



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2023 – 03:40 AM EDT

PDB ID : 3POX  
Title : Crystal Structure of E.coli OmpF porin in lipidic cubic phase: space group P1  
Authors : Efremov, R.G.; Sazanov, L.A.  
Deposited on : 2010-11-23  
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.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

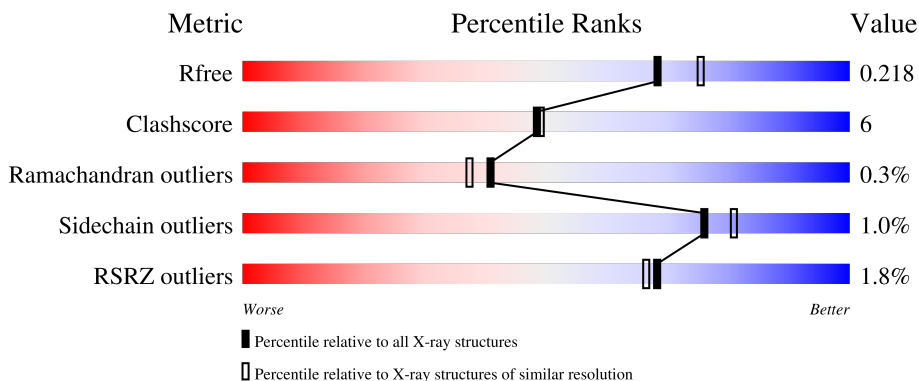
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


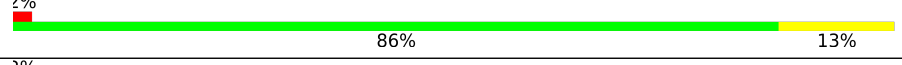
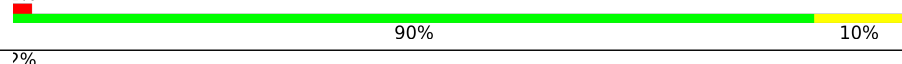
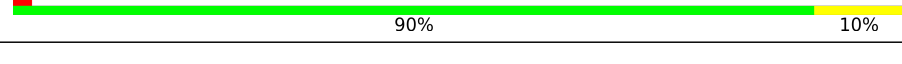
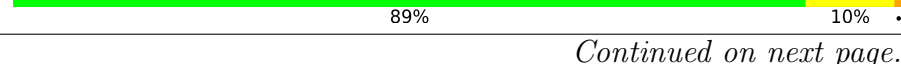
The reported resolution of this entry is 2.00 Å.

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	340	 88% 12%
1	B	340	 86% 13%
1	C	340	 90% 10%
1	D	340	 90% 10%
1	E	340	 89% 10%

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Mol	Chain	Length	Quality of chain
1	F	340	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a small red segment on the left labeled '3%', a large green segment in the middle labeled '89%', and a small yellow segment on the right labeled '11%'.</p>

## 2 Entry composition i

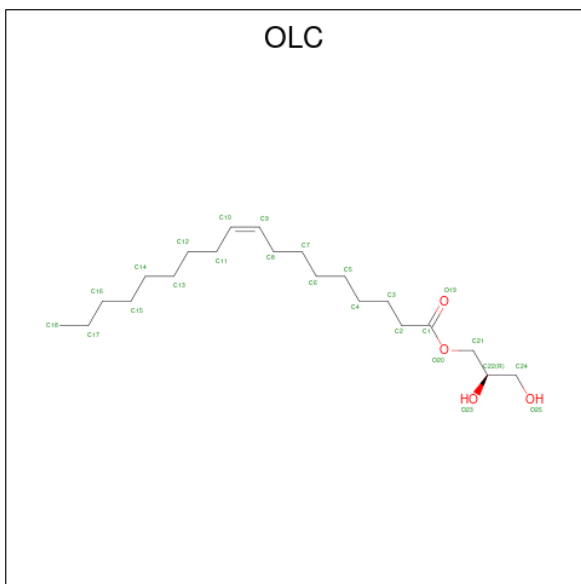
There are 5 unique types of molecules in this entry. The entry contains 18507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OmpF protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	Total 2627	C 1654	N 438	O 532	S 3	0	0	0
1	B	340	Total 2627	C 1654	N 438	O 532	S 3	0	0	0
1	C	340	Total 2627	C 1654	N 438	O 532	S 3	0	0	0
1	D	340	Total 2627	C 1654	N 438	O 532	S 3	0	0	0
1	E	340	Total 2627	C 1654	N 438	O 532	S 3	0	0	0
1	F	340	Total 2627	C 1654	N 438	O 532	S 3	0	0	0

- 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 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 14 14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 8 8	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 8 8	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 14 14	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 14 14	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C 12 12	0	0
2	D	1	Total C 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 25 21 4	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C 12 12	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 8 8	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 12 12	0	0
2	E	1	Total C 12 12	0	0
2	E	1	Total C 14 14	0	0
2	E	1	Total C 10 10	0	0
2	E	1	Total C O 25 21 4	0	0
2	E	1	Total C 12 12	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C 14 14	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C 10 10	0	0
2	F	1	Total C 12 12	0	0

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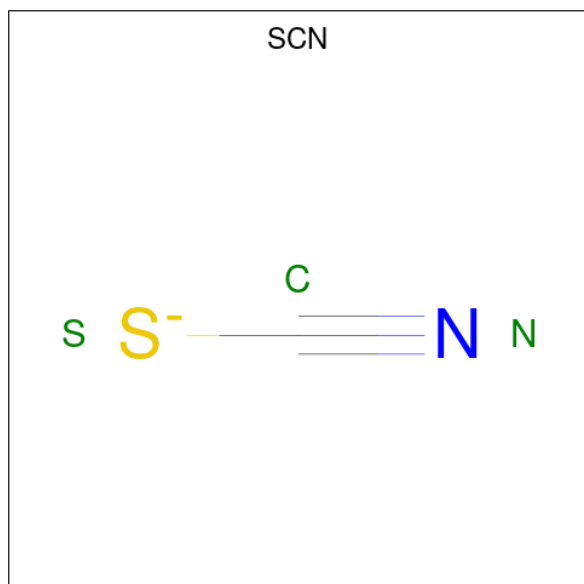
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C 8 8	0	0
2	F	1	Total C 14 14	0	0
2	F	1	Total C 14 14	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total K 3 3	0	0
3	B	3	Total K 3 3	0	0
3	C	4	Total K 4 4	0	0
3	D	4	Total K 4 4	0	0
3	E	3	Total K 3 3	0	0
3	F	3	Total K 3 3	0	0

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 3	C 1	N 1	S 1	0	0
4	B	1	Total 3	C 1	N 1	S 1	0	0
4	D	1	Total 3	C 1	N 1	S 1	0	0
4	E	1	Total 3	C 1	N 1	S 1	0	0
4	E	1	Total 3	C 1	N 1	S 1	0	0
4	F	1	Total 3	C 1	N 1	S 1	0	0

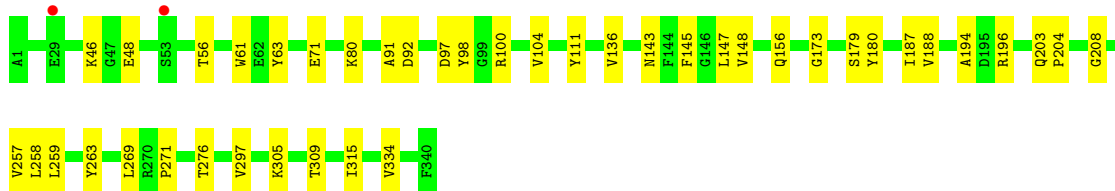
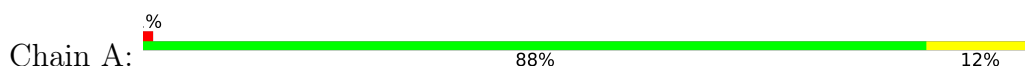
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	267	Total 267	O 267	0	0
5	B	236	Total 236	O 236	0	0
5	C	257	Total 257	O 257	0	0
5	D	272	Total 272	O 272	0	0
5	E	278	Total 278	O 278	0	0
5	F	212	Total 212	O 212	0	0

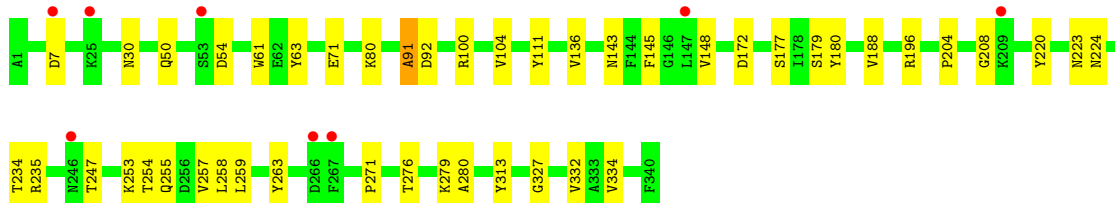
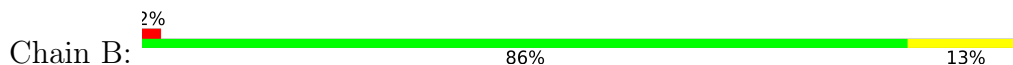
### 3 Residue-property plots

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.

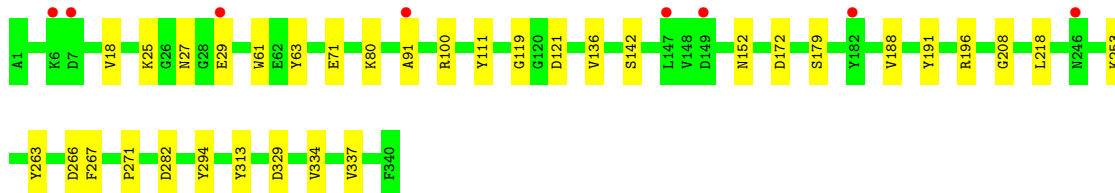
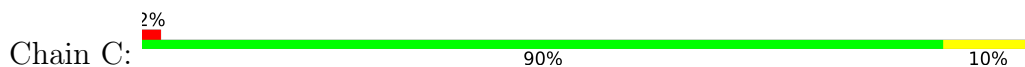
- Molecule 1: OmpF protein



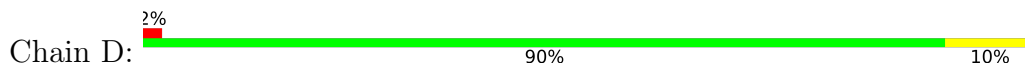
- Molecule 1: OmpF protein



- Molecule 1: OmpF protein

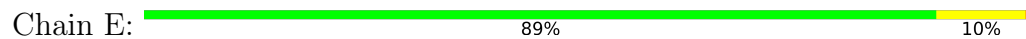


- Molecule 1: OmpF protein

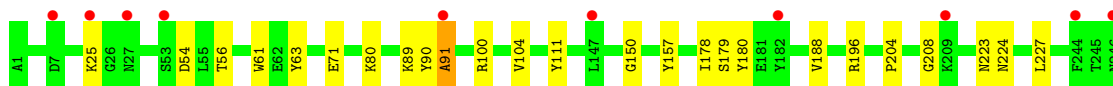
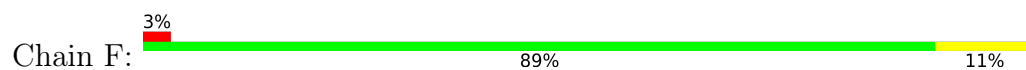




- Molecule 1: OmpF protein



- Molecule 1: OmpF protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.57Å 86.02Å 116.56Å 83.28° 78.46° 89.89°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-2.00) 96.6 (20.00-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.01Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, $R_{free}$	0.188 , 0.225 0.181 , 0.218	Depositor DCC
$R_{free}$ test set	9832 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 62.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, SCN, K

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	0.44	0/2683	0.56	0/3628
1	B	0.39	0/2683	0.54	0/3628
1	C	0.40	0/2683	0.55	0/3628
1	D	0.40	0/2683	0.55	0/3628
1	E	0.43	0/2683	0.57	0/3628
1	F	0.36	0/2683	0.53	0/3628
All	All	0.40	0/16098	0.55	0/21768

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2444	35	0
1	B	2627	0	2444	36	0
1	C	2627	0	2444	27	0
1	D	2627	0	2444	26	0
1	E	2627	0	2444	26	0
1	F	2627	0	2444	28	0
2	A	342	0	531	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	205	0	321	5	0
2	C	323	0	499	18	0
2	D	109	0	167	8	0
2	E	118	0	183	19	0
2	F	88	0	135	9	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	D	3	0	0	0	0
4	E	6	0	0	0	0
4	F	3	0	0	0	0
5	A	267	0	0	2	0
5	B	236	0	0	4	0
5	C	257	0	0	1	0
5	D	272	0	0	1	0
5	E	278	0	0	2	0
5	F	212	0	0	0	0
All	All	18507	0	16500	201	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 6.

The worst 5 of 201 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:SER:HB2	1:B:188:VAL:HG22	1.53	0.90
2:A:341:OLC:H2	2:A:361:OLC:O19	1.73	0.88
1:A:297:VAL:HG12	2:A:361:OLC:H13	1.58	0.85
1:A:258:LEU:CD1	1:A:276:THR:HG23	2.07	0.84
2:A:359:OLC:H24	1:B:172:ASP:OD1	1.79	0.83

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	338/340 (99%)	325 (96%)	12 (4%)	1 (0%)	41	37
1	B	338/340 (99%)	323 (96%)	14 (4%)	1 (0%)	41	37
1	C	338/340 (99%)	324 (96%)	13 (4%)	1 (0%)	41	37
1	D	338/340 (99%)	327 (97%)	10 (3%)	1 (0%)	41	37
1	E	338/340 (99%)	325 (96%)	12 (4%)	1 (0%)	41	37
1	F	338/340 (99%)	321 (95%)	16 (5%)	1 (0%)	41	37
All	All	2028/2040 (99%)	1945 (96%)	77 (4%)	6 (0%)	41	37

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	91	ALA
1	A	91	ALA
1	F	91	ALA
1	D	91	ALA
1	B	91	ALA

### 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	263/263 (100%)	260 (99%)	3 (1%)	73	78
1	B	263/263 (100%)	261 (99%)	2 (1%)	81	86
1	C	263/263 (100%)	260 (99%)	3 (1%)	73	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	263/263 (100%)	262 (100%)	1 (0%)	91	93
1	E	263/263 (100%)	260 (99%)	3 (1%)	73	78
1	F	263/263 (100%)	260 (99%)	3 (1%)	73	78
All	All	1578/1578 (100%)	1563 (99%)	15 (1%)	76	81

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	313	TYR
1	F	104	VAL
1	D	136	VAL
1	F	313	TYR
1	E	210	LYS

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

Mol	Chain	Res	Type
1	C	60	GLN
1	D	30	ASN
1	F	60	GLN
1	E	60	GLN
1	F	30	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 114 ligands modelled in this entry, 20 are monoatomic - leaving 94 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	A	356	-	24,24,24	1.35	4 (16%)	25,25,25	1.27	3 (12%)
4	SCN	F	352	-	1,2,2	0.90	0	0,1,1	-	-
2	OLC	C	364	-	11,11,24	1.19	1 (9%)	9,10,25	0.84	0
2	OLC	B	347	-	13,13,24	1.07	1 (7%)	12,12,25	0.90	1 (8%)
4	SCN	D	354	-	1,2,2	1.14	0	0,1,1	-	-
2	OLC	B	354	-	7,7,24	0.44	0	6,6,25	0.69	0
2	OLC	B	342	-	13,13,24	1.06	1 (7%)	12,12,25	0.86	0
2	OLC	C	341	-	9,9,24	1.19	1 (11%)	8,8,25	1.00	1 (12%)
2	OLC	B	346	-	24,24,24	1.36	4 (16%)	25,25,25	1.42	3 (12%)
2	OLC	C	352	-	11,11,24	1.16	1 (9%)	9,10,25	0.69	0
2	OLC	A	344	-	9,9,24	1.24	1 (11%)	8,8,25	0.96	1 (12%)
2	OLC	E	344	-	11,11,24	1.14	1 (9%)	9,10,25	0.83	0
2	OLC	A	353	-	7,7,24	0.20	0	6,6,25	0.55	0
2	OLC	E	345	-	13,13,24	1.09	1 (7%)	12,12,25	0.79	0
2	OLC	C	351	-	7,7,24	0.24	0	6,6,25	0.49	0
2	OLC	A	354	-	7,7,24	0.24	0	6,6,25	0.53	0
2	OLC	D	341	-	4,4,24	0.26	0	3,3,25	0.35	0
2	OLC	A	349	-	24,24,24	1.33	4 (16%)	25,25,25	1.10	2 (8%)
2	OLC	C	345	-	11,11,24	1.18	1 (9%)	9,10,25	0.63	0
2	OLC	C	347	-	9,9,24	1.20	1 (11%)	8,8,25	1.08	1 (12%)
2	OLC	C	357	-	13,13,24	1.13	1 (7%)	12,12,25	0.72	0
4	SCN	E	352	-	1,2,2	1.00	0	0,1,1	-	-
2	OLC	F	347	-	13,13,24	1.07	1 (7%)	12,12,25	0.84	0
2	OLC	A	358	-	24,24,24	1.35	4 (16%)	25,25,25	1.13	2 (8%)
2	OLC	A	361	-	24,24,24	1.46	4 (16%)	25,25,25	1.34	2 (8%)
2	OLC	B	341	-	4,4,24	0.22	0	3,3,25	0.44	0
2	OLC	D	344	-	7,7,24	0.22	0	6,6,25	0.50	0
2	OLC	B	344	-	9,9,24	1.22	1 (11%)	8,8,25	0.92	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	F	341	-	7,7,24	0.25	0	6,6,25	0.47	0
2	OLC	F	345	-	11,11,24	1.16	1 (9%)	9,10,25	0.76	0
4	SCN	A	369	-	1,2,2	1.09	0	0,1,1	-	-
2	OLC	D	343	-	7,7,24	0.22	0	6,6,25	0.56	0
4	SCN	E	353	-	1,2,2	1.05	0	0,1,1	-	-
2	OLC	B	350	-	24,24,24	1.35	4 (16%)	25,25,25	1.05	1 (4%)
2	OLC	E	348	-	11,11,24	1.26	1 (9%)	9,10,25	0.59	0
2	OLC	E	346	-	9,9,24	1.20	1 (11%)	8,8,25	0.99	1 (12%)
2	OLC	A	364	-	11,11,24	1.20	1 (9%)	9,10,25	0.75	0
2	OLC	C	354	-	9,9,24	1.20	1 (11%)	8,8,25	1.01	1 (12%)
2	OLC	D	342	-	24,24,24	1.37	4 (16%)	25,25,25	1.05	2 (8%)
2	OLC	A	359	-	24,24,24	1.30	4 (16%)	25,25,25	1.01	2 (8%)
2	OLC	B	345	-	24,24,24	1.36	4 (16%)	25,25,25	1.04	2 (8%)
2	OLC	A	362	-	13,13,24	1.11	1 (7%)	12,12,25	0.92	1 (8%)
2	OLC	F	348	-	13,13,24	1.15	1 (7%)	12,12,25	0.85	0
2	OLC	D	346	-	11,11,24	1.19	1 (9%)	9,10,25	0.83	0
2	OLC	E	341	-	24,24,24	1.33	4 (16%)	25,25,25	1.41	3 (12%)
2	OLC	A	357	-	9,9,24	1.21	1 (11%)	8,8,25	0.92	1 (12%)
2	OLC	B	351	-	24,24,24	1.28	4 (16%)	25,25,25	1.07	1 (4%)
2	OLC	C	355	-	9,9,24	1.19	1 (11%)	8,8,25	1.00	1 (12%)
2	OLC	A	352	-	9,9,24	1.21	1 (11%)	8,8,25	0.94	1 (12%)
2	OLC	C	343	-	7,7,24	0.22	0	6,6,25	0.53	0
2	OLC	F	343	-	7,7,24	0.22	0	6,6,25	0.63	0
2	OLC	C	361	-	11,11,24	1.20	1 (9%)	9,10,25	0.77	0
2	OLC	C	349	-	9,9,24	1.19	1 (11%)	8,8,25	1.13	1 (12%)
2	OLC	C	350	-	13,13,24	1.06	1 (7%)	12,12,25	0.89	0
2	OLC	B	348	-	13,13,24	1.05	1 (7%)	12,12,25	0.89	1 (8%)
2	OLC	C	358	-	24,24,24	1.34	4 (16%)	25,25,25	1.17	1 (4%)
2	OLC	B	352	-	15,15,24	0.97	1 (6%)	14,14,25	1.12	1 (7%)
2	OLC	A	345	-	7,7,24	0.27	0	6,6,25	0.48	0
2	OLC	E	342	-	7,7,24	0.23	0	6,6,25	0.61	0
2	OLC	F	344	-	9,9,24	1.19	1 (11%)	8,8,25	1.03	1 (12%)
2	OLC	C	353	-	9,9,24	1.20	1 (11%)	8,8,25	1.00	1 (12%)
2	OLC	B	343	-	7,7,24	0.23	0	6,6,25	0.46	0
2	OLC	E	347	-	24,24,24	1.38	4 (16%)	25,25,25	1.15	2 (8%)
2	OLC	A	347	-	7,7,24	0.24	0	6,6,25	0.52	0
2	OLC	C	356	-	7,7,24	0.26	0	6,6,25	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	C	363	-	24,24,24	1.33	4 (16%)	25,25,25	1.37	2 (8%)
2	OLC	A	348	-	9,9,24	1.20	1 (11%)	8,8,25	0.97	1 (12%)
2	OLC	C	359	-	24,24,24	1.34	4 (16%)	25,25,25	1.27	3 (12%)
2	OLC	F	342	-	13,13,24	1.10	1 (7%)	12,12,25	0.79	1 (8%)
4	SCN	B	358	-	1,2,2	0.99	0	0,1,1	-	-
2	OLC	B	349	-	7,7,24	0.24	0	6,6,25	0.47	0
2	OLC	A	351	-	13,13,24	1.06	1 (7%)	12,12,25	0.82	0
2	OLC	A	342	-	7,7,24	0.22	0	6,6,25	0.58	0
2	OLC	C	348	-	11,11,24	1.17	1 (9%)	9,10,25	0.72	0
2	OLC	C	342	-	7,7,24	0.22	0	6,6,25	0.58	0
2	OLC	A	360	-	11,11,24	1.15	1 (9%)	9,10,25	0.75	0
2	OLC	E	343	-	11,11,24	1.19	1 (9%)	9,10,25	0.76	0
2	OLC	B	353	-	7,7,24	0.34	0	6,6,25	0.46	0
2	OLC	A	343	-	7,7,24	0.23	0	6,6,25	0.57	0
2	OLC	D	345	-	9,9,24	1.19	1 (11%)	8,8,25	1.05	1 (12%)
2	OLC	D	347	-	7,7,24	0.31	0	6,6,25	0.50	0
2	OLC	A	346	-	24,24,24	1.37	4 (16%)	25,25,25	1.21	3 (12%)
2	OLC	C	360	3	24,24,24	1.39	4 (16%)	25,25,25	1.01	2 (8%)
2	OLC	A	341	-	7,7,24	0.23	0	6,6,25	0.45	0
2	OLC	D	349	3	24,24,24	1.29	4 (16%)	25,25,25	1.22	3 (12%)
2	OLC	C	344	-	7,7,24	0.28	0	6,6,25	0.45	0
2	OLC	A	355	-	9,9,24	1.21	1 (11%)	8,8,25	1.01	1 (12%)
2	OLC	A	363	-	11,11,24	1.26	1 (9%)	9,10,25	0.66	0
2	OLC	C	346	-	9,9,24	1.19	1 (11%)	8,8,25	1.10	1 (12%)
2	OLC	D	348	-	7,7,24	0.17	0	6,6,25	0.84	0
2	OLC	A	350	-	13,13,24	1.09	1 (7%)	12,12,25	0.83	0
2	OLC	A	365	-	7,7,24	0.45	0	6,6,25	0.79	0
2	OLC	F	346	-	7,7,24	0.22	0	6,6,25	0.65	0
2	OLC	C	362	-	24,24,24	1.35	4 (16%)	25,25,25	1.39	3 (12%)

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	A	356	-	-	5/24/24/24	-
2	OLC	C	364	-	-	5/9/9/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	347	-	-	1/11/11/24	-
2	OLC	B	354	-	-	2/5/5/24	-
2	OLC	B	342	-	-	3/11/11/24	-
2	OLC	C	341	-	-	1/7/7/24	-
2	OLC	B	346	-	-	10/24/24/24	-
2	OLC	C	352	-	-	6/9/9/24	-
2	OLC	A	344	-	-	0/7/7/24	-
2	OLC	E	344	-	-	4/9/9/24	-
2	OLC	A	353	-	-	0/5/5/24	-
2	OLC	E	345	-	-	7/11/11/24	-
2	OLC	C	351	-	-	0/5/5/24	-
2	OLC	A	354	-	-	4/5/5/24	-
2	OLC	D	341	-	-	0/2/2/24	-
2	OLC	A	349	-	-	11/24/24/24	-
2	OLC	C	345	-	-	1/9/9/24	-
2	OLC	C	347	-	-	2/7/7/24	-
2	OLC	C	357	-	-	2/11/11/24	-
2	OLC	F	347	-	-	4/11/11/24	-
2	OLC	A	358	-	-	16/24/24/24	-
2	OLC	A	361	-	-	15/24/24/24	-
2	OLC	B	341	-	-	1/2/2/24	-
2	OLC	D	344	-	-	2/5/5/24	-
2	OLC	B	344	-	-	2/7/7/24	-
2	OLC	F	341	-	-	0/5/5/24	-
2	OLC	F	345	-	-	4/9/9/24	-
2	OLC	D	343	-	-	0/5/5/24	-
2	OLC	B	350	-	-	18/24/24/24	-
2	OLC	E	348	-	-	6/9/9/24	-
2	OLC	E	346	-	-	2/7/7/24	-
2	OLC	A	364	-	-	6/9/9/24	-
2	OLC	C	354	-	-	1/7/7/24	-
2	OLC	D	342	-	-	11/24/24/24	-
2	OLC	A	359	-	-	10/24/24/24	-
2	OLC	B	345	-	-	9/24/24/24	-
2	OLC	A	362	-	-	6/11/11/24	-
2	OLC	F	348	-	-	6/11/11/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	D	346	-	-	4/9/9/24	-
2	OLC	E	341	-	-	11/24/24/24	-
2	OLC	A	357	-	-	4/7/7/24	-
2	OLC	B	351	-	-	16/24/24/24	-
2	OLC	C	355	-	-	1/7/7/24	-
2	OLC	A	352	-	-	3/7/7/24	-
2	OLC	C	343	-	-	0/5/5/24	-
2	OLC	F	343	-	-	0/5/5/24	-
2	OLC	C	361	-	-	4/9/9/24	-
2	OLC	C	349	-	-	4/7/7/24	-
2	OLC	C	350	-	-	3/11/11/24	-
2	OLC	B	348	-	-	3/11/11/24	-
2	OLC	C	358	-	-	8/24/24/24	-
2	OLC	B	352	-	-	9/13/13/24	-
2	OLC	A	345	-	-	1/5/5/24	-
2	OLC	E	342	-	-	2/5/5/24	-
2	OLC	F	344	-	-	1/7/7/24	-
2	OLC	C	353	-	-	3/7/7/24	-
2	OLC	B	343	-	-	0/5/5/24	-
2	OLC	E	347	-	-	8/24/24/24	-
2	OLC	A	347	-	-	3/5/5/24	-
2	OLC	C	356	-	-	0/5/5/24	-
2	OLC	C	363	-	-	12/24/24/24	-
2	OLC	A	348	-	-	5/7/7/24	-
2	OLC	C	359	-	-	12/24/24/24	-
2	OLC	F	342	-	-	4/11/11/24	-
2	OLC	B	349	-	-	0/5/5/24	-
2	OLC	A	351	-	-	1/11/11/24	-
2	OLC	A	342	-	-	1/5/5/24	-
2	OLC	C	348	-	-	2/9/9/24	-
2	OLC	C	342	-	-	2/5/5/24	-
2	OLC	A	360	-	-	2/9/9/24	-
2	OLC	E	343	-	-	4/9/9/24	-
2	OLC	B	353	-	-	1/5/5/24	-
2	OLC	A	343	-	-	2/5/5/24	-
2	OLC	D	345	-	-	1/7/7/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	D	347	-	-	3/5/5/24	-
2	OLC	A	346	-	-	7/24/24/24	-
2	OLC	C	360	3	-	17/24/24/24	-
2	OLC	A	341	-	-	0/5/5/24	-
2	OLC	D	349	3	-	14/24/24/24	-
2	OLC	C	344	-	-	1/5/5/24	-
2	OLC	A	355	-	-	2/7/7/24	-
2	OLC	A	363	-	-	6/9/9/24	-
2	OLC	C	346	-	-	3/7/7/24	-
2	OLC	D	348	-	-	3/5/5/24	-
2	OLC	A	350	-	-	4/11/11/24	-
2	OLC	A	365	-	-	3/5/5/24	-
2	OLC	F	346	-	-	0/5/5/24	-
2	OLC	C	362	-	-	15/24/24/24	-

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	361	OLC	O20-C1	4.89	1.47	1.33
2	C	360	OLC	O20-C1	4.66	1.47	1.33
2	E	347	OLC	O20-C1	4.56	1.46	1.33
2	D	342	OLC	O20-C1	4.50	1.46	1.33
2	B	346	OLC	O20-C1	4.45	1.46	1.33

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	OLC	O20-C1-C2	4.60	126.35	111.91
2	C	362	OLC	O20-C1-C2	4.09	124.75	111.91
2	E	341	OLC	O20-C1-C2	4.07	124.68	111.91
2	B	346	OLC	O20-C1-C2	3.99	124.42	111.91
2	C	363	OLC	O20-C1-C2	3.80	123.85	111.91

There are no chirality outliers.

5 of 398 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	349	OLC	O20-C21-C22-C24
2	A	349	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
2	A	358	OLC	O20-C21-C22-C24
2	A	358	OLC	O20-C21-C22-O23
2	A	361	OLC	C11-C10-C9-C8

There are no ring outliers.

44 monomers are involved in 81 short contacts:

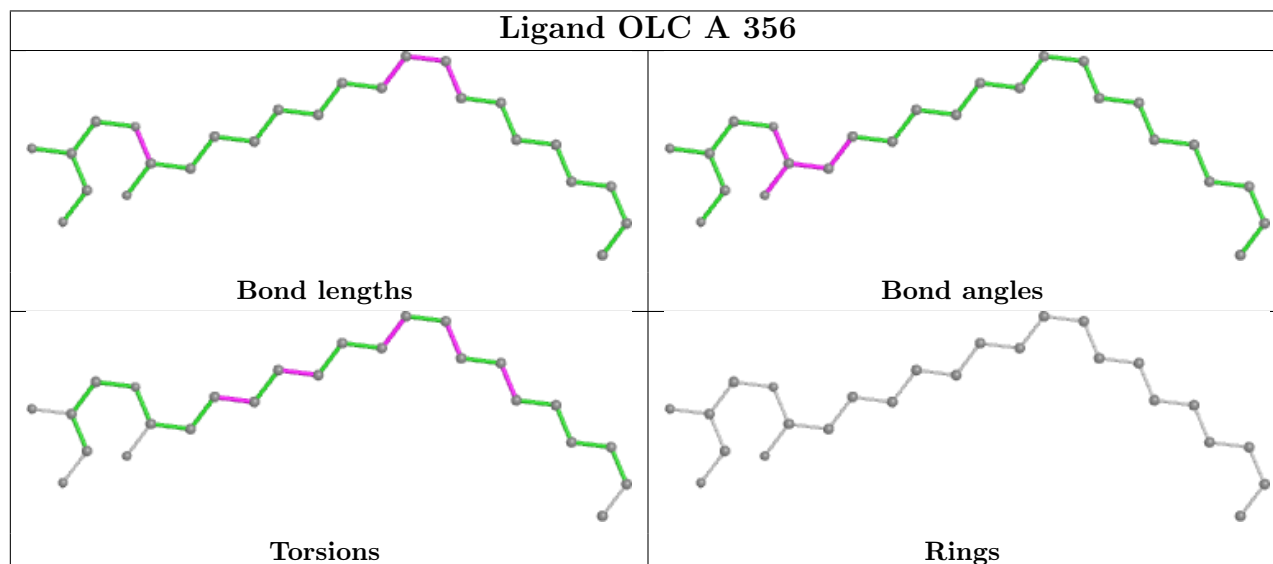
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	356	OLC	2	0
2	C	352	OLC	3	0
2	A	344	OLC	1	0
2	E	344	OLC	3	0
2	A	353	OLC	1	0
2	A	349	OLC	3	0
2	C	347	OLC	2	0
2	F	347	OLC	3	0
2	A	361	OLC	8	0
2	B	344	OLC	1	0
2	F	341	OLC	1	0
2	F	345	OLC	1	0
2	B	350	OLC	1	0
2	E	348	OLC	6	0
2	E	346	OLC	2	0
2	D	342	OLC	4	0
2	A	359	OLC	3	0
2	B	345	OLC	2	0
2	A	362	OLC	1	0
2	D	346	OLC	1	0
2	E	341	OLC	1	0
2	B	351	OLC	2	0
2	F	343	OLC	1	0
2	C	349	OLC	3	0
2	C	358	OLC	2	0
2	A	345	OLC	1	0
2	E	342	OLC	1	0
2	F	344	OLC	1	0
2	C	353	OLC	1	0
2	E	347	OLC	11	0
2	C	363	OLC	4	0
2	C	359	OLC	3	0
2	F	342	OLC	3	0
2	C	348	OLC	2	0

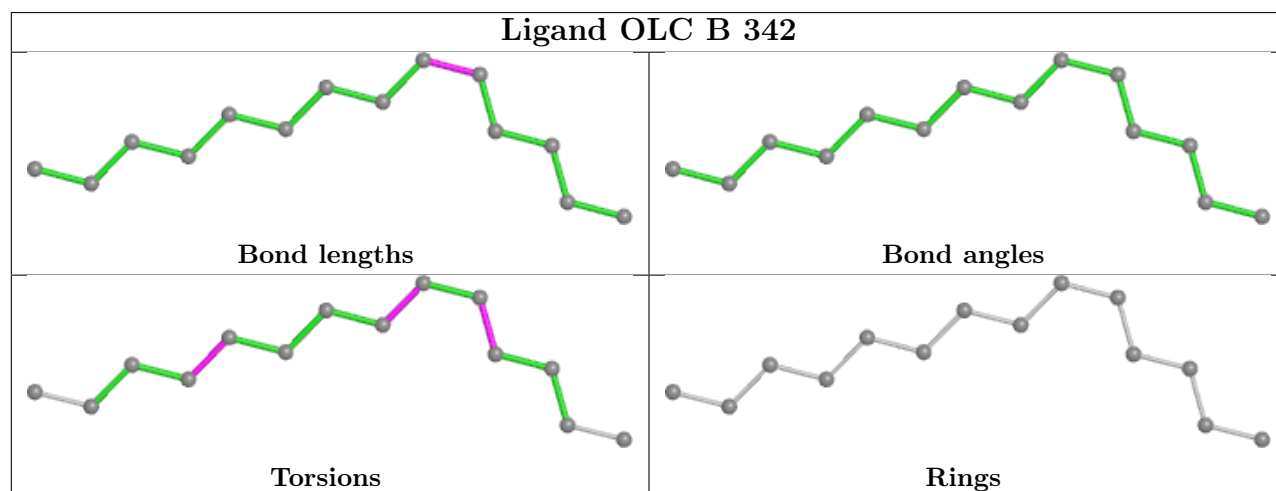
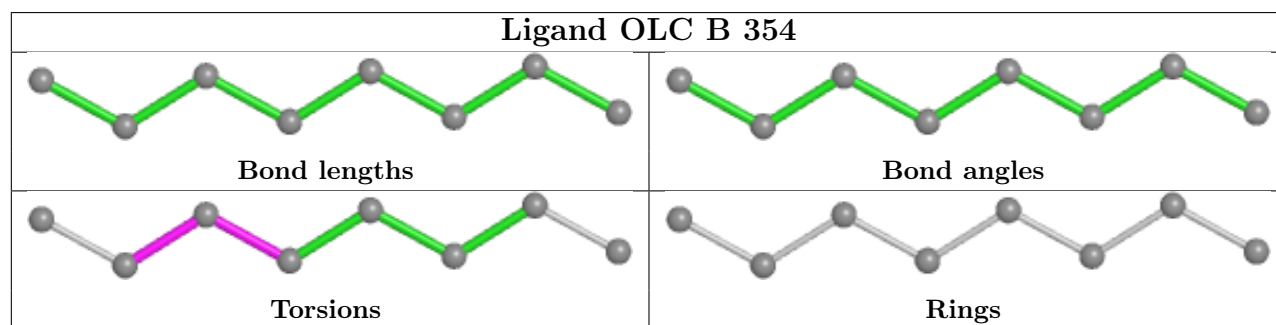
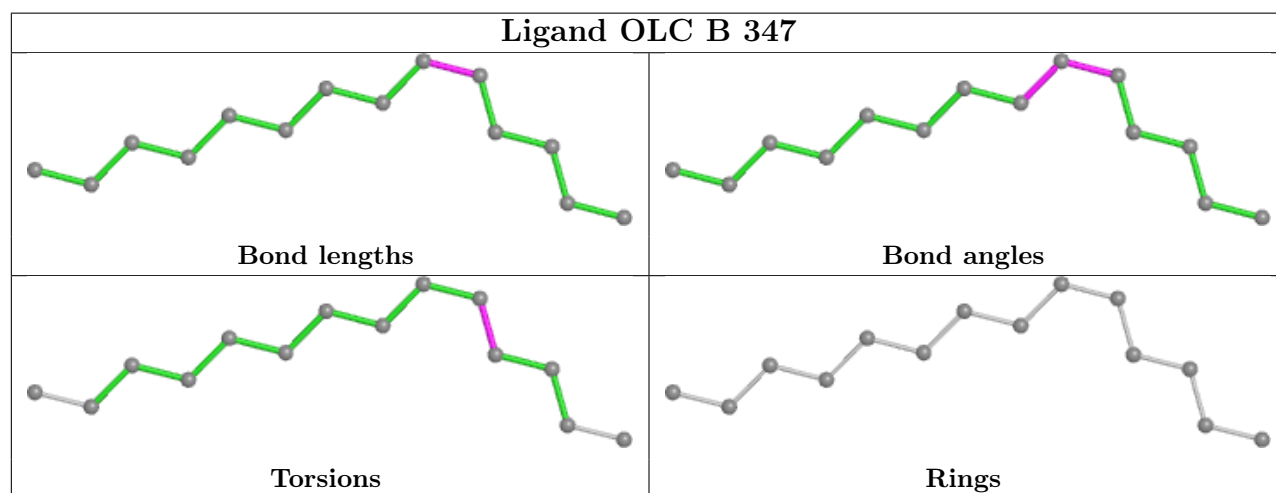
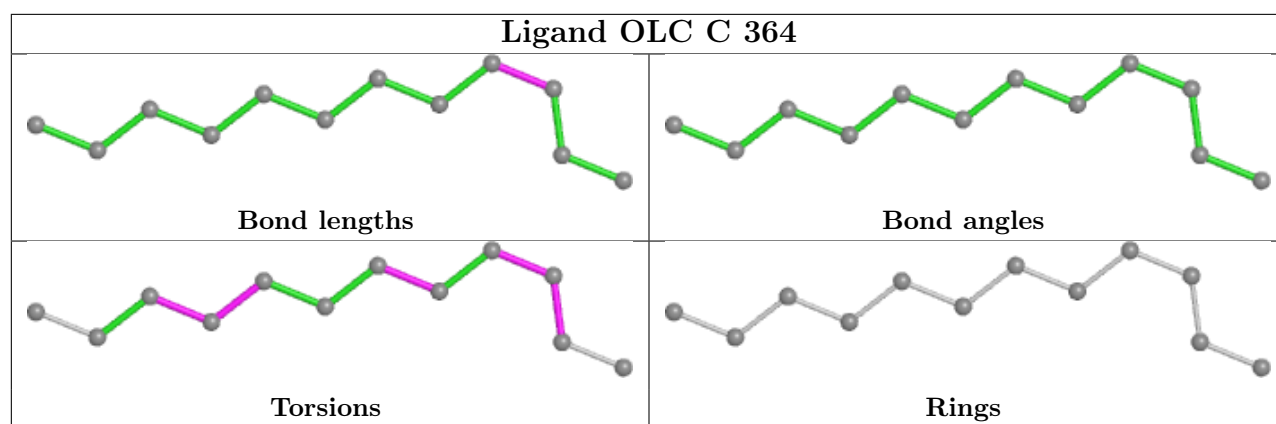
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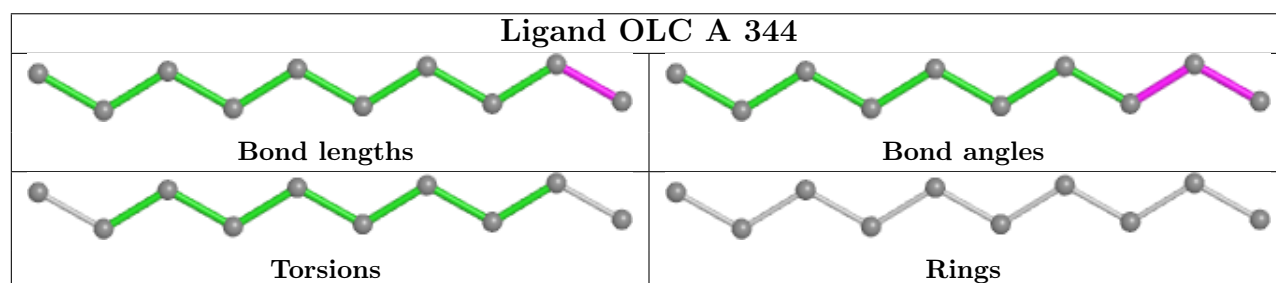
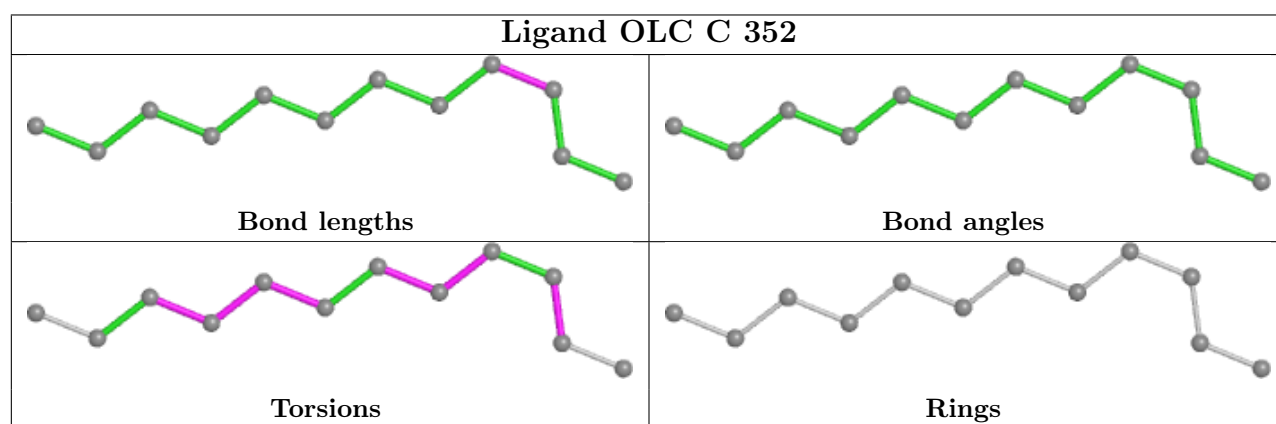
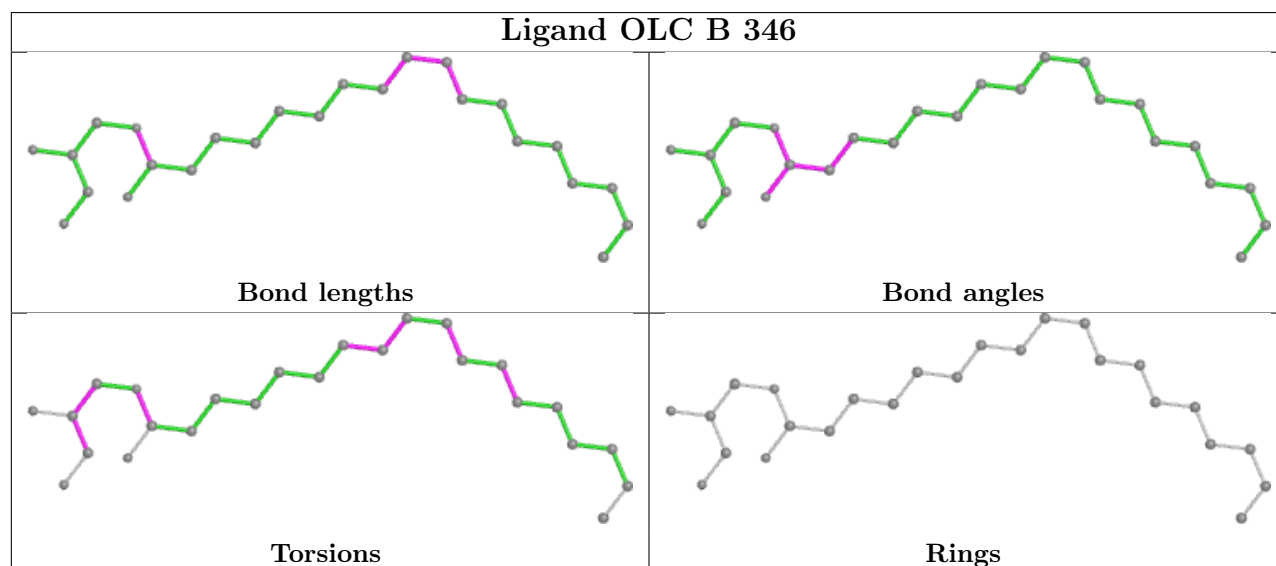
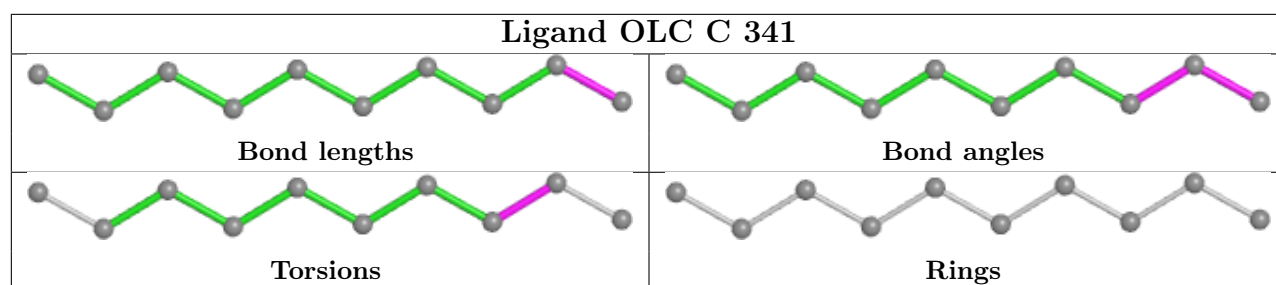
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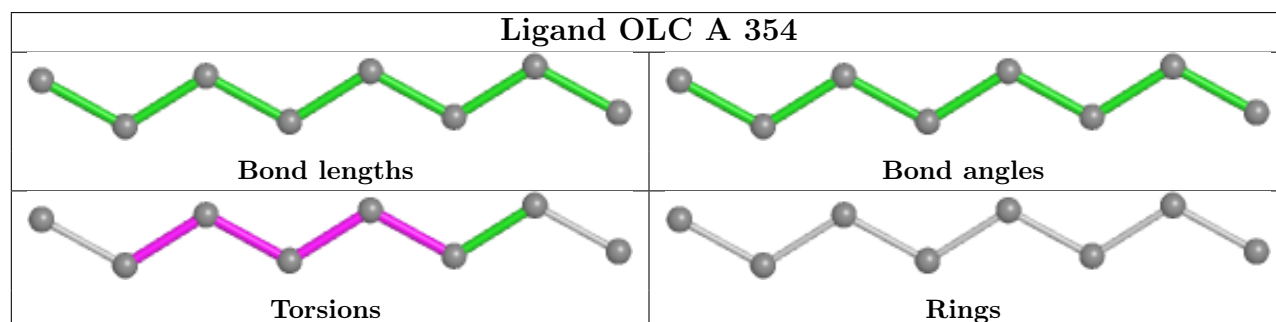
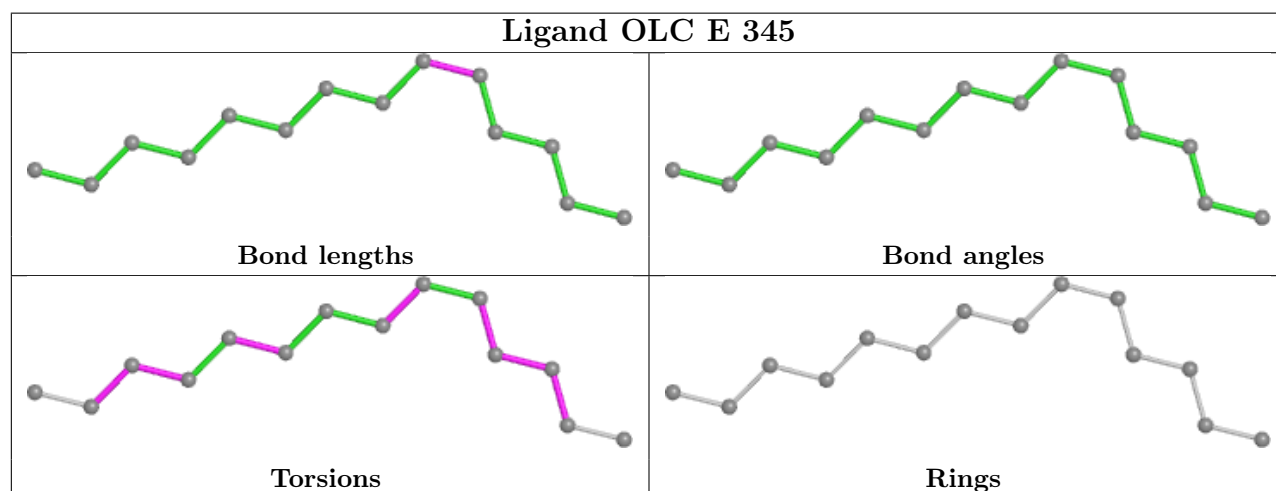
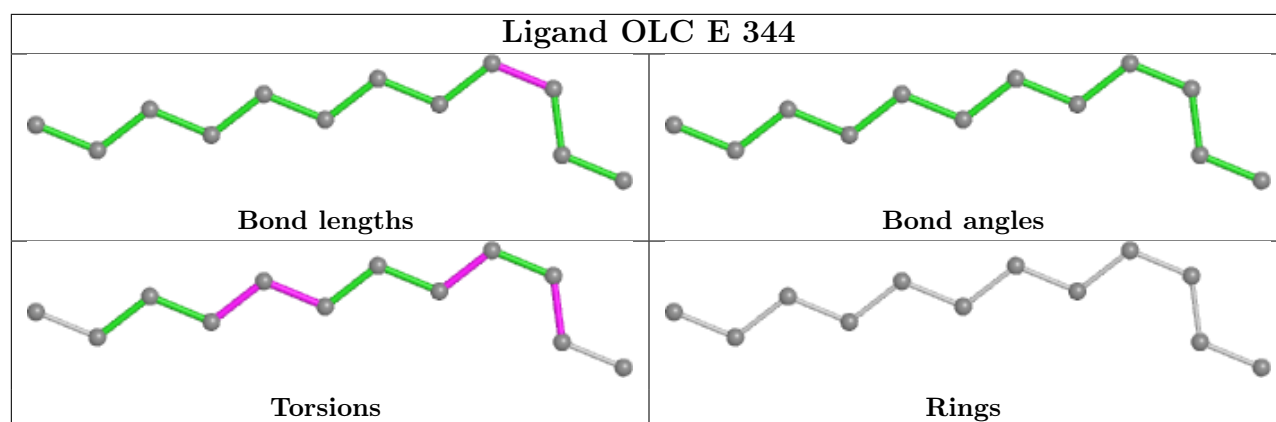
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	360	OLC	4	0
2	E	343	OLC	1	0
2	A	343	OLC	1	0
2	D	345	OLC	1	0
2	C	360	OLC	2	0
2	A	341	OLC	2	0
2	D	349	OLC	1	0
2	D	348	OLC	1	0
2	A	365	OLC	5	0
2	C	362	OLC	2	0

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

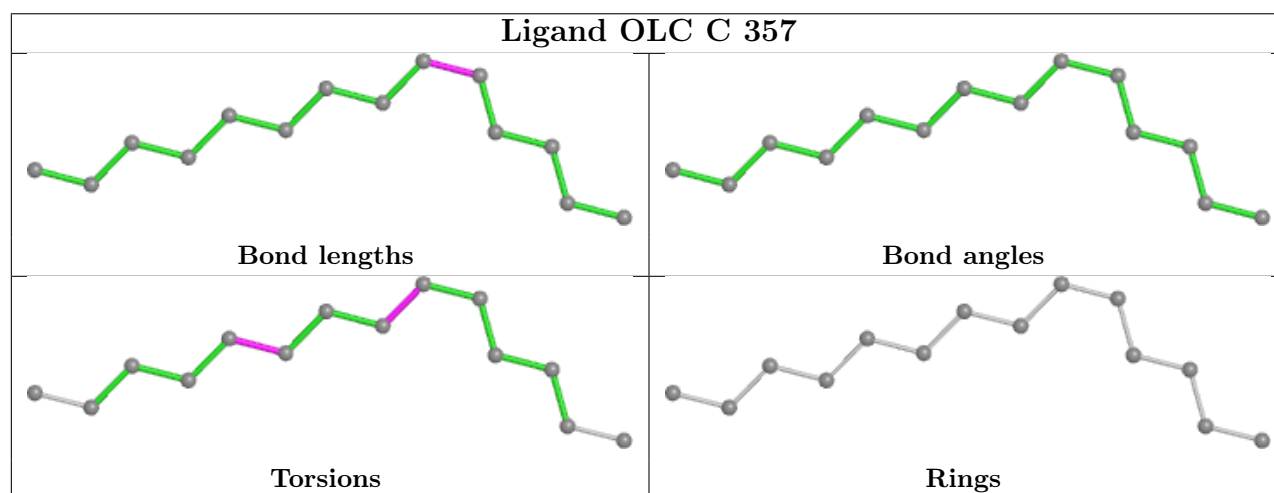
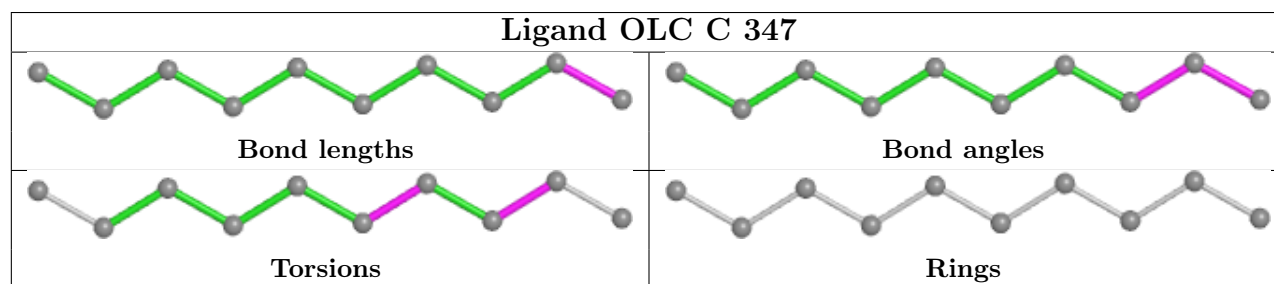
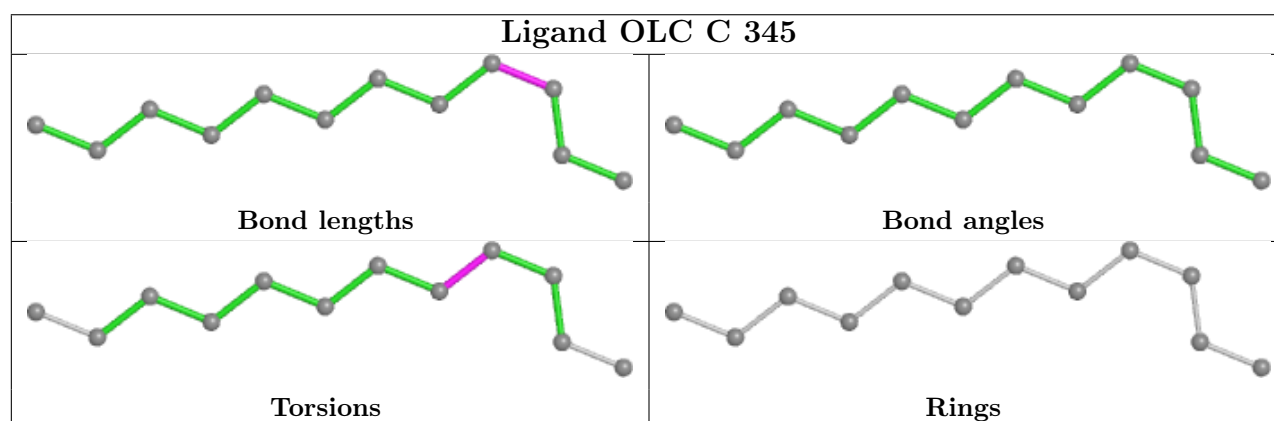
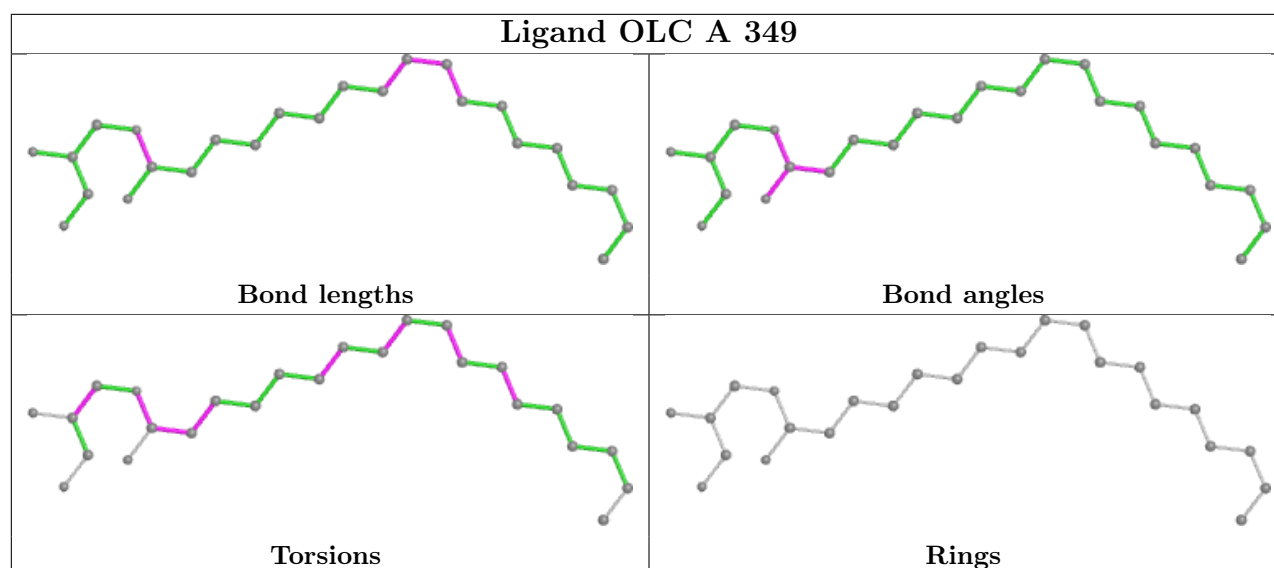


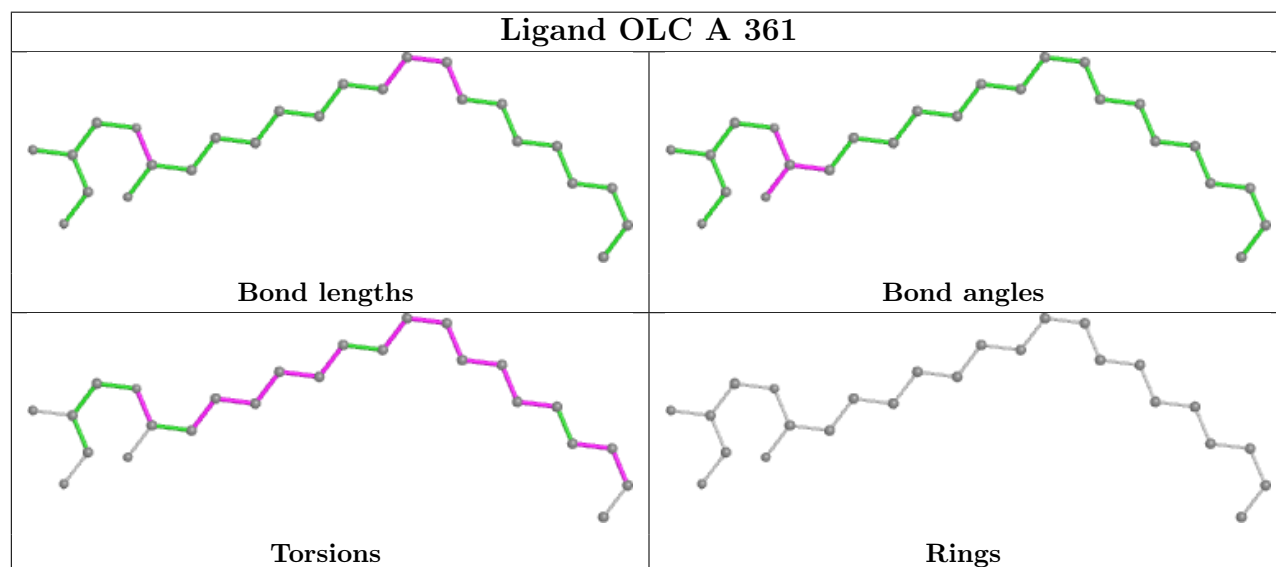
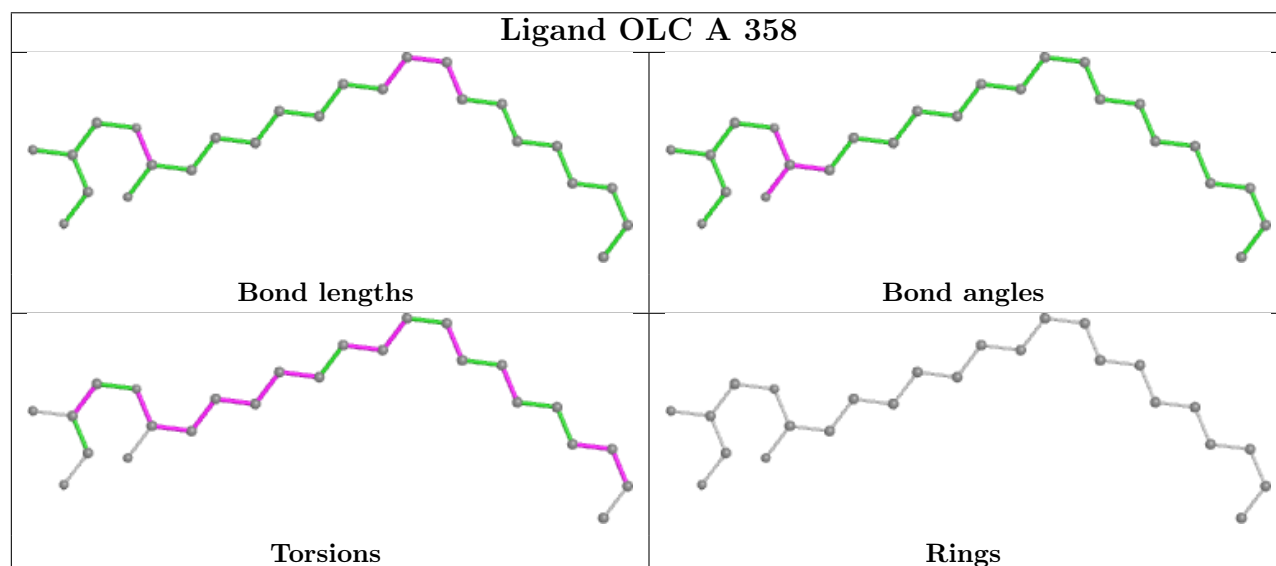
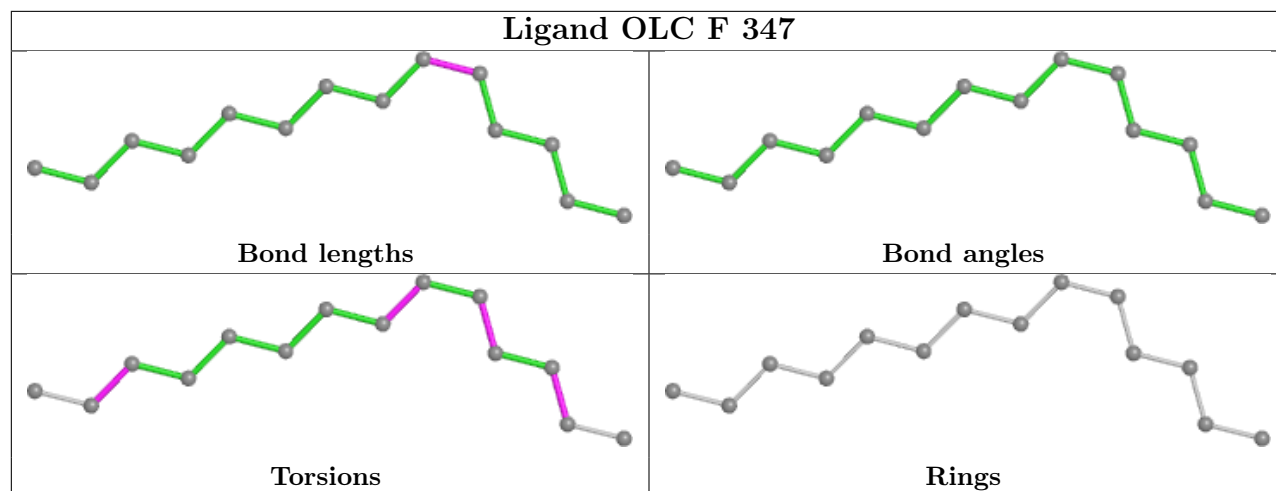


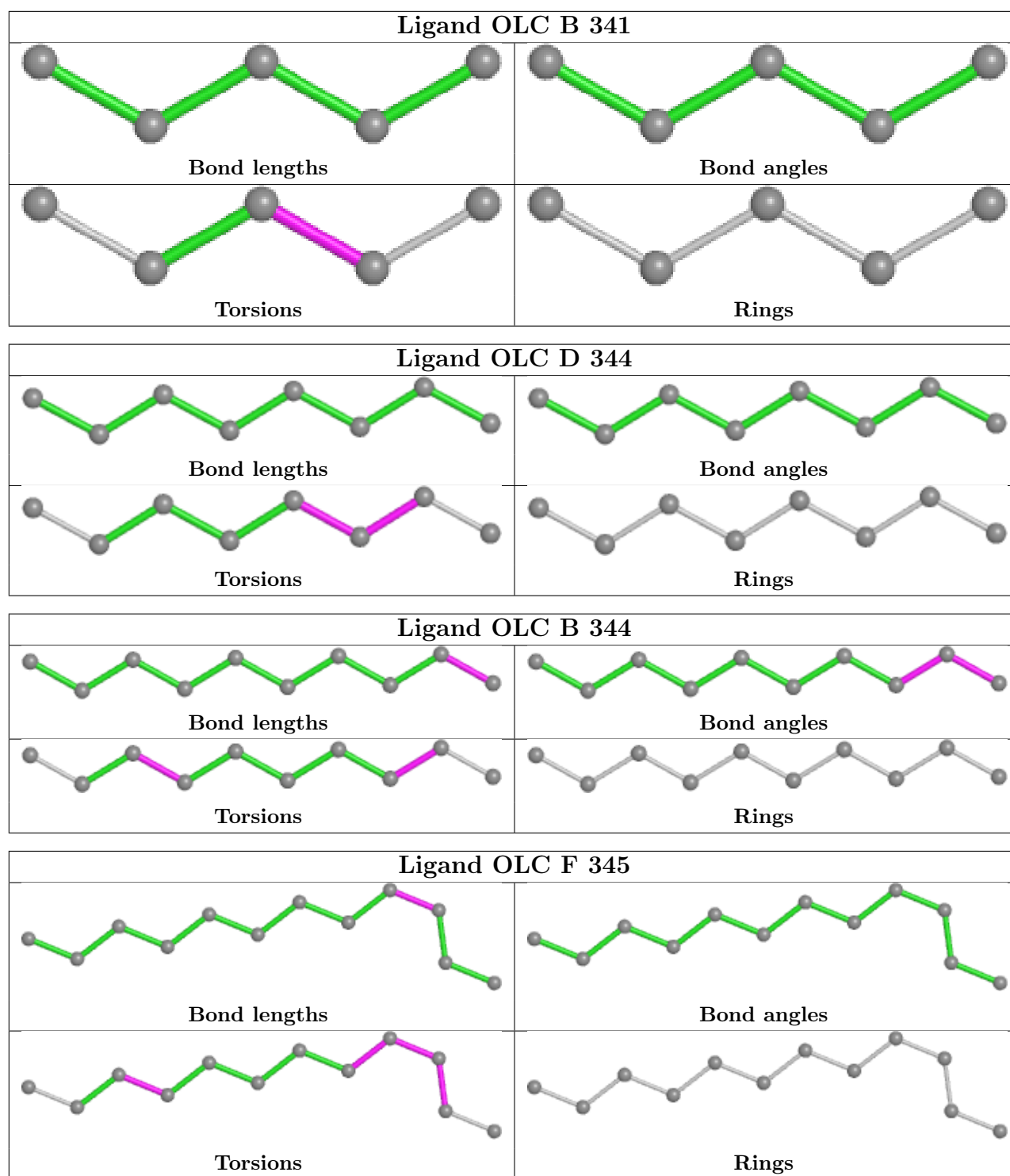


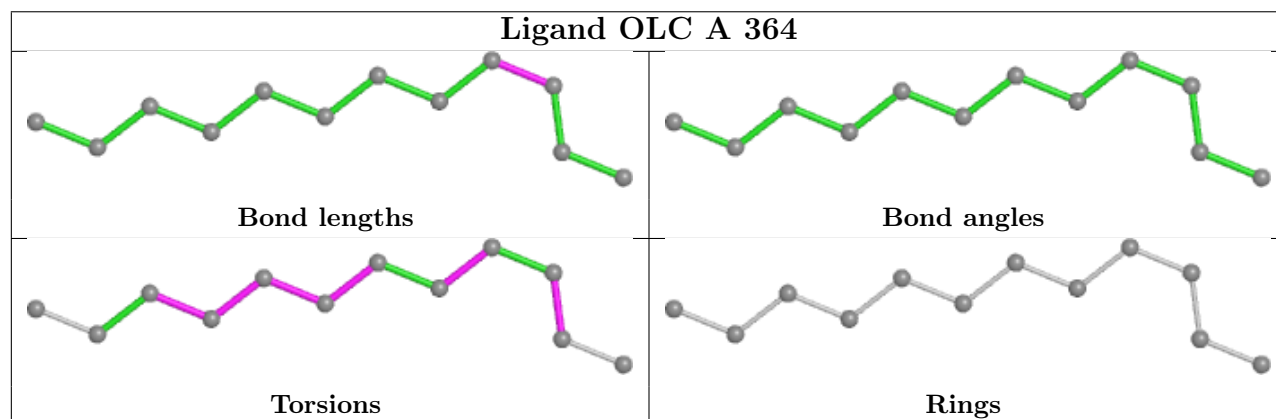
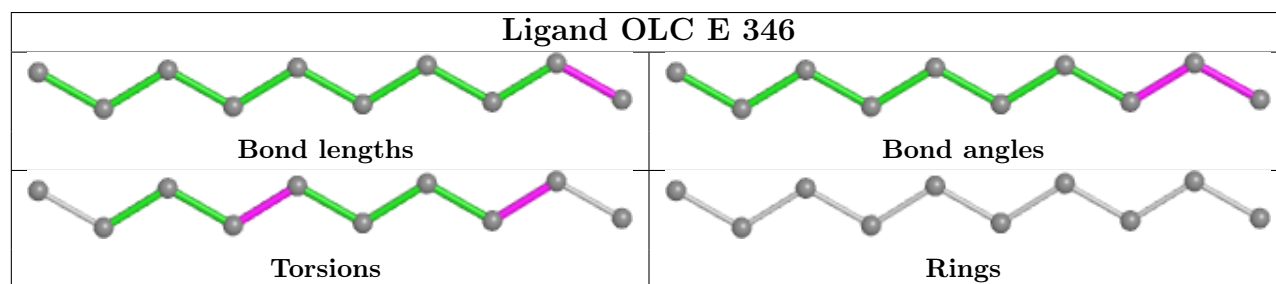
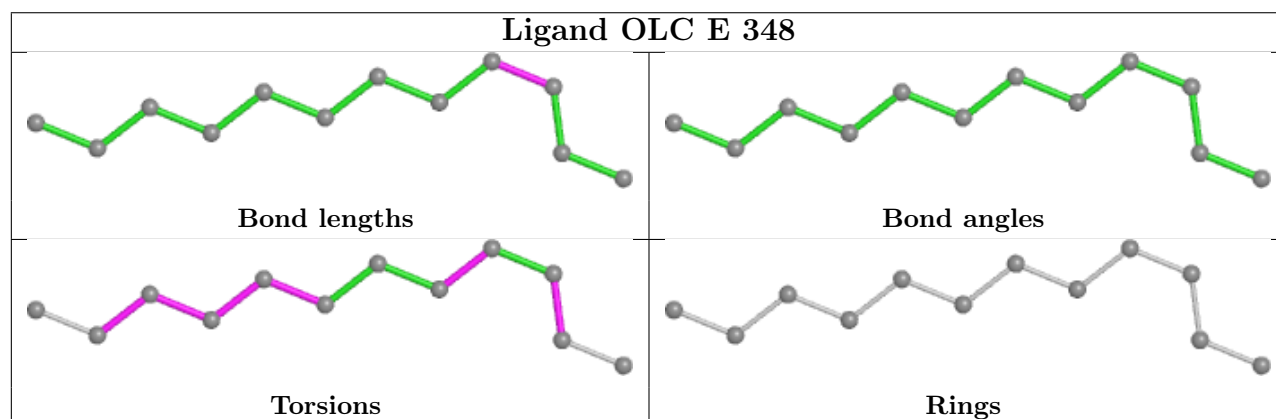
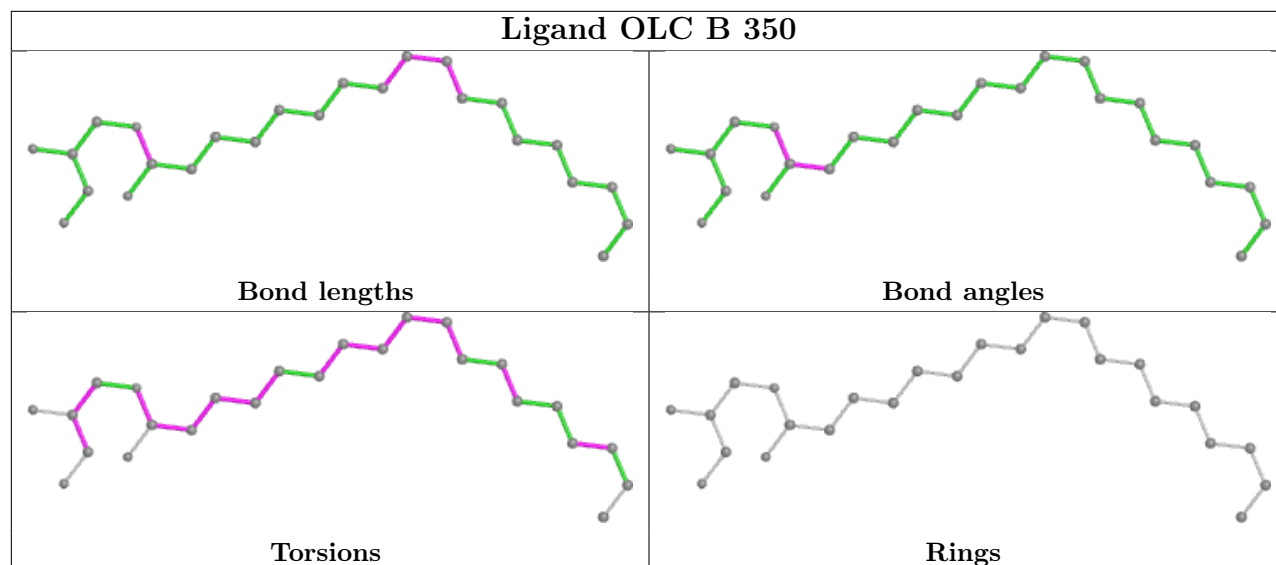


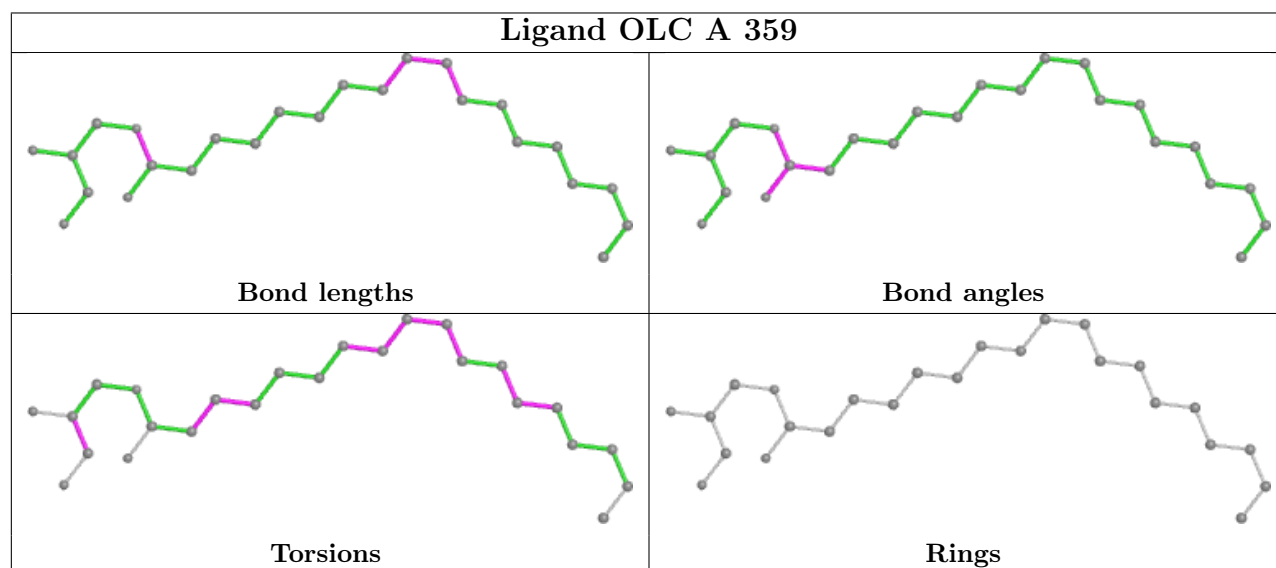
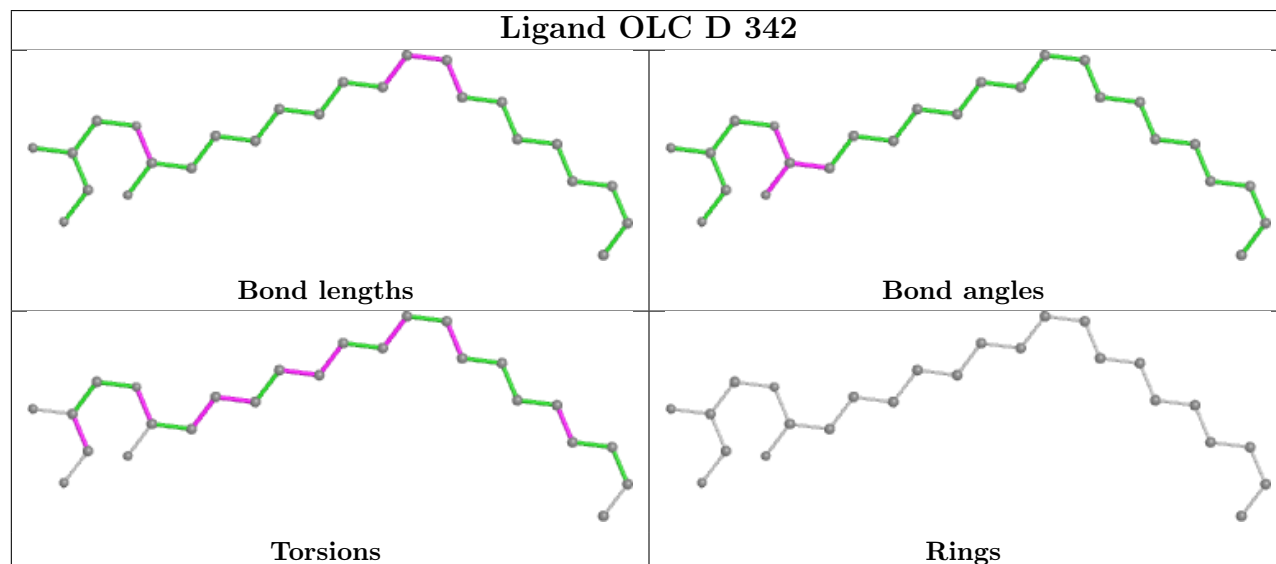
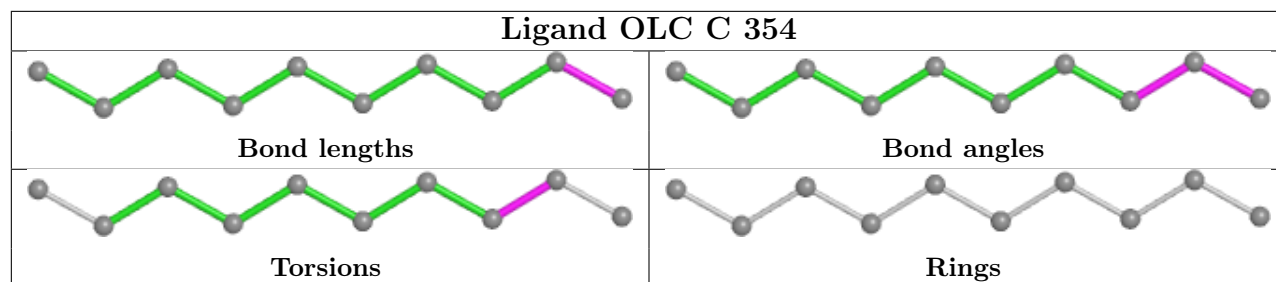


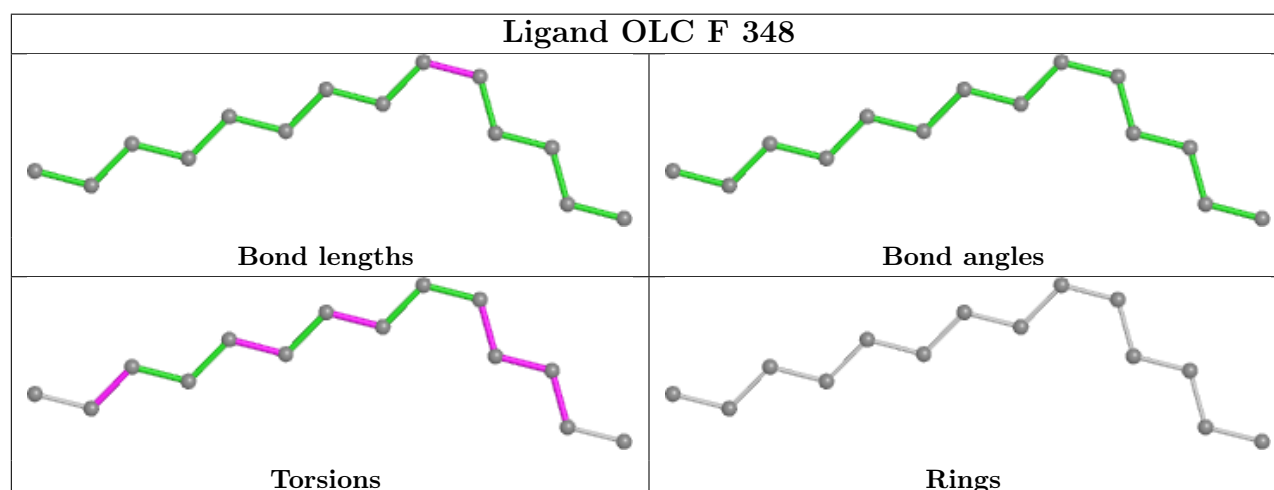
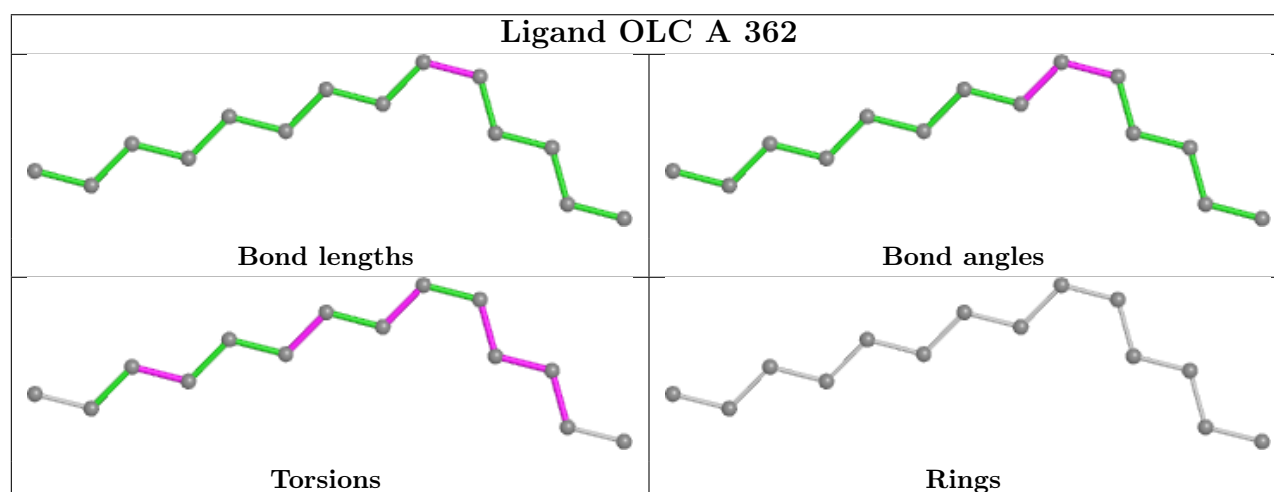
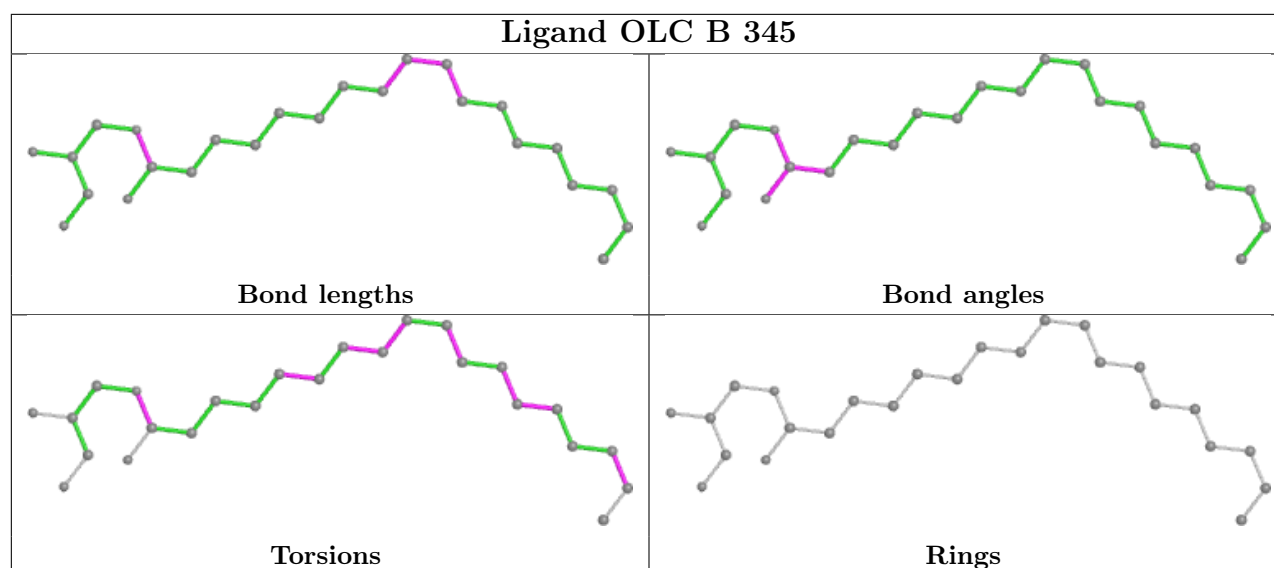


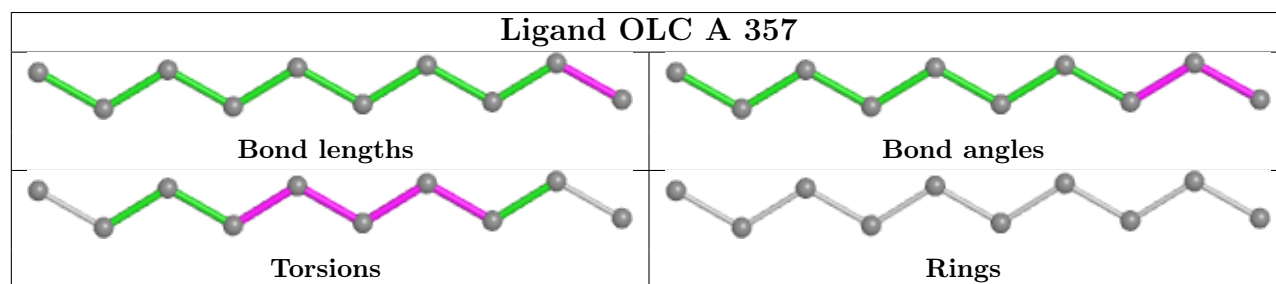
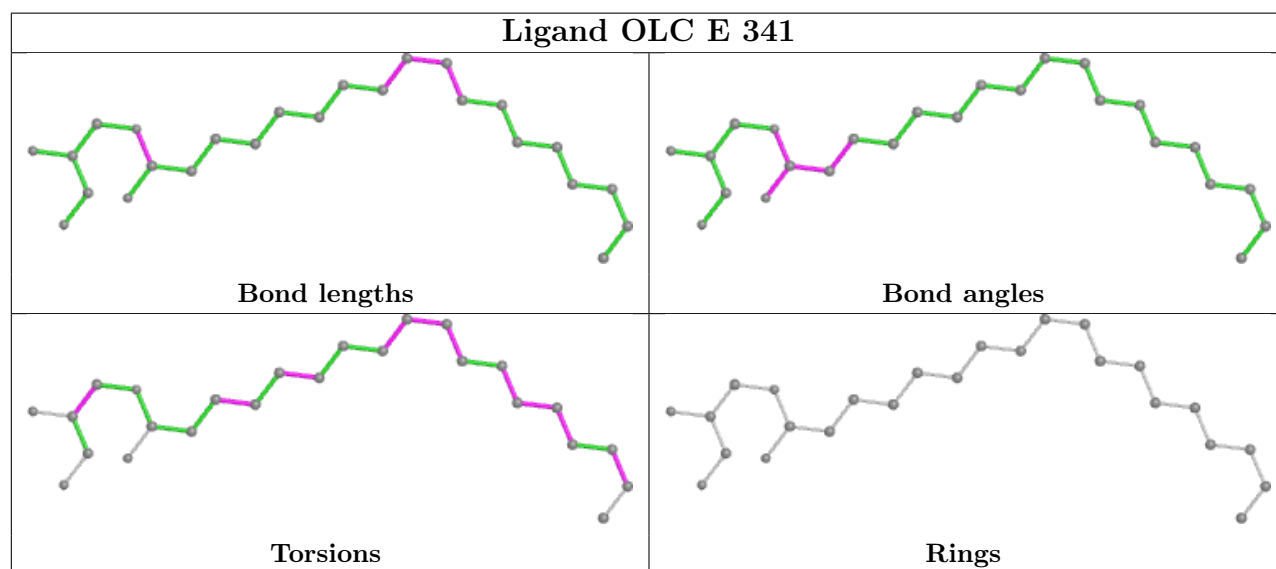
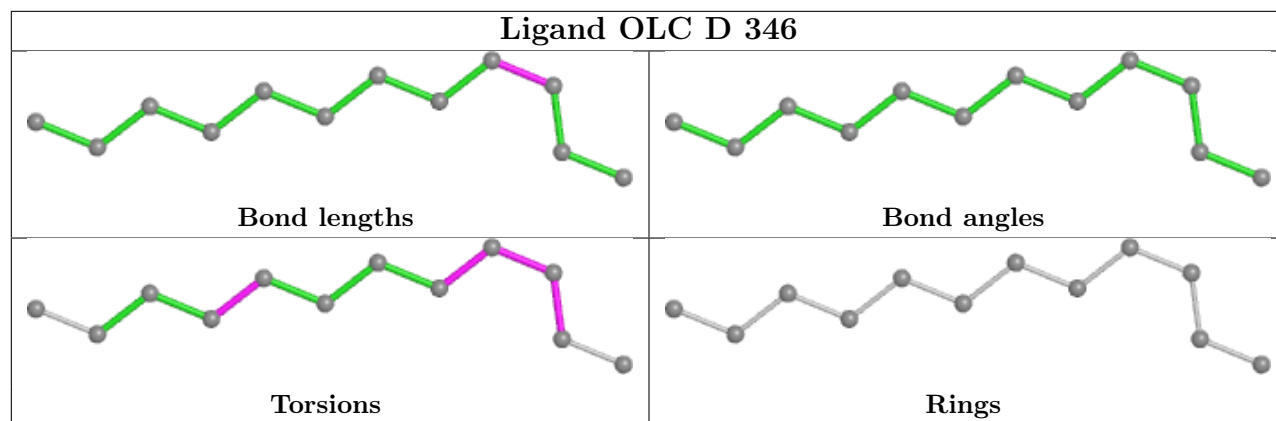


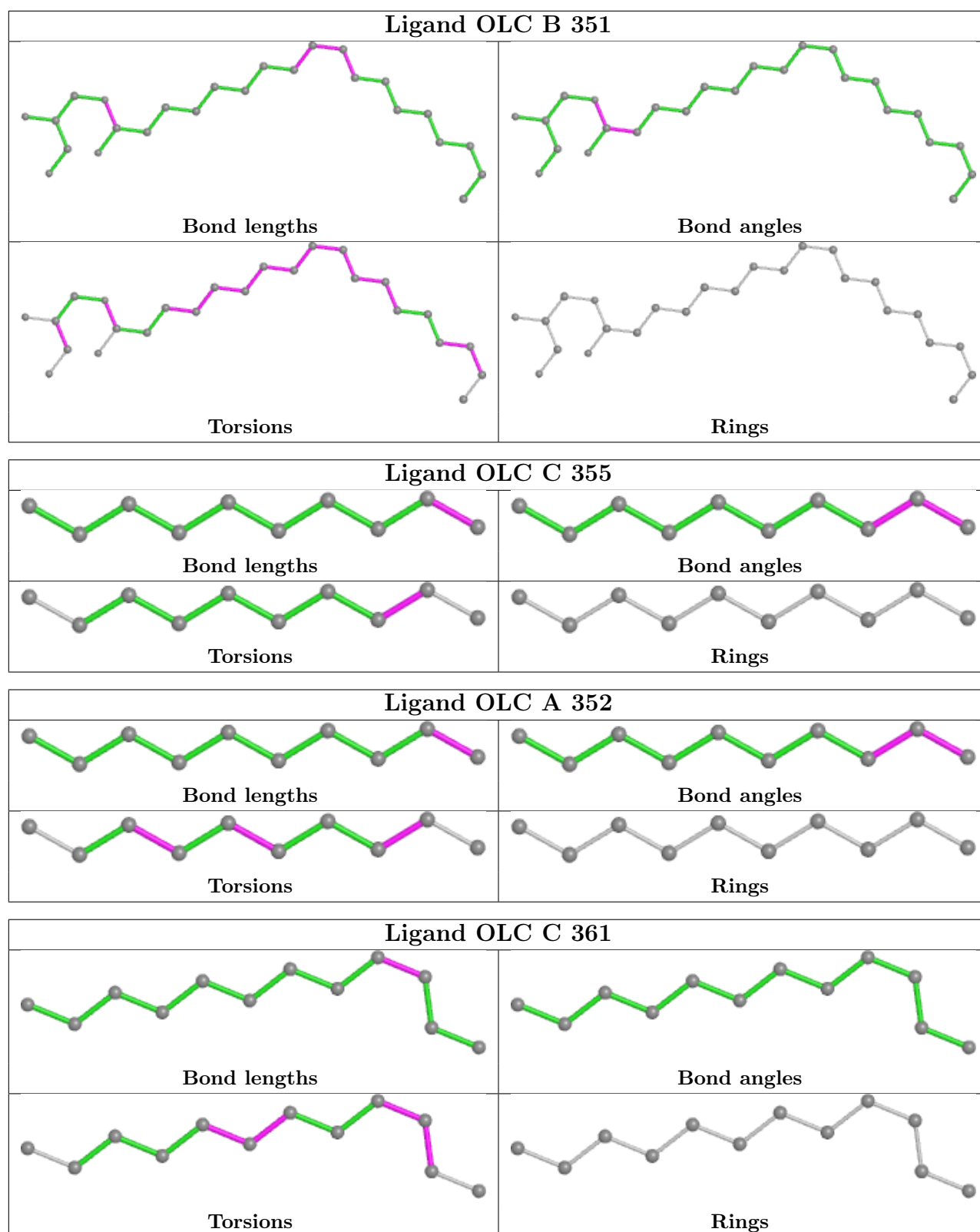




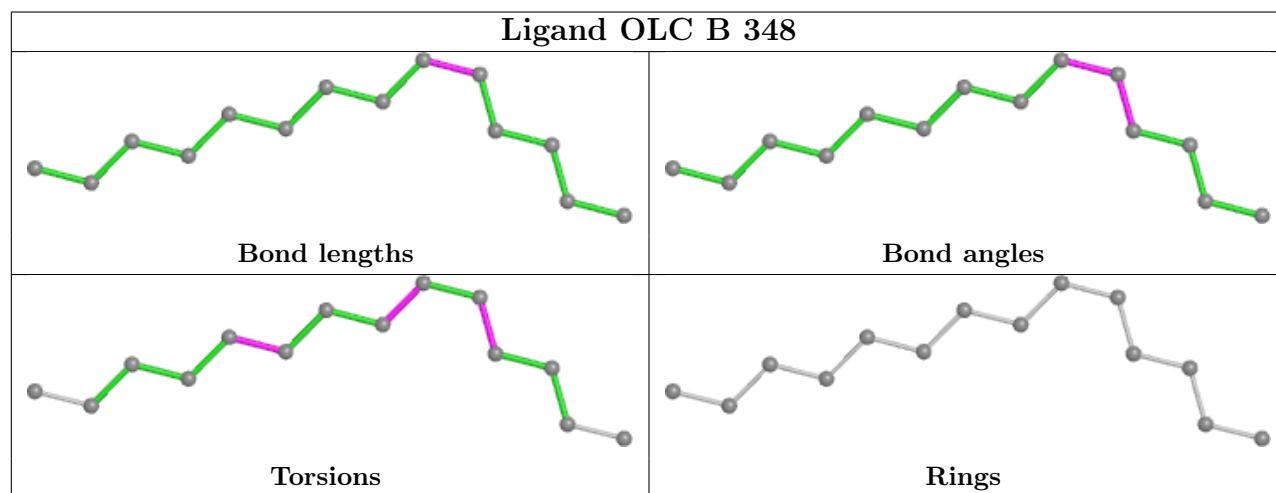
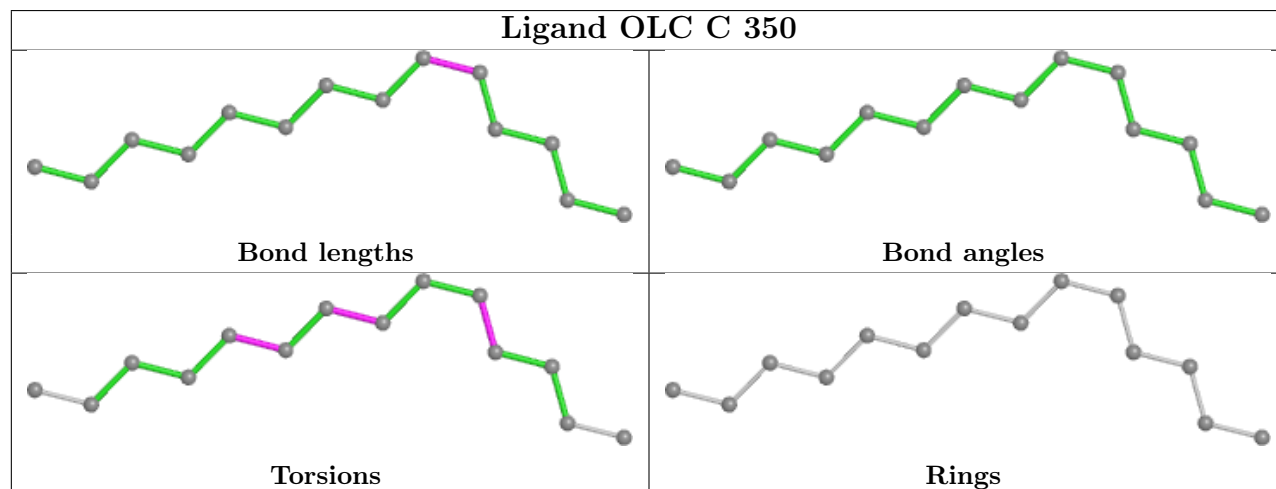
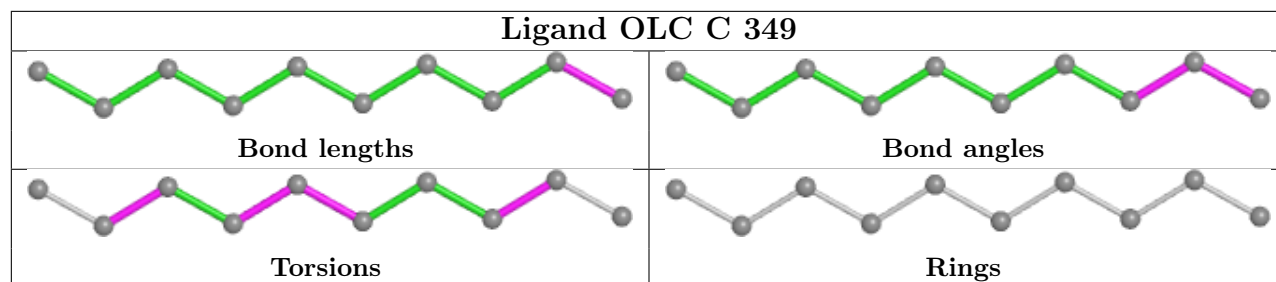


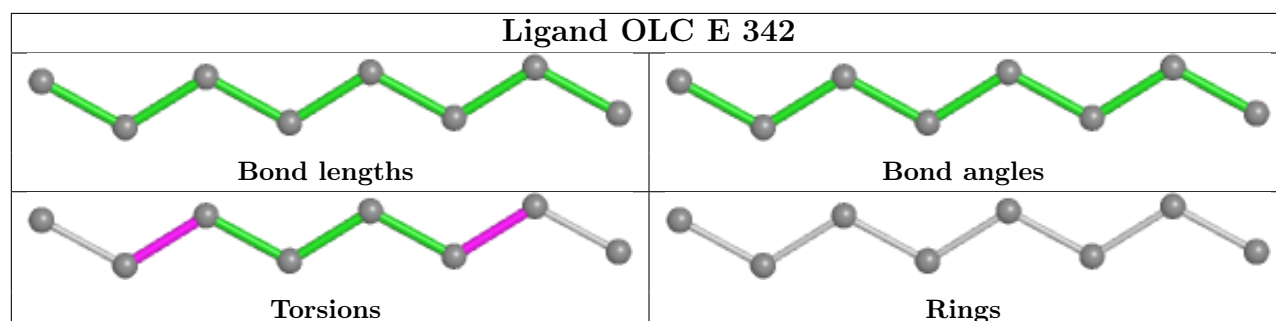
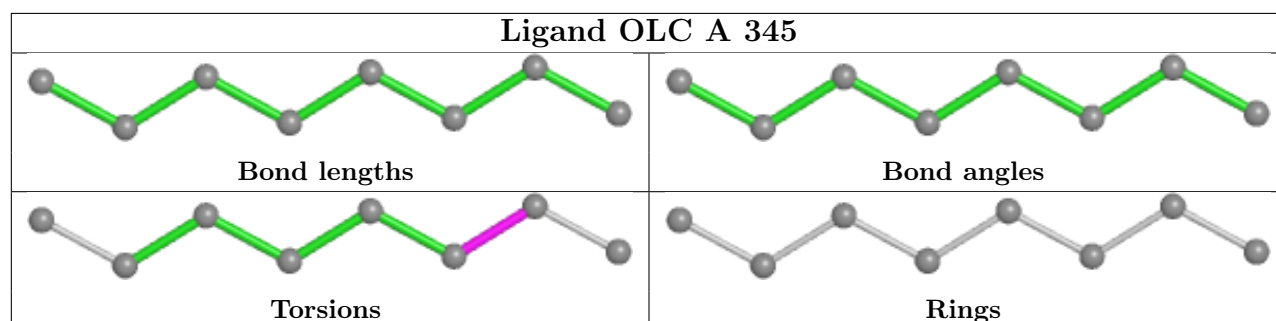
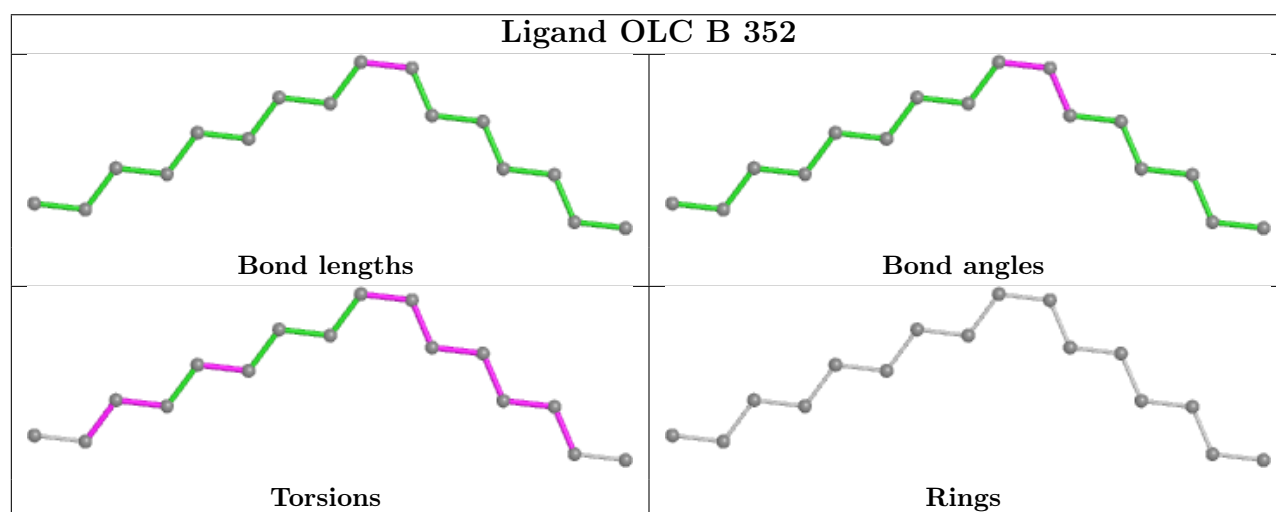
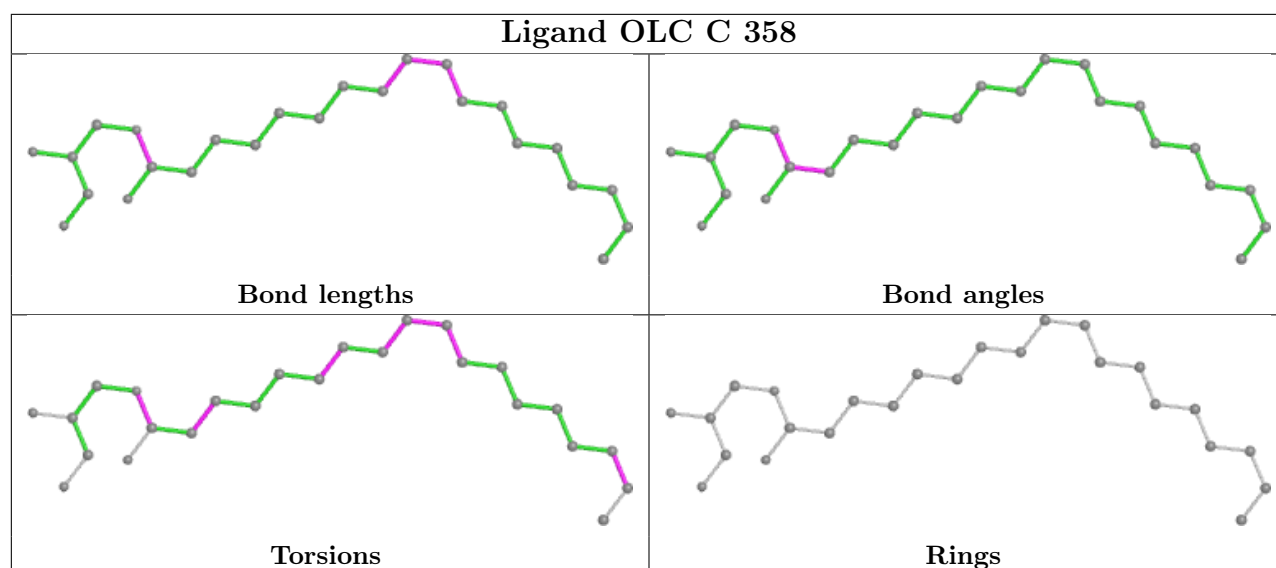


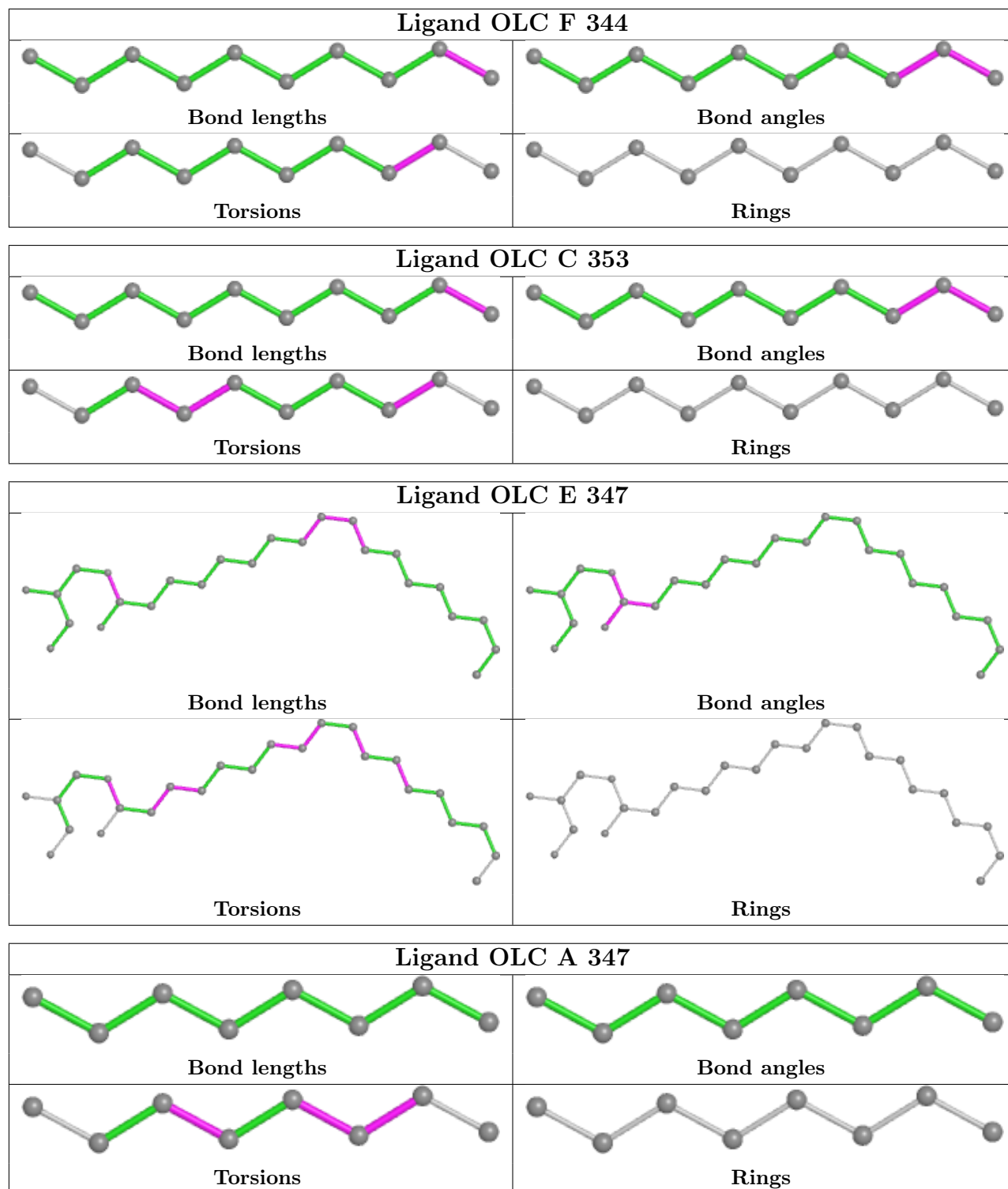


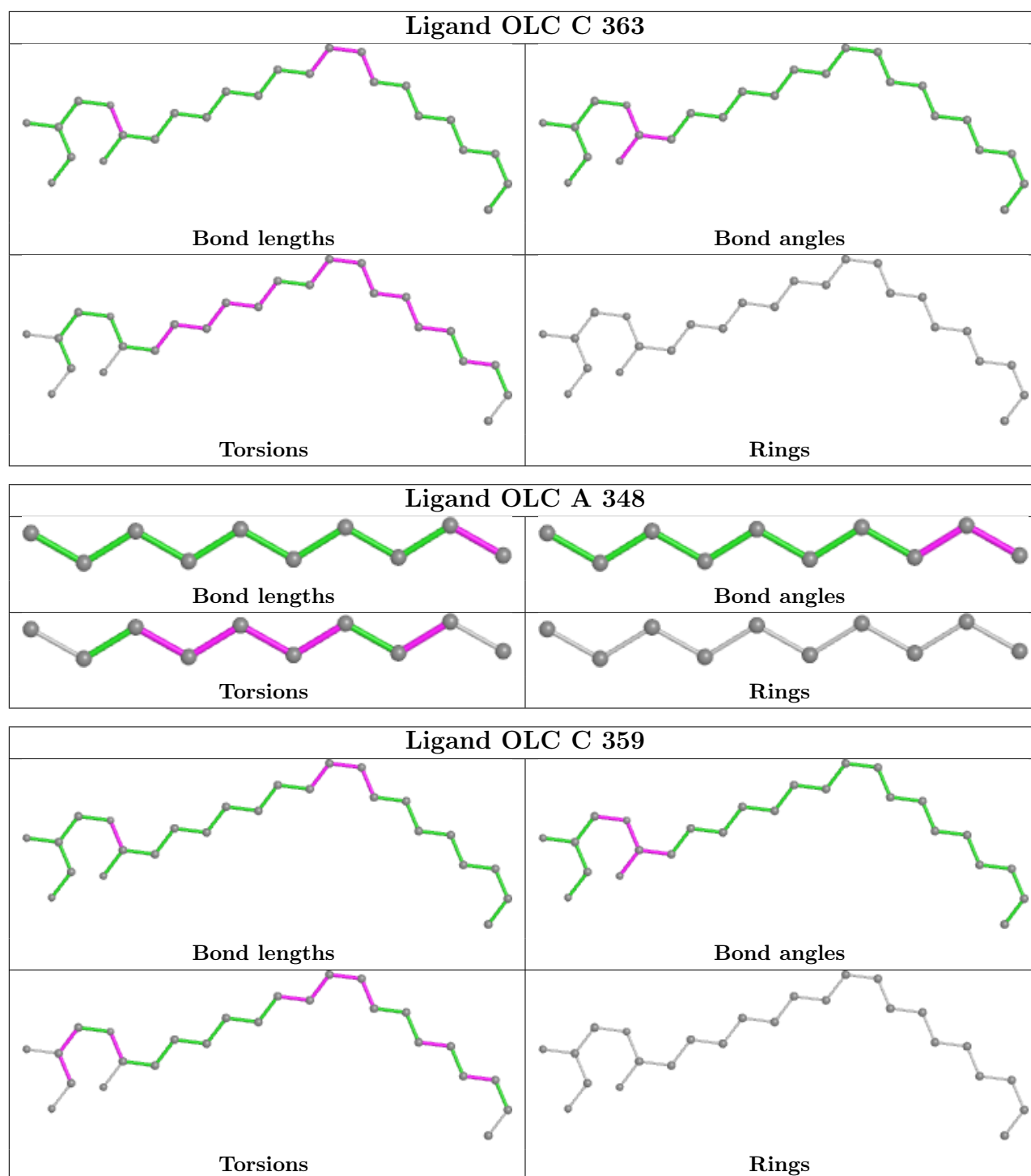


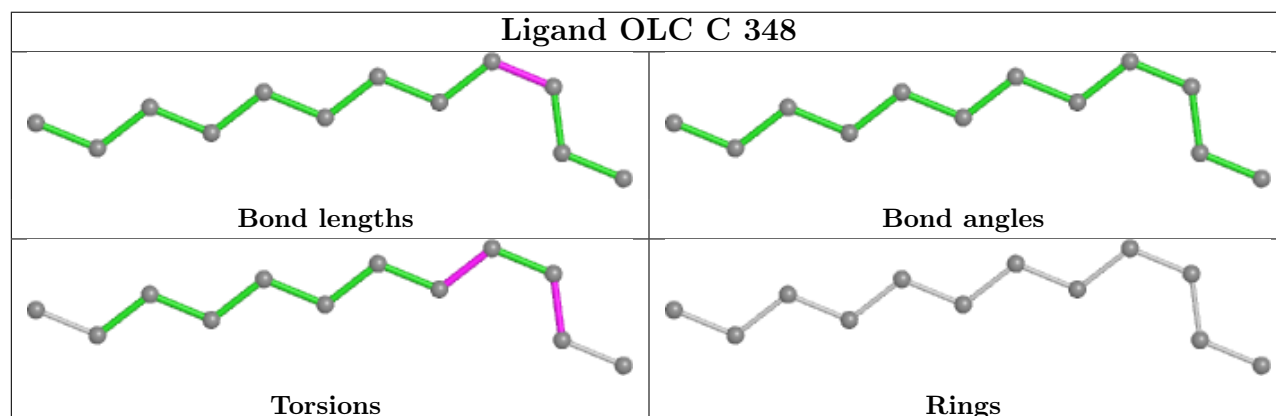
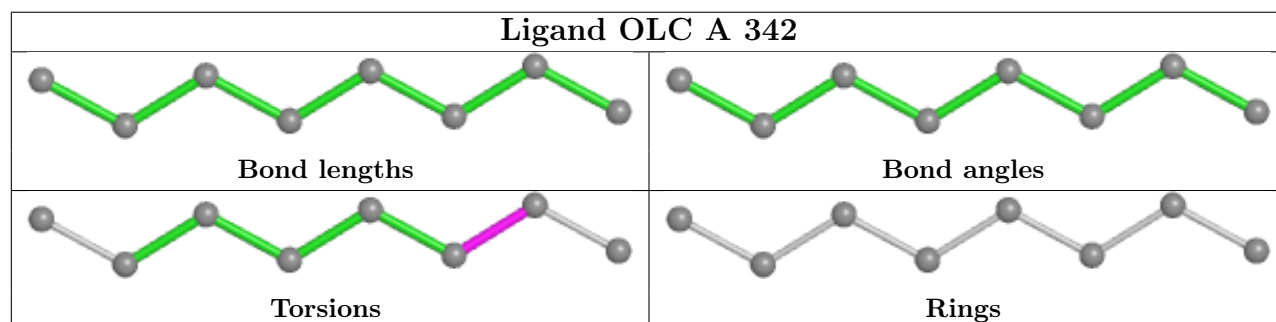
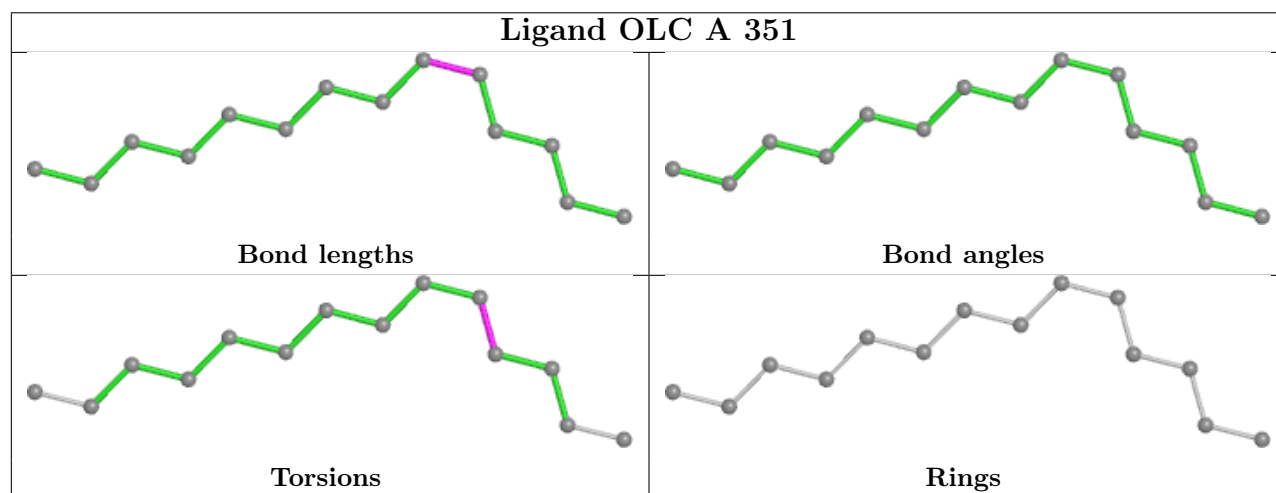
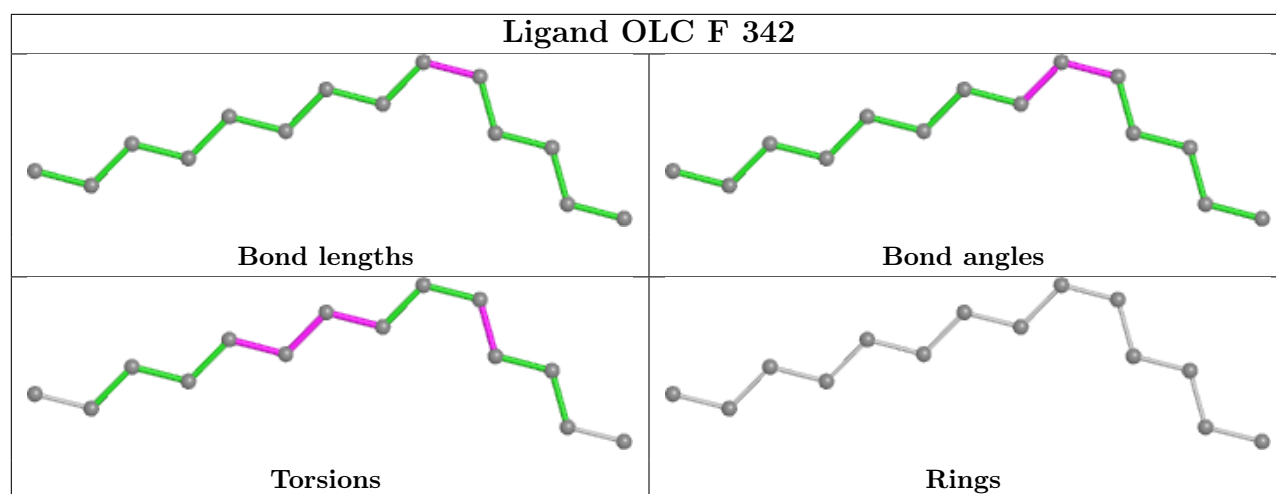


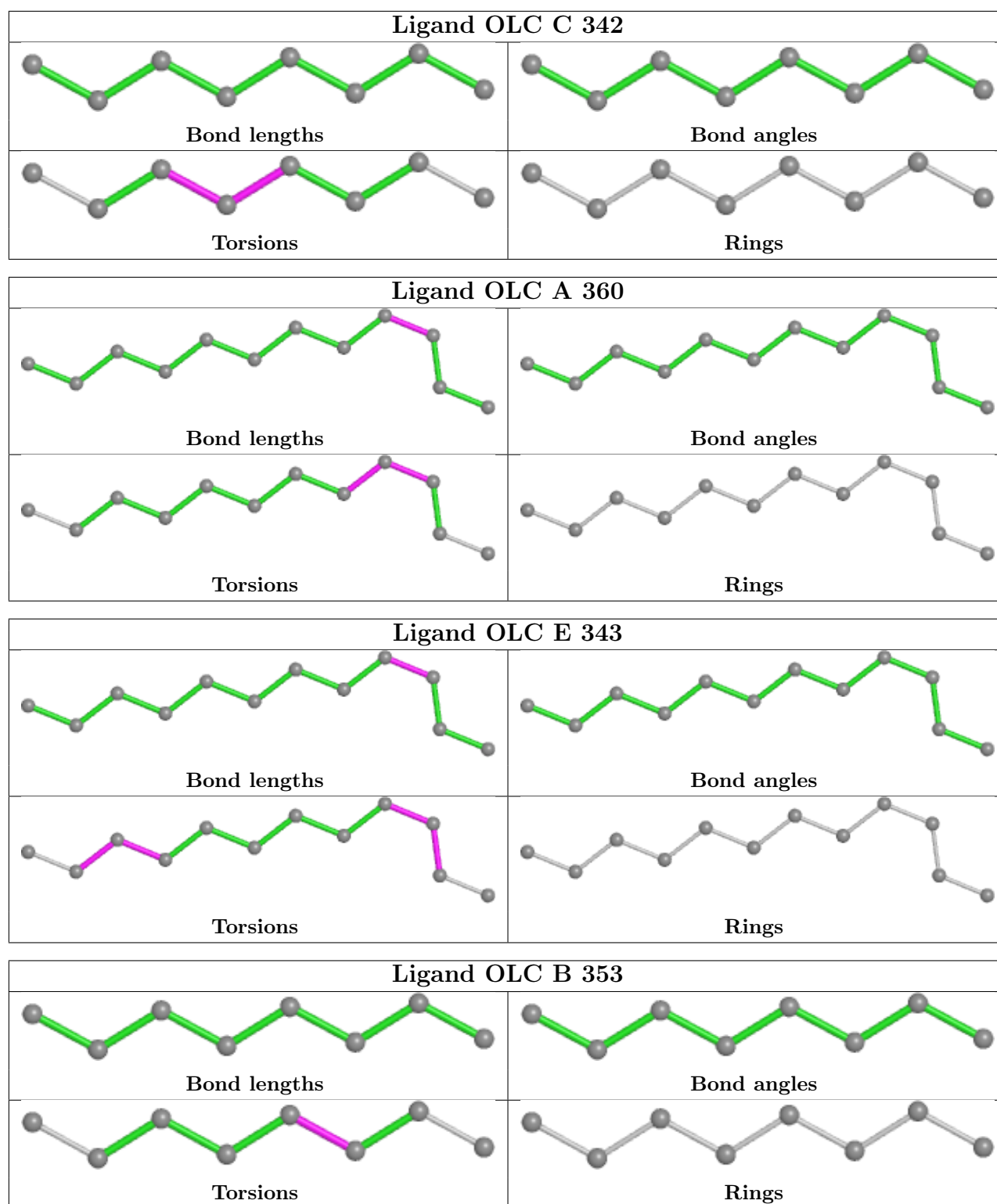


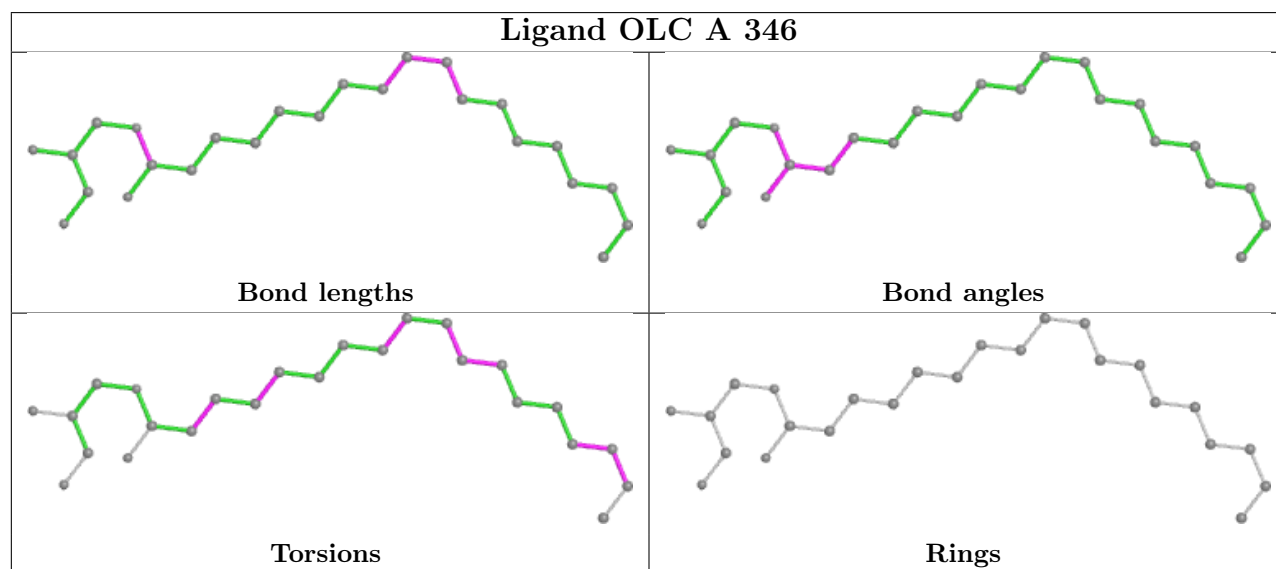
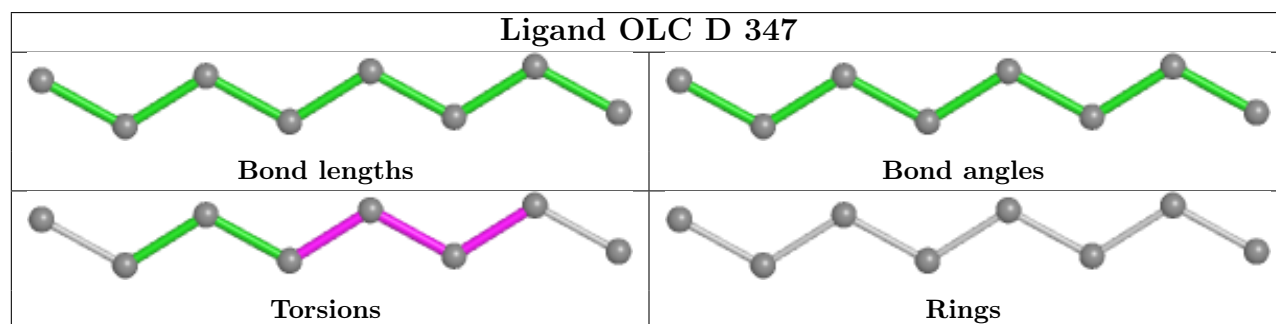
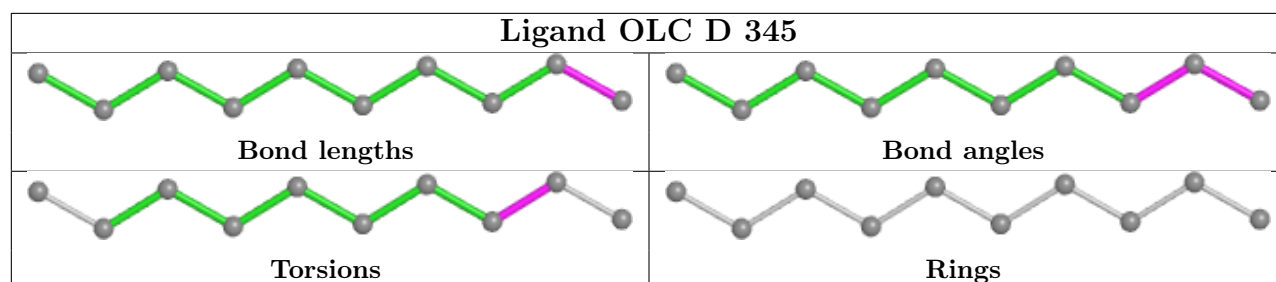
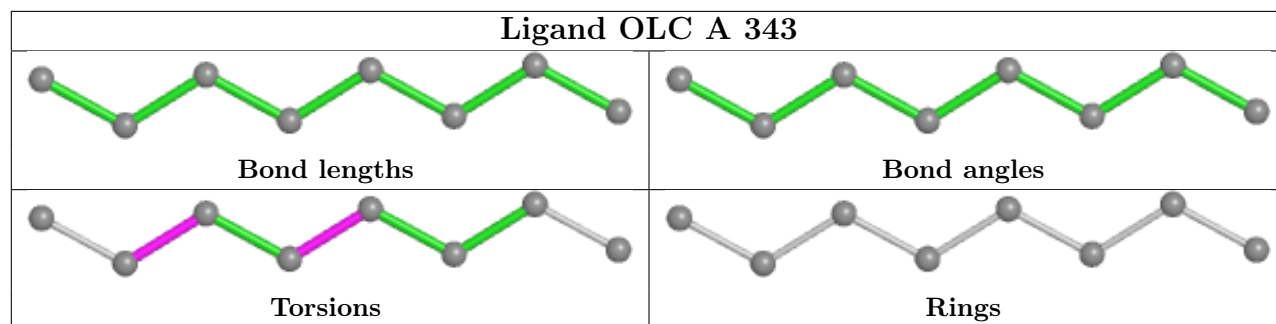


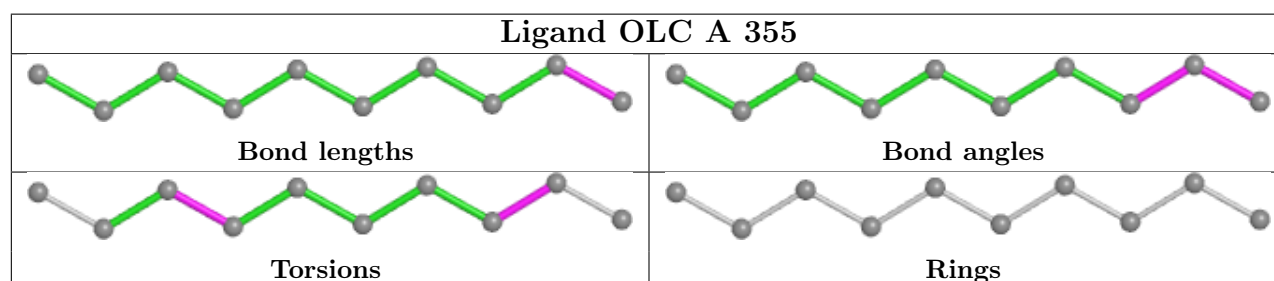
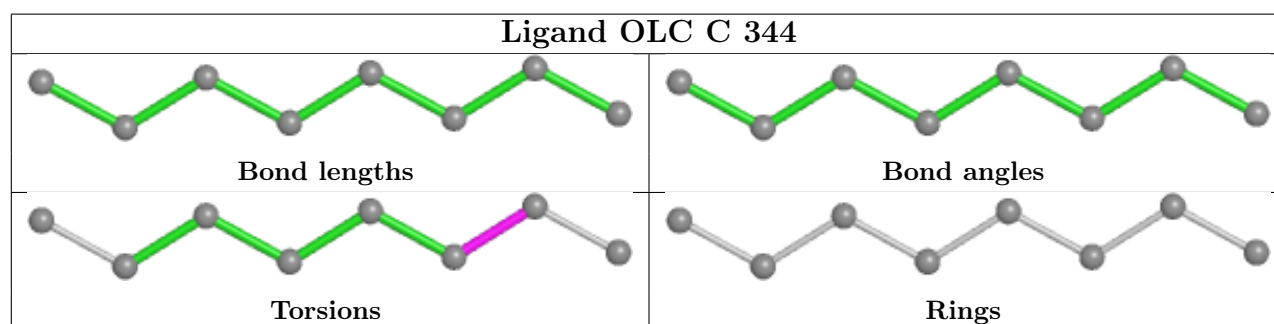
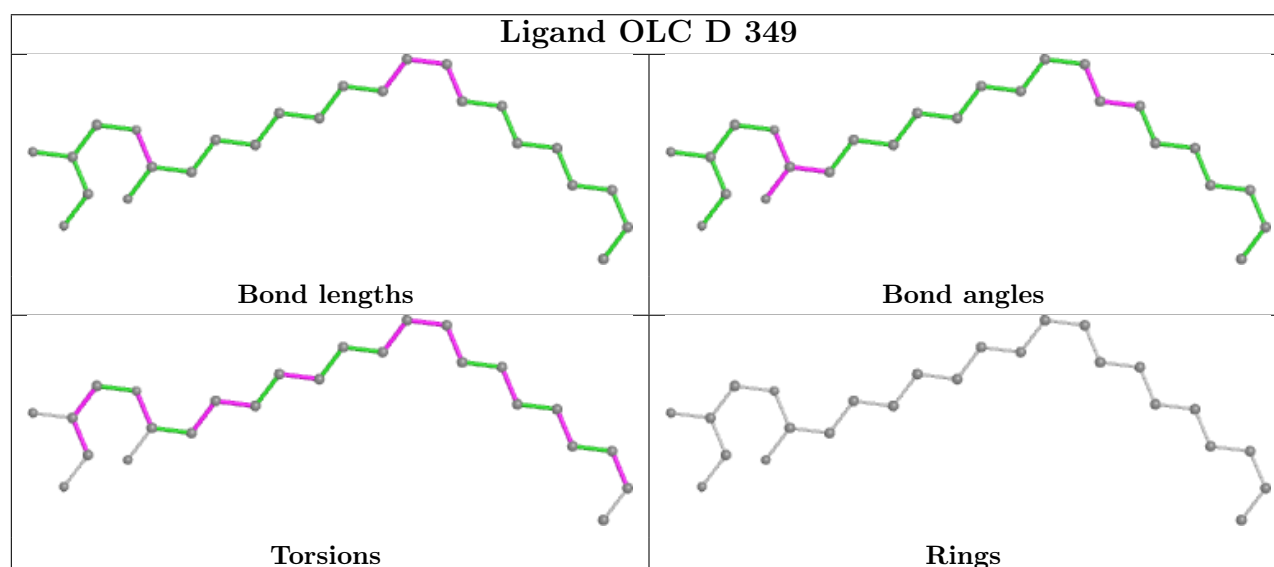
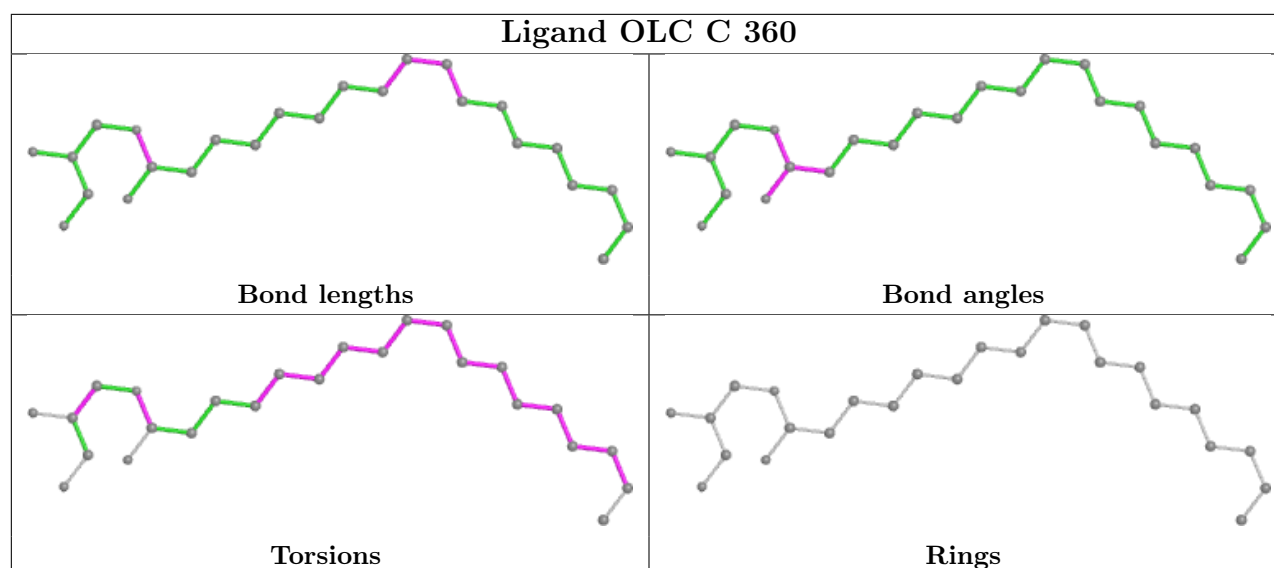




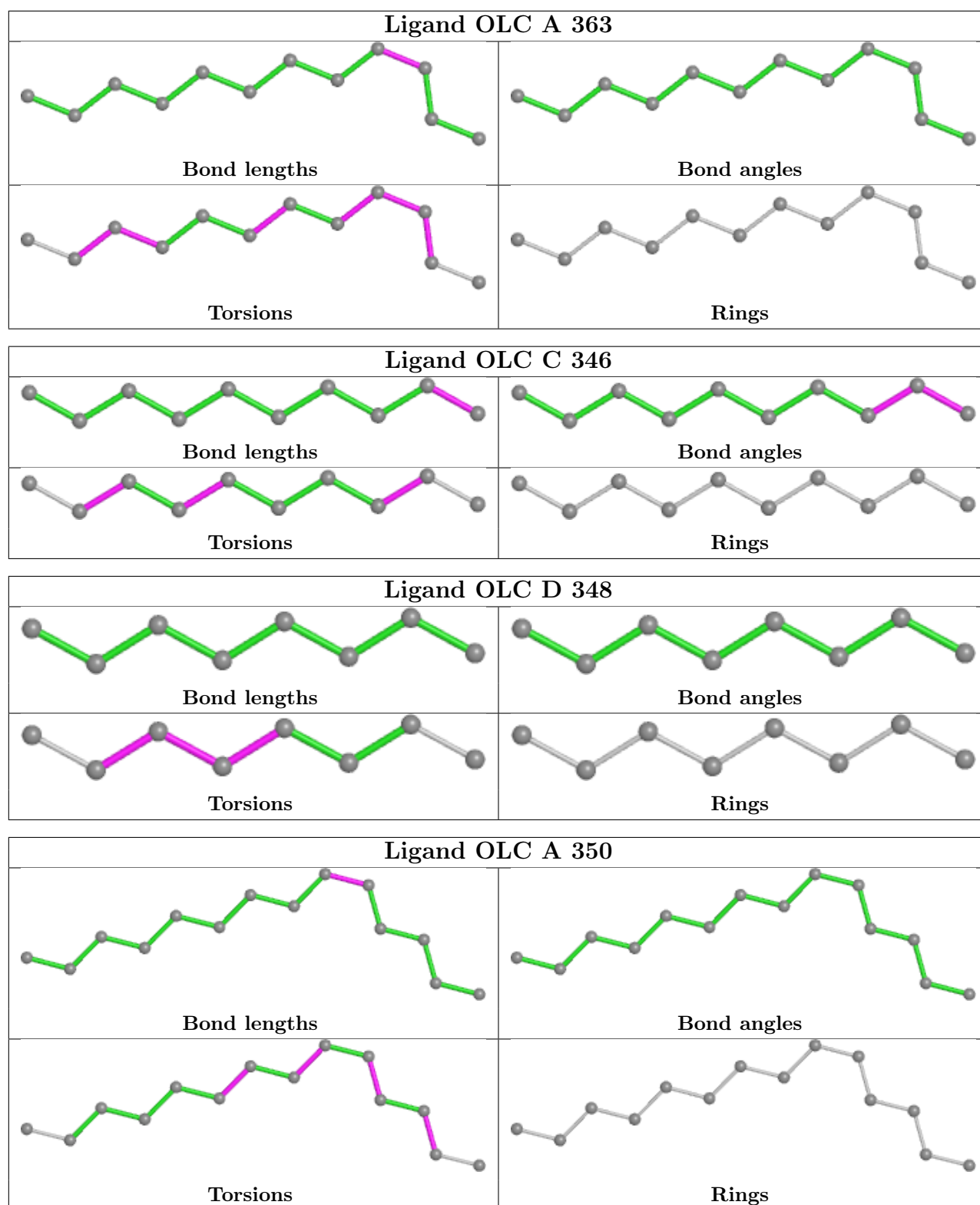


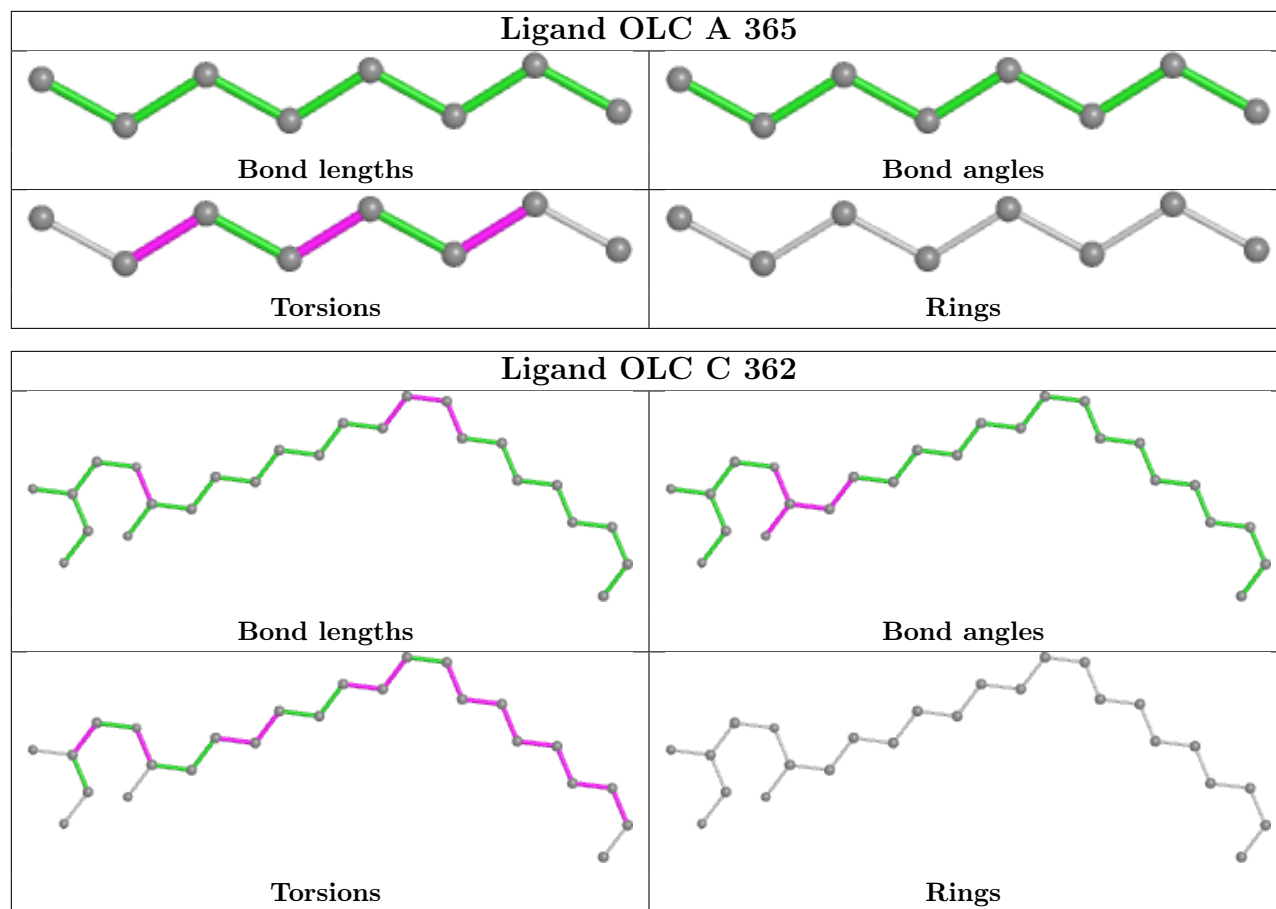












## 5.7 Other polymers [i](#)

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	340/340 (100%)	-0.50	2 (0%) 89 88	11, 19, 38, 53	0
1	B	340/340 (100%)	-0.32	8 (2%) 59 57	14, 25, 46, 59	0
1	C	340/340 (100%)	-0.37	8 (2%) 59 57	13, 22, 40, 53	0
1	D	340/340 (100%)	-0.41	6 (1%) 68 66	12, 21, 42, 56	0
1	E	340/340 (100%)	-0.50	1 (0%) 94 93	11, 20, 38, 51	0
1	F	340/340 (100%)	-0.21	11 (3%) 47 46	13, 27, 49, 65	0
All	All	2040/2040 (100%)	-0.39	36 (1%) 68 66	11, 22, 44, 65	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	ASN	3.6
1	F	246	ASN	3.3
1	F	147	LEU	3.3
1	F	182	TYR	3.2
1	C	147	LEU	3.1

### 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	E	345	14/25	0.60	0.21	32,50,57,59	0
2	OLC	B	348	14/25	0.63	0.27	50,58,61,61	0
2	OLC	F	342	14/25	0.63	0.24	50,52,58,59	0
2	OLC	D	342	25/25	0.64	0.23	45,51,70,75	0
2	OLC	B	351	25/25	0.68	0.21	37,46,61,68	0
2	OLC	A	358	25/25	0.68	0.24	49,55,61,64	0
2	OLC	D	349	25/25	0.69	0.18	39,49,54,55	0
2	OLC	A	360	12/25	0.70	0.32	49,54,68,68	0
2	OLC	B	341	5/25	0.70	0.18	42,44,47,47	0
2	OLC	B	342	14/25	0.70	0.30	51,56,62,64	0
2	OLC	B	350	25/25	0.71	0.22	34,49,60,71	0
2	OLC	A	365	8/25	0.71	0.26	44,48,60,60	0
2	OLC	C	352	12/25	0.72	0.25	51,56,59,59	0
2	OLC	E	344	12/25	0.73	0.29	29,54,59,59	0
2	OLC	C	351	8/25	0.73	0.27	53,56,60,60	0
2	OLC	C	348	12/25	0.73	0.26	50,55,59,59	0
2	OLC	C	363	25/25	0.74	0.21	38,46,56,66	0
2	OLC	C	356	8/25	0.74	0.27	35,50,58,59	0
2	OLC	C	357	14/25	0.74	0.18	28,46,50,51	0
2	OLC	F	344	10/25	0.74	0.22	49,57,62,63	0
2	OLC	D	345	10/25	0.75	0.18	39,45,49,51	0
2	OLC	E	346	10/25	0.75	0.21	58,60,62,62	0
2	OLC	A	361	25/25	0.76	0.23	40,53,64,67	0
2	OLC	C	354	10/25	0.76	0.34	60,64,67,67	0
2	OLC	C	362	25/25	0.76	0.22	27,41,58,60	0
2	OLC	C	347	10/25	0.77	0.23	49,50,62,63	0
2	OLC	B	354	8/25	0.77	0.15	36,48,60,64	0
2	OLC	C	350	14/25	0.77	0.19	37,49,53,55	0
2	OLC	A	344	10/25	0.78	0.18	29,42,49,49	0
2	OLC	F	341	8/25	0.78	0.22	40,44,48,52	0
2	OLC	C	345	12/25	0.78	0.17	37,43,49,49	0
2	OLC	D	346	12/25	0.78	0.16	32,36,41,43	0
2	OLC	A	355	10/25	0.79	0.22	40,51,66,66	0
2	OLC	A	345	8/25	0.79	0.14	35,44,47,49	0
2	OLC	F	347	14/25	0.79	0.34	49,60,63,64	0
2	OLC	C	344	8/25	0.80	0.18	40,44,53,55	0
2	OLC	B	349	8/25	0.80	0.14	43,45,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLC	C	360	25/25	0.80	0.16	23,40,72,74	0
2	OLC	B	353	8/25	0.80	0.22	35,41,49,50	0
2	OLC	E	343	12/25	0.80	0.15	40,48,52,54	0
2	OLC	F	345	12/25	0.80	0.19	37,46,57,57	0
2	OLC	A	350	14/25	0.80	0.17	31,35,46,47	0
2	OLC	F	348	14/25	0.80	0.16	36,43,50,50	0
2	OLC	F	343	8/25	0.81	0.22	48,55,61,61	0
2	OLC	A	351	14/25	0.81	0.16	42,50,56,56	0
2	OLC	A	363	12/25	0.81	0.15	31,39,47,48	0
2	OLC	F	346	8/25	0.81	0.15	40,45,50,51	0
2	OLC	A	349	25/25	0.81	0.19	36,42,56,63	0
2	OLC	C	353	10/25	0.81	0.28	54,56,62,63	0
2	OLC	C	358	25/25	0.82	0.18	31,39,63,66	0
2	OLC	C	341	10/25	0.82	0.13	36,40,55,59	0
2	OLC	A	346	25/25	0.82	0.17	35,44,57,61	0
2	OLC	A	362	14/25	0.82	0.15	38,44,49,49	0
2	OLC	E	347	25/25	0.83	0.17	26,45,53,57	0
2	OLC	E	348	12/25	0.83	0.13	42,49,52,52	0
2	OLC	A	348	10/25	0.83	0.15	40,44,49,50	0
2	OLC	C	361	12/25	0.83	0.15	24,32,37,37	0
2	OLC	A	359	25/25	0.83	0.18	28,40,54,54	0
2	OLC	A	357	10/25	0.84	0.17	26,37,44,46	0
2	OLC	E	341	25/25	0.84	0.17	21,39,49,53	0
2	OLC	B	345	25/25	0.85	0.17	33,43,52,60	0
2	OLC	D	347	8/25	0.85	0.14	28,36,41,41	0
2	OLC	C	343	8/25	0.85	0.42	56,62,66,66	0
2	OLC	B	344	10/25	0.86	0.12	42,44,53,54	0
2	OLC	A	364	12/25	0.86	0.32	48,54,56,56	0
2	OLC	B	347	14/25	0.86	0.13	30,38,47,49	0
2	OLC	D	348	8/25	0.86	0.17	37,43,44,46	0
2	OLC	B	352	16/25	0.86	0.16	32,41,46,47	0
2	OLC	A	352	10/25	0.86	0.17	38,47,51,51	0
2	OLC	E	342	8/25	0.86	0.17	40,41,43,45	0
2	OLC	B	346	25/25	0.87	0.16	29,39,54,61	0
2	OLC	C	359	25/25	0.87	0.14	30,38,57,63	0
2	OLC	C	349	10/25	0.87	0.21	36,44,52,56	0
2	OLC	A	342	8/25	0.87	0.12	48,50,58,60	0
2	OLC	C	364	12/25	0.88	0.14	37,44,47,47	0
2	OLC	C	355	10/25	0.89	0.13	33,41,50,51	0
2	OLC	A	347	8/25	0.89	0.13	25,29,36,39	0
2	OLC	A	356	25/25	0.90	0.16	22,36,53,65	0
2	OLC	C	346	10/25	0.90	0.12	34,44,54,57	0

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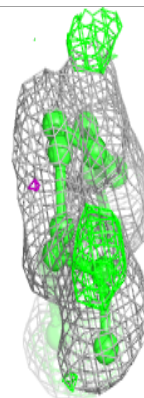
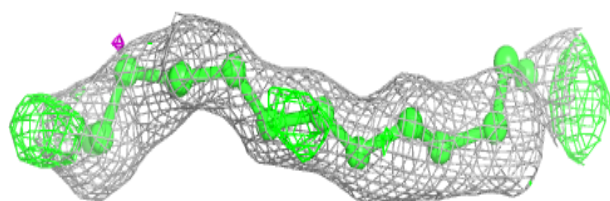
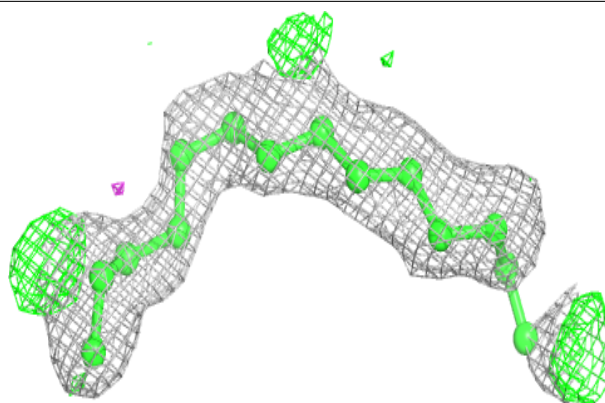
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLC	A	343	8/25	0.91	0.17	32,36,42,43	0
2	OLC	A	354	8/25	0.91	0.15	28,35,39,44	0
2	OLC	D	343	8/25	0.91	0.22	39,44,48,53	0
2	OLC	D	341	5/25	0.93	0.11	36,39,44,45	0
2	OLC	B	343	8/25	0.93	0.14	30,37,44,48	0
2	OLC	C	342	8/25	0.93	0.11	26,35,46,48	0
2	OLC	A	341	8/25	0.94	0.10	28,32,41,43	0
2	OLC	A	353	8/25	0.94	0.09	32,34,43,44	0
2	OLC	D	344	8/25	0.95	0.12	27,31,47,51	0
3	K	F	350	1/1	0.95	0.18	42,42,42,42	0
4	SCN	B	358	3/3	0.95	0.08	25,25,26,37	0
4	SCN	E	352	3/3	0.95	0.11	20,20,21,35	0
4	SCN	A	369	3/3	0.96	0.08	23,23,25,32	0
3	K	C	367	1/1	0.96	0.06	38,38,38,38	0
4	SCN	D	354	3/3	0.96	0.06	25,25,25,36	0
3	K	B	356	1/1	0.96	0.15	38,38,38,38	0
4	SCN	E	353	3/3	0.96	0.12	40,40,44,49	0
4	SCN	F	352	3/3	0.97	0.09	21,21,23,34	0
3	K	D	353	1/1	0.98	0.08	38,38,38,38	0
3	K	E	350	1/1	0.98	0.03	26,26,26,26	0
3	K	E	351	1/1	0.98	0.11	33,33,33,33	0
3	K	A	368	1/1	0.98	0.07	32,32,32,32	0
3	K	B	355	1/1	0.98	0.07	34,34,34,34	0
3	K	F	349	1/1	0.99	0.08	30,30,30,30	0
3	K	A	367	1/1	0.99	0.05	27,27,27,27	0
3	K	F	351	1/1	0.99	0.21	44,44,44,44	0
3	K	C	368	1/1	0.99	0.11	36,36,36,36	0
3	K	D	351	1/1	0.99	0.04	29,29,29,29	0
3	K	D	352	1/1	0.99	0.09	38,38,38,38	0
3	K	B	357	1/1	0.99	0.15	41,41,41,41	0
3	K	C	365	1/1	0.99	0.04	25,25,25,25	0
3	K	C	366	1/1	0.99	0.05	28,28,28,28	0
3	K	E	349	1/1	1.00	0.02	23,23,23,23	0
3	K	D	350	1/1	1.00	0.04	23,23,23,23	0
3	K	A	366	1/1	1.00	0.05	25,25,25,25	0

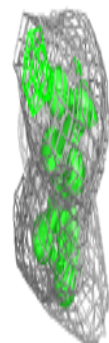
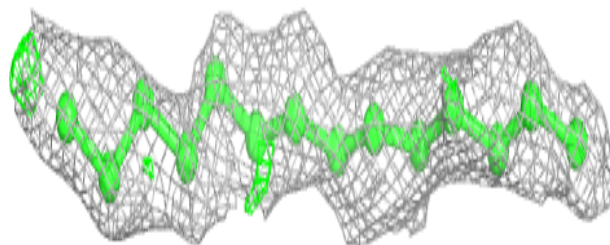
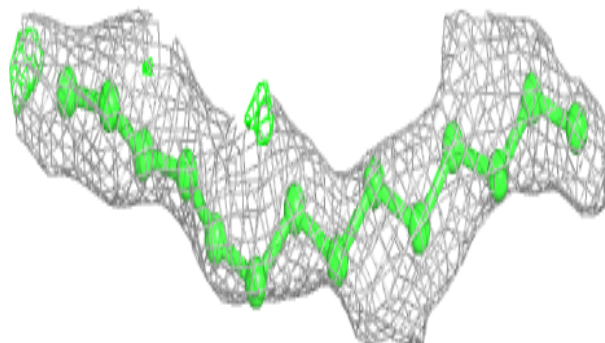
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLC E 345:**

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

**Electron density around OLC B 348:**

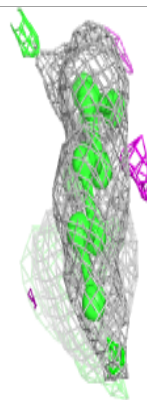
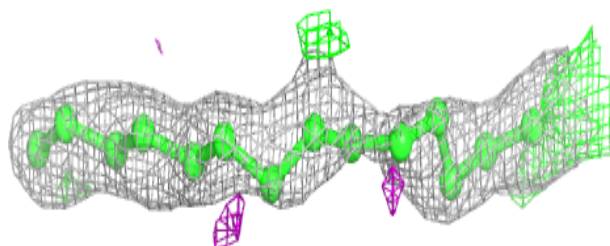
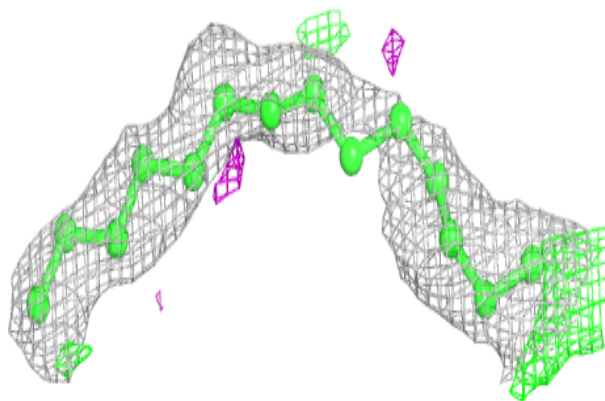
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



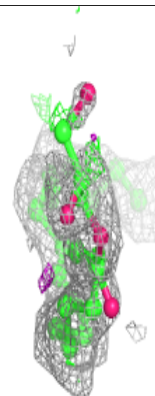
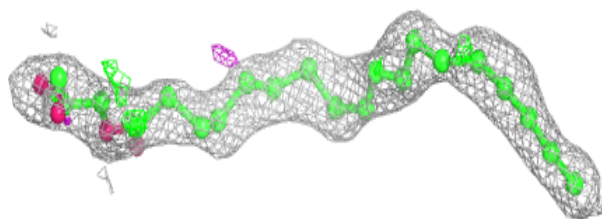
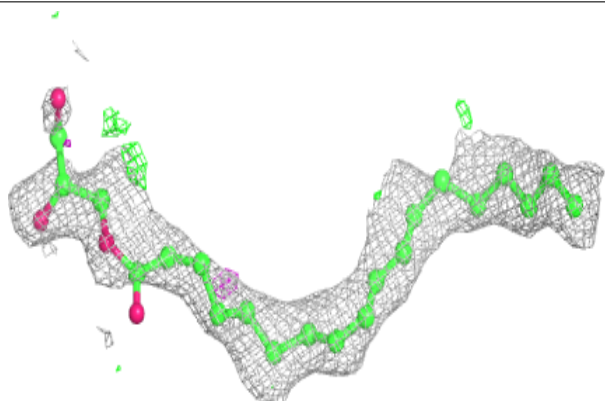


**Electron density around OLC F 342:**

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

**Electron density around OLC D 342:**

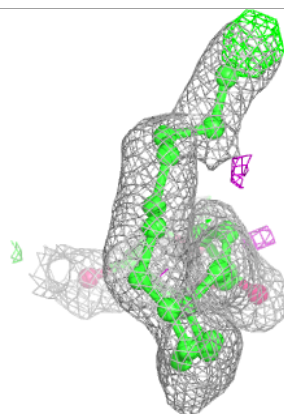
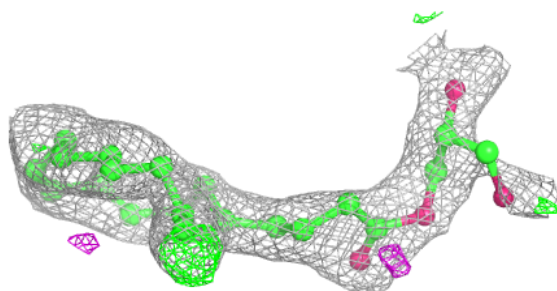
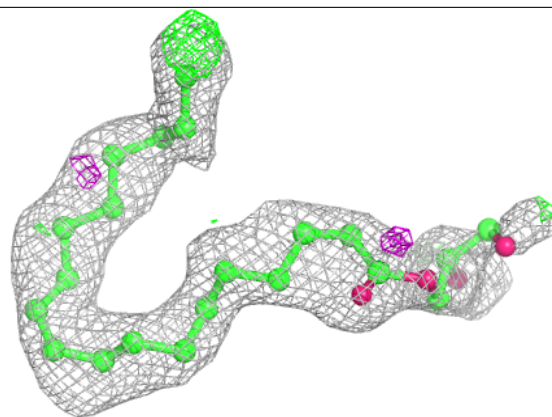
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



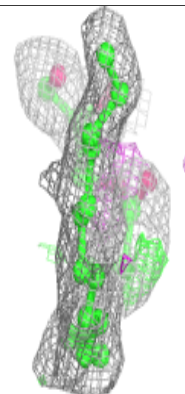
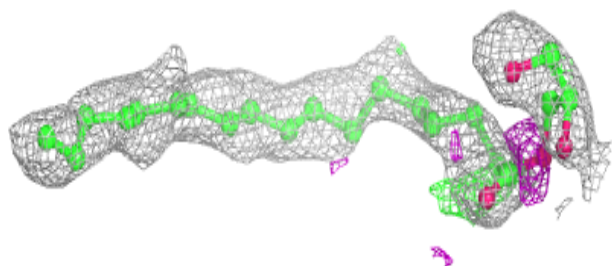
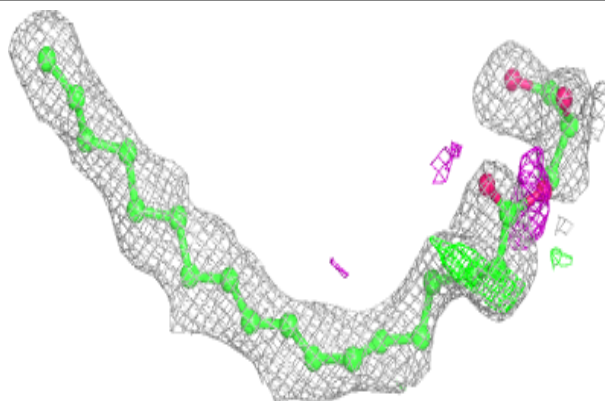


**Electron density around OLC B 351:**

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

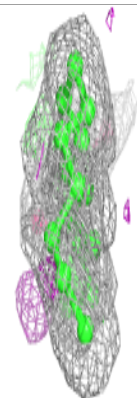
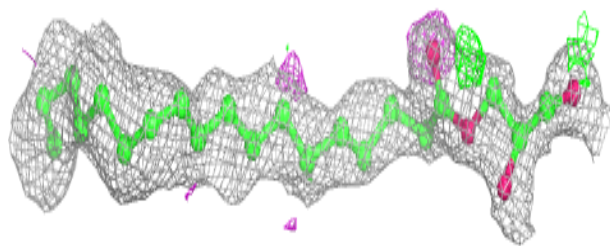
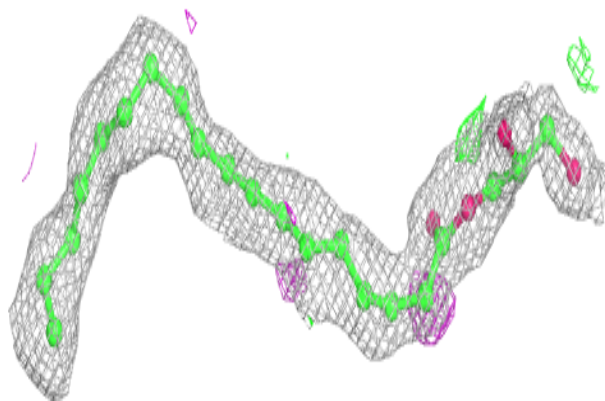
**Electron density around OLC A 358:**

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

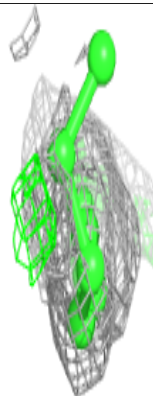
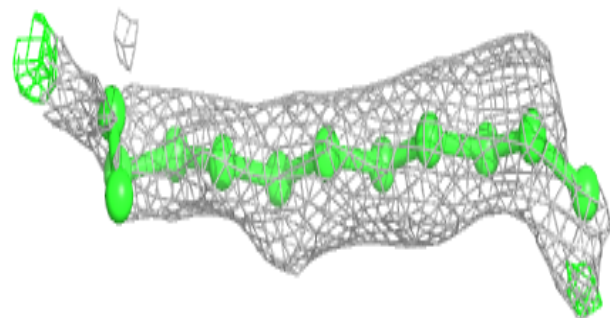
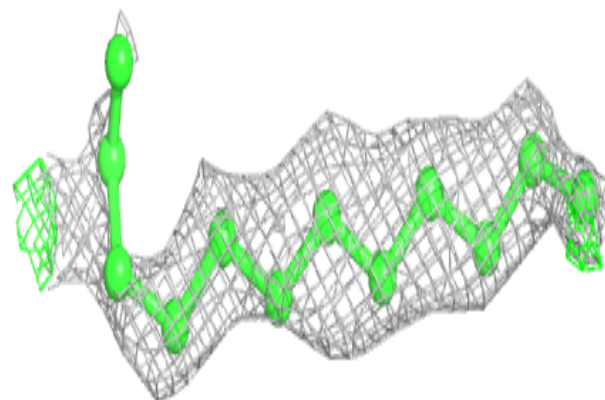


**Electron density around OLC D 349:**

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

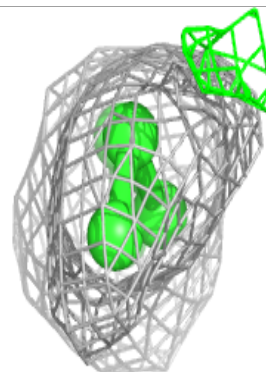
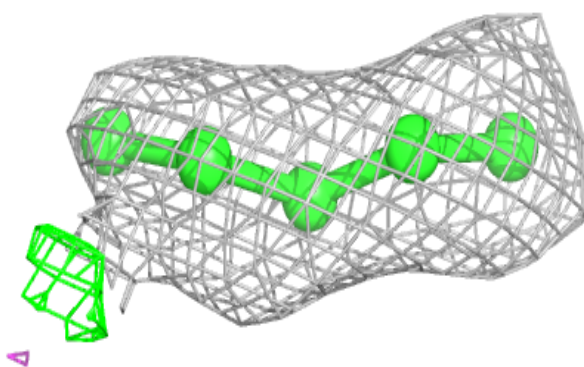
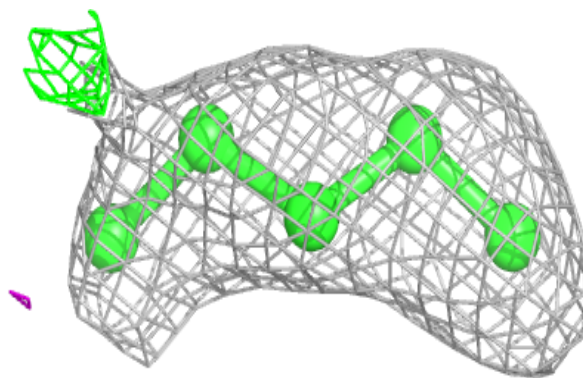
**Electron density around OLC A 360:**

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

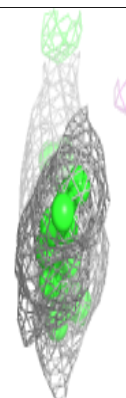
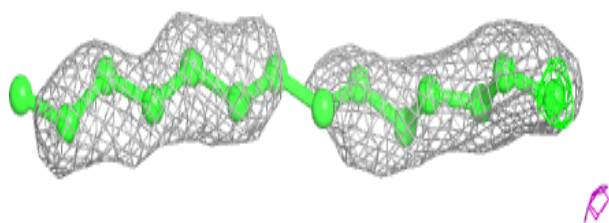
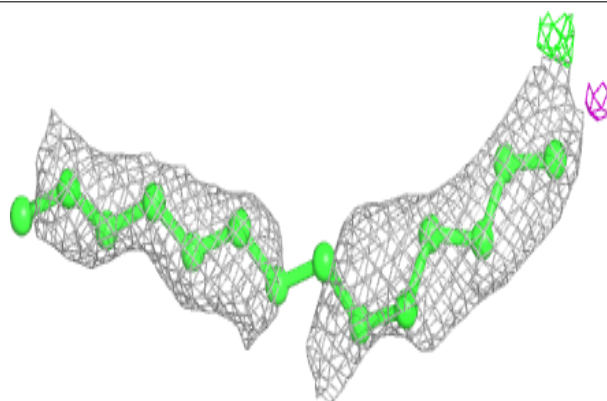


**Electron density around OLC B 341:**

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

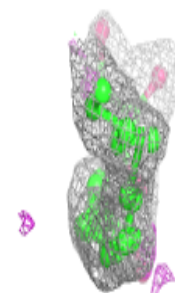
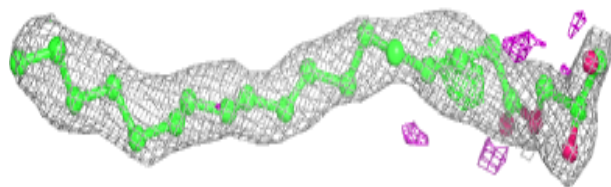
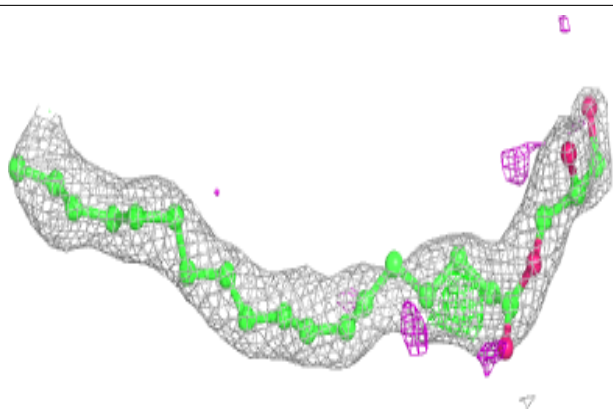
**Electron density around OLC B 342:**

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

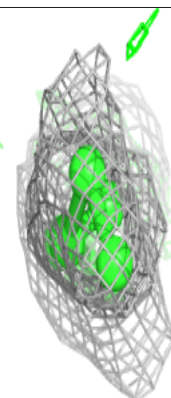
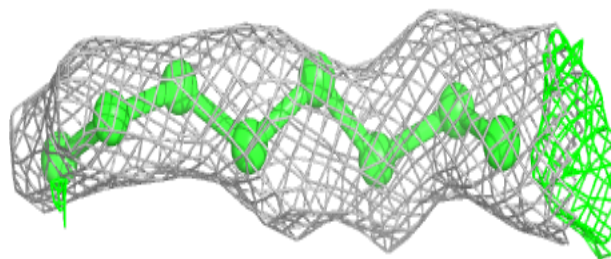
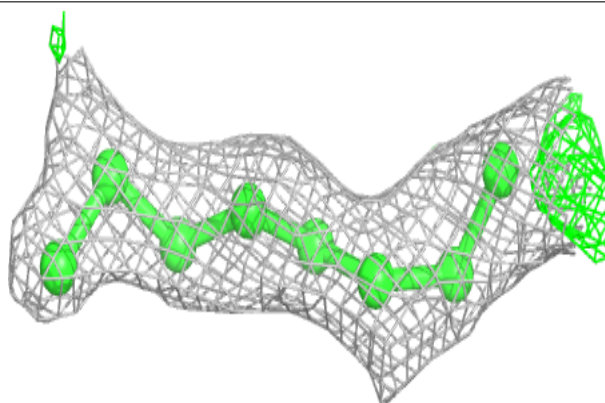


**Electron density around OLC B 350:**

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

**Electron density around OLC A 365:**

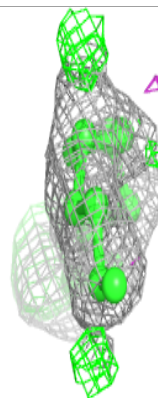
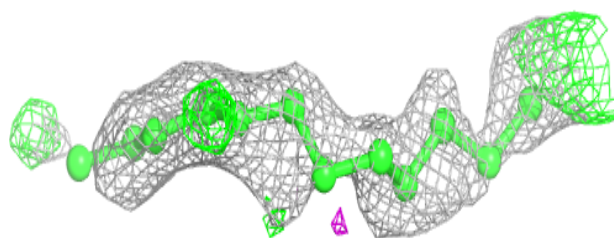
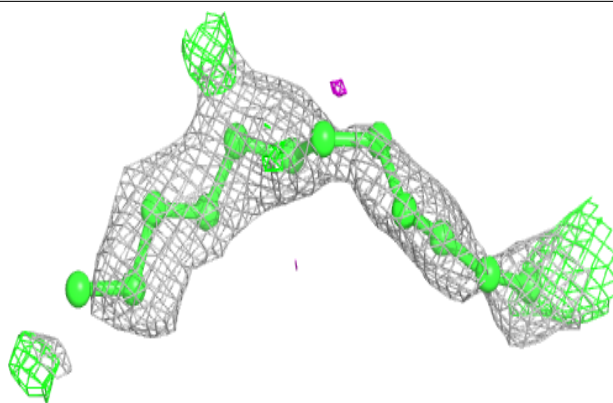
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



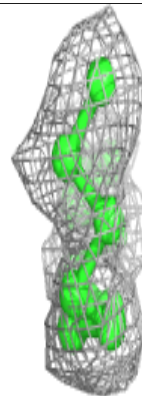
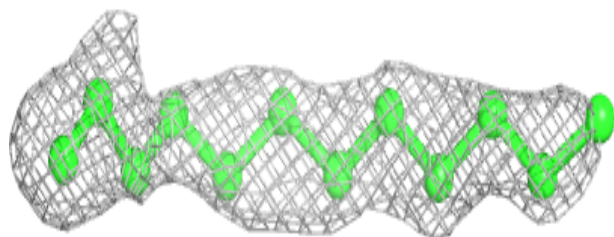
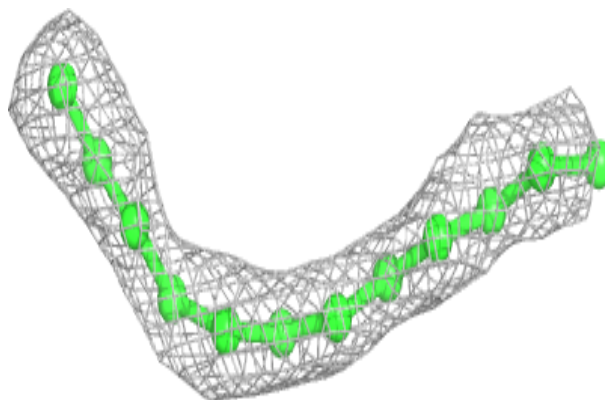


**Electron density around OLC C 352:**

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

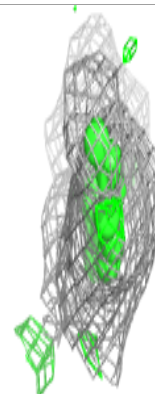
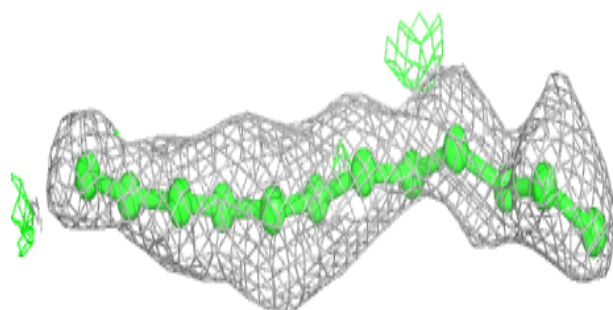
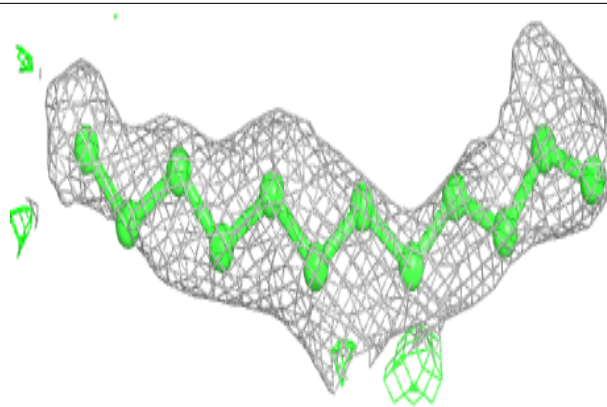
**Electron density around OLC E 344:**

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

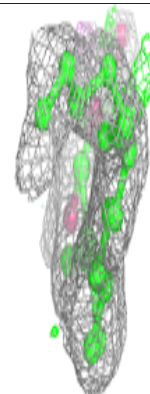
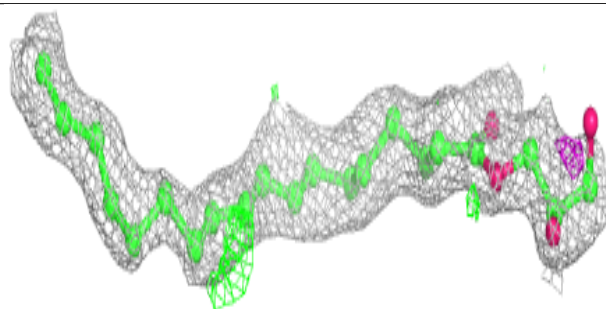
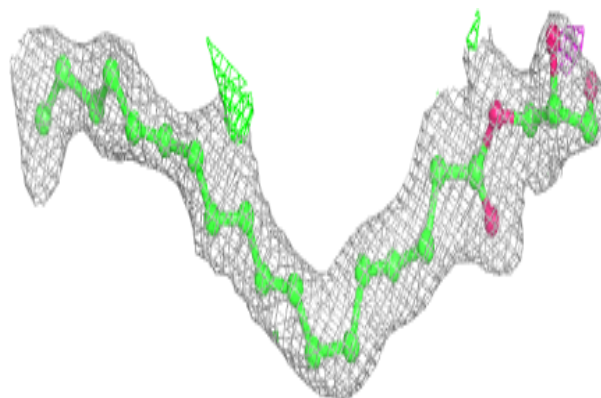


**Electron density around OLC C 348:**

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

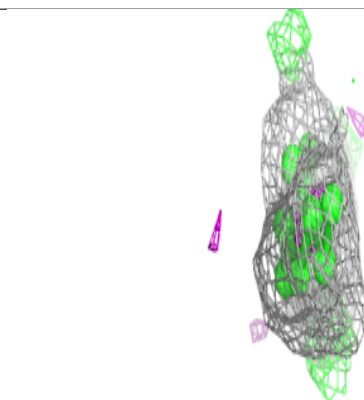
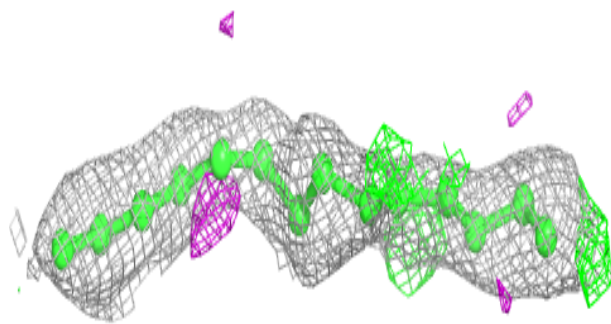
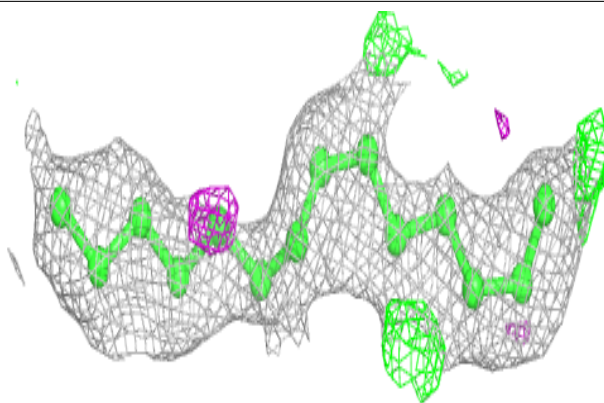
**Electron density around OLC C 363:**

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

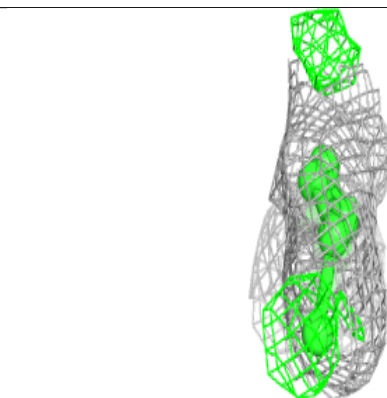
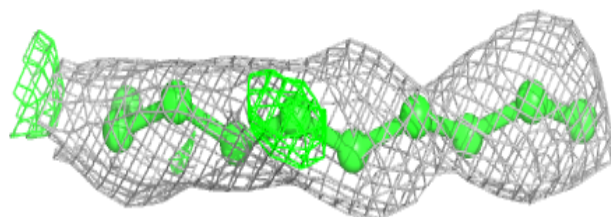
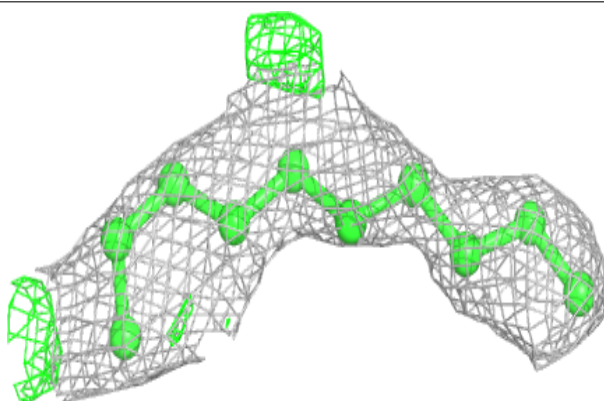


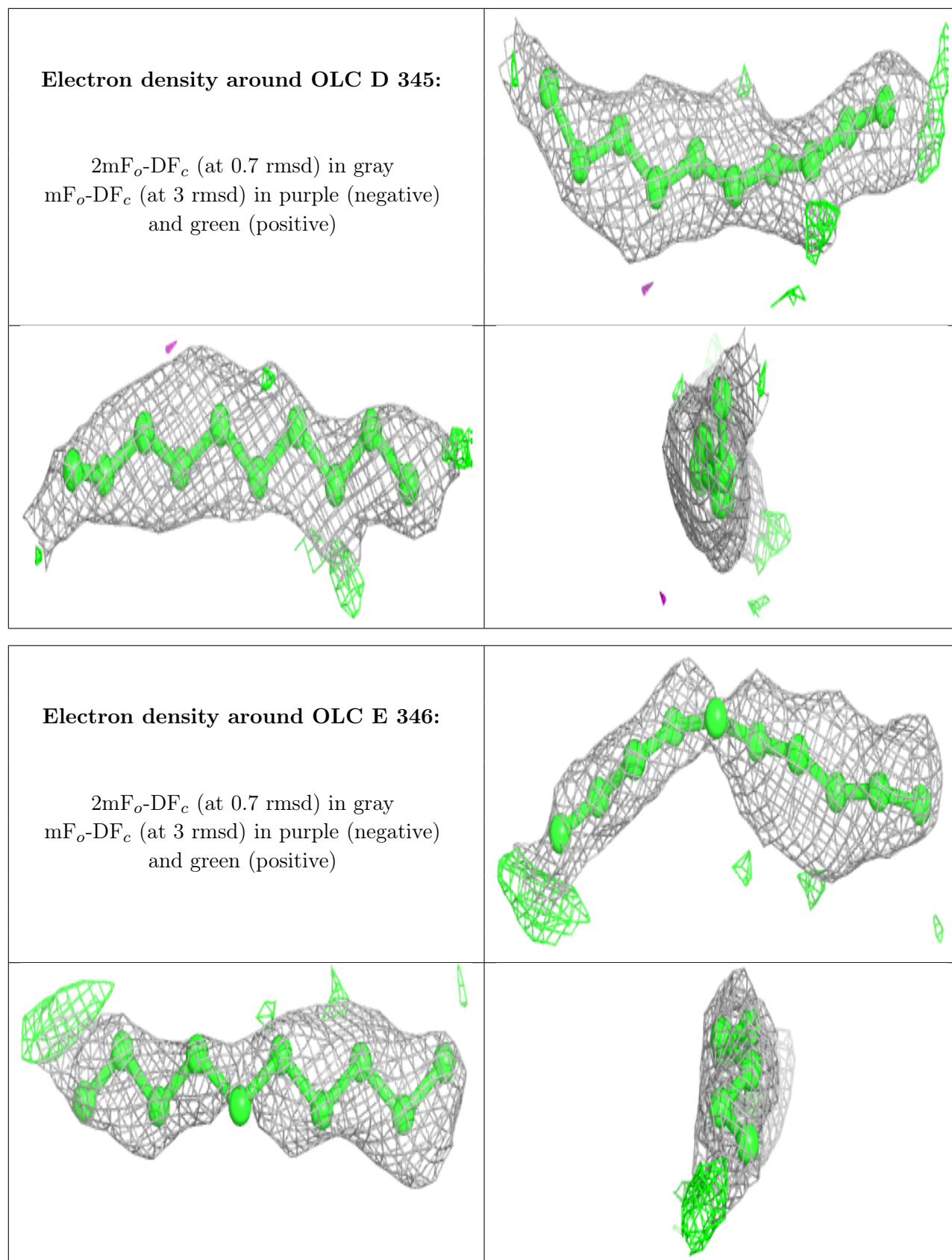
**Electron density around OLC C 357:**

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

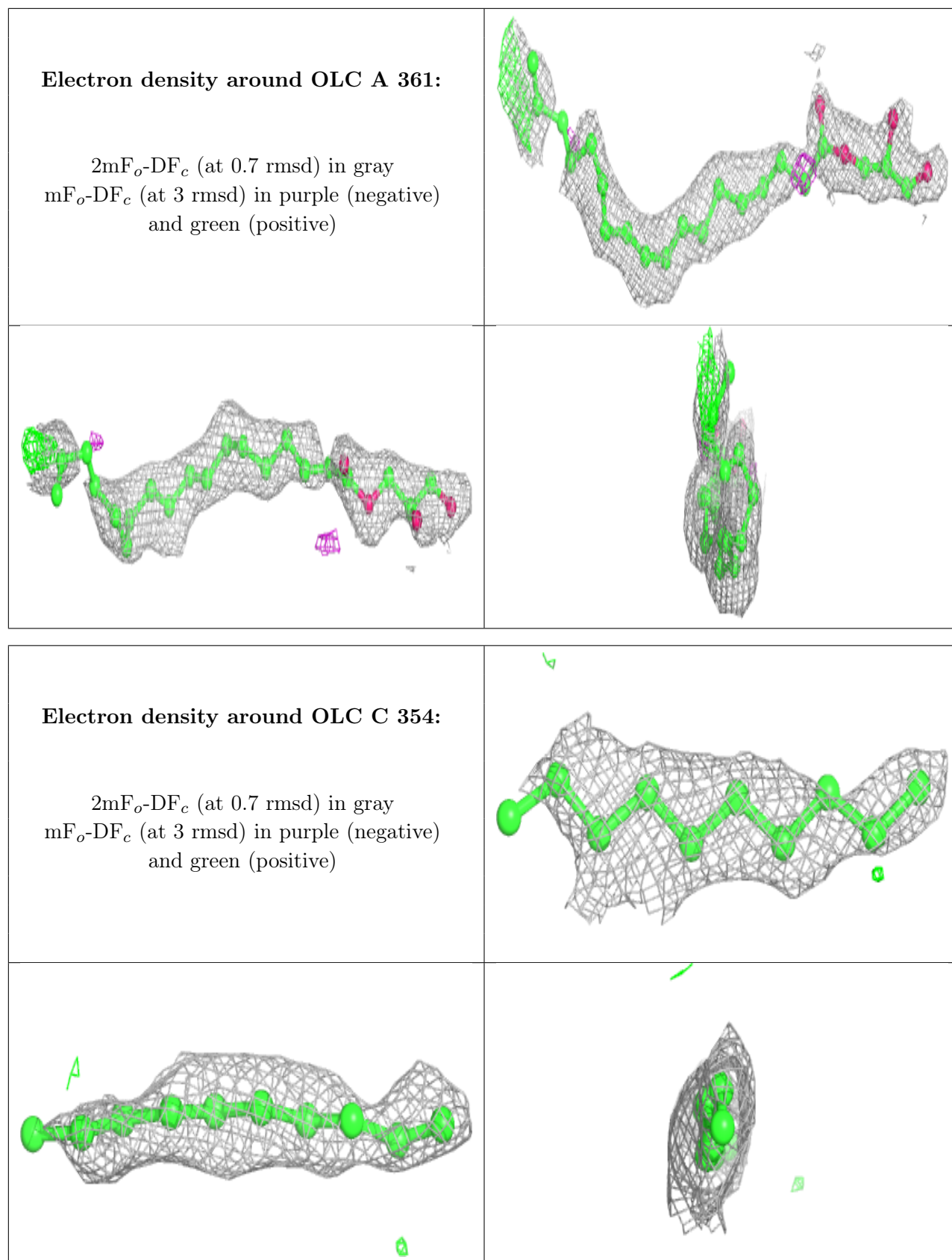
**Electron density around OLC F 344:**

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



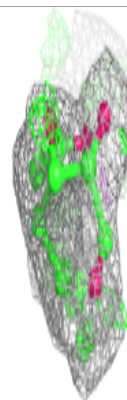
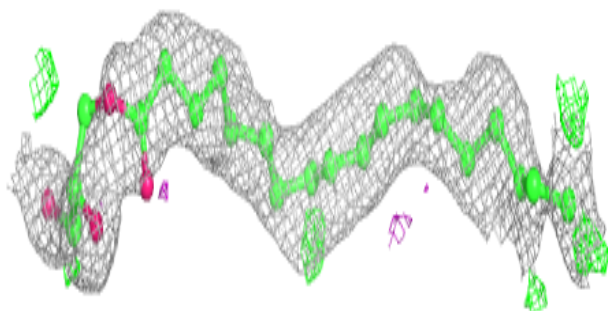
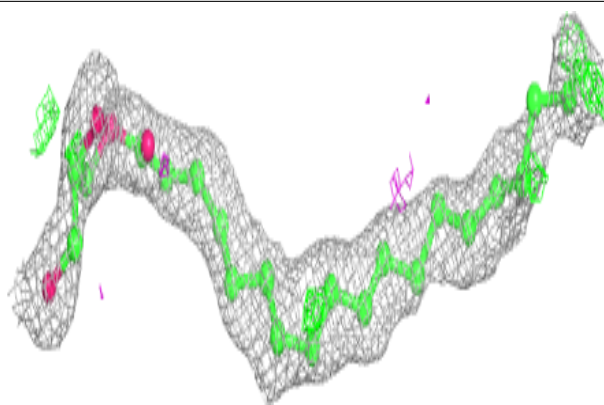




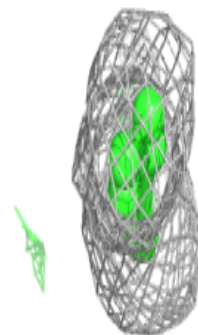
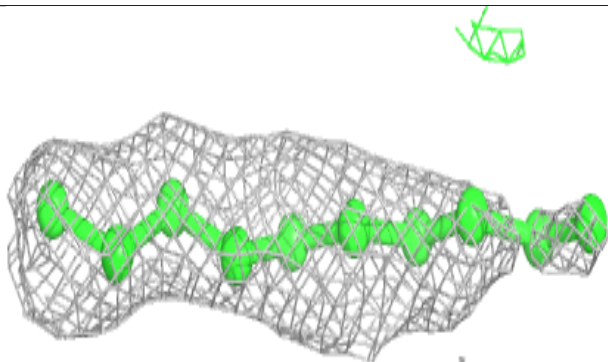
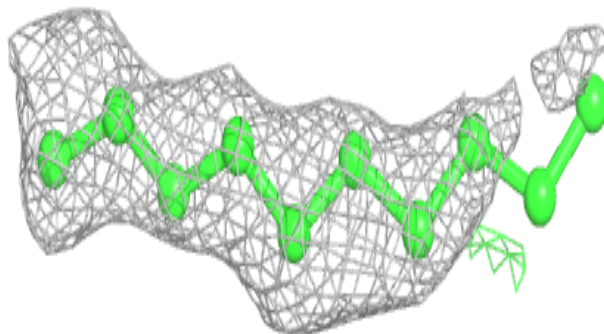


**Electron density around OLC C 362:**

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

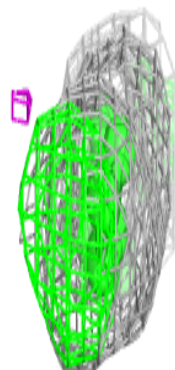
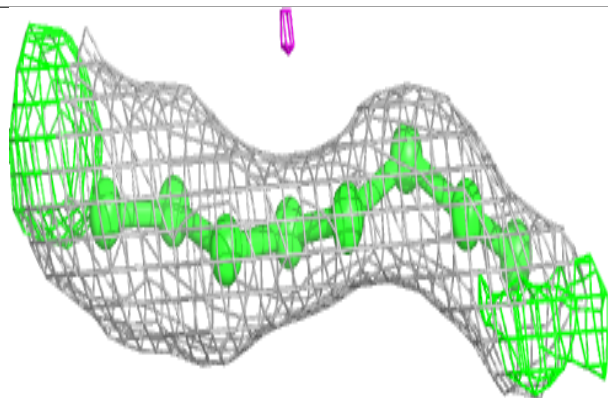
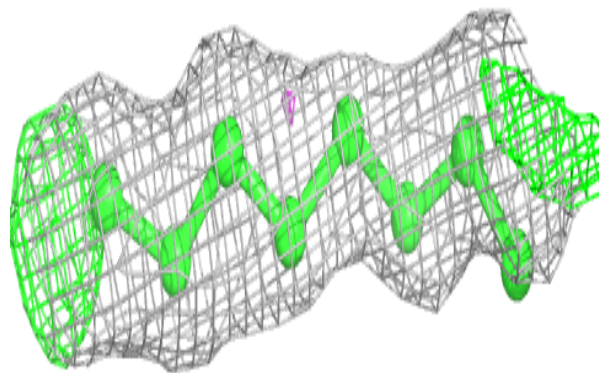
**Electron density around OLC C 347:**

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

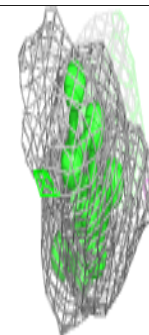
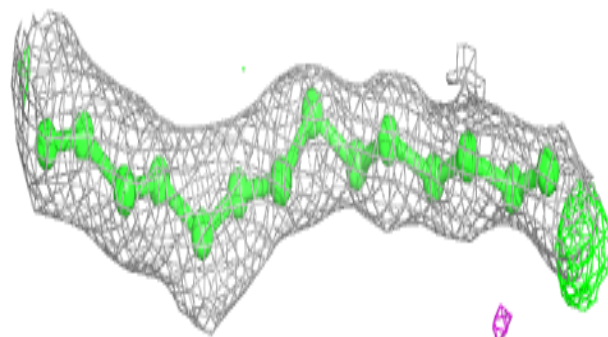
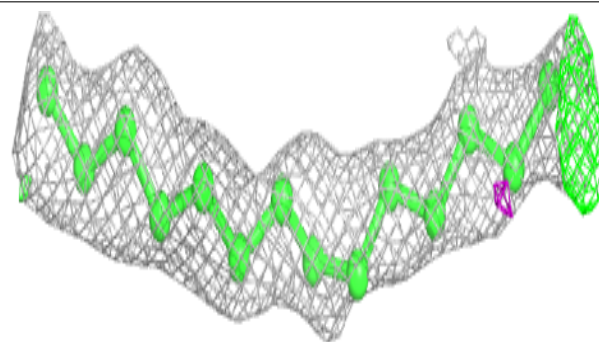


**Electron density around OLC B 354:**

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

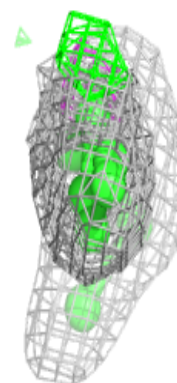
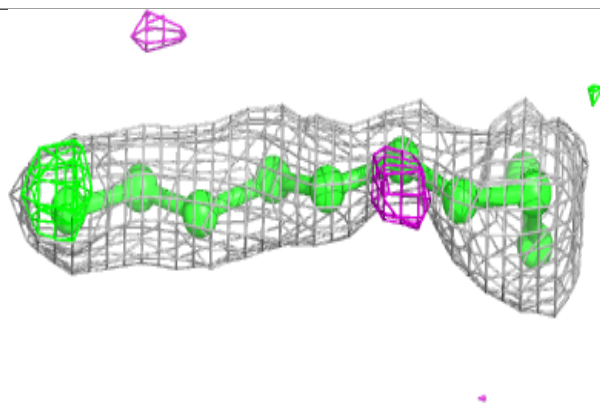
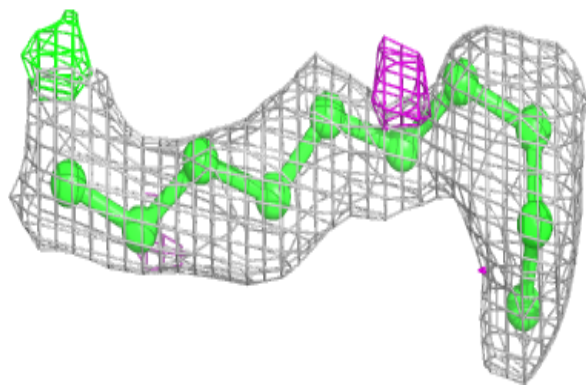
**Electron density around OLC C 350:**

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

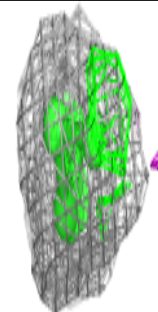
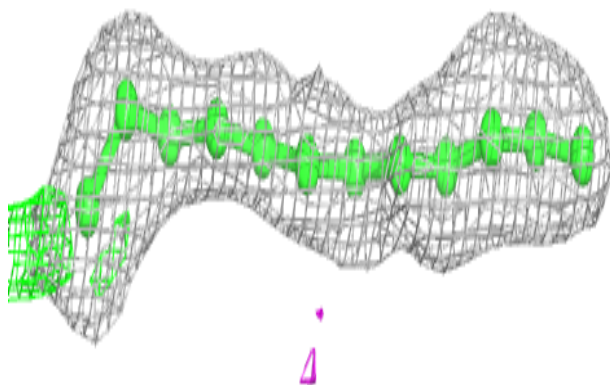
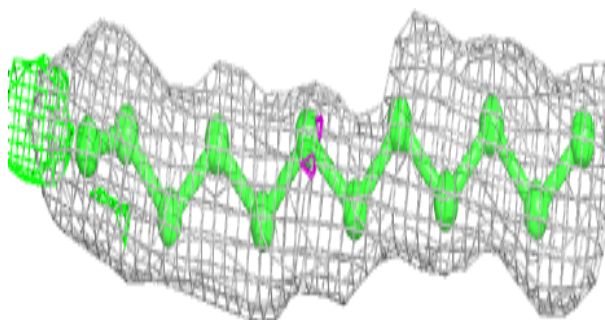


**Electron density around OLC A 344:**

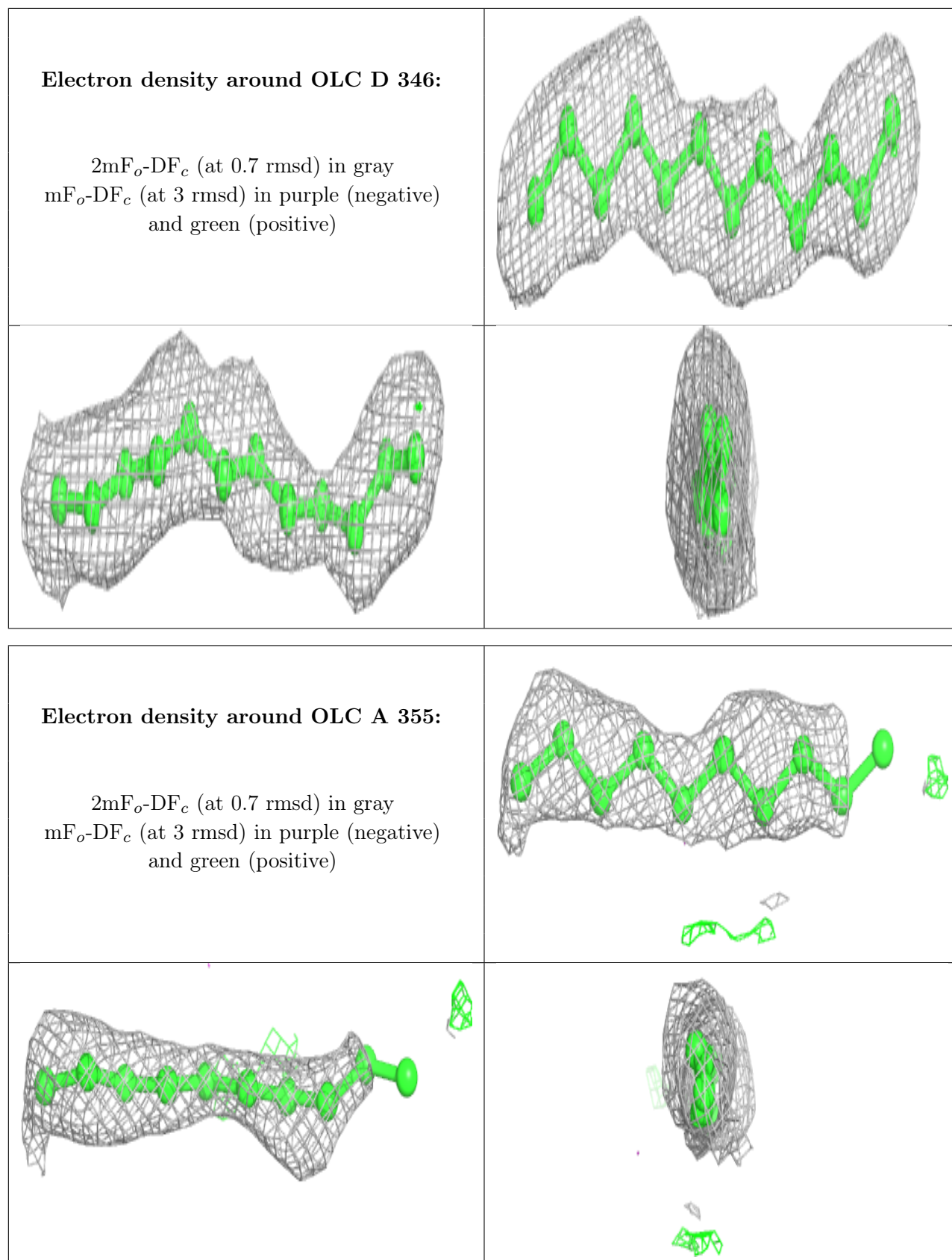
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

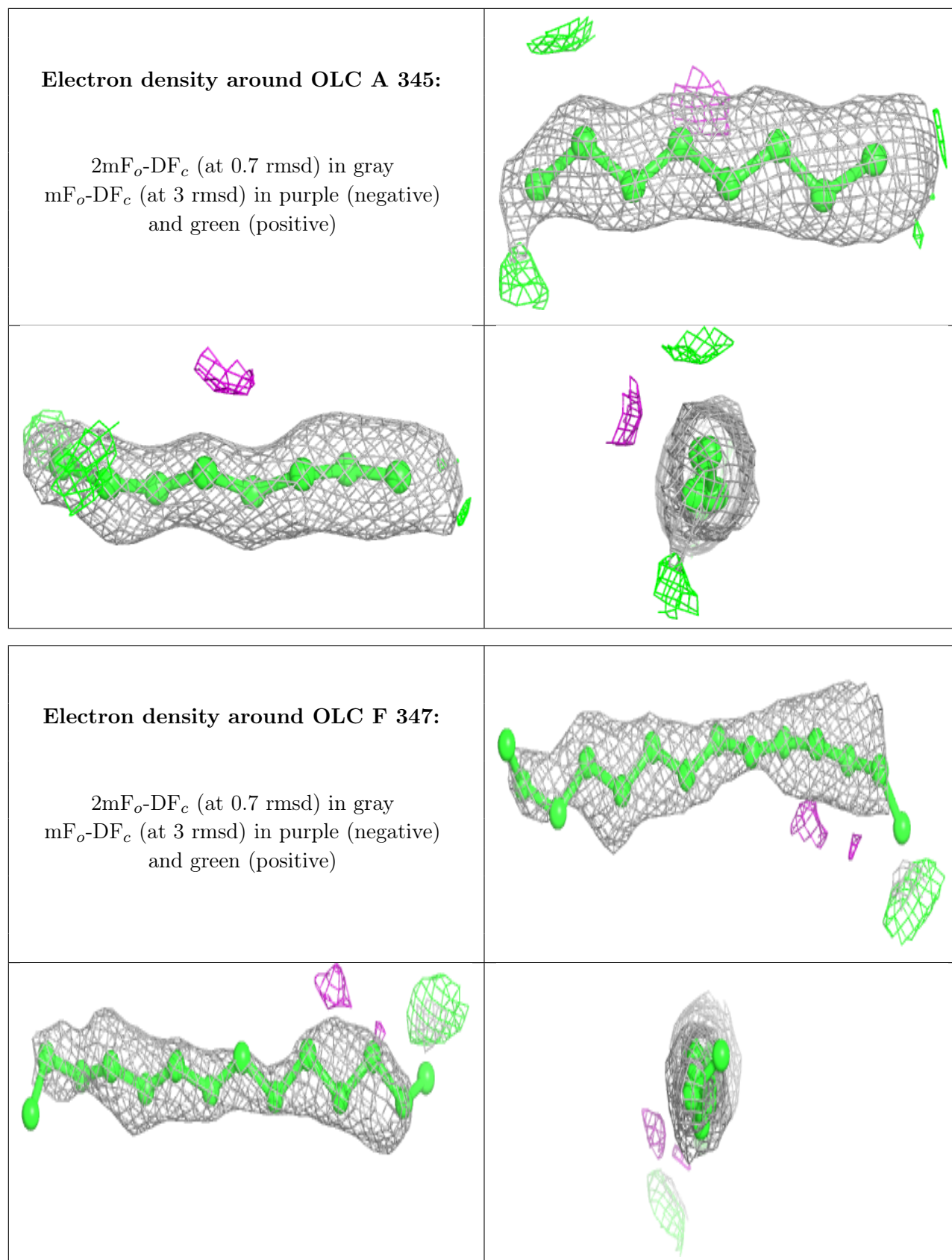
**Electron density around OLC C 345:**

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



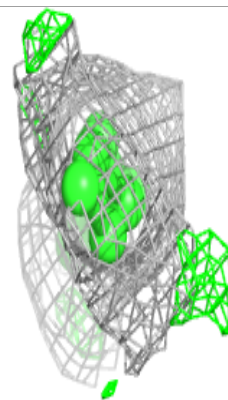
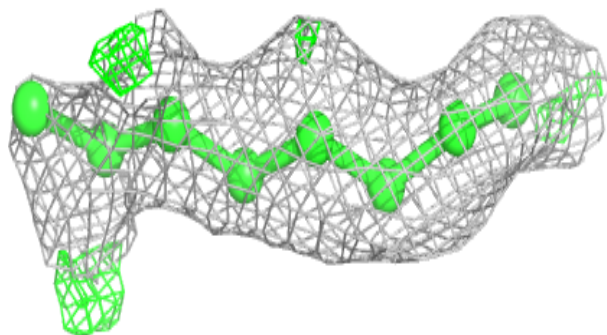
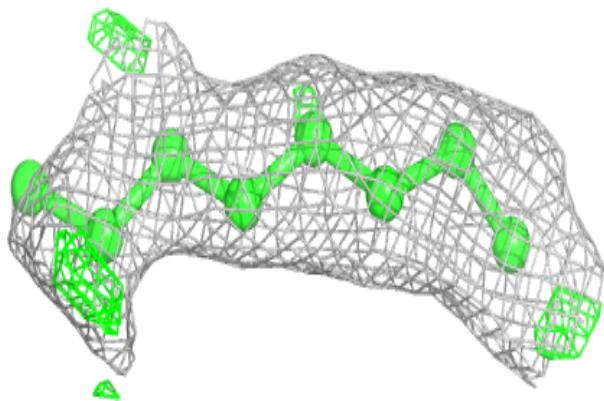




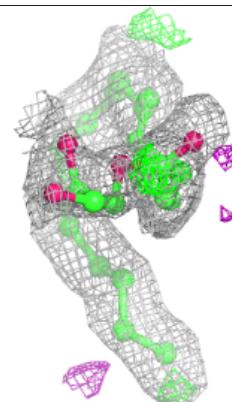
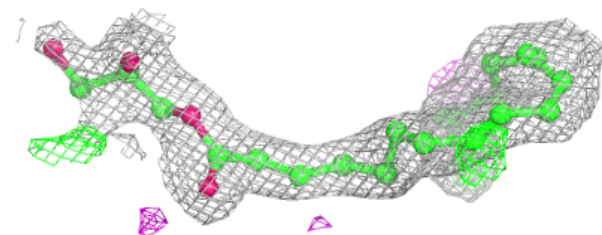
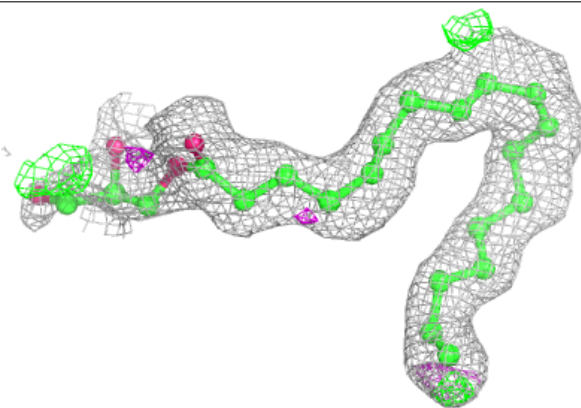


**Electron density around OLC C 344:**

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

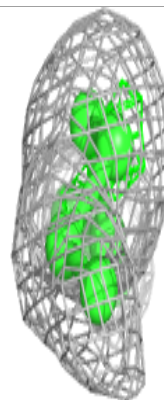
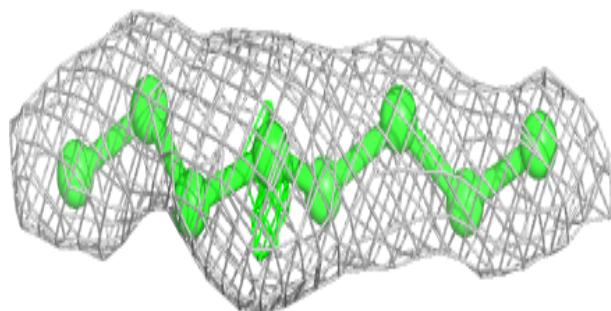
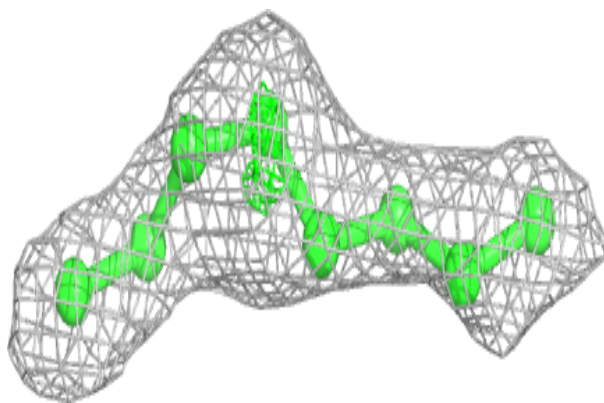
**Electron density around OLC C 360:**

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

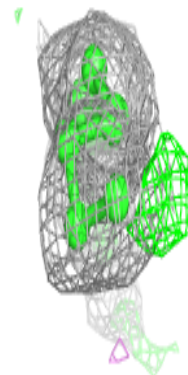
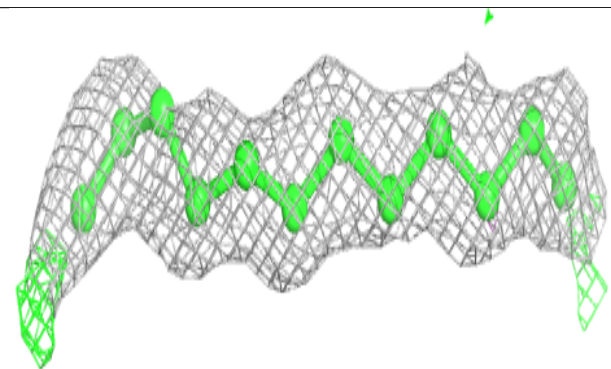
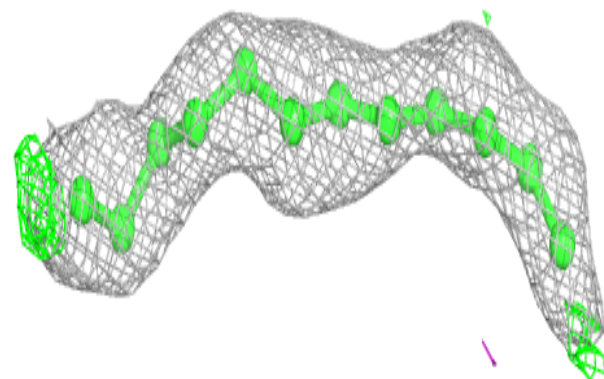


**Electron density around OLC B 353:**

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

**Electron density around OLC E 343:**

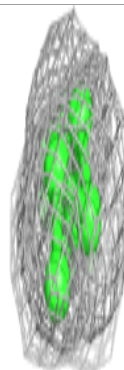
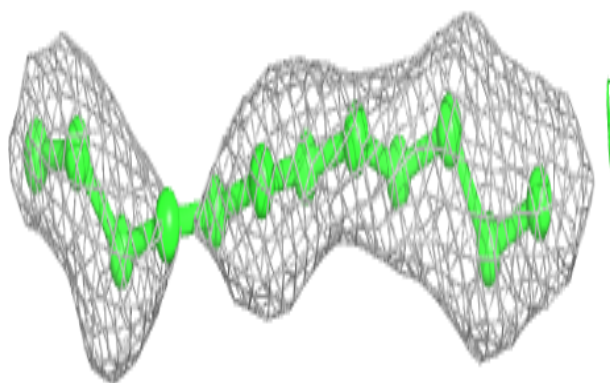
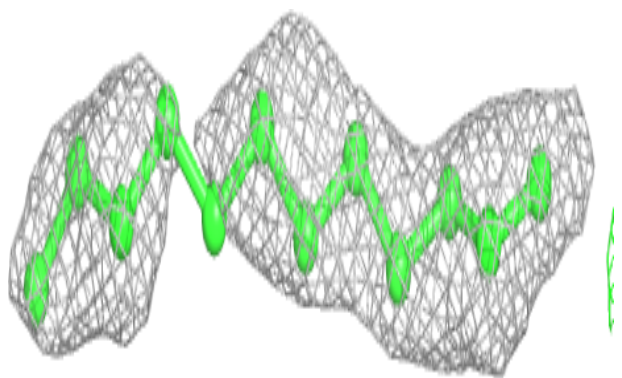
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



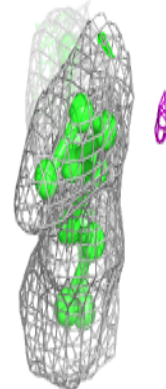
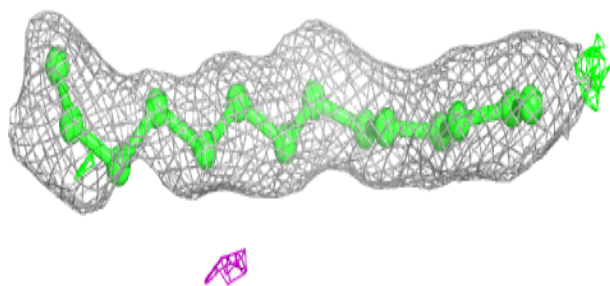
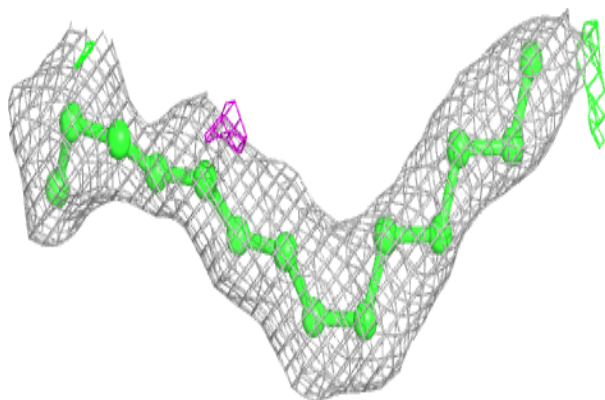


**Electron density around OLC F 345:**

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

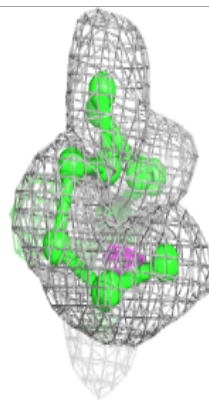
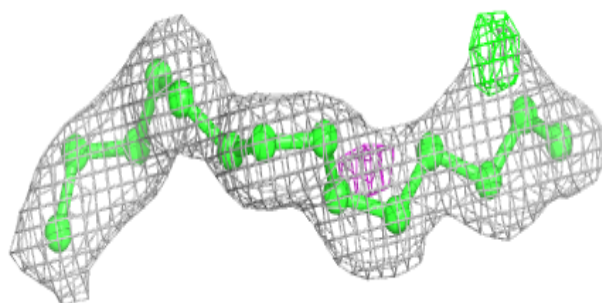
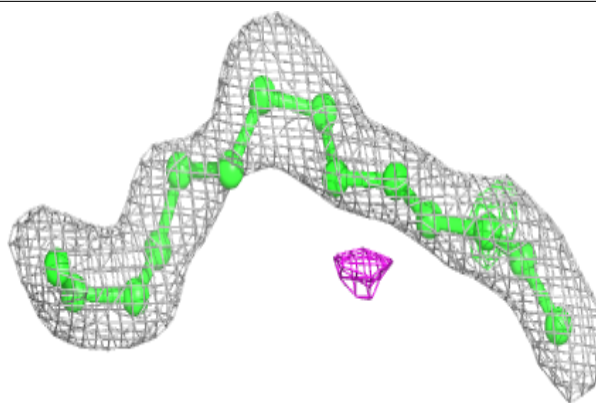
**Electron density around OLC A 350:**

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

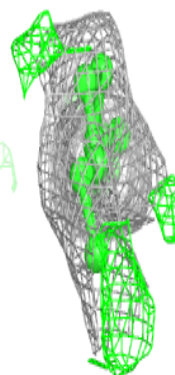
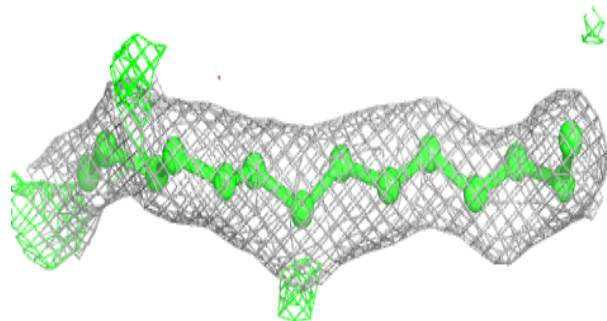
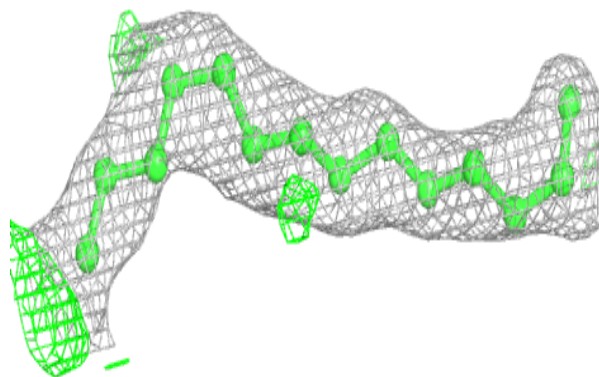


**Electron density around OLC F 348:**

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

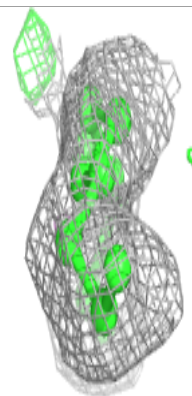
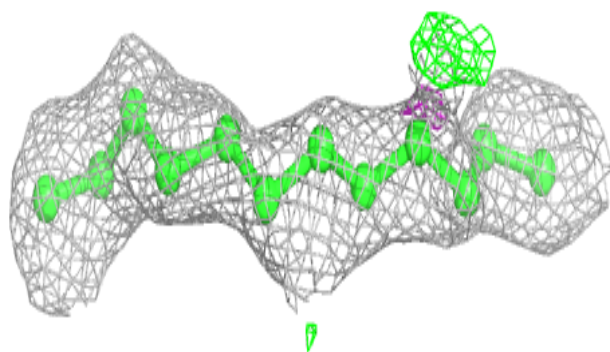
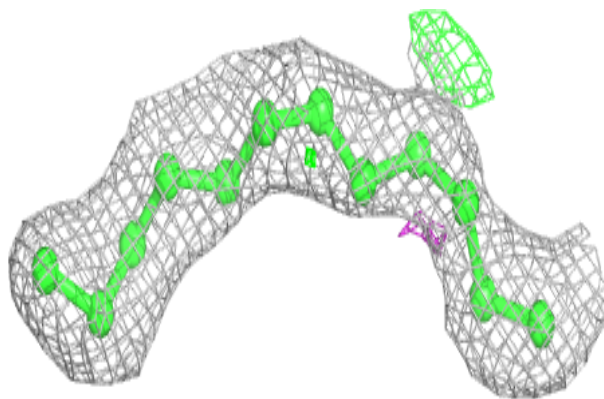
**Electron density around OLC A 351:**

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

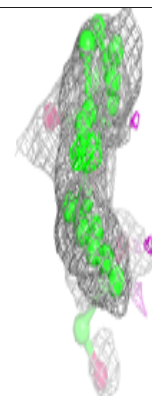
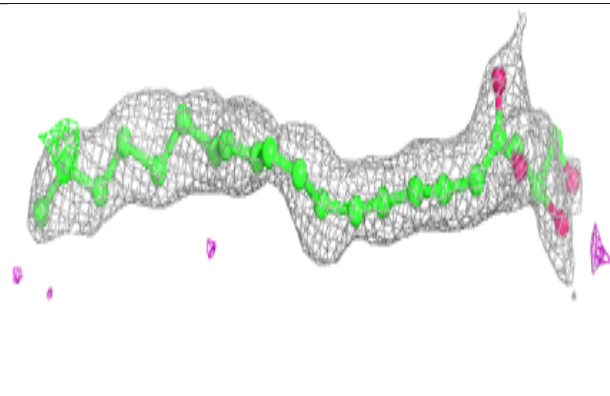
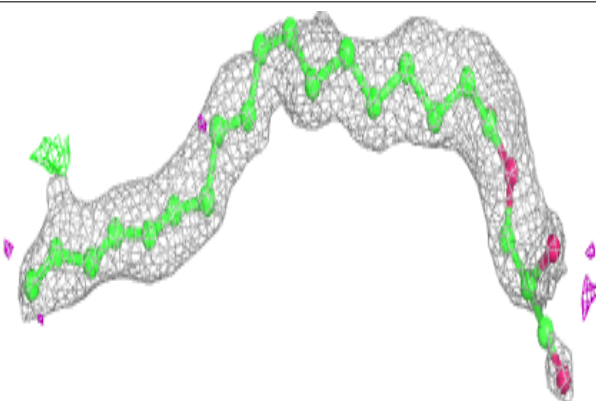


**Electron density around OLC A 363:**

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

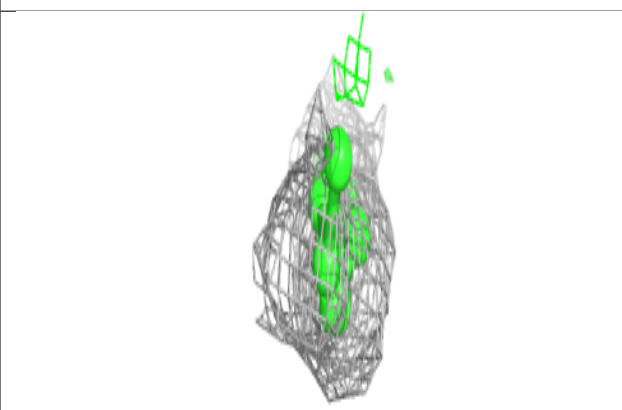
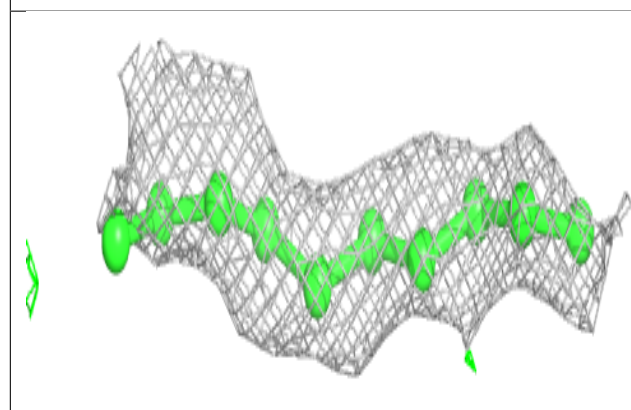
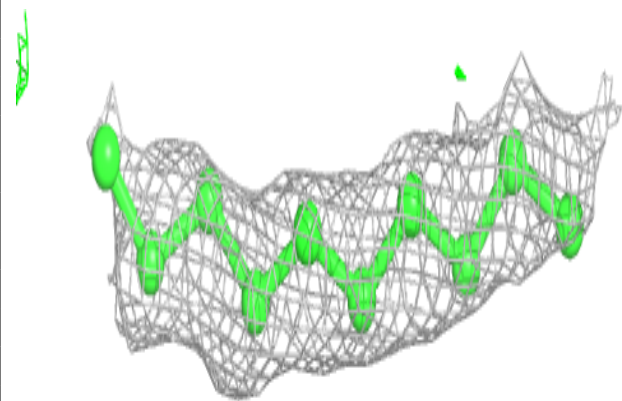
**Electron density around OLC A 349:**

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

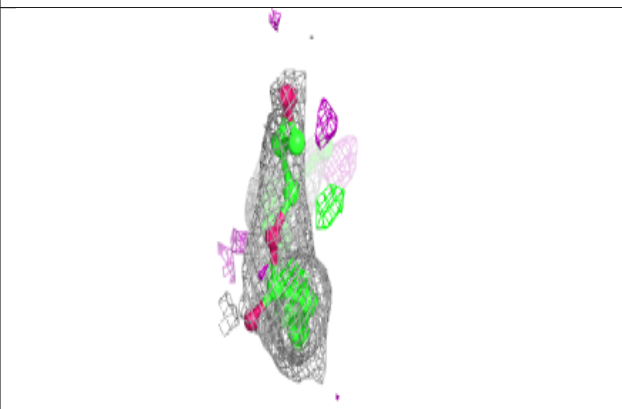
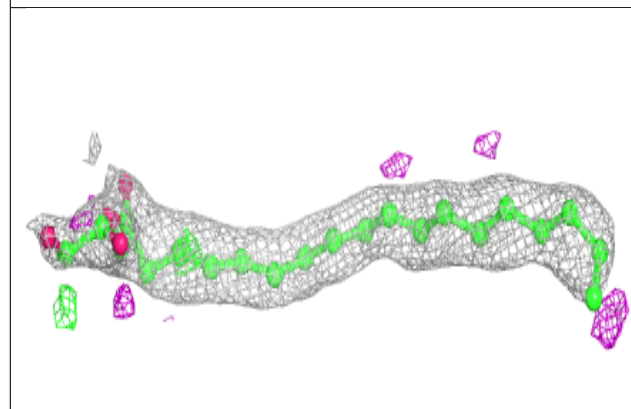
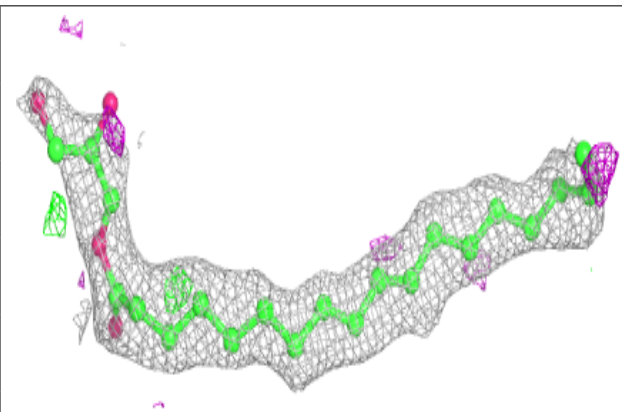


**Electron density around OLC C 353:**

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

**Electron density around OLC C 358:**

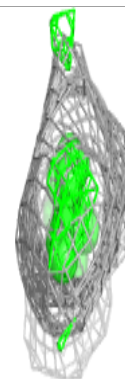
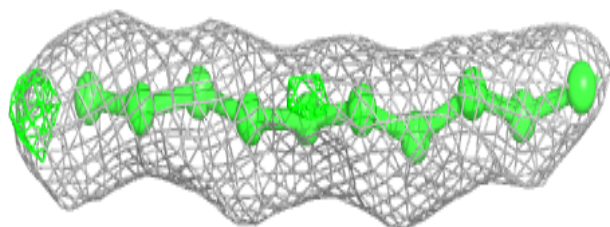
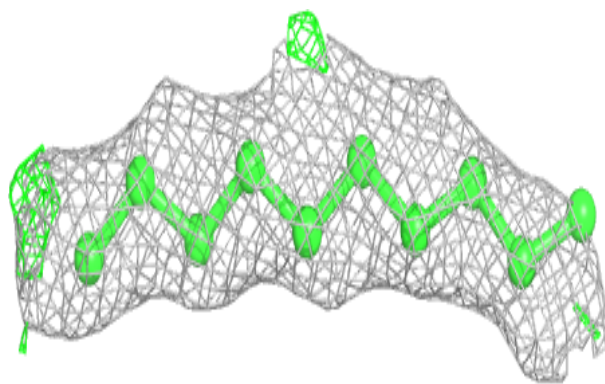
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



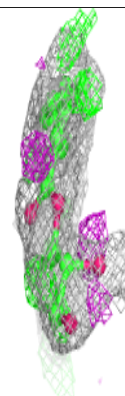
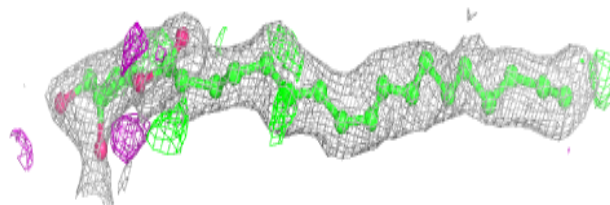
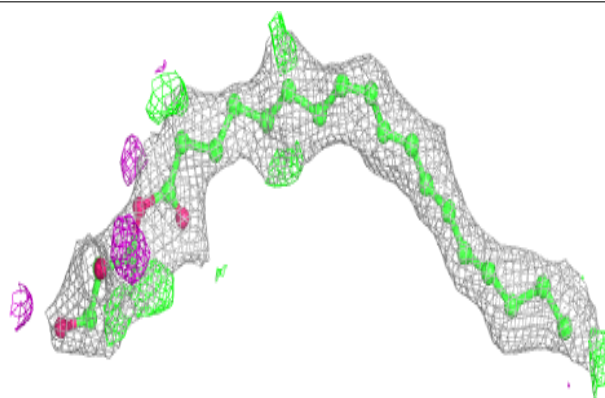


**Electron density around OLC C 341:**

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

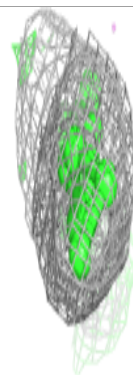
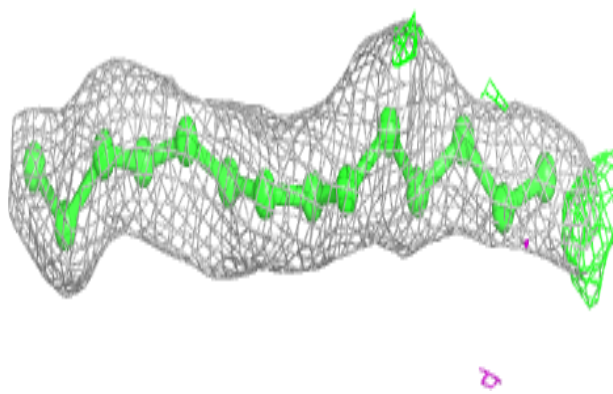
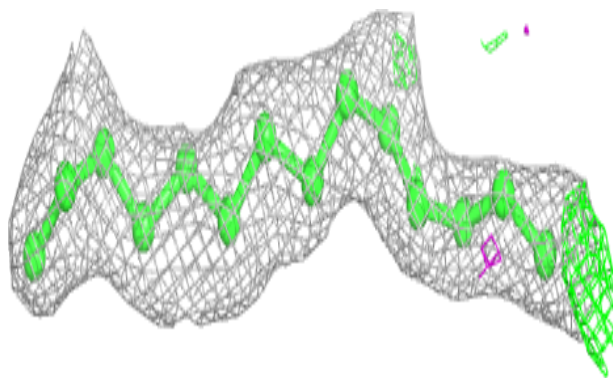
**Electron density around OLC A 346:**

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

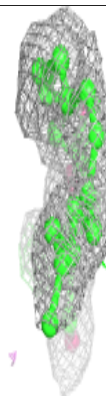
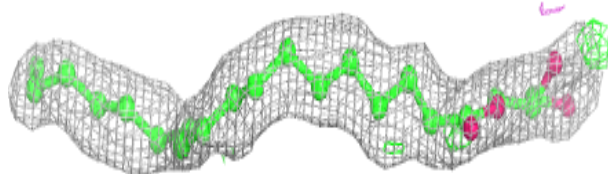
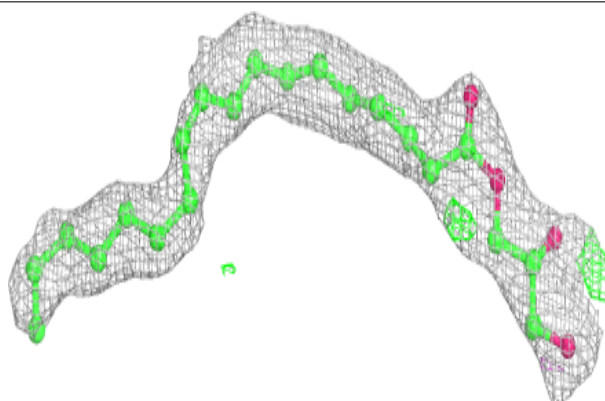


**Electron density around OLC A 362:**

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

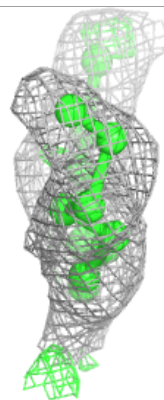
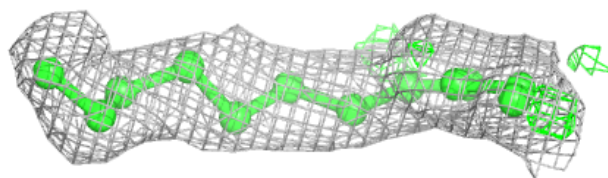
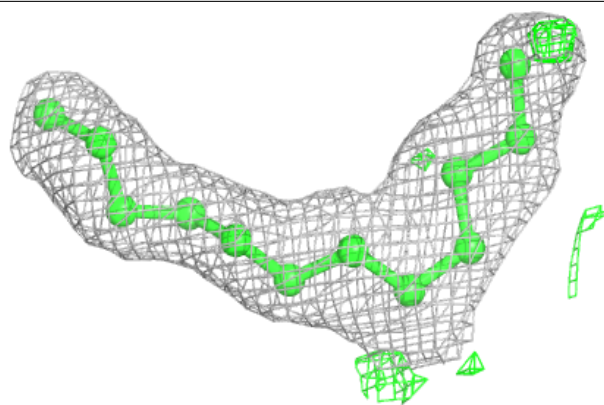
**Electron density around OLC E 347:**

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

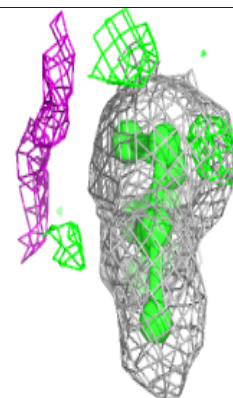
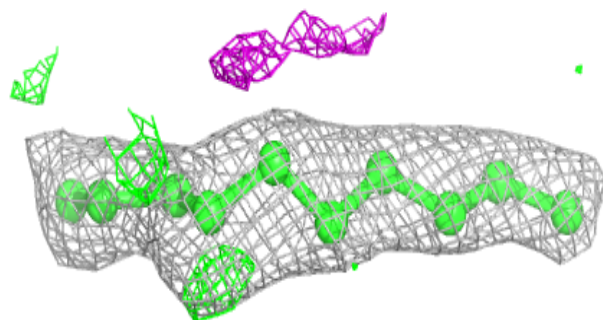
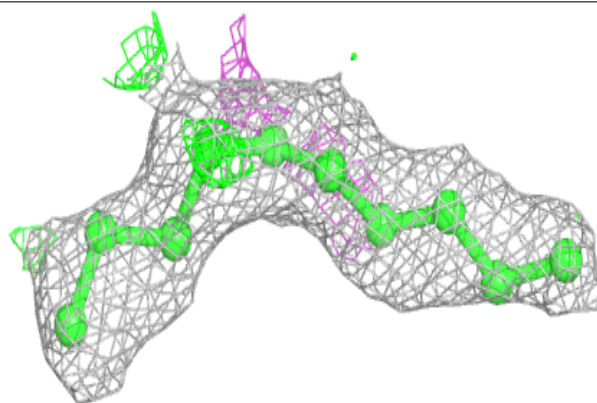


**Electron density around OLC E 348:**

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

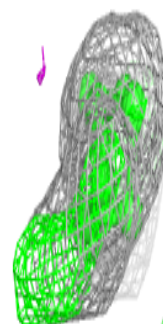
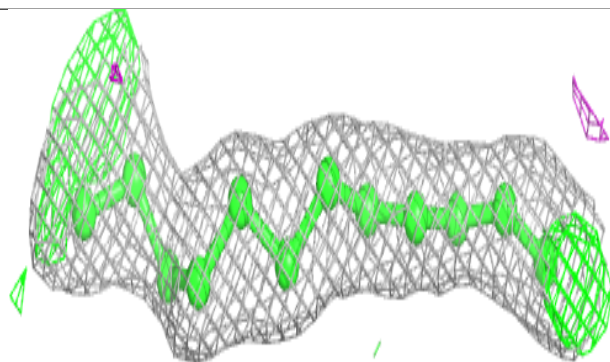
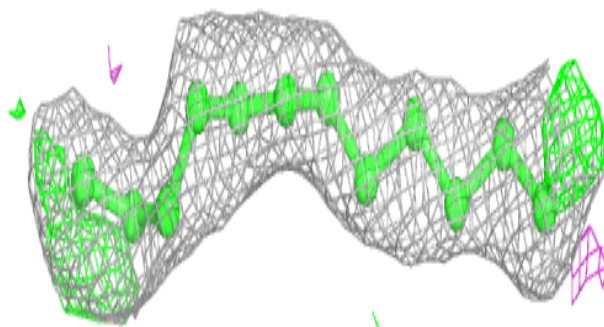
**Electron density around OLC A 348:**

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

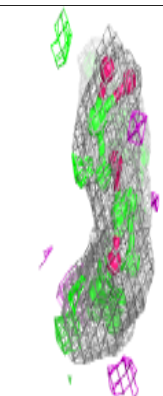
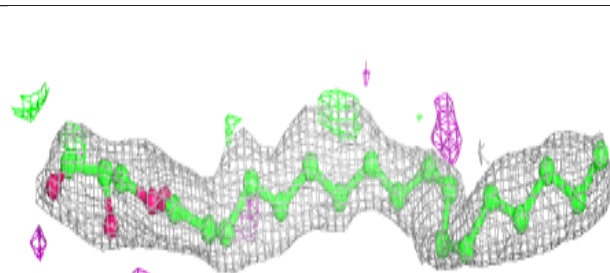
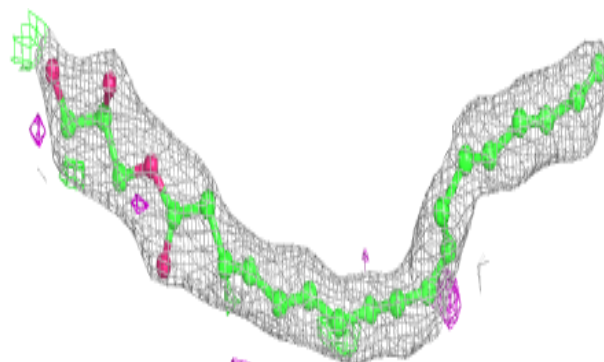


**Electron density around OLC C 361:**

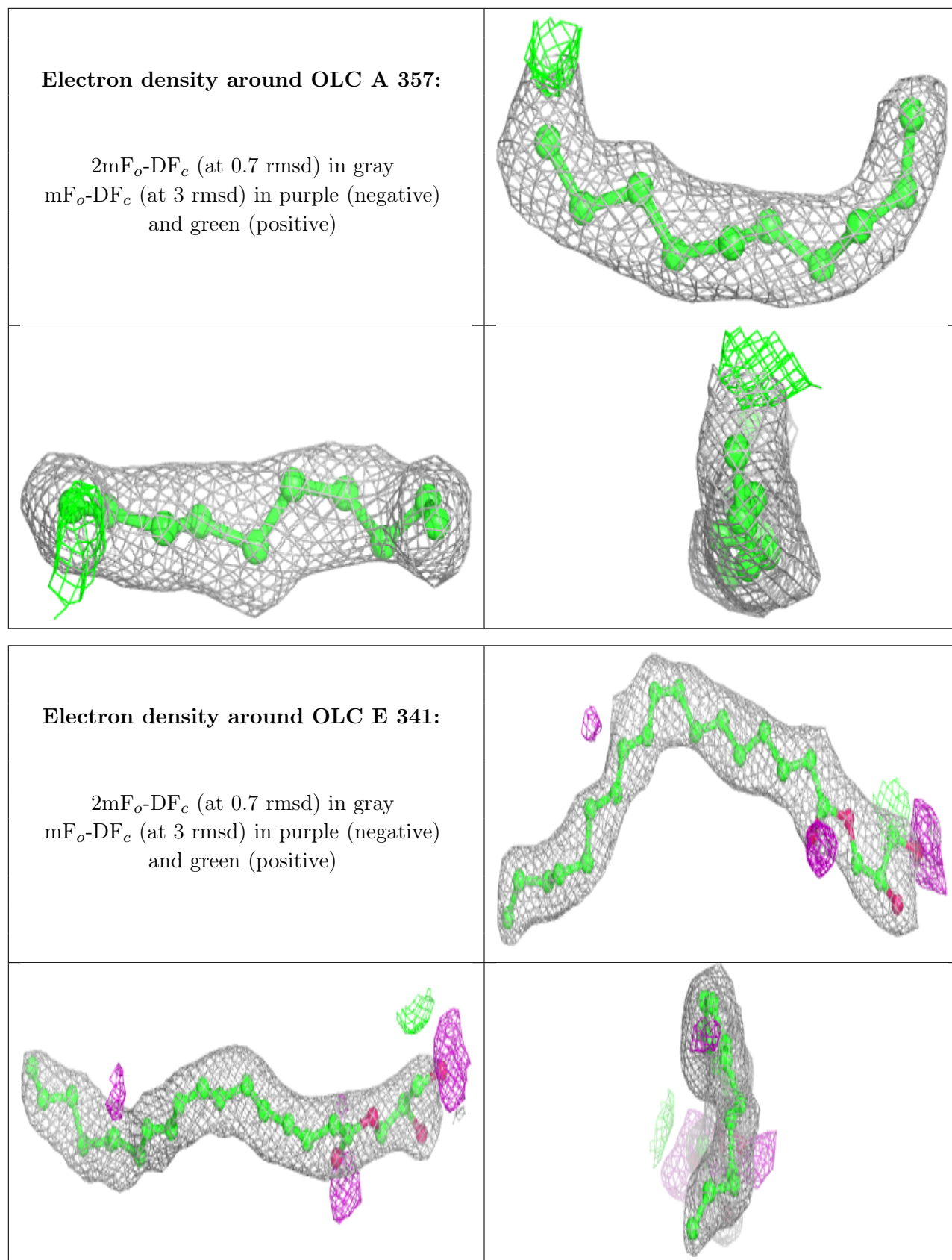
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around OLC A 359:**

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

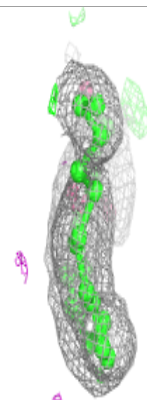
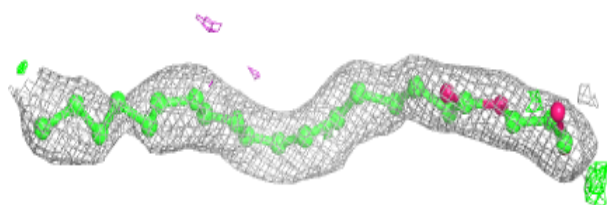
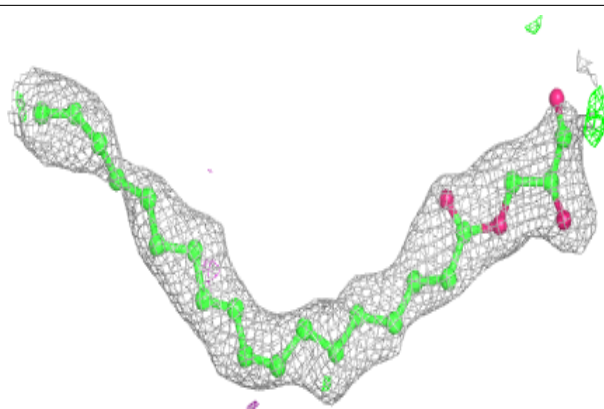




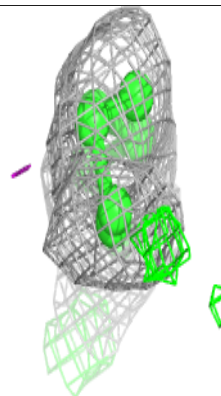
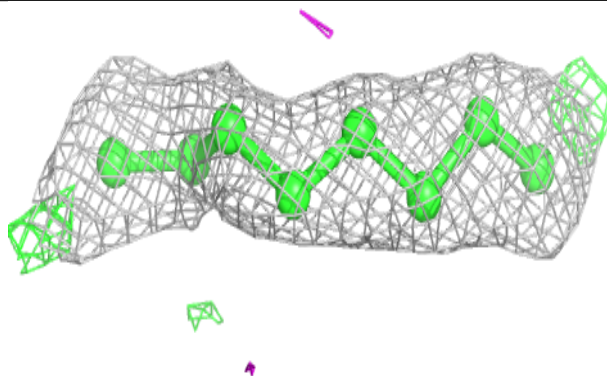
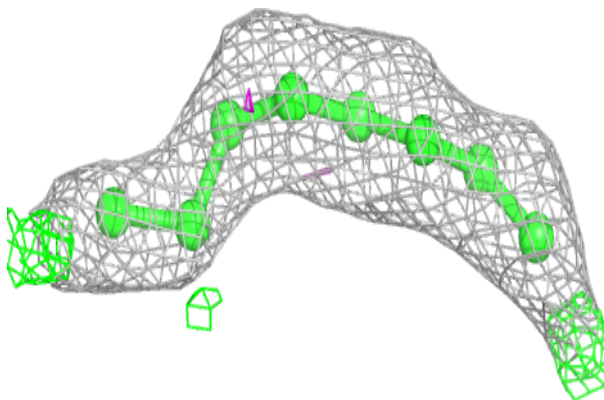


**Electron density around OLC B 345:**

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

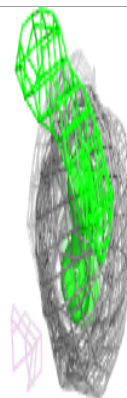
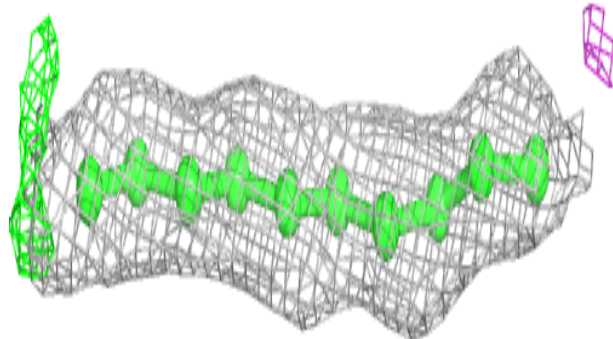
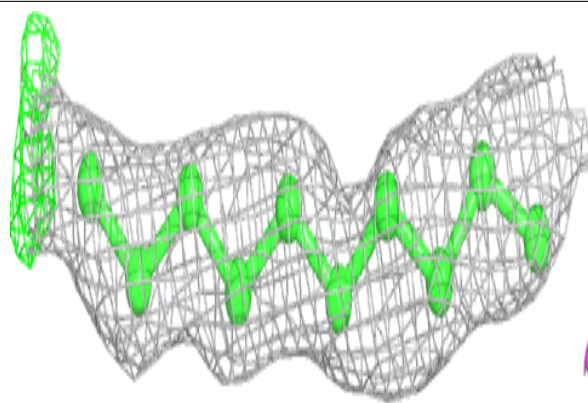
**Electron density around OLC D 347:**

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

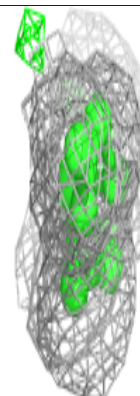
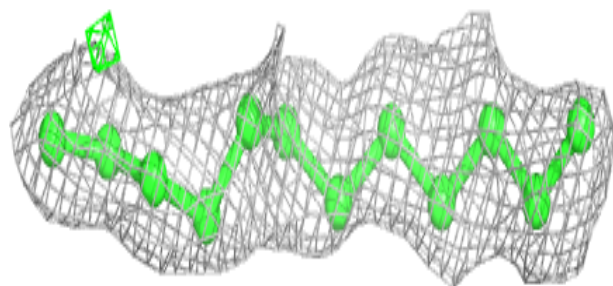
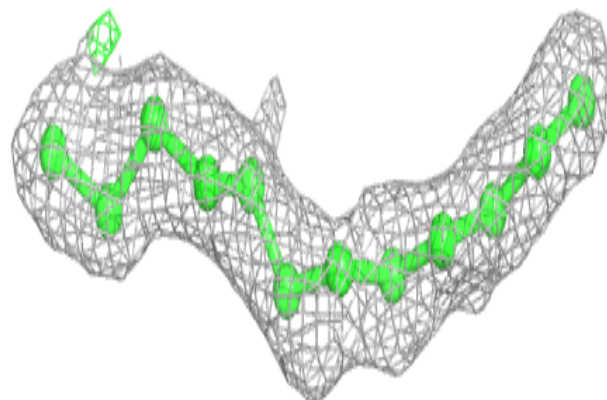


**Electron density around OLC B 344:**

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

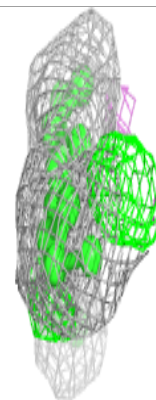
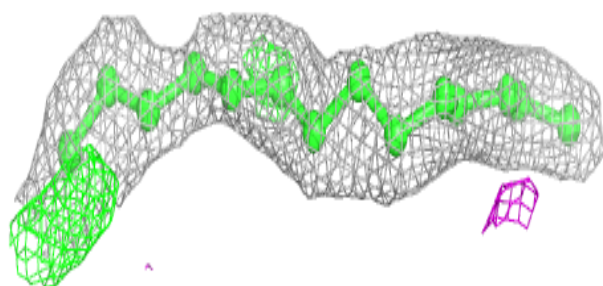
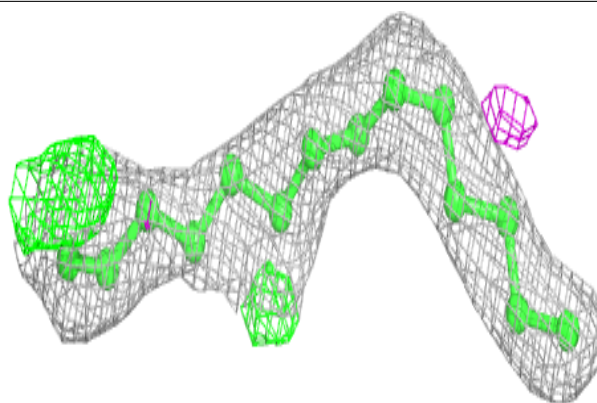
**Electron density around OLC A 364:**

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

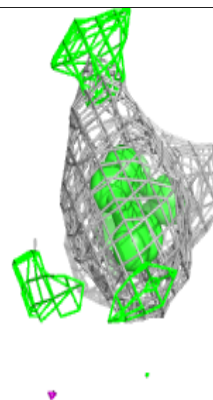
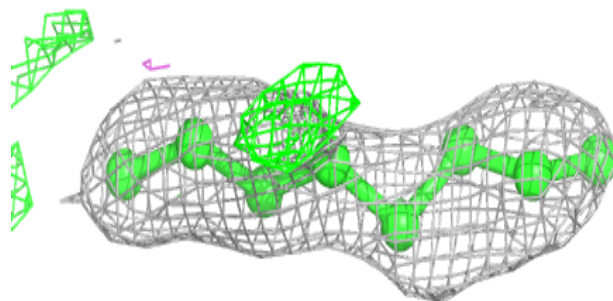
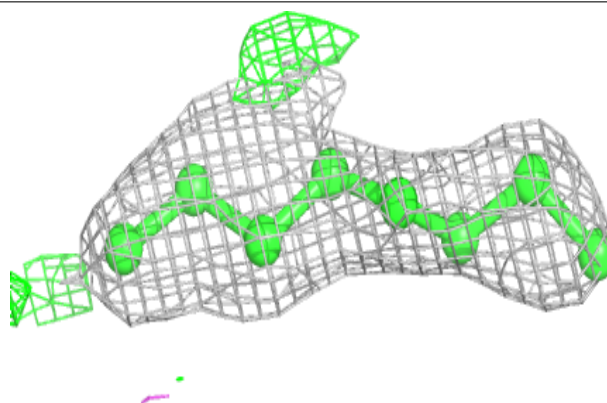


**Electron density around OLC B 347:**

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

**Electron density around OLC D 348:**

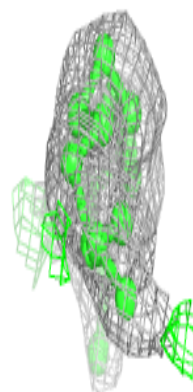
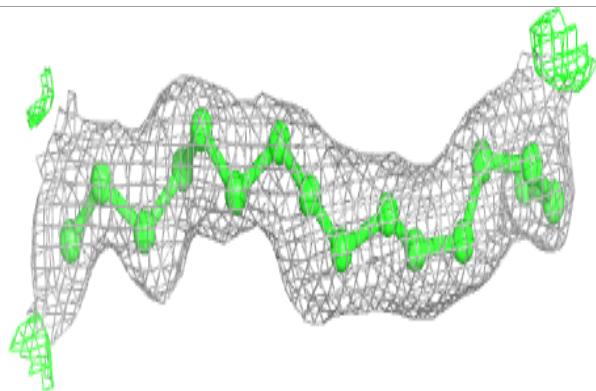
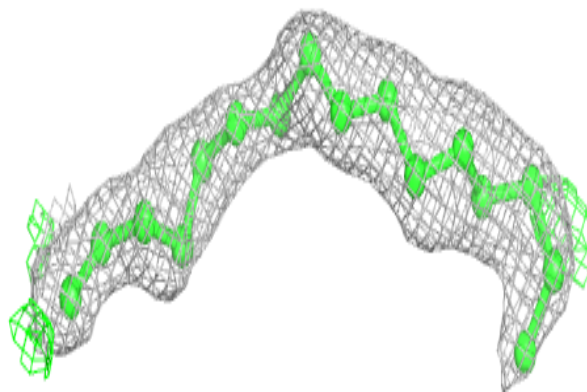
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



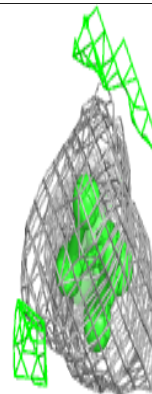
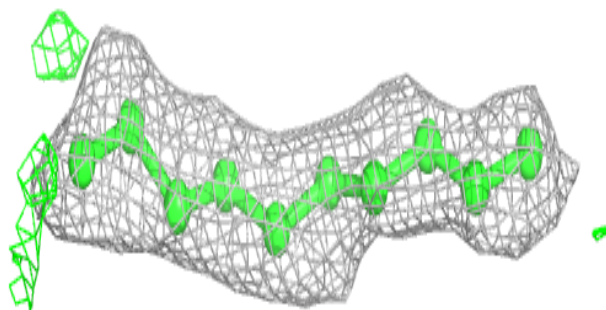
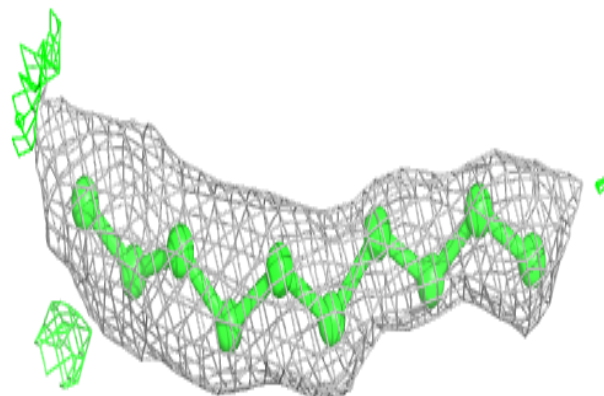


**Electron density around OLC B 352:**

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

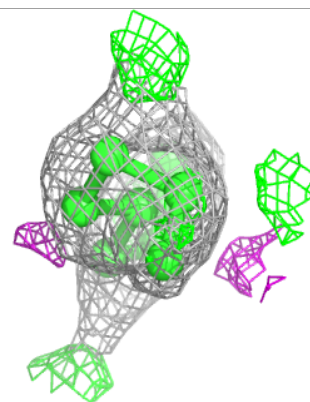
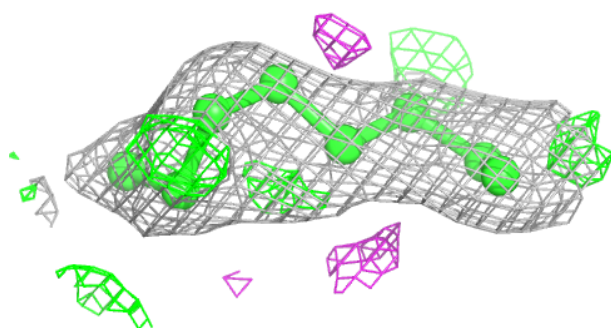
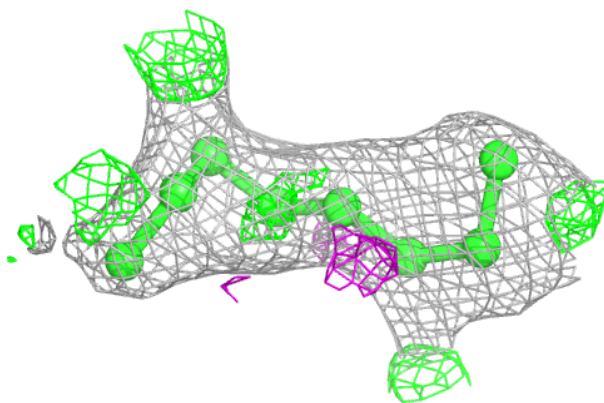
**Electron density around OLC A 352:**

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

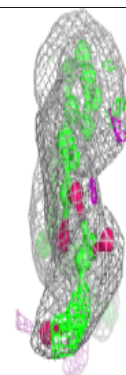
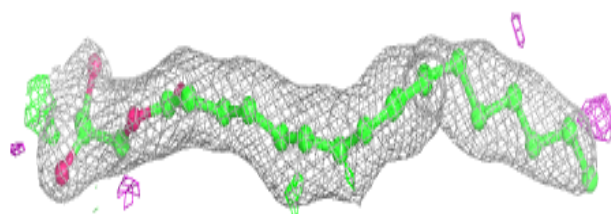
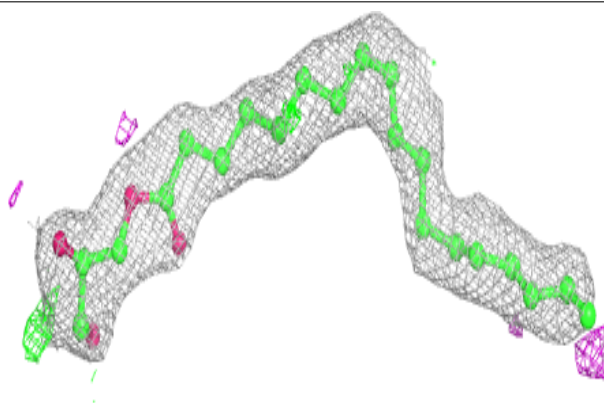


**Electron density around OLC E 342:**

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

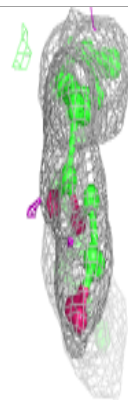
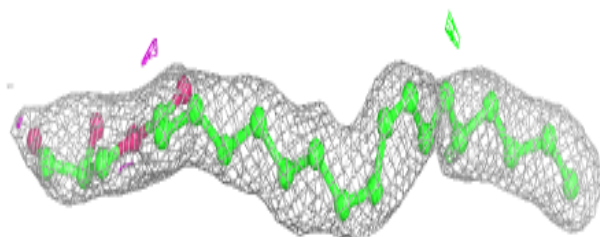
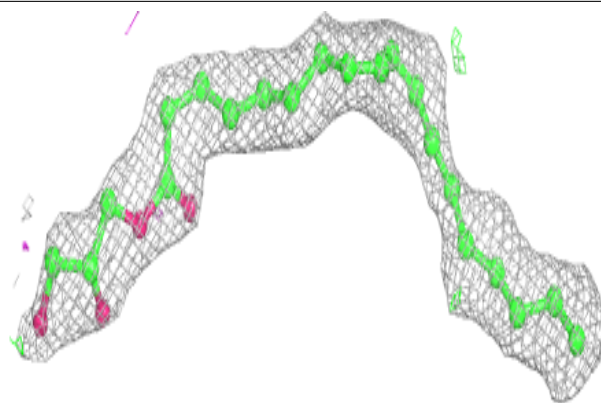
**Electron density around OLC B 346:**

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

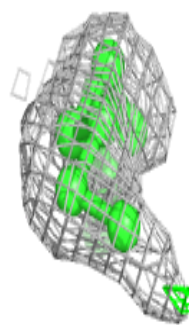
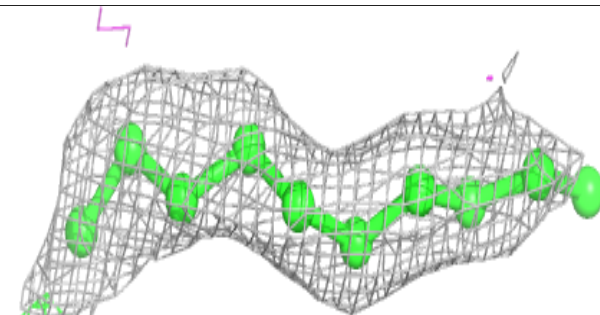
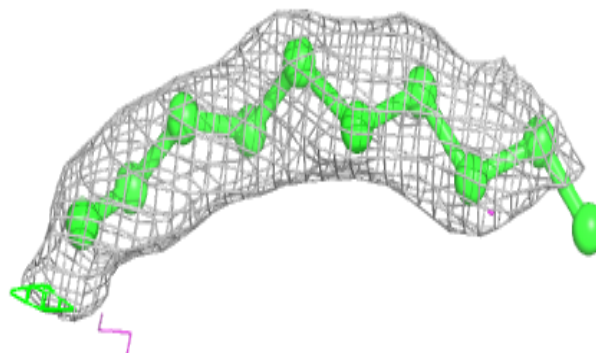


**Electron density around OLC C 359:**

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

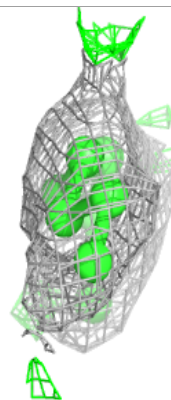
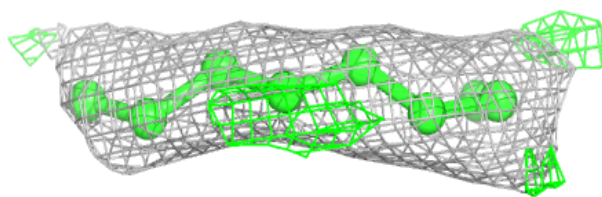
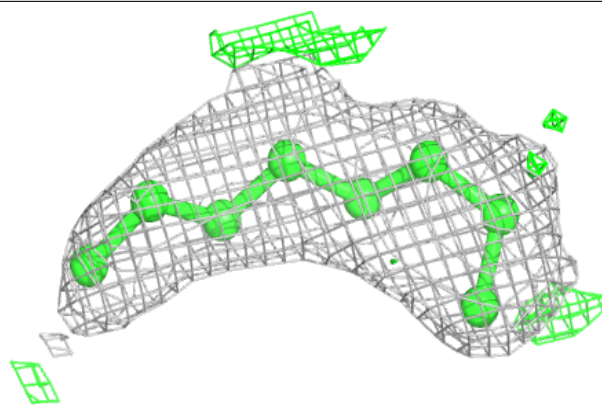
**Electron density around OLC C 349:**

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

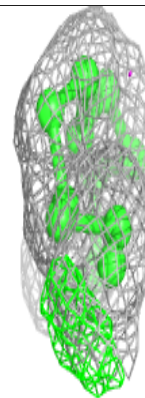
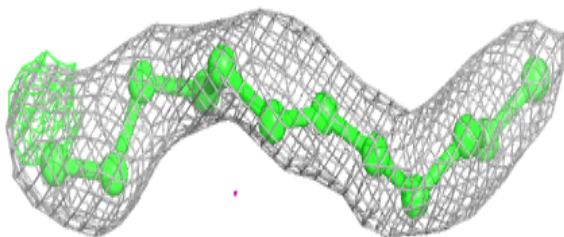
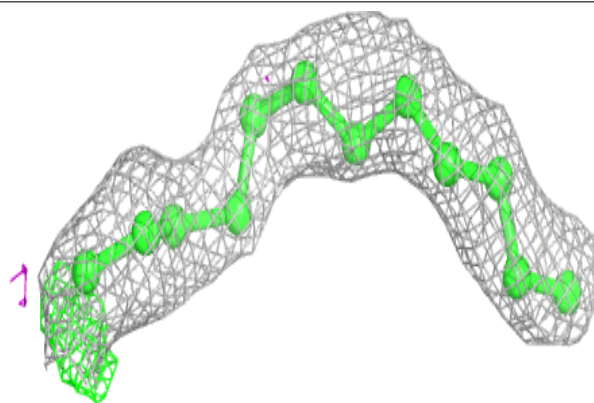


**Electron density around OLC A 342:**

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

**Electron density around OLC C 364:**

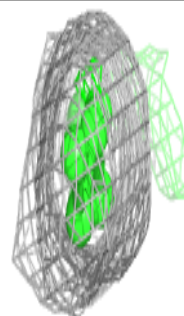
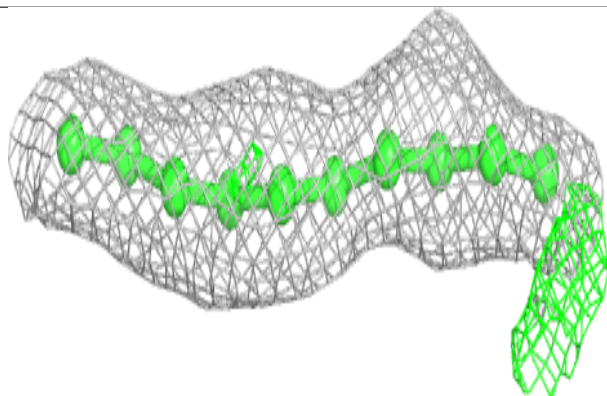
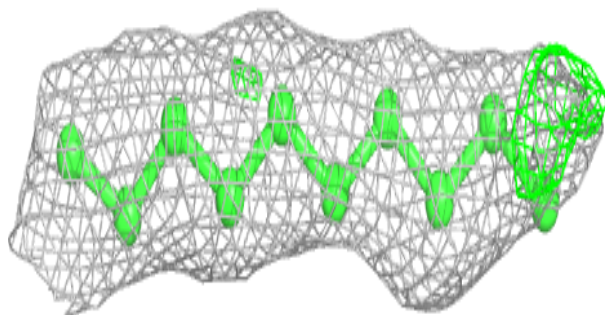
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



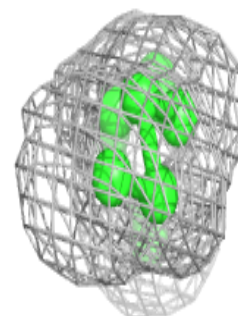
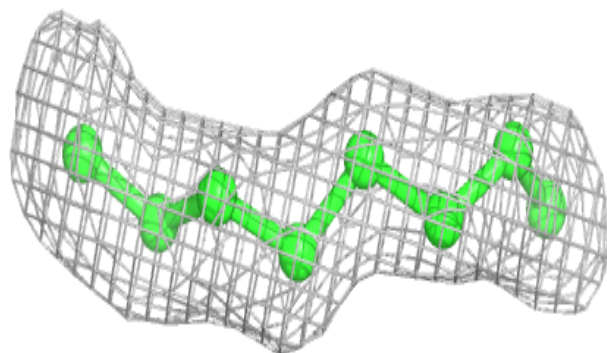
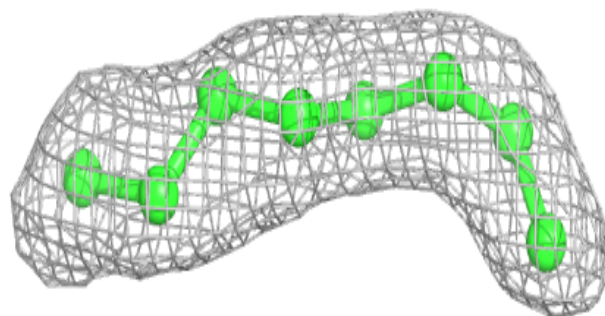


**Electron density around OLC C 355:**

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

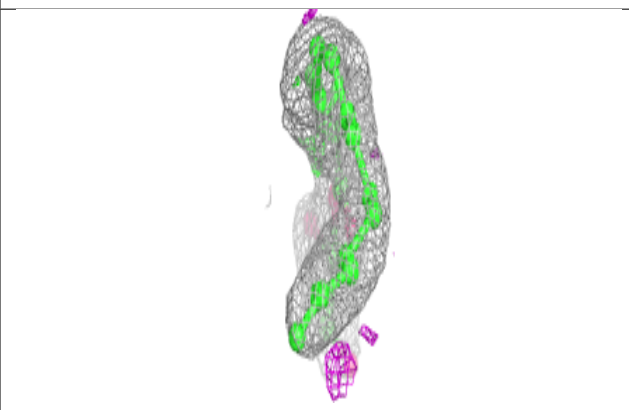
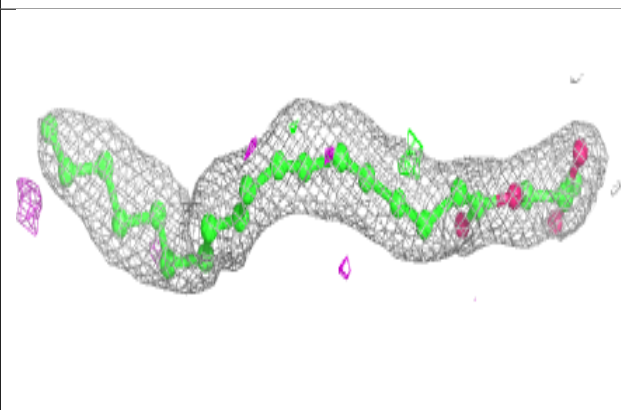
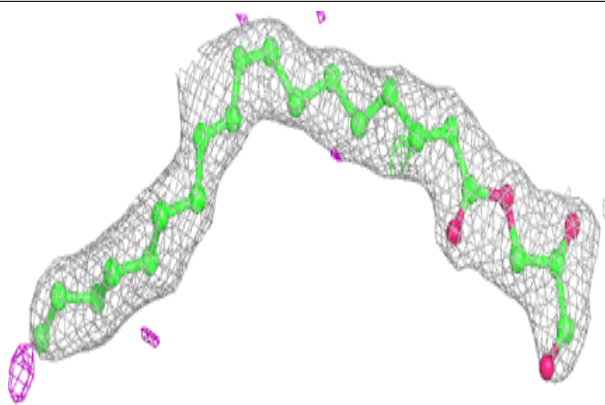
**Electron density around OLC A 347:**

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

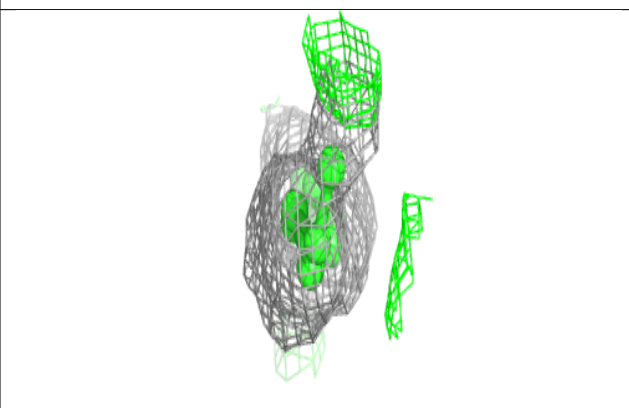
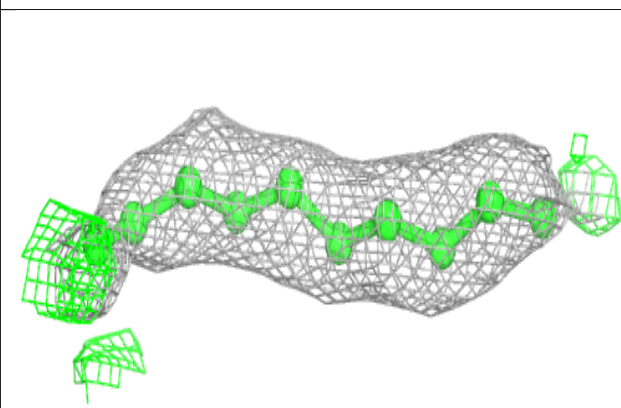
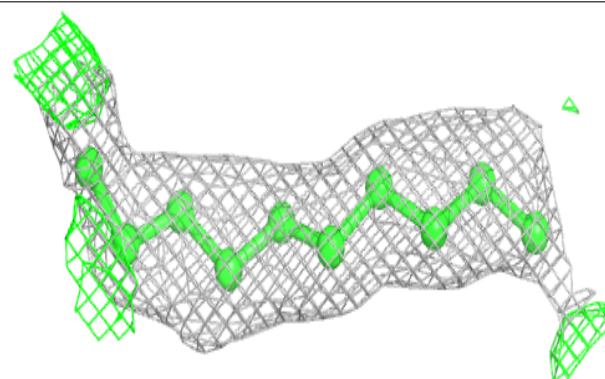


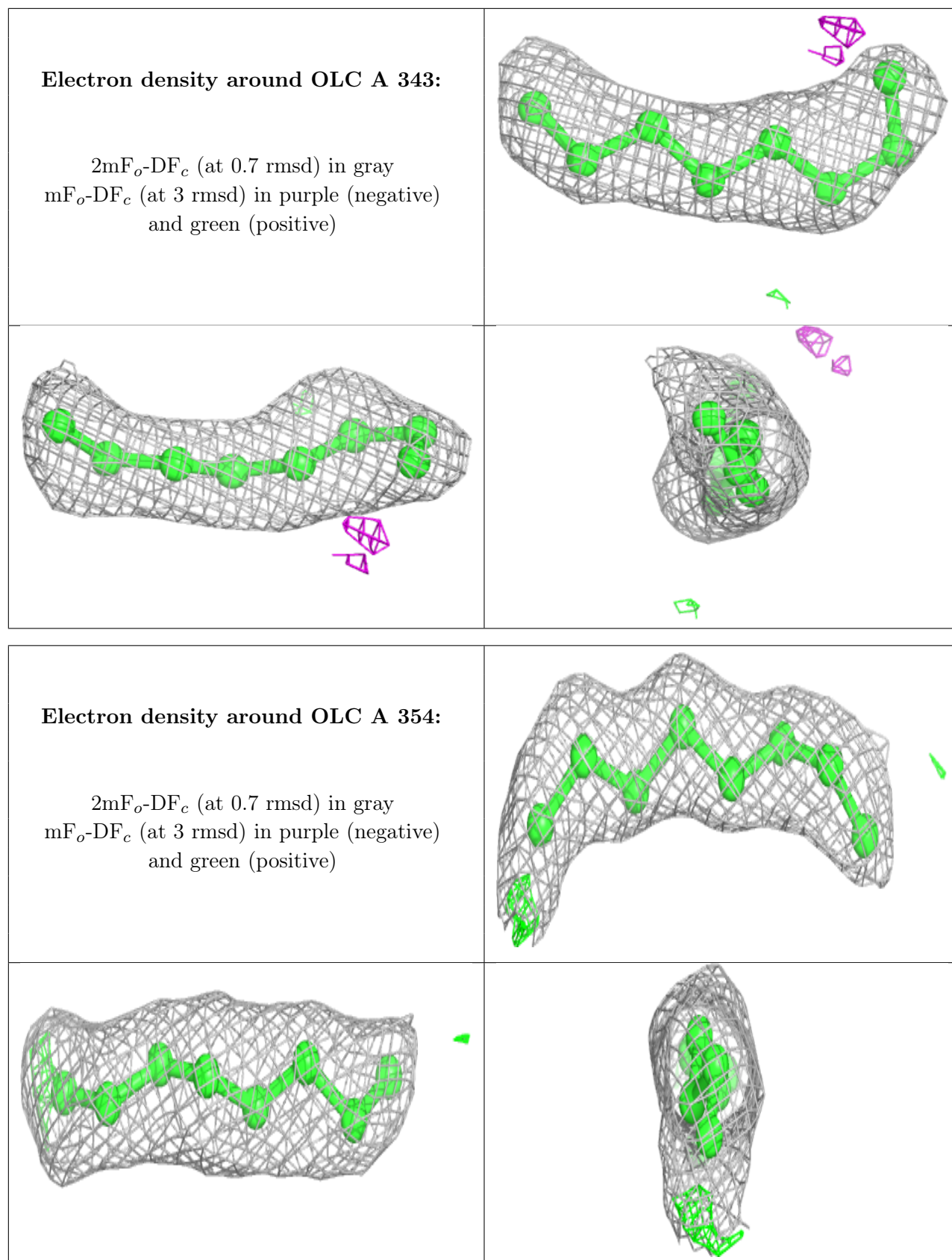
**Electron density around OLC A 356:**

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

**Electron density around OLC C 346:**

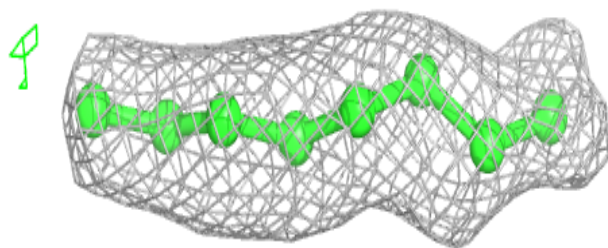
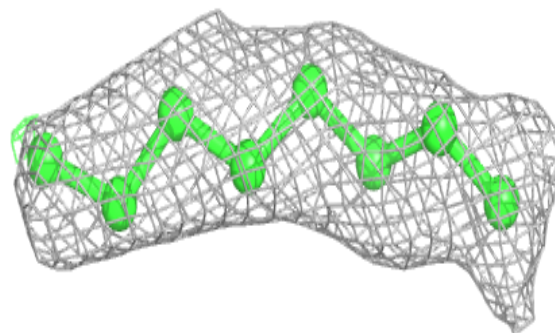
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



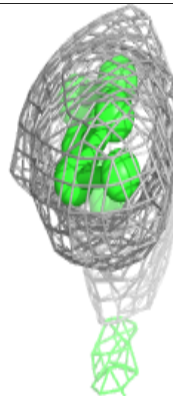
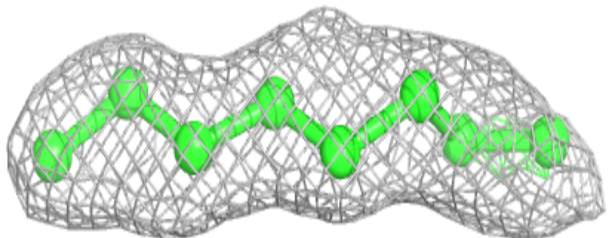
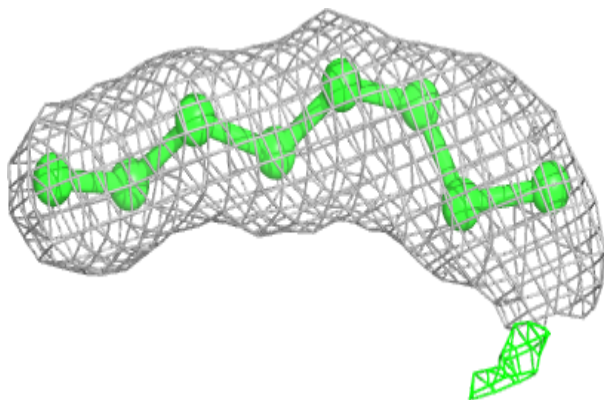


**Electron density around OLC C 342:**

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

**Electron density around OLC D 344:**

$2mF_o-DF_c$  (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.