



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 03:19 AM BST

PDB ID : 6YC3  
Title : Crystal structure of the light-driven sodium pump KR2 in the pentameric form, pH 8.0  
Authors : Kovalev, K.; Gushchin, I.; Gordeliy, V.  
Deposited on : 2020-03-18  
Resolution : 2.00 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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

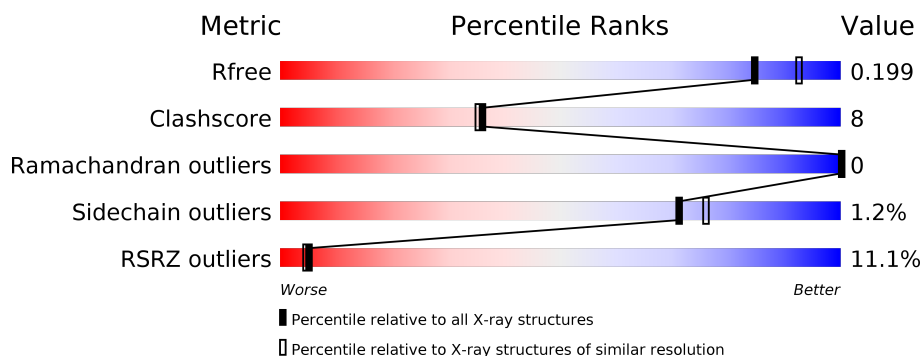
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	273	<div> <div>10%</div> <div>88%12%</div> </div>
1	B	273	<div> <div>10%</div> <div>84%15%</div> </div>
1	C	273	<div> <div>11%</div> <div>86%14%</div> </div>
1	D	273	<div> <div>14%</div> <div>86%13%</div> </div>
1	E	273	<div> <div>11%</div> <div>85%14%</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	C	308	-	-	-	X
2	OLC	E	307	-	-	-	X
2	OLC	E	311	-	-	-	X
3	LFA	A	318	-	-	-	X
3	LFA	B	302	-	-	-	X
3	LFA	C	304	-	-	-	X
3	LFA	D	301	-	-	-	X
3	LFA	E	301	-	-	-	X
3	LFA	E	303	-	-	-	X
4	BOG	A	315	-	-	-	X
4	BOG	B	312	-	-	-	X
4	BOG	C	316	-	-	-	X
4	BOG	E	316	-	-	-	X

## 2 Entry composition [i](#)

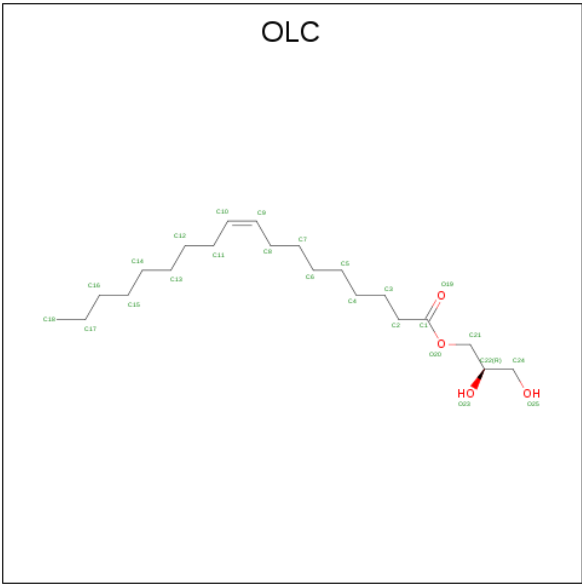
There are 7 unique types of molecules in this entry. The entry contains 12886 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	3	0
			2193	1459	333	392	9			
1	B	273	Total	C	N	O	S	0	3	0
			2194	1457	335	393	9			
1	C	273	Total	C	N	O	S	0	3	0
			2186	1455	332	390	9			
1	D	273	Total	C	N	O	S	0	3	0
			2192	1457	334	392	9			
1	E	273	Total	C	N	O	S	0	3	0
			2194	1459	334	392	9			

- 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	0	0
			9	9		

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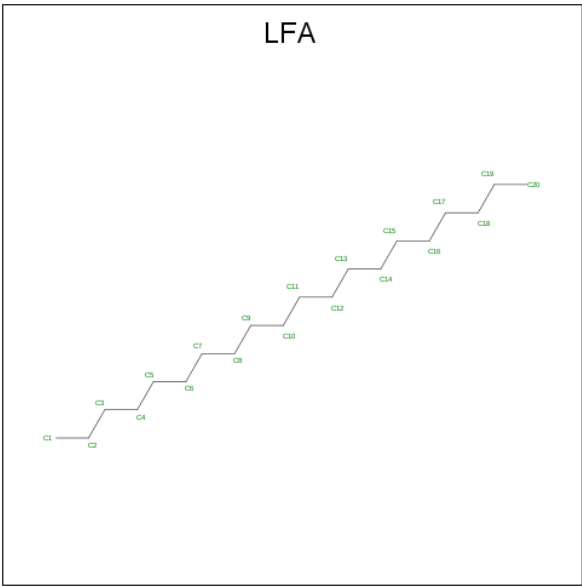
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	18	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			13	9	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			15	11	4		
2	A	1	Total	C		0	0
			7	7			
2	A	1	Total	C	O	0	0
			16	12	4		
2	A	1	Total	C	O	0	0
			19	17	2		
2	A	1	Total	C	O	0	0
			20	18	2		
2	B	1	Total	C	O	0	0
			22	18	4		
2	B	1	Total	C	O	0	0
			25	21	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		0	0
			7	7			
2	C	1	Total	C	O	0	0
			21	17	4		
2	C	1	Total	C	O	0	0
			20	16	4		
2	C	1	Total	C	O	0	0
			12	8	4		
2	C	1	Total	C	O	0	0
			23	19	4		
2	C	1	Total	C	O	0	0
			22	18	4		
2	C	1	Total	C	O	0	0
			20	16	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C O 18 14 4	0	0
2	D	1	Total C O 16 12 4	0	0
2	D	1	Total C O 13 9 4	0	0
2	D	1	Total C O 25 21 4	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C O 18 16 2	0	0
2	D	1	Total C O 14 10 4	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C O 25 21 4	0	0
2	E	1	Total C O 25 21 4	0	0
2	E	1	Total C 8 8	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 20 16 4	0	0
2	E	1	Total C O 15 11 4	0	0
2	E	1	Total C O 15 11 4	0	0
2	E	1	Total C 6 6	0	0
2	E	1	Total C O 22 18 4	0	0
2	E	1	Total C O 20 16 4	0	0

- Molecule 3 is EICOSANE (three-letter code: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).



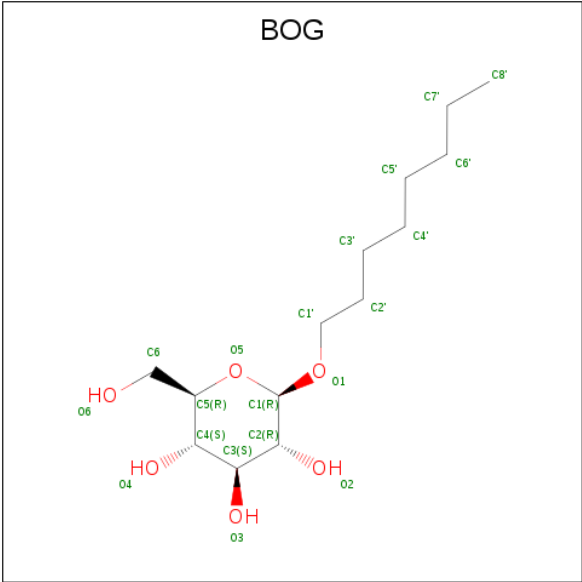
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 20 20	0	0
3	A	1	Total C 9 9	0	0
3	B	1	Total C 20 20	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 7 7	0	0

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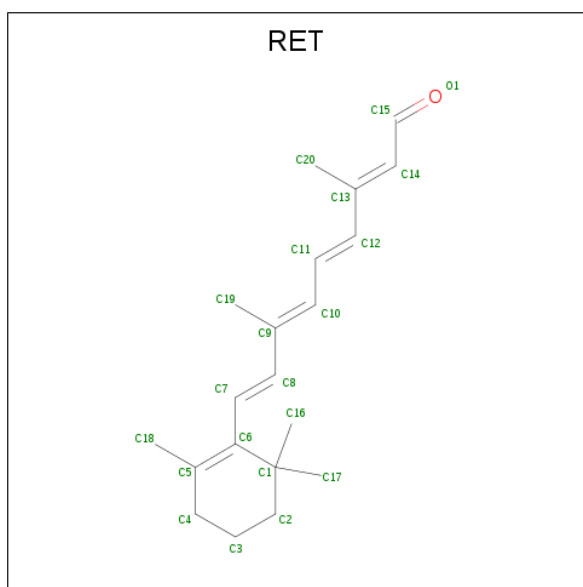
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 4 4	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 4 4	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total 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 14 14	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
3	E	1	Total C 4 4	0	0
3	E	1	Total C 5 5	0	0

- Molecule 4 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
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	D	1	Total	C	O	0	0
			20	14	6		
4	E	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O) (labeled as "Ligand of Interest" by author).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Na 2 2	0	0
6	A	2	Total Na 2 2	0	0
6	D	2	Total Na 2 2	0	0
6	C	2	Total Na 2 2	0	0
6	E	2	Total Na 2 2	0	0

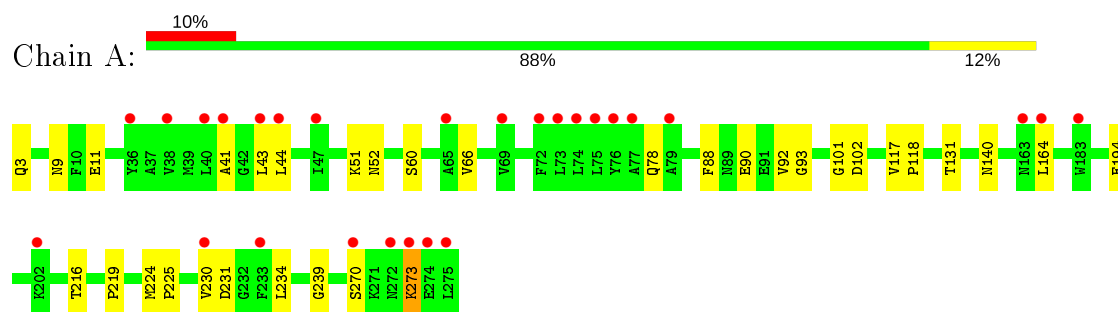
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	123	Total 123	O 123	0	0
7	B	123	Total 123	O 123	0	0
7	C	123	Total 123	O 123	0	0
7	D	107	Total 107	O 107	0	0
7	E	131	Total 131	O 131	0	0

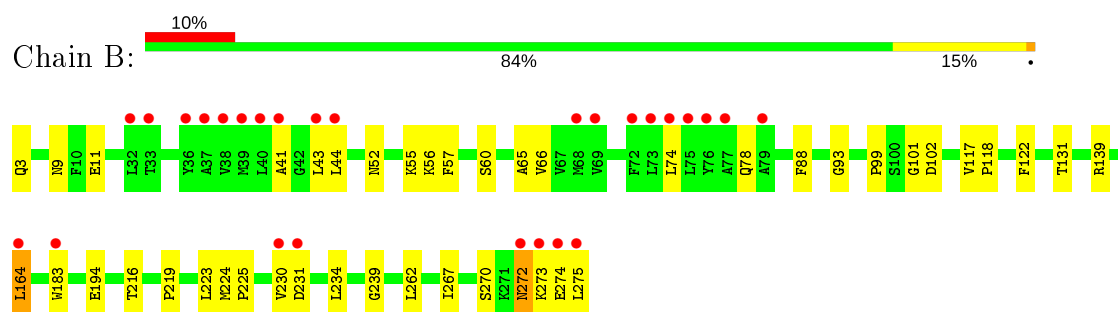
### 3 Residue-property plots

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

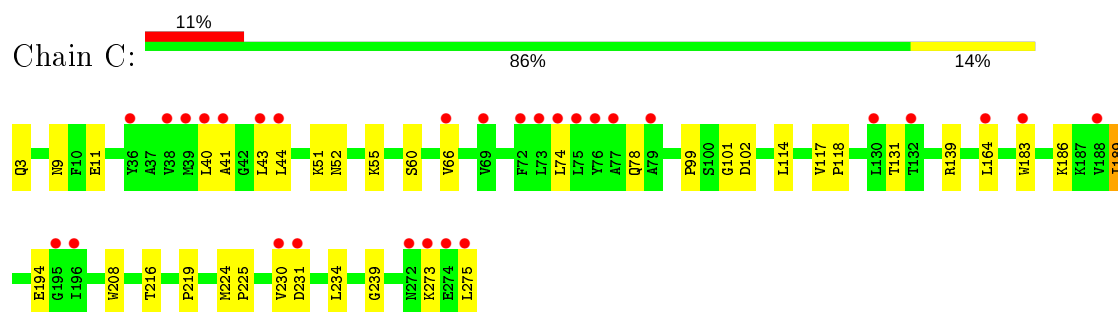
#### • Molecule 1: Sodium pumping rhodopsin



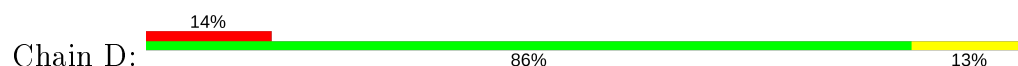
#### • Molecule 1: Sodium pumping rhodopsin



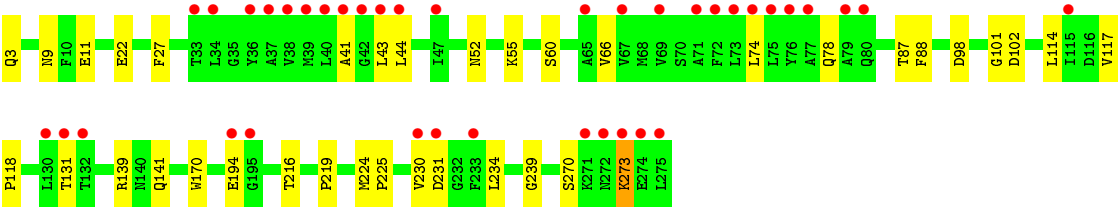
#### • Molecule 1: Sodium pumping rhodopsin



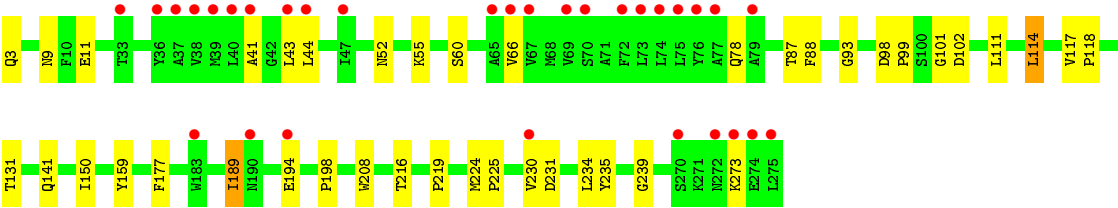
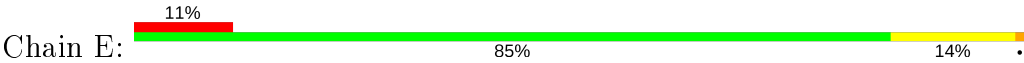
#### • Molecule 1: Sodium pumping rhodopsin







● 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, $\alpha$ , $\beta$ , $\gamma$	131.87Å 240.32Å 135.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 48.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 99.9 (48.16-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.168 , 0.195 0.172 , 0.199	Depositor DCC
$R_{free}$ test set	7215 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 73.8	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	0.97	EDS
Total number of atoms	12886	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NA, OLC, LFA, RET, 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	0.63	0/2251	0.61	0/3060
1	B	0.63	0/2252	0.61	0/3062
1	C	0.63	0/2244	0.61	0/3051
1	D	0.62	0/2250	0.62	0/3059
1	E	0.63	0/2252	0.61	0/3062
All	All	0.63	0/11249	0.61	0/15294

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2193	0	2162	26	0
1	B	2194	0	2165	51	0
1	C	2186	0	2155	34	0
1	D	2192	0	2160	37	0
1	E	2194	0	2167	38	0
2	A	171	0	249	4	0
2	B	111	0	157	3	0
2	C	181	0	245	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	136	0	192	5	0
2	E	147	0	209	7	0
3	A	78	0	151	0	0
3	B	58	0	113	5	0
3	C	65	0	127	7	0
3	D	98	0	198	4	0
3	E	65	0	127	3	0
4	A	20	0	28	2	0
4	B	20	0	28	3	0
4	C	20	0	28	3	0
4	D	20	0	28	2	0
4	E	20	0	28	4	0
5	A	20	0	27	3	0
5	B	20	0	27	2	0
5	C	20	0	27	4	0
5	D	20	0	27	3	0
5	E	20	0	27	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
7	A	123	0	0	6	0
7	B	123	0	0	6	0
7	C	123	0	0	7	0
7	D	107	0	0	7	0
7	E	131	0	0	11	0
All	All	12886	0	12852	200	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 8.

The worst 5 of 200 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)
7:B:494:HOH:O	1:C:99:PRO:HG2	1.56	1.03
1:B:272:ASN:N	1:B:272:ASN:HD22	1.56	1.03
1:C:55:LYS:NZ	7:C:401:HOH:O	1.94	0.98
1:B:272:ASN:H	1:B:272:ASN:HD22	0.92	0.89
1:D:52:ASN:O	1:D:273:LYS:HG3	1.73	0.89

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	275/273 (101%)	269 (98%)	6 (2%)	0	100	100
1	B	275/273 (101%)	267 (97%)	8 (3%)	0	100	100
1	C	274/273 (100%)	268 (98%)	6 (2%)	0	100	100
1	D	275/273 (101%)	270 (98%)	5 (2%)	0	100	100
1	E	275/273 (101%)	269 (98%)	6 (2%)	0	100	100
All	All	1374/1365 (101%)	1343 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/234 (99%)	229 (99%)	3 (1%)	69	74
1	B	234/234 (100%)	231 (99%)	3 (1%)	69	74
1	C	231/234 (99%)	228 (99%)	3 (1%)	69	74
1	D	232/234 (99%)	230 (99%)	2 (1%)	78	83
1	E	233/234 (100%)	230 (99%)	3 (1%)	69	74
All	All	1162/1170 (99%)	1148 (99%)	14 (1%)	71	76

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	189	ILE
1	C	230	VAL
1	E	114	LEU
1	B	272	ASN
1	D	273	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	B	141	GLN
1	B	272	ASN
1	C	3	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 96 ligands modelled in this entry, 10 are monoatomic - leaving 86 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	E	308	-	14,14,24	1.16	1 (7%)	15,15,25	0.97	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	E	310	-	21,21,24	1.03	1 (4%)	22,22,25	0.86	1 (4%)
2	OLC	A	317	-	16,19,24	0.26	0	15,19,25	0.55	0
2	OLC	E	307	-	14,14,24	1.21	1 (7%)	15,15,25	1.04	1 (6%)
3	LFA	B	302	-	19,19,19	0.12	0	18,18,18	0.09	0
2	OLC	B	303	-	24,24,24	0.94	1 (4%)	25,25,25	0.85	1 (4%)
2	OLC	A	307	-	6,6,24	0.27	0	5,5,25	0.44	0
2	OLC	C	309	-	15,15,24	1.16	1 (6%)	16,16,25	0.85	1 (6%)
2	OLC	A	302	-	21,21,24	0.96	1 (4%)	22,22,25	0.90	2 (9%)
2	OLC	D	304	-	24,24,24	0.93	1 (4%)	25,25,25	0.82	1 (4%)
3	LFA	E	313	-	13,13,19	0.08	0	12,12,18	0.05	0
3	LFA	B	309	-	7,7,19	0.11	0	6,6,18	0.06	0
3	LFA	B	308	-	8,8,19	0.11	0	7,7,18	0.07	0
2	OLC	C	305	-	22,22,24	0.94	1 (4%)	23,23,25	0.92	1 (4%)
3	LFA	E	312	-	7,7,19	0.10	0	6,6,18	0.07	0
2	OLC	D	307	-	13,13,24	1.21	1 (7%)	14,14,25	0.95	2 (14%)
3	LFA	C	314	-	5,5,19	0.13	0	4,4,18	0.10	0
2	OLC	D	302	-	15,15,24	1.25	1 (6%)	16,16,25	1.09	2 (12%)
2	OLC	D	306	-	14,17,24	0.26	0	13,17,25	0.54	0
5	RET	D	317	1	20,20,21	2.22	3 (15%)	27,27,28	1.22	2 (7%)
3	LFA	D	313	-	16,16,19	0.07	0	15,15,18	0.07	0
5	RET	A	320	1	20,20,21	2.39	4 (20%)	27,27,28	1.19	2 (7%)
3	LFA	A	309	-	6,6,19	0.12	0	5,5,18	0.08	0
2	OLC	A	308	-	15,15,24	1.22	1 (6%)	16,16,25	1.01	1 (6%)
4	BOG	B	312	-	20,20,20	0.55	0	25,25,25	0.67	0
2	OLC	B	306	-	15,15,24	1.13	1 (6%)	16,16,25	1.02	2 (12%)
4	BOG	D	316	-	20,20,20	0.52	0	25,25,25	0.63	0
3	LFA	E	314	-	3,3,19	0.23	0	2,2,18	0.44	0
2	OLC	E	305	-	15,15,24	0.28	0	14,14,25	0.49	0
2	OLC	A	306	-	14,14,24	1.20	1 (7%)	15,15,25	1.08	2 (13%)
3	LFA	B	310	-	9,9,19	0.10	0	8,8,18	0.07	0
3	LFA	C	312	-	7,7,19	0.10	0	6,6,18	0.07	0
3	LFA	E	303	-	19,19,19	0.13	0	18,18,18	0.10	0
3	LFA	B	311	-	6,6,19	0.11	0	5,5,18	0.08	0
2	OLC	D	309	-	24,24,24	0.93	1 (4%)	25,25,25	0.80	1 (4%)
2	OLC	E	306	-	19,19,24	1.04	1 (5%)	20,20,25	1.00	2 (10%)
3	LFA	B	314	-	3,3,19	0.23	0	2,2,18	0.44	0
2	OLC	B	301	-	21,21,24	0.99	1 (4%)	22,22,25	0.89	1 (4%)
5	RET	B	313	1	20,20,21	2.36	4 (20%)	27,27,28	1.19	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	C	302	-	19,19,24	1.07	1 (5%)	20,20,25	0.91	2 (10%)
2	OLC	D	308	-	6,6,24	0.33	0	5,5,25	0.36	0
2	OLC	A	301	-	8,8,24	0.35	0	6,7,25	0.51	0
2	OLC	E	311	-	19,19,24	1.07	1 (5%)	20,20,25	0.93	1 (5%)
2	OLC	C	301	-	20,20,24	1.01	1 (5%)	21,21,25	0.95	1 (4%)
3	LFA	C	304	-	19,19,19	0.10	0	18,18,18	0.09	0
5	RET	C	317	1	20,20,21	2.32	3 (15%)	27,27,28	1.12	1 (3%)
3	LFA	D	311	-	19,19,19	0.07	0	18,18,18	0.05	0
3	LFA	D	314	-	6,6,19	0.12	0	5,5,18	0.08	0
2	OLC	C	318	-	17,17,24	1.11	1 (5%)	18,18,25	1.01	1 (5%)
2	OLC	B	304	-	19,19,24	1.05	1 (5%)	20,20,25	0.96	2 (10%)
2	OLC	C	307	-	19,19,24	1.05	1 (5%)	20,20,25	0.92	1 (5%)
3	LFA	C	313	-	19,19,19	0.07	0	18,18,18	0.04	0
2	OLC	A	304	-	12,12,24	1.29	1 (8%)	13,13,25	1.22	2 (15%)
5	RET	E	317	1	20,20,21	2.29	4 (20%)	27,27,28	1.25	2 (7%)
2	OLC	E	302	-	24,24,24	0.94	1 (4%)	25,25,25	0.88	1 (4%)
2	OLC	A	316	-	15,18,24	0.22	0	14,18,25	0.55	0
2	OLC	B	307	-	6,6,24	0.44	0	5,5,25	0.58	0
2	OLC	A	303	-	24,24,24	0.96	1 (4%)	25,25,25	0.85	1 (4%)
2	OLC	E	304	-	7,7,24	0.30	0	6,6,25	0.37	0
3	LFA	A	312	-	3,3,19	0.24	0	2,2,18	0.44	0
2	OLC	C	310	-	6,6,24	0.29	0	5,5,25	0.39	0
3	LFA	D	301	-	19,19,19	0.12	0	18,18,18	0.11	0
3	LFA	C	311	-	6,6,19	0.13	0	5,5,18	0.07	0
3	LFA	A	311	-	7,7,19	0.10	0	6,6,18	0.07	0
3	LFA	A	310	-	7,7,19	0.11	0	6,6,18	0.08	0
3	LFA	D	315	-	5,5,19	0.13	0	4,4,18	0.11	0
3	LFA	E	301	-	13,13,19	0.07	0	12,12,18	0.06	0
3	LFA	A	313	-	5,5,19	0.14	0	4,4,18	0.10	0
2	OLC	C	308	-	21,21,24	1.02	1 (4%)	22,22,25	0.92	1 (4%)
3	LFA	A	318	-	19,19,19	0.12	0	18,18,18	0.10	0
3	LFA	E	315	-	4,4,19	0.15	0	3,3,18	0.22	0
3	LFA	A	319	-	8,8,19	0.11	0	7,7,18	0.07	0
2	OLC	C	306	-	21,21,24	1.01	1 (4%)	22,22,25	0.92	1 (4%)
3	LFA	D	310	-	19,19,19	0.08	0	18,18,18	0.03	0
2	OLC	D	303	-	12,12,24	1.31	1 (8%)	13,13,25	1.03	1 (7%)
4	BOG	A	315	-	20,20,20	0.54	0	25,25,25	0.59	0
2	OLC	C	303	-	11,11,24	1.42	1 (9%)	12,12,25	1.05	1 (8%)
2	OLC	E	309	-	5,5,24	0.31	0	4,4,25	0.32	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LFA	D	312	-	7,7,19	0.11	0	6,6,18	0.07	0
2	OLC	B	305	-	20,20,24	1.03	1 (5%)	21,21,25	0.95	1 (4%)
2	OLC	A	305	-	24,24,24	0.99	1 (4%)	25,25,25	0.89	1 (4%)
3	LFA	C	315	-	3,3,19	0.24	0	2,2,18	0.42	0
2	OLC	D	305	-	17,17,24	1.10	1 (5%)	18,18,25	1.15	2 (11%)
3	LFA	A	314	-	15,15,19	0.08	0	14,14,18	0.06	0
4	BOG	E	316	-	20,20,20	0.54	0	25,25,25	0.55	0
4	BOG	C	316	-	20,20,20	0.53	0	25,25,25	0.61	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	E	308	-	-	10/14/14/24	-
2	OLC	E	310	-	-	7/21/21/24	-
2	OLC	A	317	-	-	8/15/17/24	-
2	OLC	E	307	-	-	7/14/14/24	-
3	LFA	B	302	-	-	6/17/17/17	-
2	OLC	B	303	-	-	13/24/24/24	-
2	OLC	A	307	-	-	3/4/4/24	-
2	OLC	C	309	-	-	6/15/15/24	-
2	OLC	A	302	-	-	10/21/21/24	-
2	OLC	D	304	-	-	10/24/24/24	-
3	LFA	E	313	-	-	4/11/11/17	-
3	LFA	B	309	-	-	3/5/5/17	-
3	LFA	B	308	-	-	2/6/6/17	-
2	OLC	C	305	-	-	11/22/22/24	-
3	LFA	E	312	-	-	2/5/5/17	-
2	OLC	D	307	-	-	7/13/13/24	-
3	LFA	C	314	-	-	0/3/3/17	-
2	OLC	D	302	-	-	8/15/15/24	-
2	OLC	D	306	-	-	5/13/15/24	-
5	RET	D	317	1	-	2/13/30/31	0/1/1/1
3	LFA	D	313	-	-	10/14/14/17	-
5	RET	A	320	1	-	2/13/30/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	A	309	-	-	2/4/4/17	-
2	OLC	A	308	-	-	6/15/15/24	-
4	BOG	B	312	-	-	5/11/31/31	0/1/1/1
2	OLC	B	306	-	-	3/15/15/24	-
4	BOG	D	316	-	-	5/11/31/31	0/1/1/1
3	LFA	E	314	-	-	1/1/1/17	-
2	OLC	E	305	-	-	7/13/13/24	-
2	OLC	A	306	-	-	8/14/14/24	-
3	LFA	B	310	-	-	3/7/7/17	-
3	LFA	C	312	-	-	5/5/5/17	-
3	LFA	E	303	-	-	11/17/17/17	-
3	LFA	B	311	-	-	1/4/4/17	-
2	OLC	D	309	-	-	13/24/24/24	-
2	OLC	E	306	-	-	5/19/19/24	-
3	LFA	B	314	-	-	0/1/1/17	-
2	OLC	B	301	-	-	10/21/21/24	-
5	RET	B	313	1	-	2/13/30/31	0/1/1/1
2	OLC	C	302	-	-	9/19/19/24	-
2	OLC	D	308	-	-	3/4/4/24	-
2	OLC	A	301	-	-	4/6/6/24	-
2	OLC	E	311	-	-	12/19/19/24	-
2	OLC	C	301	-	-	7/20/20/24	-
3	LFA	C	304	-	-	12/17/17/17	-
5	RET	C	317	1	-	2/13/30/31	0/1/1/1
3	LFA	D	311	-	-	9/17/17/17	-
3	LFA	D	314	-	-	3/4/4/17	-
2	OLC	C	318	-	-	6/17/17/24	-
2	OLC	B	304	-	-	5/19/19/24	-
2	OLC	C	307	-	-	4/19/19/24	-
3	LFA	C	313	-	-	13/17/17/17	-
2	OLC	A	304	-	-	0/12/12/24	-
5	RET	E	317	1	-	3/13/30/31	0/1/1/1
2	OLC	E	302	-	-	15/24/24/24	-
2	OLC	A	316	-	-	6/14/16/24	-
2	OLC	B	307	-	-	2/4/4/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	303	-	-	12/24/24/24	-
2	OLC	E	304	-	-	2/5/5/24	-
3	LFA	A	312	-	-	0/1/1/17	-
2	OLC	C	310	-	-	3/4/4/24	-
3	LFA	D	301	-	-	7/17/17/17	-
3	LFA	C	311	-	-	2/4/4/17	-
3	LFA	A	311	-	-	2/5/5/17	-
3	LFA	A	310	-	-	1/5/5/17	-
3	LFA	D	315	-	-	1/3/3/17	-
3	LFA	E	301	-	-	4/11/11/17	-
3	LFA	A	313	-	-	2/3/3/17	-
2	OLC	C	308	-	-	11/21/21/24	-
3	LFA	A	318	-	-	10/17/17/17	-
3	LFA	E	315	-	-	1/2/2/17	-
3	LFA	A	319	-	-	3/6/6/17	-
2	OLC	C	306	-	-	7/21/21/24	-
3	LFA	D	310	-	-	11/17/17/17	-
2	OLC	D	303	-	-	4/12/12/24	-
4	BOG	A	315	-	-	3/11/31/31	0/1/1/1
2	OLC	C	303	-	-	5/11/11/24	-
2	OLC	E	309	-	-	1/3/3/24	-
3	LFA	D	312	-	-	4/5/5/17	-
2	OLC	B	305	-	-	11/20/20/24	-
2	OLC	A	305	-	-	17/24/24/24	-
3	LFA	C	315	-	-	1/1/1/17	-
2	OLC	D	305	-	-	7/17/17/24	-
3	LFA	A	314	-	-	9/13/13/17	-
4	BOG	E	316	-	-	9/11/31/31	0/1/1/1
4	BOG	C	316	-	-	3/11/31/31	0/1/1/1

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	320	RET	C14-C13	8.45	1.40	1.33
5	B	313	RET	C14-C13	8.41	1.40	1.33
5	C	317	RET	C14-C13	8.09	1.40	1.33
5	E	317	RET	C14-C13	7.98	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	317	RET	C14-C13	7.62	1.39	1.33

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	317	RET	C19-C9-C10	-4.18	117.06	122.92
5	D	317	RET	C19-C9-C10	-4.16	117.10	122.92
5	B	313	RET	C19-C9-C10	-4.13	117.13	122.92
5	A	320	RET	C19-C9-C10	-4.00	117.33	122.92
5	C	317	RET	C19-C9-C10	-3.72	117.71	122.92

There are no chirality outliers.

5 of 491 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	308	OLC	O20-C21-C22-C24
2	E	308	OLC	O20-C21-C22-O23
2	E	307	OLC	O20-C21-C22-O23
2	A	302	OLC	C21-C22-C24-O25
2	D	304	OLC	C21-C22-C24-O25

There are no ring outliers.

32 monomers are involved in 64 short contacts:

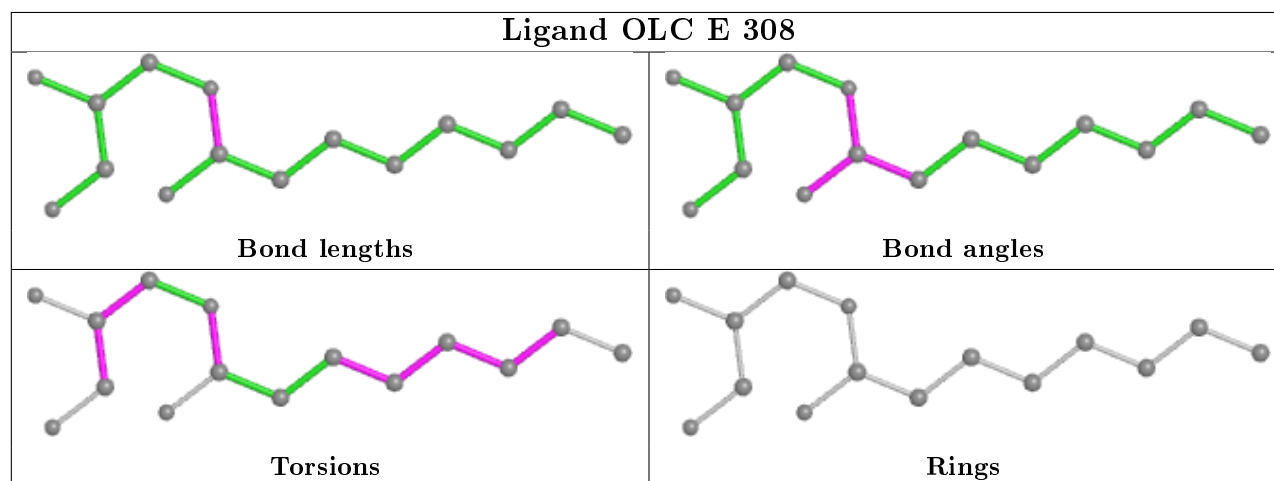
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	308	OLC	2	0
2	E	310	OLC	1	0
2	B	303	OLC	1	0
2	A	302	OLC	1	0
2	D	304	OLC	1	0
3	B	308	LFA	2	0
2	C	305	OLC	3	0
5	D	317	RET	3	0
3	D	313	LFA	3	0
5	A	320	RET	3	0
4	B	312	BOG	3	0
4	D	316	BOG	2	0
2	E	305	OLC	2	0
2	D	309	OLC	3	0
3	B	314	LFA	3	0
2	B	301	OLC	2	0

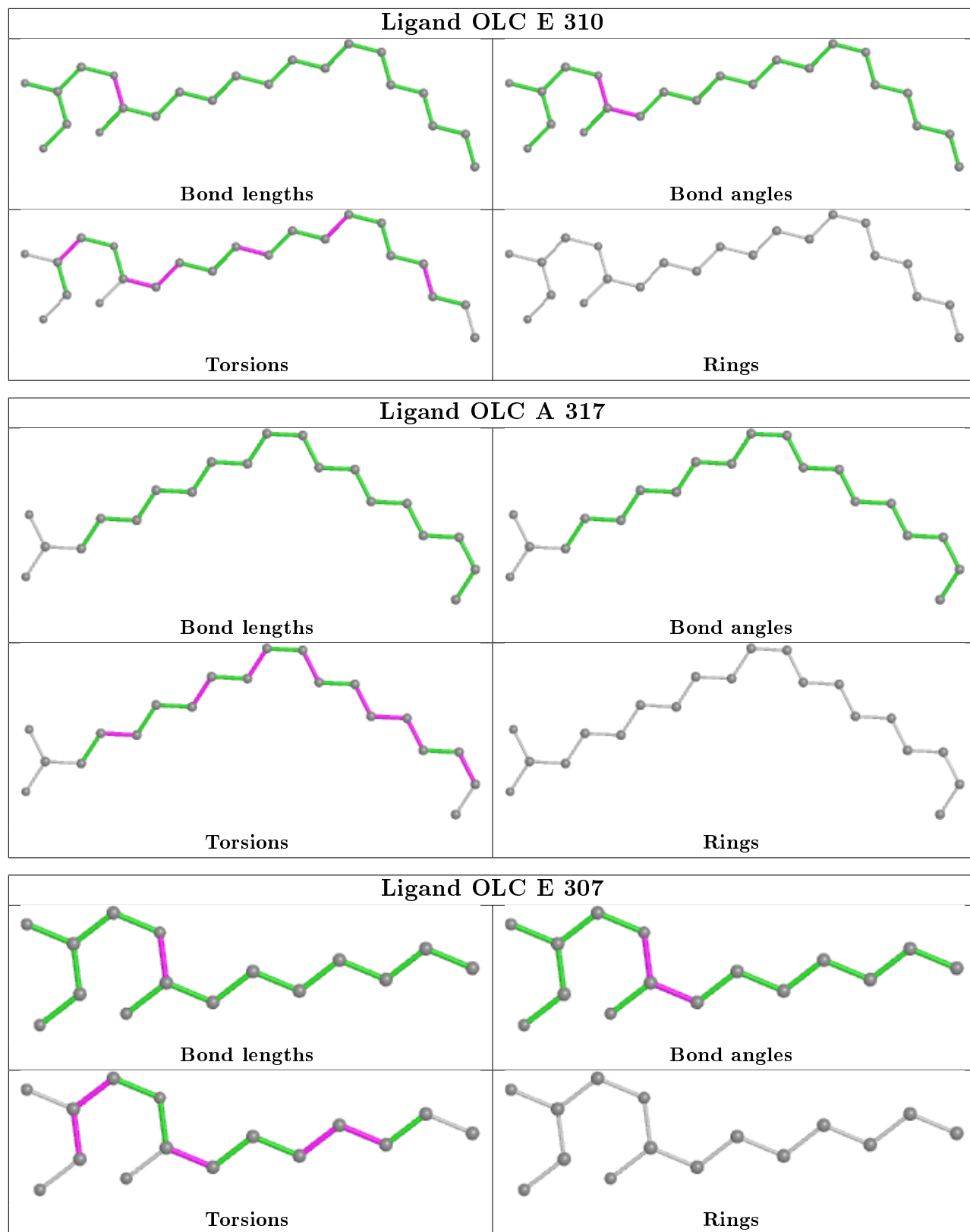
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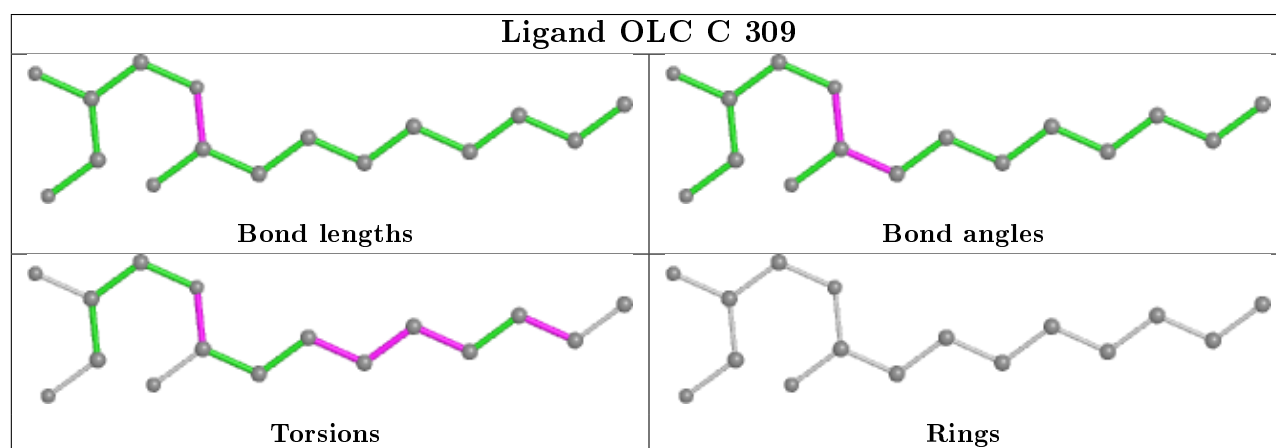
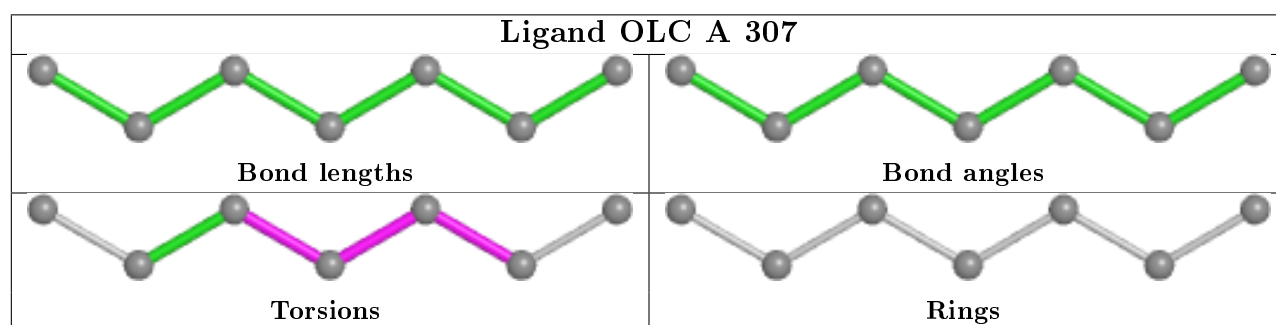
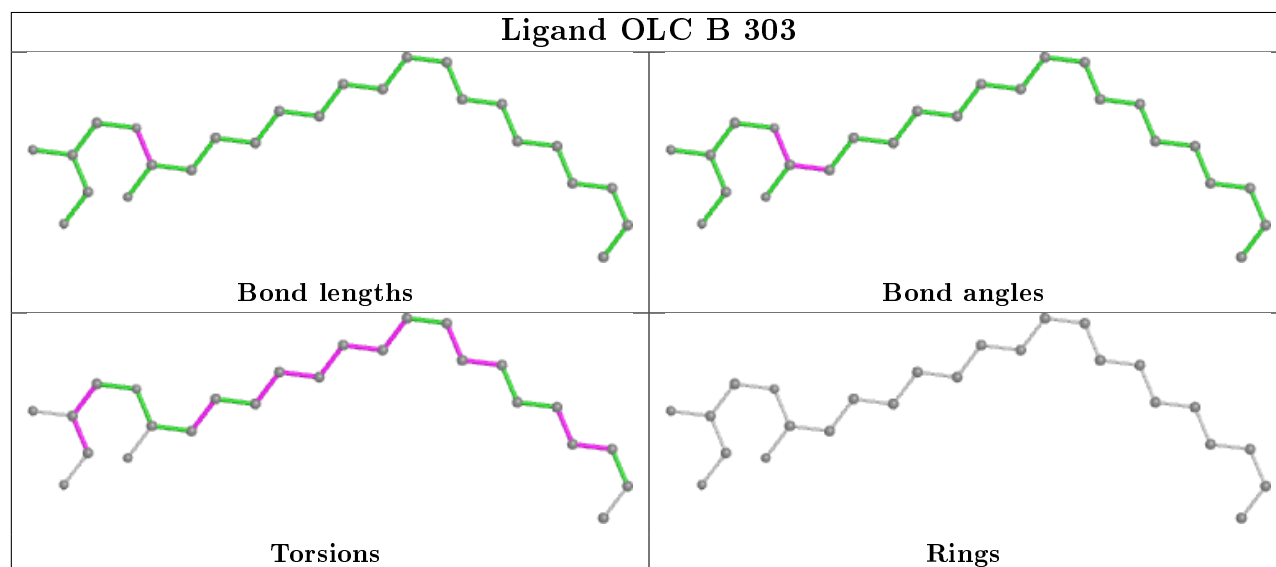
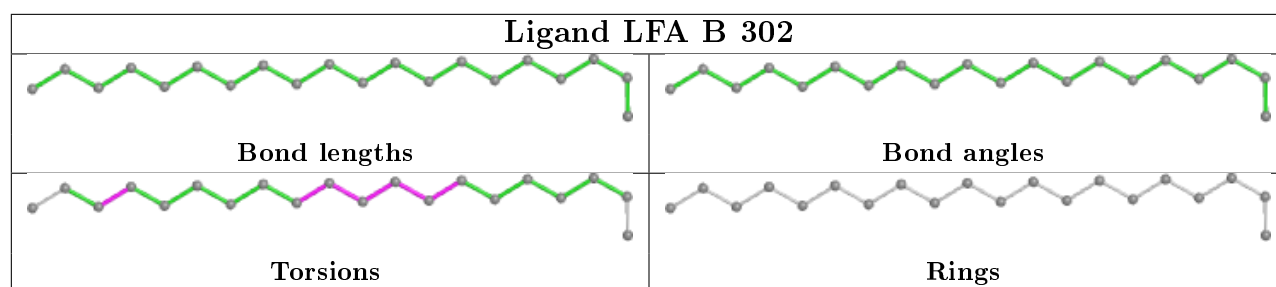
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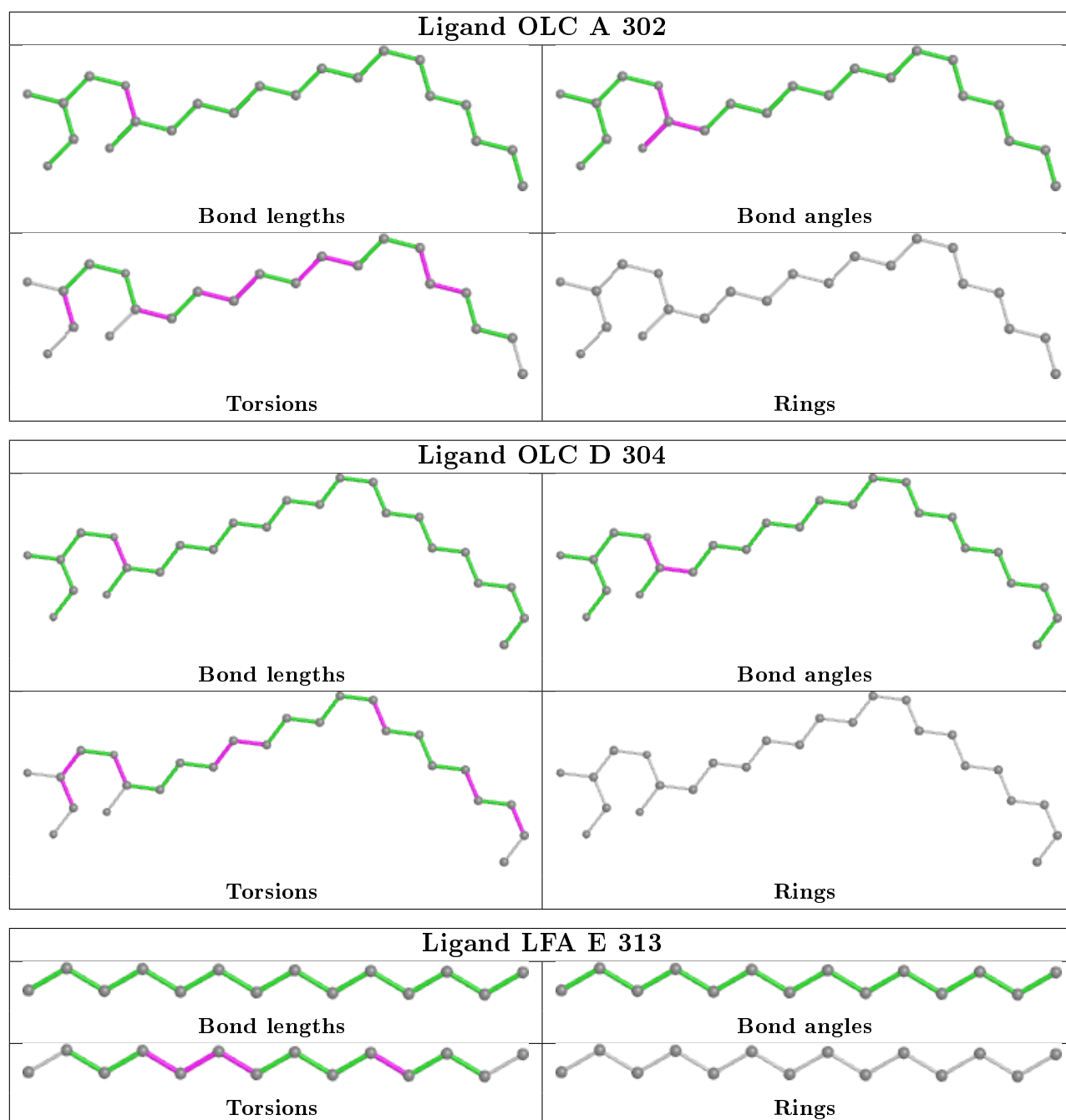
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	313	RET	2	0
3	C	304	LFA	2	0
5	C	317	RET	4	0
2	C	318	OLC	4	0
3	C	313	LFA	1	0
5	E	317	RET	3	0
2	E	302	OLC	2	0
2	A	316	OLC	1	0
2	A	303	OLC	2	0
3	D	301	LFA	1	0
3	C	311	LFA	4	0
3	E	301	LFA	3	0
4	A	315	BOG	2	0
2	D	305	OLC	1	0
4	E	316	BOG	4	0
4	C	316	BOG	3	0

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

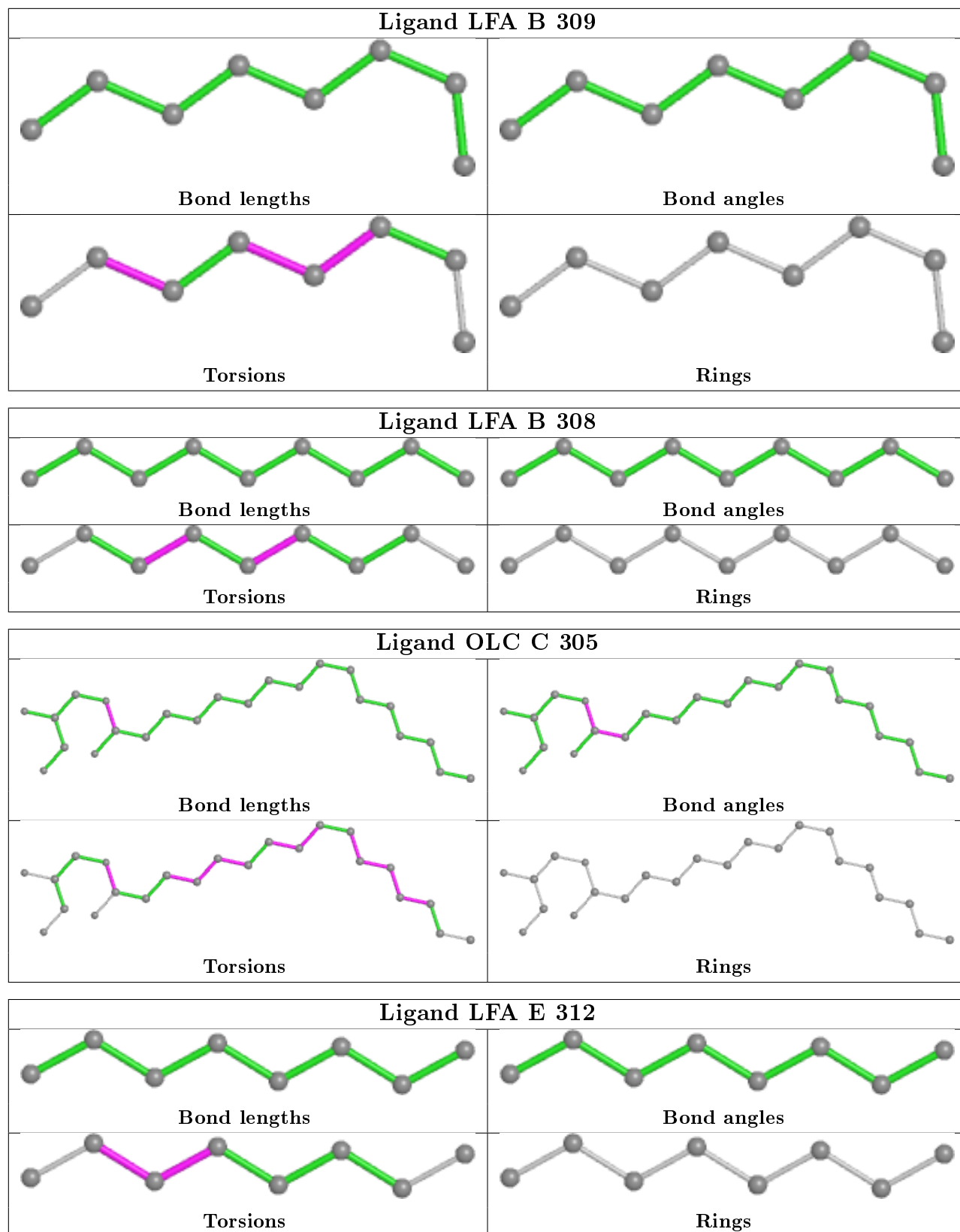


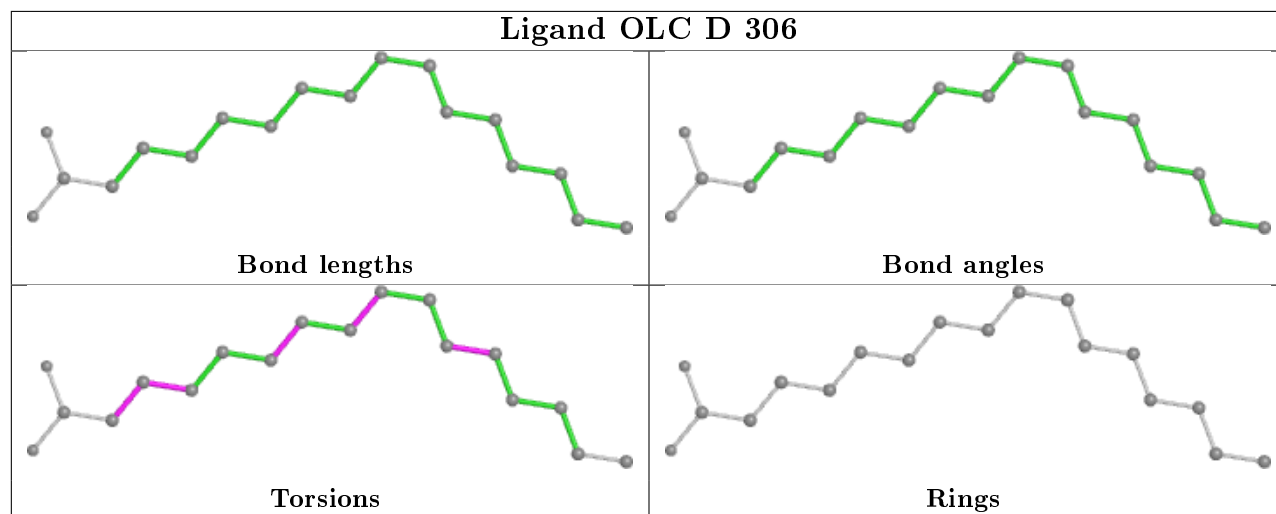
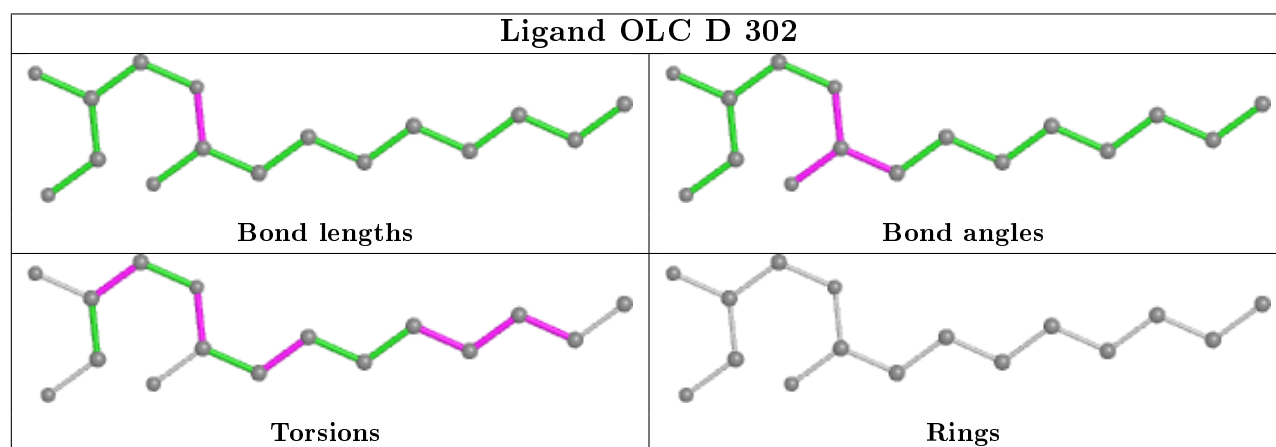
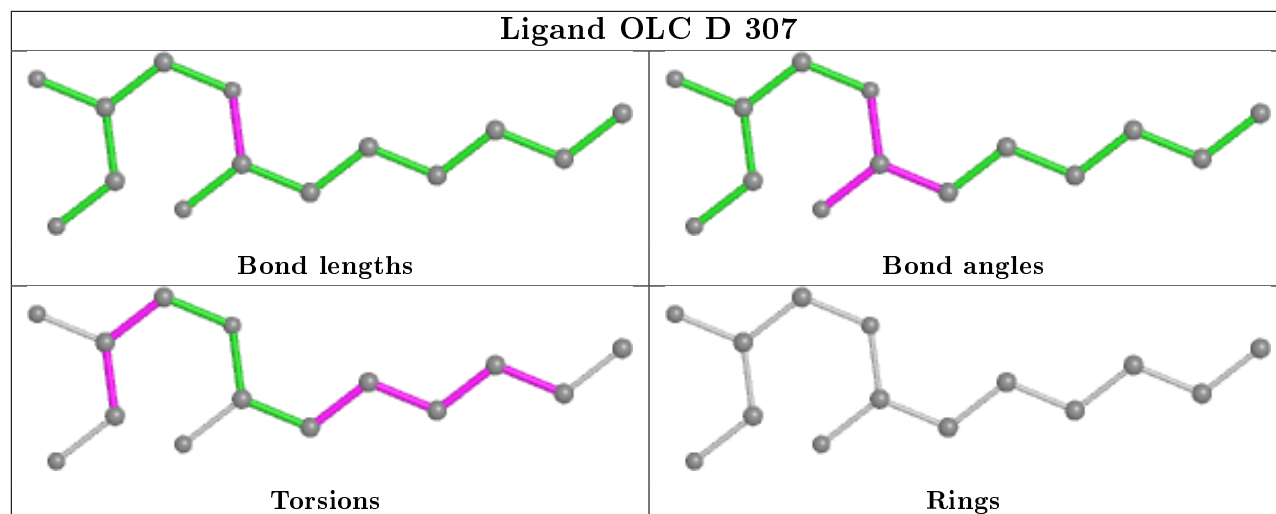


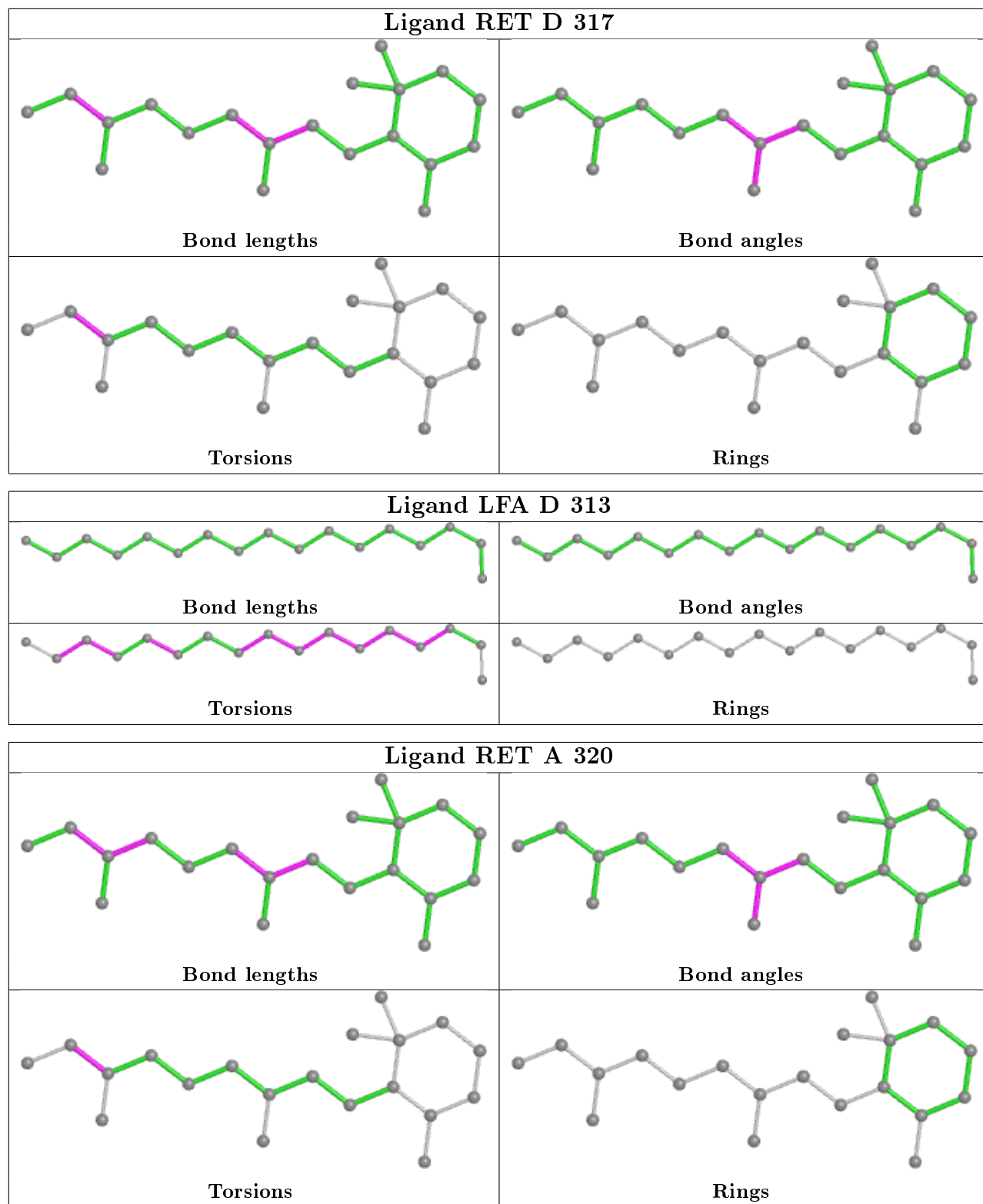


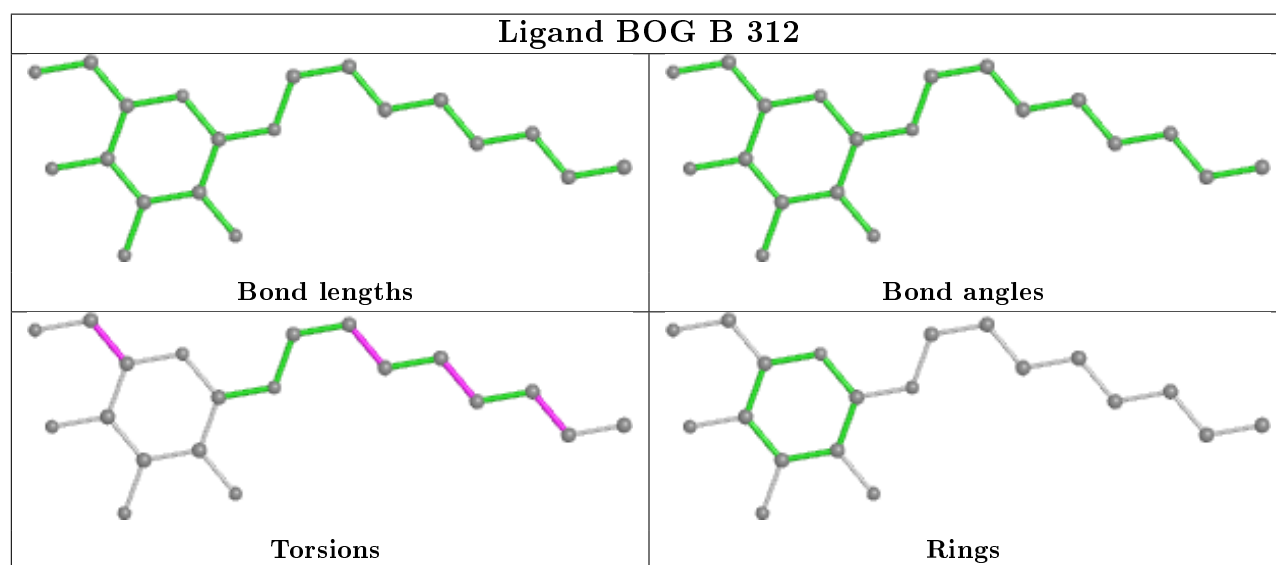
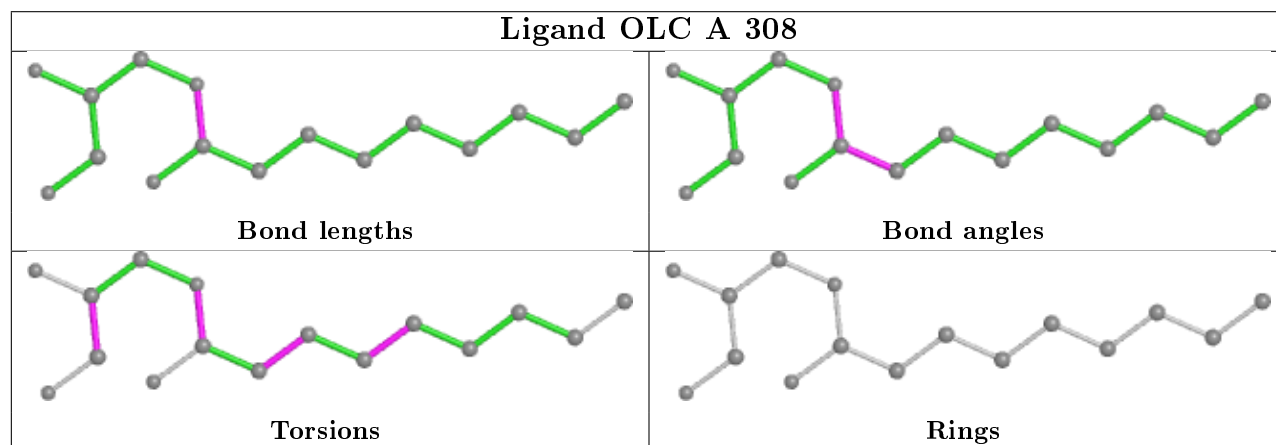
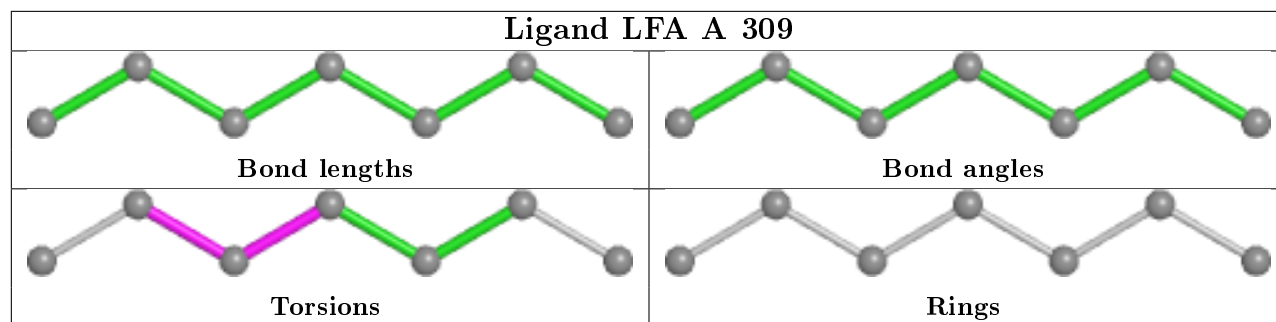


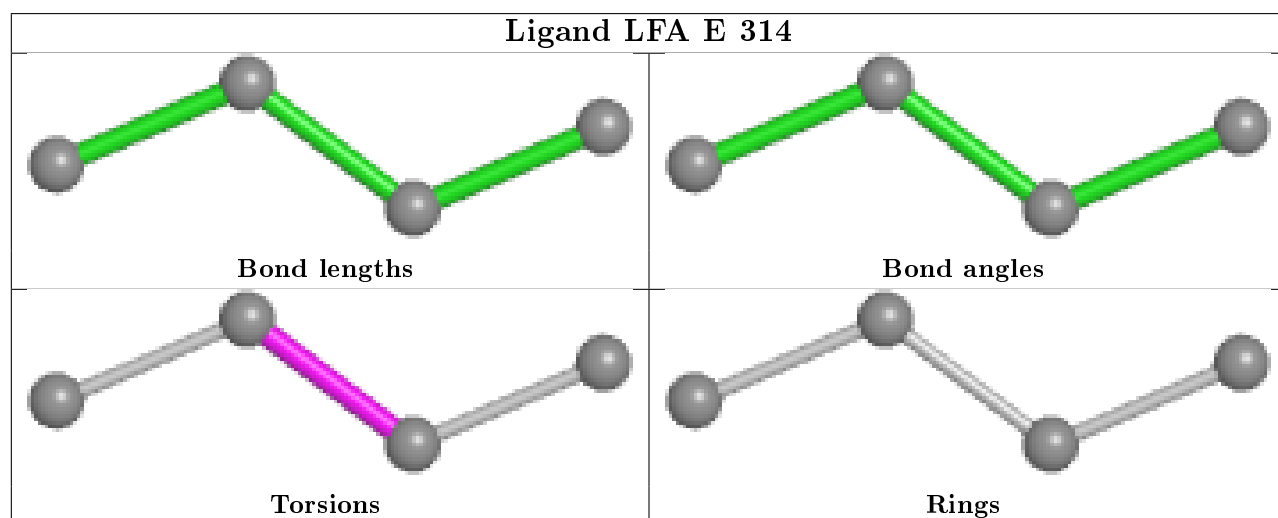
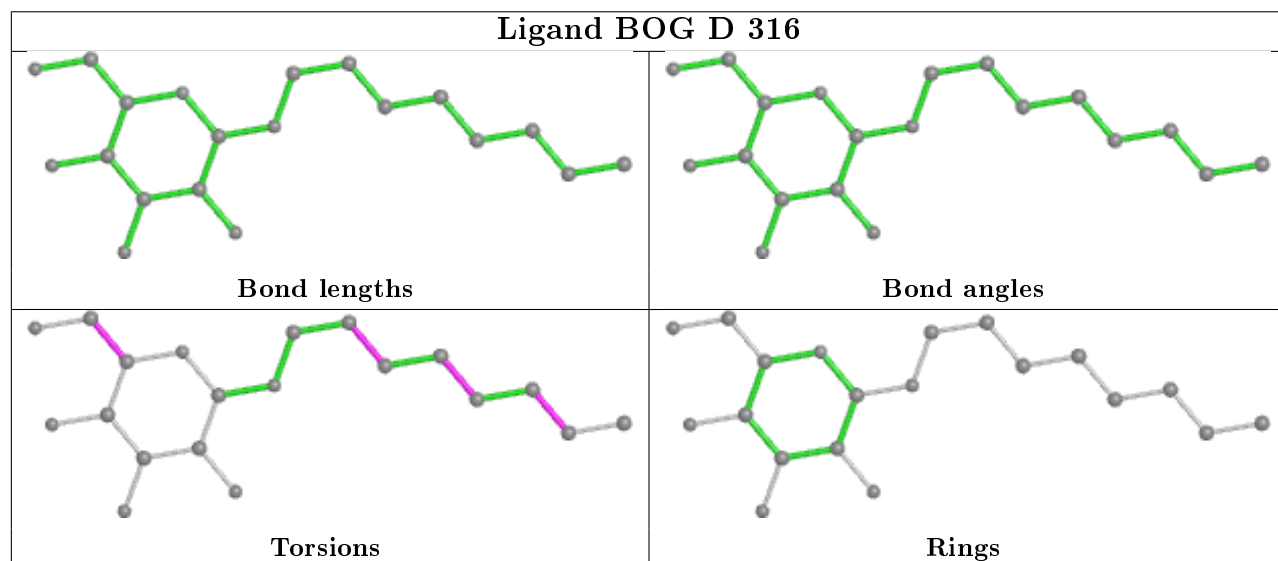
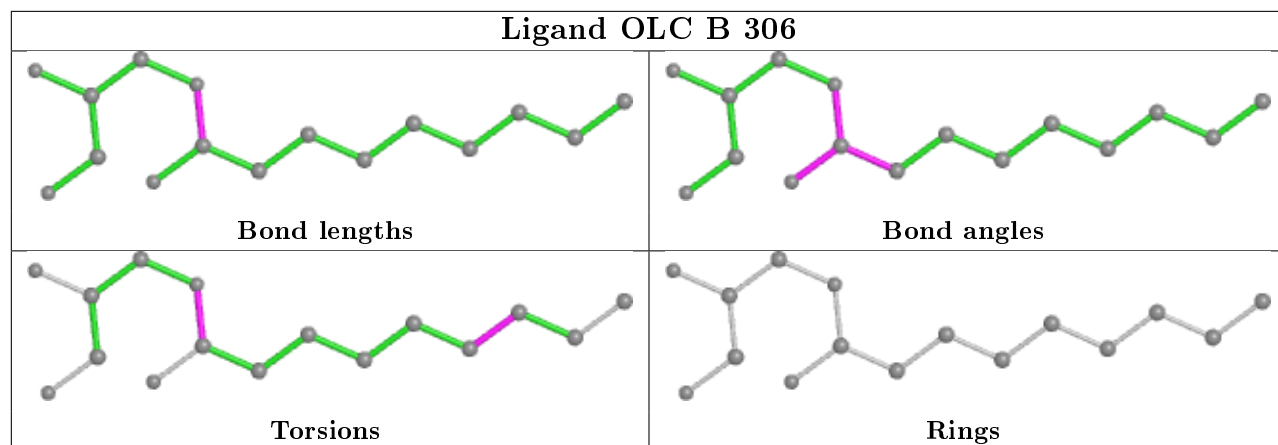


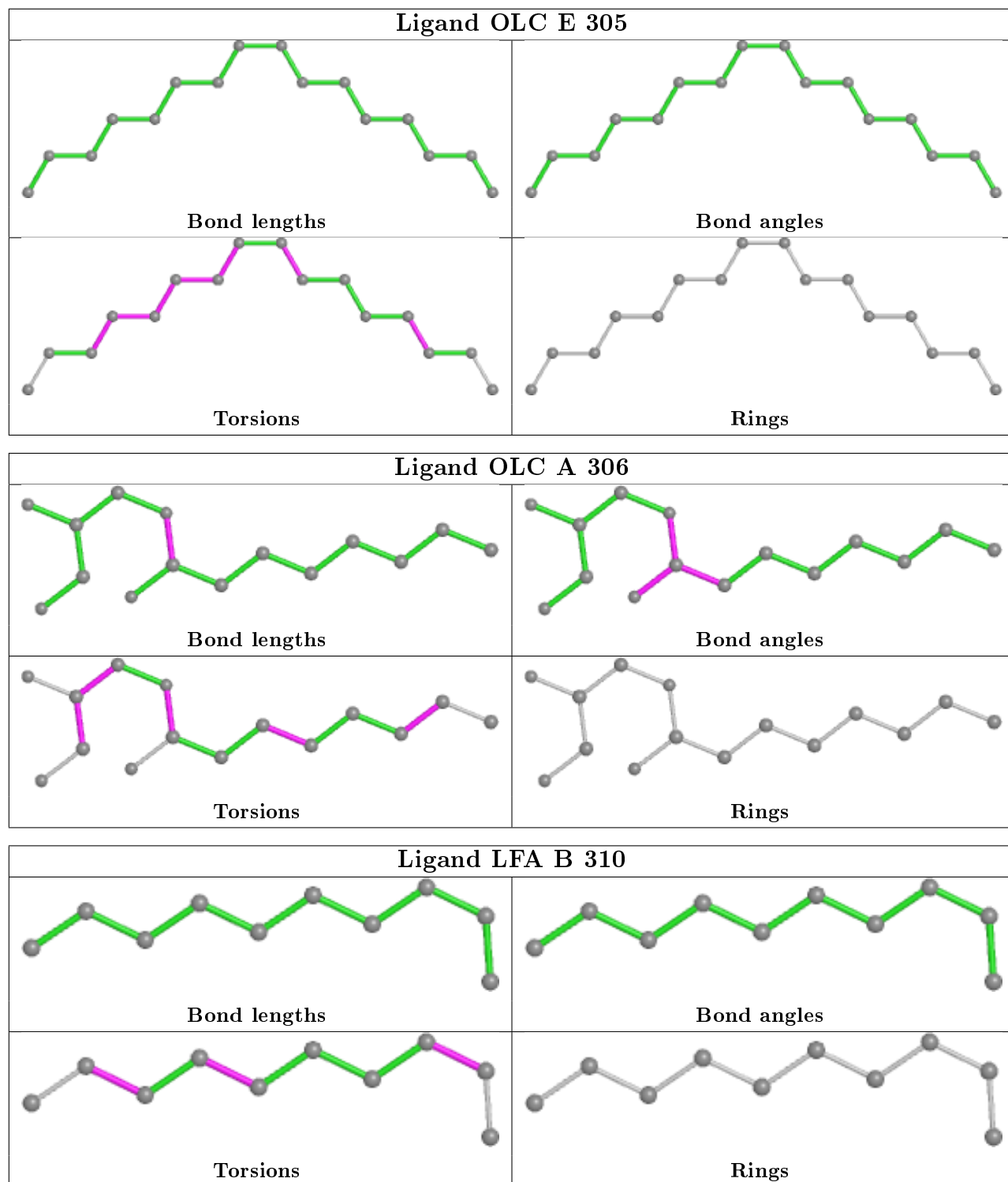


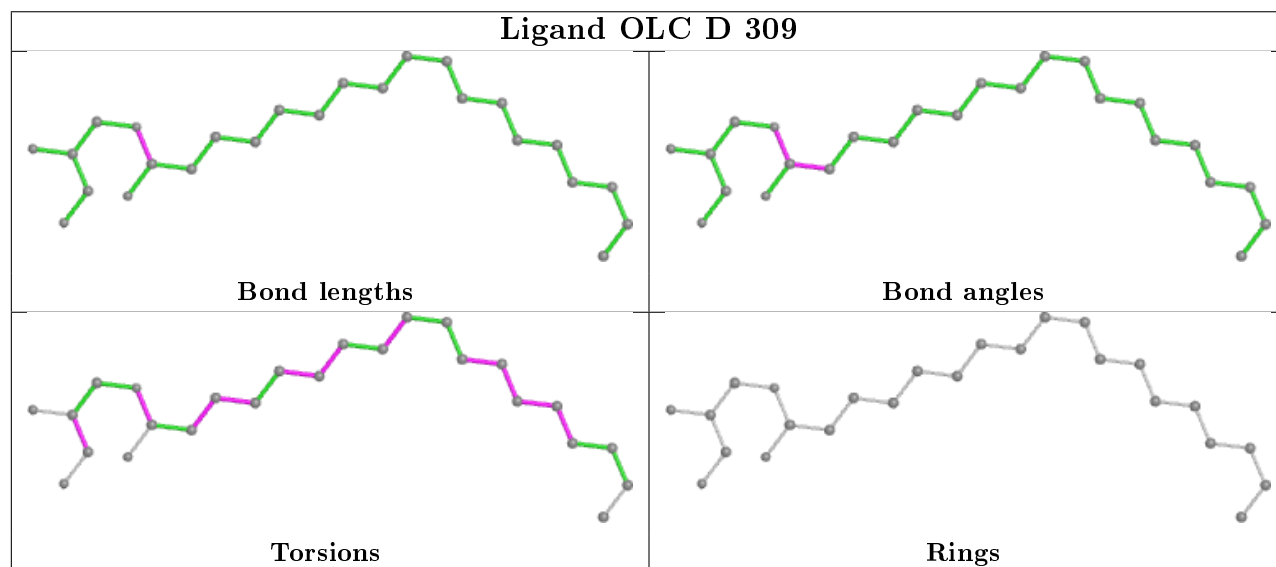
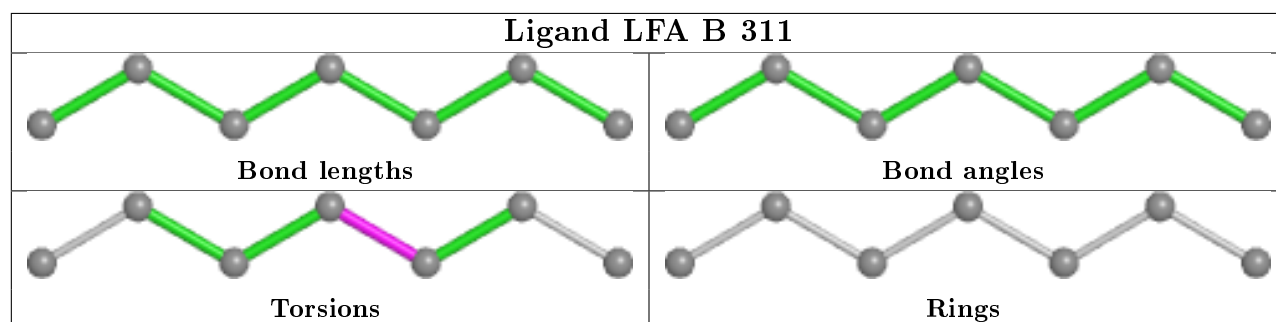
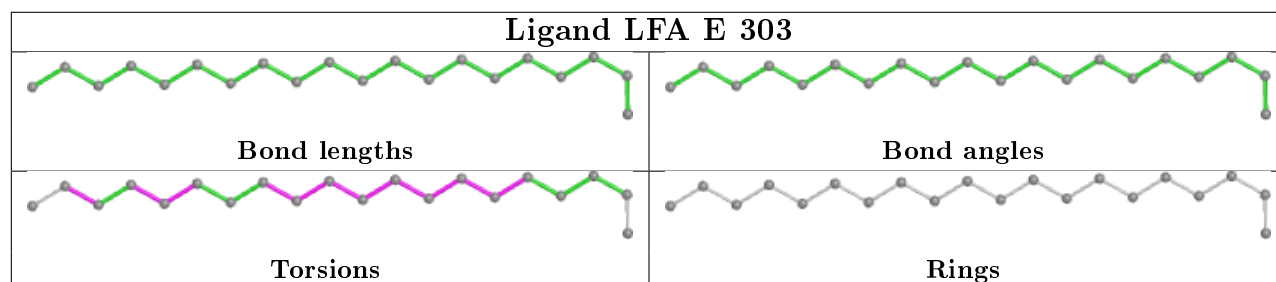
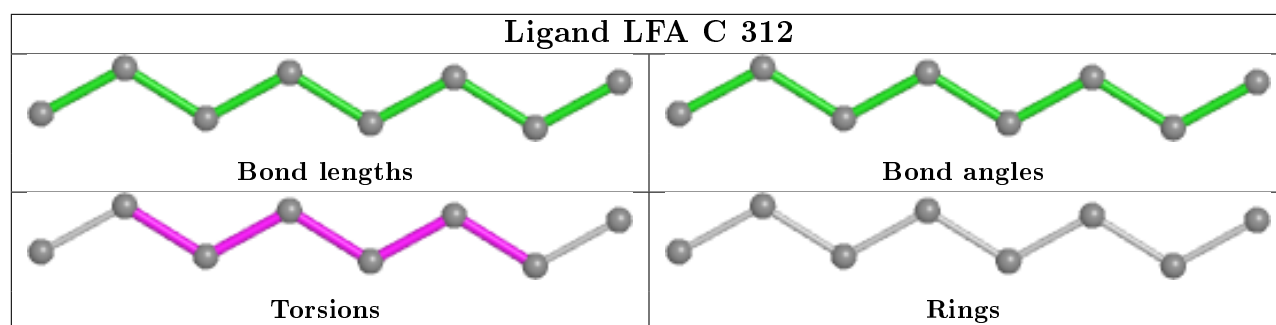


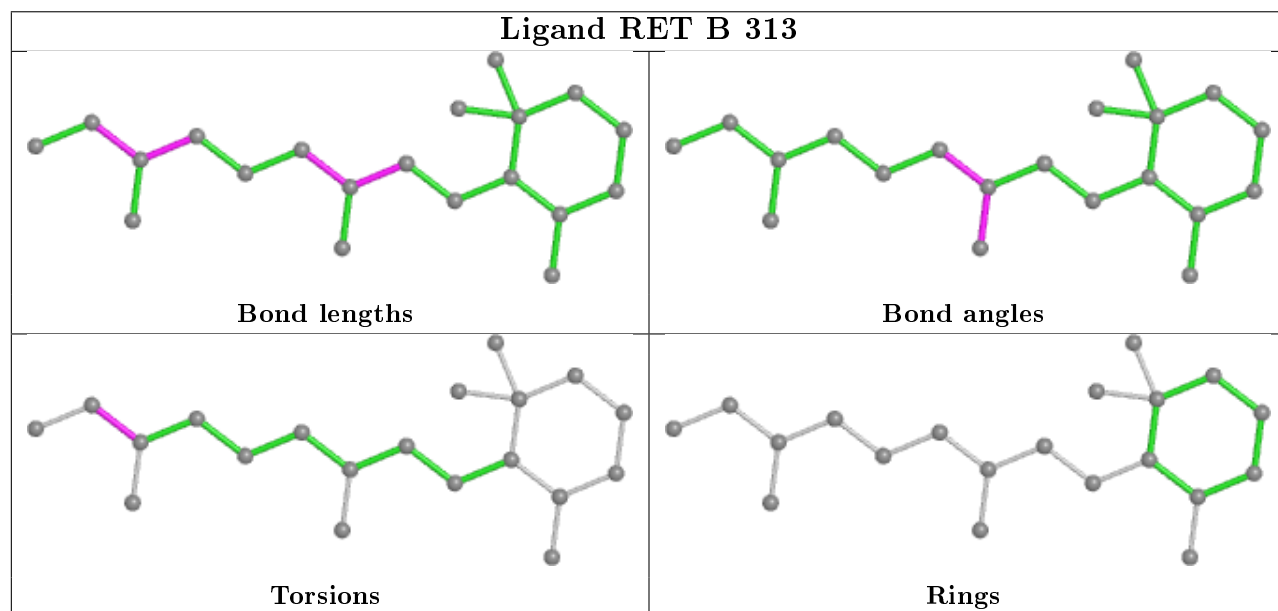
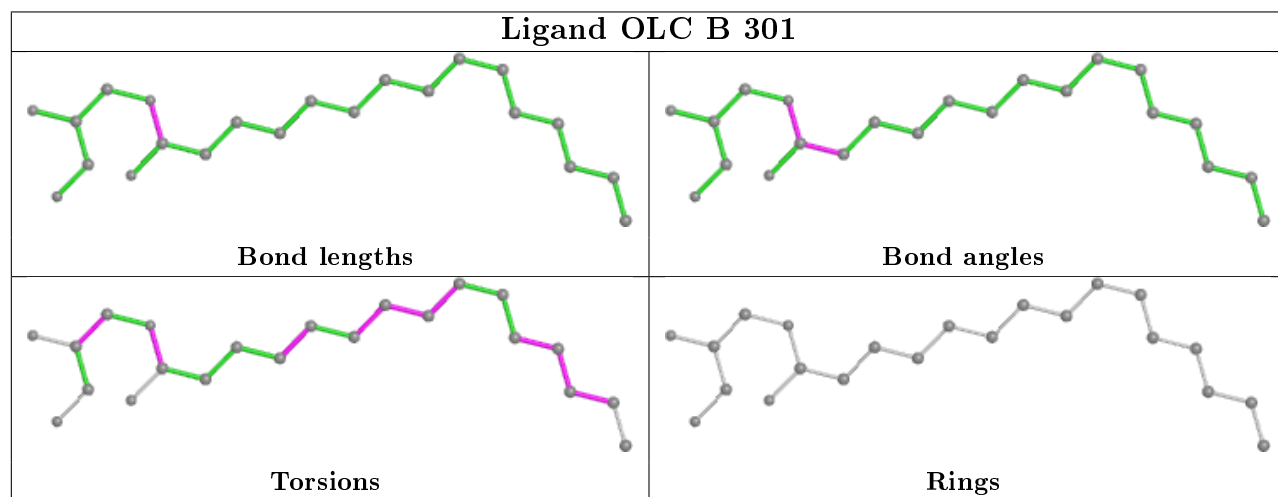
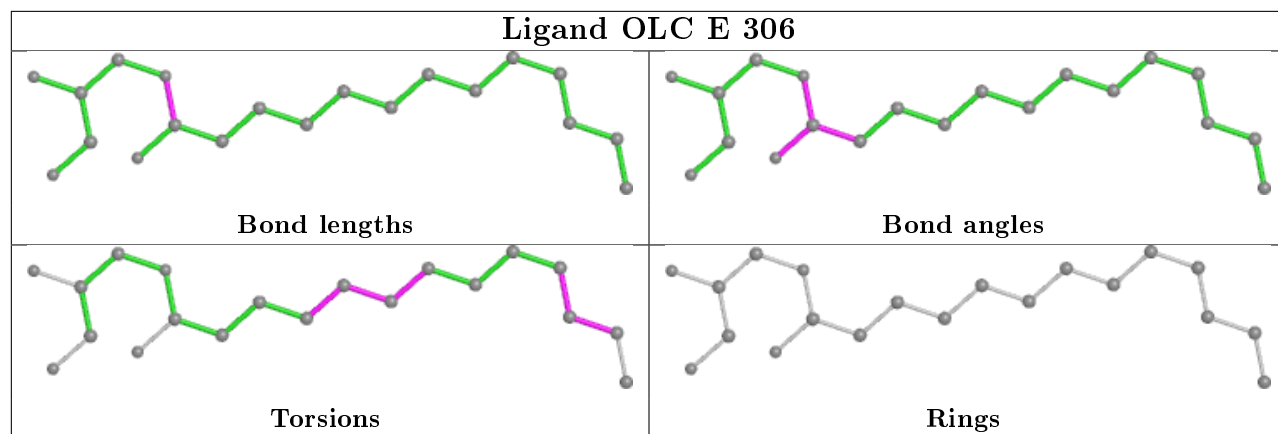




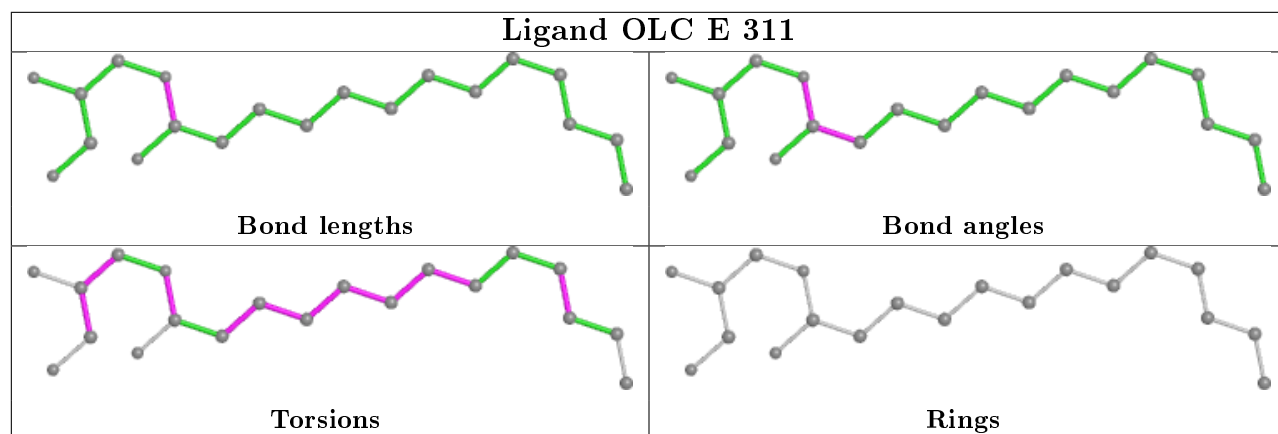
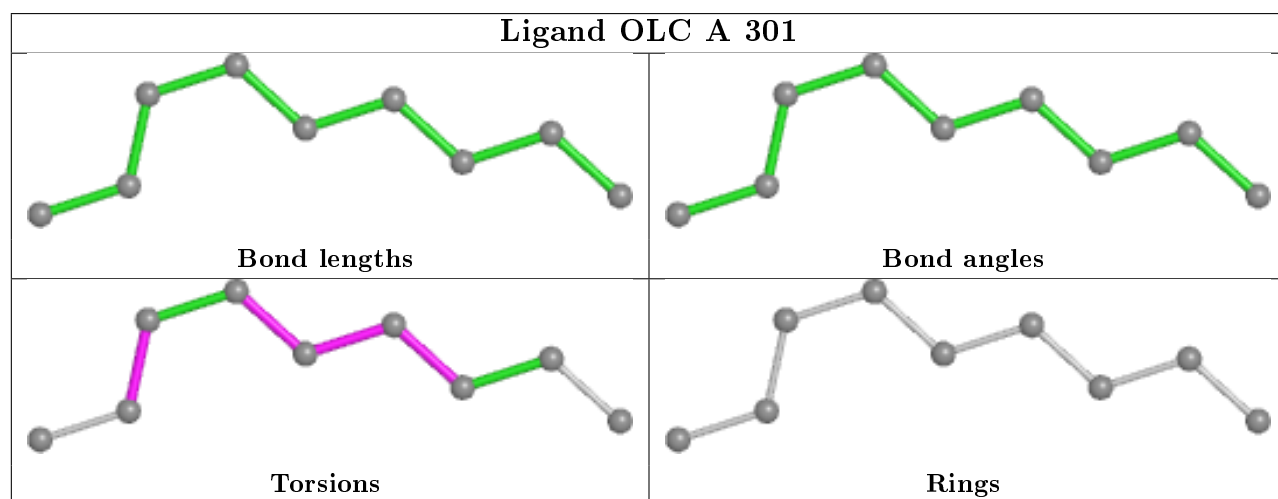
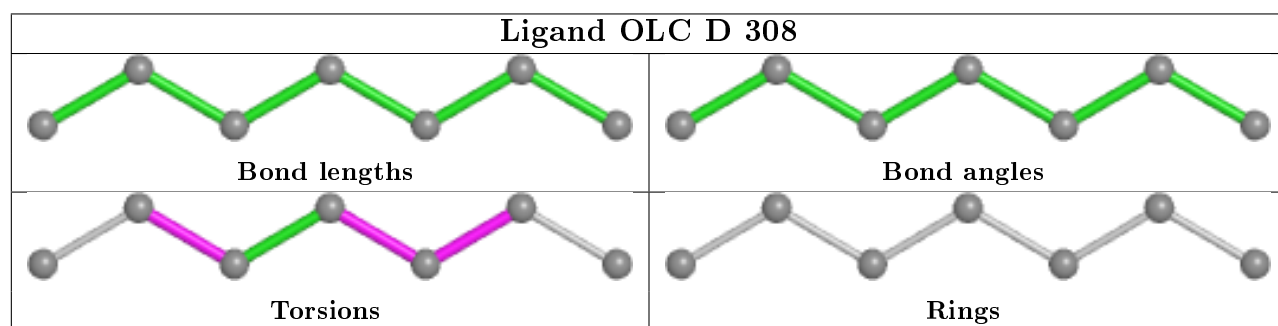
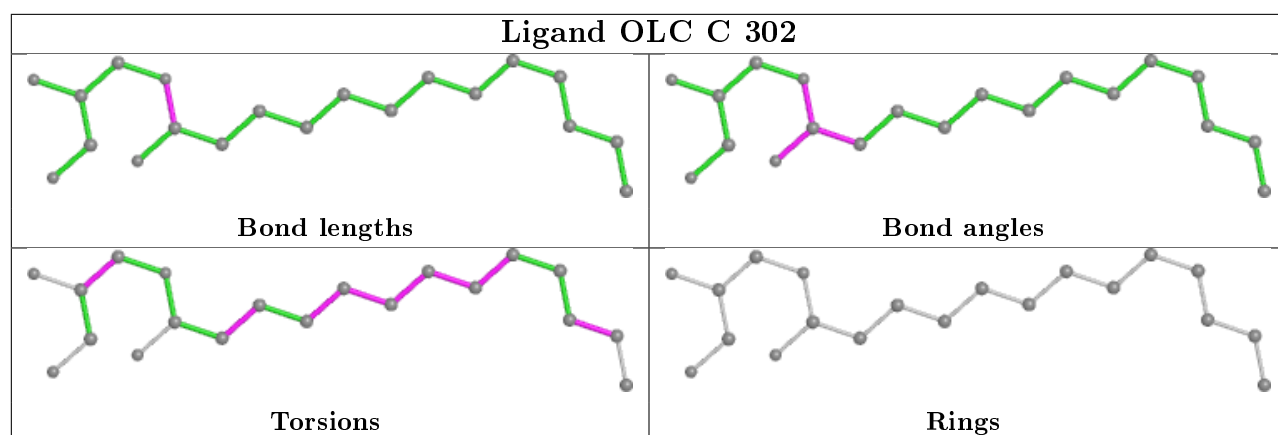


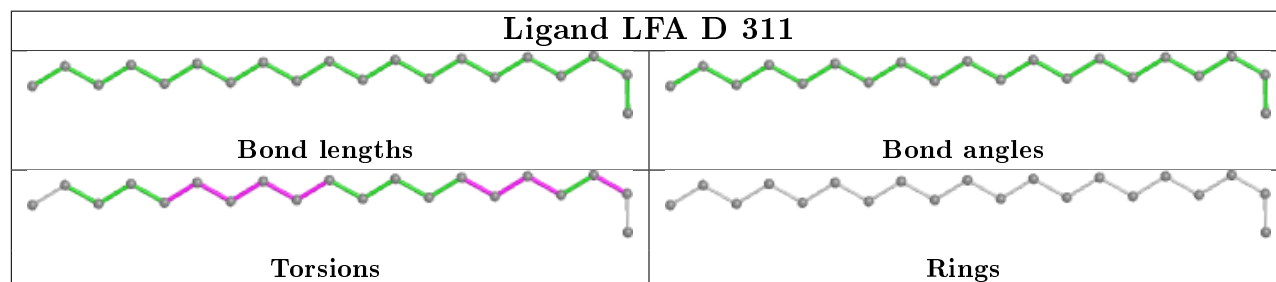
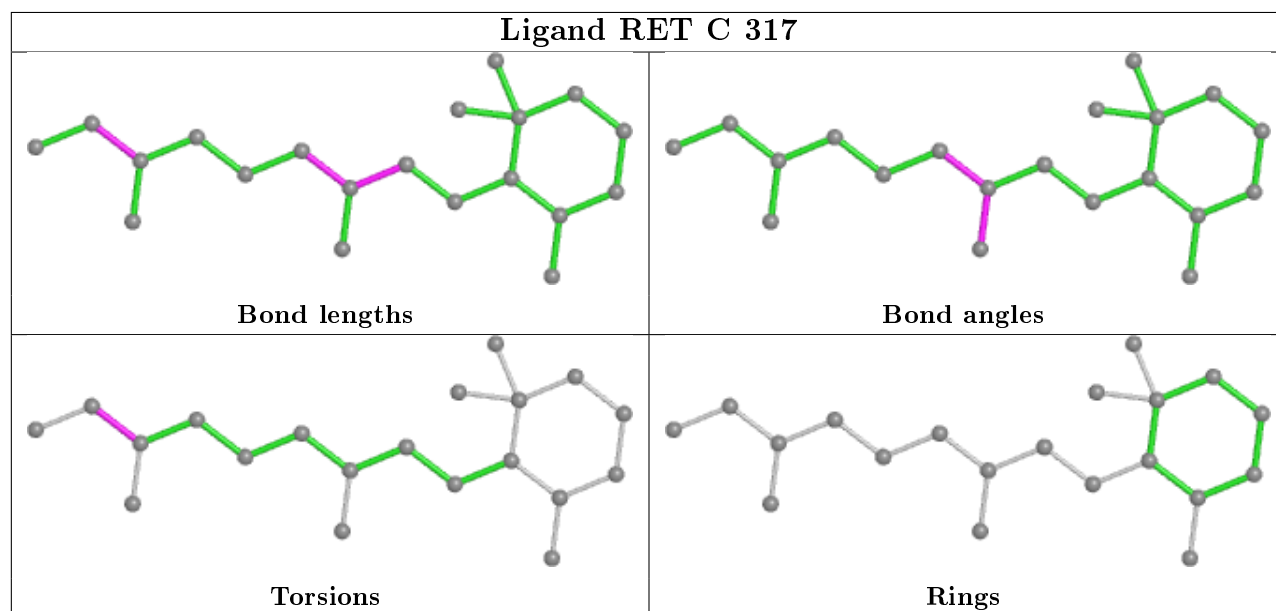
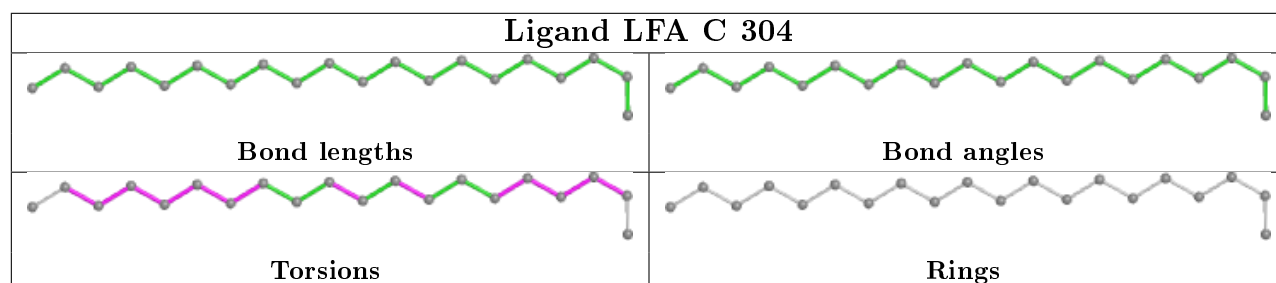
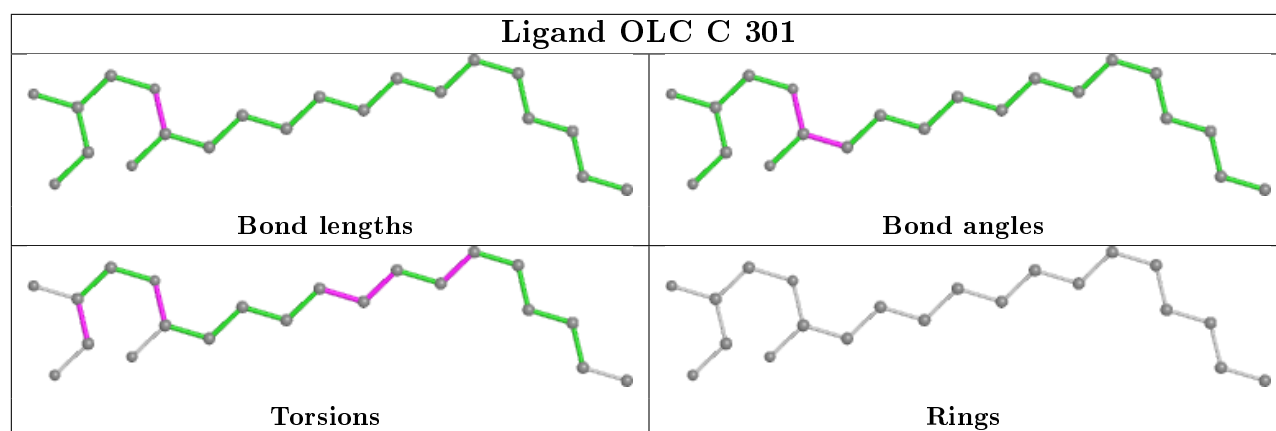


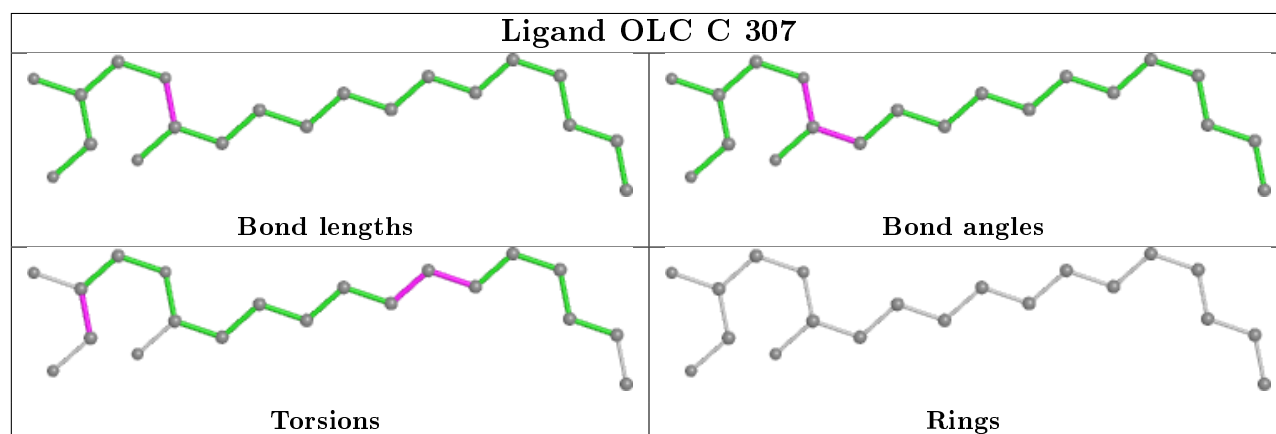
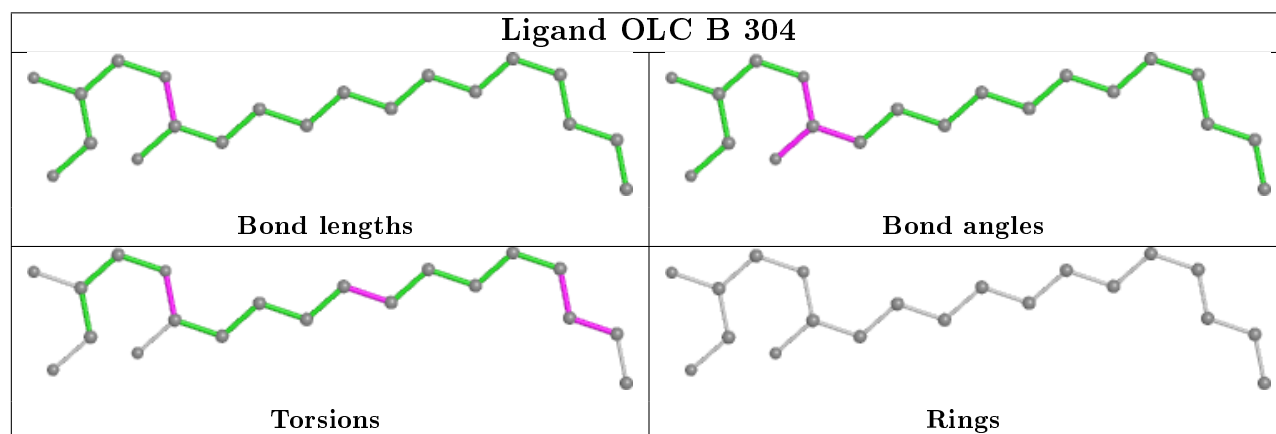
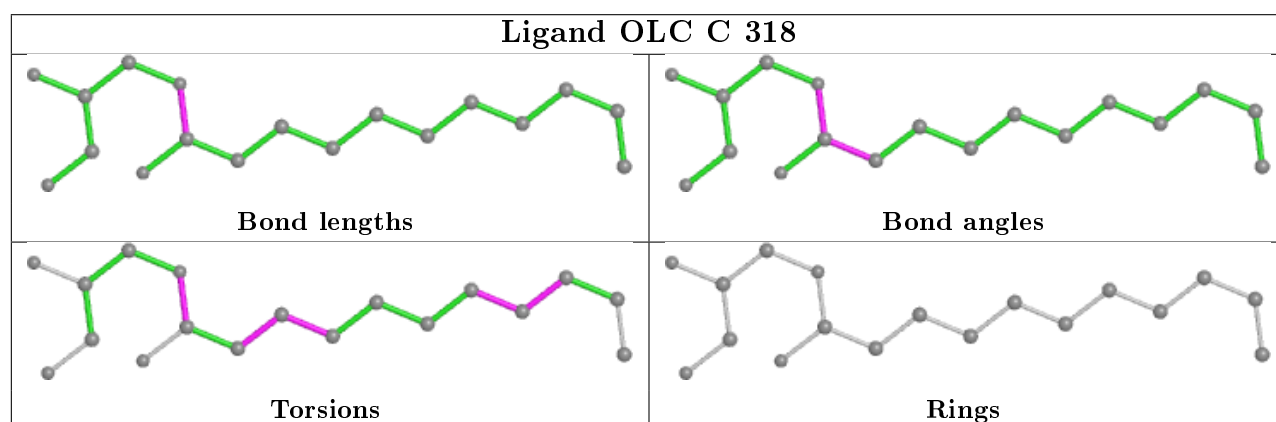
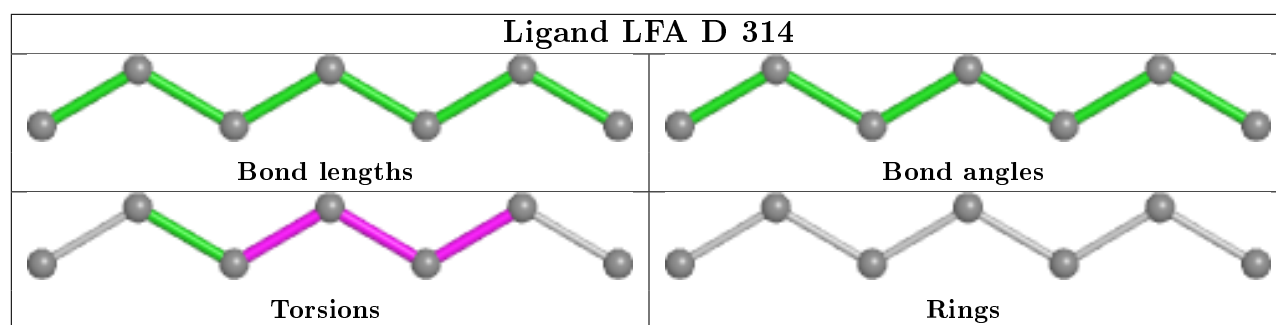


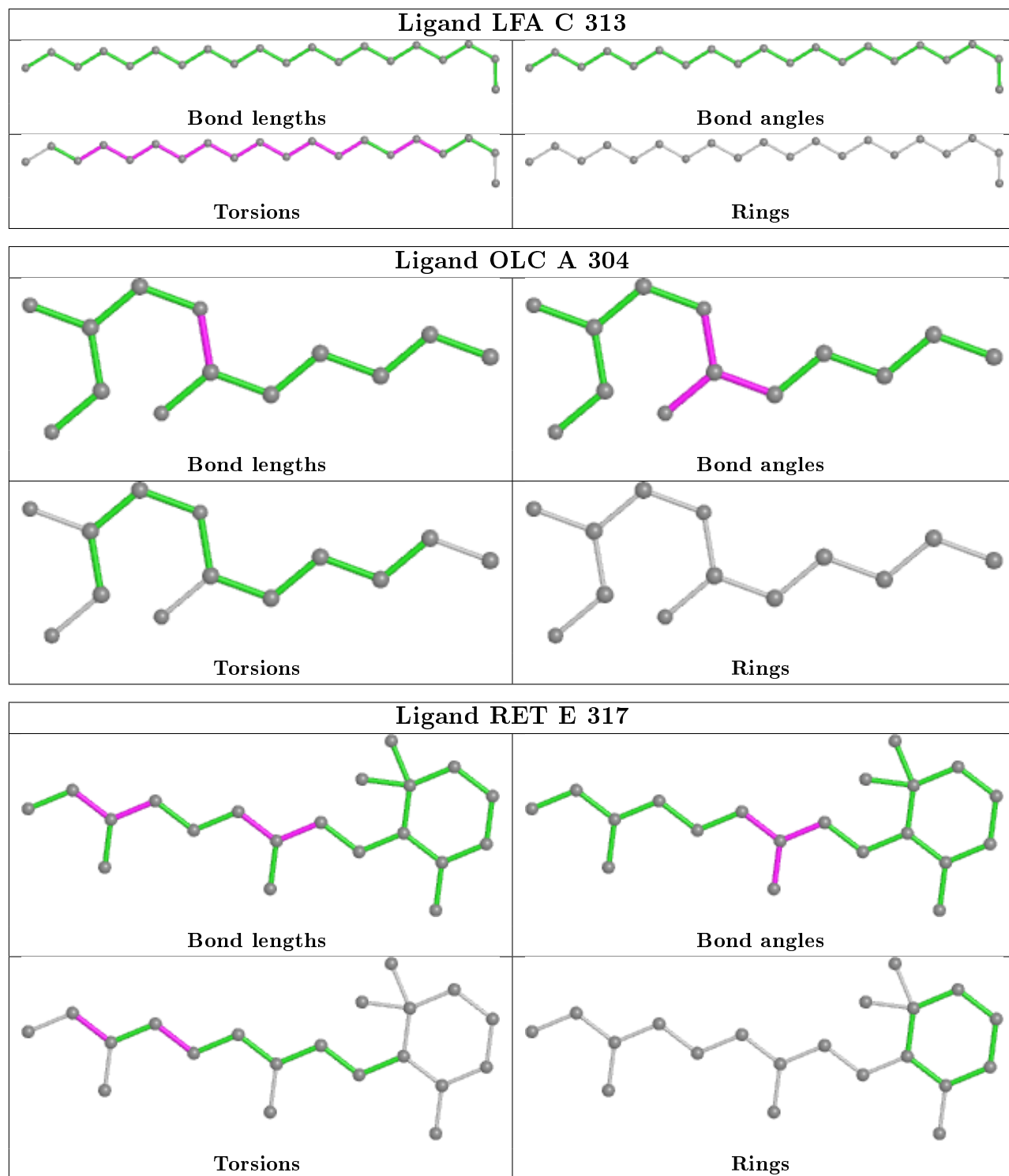


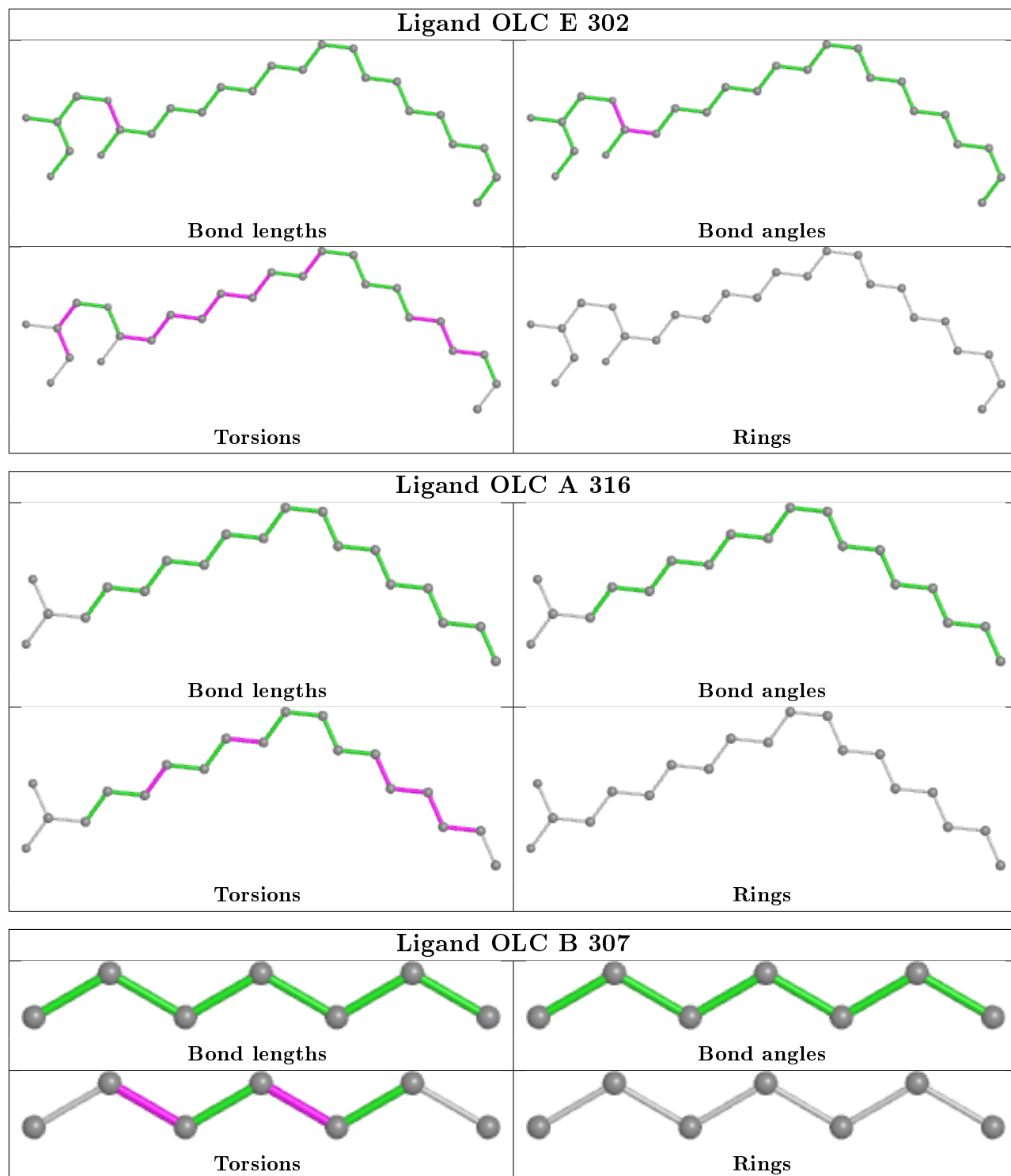


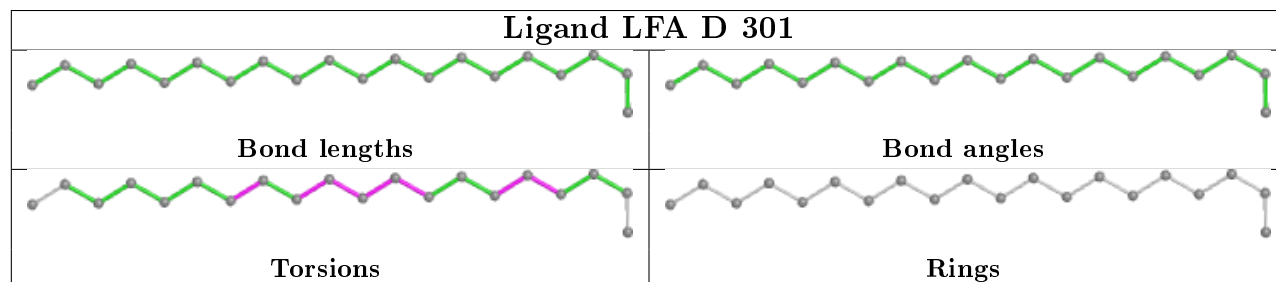
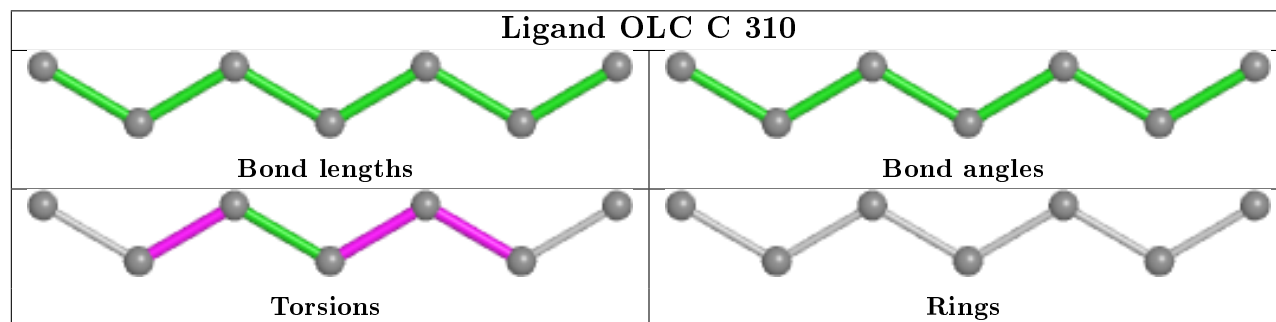
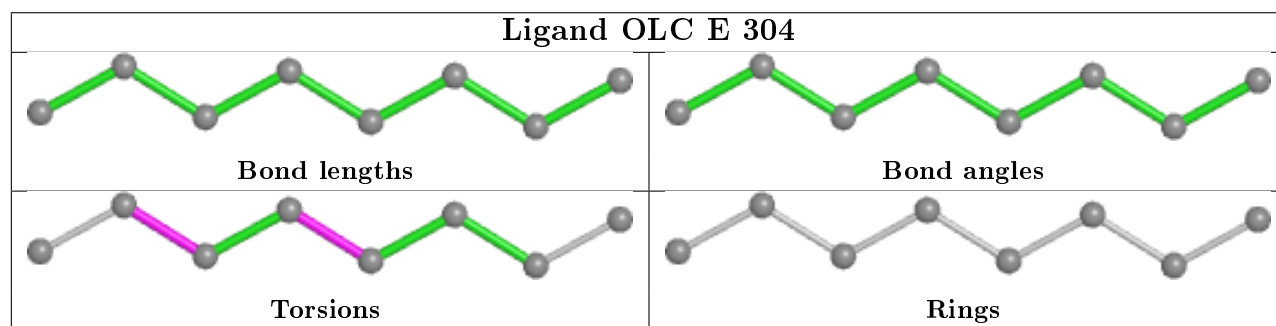
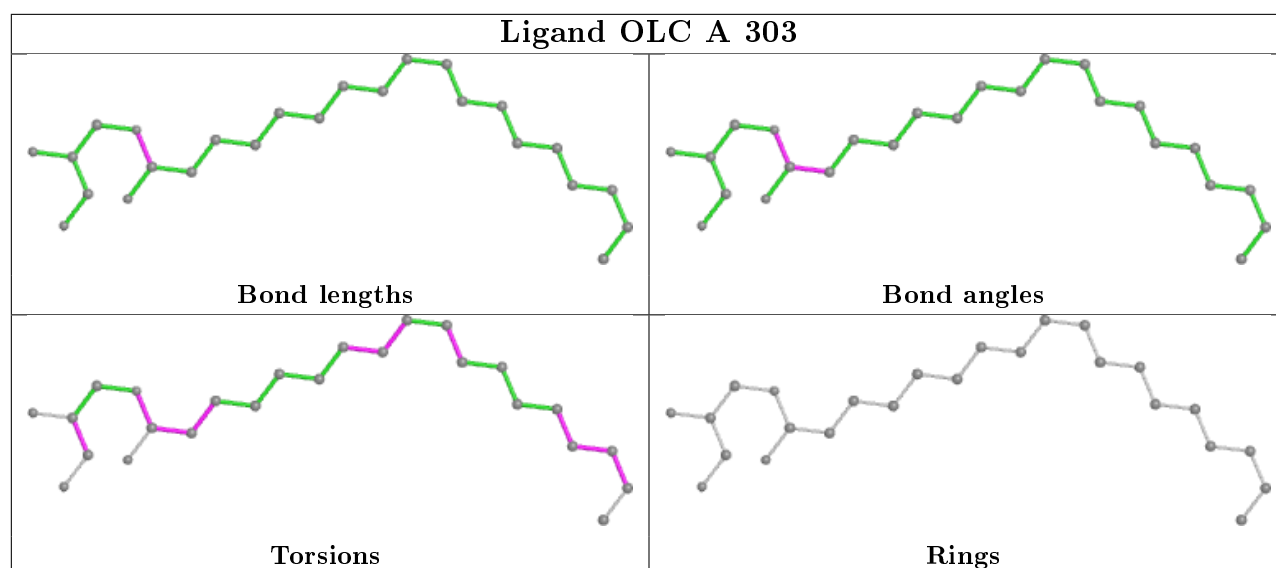


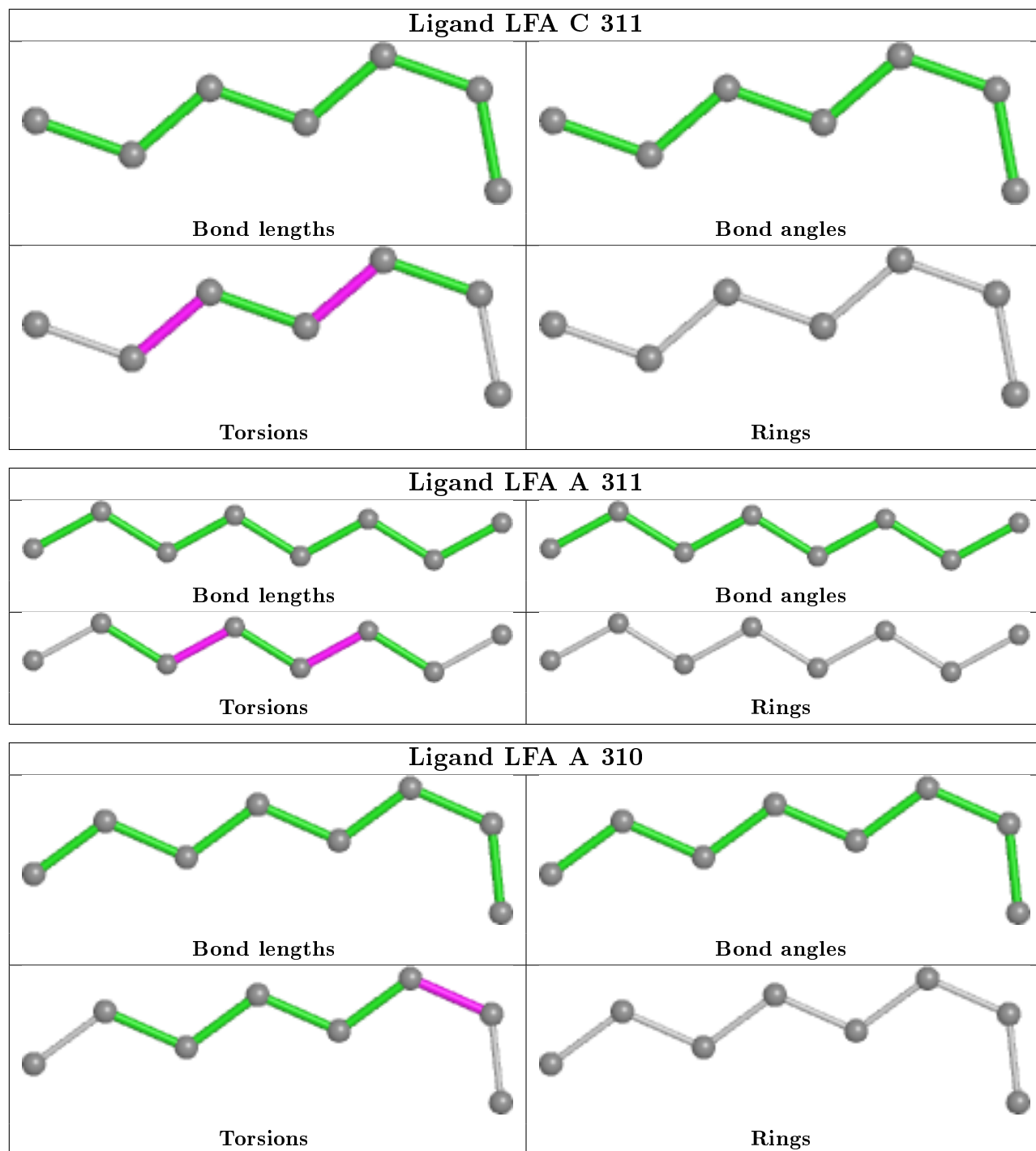


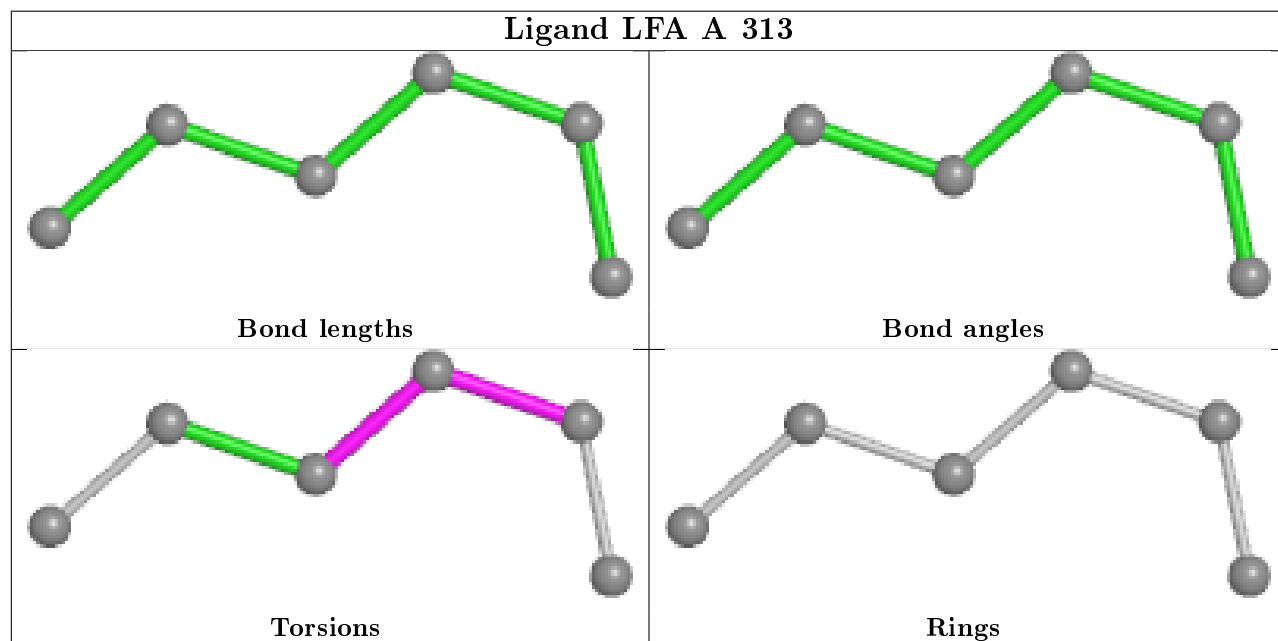
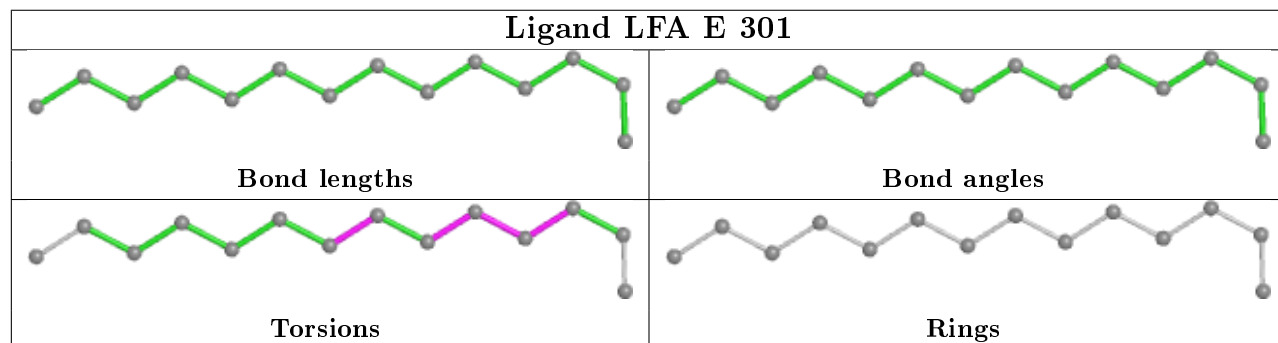
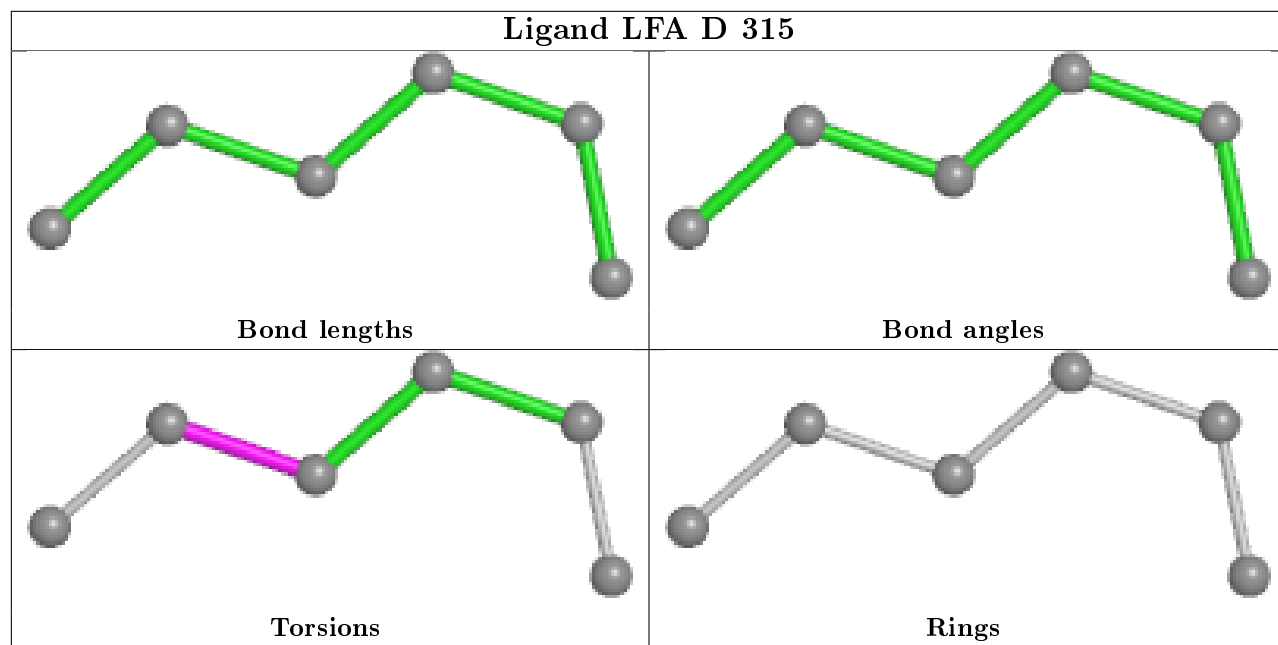




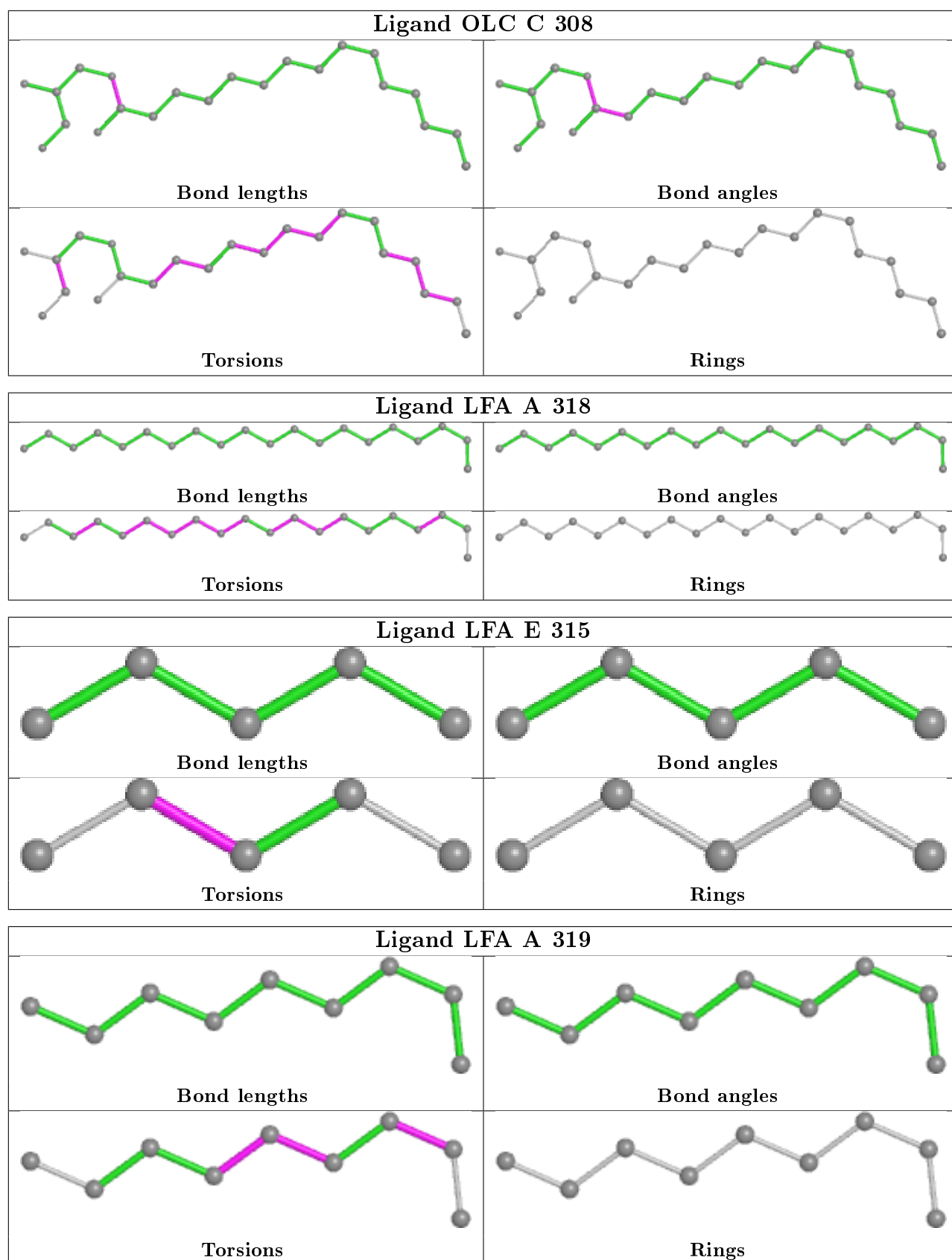


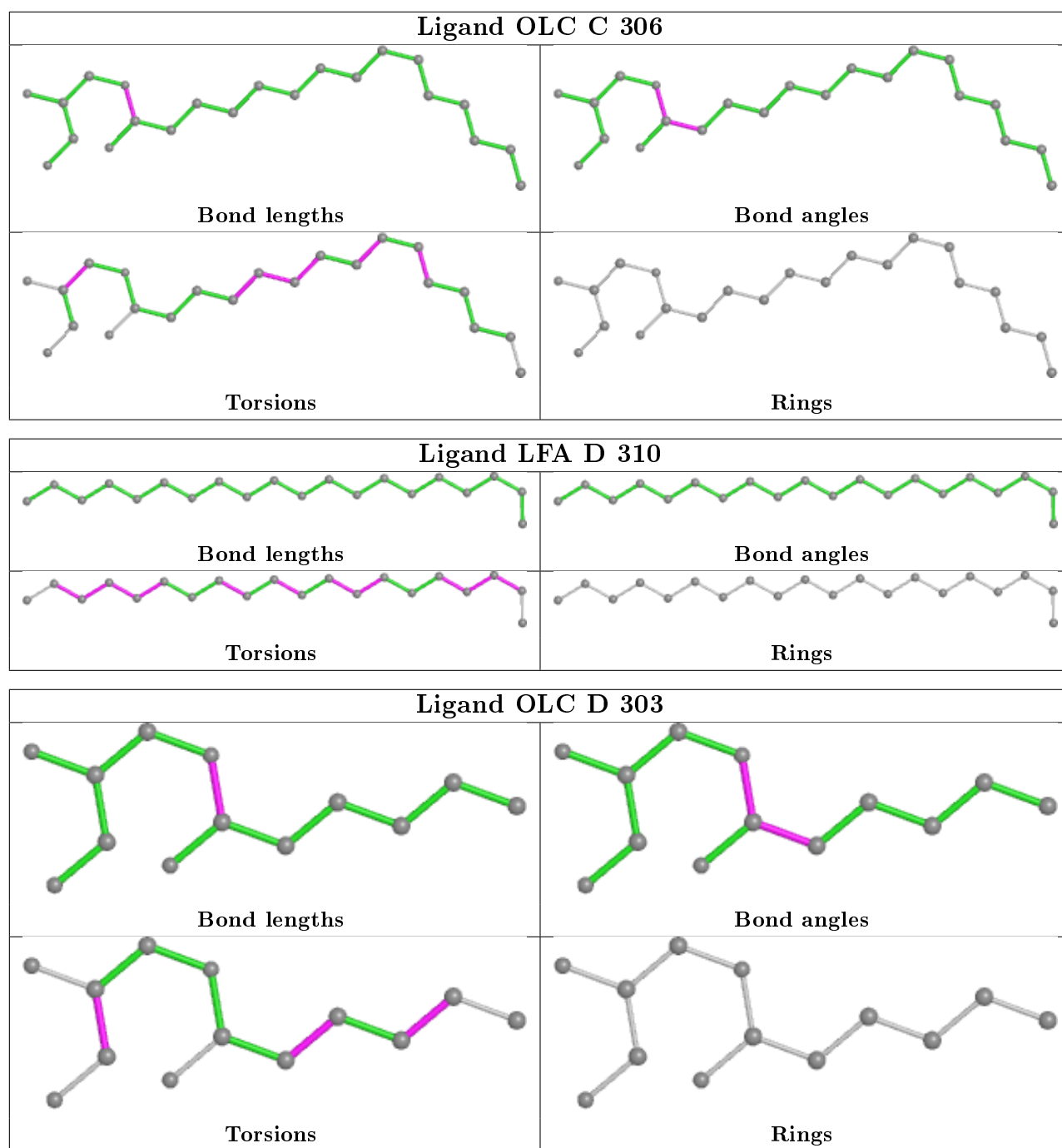


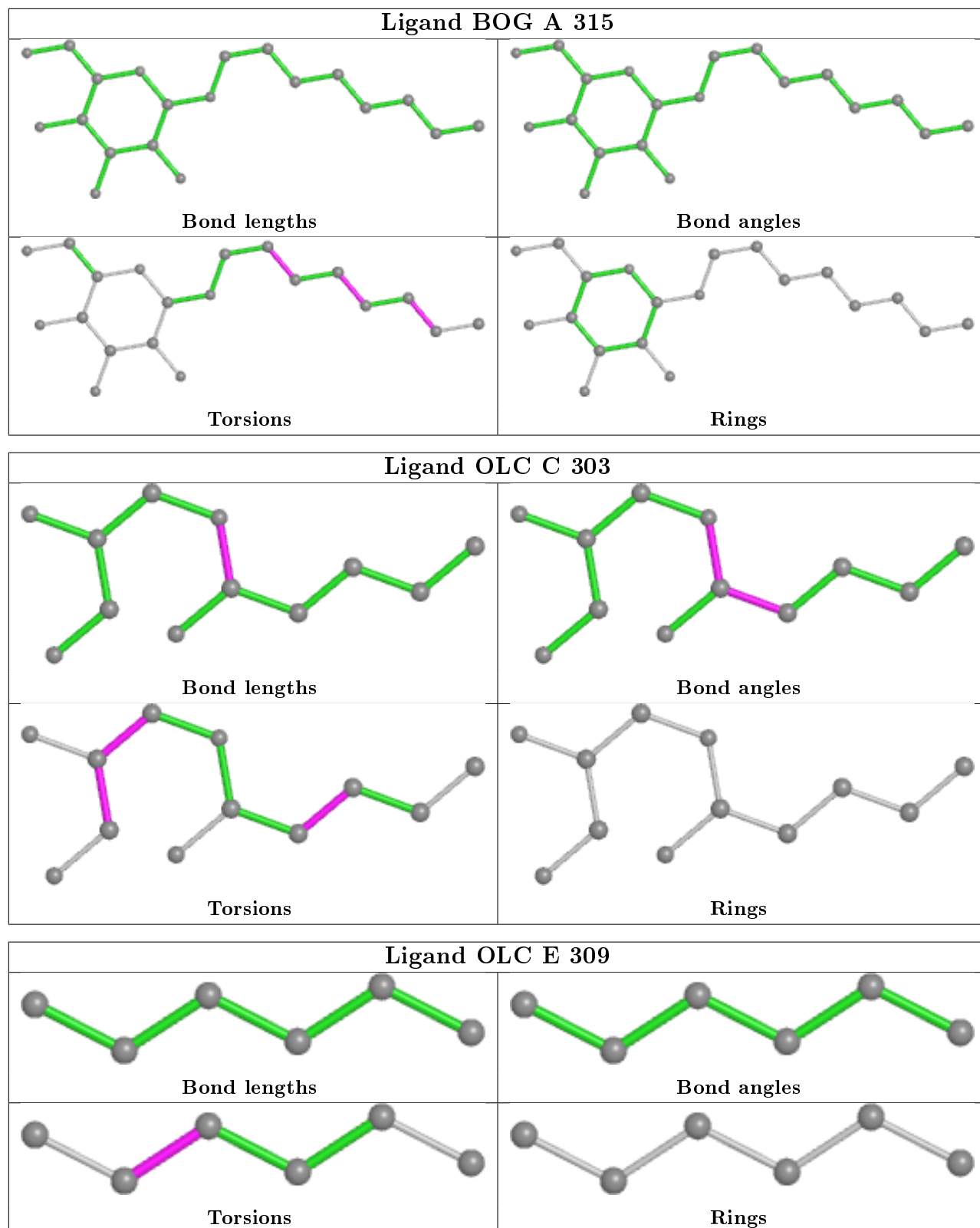


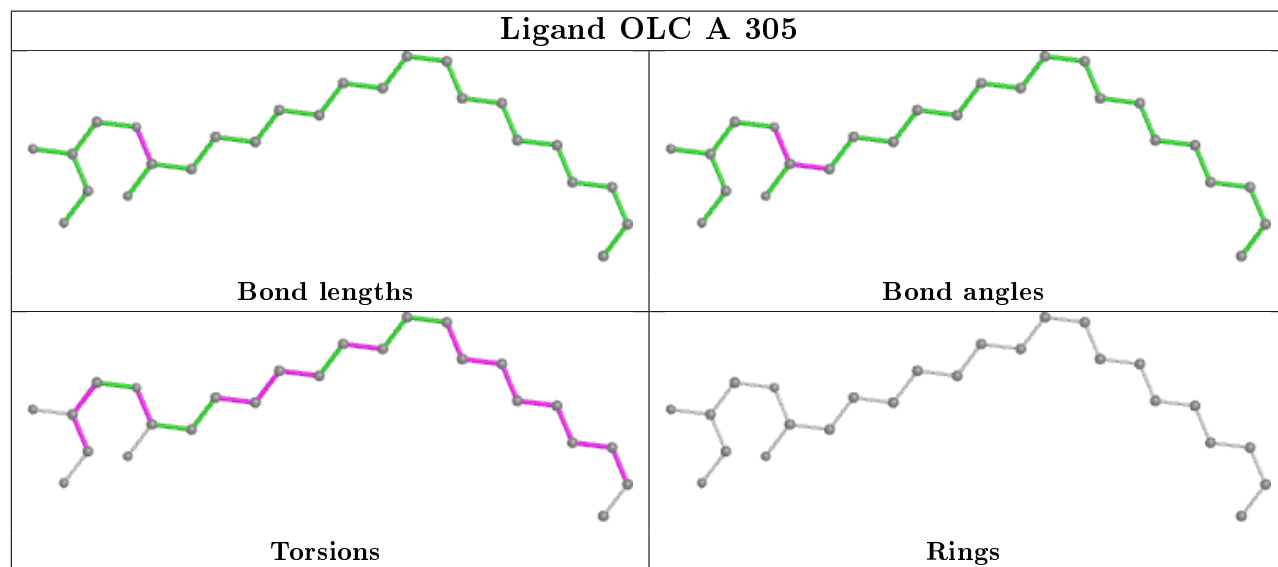
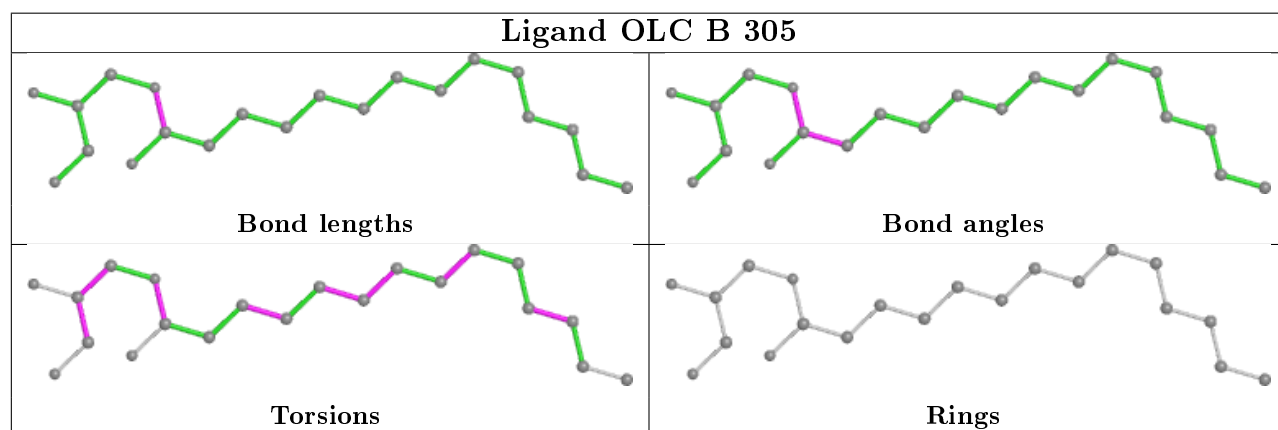
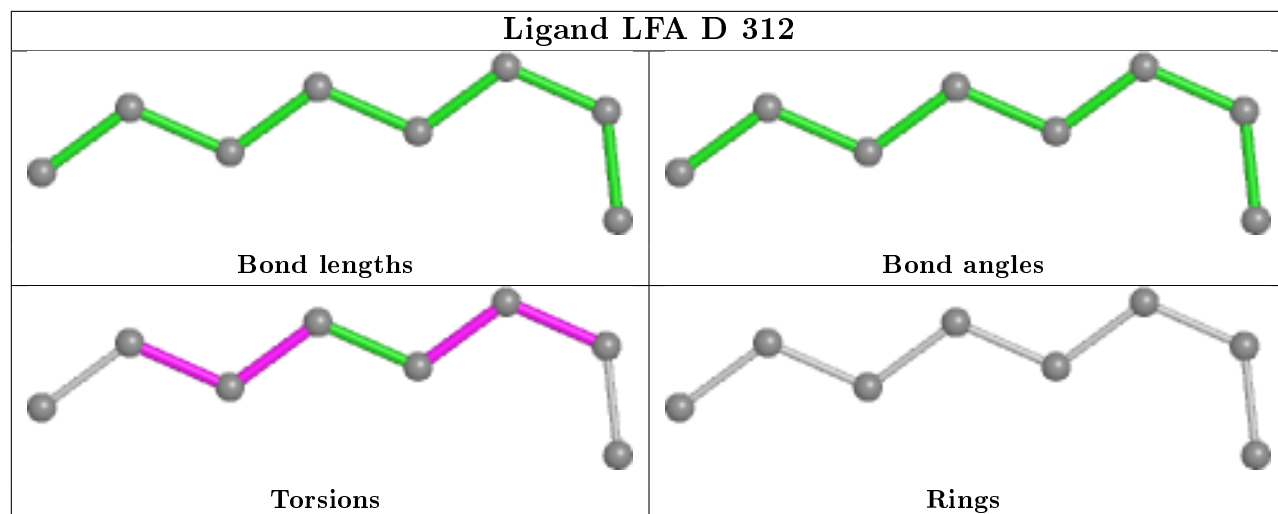


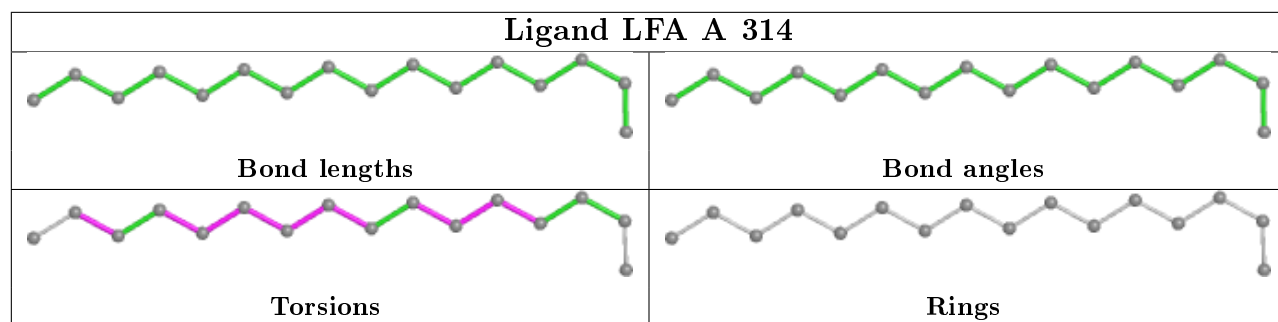
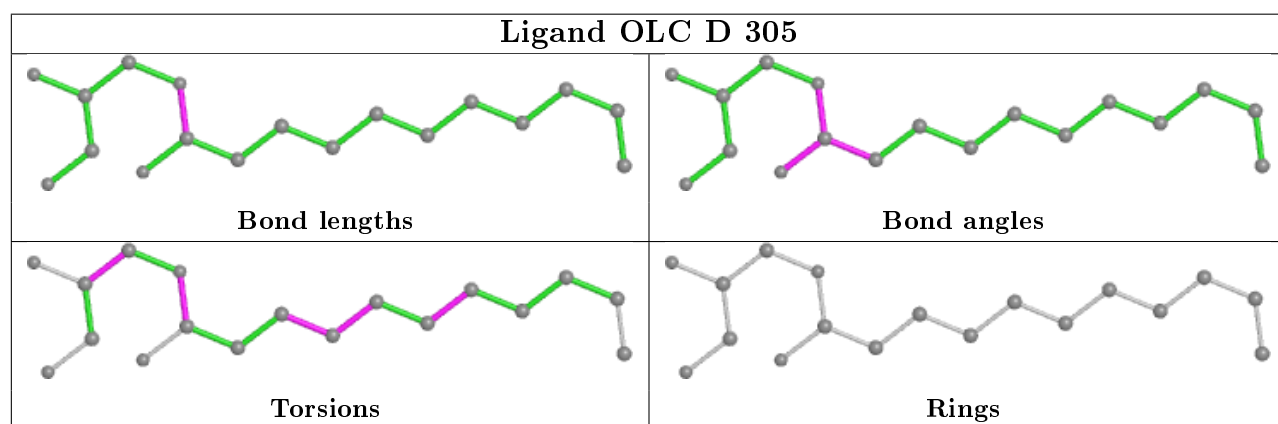
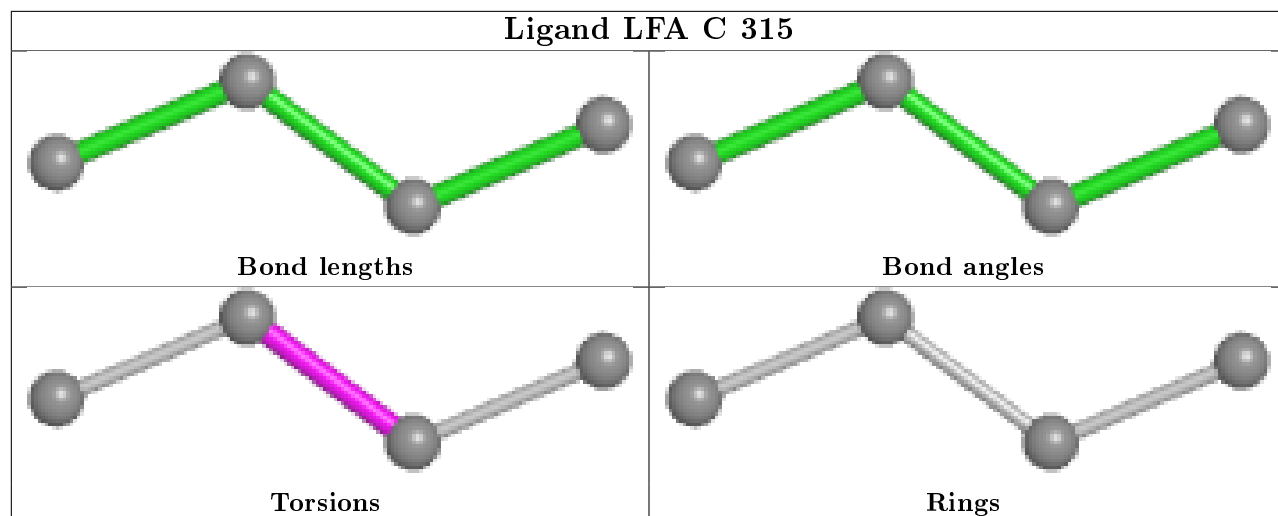


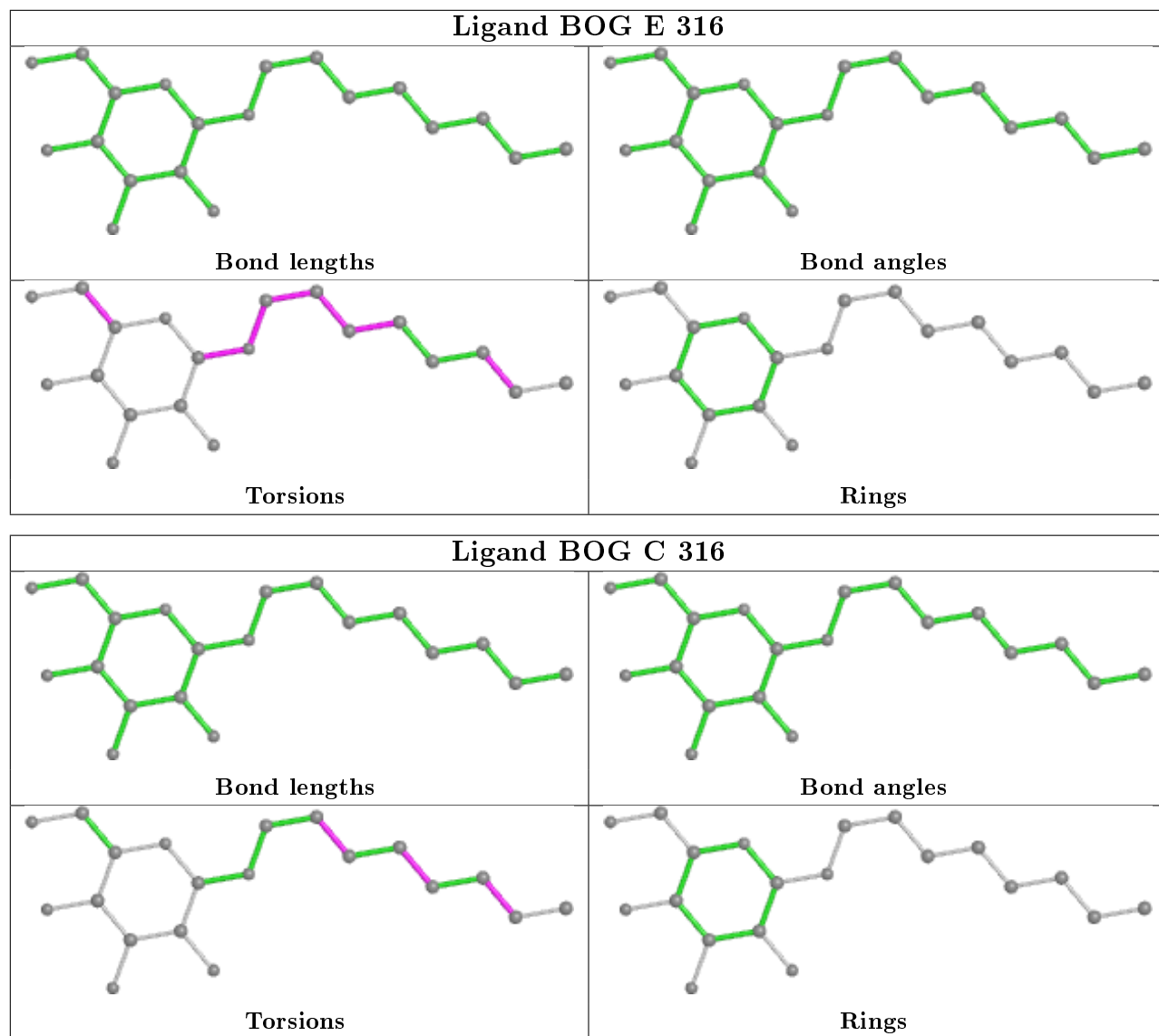












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	273/273 (100%)	0.43	27 (9%) 7 6	36, 44, 65, 122	0
1	B	273/273 (100%)	0.39	27 (9%) 7 6	36, 45, 65, 118	0
1	C	273/273 (100%)	0.42	29 (10%) 6 5	36, 44, 66, 127	0
1	D	273/273 (100%)	0.52	38 (13%) 2 2	35, 45, 70, 129	0
1	E	273/273 (100%)	0.38	31 (11%) 5 4	36, 44, 67, 124	0
All	All	1365/1365 (100%)	0.43	152 (11%) 5 4	35, 44, 67, 129	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	275	LEU	9.4
1	C	230	VAL	6.3
1	A	275	LEU	6.3
1	D	40	LEU	6.1
1	D	273	LYS	6.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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	A	305	25/25	0.43	0.32	80,98,107,111	0
3	LFA	D	315	6/20	0.52	0.30	86,90,96,102	0
3	LFA	E	312	8/20	0.61	0.23	68,85,93,94	0
2	OLC	C	308	22/25	0.62	0.41	53,90,109,116	0
3	LFA	E	301	14/20	0.62	1.51	95,104,119,121	0
2	OLC	E	311	20/25	0.65	0.54	60,105,126,126	0
2	OLC	B	303	25/25	0.66	0.24	77,96,107,113	0
3	LFA	C	311	7/20	0.66	0.37	74,84,96,99	0
2	OLC	E	310	22/25	0.67	0.32	68,88,107,117	0
3	LFA	B	302	20/20	0.67	0.94	53,73,87,97	0
3	LFA	A	318	20/20	0.67	0.92	59,69,80,83	0
3	LFA	E	303	20/20	0.67	1.02	57,73,92,92	0
3	LFA	A	319	9/20	0.68	0.34	76,79,94,95	0
4	BOG	A	315	20/20	0.68	0.53	71,97,111,113	0
3	LFA	D	314	7/20	0.68	0.20	78,84,96,98	0
3	LFA	D	312	8/20	0.69	0.20	75,93,104,107	0
3	LFA	D	301	20/20	0.69	0.98	57,70,97,97	0
3	LFA	B	310	10/20	0.70	0.19	79,95,103,105	0
2	OLC	B	305	21/25	0.70	0.39	55,87,118,133	0
4	BOG	B	312	20/20	0.70	0.56	73,89,103,104	0
2	OLC	E	302	25/25	0.71	0.28	70,82,129,140	0
3	LFA	C	304	20/20	0.71	1.01	57,72,84,88	0
2	OLC	E	307	15/25	0.72	0.54	77,93,123,123	0
2	OLC	E	305	16/25	0.72	0.32	76,88,96,99	0
3	LFA	A	311	8/20	0.72	0.25	70,85,101,103	0
2	OLC	E	309	6/25	0.73	0.20	61,74,80,86	0
2	OLC	A	303	25/25	0.73	0.38	79,90,106,137	0
3	LFA	B	311	7/20	0.73	0.23	75,77,95,108	0
3	LFA	A	310	8/20	0.73	0.20	75,80,84,84	0
4	BOG	E	316	20/20	0.73	0.42	69,89,103,112	0
2	OLC	D	302	16/25	0.74	0.28	66,88,94,111	0
2	OLC	D	308	7/25	0.74	0.20	64,75,83,85	0
2	OLC	C	303	12/25	0.74	0.28	72,88,121,133	0
3	LFA	A	314	16/20	0.74	0.38	83,98,106,108	0
3	LFA	A	309	7/20	0.74	0.27	80,82,90,92	0
2	OLC	D	303	13/25	0.75	0.29	98,114,134,162	0
2	OLC	D	306	18/25	0.75	0.31	53,86,104,111	0
3	LFA	D	310	20/20	0.75	0.21	82,93,102,106	0
3	LFA	C	314	6/20	0.76	0.22	61,70,84,84	0
2	OLC	D	309	25/25	0.76	0.26	67,86,112,130	0

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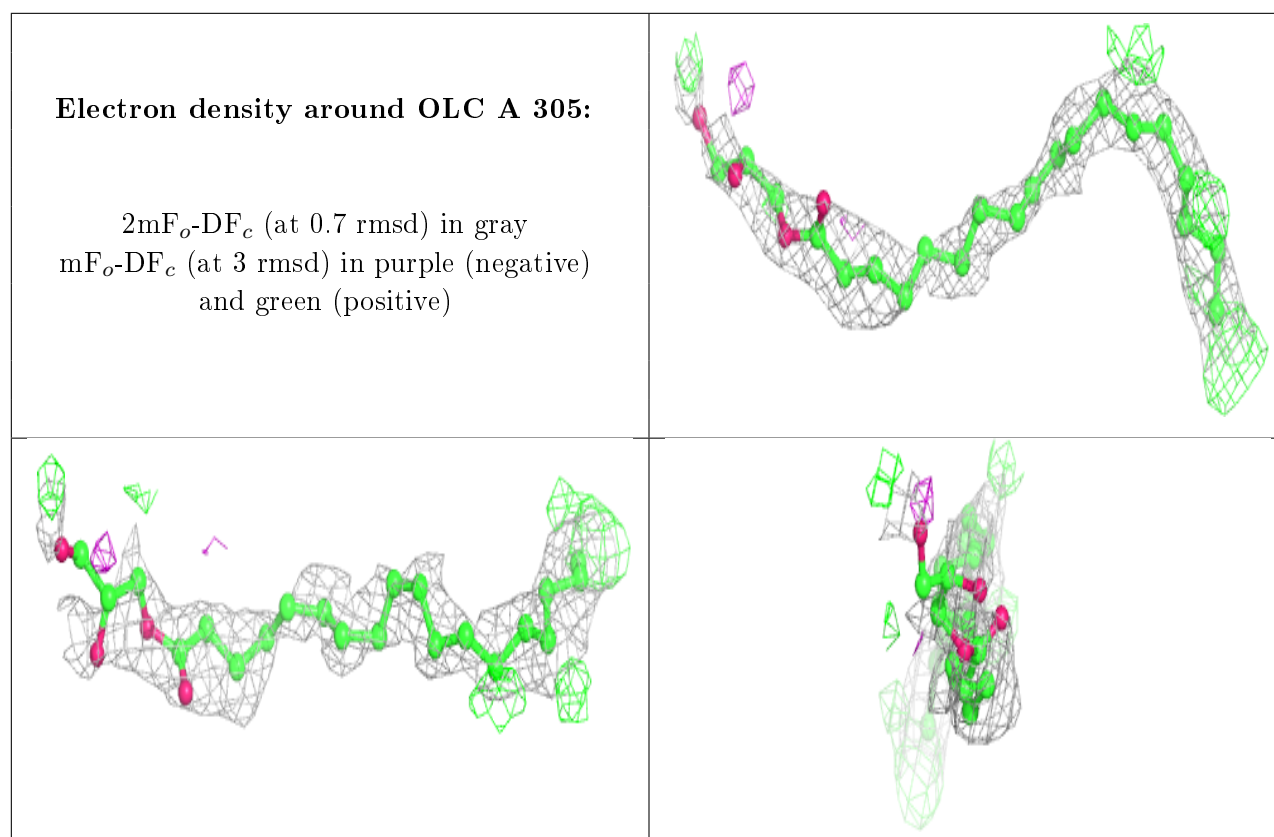
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLC	B	304	20/25	0.76	0.22	65,88,108,116	0
2	OLC	C	302	20/25	0.77	0.21	67,83,89,96	0
2	OLC	D	304	25/25	0.77	0.26	77,97,108,124	0
2	OLC	A	302	22/25	0.77	0.25	45,67,107,111	0
4	BOG	C	316	20/20	0.77	0.47	64,82,99,100	0
3	LFA	B	309	8/20	0.78	0.21	68,82,87,92	0
2	OLC	A	308	16/25	0.78	0.28	65,83,127,132	0
2	OLC	C	307	20/25	0.78	0.29	70,95,111,114	0
6	NA	B	316	1/1	0.78	0.22	76,76,76,76	0
3	LFA	D	311	20/20	0.78	0.20	78,89,99,104	0
3	LFA	C	315	4/20	0.79	0.31	76,76,81,87	0
6	NA	E	319	1/1	0.79	0.40	66,66,66,66	0
3	LFA	E	313	14/20	0.80	0.19	74,89,103,104	0
3	LFA	A	312	4/20	0.80	0.25	79,82,84,86	0
3	LFA	B	308	9/20	0.80	0.39	82,92,103,107	0
2	OLC	A	304	13/25	0.80	0.24	65,72,90,91	0
3	LFA	C	312	8/20	0.80	0.21	72,85,88,90	0
2	OLC	B	307	7/25	0.80	0.19	69,77,86,86	0
2	OLC	E	304	8/25	0.81	0.20	67,71,90,90	0
2	OLC	C	306	22/25	0.81	0.23	79,95,113,118	0
2	OLC	A	306	15/25	0.81	0.26	65,76,100,125	0
2	OLC	C	310	7/25	0.82	0.19	70,70,84,94	0
2	OLC	A	317	20/25	0.82	0.21	66,76,96,97	0
2	OLC	C	305	23/25	0.82	0.24	49,66,106,120	0
4	BOG	D	316	20/20	0.82	0.49	69,83,100,100	0
6	NA	C	320	1/1	0.83	0.12	70,70,70,70	0
2	OLC	C	318	18/25	0.83	0.21	67,81,98,110	0
2	OLC	D	305	18/25	0.84	0.23	77,90,111,125	0
2	OLC	E	306	20/25	0.84	0.32	72,89,105,116	0
3	LFA	D	313	17/20	0.85	0.42	56,62,83,91	0
2	OLC	B	301	22/25	0.85	0.17	70,82,101,108	0
2	OLC	E	308	15/25	0.85	0.28	60,73,85,86	0
2	OLC	A	307	7/25	0.86	0.15	76,81,86,88	0
2	OLC	B	306	16/25	0.86	0.27	61,85,96,116	0
2	OLC	C	301	21/25	0.87	0.24	51,64,90,96	0
3	LFA	C	313	20/20	0.87	0.16	70,88,106,108	0
2	OLC	A	301	9/25	0.87	0.17	66,77,89,92	0
3	LFA	B	314	4/20	0.88	1.80	84,87,90,92	0
3	LFA	E	315	5/20	0.88	0.21	83,85,87,91	0
6	NA	A	322	1/1	0.88	0.27	78,78,78,78	0
6	NA	D	319	1/1	0.89	0.11	71,71,71,71	0
2	OLC	C	309	16/25	0.89	0.20	61,84,92,94	0

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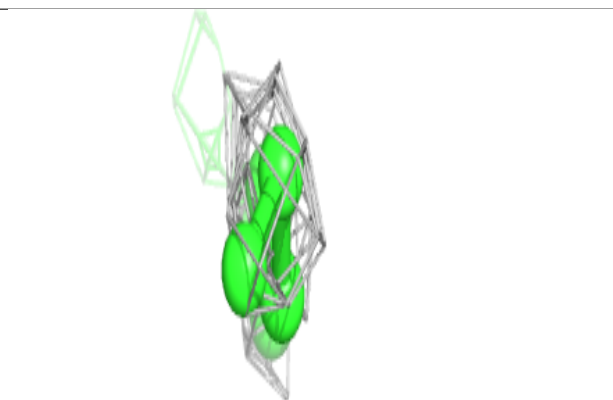
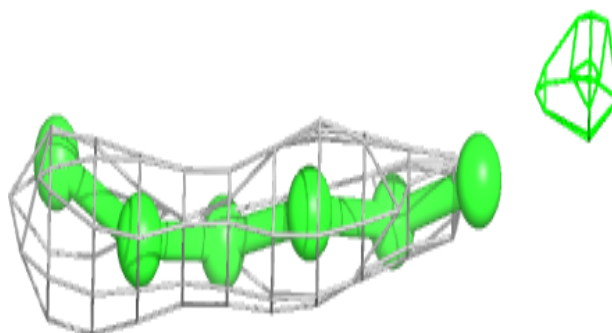
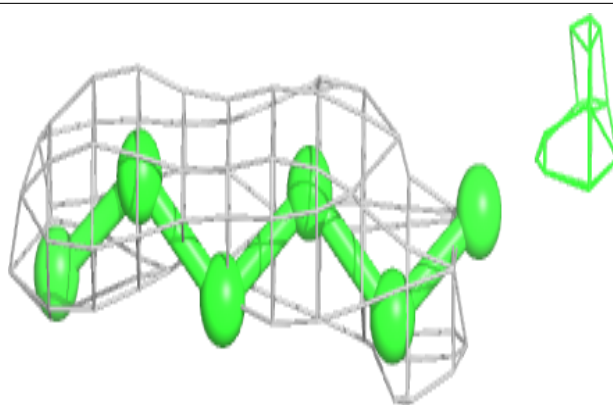
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LFA	A	313	6/20	0.90	0.20	64,69,81,93	0
2	OLC	A	316	19/25	0.91	0.24	51,59,74,75	0
3	LFA	E	314	4/20	0.93	0.20	67,70,79,79	0
5	RET	A	320	20/21	0.93	0.13	38,43,45,46	0
5	RET	D	317	20/21	0.94	0.12	39,43,48,49	0
5	RET	B	313	20/21	0.94	0.10	37,43,49,52	0
5	RET	C	317	20/21	0.94	0.12	36,43,47,49	0
2	OLC	D	307	14/25	0.94	0.15	59,76,94,97	0
5	RET	E	317	20/21	0.95	0.11	37,43,45,49	0
6	NA	E	318	1/1	0.97	0.05	39,39,39,39	0
6	NA	A	321	1/1	0.97	0.06	39,39,39,39	0
6	NA	D	318	1/1	0.98	0.07	38,38,38,38	0
6	NA	B	315	1/1	0.98	0.09	39,39,39,39	0
6	NA	C	319	1/1	0.98	0.05	39,39,39,39	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.

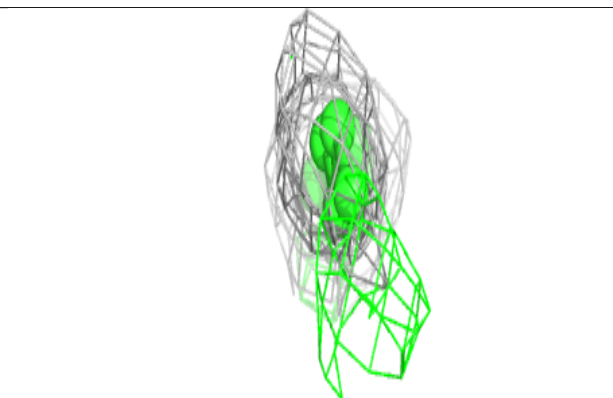
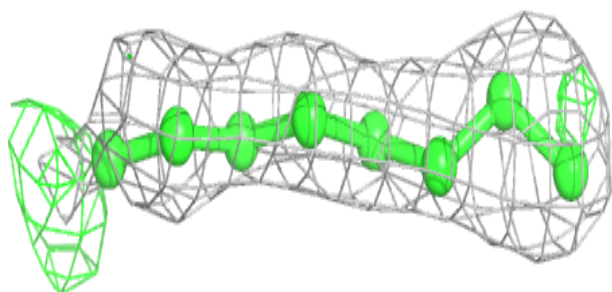
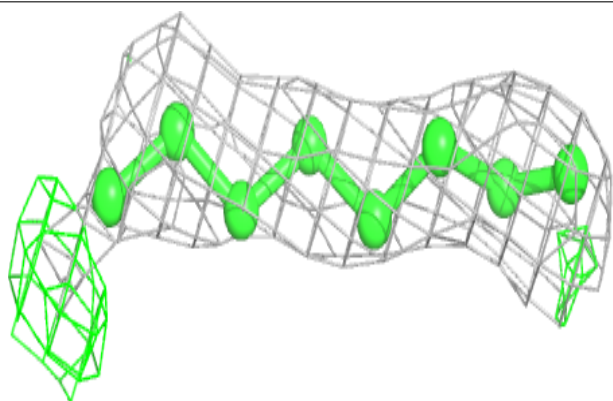


**Electron density around LFA D 315:**

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

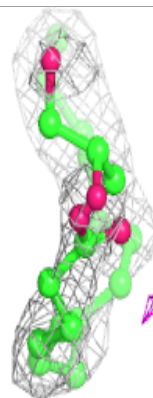
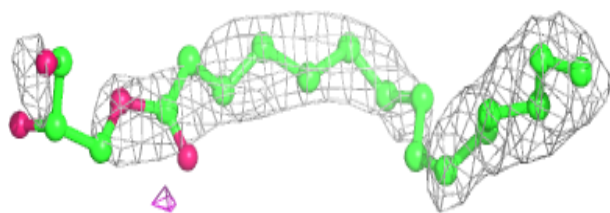
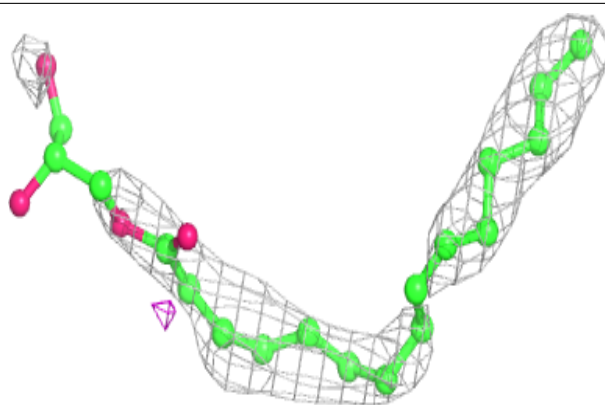
**Electron density around LFA E 312:**

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

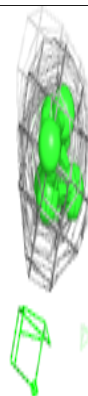
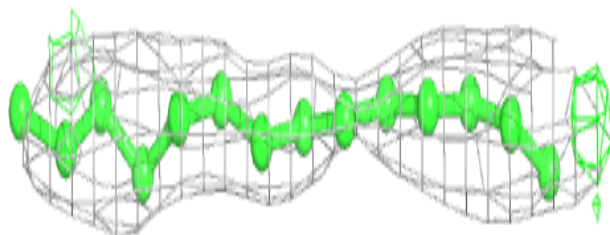
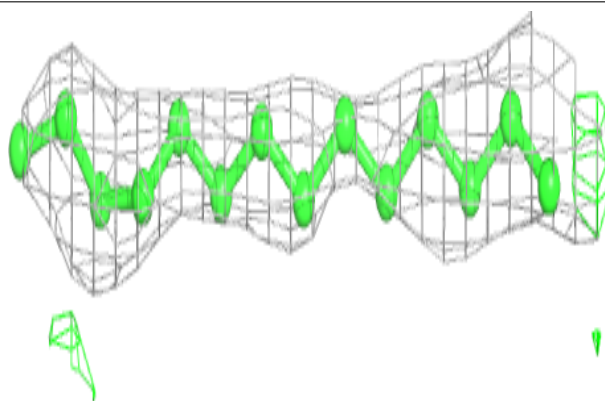


**Electron density around OLC C 308:**

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

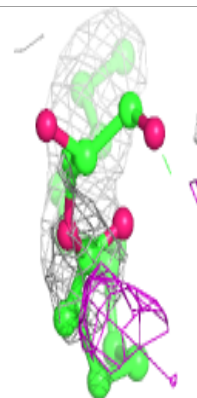
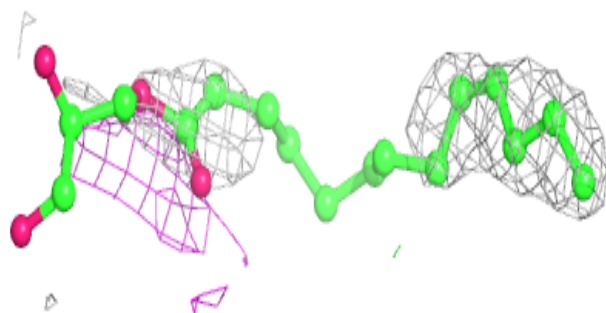
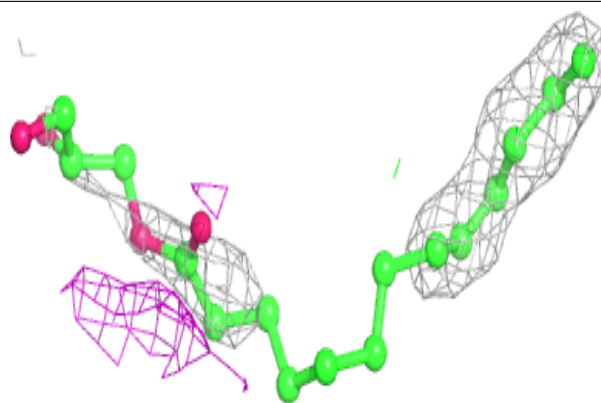
**Electron density around LFA E 301:**

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

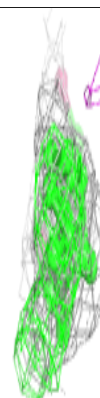
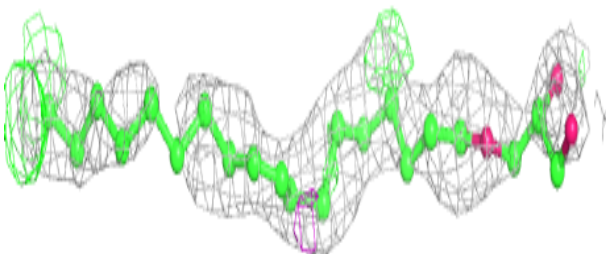
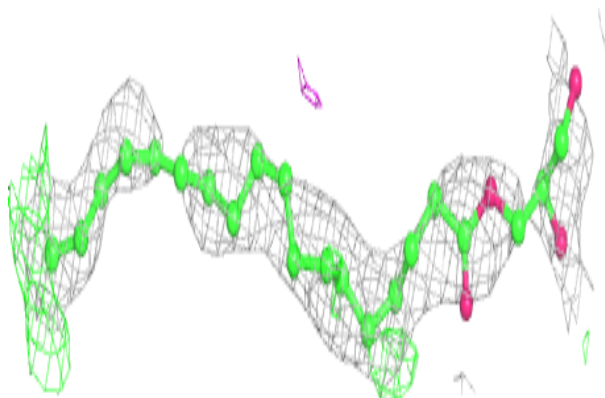


**Electron density around OLC E 311:**

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

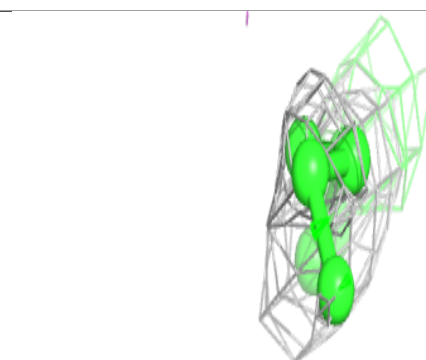
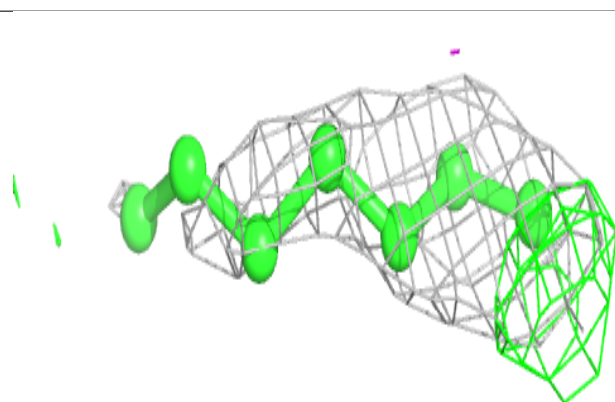
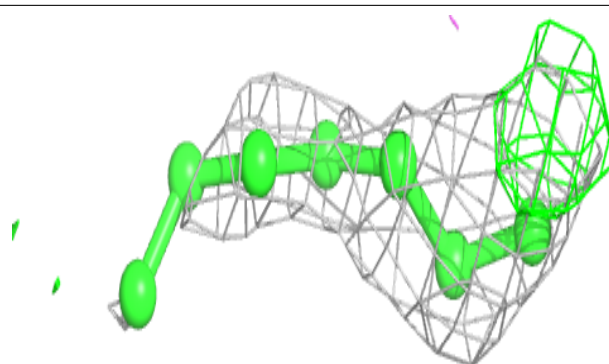
**Electron density around OLC B 303:**

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

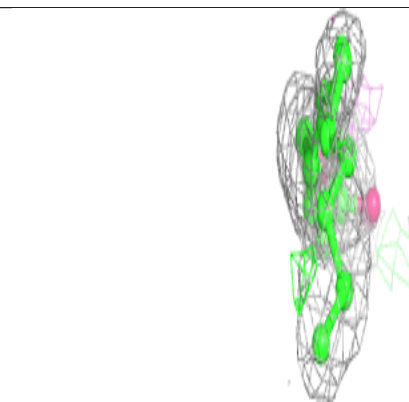
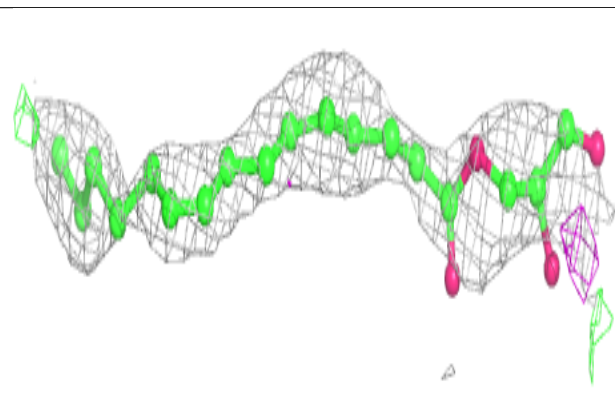
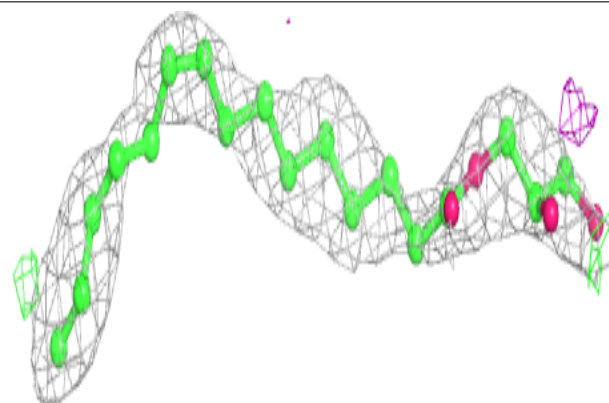


**Electron density around LFA C 311:**

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

**Electron density around OLC E 310:**

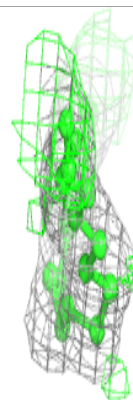
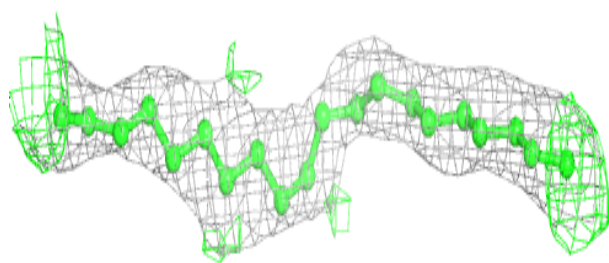
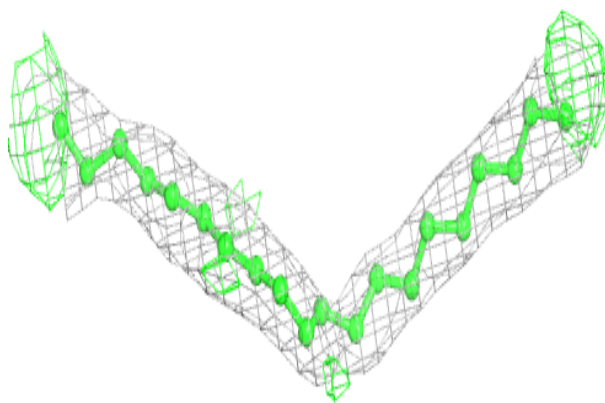
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



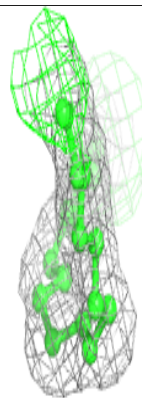
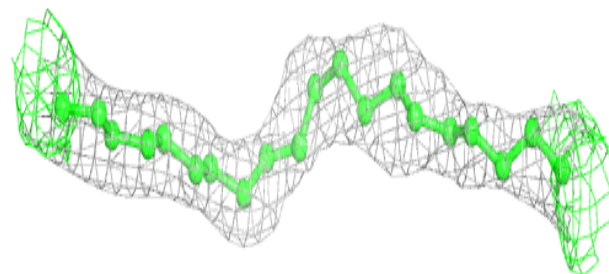
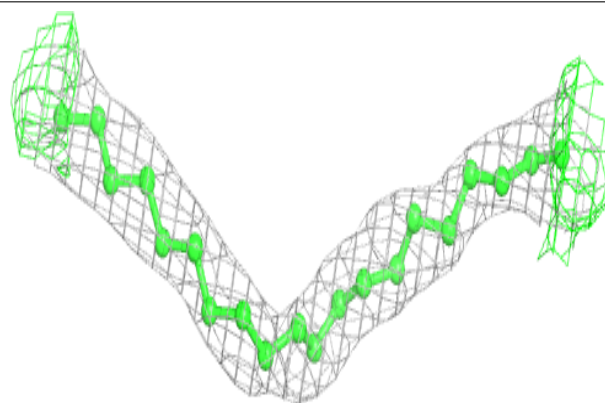


**Electron density around LFA B 302:**

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

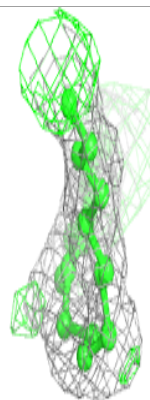
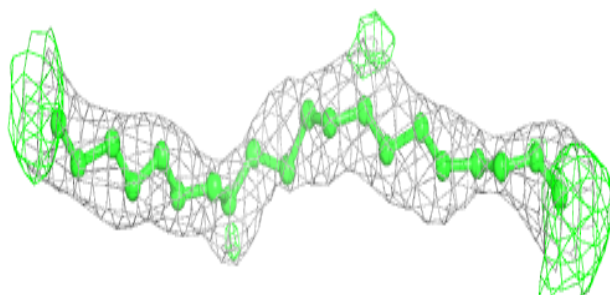
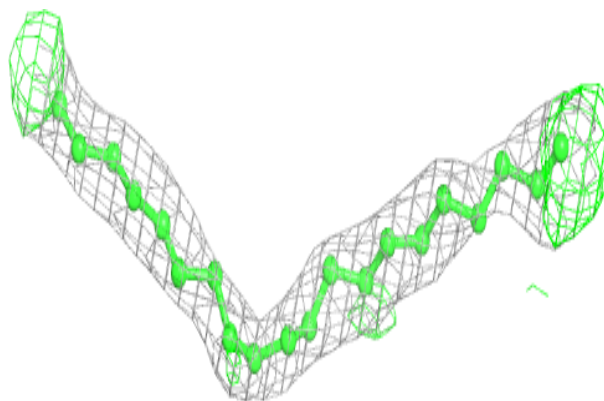
**Electron density around LFA A 318:**

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

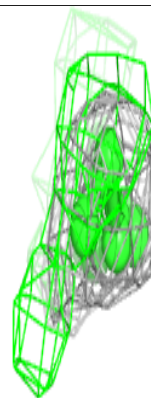
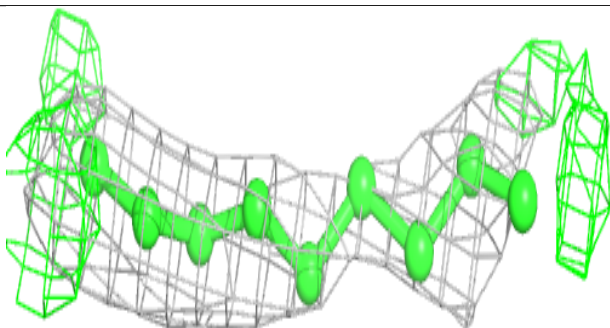
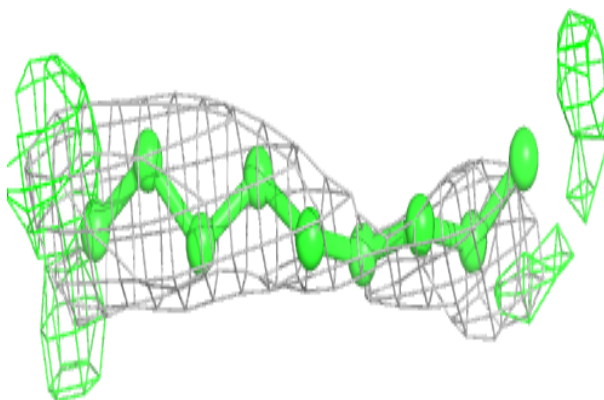


**Electron density around LFA E 303:**

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

**Electron density around LFA A 319:**

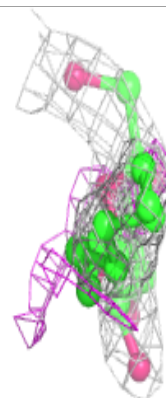
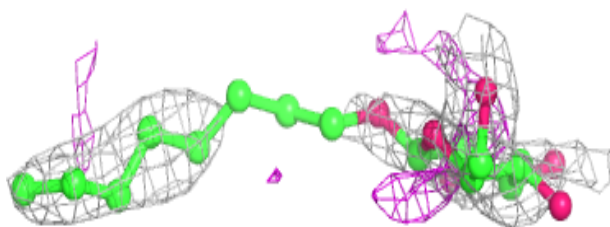
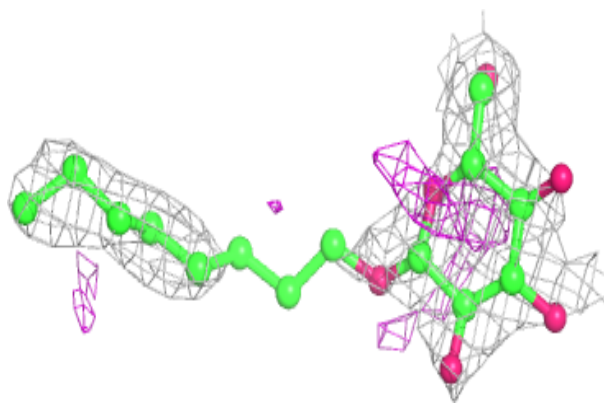
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



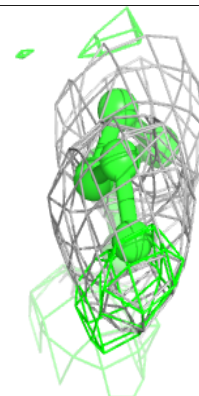
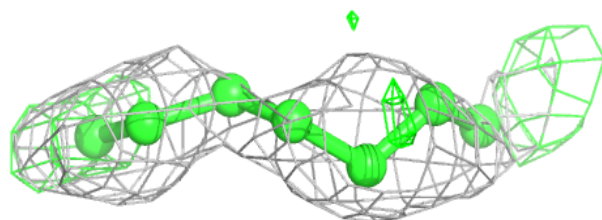
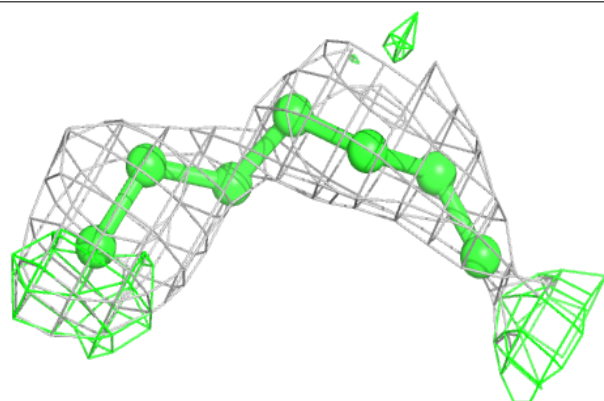


**Electron density around BOG A 315:**

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

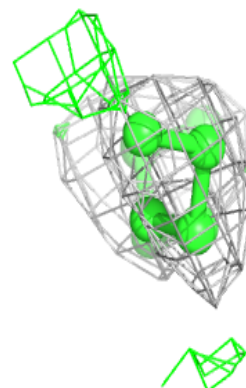
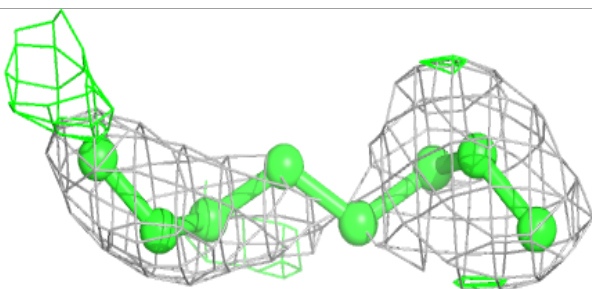
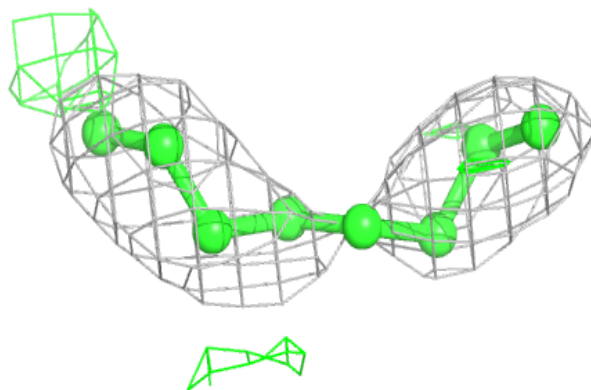
**Electron density around LFA D 314:**

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

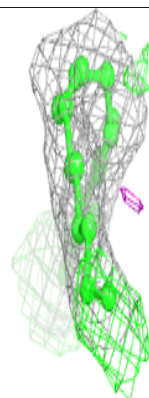
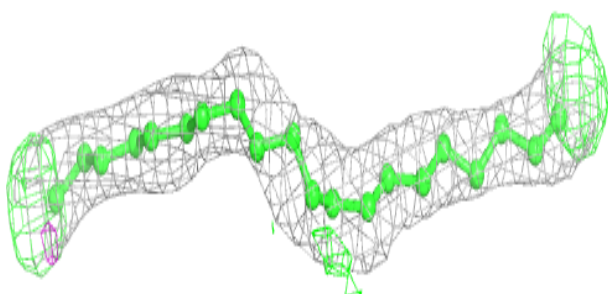
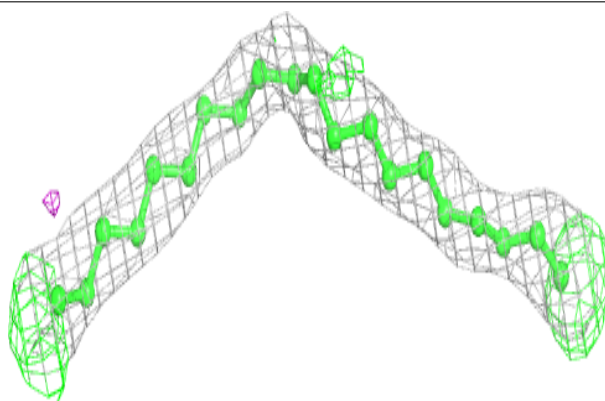


**Electron density around LFA D 312:**

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

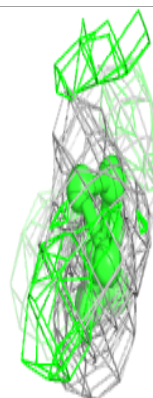
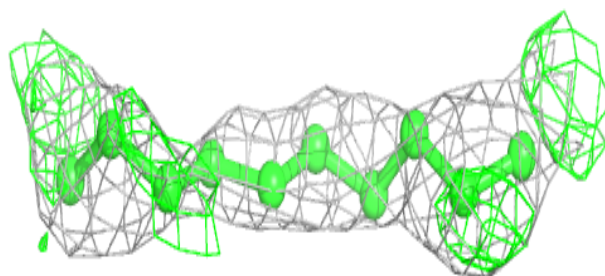
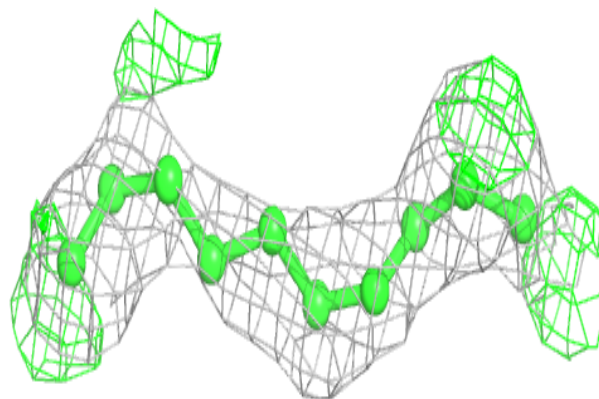
**Electron density around LFA D 301:**

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

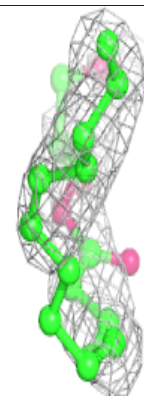
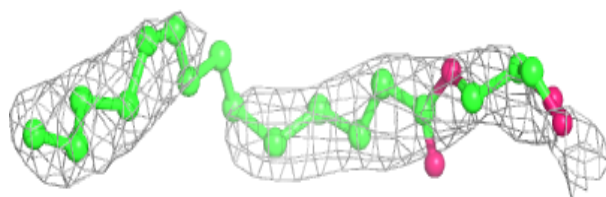
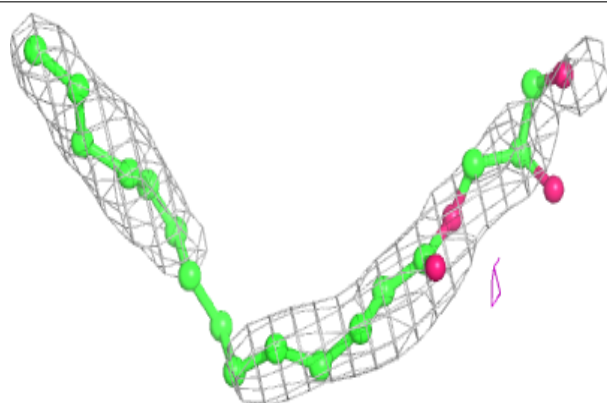


**Electron density around LFA B 310:**

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

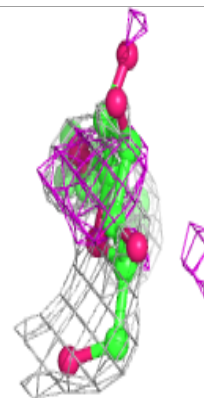
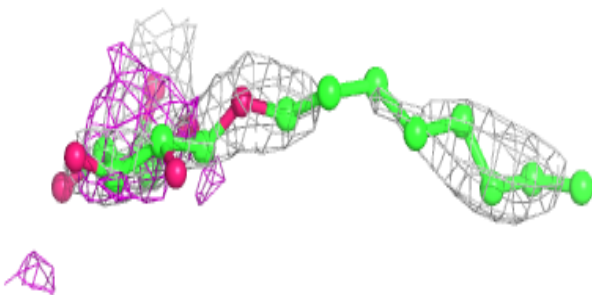
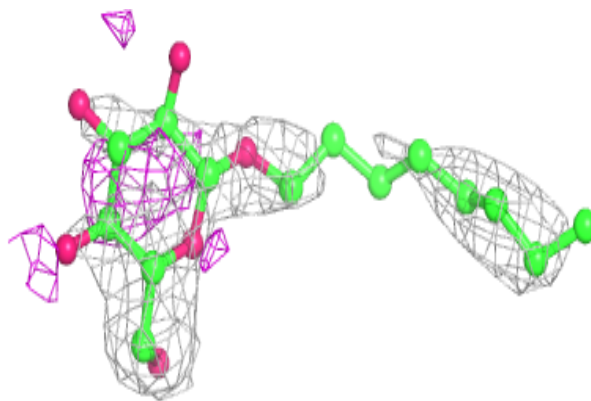
**Electron density around OLC B 305:**

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

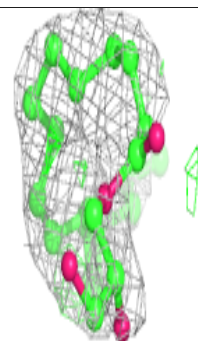
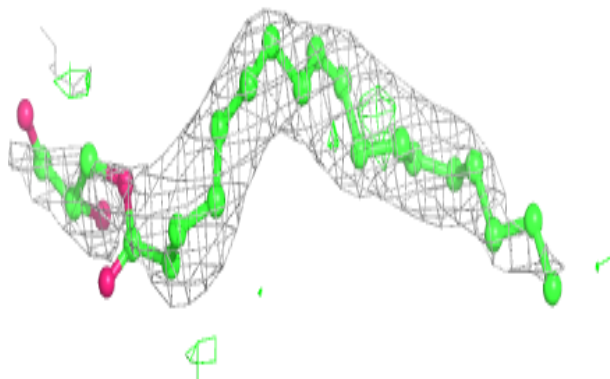
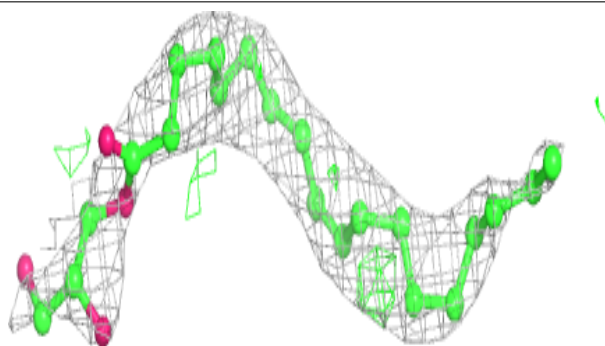


**Electron density around BOG B 312:**

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

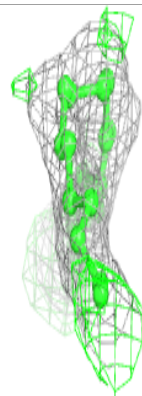
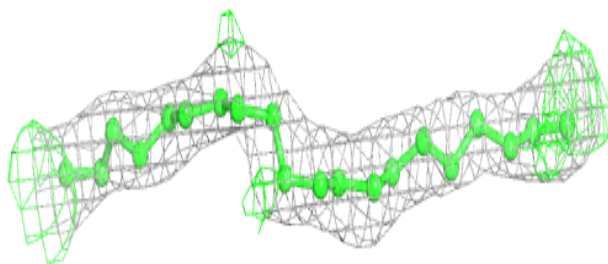
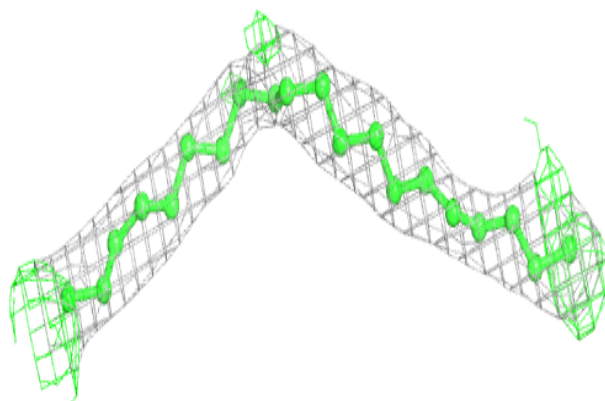
**Electron density around OLC E 302:**

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

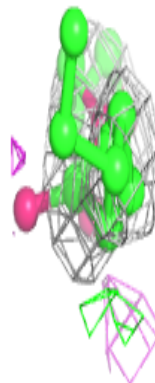
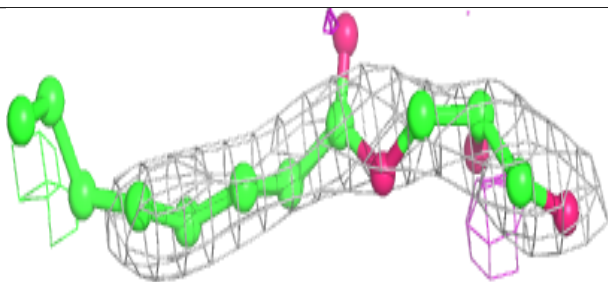
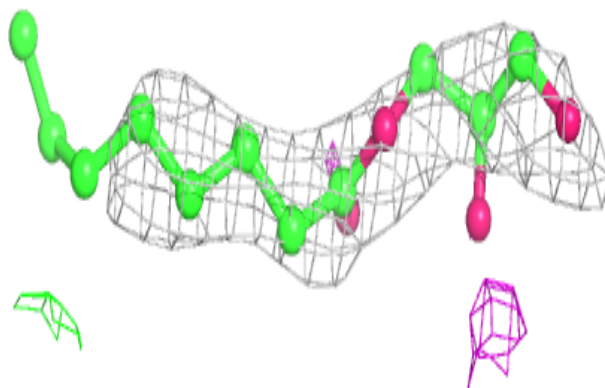


**Electron density around LFA C 304:**

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

**Electron density around OLC E 307:**

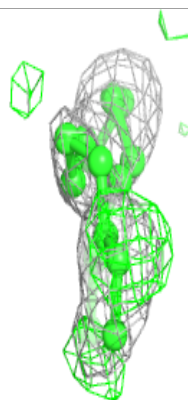
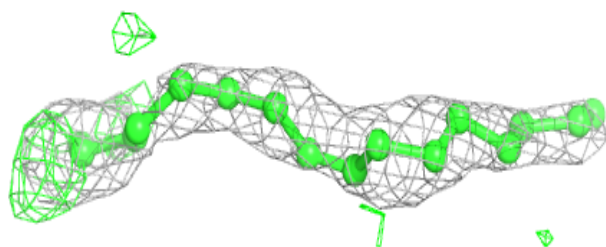
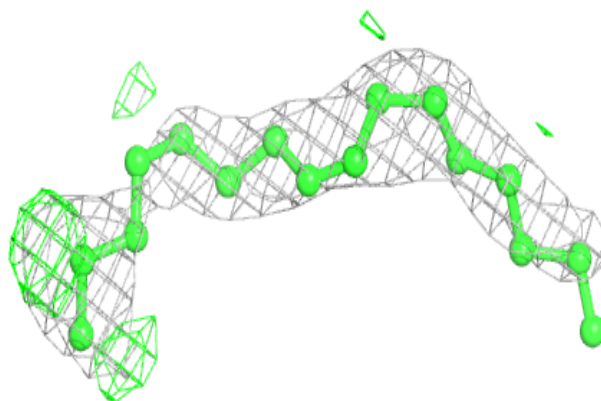
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



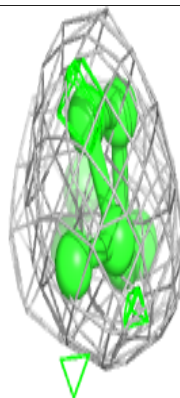
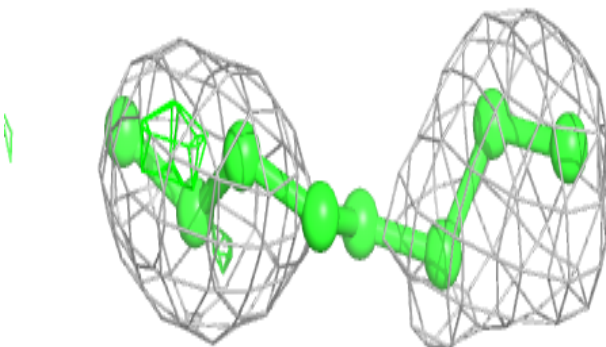
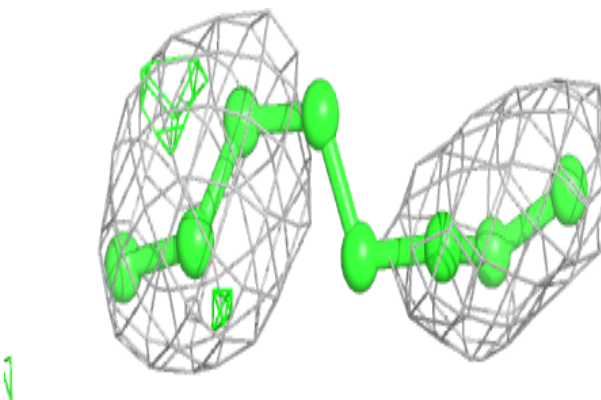


**Electron density around OLC E 305:**

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

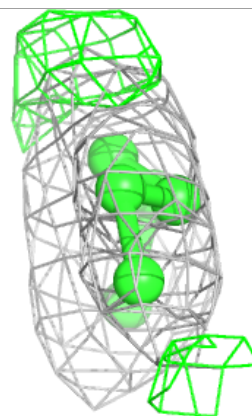
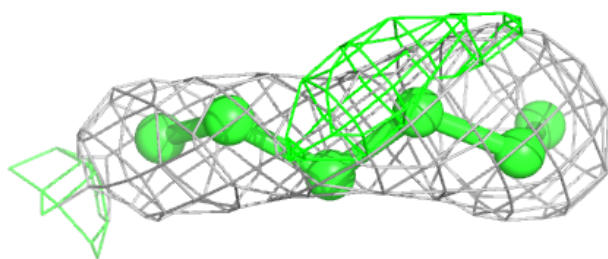
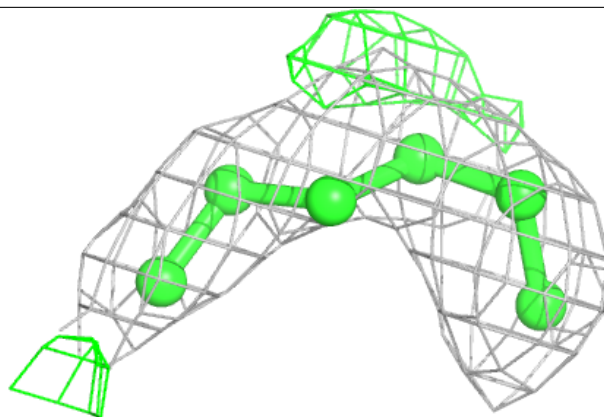
**Electron density around LFA A 311:**

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

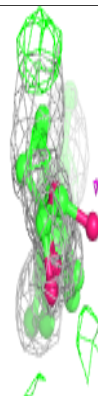
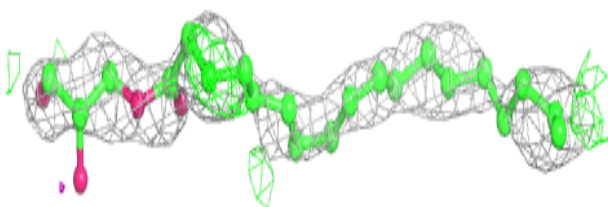
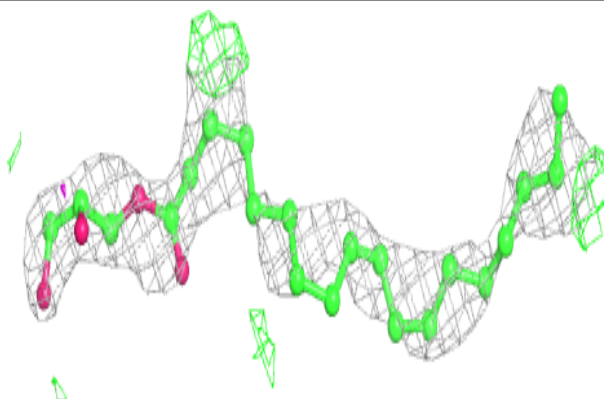


**Electron density around OLC E 309:**

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

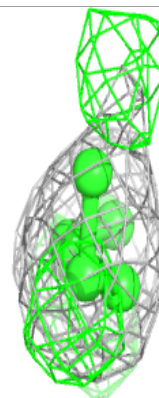
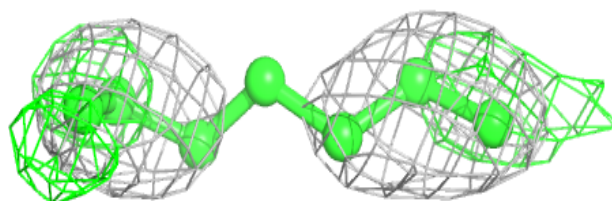
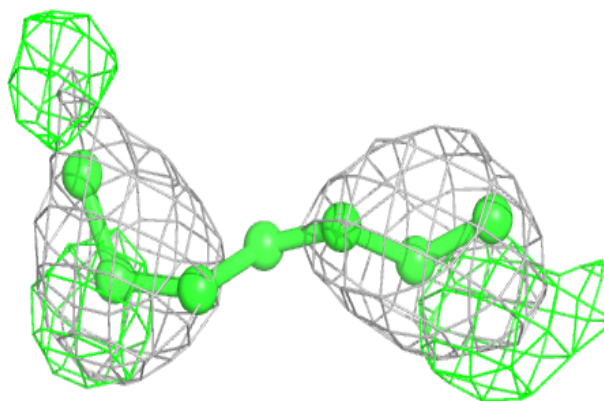
**Electron density around OLC A 303:**

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

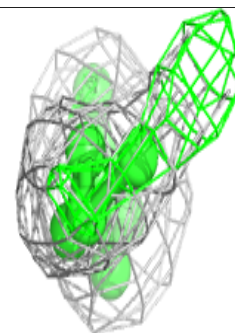
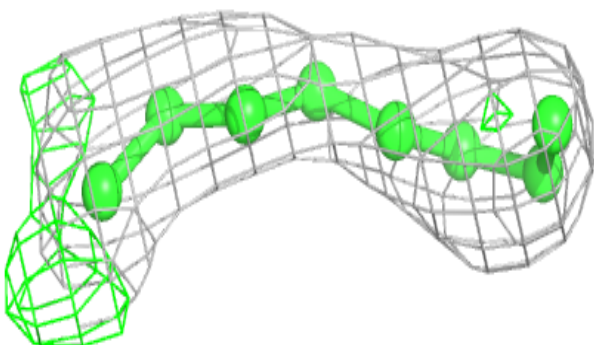
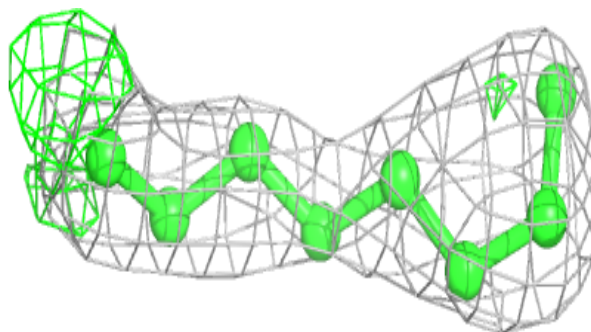


**Electron density around LFA B 311:**

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

**Electron density around LFA A 310:**

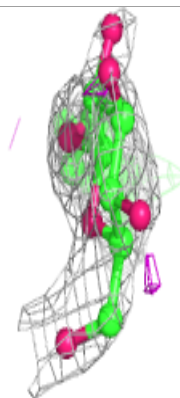
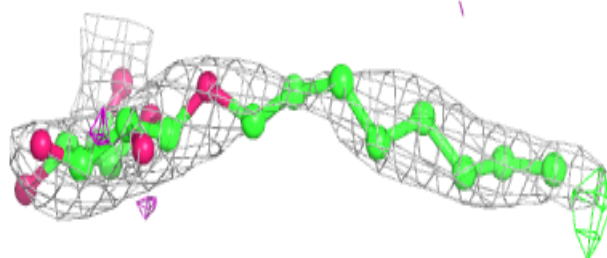
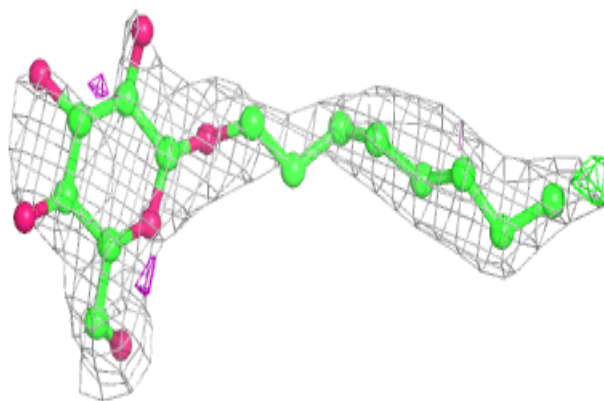
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



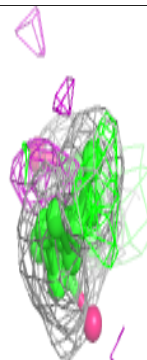
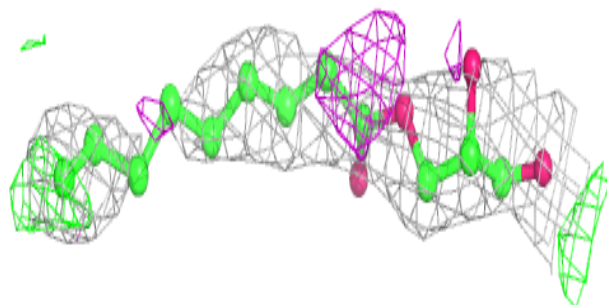
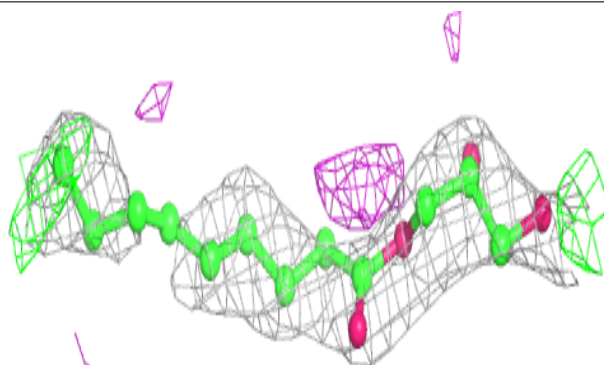


**Electron density around BOG E 316:**

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

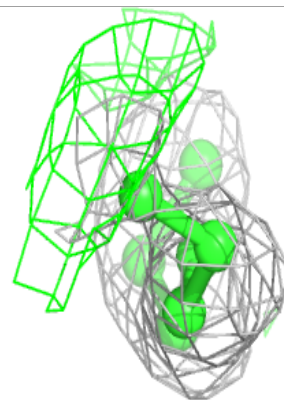
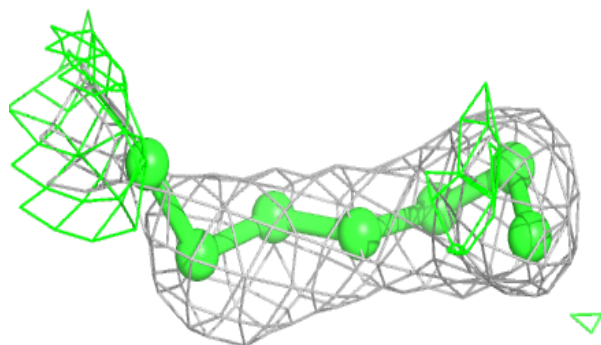
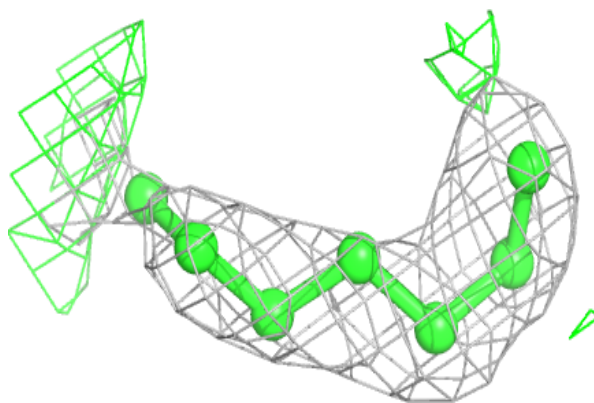
**Electron density around OLC D 302:**

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

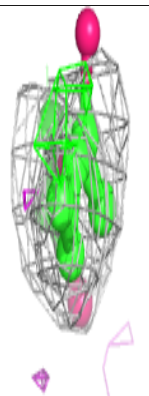
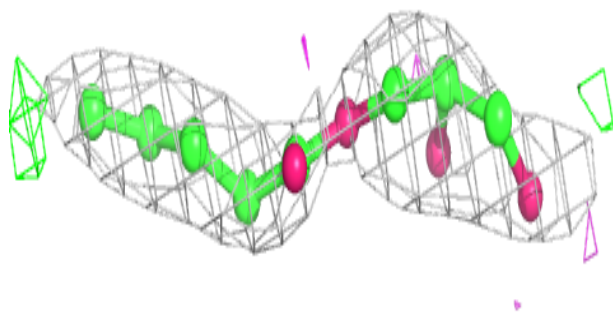
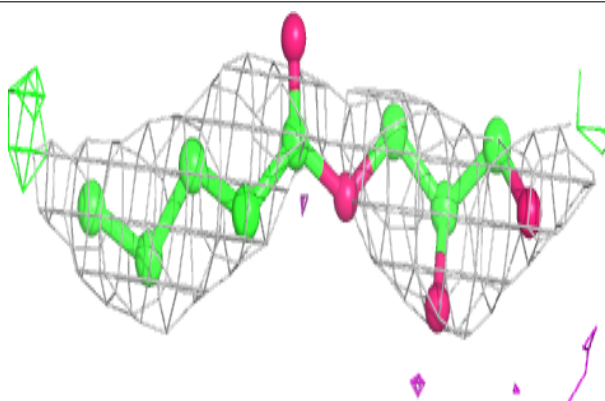


**Electron density around OLC D 308:**

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

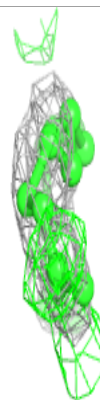
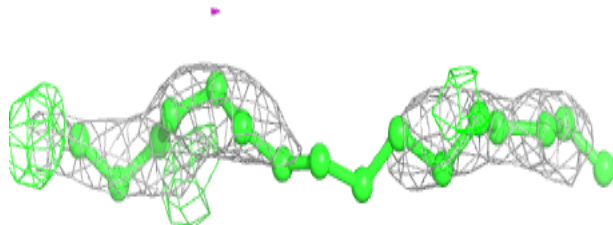
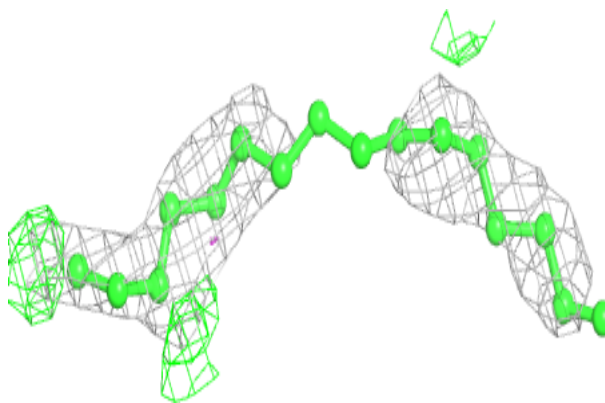
**Electron density around OLC C 303:**

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

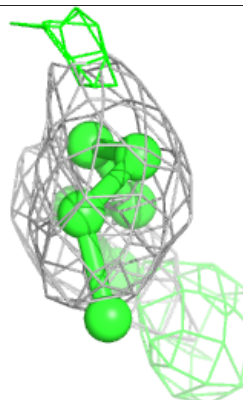
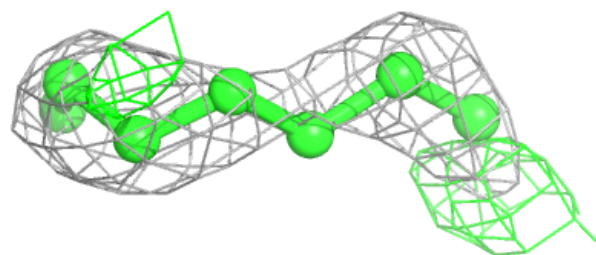
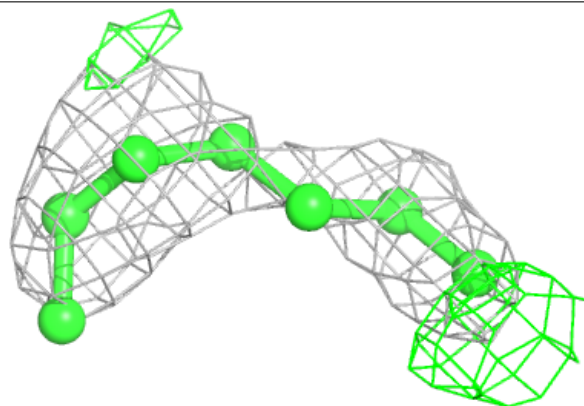


**Electron density around LFA A 314:**

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

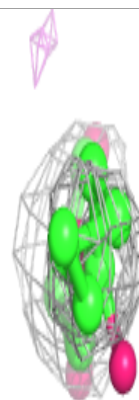
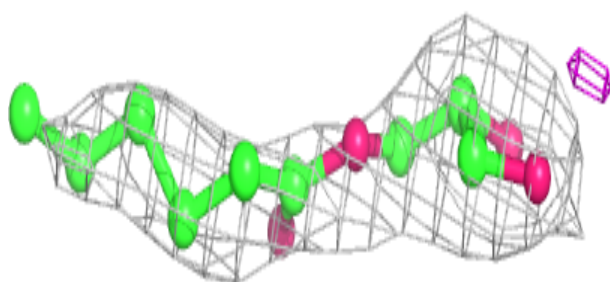
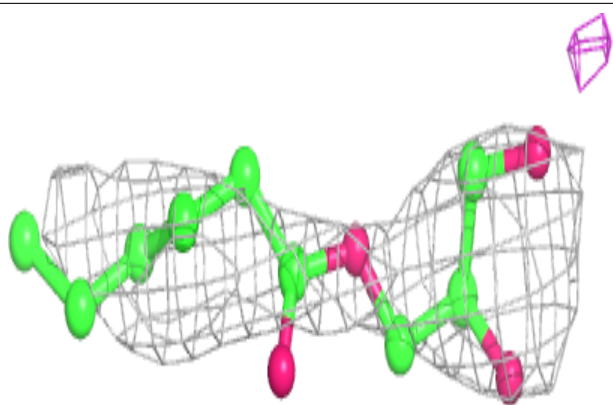
**Electron density around LFA A 309:**

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

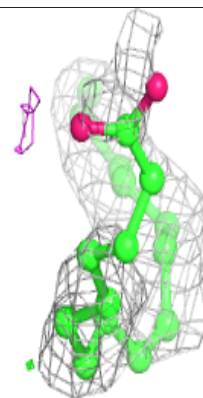
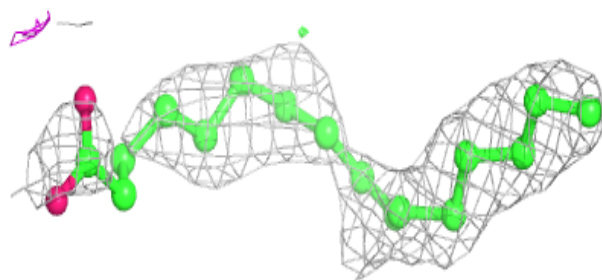
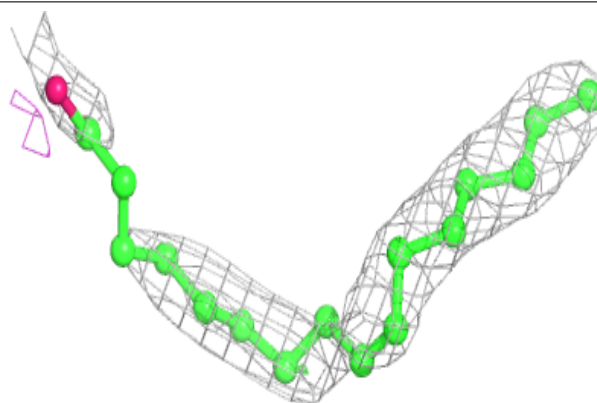


**Electron density around OLC D 303:**

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

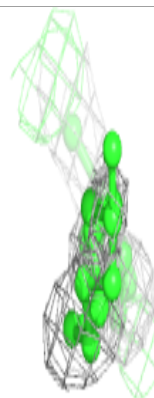
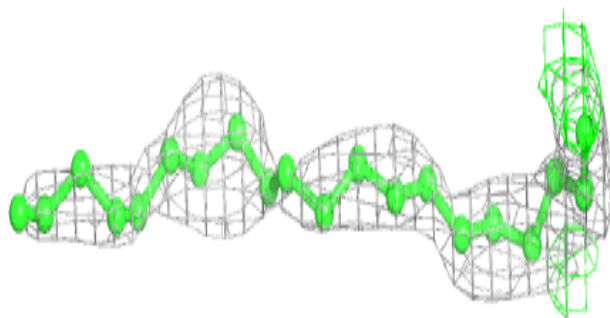
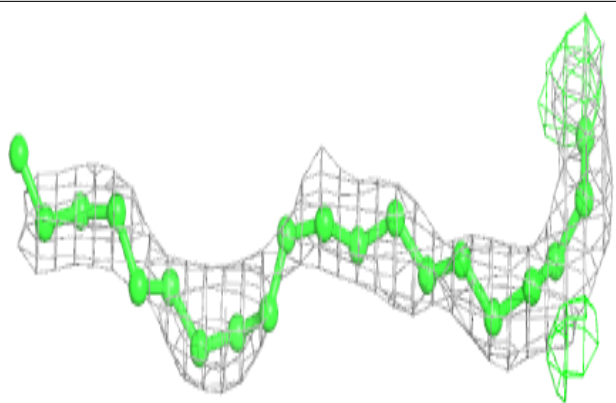
**Electron density around OLC D 306:**

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

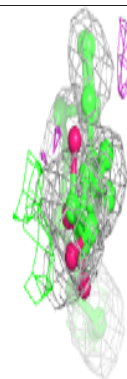
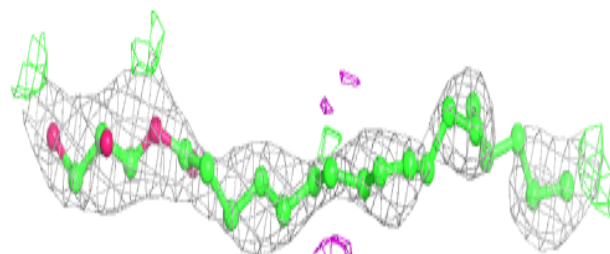
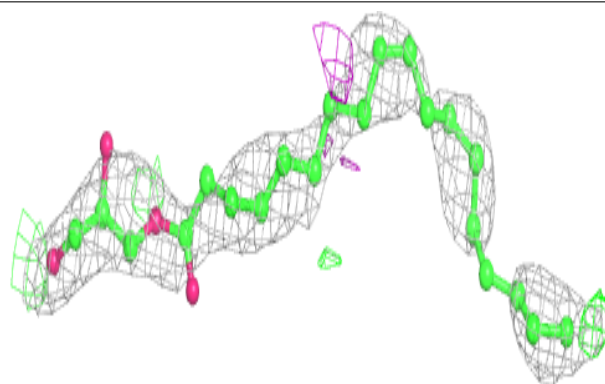


**Electron density around LFA D 310:**

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

**Electron density around OLC D 309:**

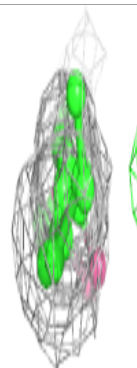
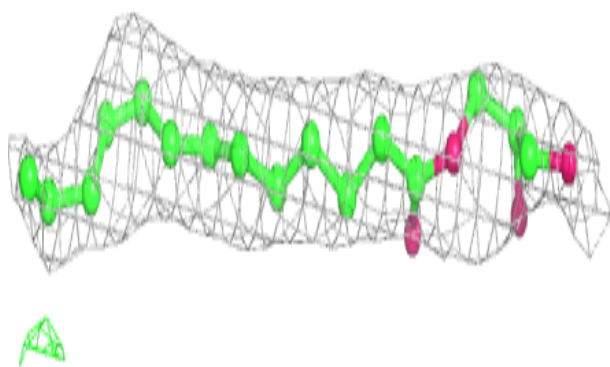
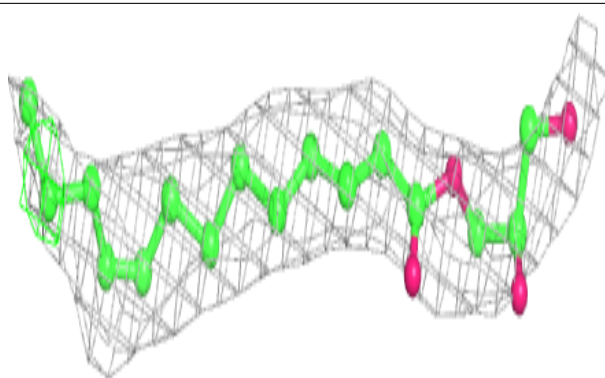
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



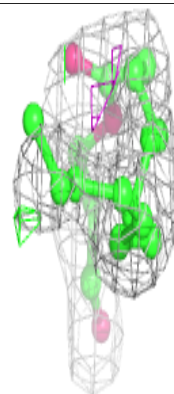
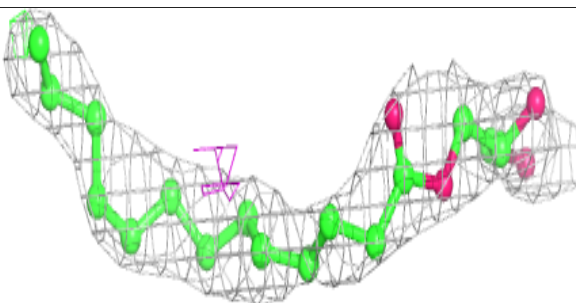
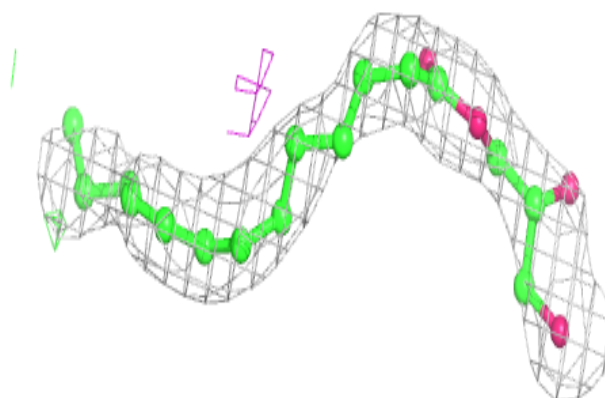


**Electron density around OLC B 304:**

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

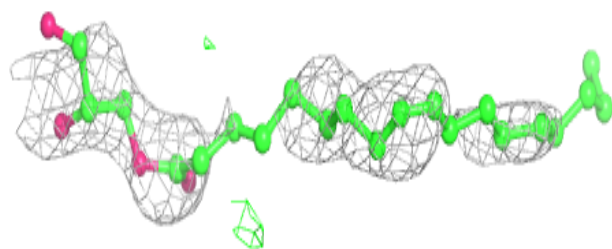
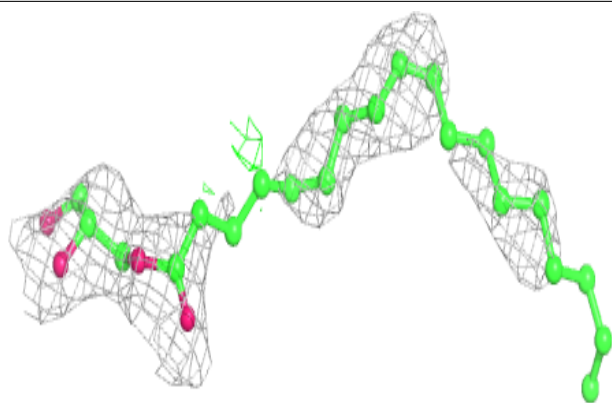
**Electron density around OLC C 302:**

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

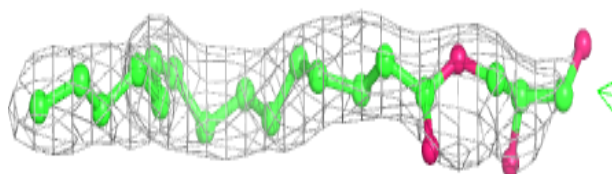
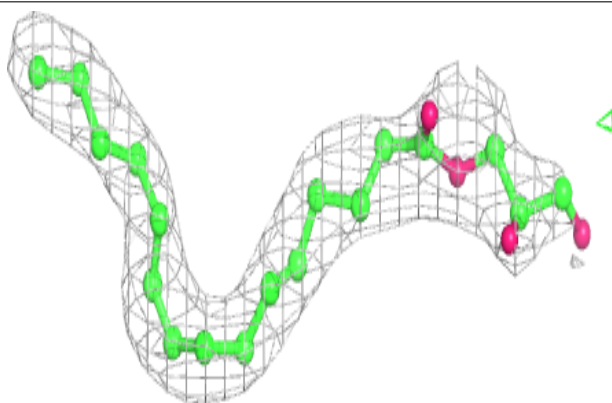


**Electron density around OLC D 304:**

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

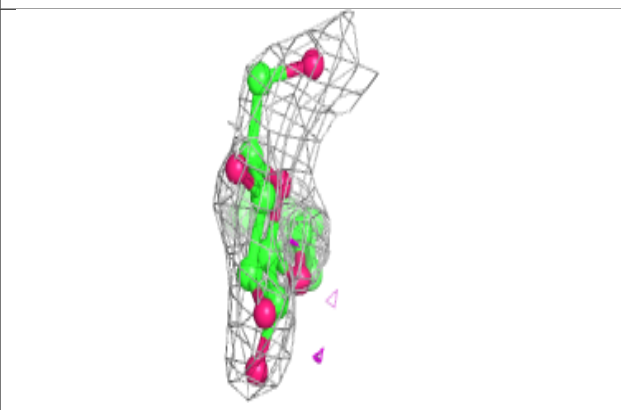
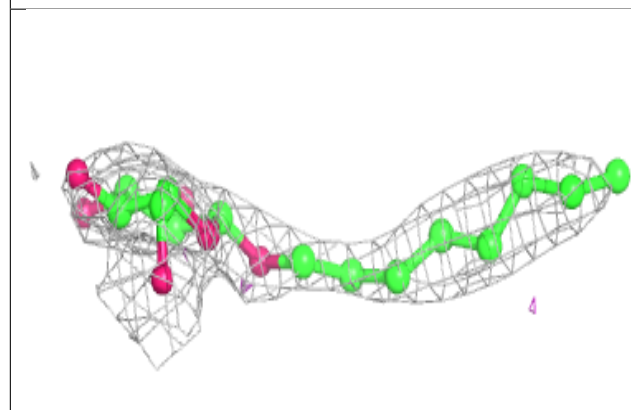
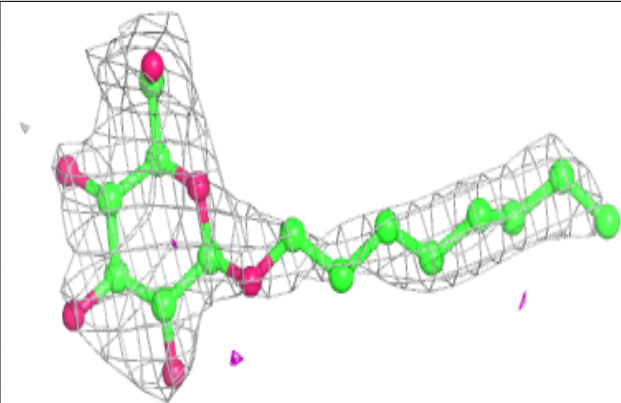
**Electron density around OLC A 302:**

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

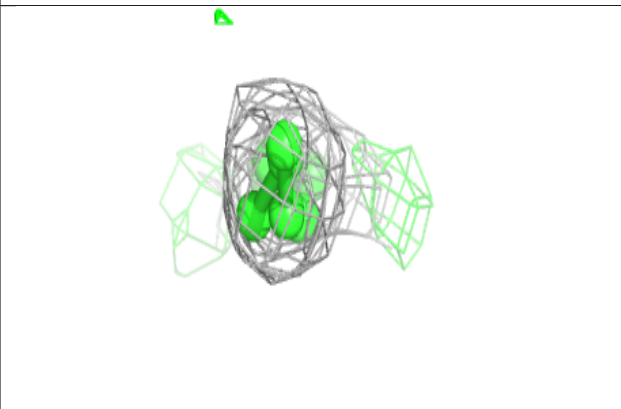
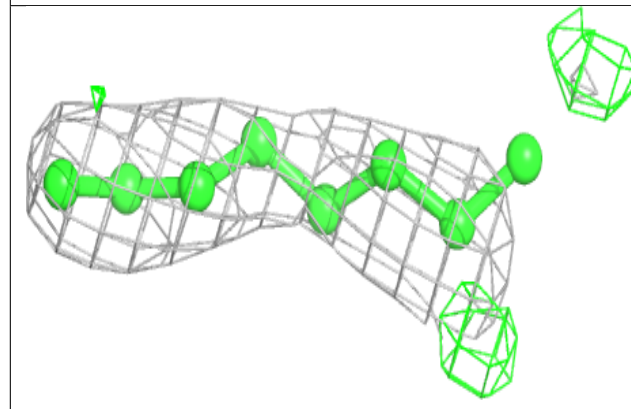
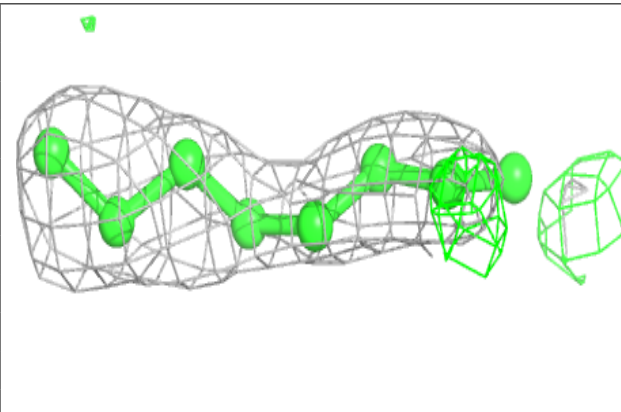


**Electron density around BOG C 316:**

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

**Electron density around LFA B 309:**

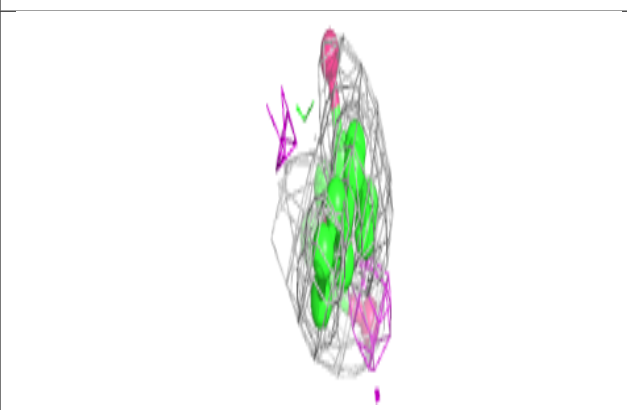
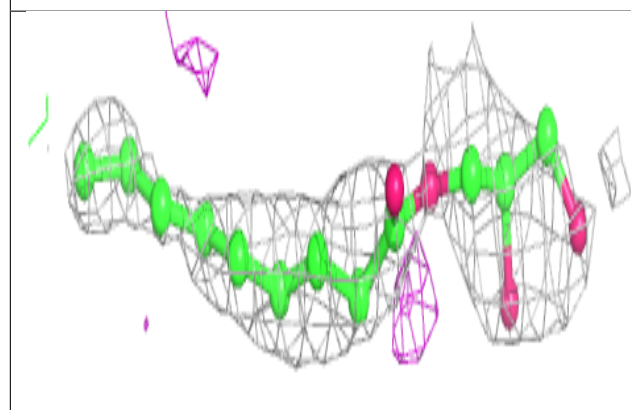
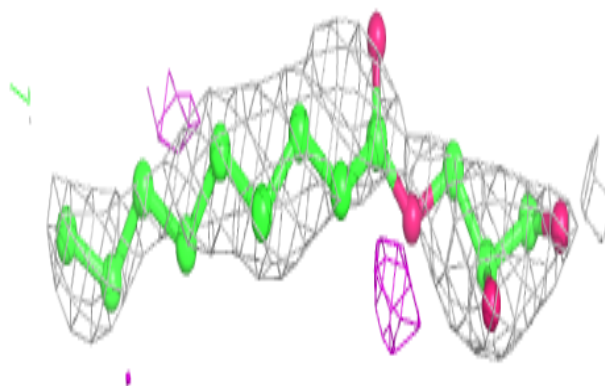
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



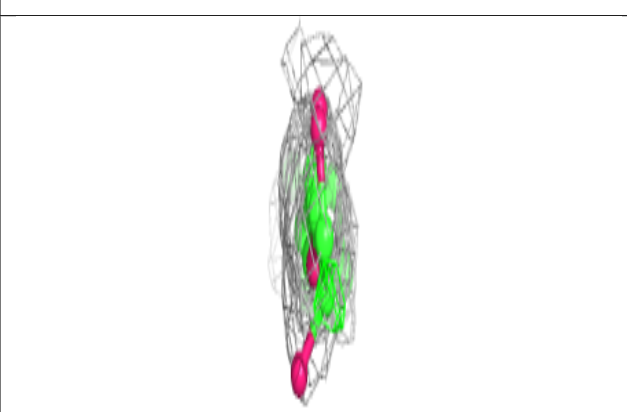
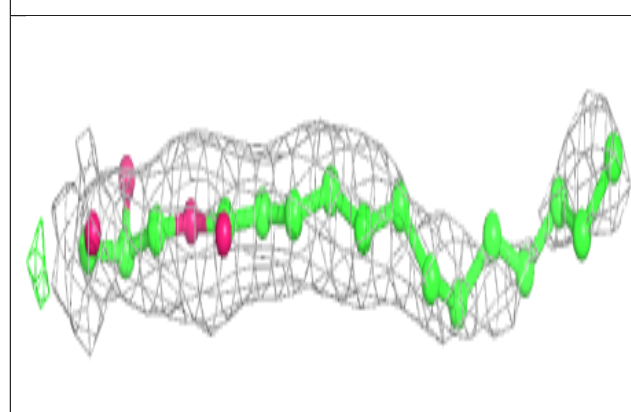
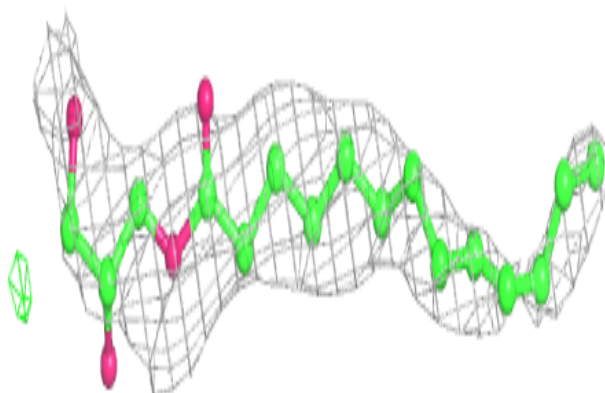


**Electron density around OLC A 308:**

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

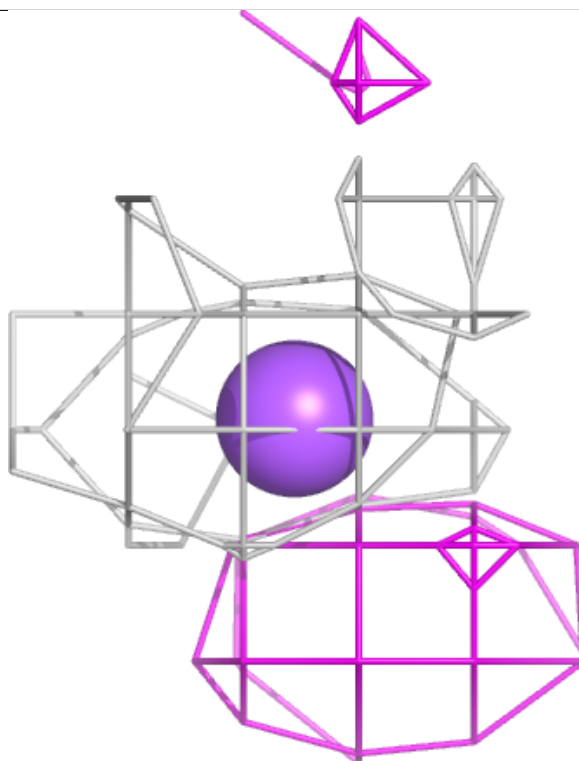
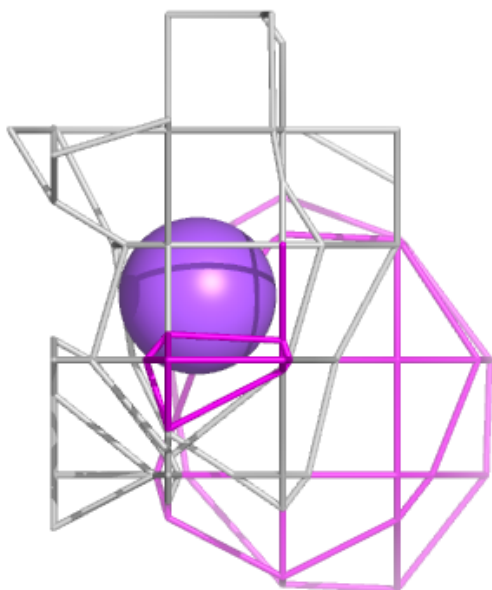
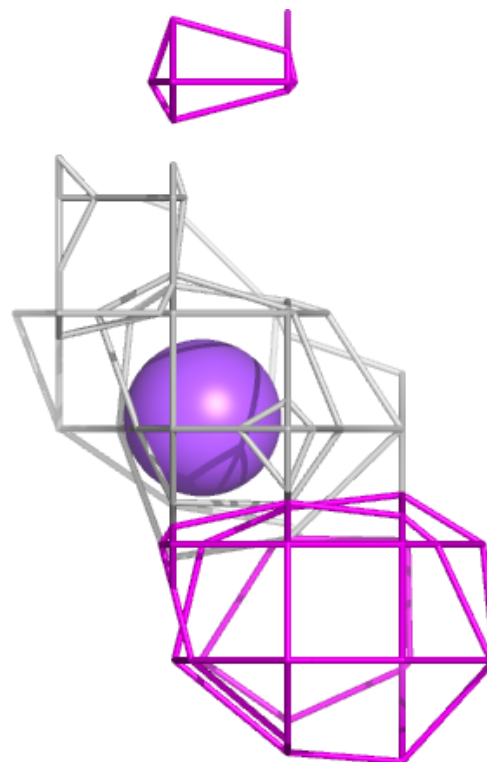
**Electron density around OLC C 307:**

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



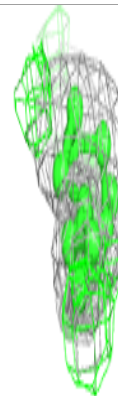
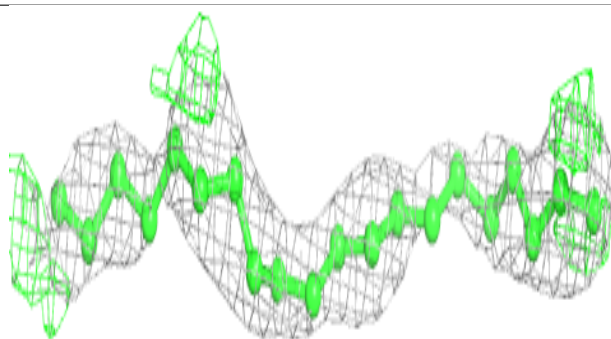
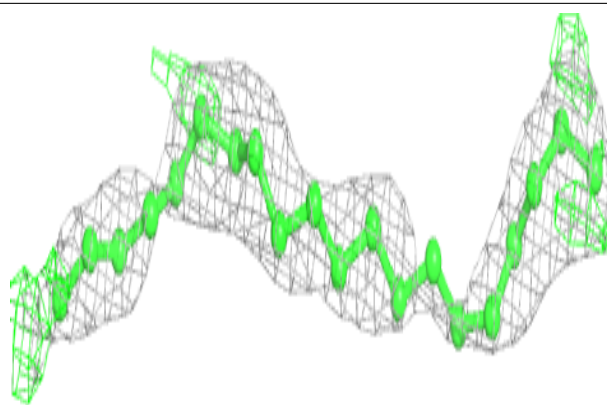
**Electron density around NA B 316:**

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

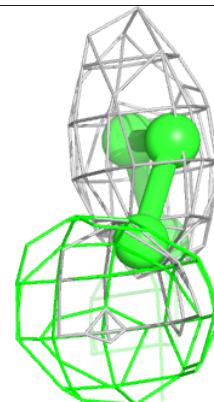
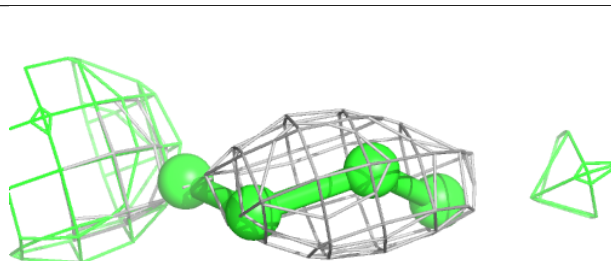
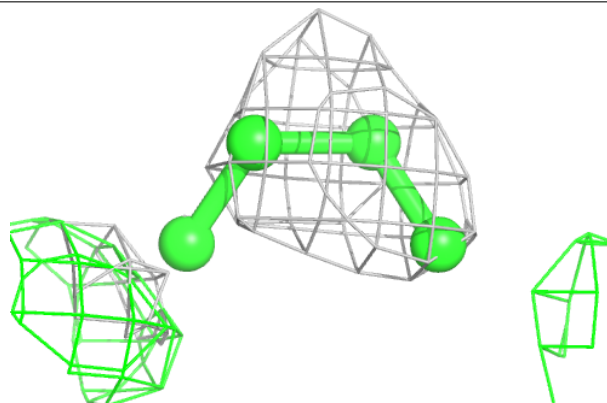


**Electron density around LFA D 311:**

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

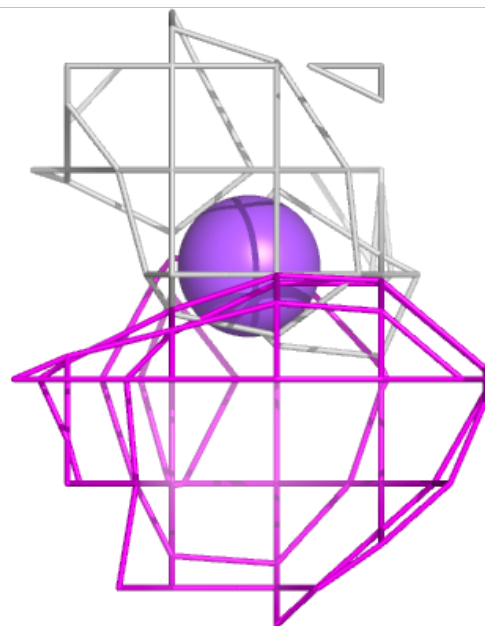
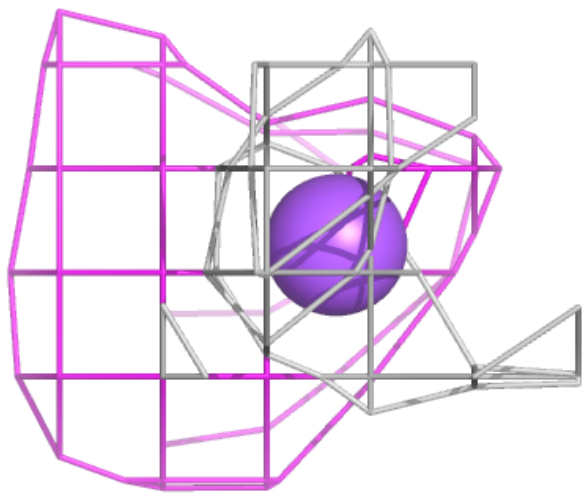
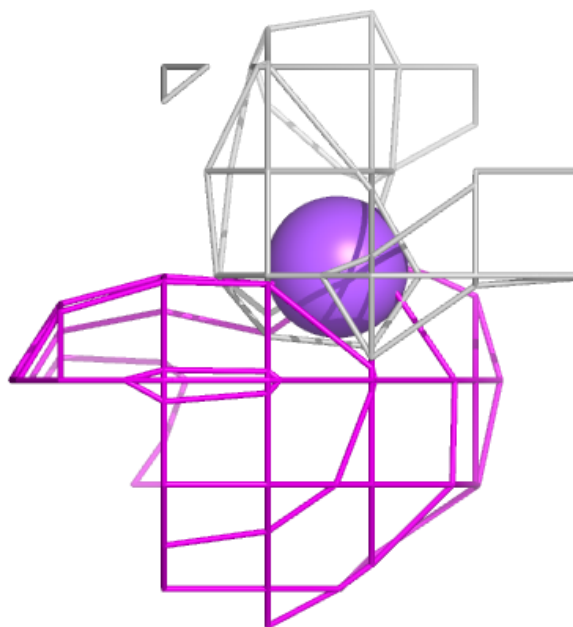
**Electron density around LFA C 315:**

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



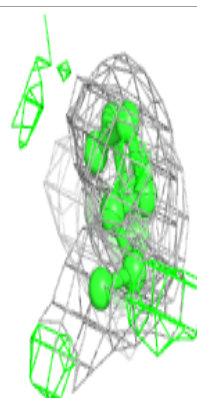
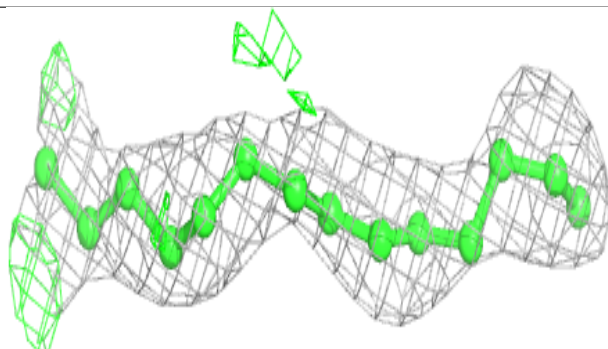
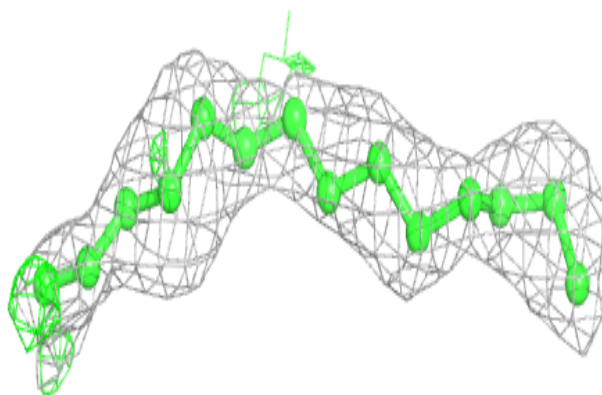
**Electron density around NA E 319:**

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

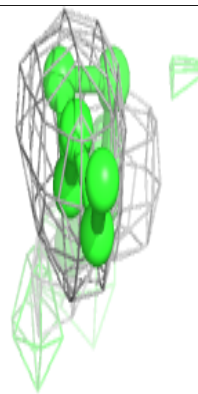
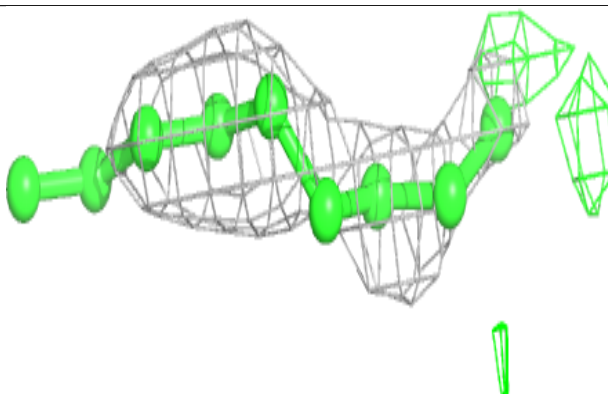
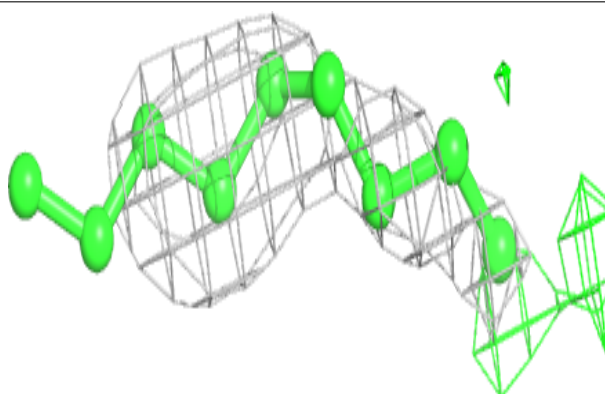


**Electron density around LFA E 313:**

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

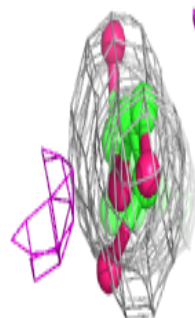
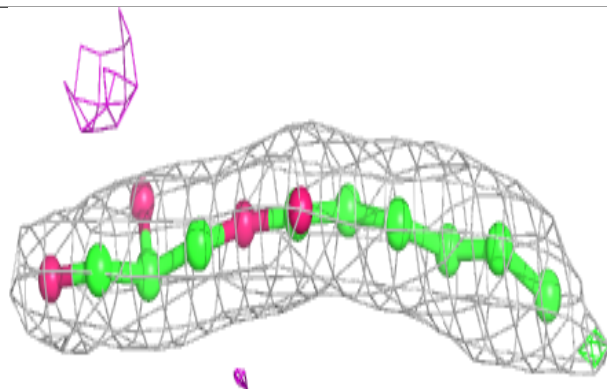
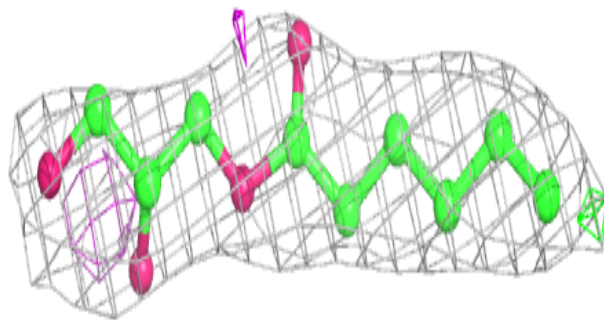
**Electron density around LFA B 308:**

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

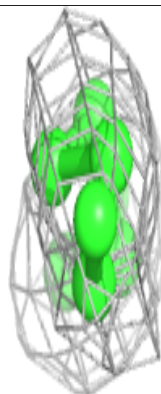
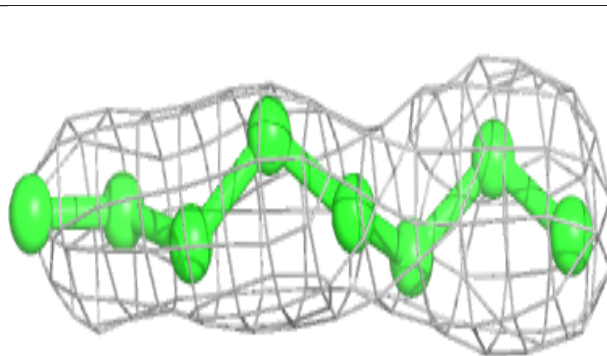
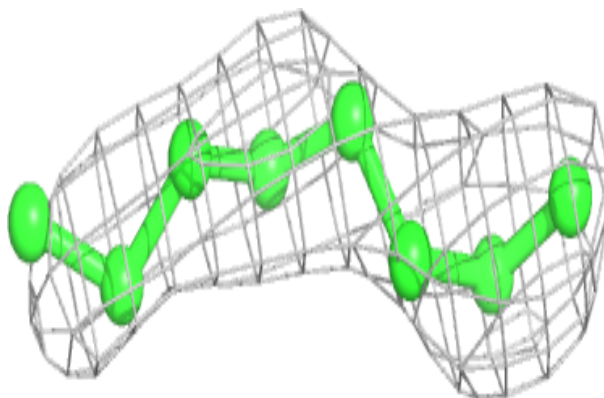


**Electron density around OLC A 304:**

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

**Electron density around LFA C 312:**

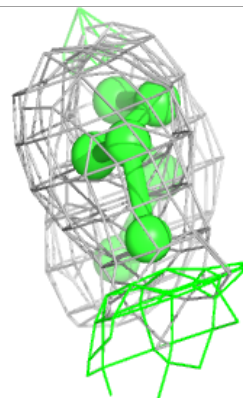
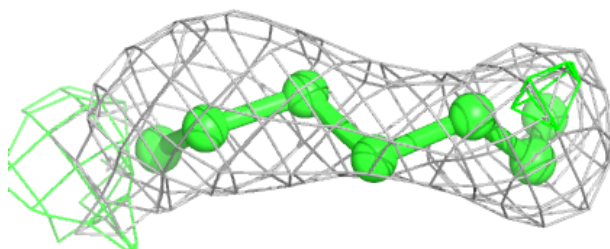
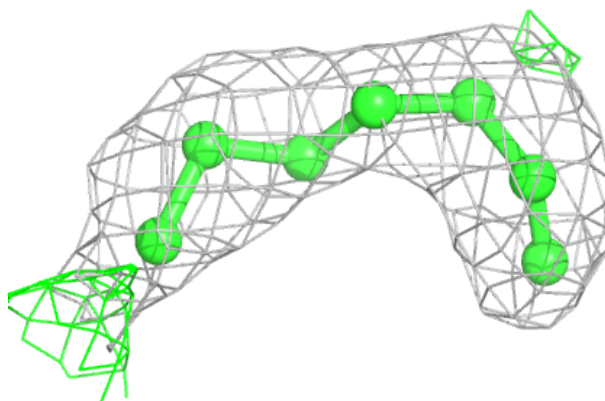
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



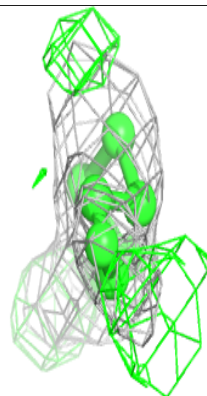
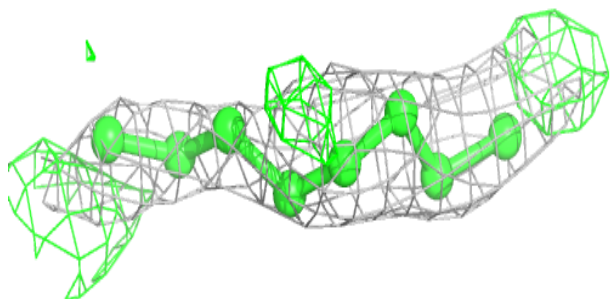
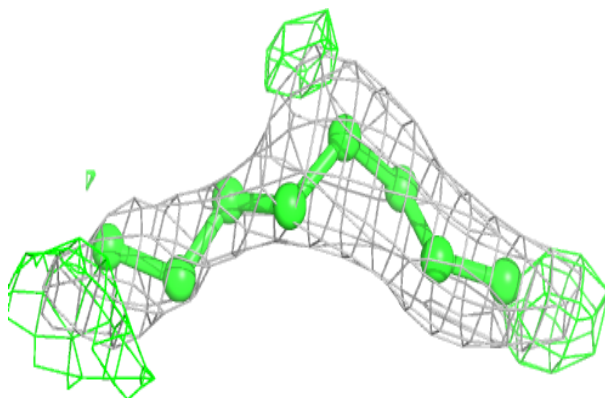


**Electron density around OLC B 307:**

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

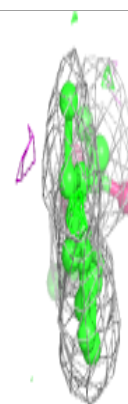
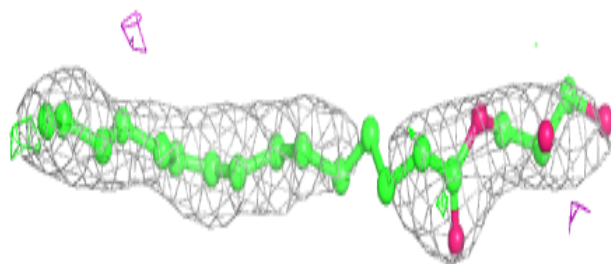
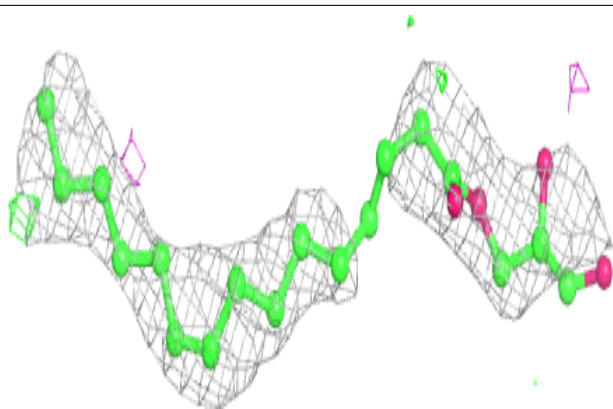
**Electron density around OLC E 304:**

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

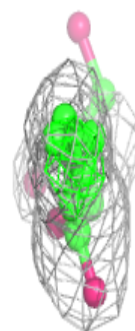
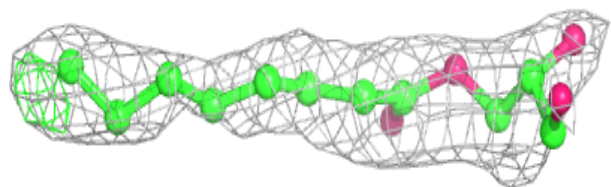
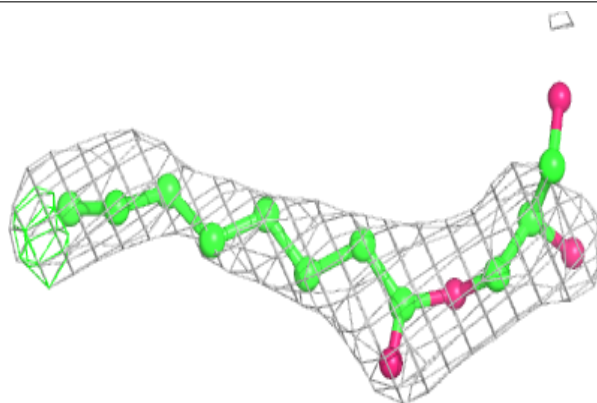


**Electron density around OLC C 306:**

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

**Electron density around OLC A 306:**

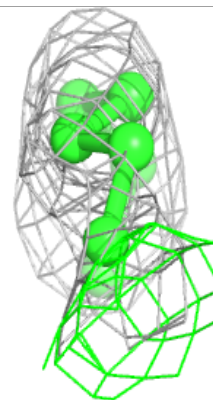
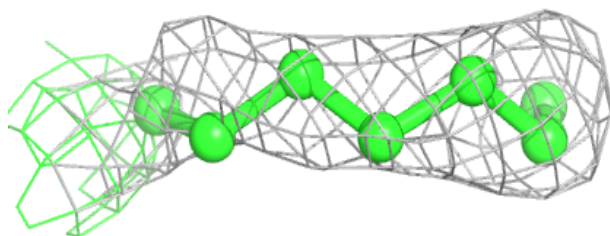
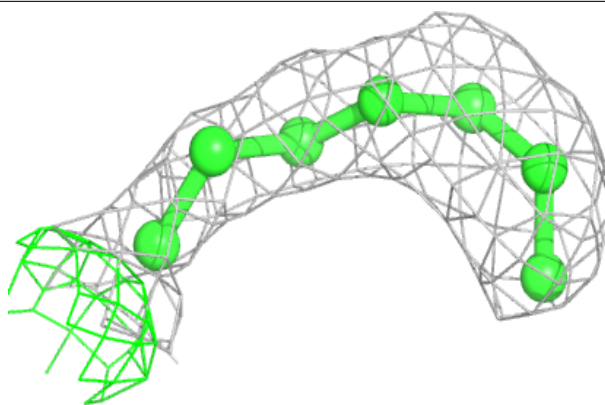
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



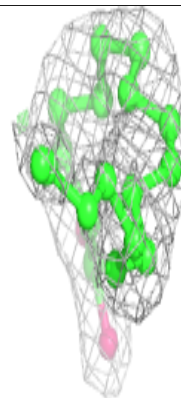
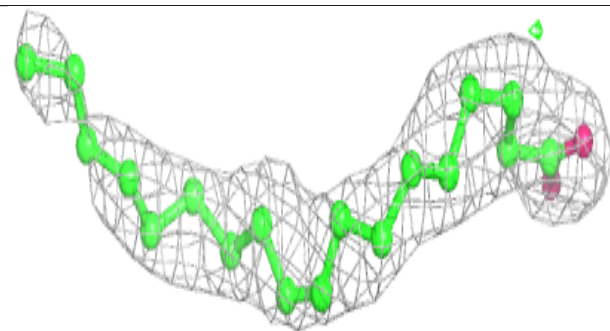
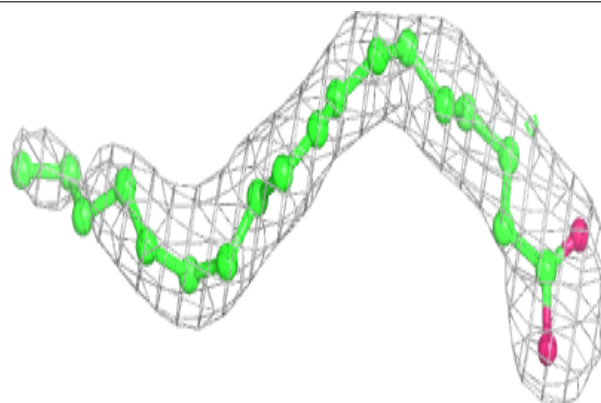


**Electron density around OLC C 310:**

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

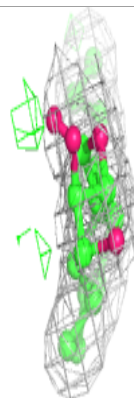
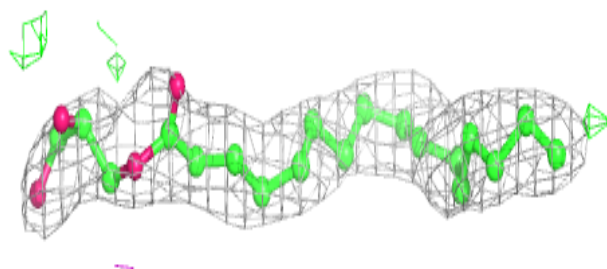
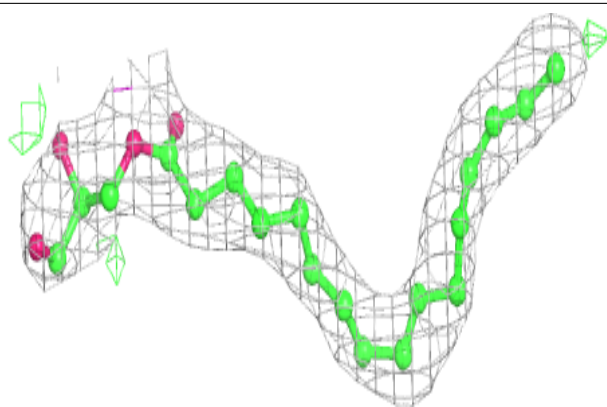
**Electron density around OLC A 317:**

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

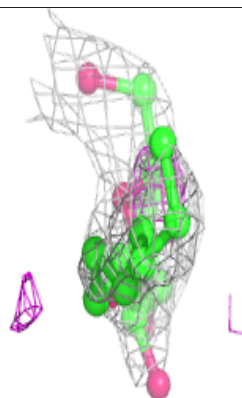
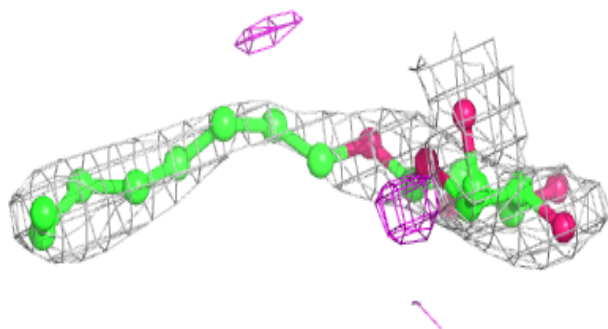
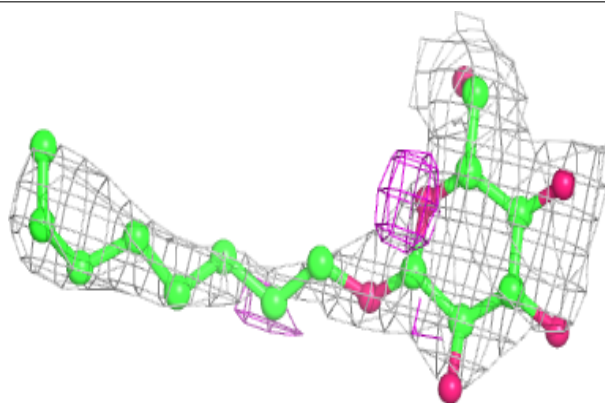


**Electron density around OLC C 305:**

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

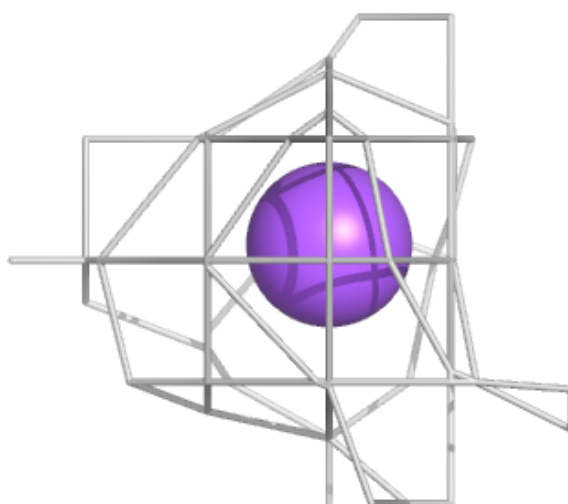
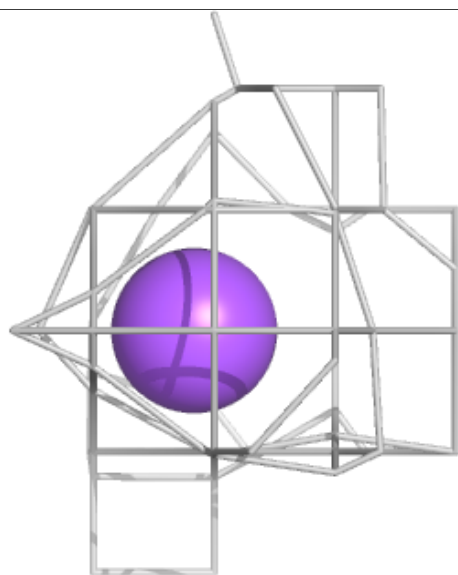
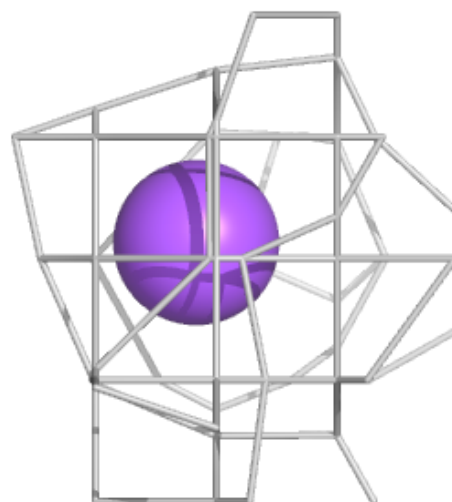
**Electron density around BOG D 316:**

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



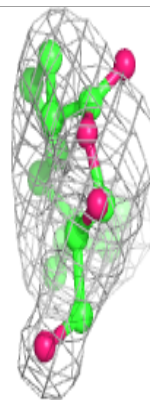
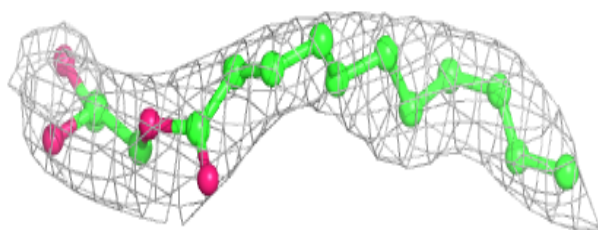
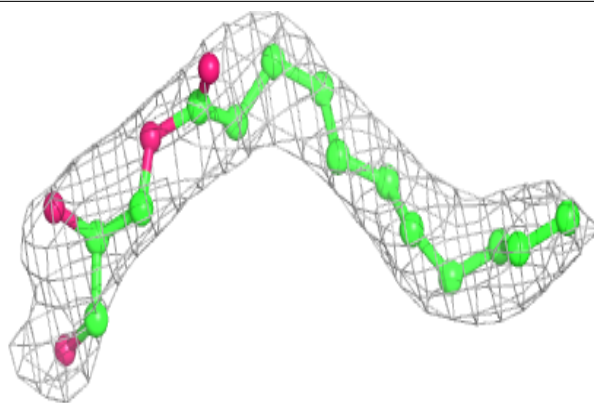
**Electron density around NA C 320:**

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

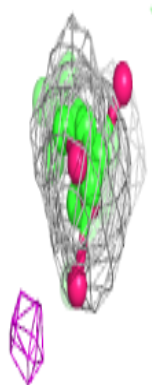
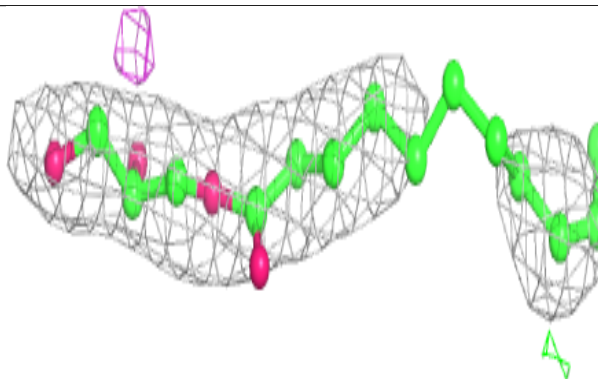
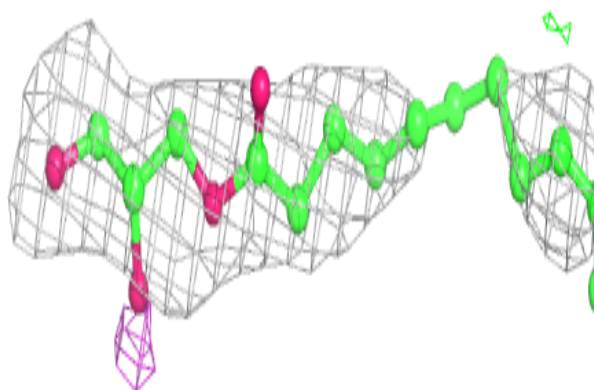


**Electron density around OLC C 318:**

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

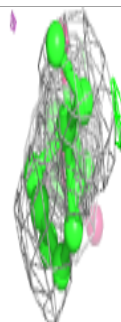
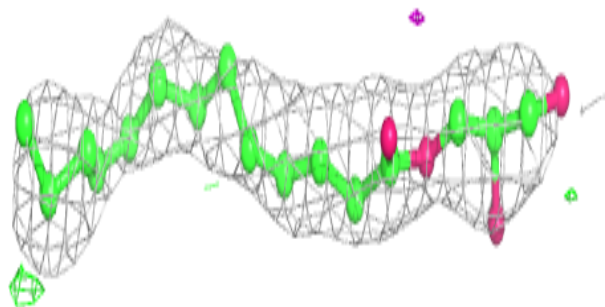
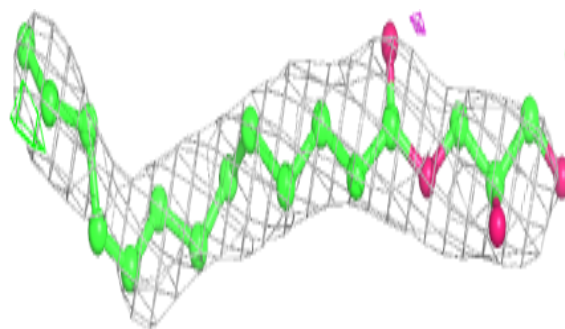
**Electron density around OLC D 305:**

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

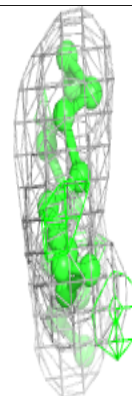
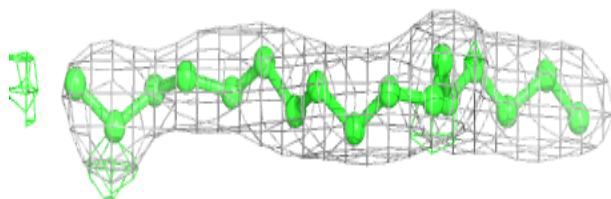
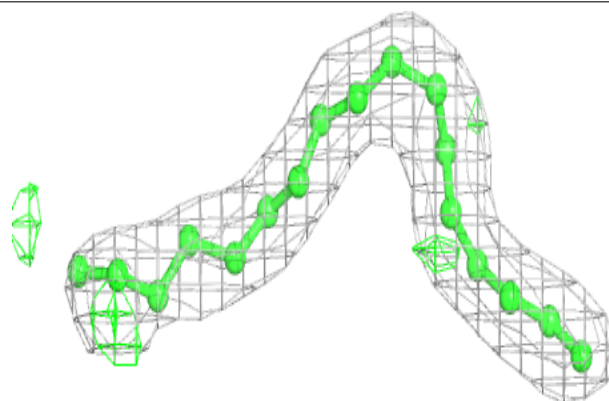


**Electron density around OLC E 306:**

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

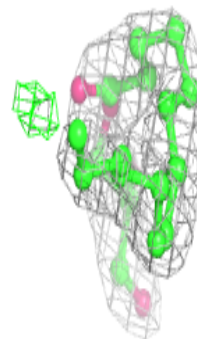
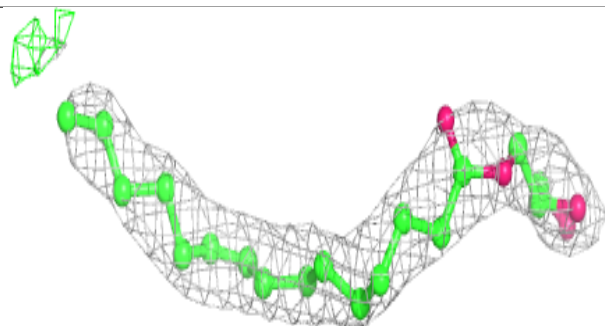
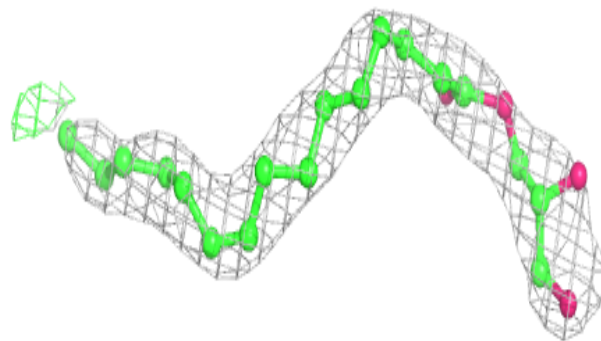
**Electron density around LFA D 313:**

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

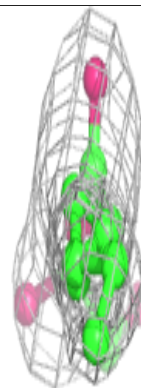
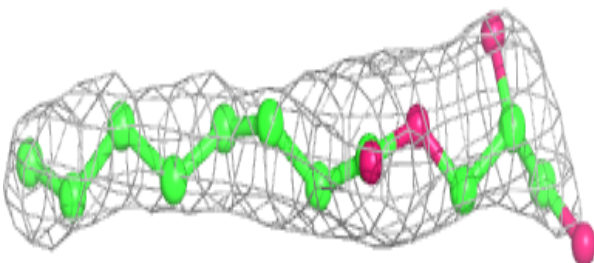
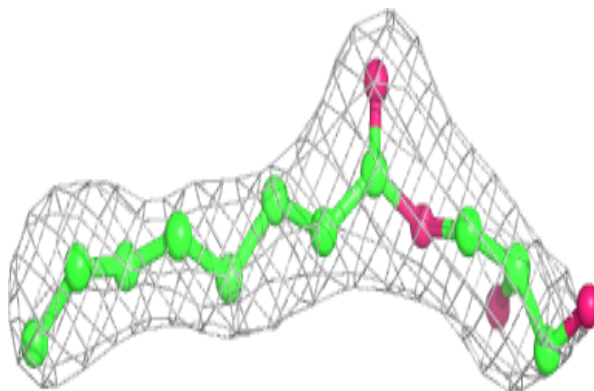


**Electron density around OLC B 301:**

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

**Electron density around OLC E 308:**

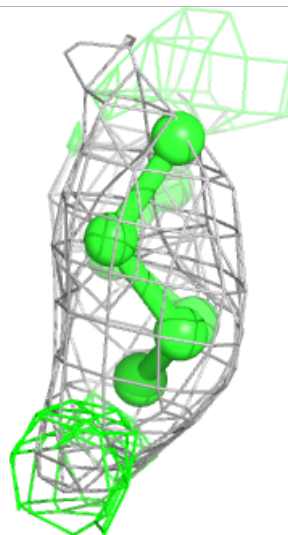
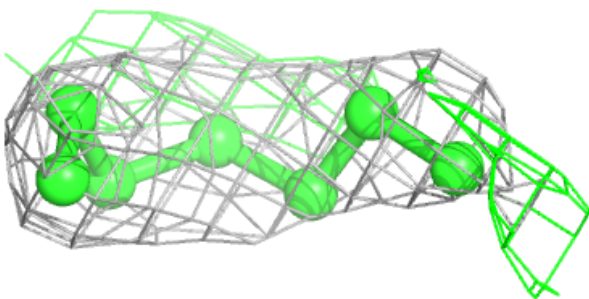
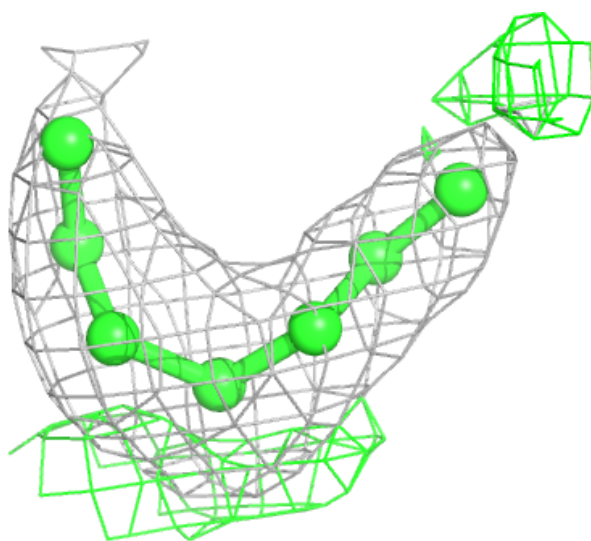
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





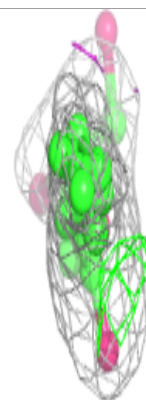
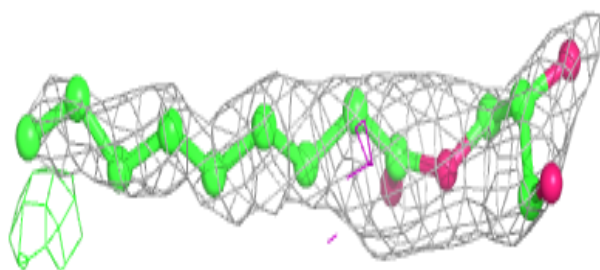
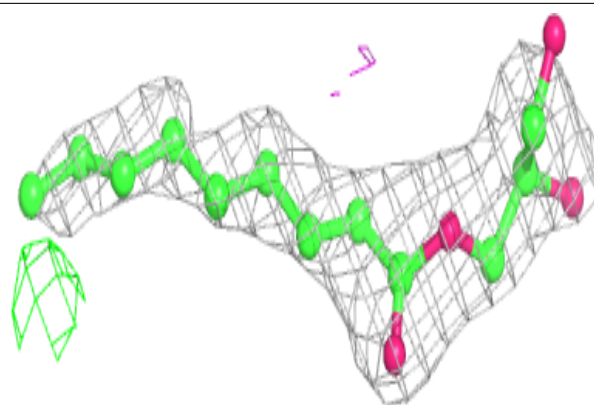
**Electron density around OLC A 307:**

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

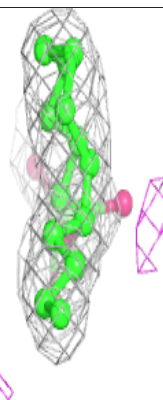
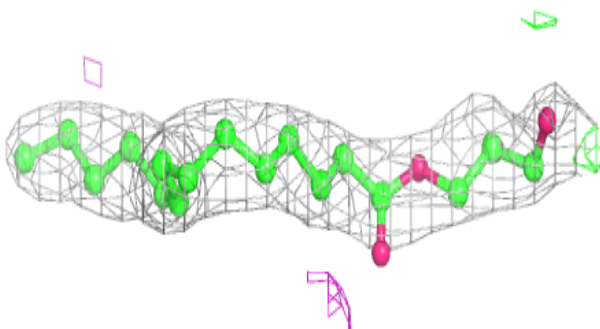
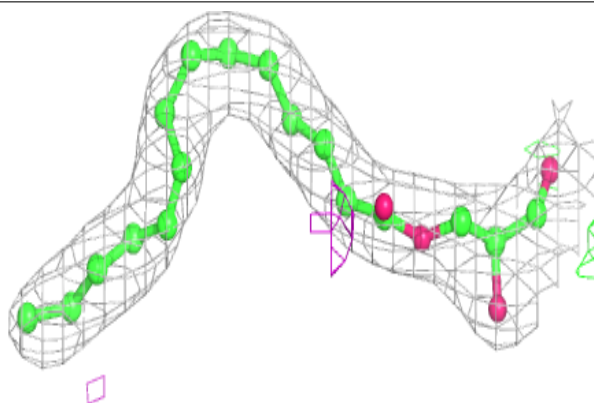


**Electron density around OLC B 306:**

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

**Electron density around OLC C 301:**

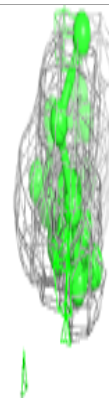
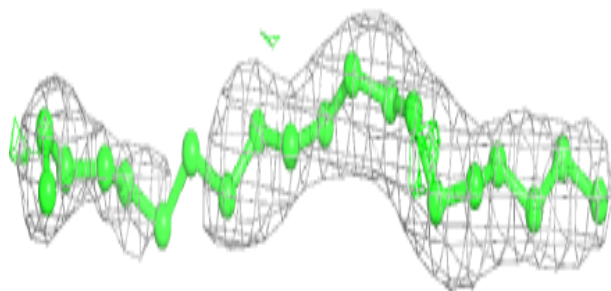
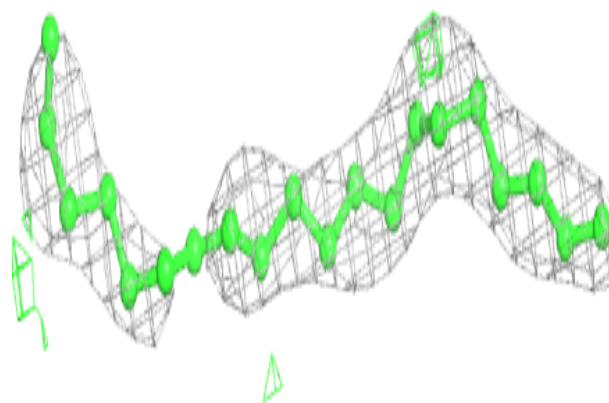
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



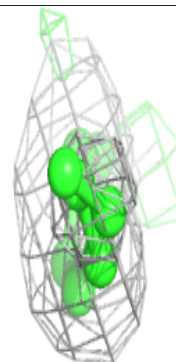
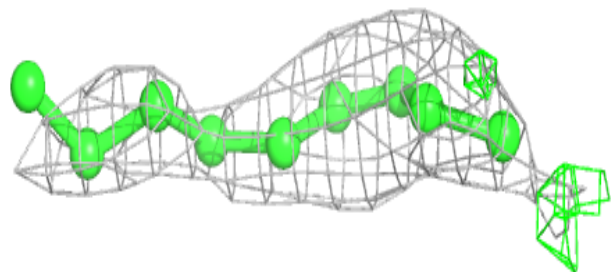
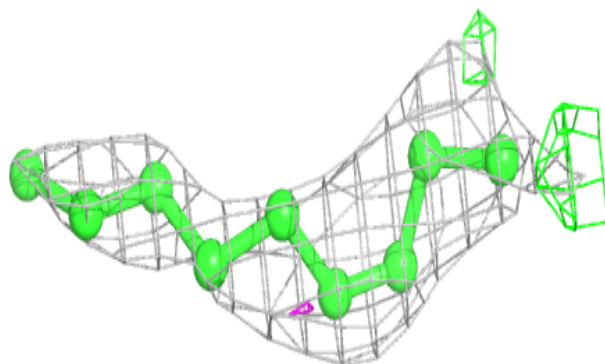


**Electron density around LFA C 313:**

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

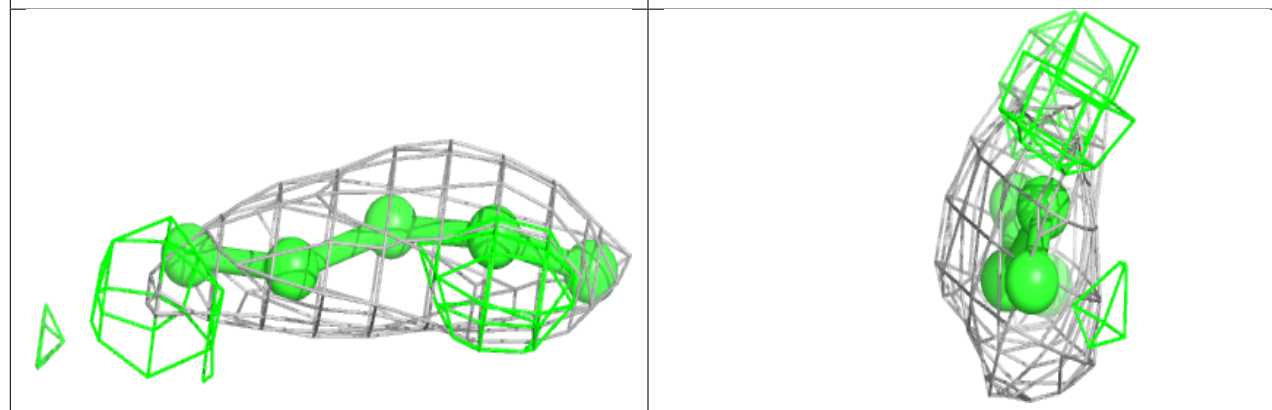
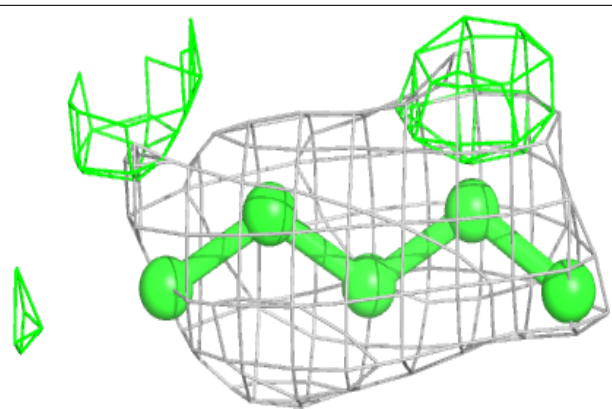
**Electron density around OLC A 301:**

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



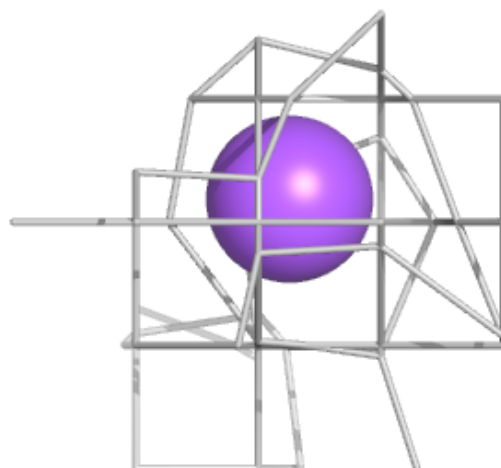
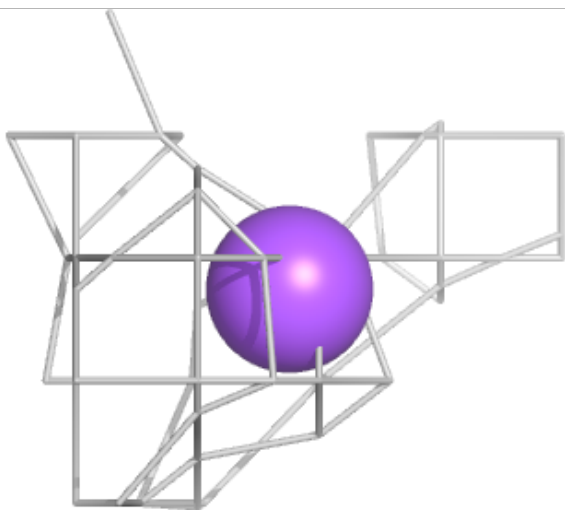
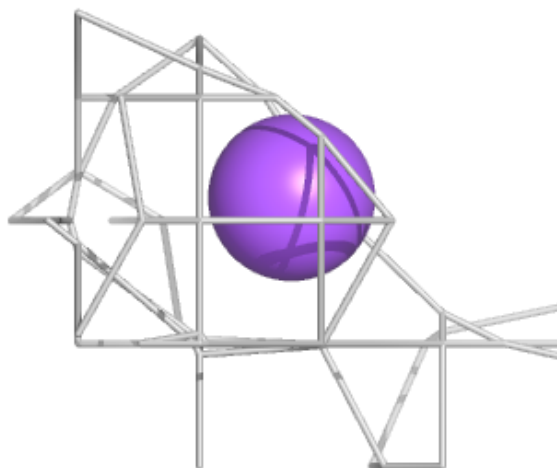
**Electron density around LFA E 315:**

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



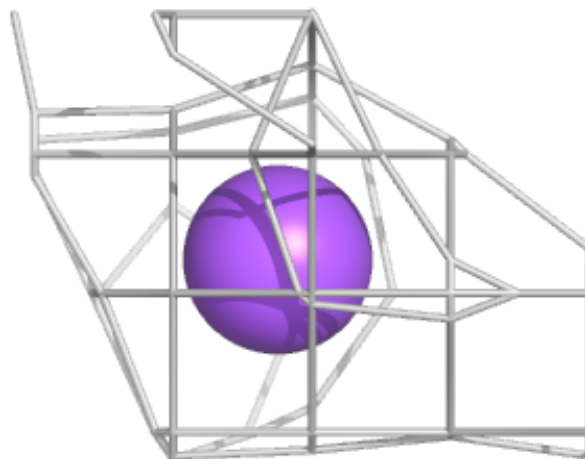
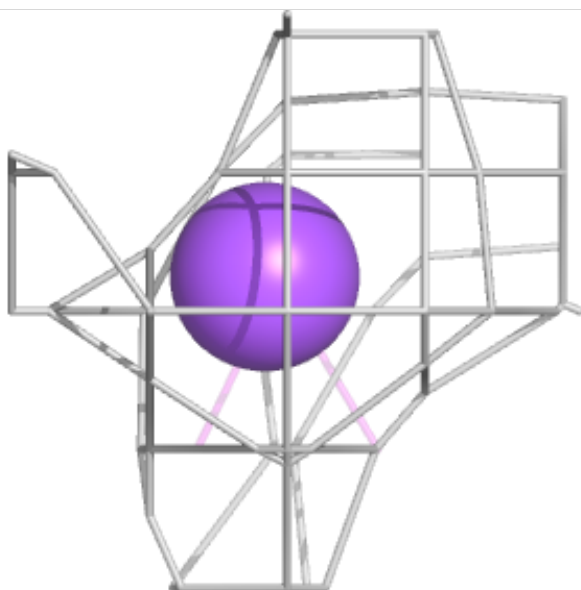
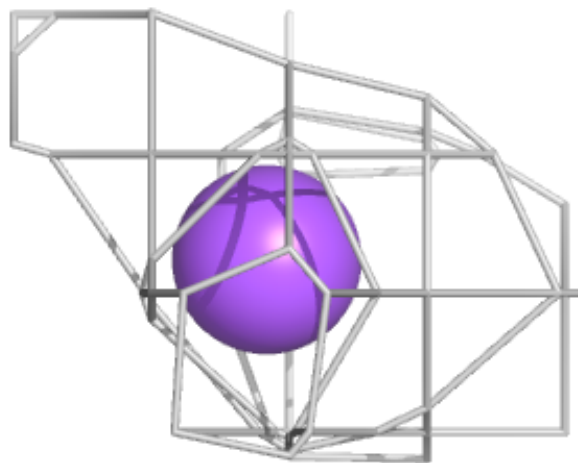
**Electron density around NA A 322:**

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



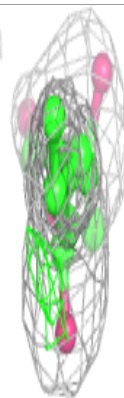
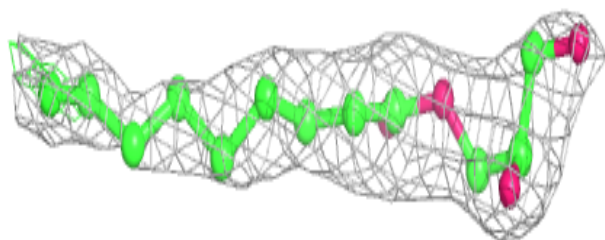
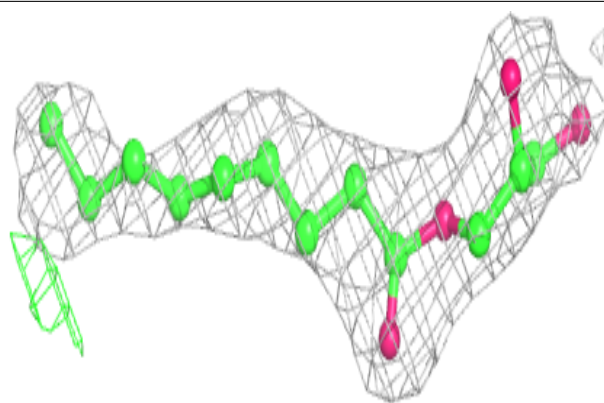
**Electron density around NA D 319:**

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

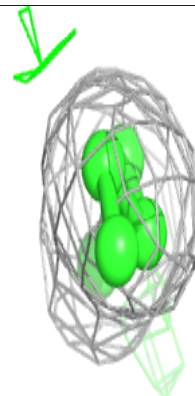
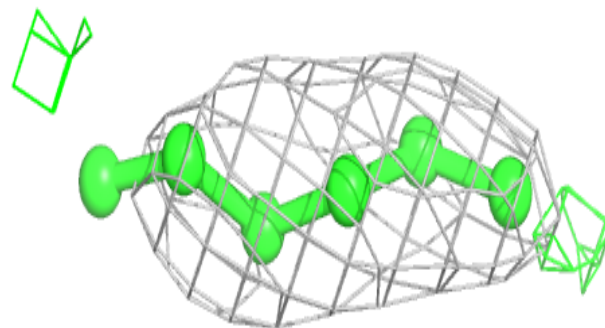
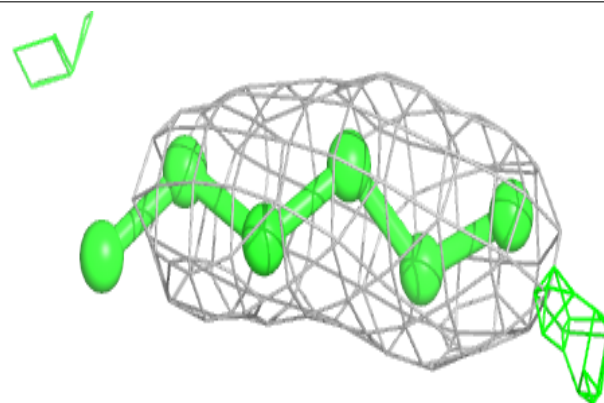


**Electron density around OLC C 309:**

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

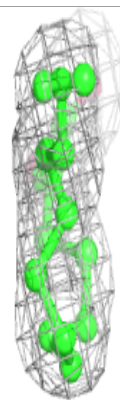
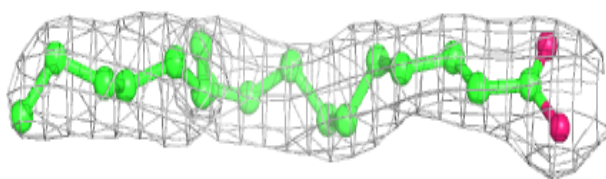
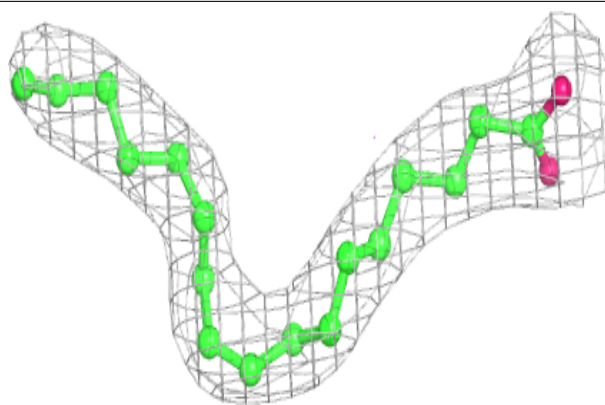
**Electron density around LFA A 313:**

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



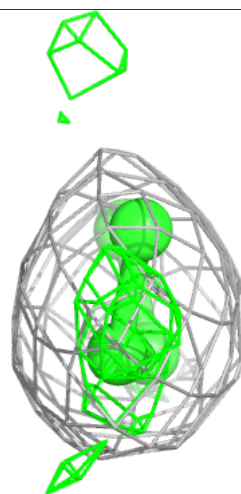
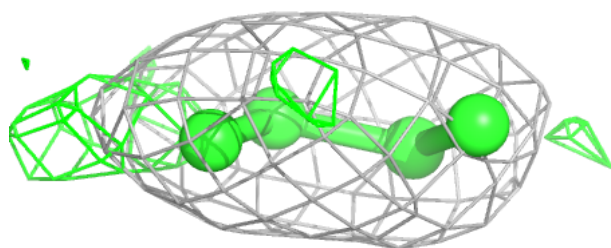
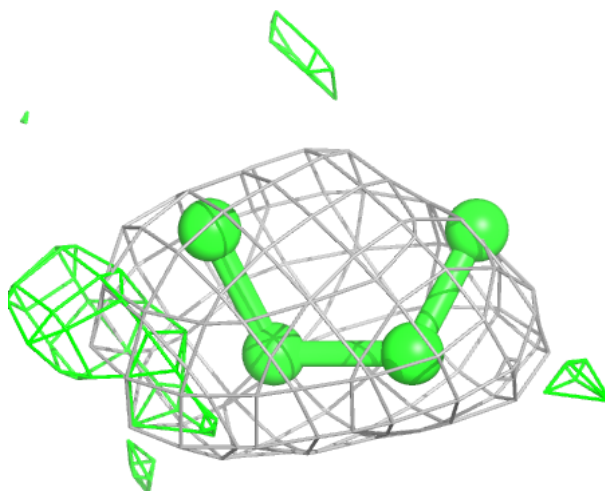
**Electron density around OLC A 316:**

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



**Electron density around LFA E 314:**

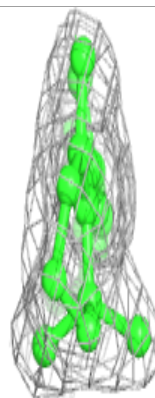
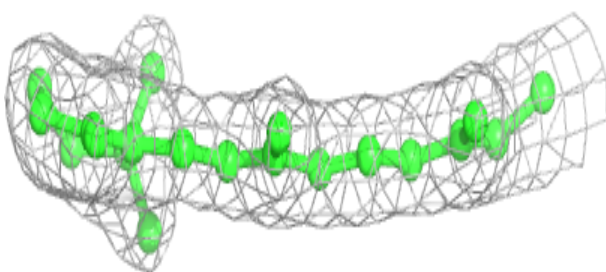
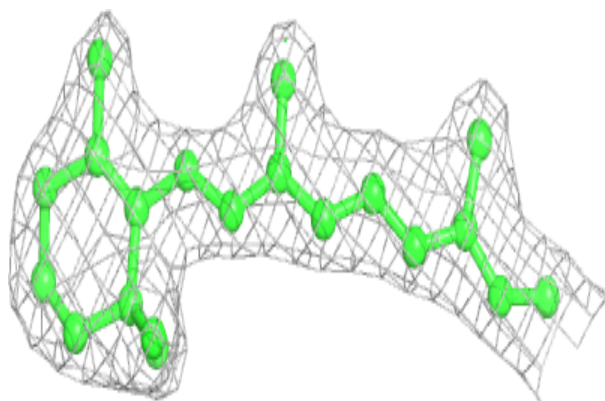
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



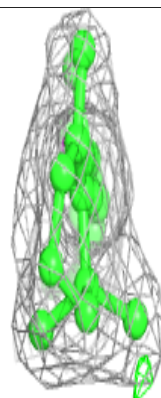
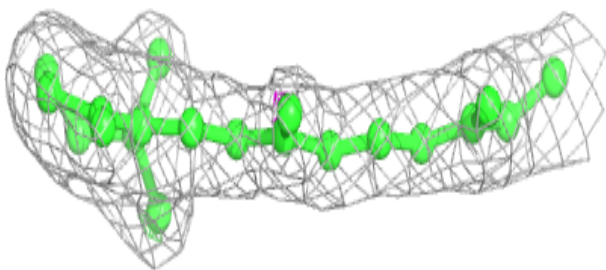
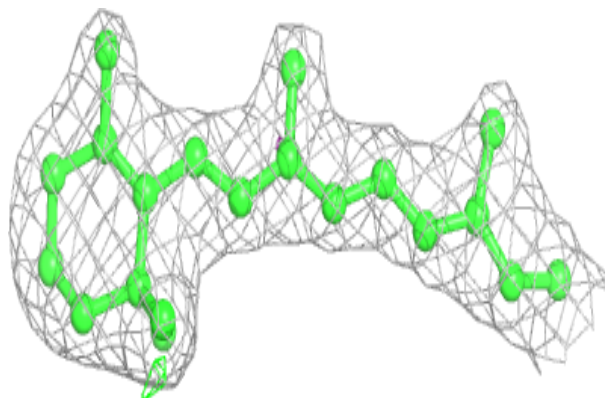


**Electron density around RET A 320:**

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

**Electron density around RET D 317:**

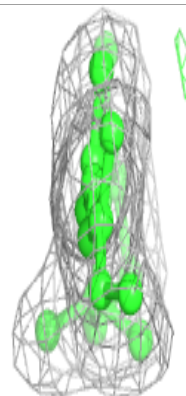
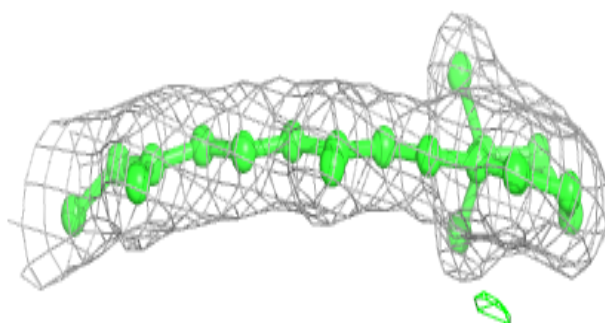
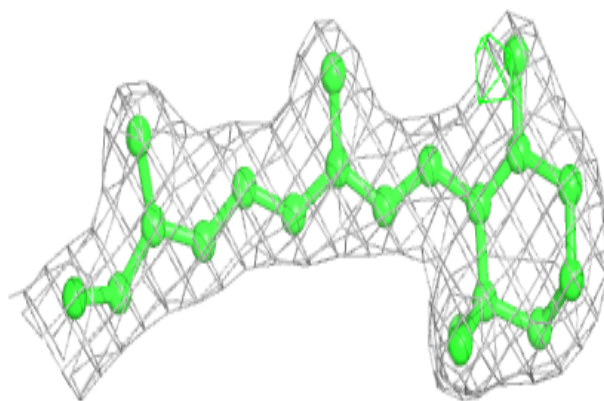
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



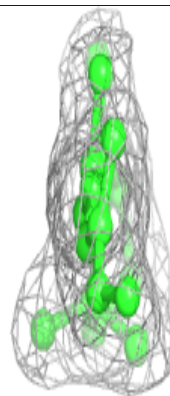
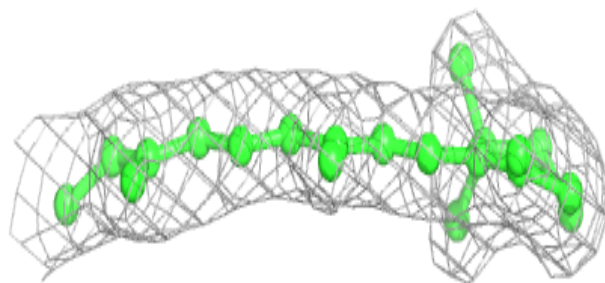
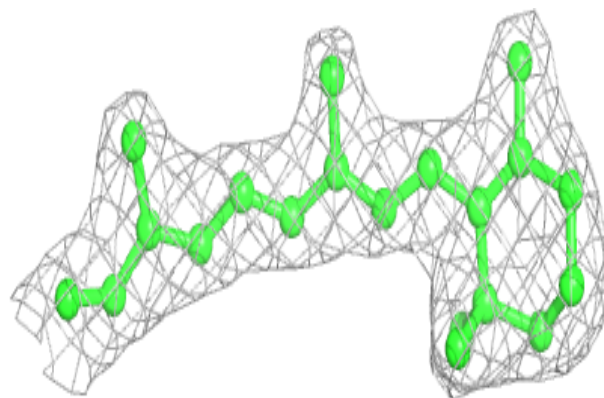


**Electron density around RET B 313:**

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

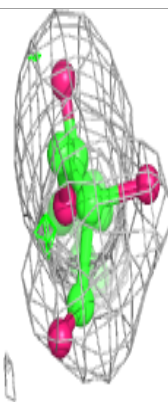
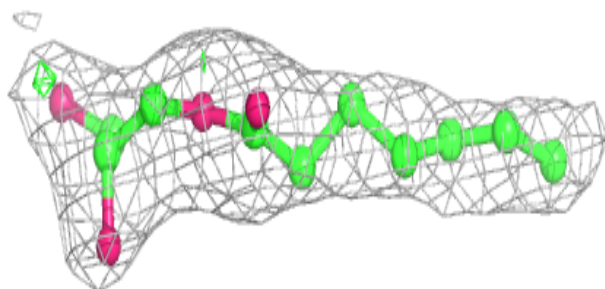
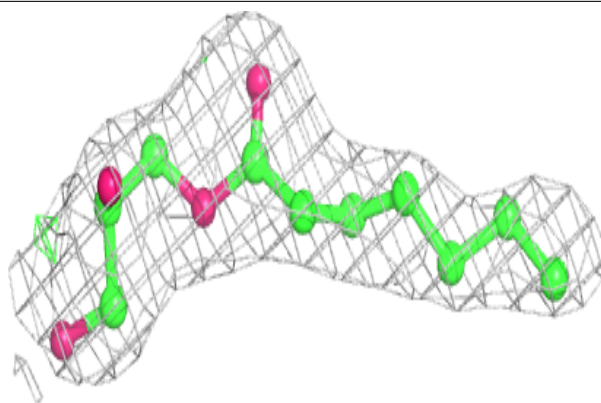
**Electron density around RET C 317:**

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

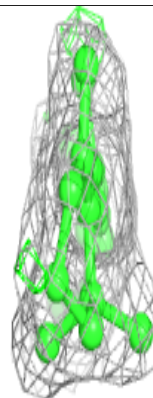
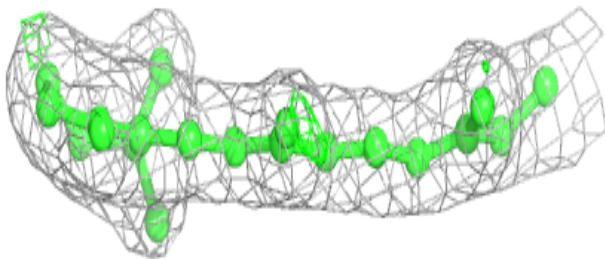
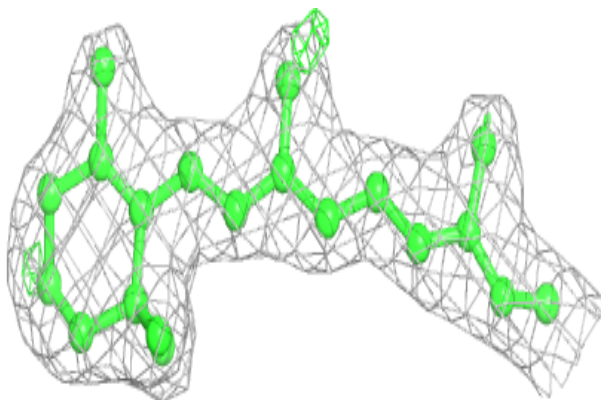


**Electron density around OLC D 307:**

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

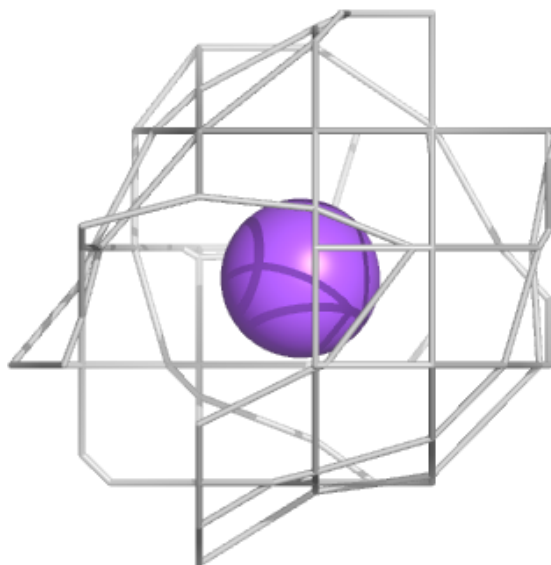
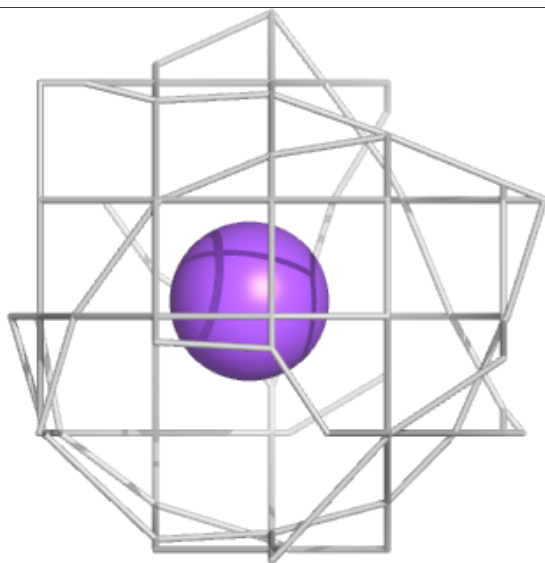
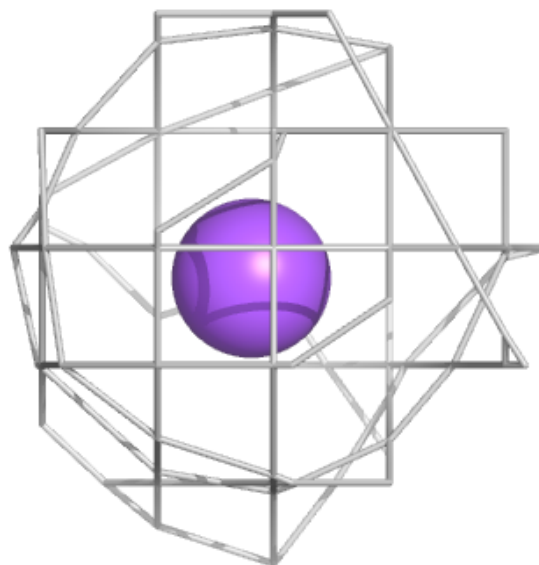
**Electron density around RET E 317:**

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



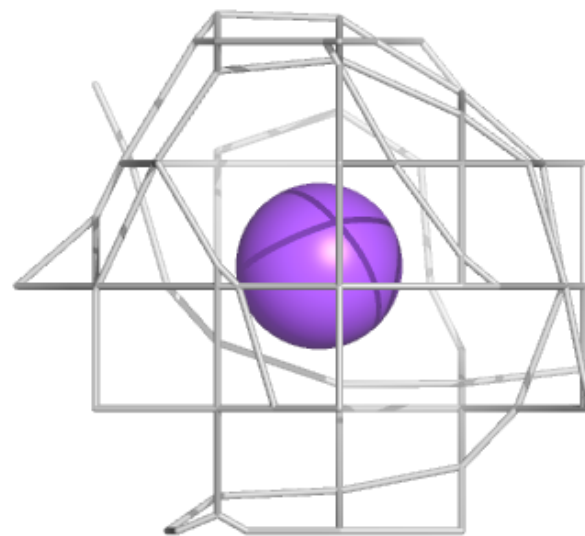
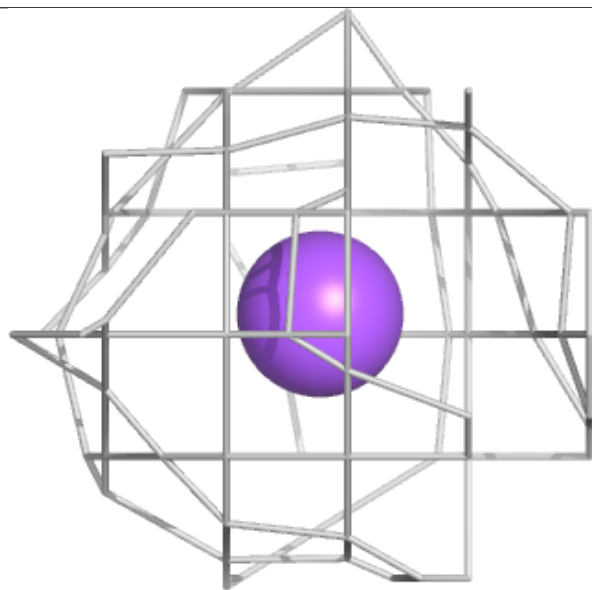
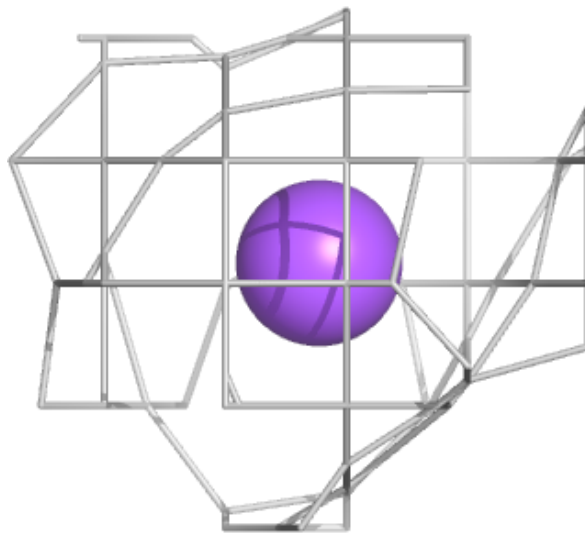
**Electron density around NA E 318:**

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



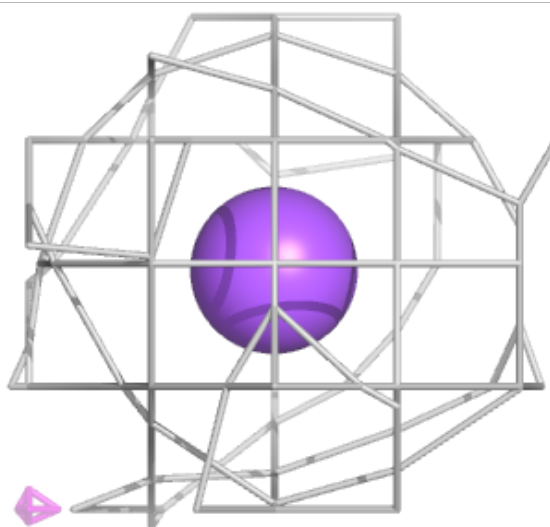
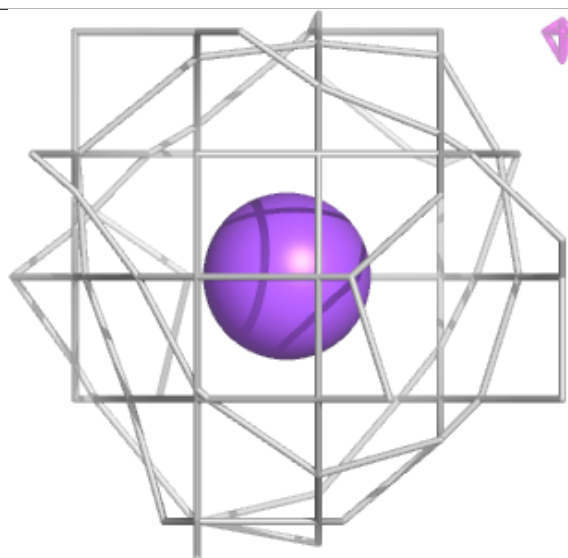
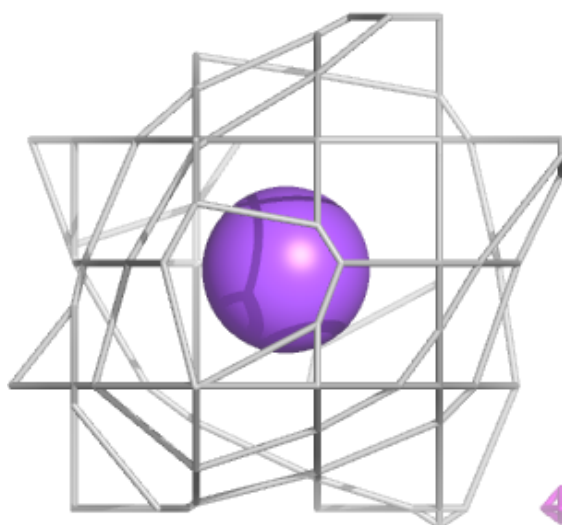
**Electron density around NA A 321:**

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



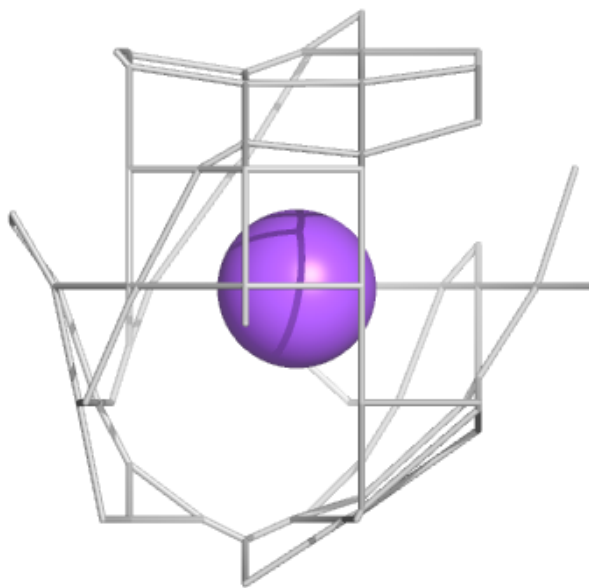
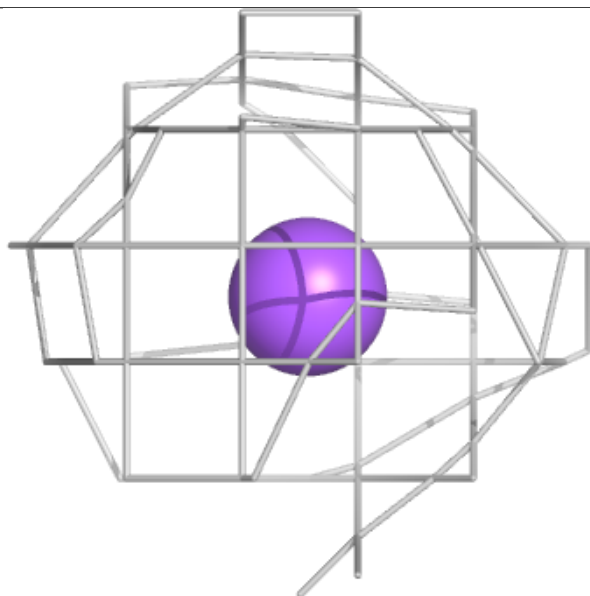
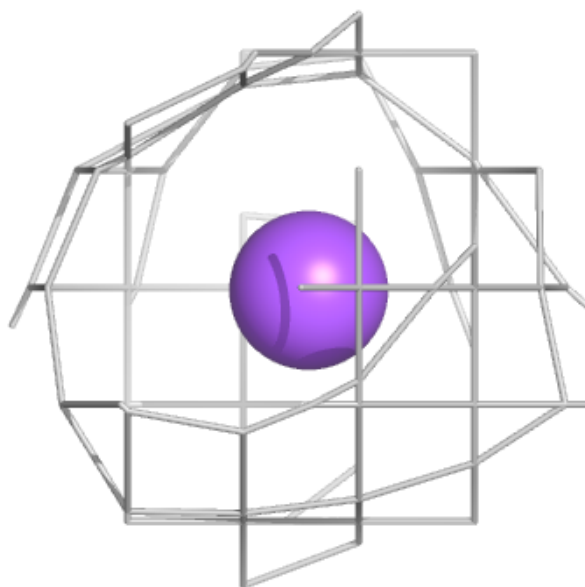
**Electron density around NA D 318:**

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



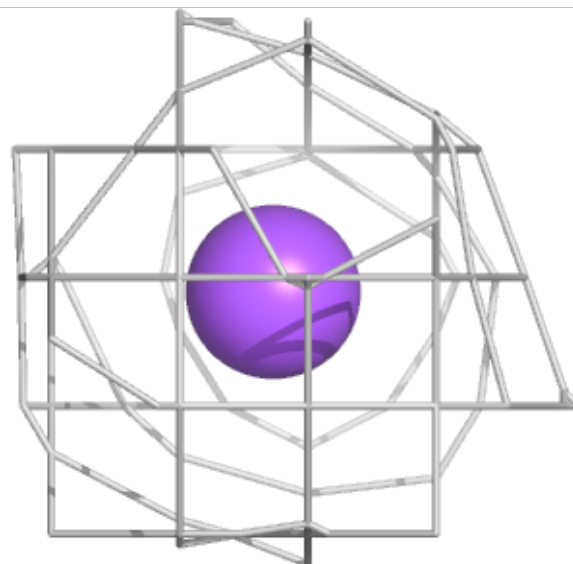
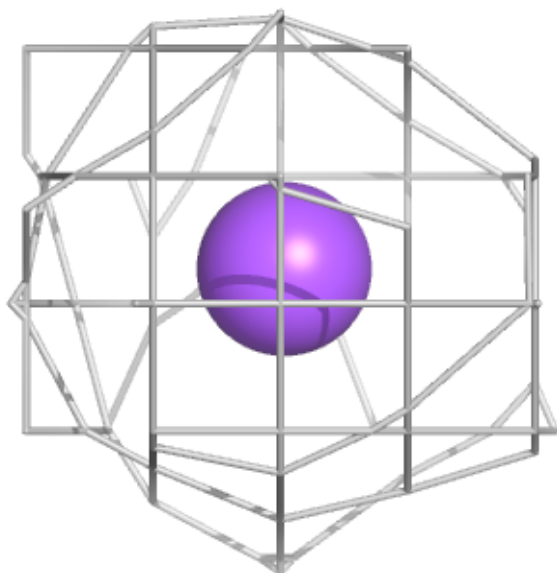
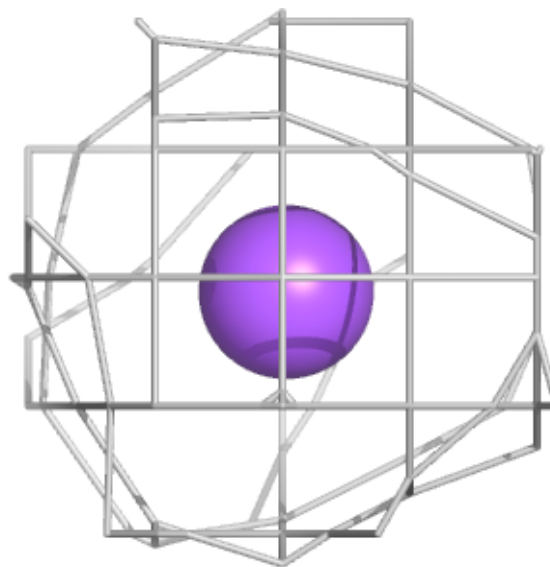
**Electron density around NA B 315:**

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



**Electron density around NA 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.