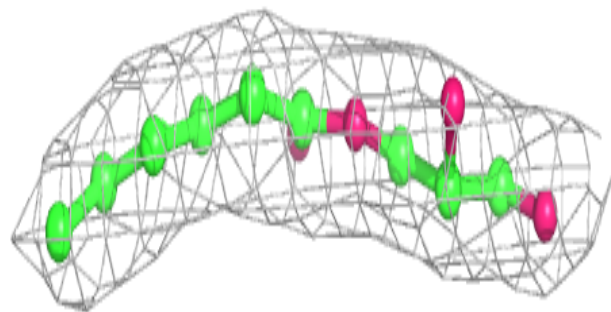
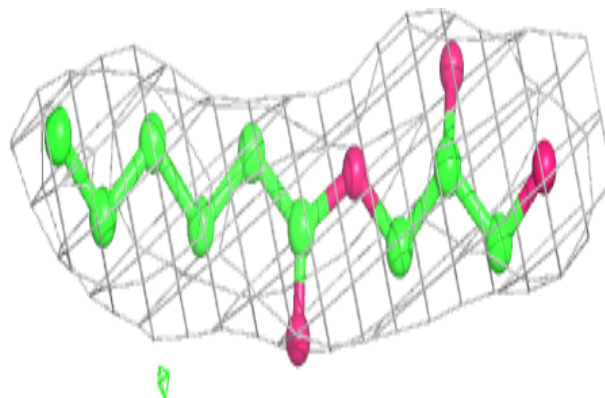


**Electron density around LFA D 311:**

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

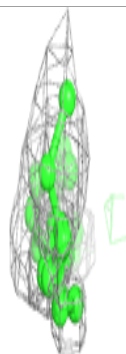
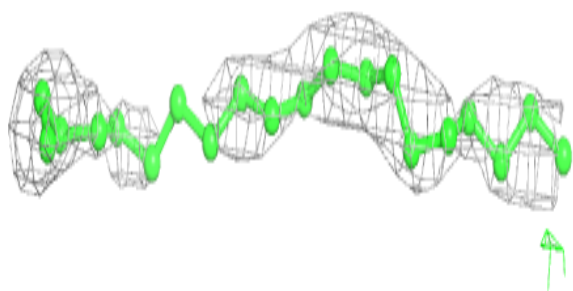
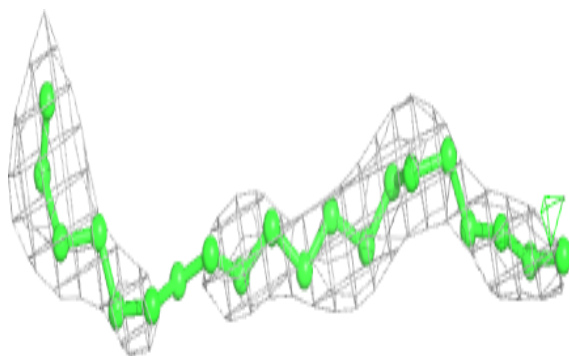
**Electron density around OLC A 305:**

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

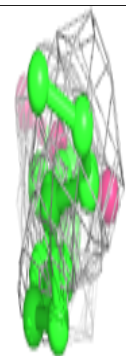
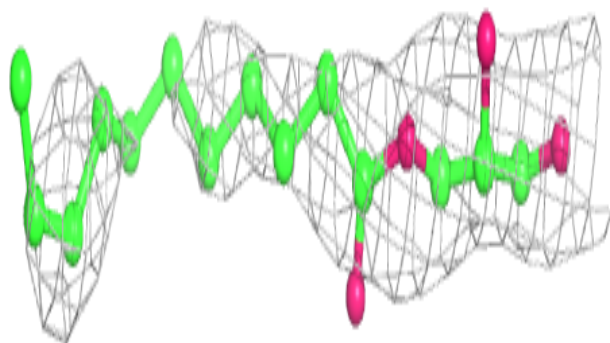
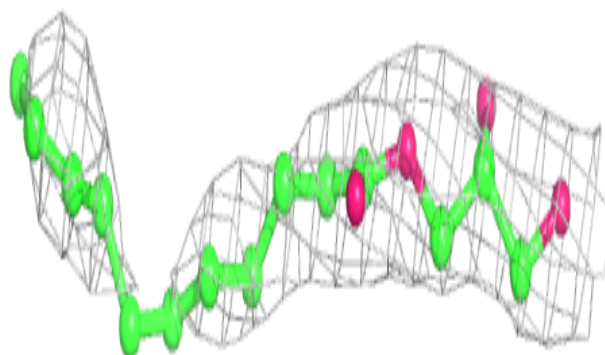


**Electron density around LFA C 316:**

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

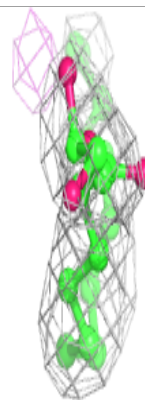
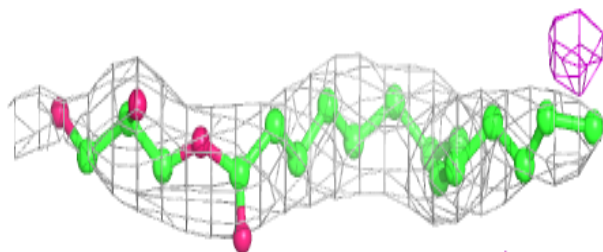
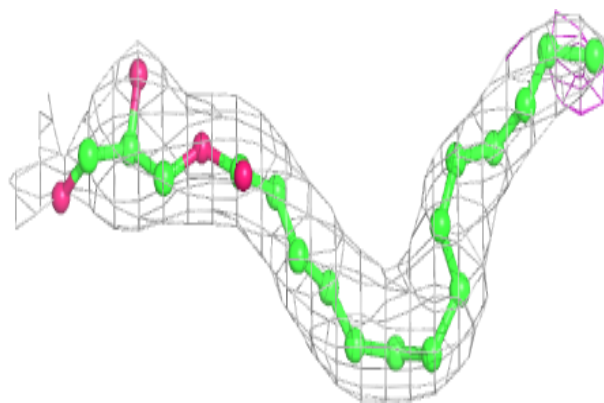
**Electron density around OLC D 304:**

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

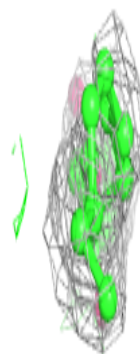
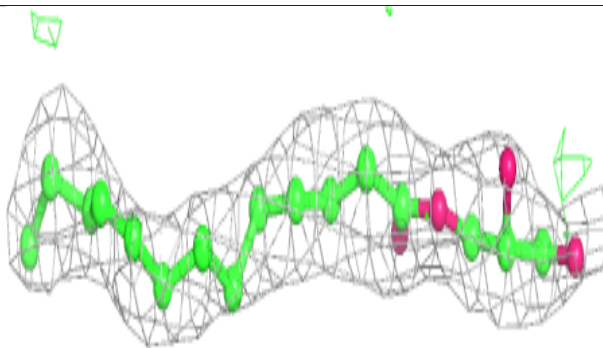
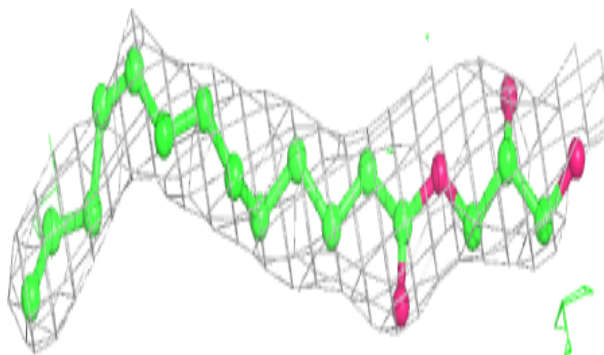


**Electron density around OLC C 301:**

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

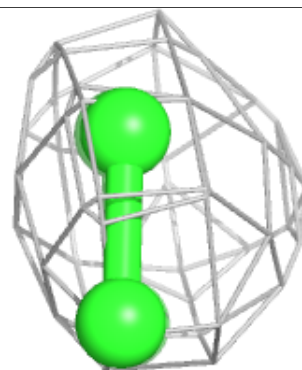
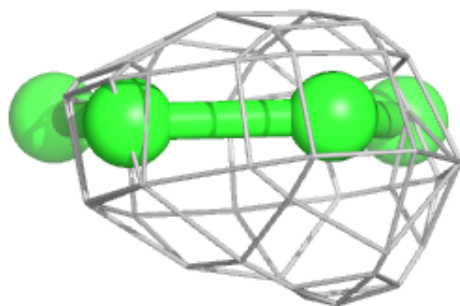
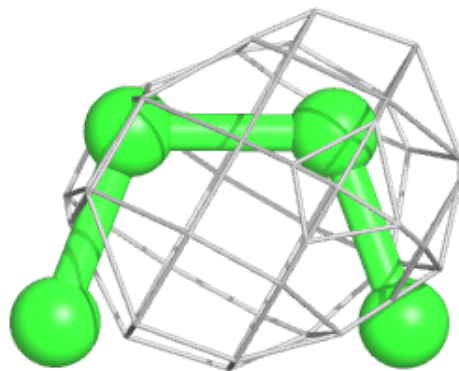
**Electron density around OLC E 307:**

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



**Electron density around LFA C 318:**

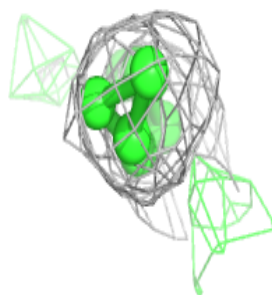
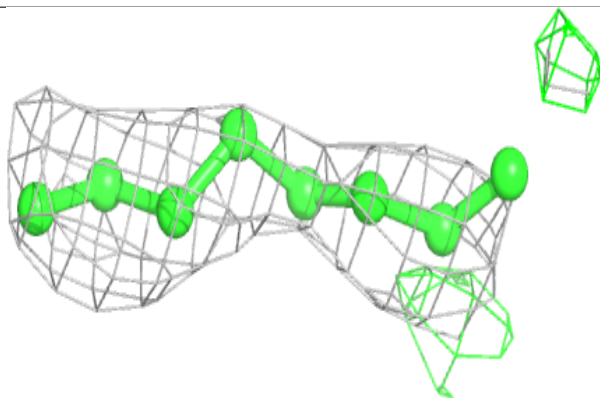
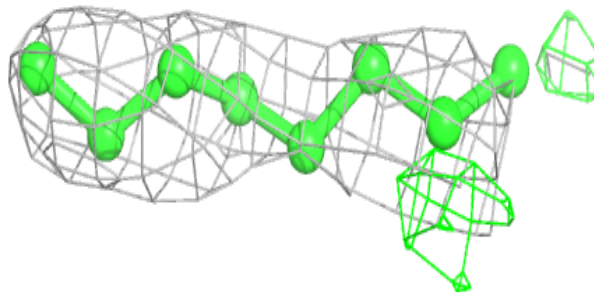
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



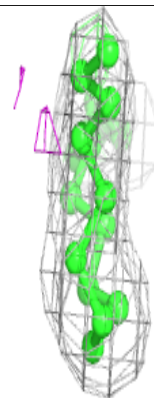
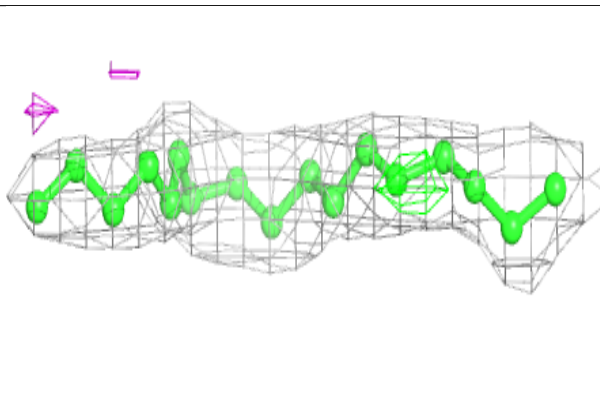
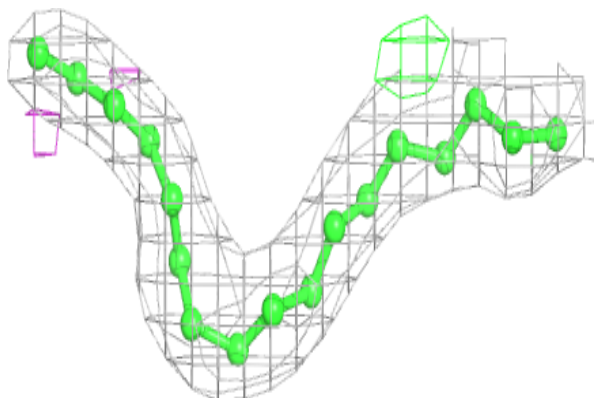


**Electron density around LFA B 317:**

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

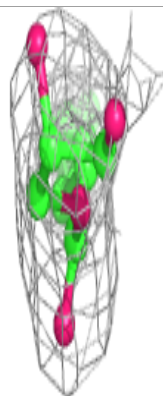
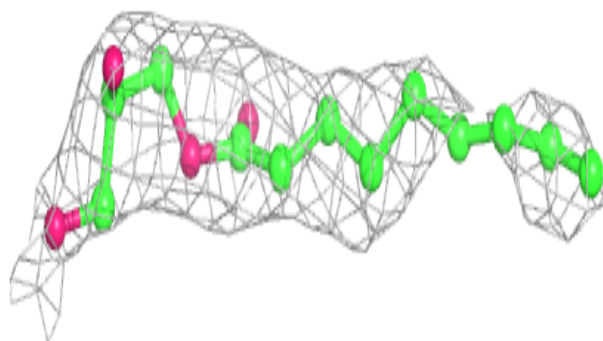
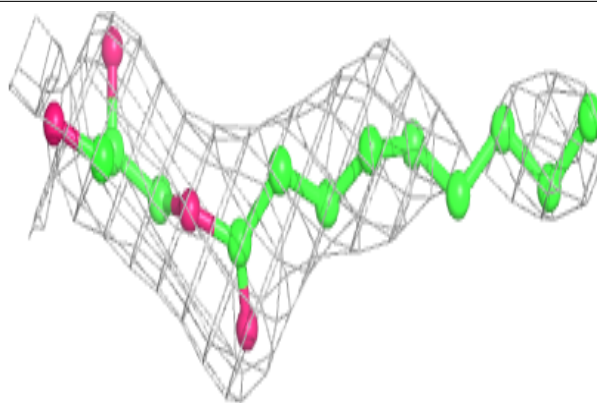
**Electron density around LFA D 313:**

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

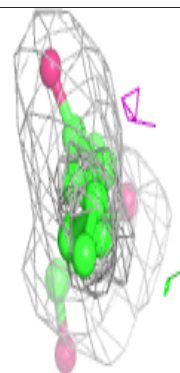
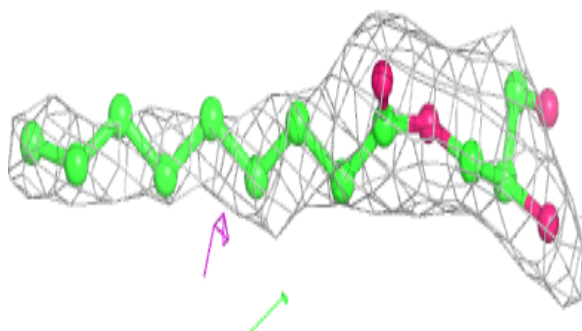
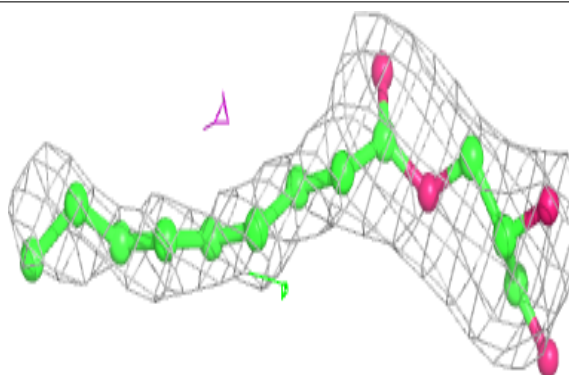


**Electron density around OLC C 311:**

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

**Electron density around OLC B 312:**

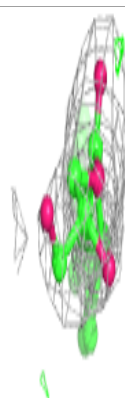
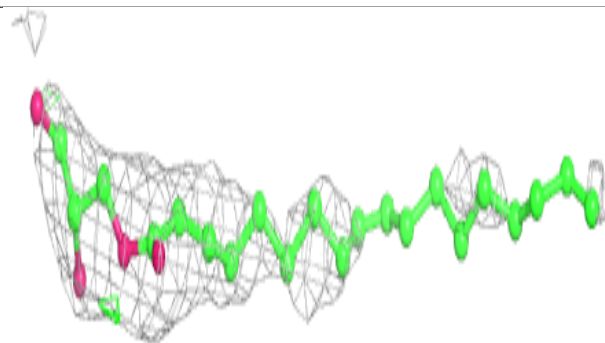
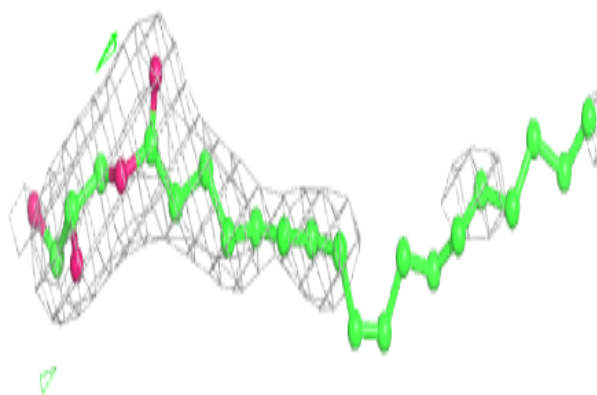
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



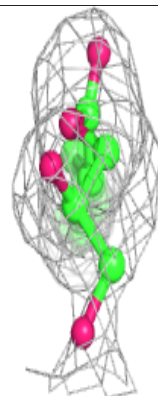
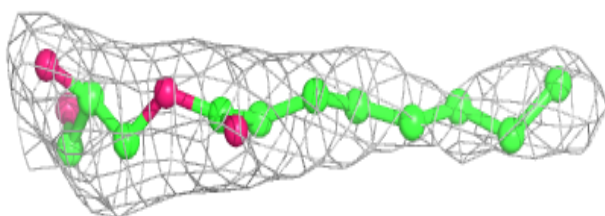
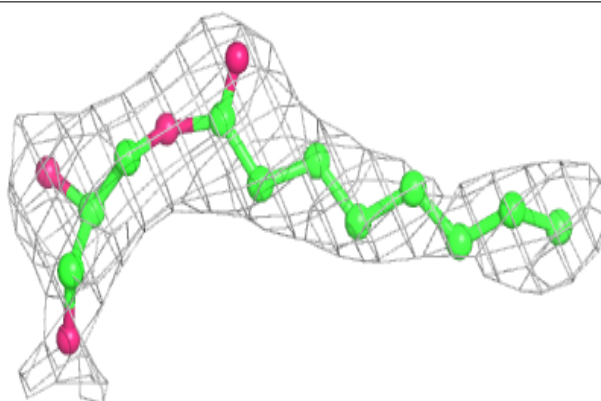


**Electron density around OLC E 309:**

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

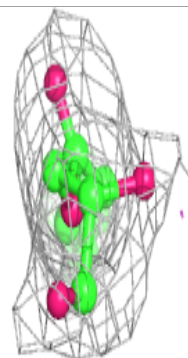
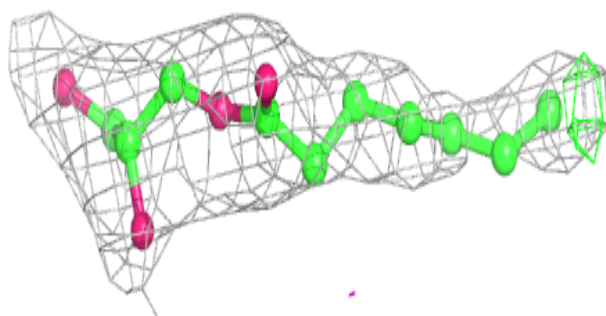
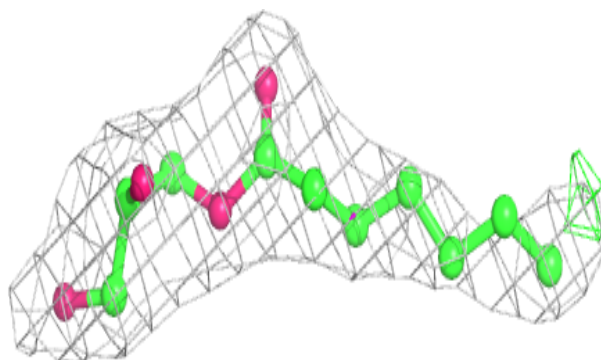
**Electron density around OLC A 309:**

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

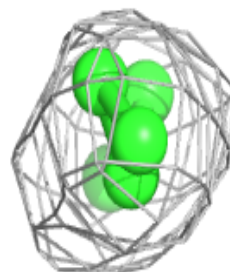
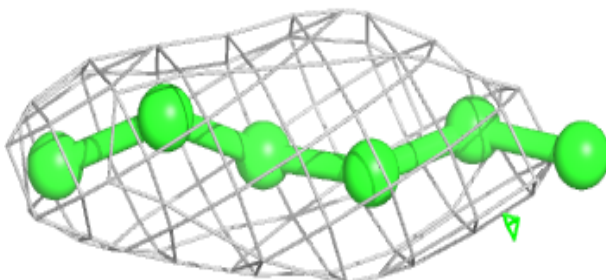
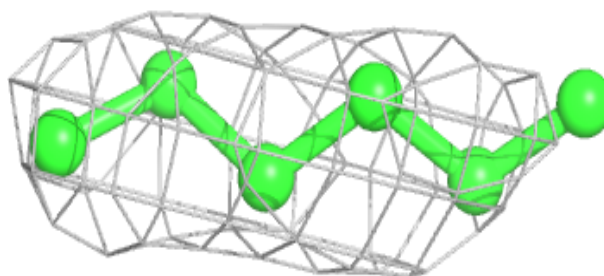


**Electron density around OLC D 307:**

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

**Electron density around LFA A 317:**

$2mF_o-DF_c$  (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.