



# wwPDB X-ray Structure Validation Summary Report

Mar 15, 2026 – 12:52 PM UTC

PDB ID : 6RF4 / pdb\_00006rf4  
Title : Crystal structure of the potassium-pumping S254A mutant of the light-driven sodium pump KR2 in the pentameric form, pH 8.0  
Authors : Kovalev, K.; Polovinkin, V.; Gushchin, I.; Borshchevskiy, V.; Gordeliy, V.  
Deposited on : 2019-04-12  
Resolution : 2.40 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

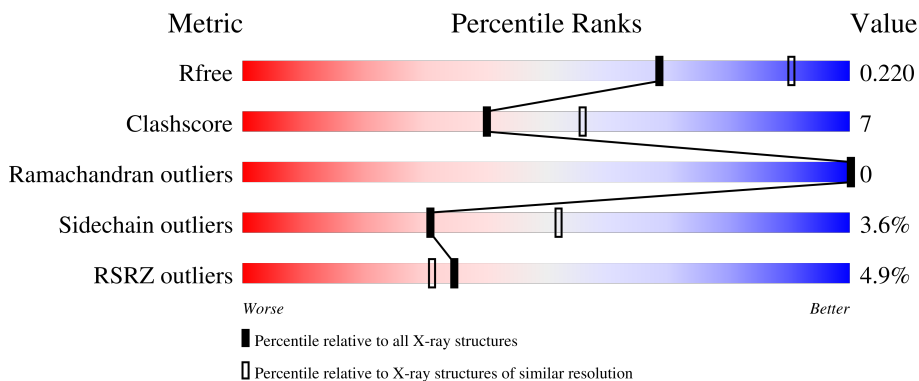
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	288	 3% 82% 11% • 5%
1	B	288	 6% 81% 14% 5%
1	C	288	 4% 79% 14% • 5%
1	D	288	 6% 83% 11% • 5%
1	E	288	 4% 81% 12% • 5%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	Total 2178	C 1451	N 330	O 388	S 9	0	1	0
1	B	273	Total 2172	C 1446	N 331	O 386	S 9	0	1	0
1	C	273	Total 2177	C 1450	N 330	O 388	S 9	0	1	0
1	D	273	Total 2169	C 1445	N 330	O 385	S 9	0	1	0
1	E	273	Total 2171	C 1447	N 330	O 385	S 9	0	1	0

There are 45 discrepancies between the modelled and reference sequences:

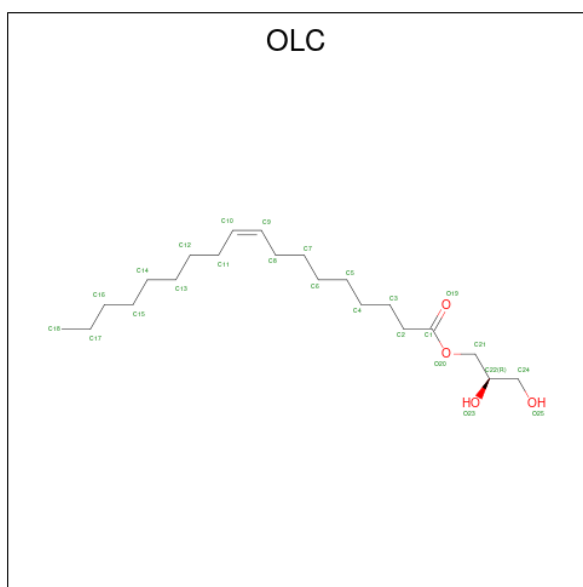
Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ALA	SER	engineered mutation	UNP N0DKS8
A	281	LEU	-	expression tag	UNP N0DKS8
A	282	GLU	-	expression tag	UNP N0DKS8
A	283	HIS	-	expression tag	UNP N0DKS8
A	284	HIS	-	expression tag	UNP N0DKS8
A	285	HIS	-	expression tag	UNP N0DKS8
A	286	HIS	-	expression tag	UNP N0DKS8
A	287	HIS	-	expression tag	UNP N0DKS8
A	288	HIS	-	expression tag	UNP N0DKS8
B	254	ALA	SER	engineered mutation	UNP N0DKS8
B	281	LEU	-	expression tag	UNP N0DKS8
B	282	GLU	-	expression tag	UNP N0DKS8
B	283	HIS	-	expression tag	UNP N0DKS8
B	284	HIS	-	expression tag	UNP N0DKS8
B	285	HIS	-	expression tag	UNP N0DKS8
B	286	HIS	-	expression tag	UNP N0DKS8
B	287	HIS	-	expression tag	UNP N0DKS8
B	288	HIS	-	expression tag	UNP N0DKS8
C	254	ALA	SER	engineered mutation	UNP N0DKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	281	LEU	-	expression tag	UNP N0DKS8
C	282	GLU	-	expression tag	UNP N0DKS8
C	283	HIS	-	expression tag	UNP N0DKS8
C	284	HIS	-	expression tag	UNP N0DKS8
C	285	HIS	-	expression tag	UNP N0DKS8
C	286	HIS	-	expression tag	UNP N0DKS8
C	287	HIS	-	expression tag	UNP N0DKS8
C	288	HIS	-	expression tag	UNP N0DKS8
D	254	ALA	SER	engineered mutation	UNP N0DKS8
D	281	LEU	-	expression tag	UNP N0DKS8
D	282	GLU	-	expression tag	UNP N0DKS8
D	283	HIS	-	expression tag	UNP N0DKS8
D	284	HIS	-	expression tag	UNP N0DKS8
D	285	HIS	-	expression tag	UNP N0DKS8
D	286	HIS	-	expression tag	UNP N0DKS8
D	287	HIS	-	expression tag	UNP N0DKS8
D	288	HIS	-	expression tag	UNP N0DKS8
E	254	ALA	SER	engineered mutation	UNP N0DKS8
E	281	LEU	-	expression tag	UNP N0DKS8
E	282	GLU	-	expression tag	UNP N0DKS8
E	283	HIS	-	expression tag	UNP N0DKS8
E	284	HIS	-	expression tag	UNP N0DKS8
E	285	HIS	-	expression tag	UNP N0DKS8
E	286	HIS	-	expression tag	UNP N0DKS8
E	287	HIS	-	expression tag	UNP N0DKS8
E	288	HIS	-	expression tag	UNP N0DKS8

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



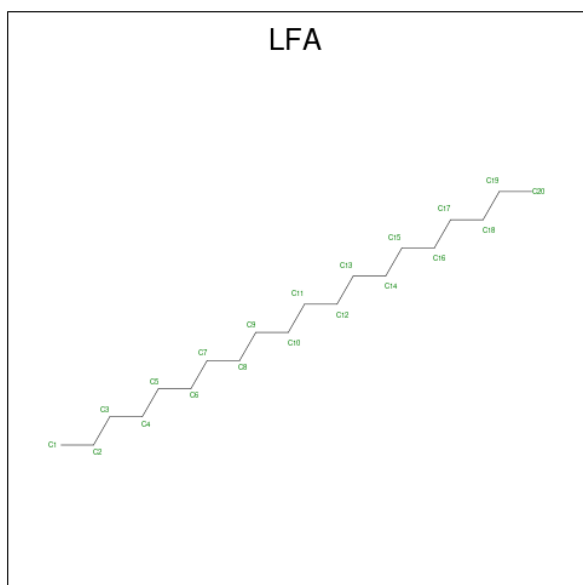
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 14 14	0	0
2	A	1	Total C O 13 9 4	0	0
2	A	1	Total C O 15 11 4	0	0
2	A	1	Total C 14 14	0	0
2	B	1	Total C O 22 18 4	0	0
2	B	1	Total C O 20 16 4	0	0
2	B	1	Total C O 16 12 4	0	0
2	C	1	Total C O 21 17 4	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 14 10 4	0	0
2	C	1	Total C O 21 17 4	0	0
2	C	1	Total C O 23 19 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C O 14 10 4	0	0
2	E	1	Total C 12 12	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 25 21 4	0	0

- Molecule 3 is EICOSANE (CCD ID: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 20 20	0	0
3	B	1	Total C 20 20	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 11 11	0	0
3	C	1	Total C 4 4	0	0
3	C	1	Total C 4 4	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 17 17	0	0
3	D	1	Total C 7 7	0	0

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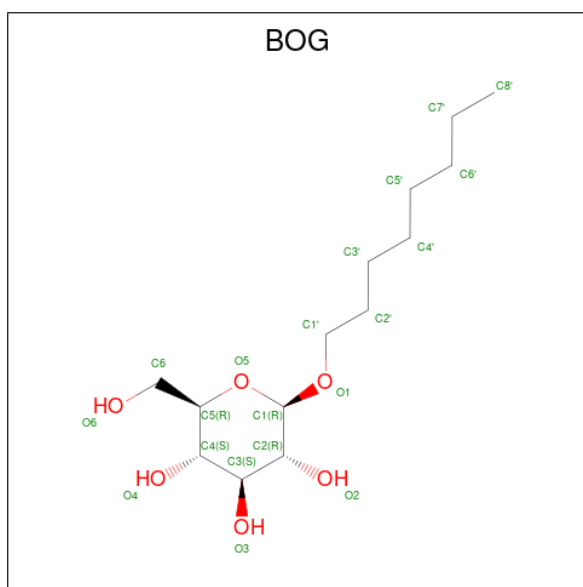
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C 6 6	0	0
3	E	1	Total C 20 20	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 14 14	0	0
3	E	1	Total C 4 4	0	0
3	E	1	Total C 5 5	0	0
3	E	1	Total C 14 14	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

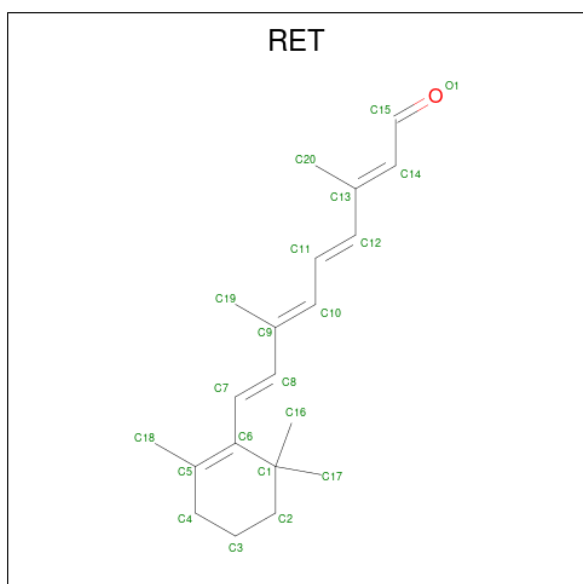
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

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



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

- Molecule 6 is RETINAL (CCD ID: RET) (formula:  $C_{20}H_{28}O$ ).



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

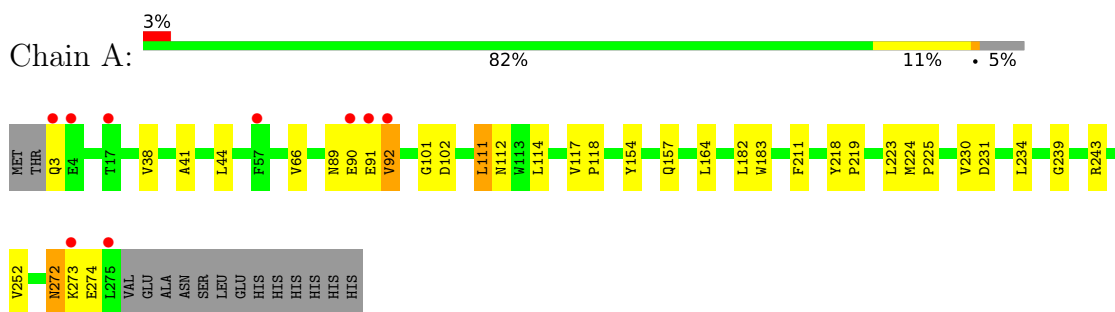
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	62	Total O 62 62	0	0
7	B	69	Total O 69 69	0	0
7	C	75	Total O 75 75	0	0
7	D	59	Total O 59 59	0	0
7	E	63	Total O 63 63	0	0

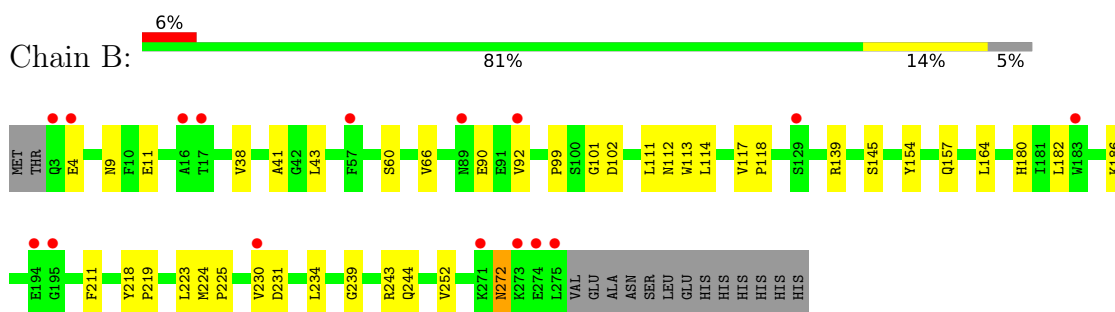
### 3 Residue-property plots [i](#)

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

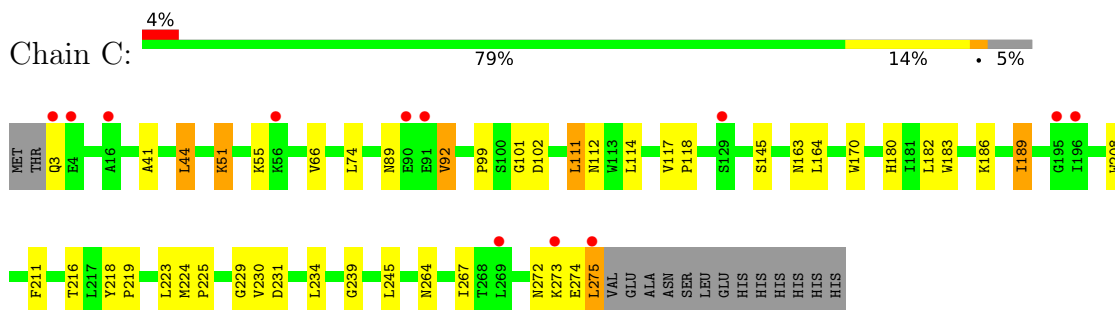
- Molecule 1: Sodium pumping rhodopsin



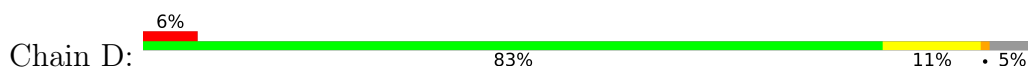
- Molecule 1: Sodium pumping rhodopsin

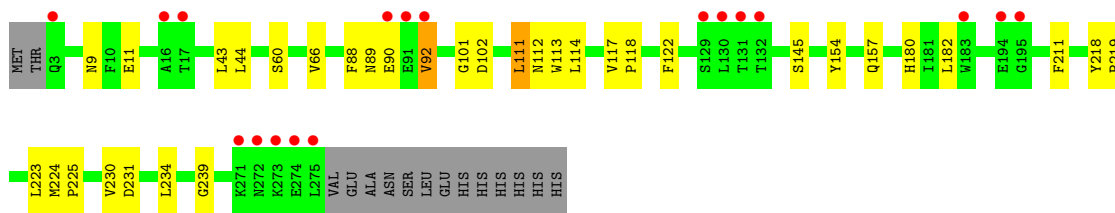


- Molecule 1: Sodium pumping rhodopsin

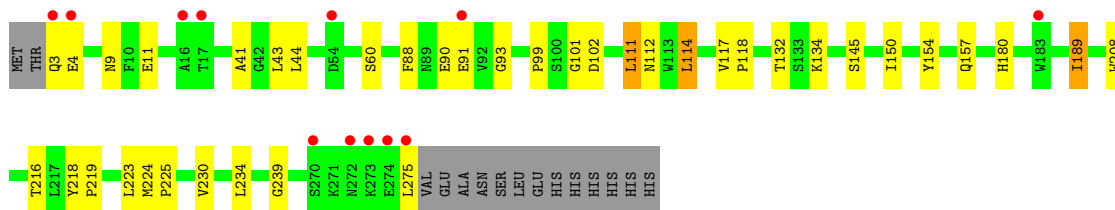
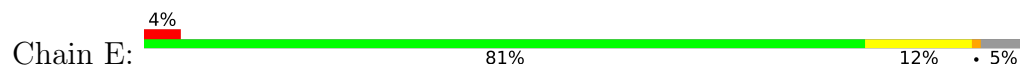


- Molecule 1: Sodium pumping rhodopsin





• Molecule 1: Sodium pumping rhodopsin



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.40Å 240.04Å 135.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.91 – 2.40 44.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.91-2.40) 99.8 (44.91-2.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.181 , 0.212 0.190 , 0.220	Depositor DCC
$R_{free}$ test set	4223 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	0.47	0/2236	0.91	0/3040
1	B	0.47	0/2230	0.90	0/3033
1	C	0.47	0/2235	0.90	0/3039
1	D	0.46	0/2227	0.92	0/3028
1	E	0.47	0/2229	0.90	0/3031
All	All	0.47	0/11157	0.91	0/15171

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Sidechain
1	B	243	ARG	Sidechain
1	C	272	ASN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2178	0	2154	25	0
1	B	2172	0	2149	33	0
1	C	2177	0	2152	35	0
1	D	2169	0	2142	25	0
1	E	2171	0	2149	24	0
2	A	56	0	78	0	0
2	B	58	0	79	4	0
2	C	260	0	370	9	0
2	D	32	0	40	0	0
2	E	53	0	84	1	0
3	A	61	0	119	1	0
3	B	37	0	74	1	0
3	C	74	0	147	5	0
3	D	98	0	198	0	0
3	E	65	0	127	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	20	0	28	2	0
5	B	20	0	28	2	0
5	C	20	0	28	3	0
5	D	20	0	28	2	0
5	E	20	0	28	0	0
6	A	20	0	27	6	0
6	B	20	0	27	5	0
6	C	20	0	27	5	0
6	D	20	0	27	6	0
6	E	20	0	27	5	0
7	A	62	0	0	0	0
7	B	69	0	0	2	0
7	C	75	0	0	2	0
7	D	59	0	0	2	0
7	E	63	0	0	1	0
All	All	12194	0	12337	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 159 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:272:ASN:HD22	1:B:272:ASN:N	1.69	0.87
1:A:272:ASN:HD22	1:A:272:ASN:N	1.71	0.87
6:D:312:RET:H161	6:D:312:RET:H8	1.60	0.83
6:B:309:RET:H161	6:B:309:RET:H8	1.59	0.82
6:A:313:RET:H8	6:A:313:RET:H161	1.62	0.82

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	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
1	B	272/288 (94%)	265 (97%)	7 (3%)	0	100	100
1	C	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
1	D	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
1	E	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
All	All	1360/1440 (94%)	1329 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/247 (93%)	222 (96%)	8 (4%)	32	53
1	B	230/247 (93%)	223 (97%)	7 (3%)	36	58
1	C	230/247 (93%)	219 (95%)	11 (5%)	23	40
1	D	228/247 (92%)	224 (98%)	4 (2%)	51	73
1	E	229/247 (93%)	218 (95%)	11 (5%)	23	40
All	All	1147/1235 (93%)	1106 (96%)	41 (4%)	31	52

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	112	ASN
1	E	114	LEU
1	D	230	VAL
1	E	91	GLU
1	E	134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	141	GLN
1	D	180	HIS
1	E	180	HIS
1	B	272	ASN
1	C	3	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 69 ligands modelled in this entry, 5 are monoatomic - leaving 64 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
3	LFA	E	306	-	13,13,19	0.30	0	12,12,18	0.48	0
3	LFA	D	304	-	19,19,19	0.27	0	18,18,18	0.53	0
3	LFA	D	306	-	7,7,19	0.31	0	6,6,18	0.36	0
2	OLC	A	303	-	14,14,24	1.21	1 (7%)	15,15,25	1.15	2 (13%)
3	LFA	E	305	-	7,7,19	0.29	0	6,6,18	0.44	0
5	BOG	E	310	-	20,20,20	0.54	0	25,25,25	0.57	0
2	OLC	E	301	-	11,11,24	0.28	0	10,10,25	0.52	0
2	OLC	C	314	-	15,15,24	1.22	1 (6%)	16,16,25	1.02	1 (6%)
3	LFA	B	302	-	19,19,19	0.36	0	18,18,18	0.39	0
2	OLC	C	304	-	13,13,24	1.29	1 (7%)	14,14,25	1.06	1 (7%)
2	OLC	D	301	-	17,17,24	1.12	1 (5%)	18,18,25	1.01	1 (5%)
2	OLC	B	301	-	21,21,24	1.00	1 (4%)	22,22,25	0.94	1 (4%)
3	LFA	D	308	-	6,6,19	0.31	0	5,5,18	0.40	0
2	OLC	C	301	-	20,20,24	1.02	1 (5%)	21,21,25	1.01	1 (4%)
2	OLC	C	310	-	15,15,24	1.22	1 (6%)	16,16,25	1.07	1 (6%)
6	RET	C	323	1	20,20,21	0.72	0	27,27,28	1.64	5 (18%)
2	OLC	C	307	-	24,24,24	0.97	1 (4%)	25,25,25	0.87	1 (4%)
2	OLC	C	312	-	15,15,24	1.19	1 (6%)	16,16,25	0.95	1 (6%)
2	OLC	E	304	-	24,24,24	0.91	1 (4%)	25,25,25	0.92	2 (8%)
2	OLC	B	304	-	15,15,24	1.11	1 (6%)	16,16,25	1.01	2 (12%)
3	LFA	C	303	-	19,19,19	0.39	0	18,18,18	0.32	0
3	LFA	D	309	-	5,5,19	0.31	0	4,4,18	0.29	0
2	OLC	A	302	-	12,12,24	1.32	1 (8%)	13,13,25	1.23	2 (15%)
3	LFA	A	304	-	6,6,19	0.30	0	5,5,18	0.39	0
2	OLC	B	303	-	19,19,24	1.06	1 (5%)	20,20,25	0.90	1 (5%)
3	LFA	D	307	-	16,16,19	0.30	0	15,15,18	0.48	0
6	RET	E	312	1	20,20,21	0.82	1 (5%)	27,27,28	1.57	5 (18%)
3	LFA	C	315	-	6,6,19	0.31	0	5,5,18	0.38	0
2	OLC	A	301	-	13,13,24	0.33	0	12,12,25	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LFA	A	308	-	5,5,19	0.30	0	4,4,18	0.34	0
2	OLC	C	311	-	24,24,24	0.96	1 (4%)	25,25,25	0.84	1 (4%)
3	LFA	B	306	-	7,7,19	0.31	0	6,6,18	0.41	0
2	OLC	C	308	-	24,24,24	0.96	1 (4%)	25,25,25	0.86	1 (4%)
3	LFA	E	307	-	3,3,19	0.33	0	2,2,18	0.62	0
3	LFA	C	322	-	3,3,19	0.38	0	2,2,18	0.57	0
3	LFA	A	312	-	19,19,19	0.38	0	18,18,18	0.34	0
3	LFA	E	302	-	19,19,19	0.38	0	18,18,18	0.37	0
2	OLC	A	311	-	13,13,24	0.36	0	12,12,25	0.46	0
3	LFA	C	317	-	19,19,19	0.27	0	18,18,18	0.51	0
5	BOG	A	310	-	20,20,20	0.55	0	25,25,25	0.58	0
3	LFA	D	305	-	19,19,19	0.25	0	18,18,18	0.56	0
2	OLC	C	302	-	19,19,24	1.06	1 (5%)	20,20,25	0.93	2 (10%)
2	OLC	E	303	-	15,15,24	0.31	0	14,14,25	0.46	0
3	LFA	B	305	-	8,8,19	0.30	0	7,7,18	0.44	0
2	OLC	C	306	-	22,22,24	0.97	1 (4%)	23,23,25	0.89	2 (8%)
2	OLC	C	305	-	20,20,24	1.04	1 (5%)	21,21,25	0.88	1 (4%)
6	RET	B	309	1	20,20,21	0.69	0	27,27,28	1.61	6 (22%)
2	OLC	C	309	-	21,21,24	1.04	1 (4%)	22,22,25	0.91	1 (4%)
3	LFA	E	308	-	4,4,19	0.30	0	3,3,18	0.37	0
5	BOG	B	308	-	20,20,20	0.58	1 (5%)	25,25,25	0.54	0
3	LFA	A	306	-	7,7,19	0.30	0	6,6,18	0.43	0
3	LFA	D	302	-	19,19,19	0.37	0	18,18,18	0.37	0
3	LFA	C	319	-	3,3,19	0.34	0	2,2,18	0.63	0
5	BOG	D	311	-	20,20,20	0.53	0	25,25,25	0.64	0
2	OLC	D	303	-	13,13,24	1.22	1 (7%)	14,14,25	0.99	2 (14%)
6	RET	A	313	1	20,20,21	0.76	0	27,27,28	1.64	5 (18%)
5	BOG	C	321	-	20,20,20	0.56	0	25,25,25	0.71	0
3	LFA	A	307	-	11,11,19	0.31	0	10,10,18	0.40	0
6	RET	D	312	1	20,20,21	0.70	0	27,27,28	1.65	6 (22%)
3	LFA	E	311	-	13,13,19	0.27	0	12,12,18	0.51	0
3	LFA	C	316	-	7,7,19	0.29	0	6,6,18	0.38	0
3	LFA	C	318	-	10,10,19	0.29	0	9,9,18	0.49	0
3	LFA	A	305	-	7,7,19	0.31	0	6,6,18	0.43	0
2	OLC	C	313	-	15,15,24	1.22	1 (6%)	16,16,25	1.04	2 (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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	E	306	-	-	5/11/11/17	-
3	LFA	D	304	-	-	9/17/17/17	-
3	LFA	D	306	-	-	4/5/5/17	-
2	OLC	A	303	-	-	7/14/14/24	-
3	LFA	E	305	-	-	1/5/5/17	-
5	BOG	E	310	-	-	9/11/31/31	0/1/1/1
2	OLC	E	301	-	-	4/9/9/24	-
2	OLC	C	314	-	-	9/15/15/24	-
3	LFA	B	302	-	-	7/17/17/17	-
2	OLC	C	304	-	-	8/13/13/24	-
2	OLC	D	301	-	-	7/17/17/24	-
2	OLC	B	301	-	-	7/21/21/24	-
3	LFA	D	308	-	-	4/4/4/17	-
2	OLC	C	301	-	-	10/20/20/24	-
2	OLC	C	310	-	-	6/15/15/24	-
6	RET	C	323	1	-	0/13/30/31	0/1/1/1
2	OLC	C	307	-	-	13/24/24/24	-
2	OLC	C	312	-	-	7/15/15/24	-
2	OLC	E	304	-	-	15/24/24/24	-
2	OLC	B	304	-	-	2/15/15/24	-
3	LFA	C	303	-	-	11/17/17/17	-
3	LFA	D	309	-	-	0/3/3/17	-
2	OLC	A	302	-	-	1/12/12/24	-
3	LFA	A	304	-	-	1/4/4/17	-
2	OLC	B	303	-	-	7/19/19/24	-
3	LFA	D	307	-	-	7/14/14/17	-
6	RET	E	312	1	-	0/13/30/31	0/1/1/1
3	LFA	C	315	-	-	3/4/4/17	-
2	OLC	A	301	-	-	6/11/11/24	-
3	LFA	A	308	-	-	1/3/3/17	-
2	OLC	C	311	-	-	13/24/24/24	-
3	LFA	B	306	-	-	2/5/5/17	-
2	OLC	C	308	-	-	6/24/24/24	-
3	LFA	E	307	-	-	1/1/1/17	-
3	LFA	C	322	-	-	0/1/1/17	-
3	LFA	A	312	-	-	10/17/17/17	-
3	LFA	E	302	-	-	6/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	311	-	-	6/11/11/24	-
3	LFA	C	317	-	-	13/17/17/17	-
5	BOG	A	310	-	-	5/11/31/31	0/1/1/1
3	LFA	D	305	-	-	9/17/17/17	-
2	OLC	C	302	-	-	11/19/19/24	-
2	OLC	E	303	-	-	5/13/13/24	-
3	LFA	B	305	-	-	3/6/6/17	-
2	OLC	C	306	-	-	12/22/22/24	-
2	OLC	C	305	-	-	12/20/20/24	-
6	RET	B	309	1	-	0/13/30/31	0/1/1/1
2	OLC	C	309	-	-	13/21/21/24	-
3	LFA	E	308	-	-	1/2/2/17	-
5	BOG	B	308	-	-	6/11/31/31	0/1/1/1
3	LFA	A	306	-	-	3/5/5/17	-
3	LFA	D	302	-	-	7/17/17/17	-
3	LFA	C	319	-	-	1/1/1/17	-
5	BOG	D	311	-	-	2/11/31/31	0/1/1/1
2	OLC	D	303	-	-	4/13/13/24	-
6	RET	A	313	1	-	0/13/30/31	0/1/1/1
5	BOG	C	321	-	-	3/11/31/31	0/1/1/1
3	LFA	A	307	-	-	5/9/9/17	-
6	RET	D	312	1	-	0/13/30/31	0/1/1/1
3	LFA	E	311	-	-	3/11/11/17	-
3	LFA	C	316	-	-	4/5/5/17	-
3	LFA	C	318	-	-	4/8/8/17	-
3	LFA	A	305	-	-	3/5/5/17	-
2	OLC	C	313	-	-	10/15/15/24	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	310	OLC	O20-C1	4.51	1.46	1.33
2	C	313	OLC	O20-C1	4.49	1.46	1.33
2	C	314	OLC	O20-C1	4.48	1.46	1.33
2	C	307	OLC	O20-C1	4.46	1.46	1.33
2	C	309	OLC	O20-C1	4.45	1.46	1.33

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	313	RET	C18-C5-C6	-4.37	119.72	124.48
6	C	323	RET	C18-C5-C6	-4.28	119.82	124.48
6	D	312	RET	C18-C5-C6	-4.15	119.96	124.48
6	E	312	RET	C18-C5-C6	-4.07	120.05	124.48
6	B	309	RET	C18-C5-C6	-3.96	120.17	124.48

There are no chirality outliers.

5 of 354 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	OLC	O20-C21-C22-C24
2	C	301	OLC	C21-C22-C24-O25
2	C	304	OLC	C21-C22-C24-O25
2	C	305	OLC	C21-C22-C24-O25
2	C	305	OLC	O20-C21-C22-O23

There are no ring outliers.

26 monomers are involved in 58 short contacts:

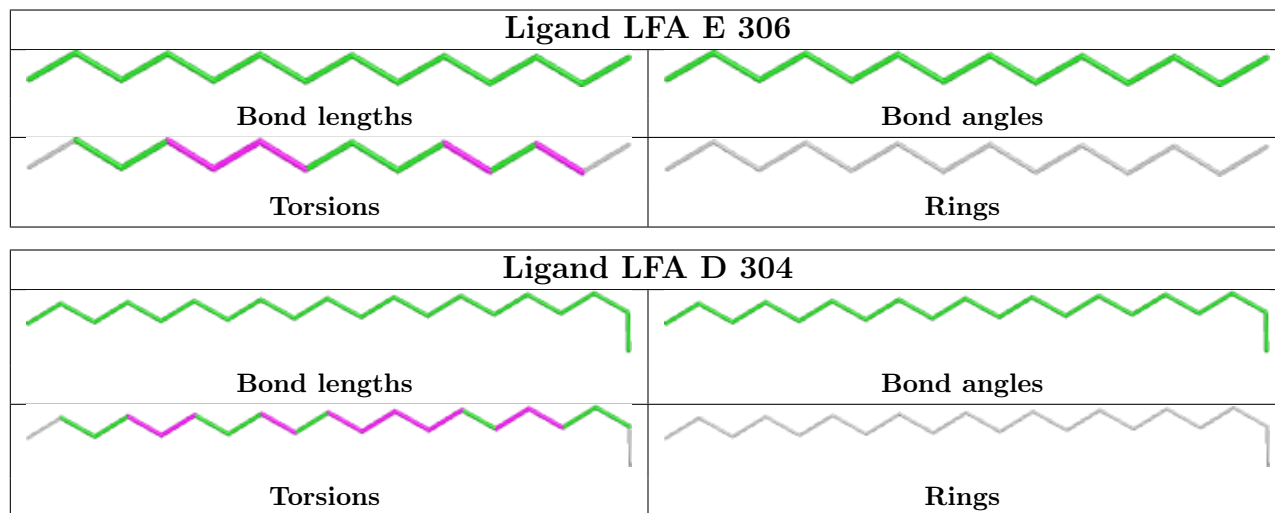
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	306	LFA	2	0
2	C	314	OLC	1	0
2	C	304	OLC	1	0
2	B	301	OLC	4	0
2	C	310	OLC	1	0
6	C	323	RET	5	0
2	C	307	OLC	1	0
2	C	312	OLC	1	0
3	A	304	LFA	1	0
6	E	312	RET	5	0
3	C	315	LFA	2	0
2	C	308	OLC	1	0
3	E	307	LFA	2	0
5	A	310	BOG	2	0
2	E	303	OLC	1	0
3	B	305	LFA	1	0
2	C	305	OLC	2	0
6	B	309	RET	5	0
5	B	308	BOG	2	0
3	C	319	LFA	2	0
5	D	311	BOG	2	0

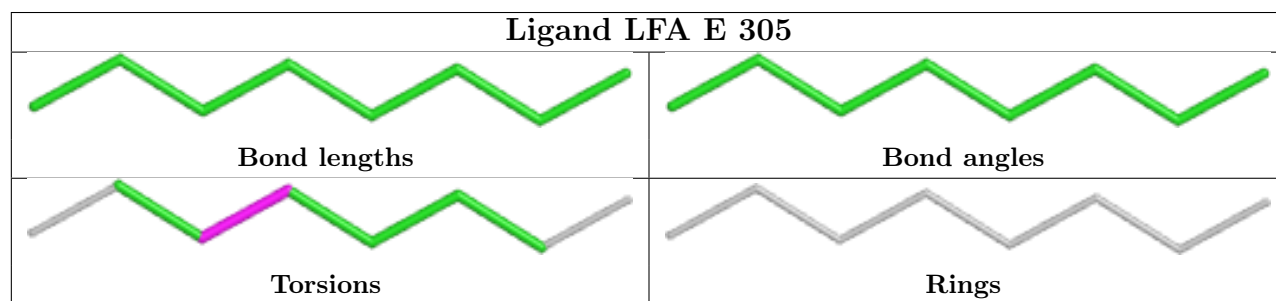
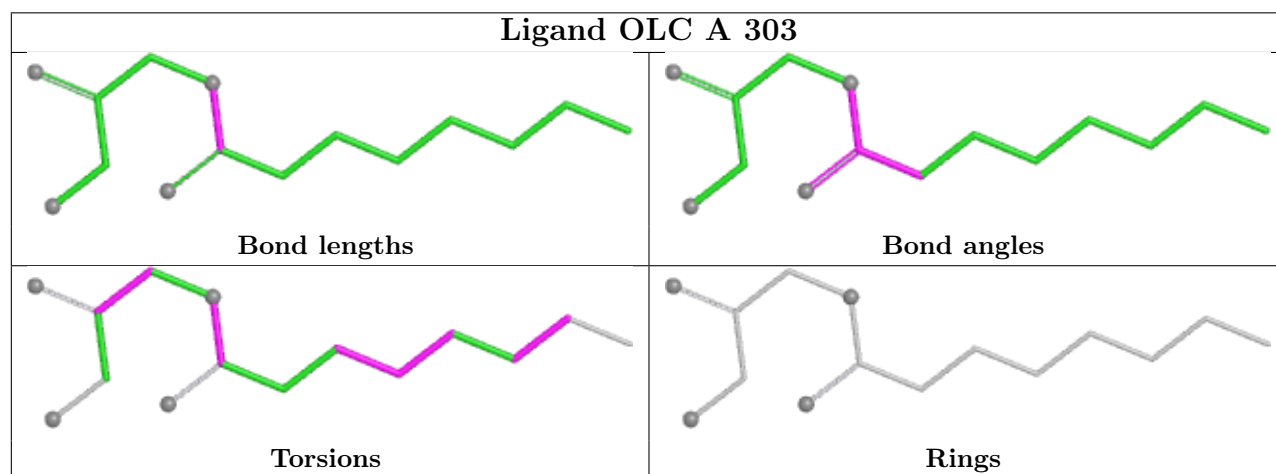
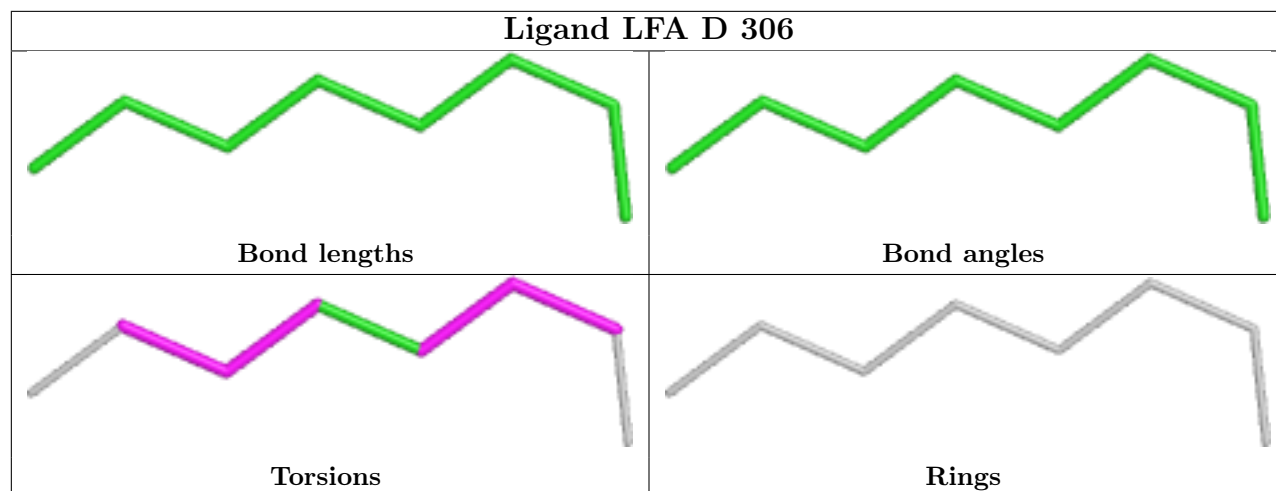
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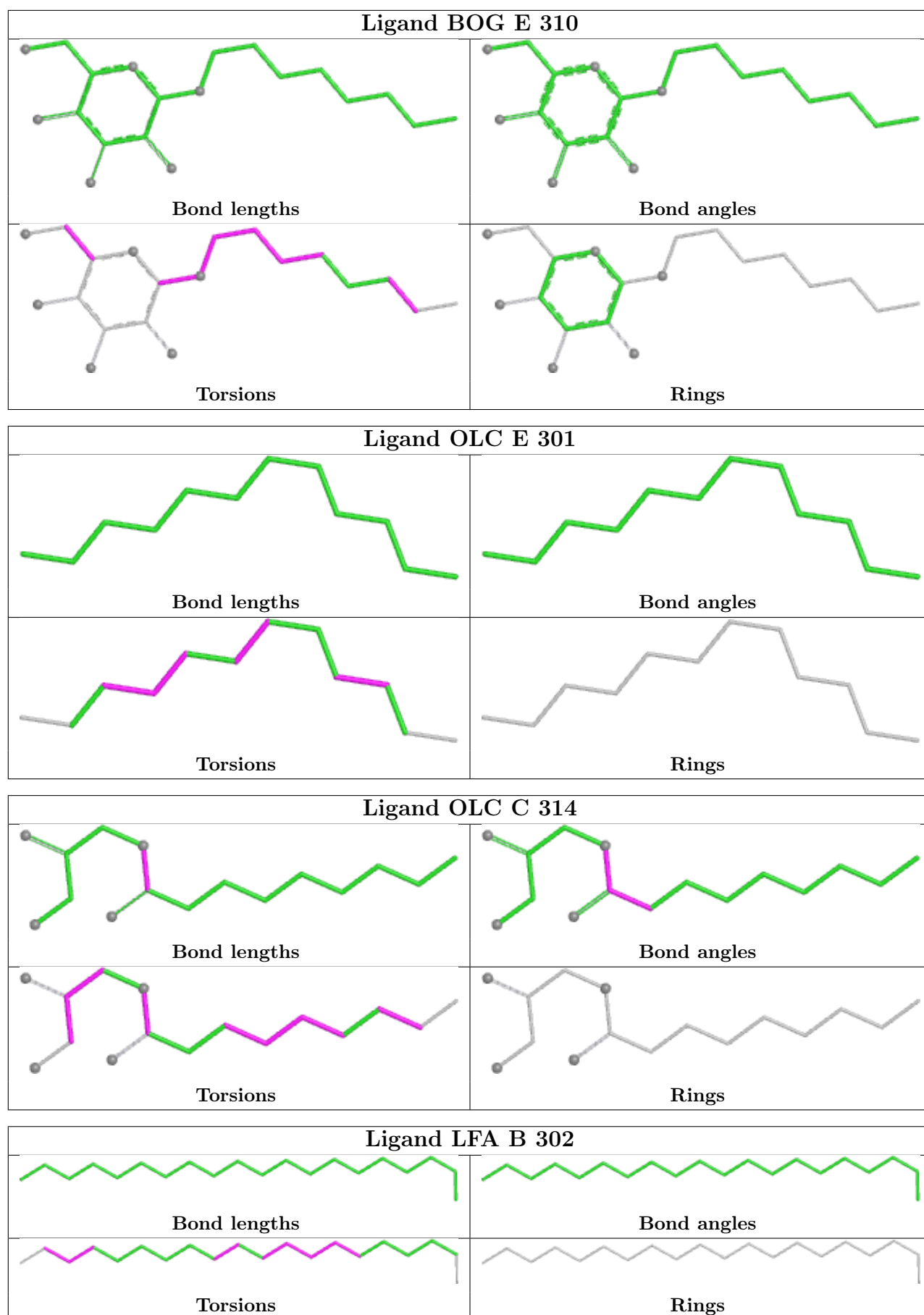
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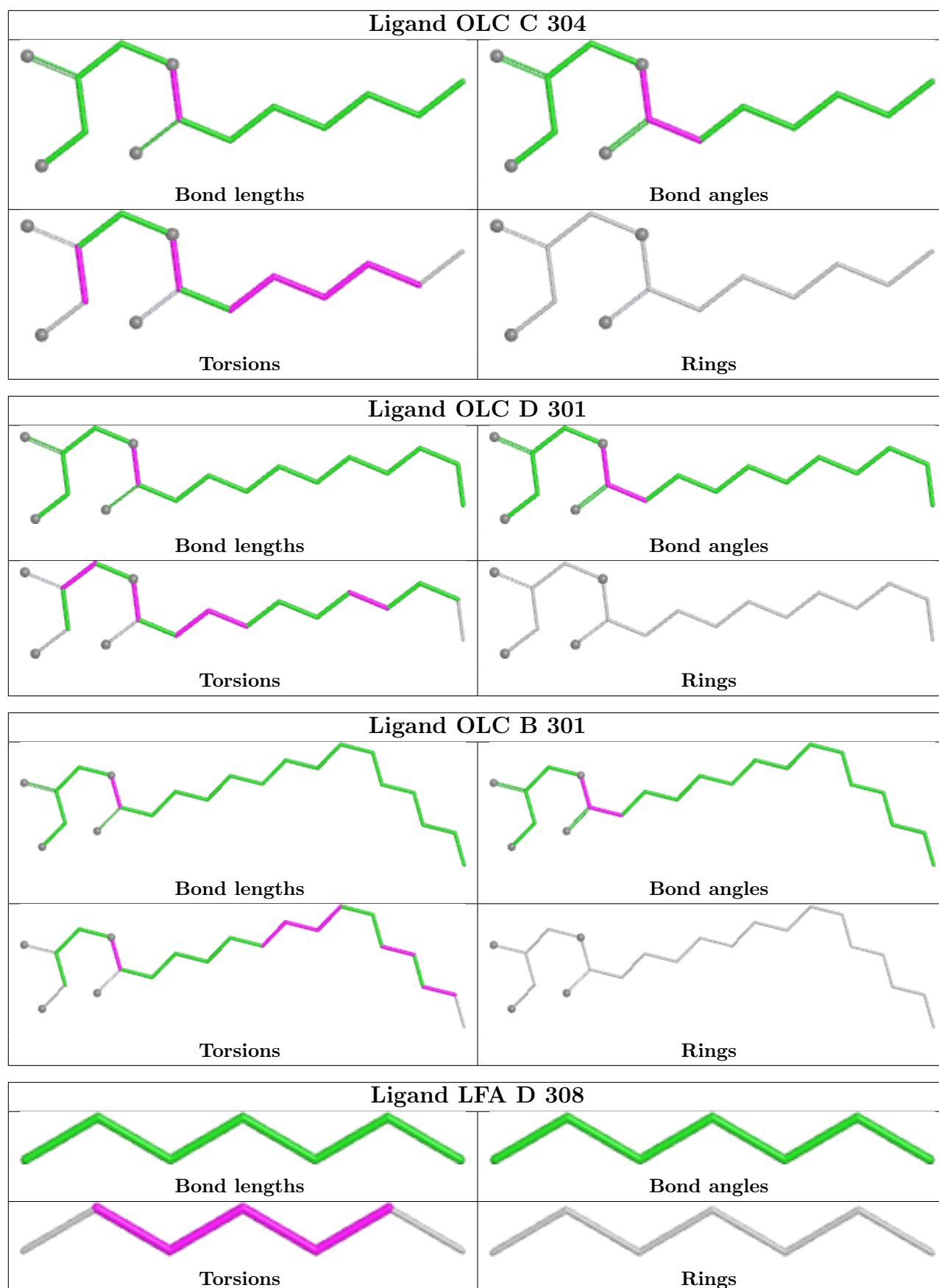
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	313	RET	6	0
5	C	321	BOG	3	0
6	D	312	RET	6	0
3	C	316	LFA	1	0
2	C	313	OLC	1	0

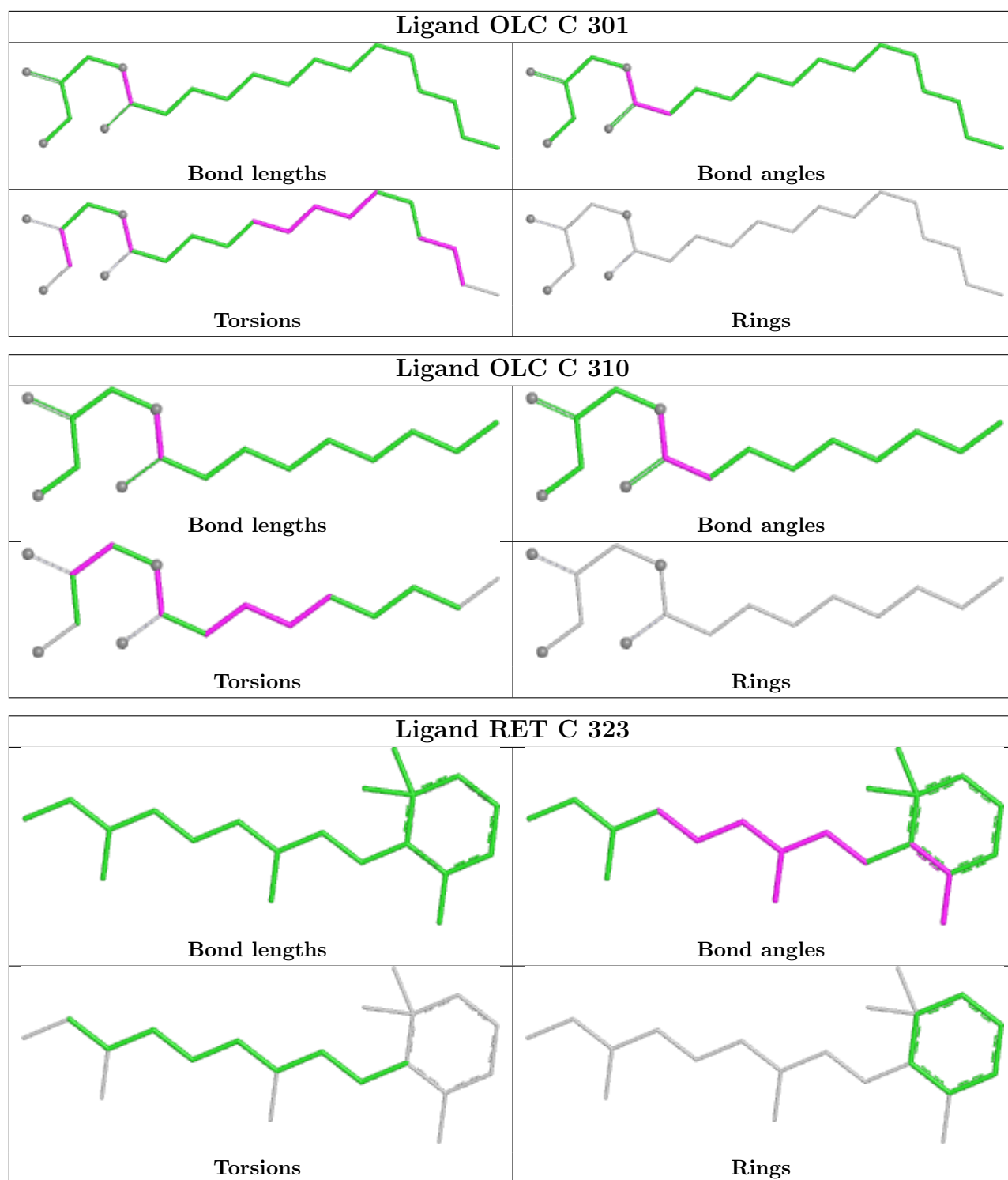
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

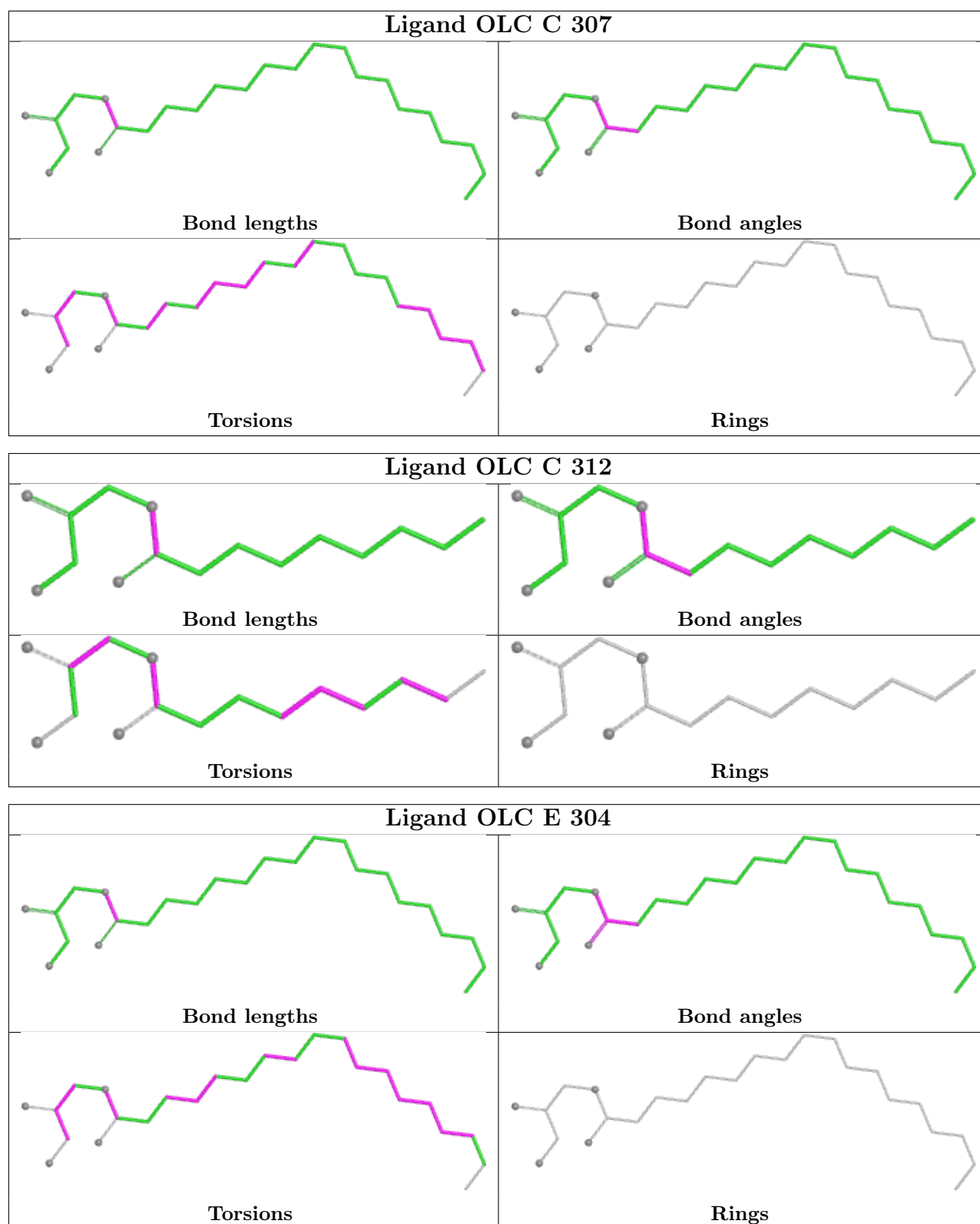


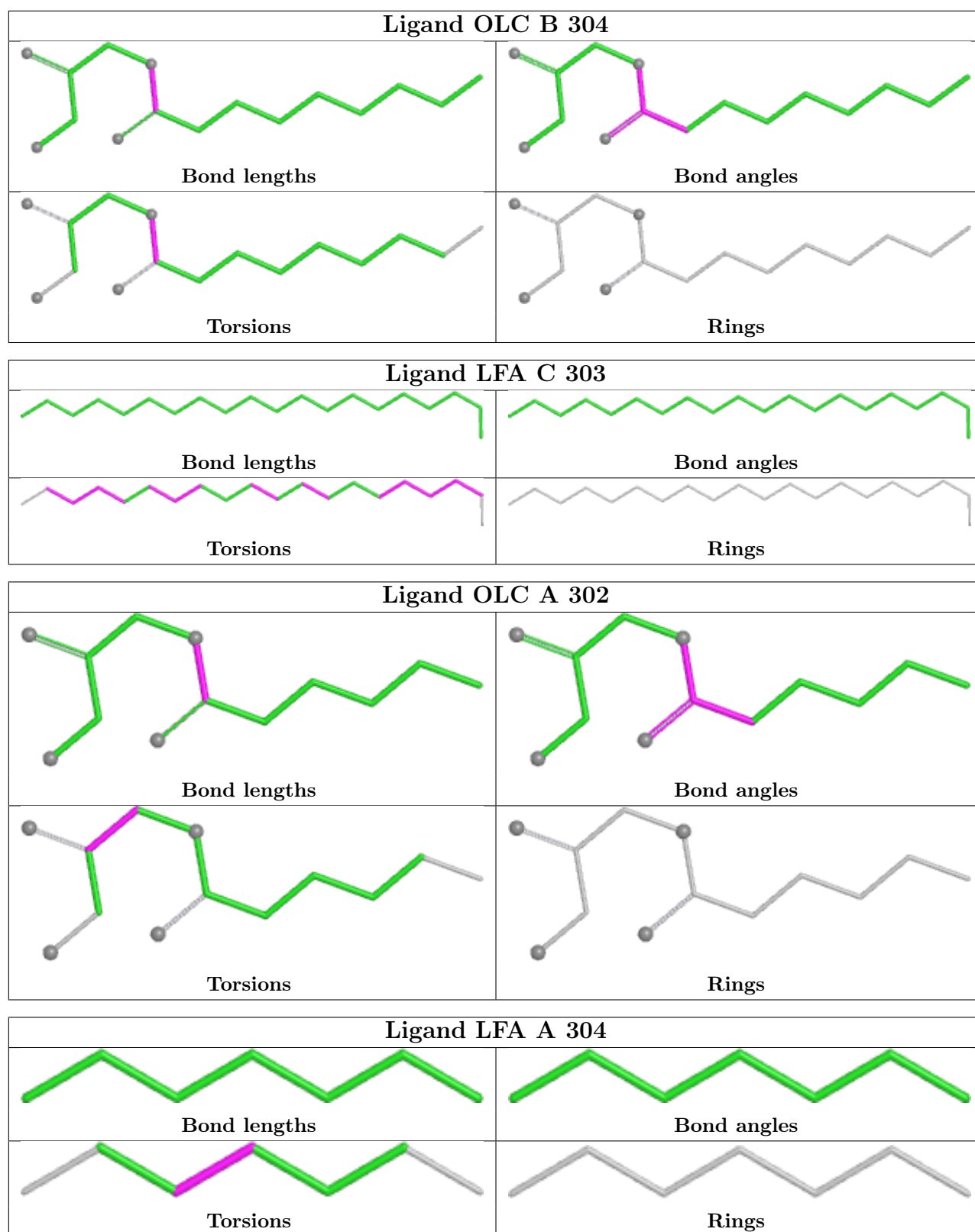


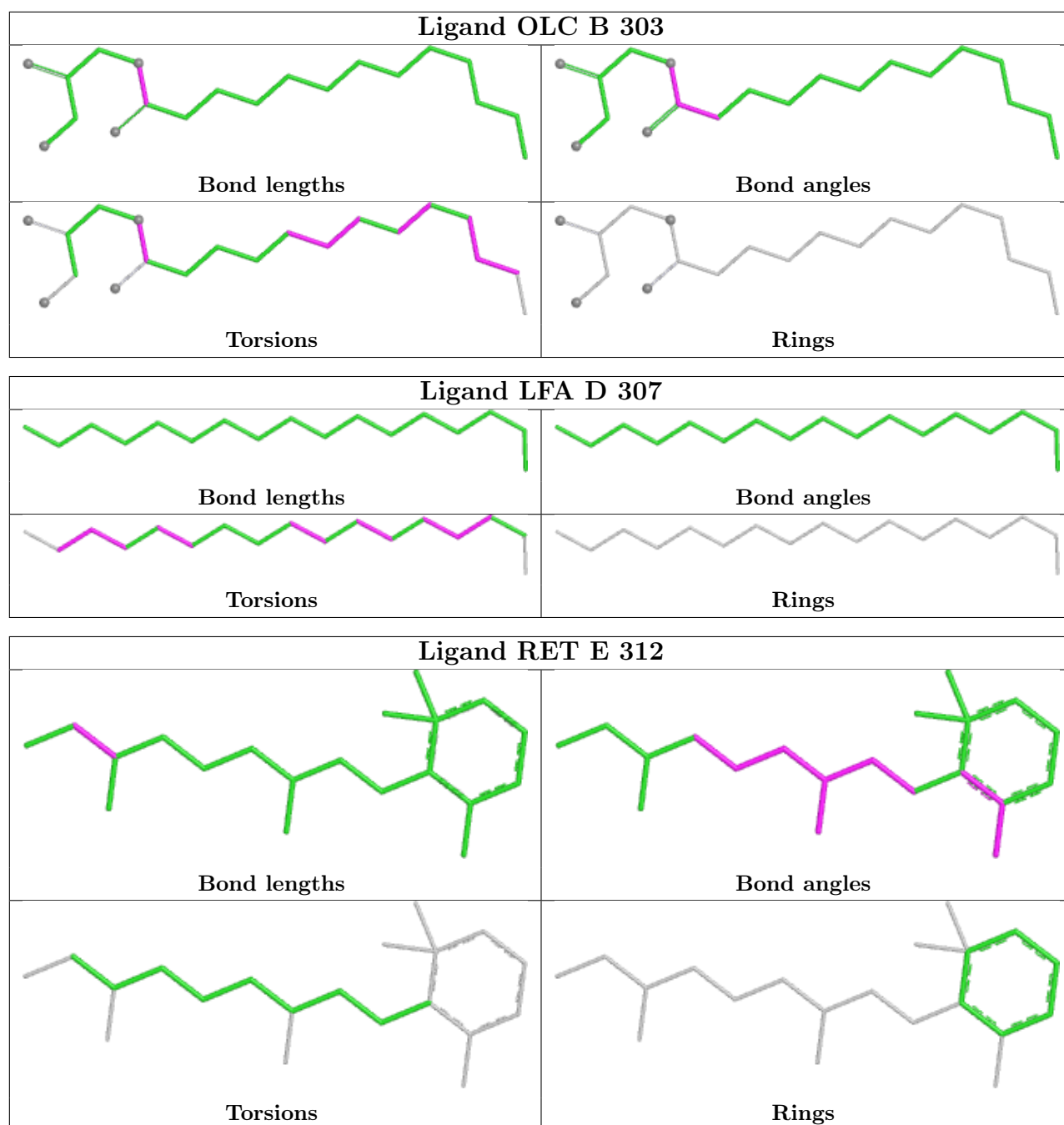


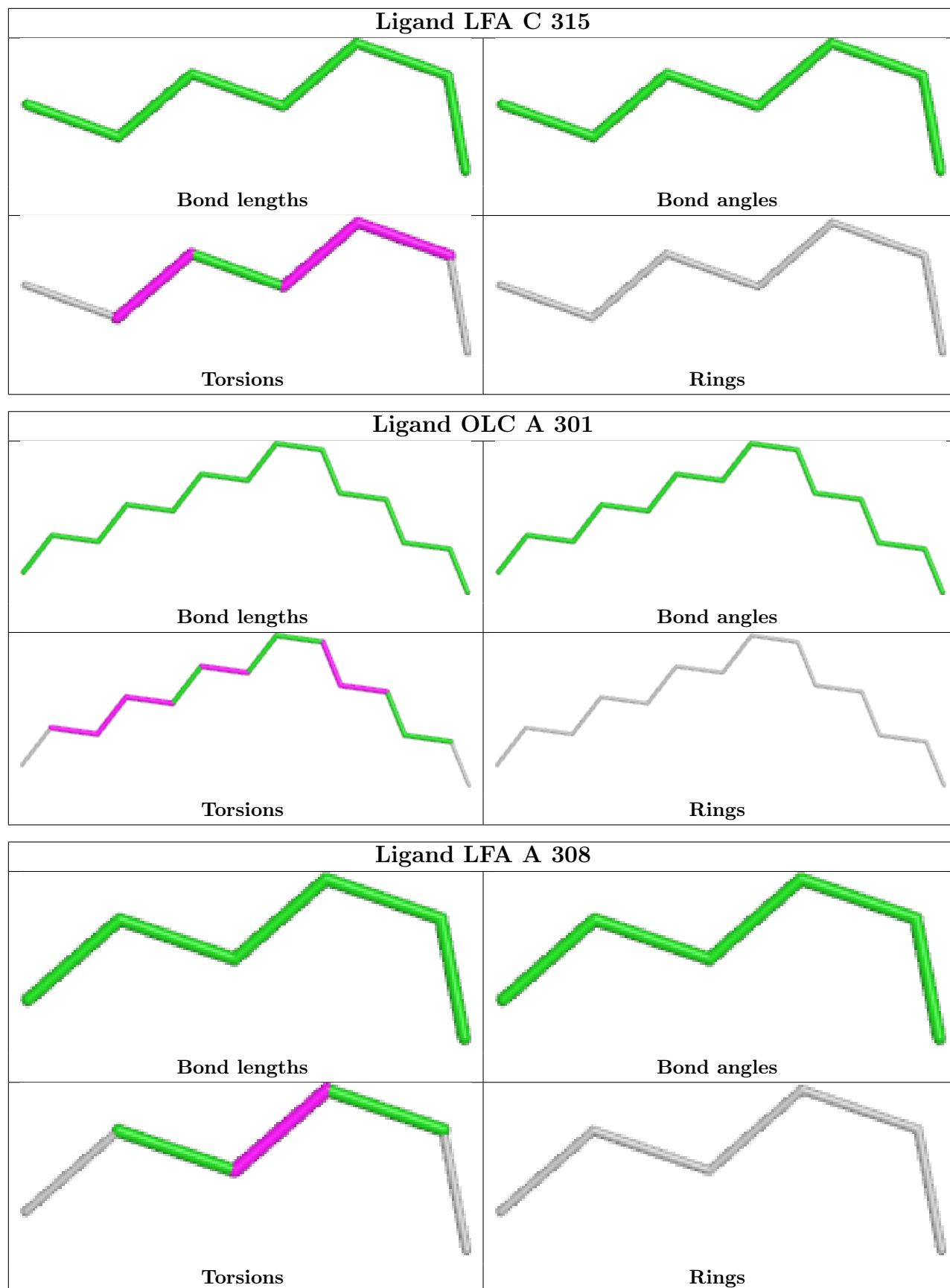


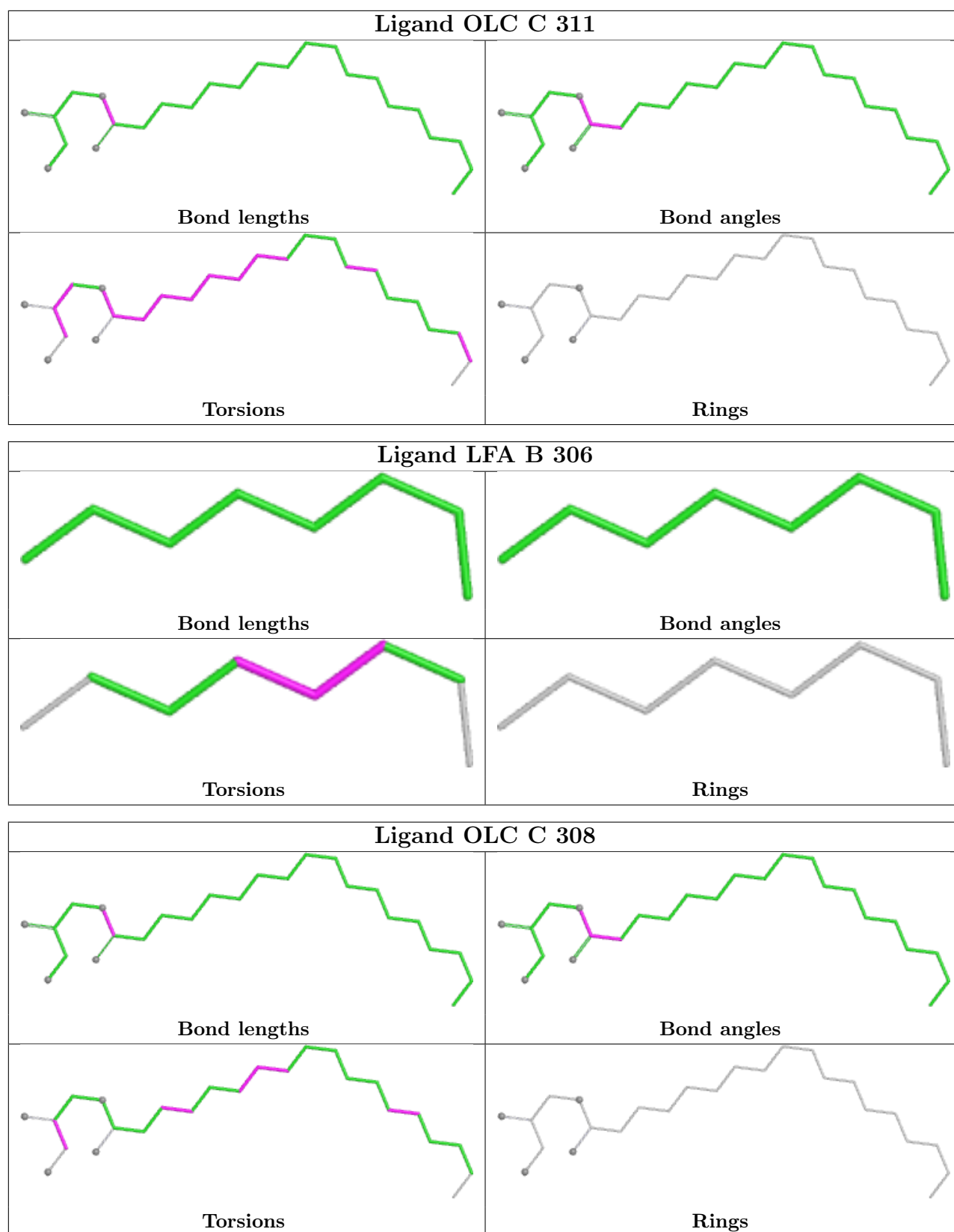


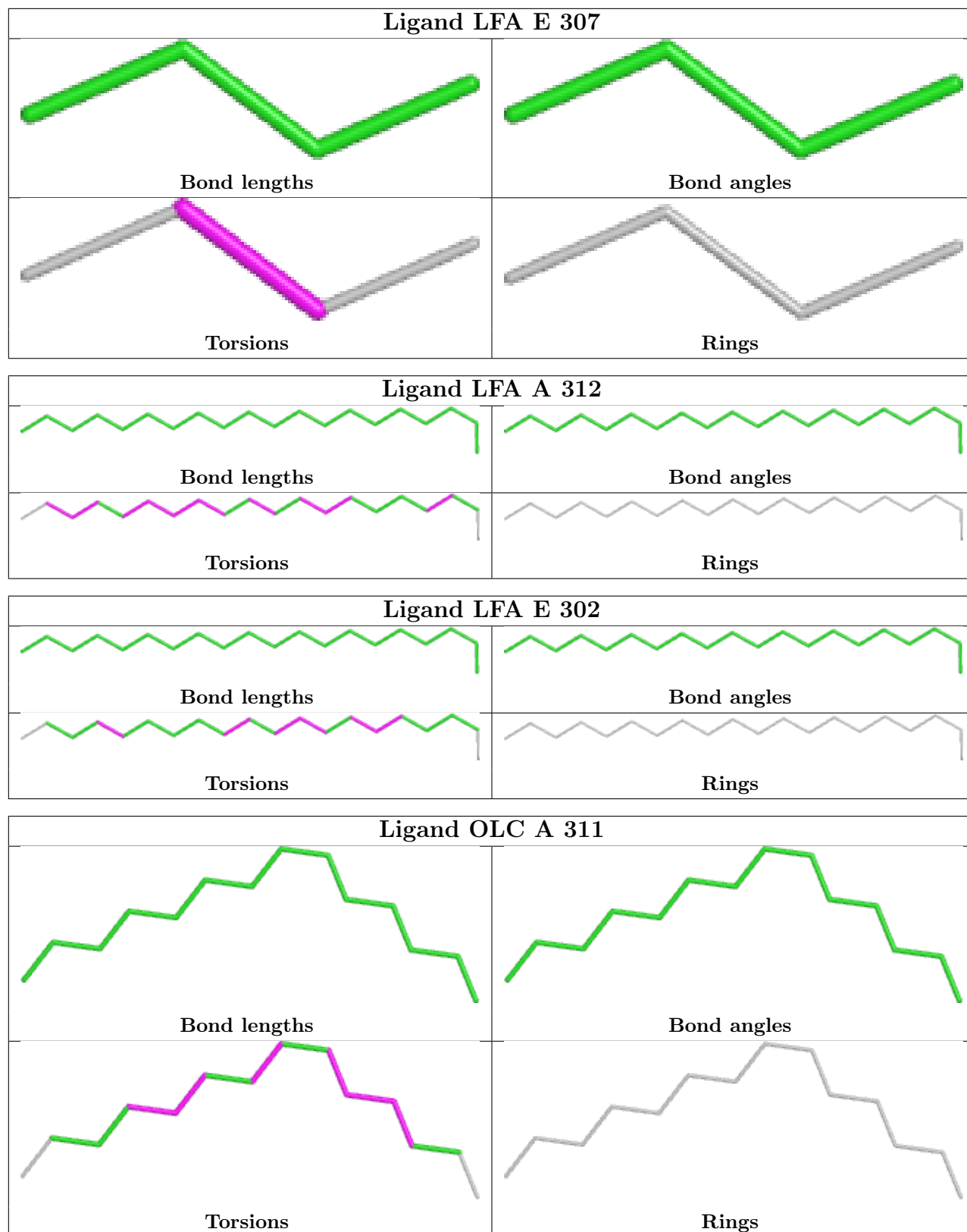


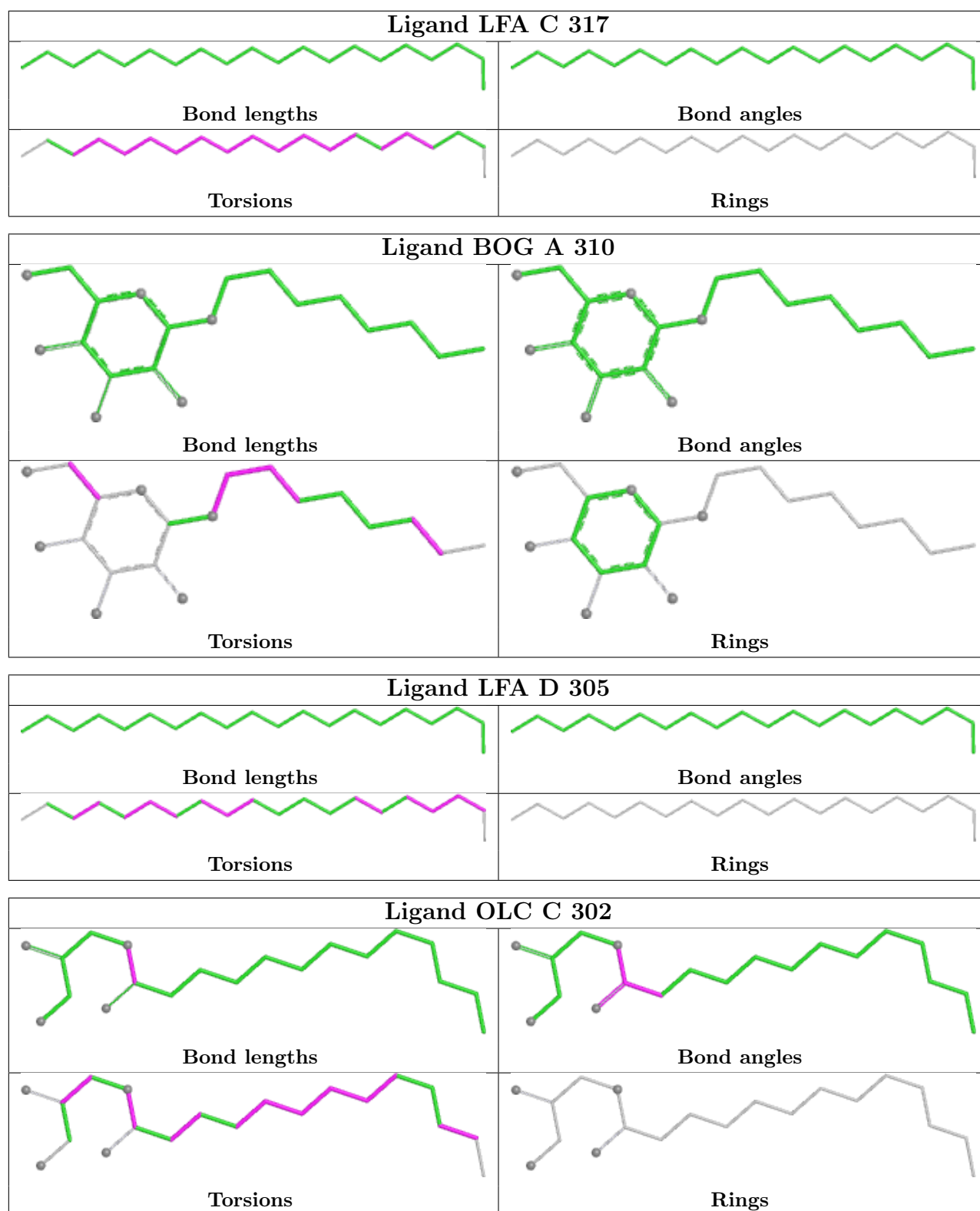


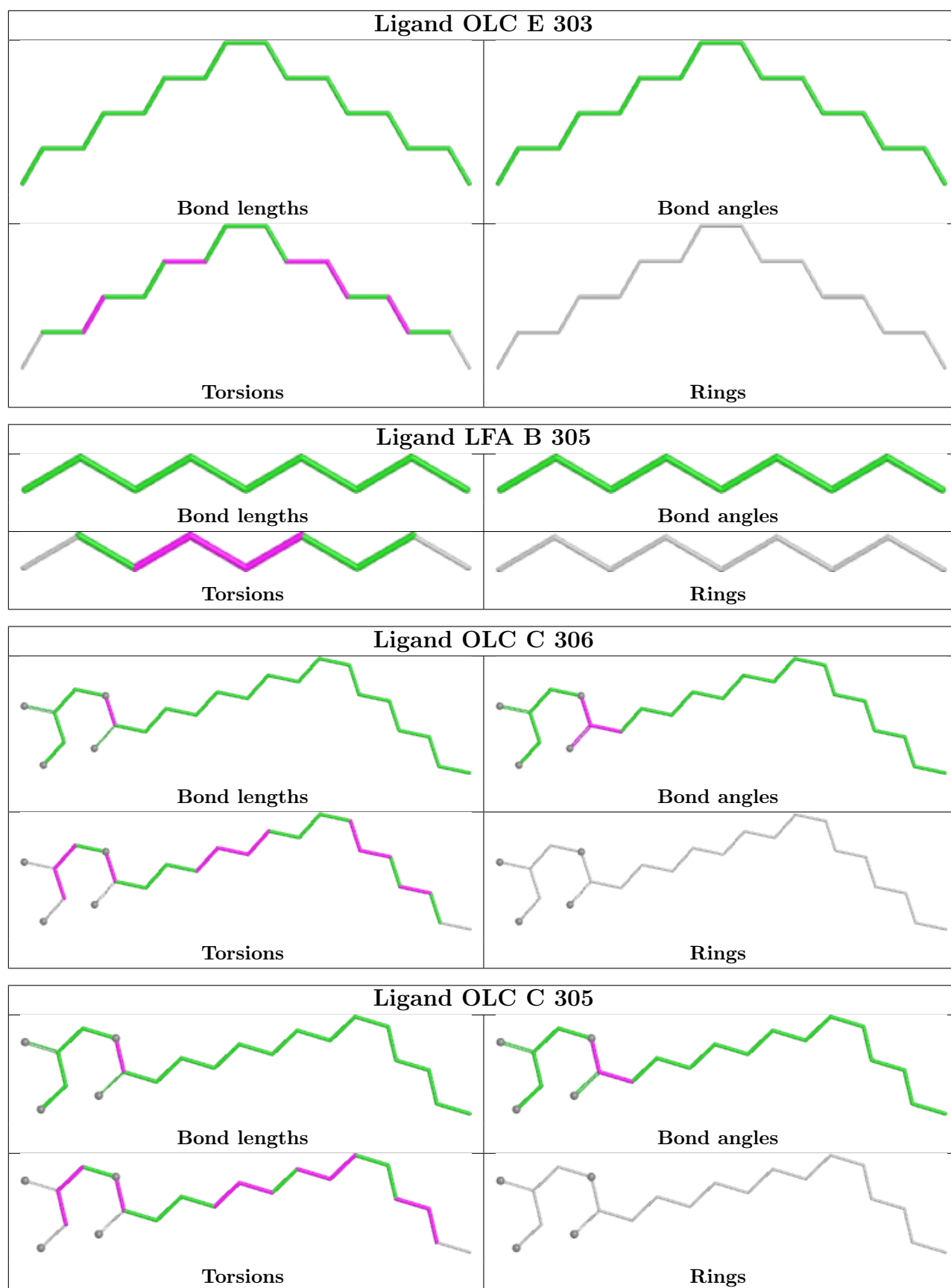


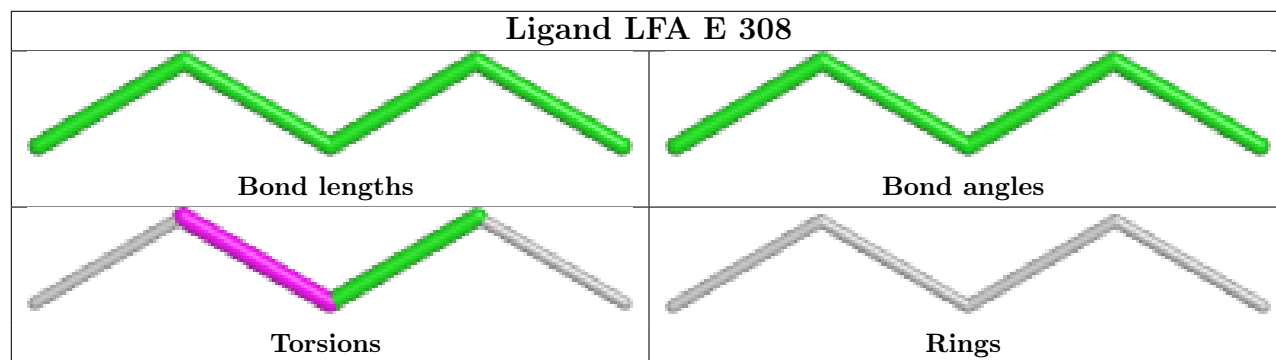
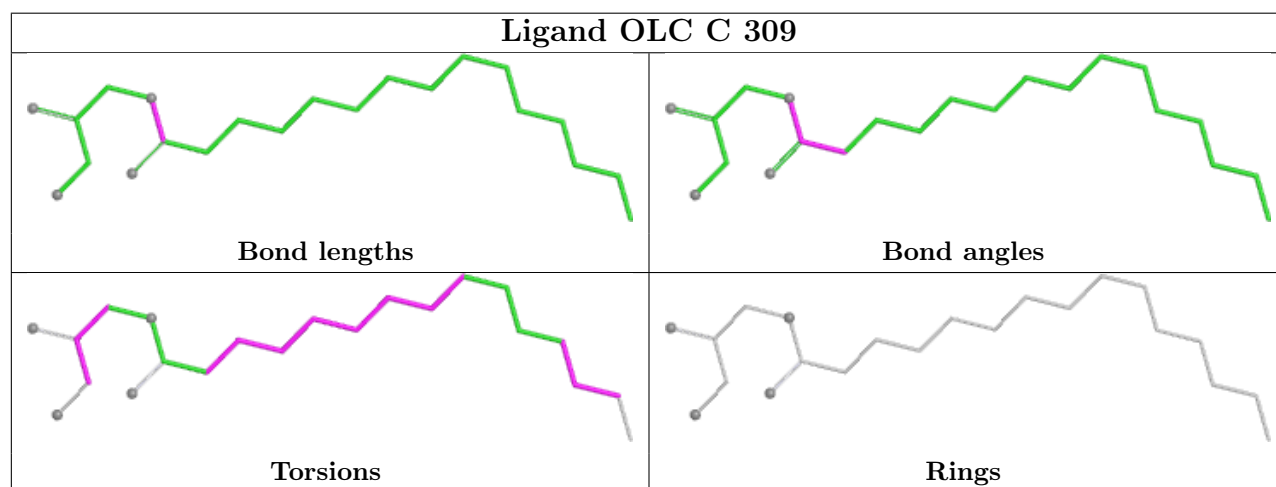
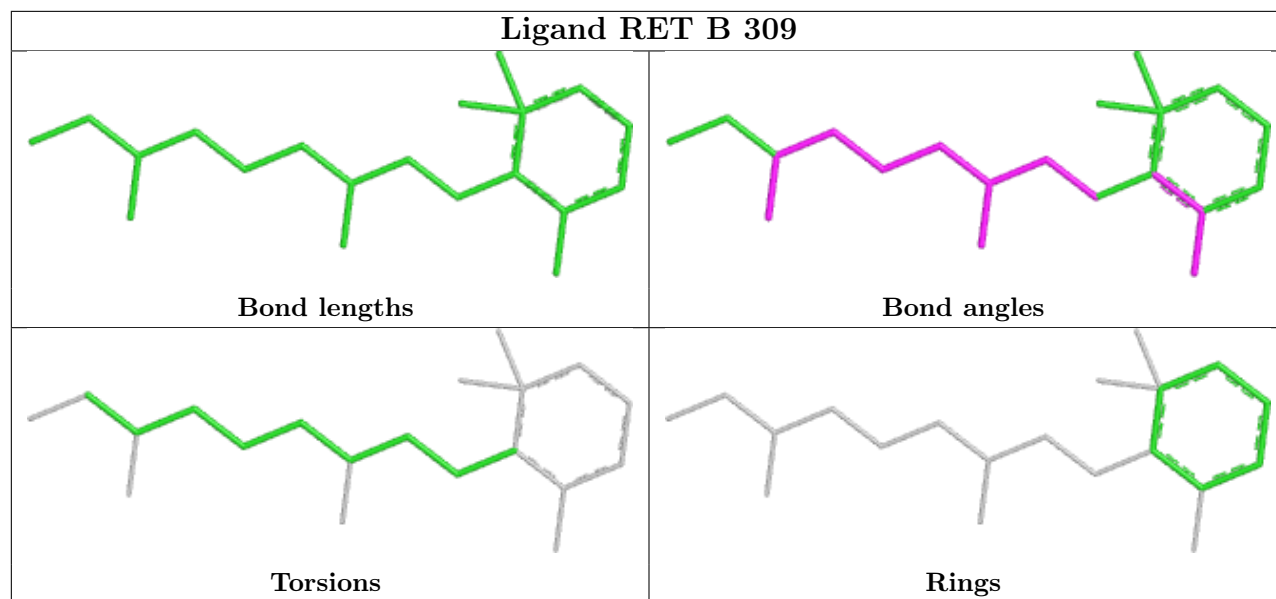


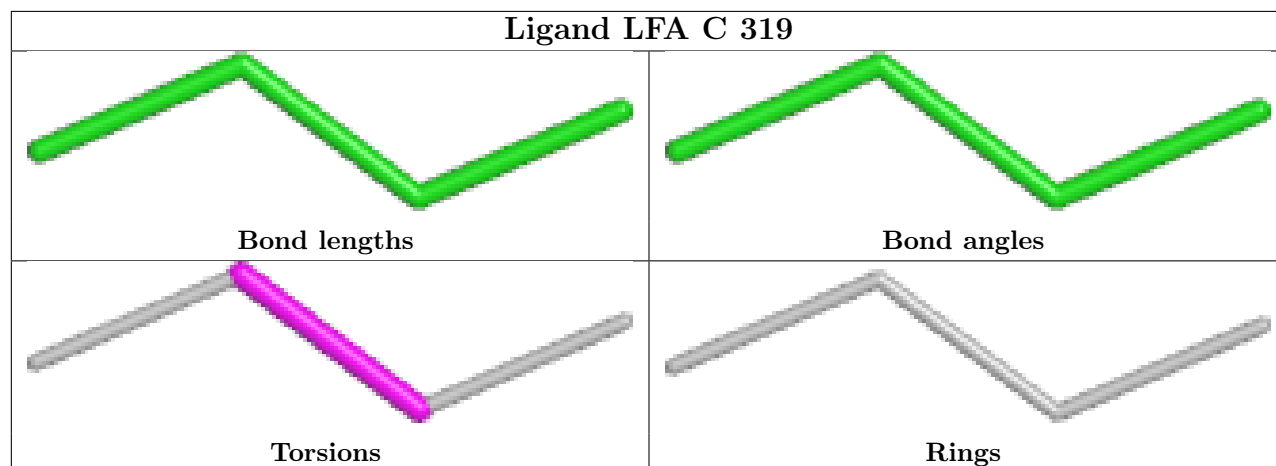
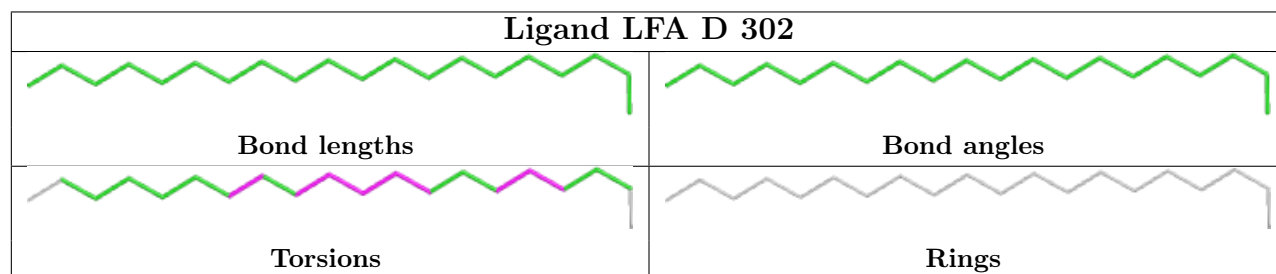
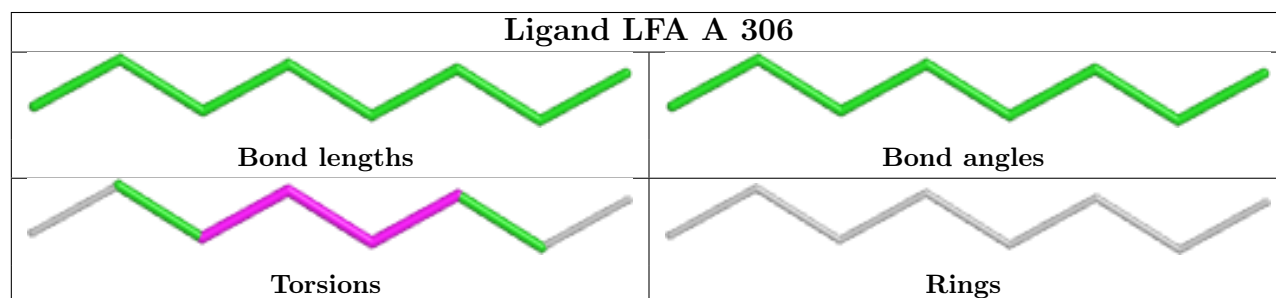
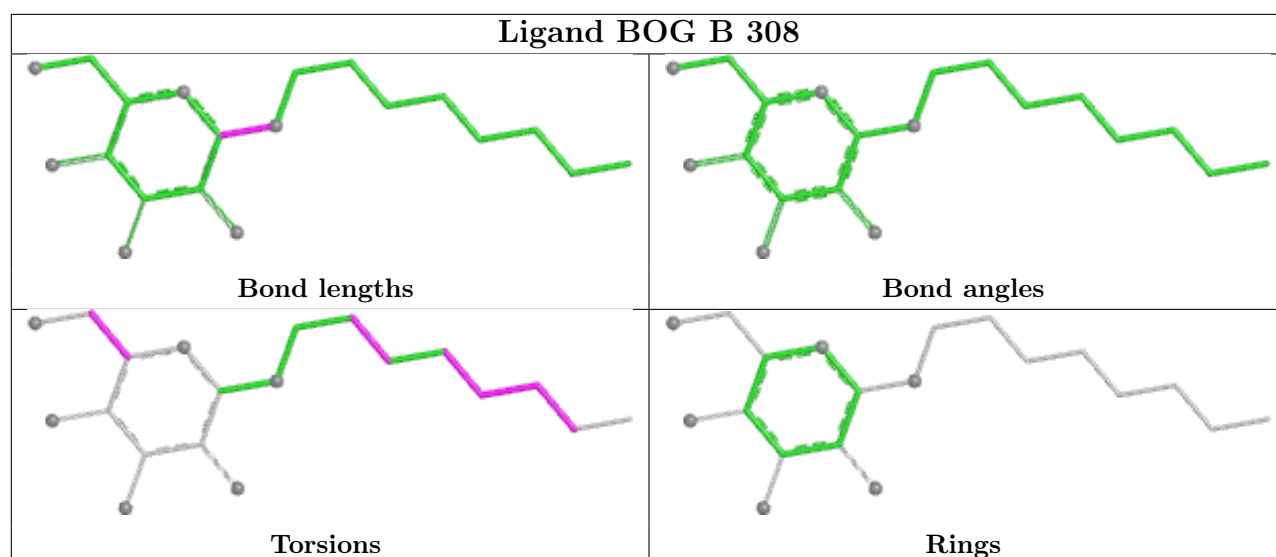


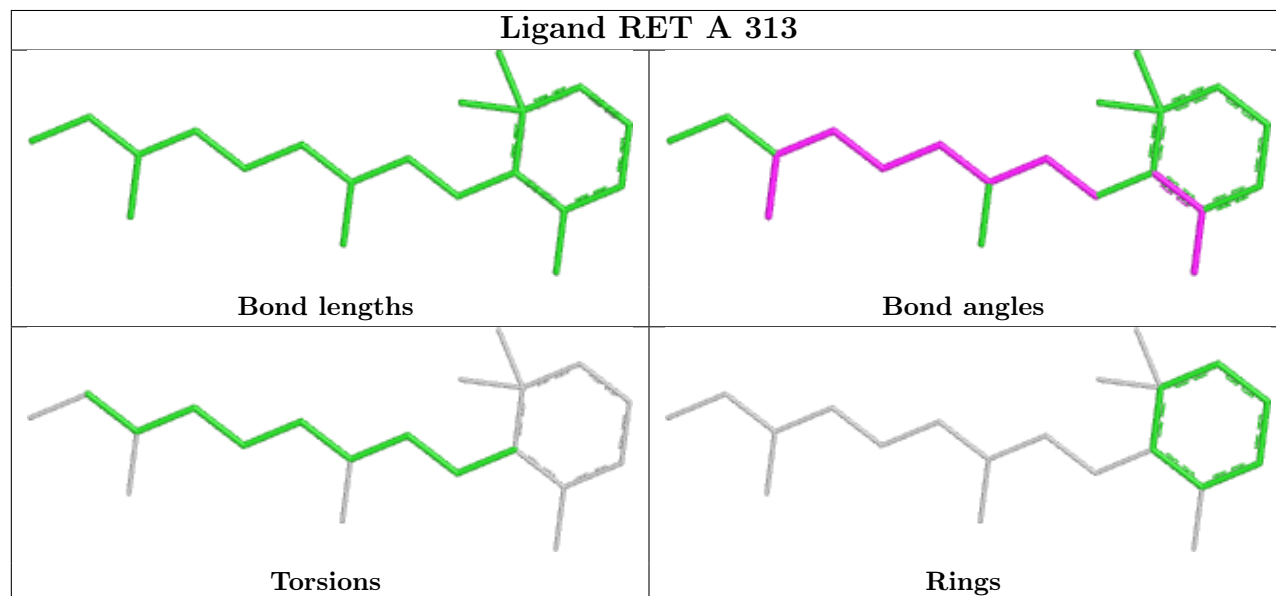
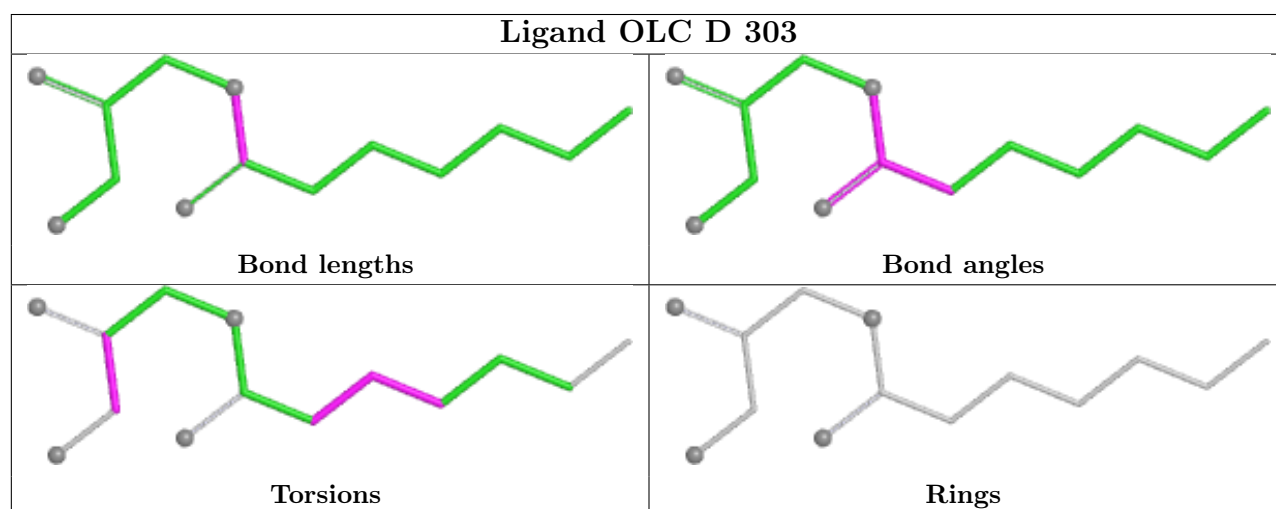
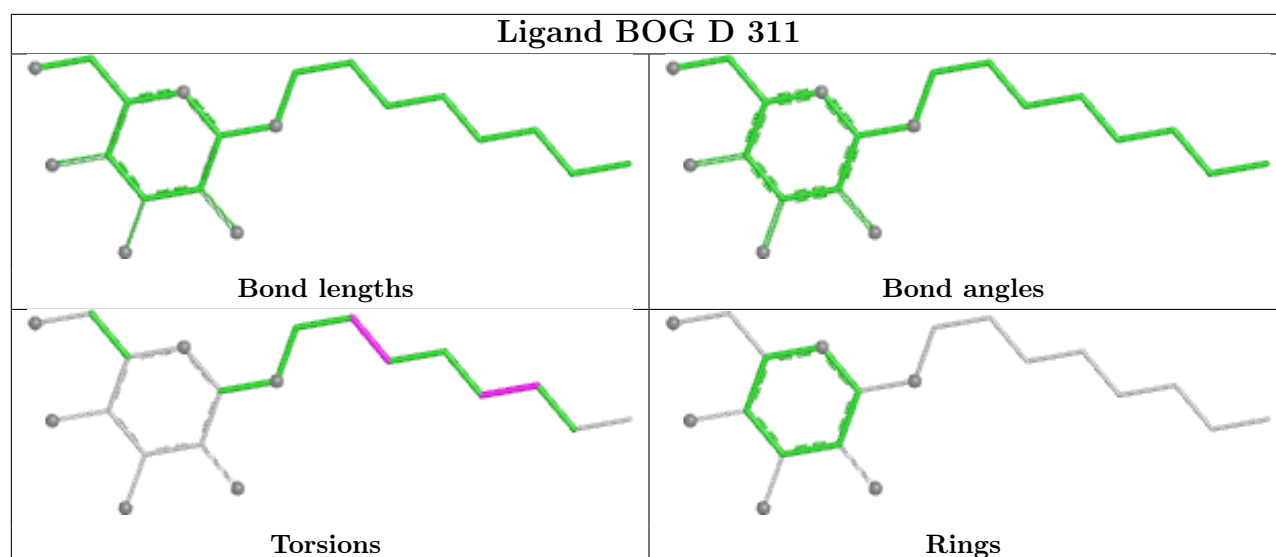


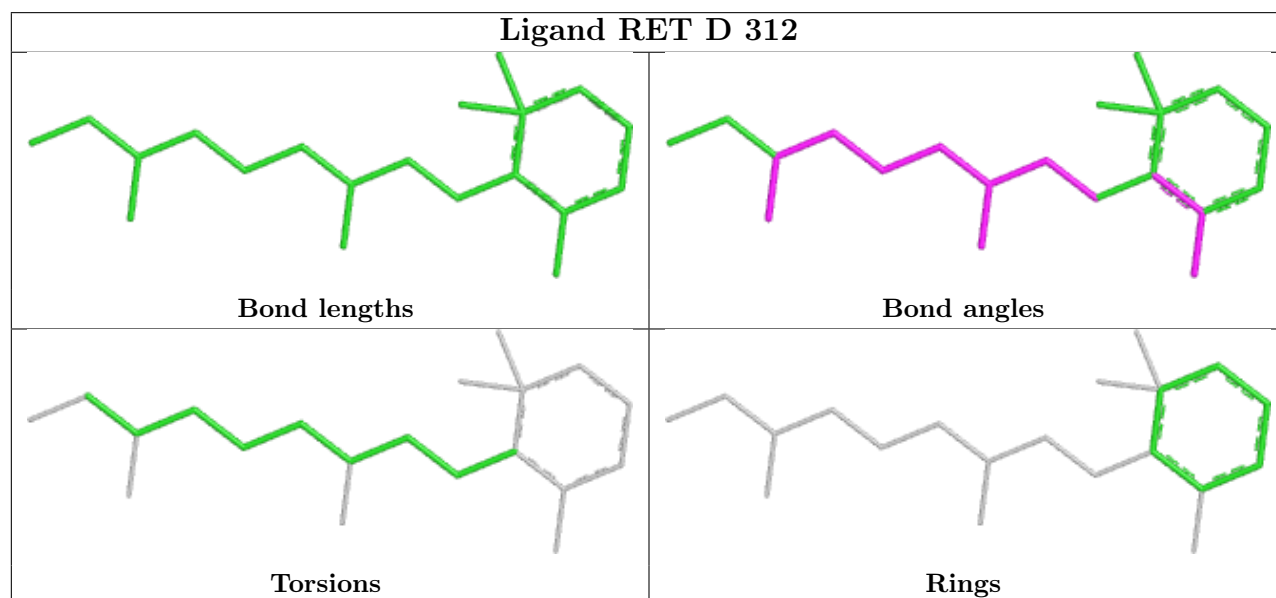
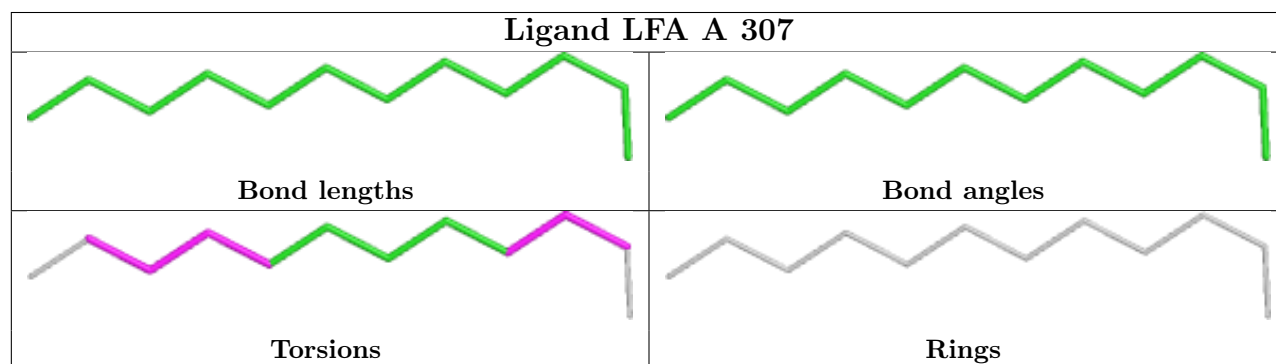
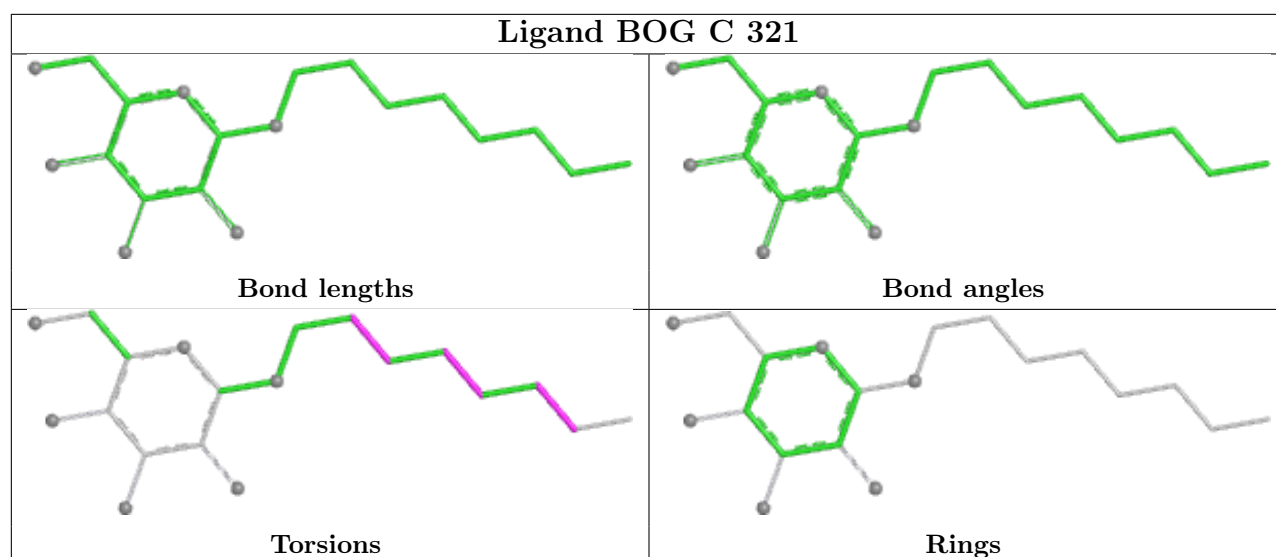


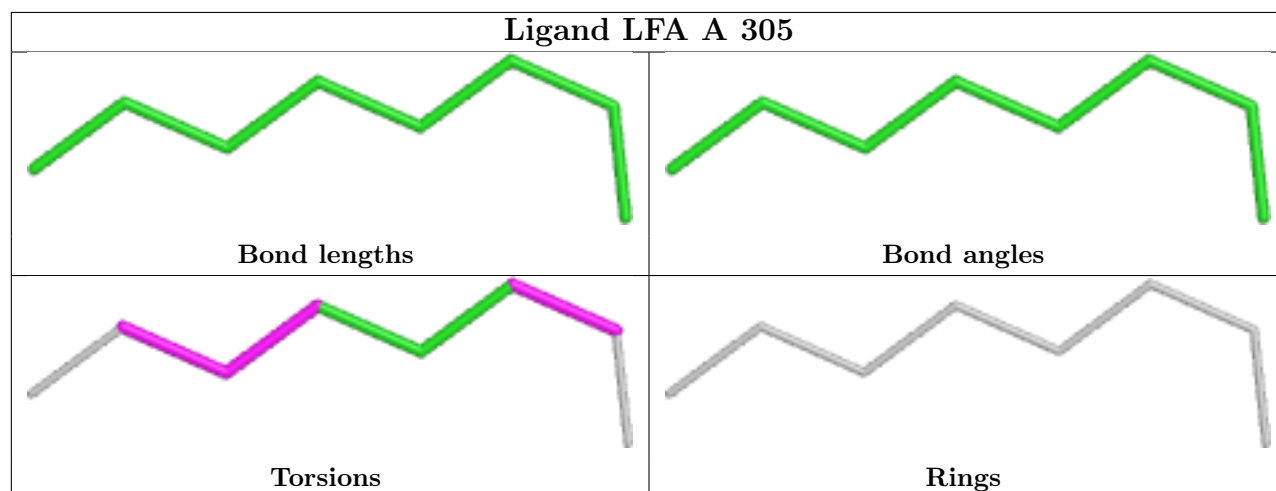
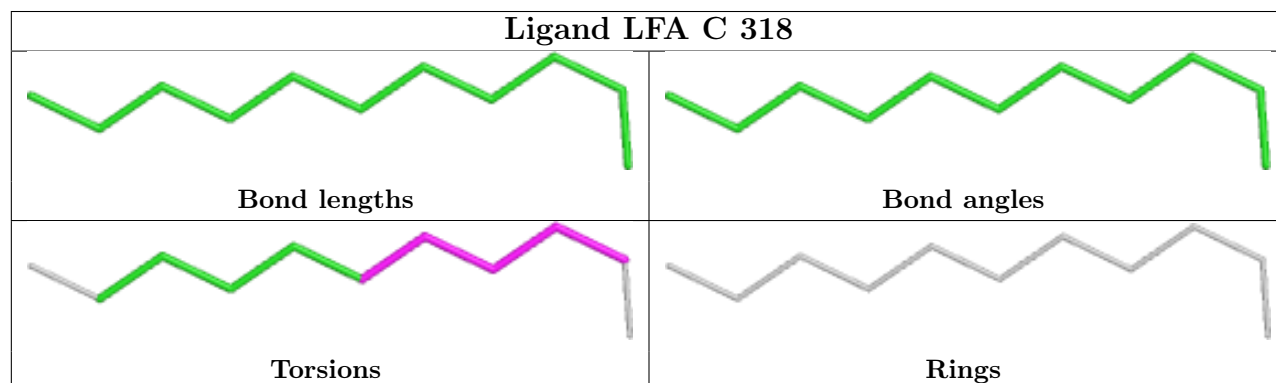
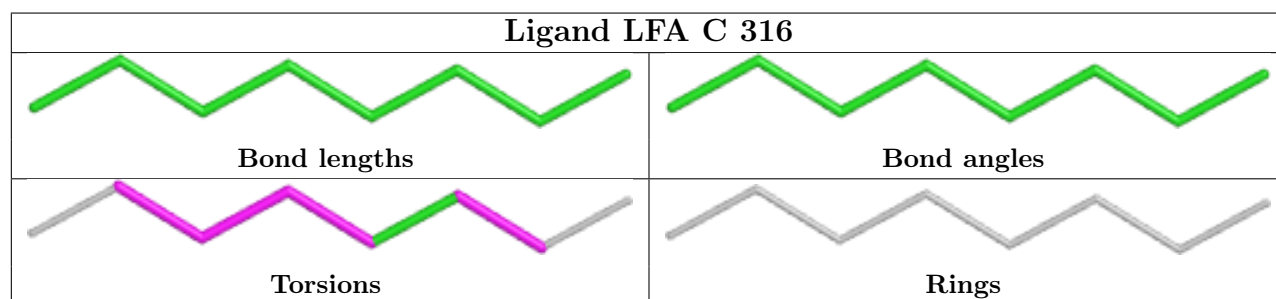
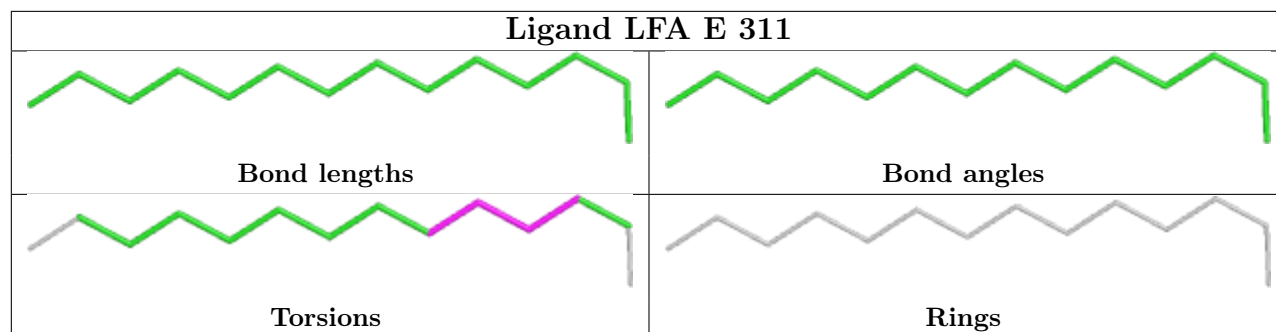


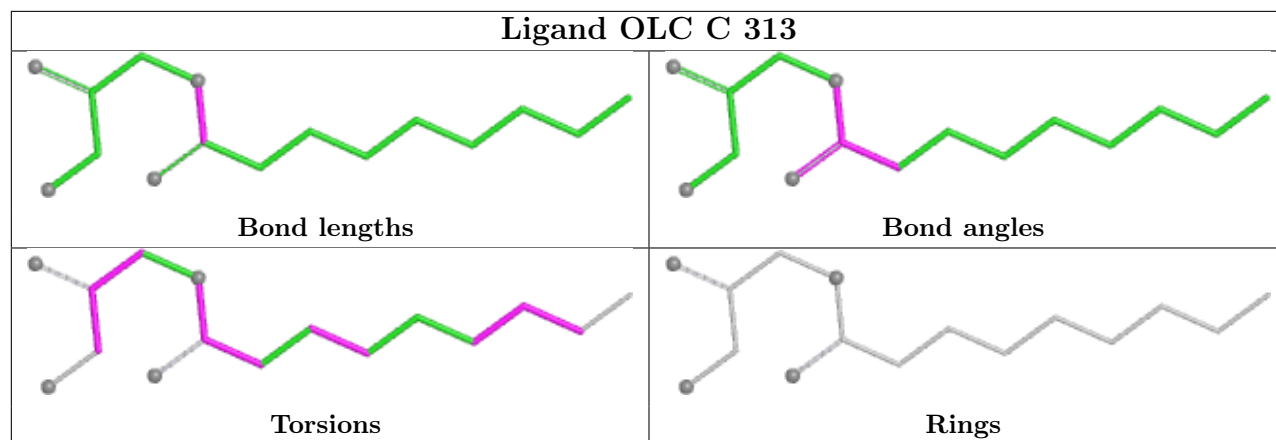












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	273/288 (94%)	0.06	9 (3%) 49 45	19, 48, 73, 154	1 (0%)
1	B	273/288 (94%)	0.16	16 (5%) 28 24	21, 48, 69, 139	1 (0%)
1	C	273/288 (94%)	0.05	12 (4%) 39 34	21, 48, 71, 152	1 (0%)
1	D	273/288 (94%)	0.11	18 (6%) 24 20	19, 50, 75, 164	1 (0%)
1	E	273/288 (94%)	0.06	12 (4%) 39 34	20, 48, 71, 169	1 (0%)
All	All	1365/1440 (94%)	0.09	67 (4%) 35 31	19, 48, 73, 169	5 (0%)

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	GLN	5.8
1	C	91	GLU	4.8
1	E	275	LEU	4.7
1	E	274	GLU	4.7
1	E	3	GLN	4.6

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

median, 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
3	LFA	D	309	6/20	0.68	0.32	80,90,93,94	0
5	BOG	B	308	20/20	0.70	0.23	80,101,109,114	0
2	OLC	C	310	16/25	0.72	0.23	91,111,137,138	0
3	LFA	B	305	9/20	0.73	0.36	82,90,110,112	0
3	LFA	C	322	4/20	0.73	0.29	72,76,78,80	0
3	LFA	C	315	7/20	0.74	0.30	75,94,106,109	0
2	OLC	C	304	14/25	0.74	0.23	95,118,144,157	0
3	LFA	E	302	20/20	0.76	0.27	61,81,101,101	0
3	LFA	C	303	20/20	0.76	0.26	59,77,86,88	0
3	LFA	A	307	12/20	0.77	0.30	89,102,110,113	0
3	LFA	B	302	20/20	0.77	0.24	60,77,100,103	0
3	LFA	D	302	20/20	0.77	0.22	54,69,89,89	0
3	LFA	A	312	20/20	0.78	0.25	64,80,91,95	0
5	BOG	A	310	20/20	0.79	0.18	81,101,112,115	0
5	BOG	E	310	20/20	0.79	0.16	71,98,112,112	0
3	LFA	A	305	8/20	0.80	0.32	77,87,92,94	0
2	OLC	C	307	25/25	0.80	0.21	74,104,118,129	0
3	LFA	E	311	14/20	0.81	0.32	102,117,127,133	0
3	LFA	D	308	7/20	0.81	0.26	74,89,98,102	0
2	OLC	C	311	25/25	0.81	0.23	87,111,133,135	0
2	OLC	C	308	25/25	0.81	0.22	67,101,124,139	0
3	LFA	D	304	20/20	0.82	0.28	81,102,113,115	0
3	LFA	A	304	7/20	0.83	0.29	79,84,94,99	0
3	LFA	C	319	4/20	0.83	0.24	78,78,78,87	0
2	OLC	B	303	20/25	0.84	0.17	69,87,106,107	0
3	LFA	E	307	4/20	0.84	0.28	67,72,78,78	0
3	LFA	C	318	11/20	0.84	0.32	65,99,118,118	0
3	LFA	C	316	8/20	0.85	0.26	76,89,94,97	0
3	LFA	E	306	14/20	0.85	0.27	73,95,106,109	0
3	LFA	D	306	8/20	0.85	0.30	81,95,117,120	0
3	LFA	E	308	5/20	0.85	0.32	78,90,101,103	0
2	OLC	A	311	14/25	0.86	0.24	67,82,92,92	0
2	OLC	C	309	22/25	0.86	0.16	60,90,121,126	0
2	OLC	E	303	16/25	0.86	0.20	56,64,80,83	0
5	BOG	C	321	20/20	0.86	0.13	71,88,104,105	0
3	LFA	C	317	20/20	0.86	0.26	73,92,103,108	0
2	OLC	E	304	25/25	0.87	0.20	55,96,127,129	0
2	OLC	A	303	15/25	0.87	0.19	64,83,106,117	0
2	OLC	C	314	16/25	0.87	0.26	79,100,117,128	0
3	LFA	B	306	8/20	0.87	0.27	76,86,100,105	0
3	LFA	A	306	8/20	0.87	0.30	70,93,119,125	0

*Continued on next page...*

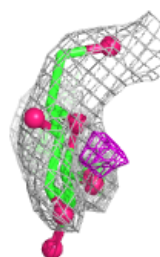
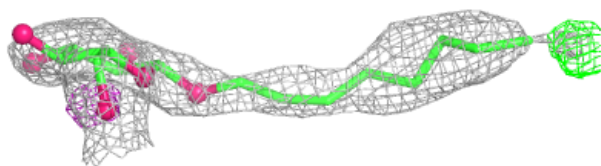
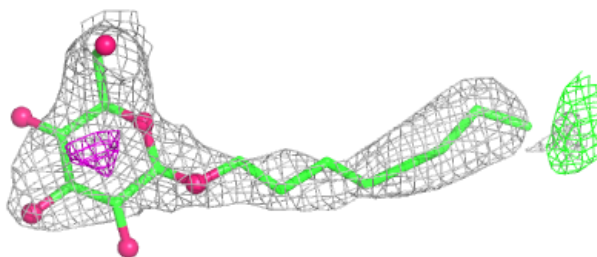
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LFA	E	305	8/20	0.87	0.28	80,86,90,92	0
5	BOG	D	311	20/20	0.87	0.15	75,96,104,105	0
2	OLC	B	301	22/25	0.87	0.18	76,85,104,111	0
2	OLC	A	302	13/25	0.88	0.13	67,74,85,88	0
2	OLC	B	304	16/25	0.88	0.17	66,89,96,108	0
2	OLC	A	301	14/25	0.88	0.18	54,64,73,73	0
2	OLC	C	312	16/25	0.89	0.15	62,83,96,101	0
2	OLC	C	305	21/25	0.89	0.22	90,116,139,140	0
2	OLC	D	303	14/25	0.89	0.16	61,82,100,102	0
3	LFA	D	305	20/20	0.90	0.24	83,103,113,115	0
2	OLC	C	313	16/25	0.90	0.17	58,99,118,123	0
2	OLC	E	301	12/25	0.90	0.21	65,76,88,92	0
3	LFA	A	308	6/20	0.90	0.20	68,71,79,86	0
2	OLC	C	302	20/25	0.90	0.16	71,91,100,101	0
3	LFA	D	307	17/20	0.93	0.14	56,65,77,77	0
2	OLC	C	301	21/25	0.94	0.14	55,72,89,104	0
6	RET	B	309	20/21	0.94	0.09	40,45,50,52	0
6	RET	E	312	20/21	0.94	0.10	37,44,48,49	0
2	OLC	C	306	23/25	0.95	0.14	59,73,107,144	0
6	RET	D	312	20/21	0.95	0.09	44,52,59,64	0
2	OLC	D	301	18/25	0.95	0.13	79,91,107,119	0
6	RET	C	323	20/21	0.96	0.08	42,49,55,56	0
4	NA	D	310	1/1	0.97	0.05	46,46,46,46	0
6	RET	A	313	20/21	0.97	0.08	37,47,51,52	0
4	NA	A	309	1/1	0.98	0.04	47,47,47,47	0
4	NA	E	309	1/1	0.98	0.04	38,38,38,38	0
4	NA	B	307	1/1	0.99	0.04	41,41,41,41	0
4	NA	C	320	1/1	1.00	0.03	40,40,40,40	0

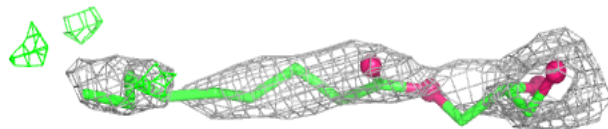
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BOG B 308:**

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

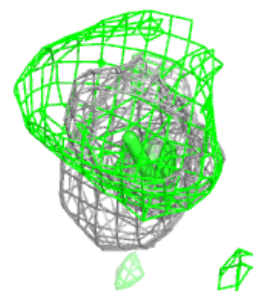
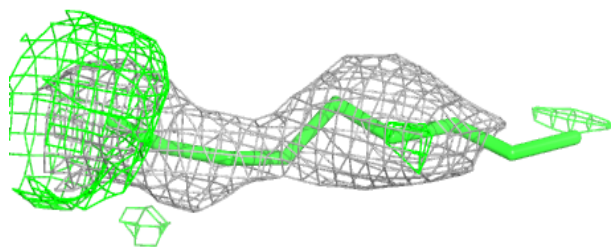
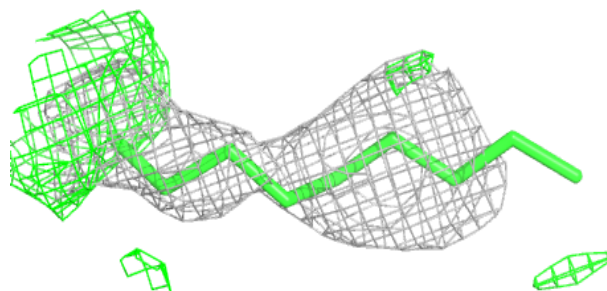
**Electron density around OLC C 310:**

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

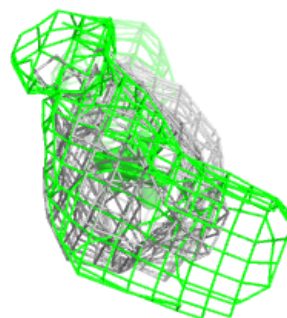
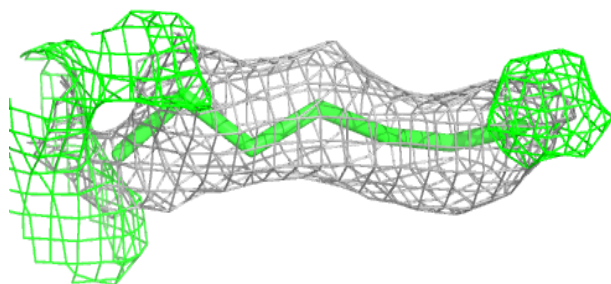
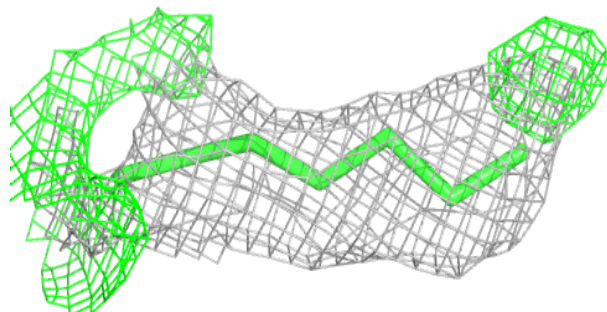


**Electron density around LFA B 305:**

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

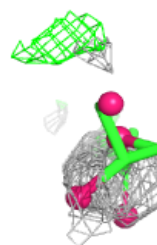
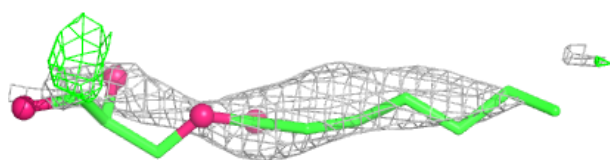
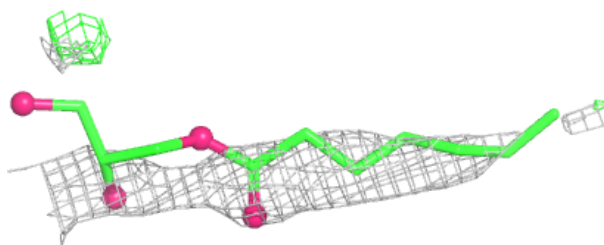
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

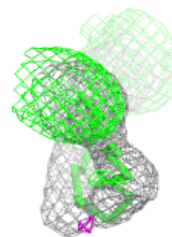
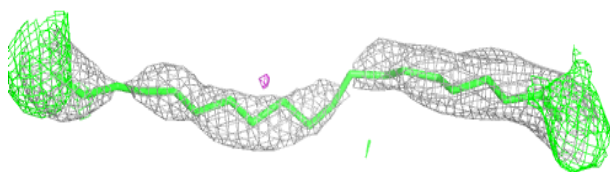
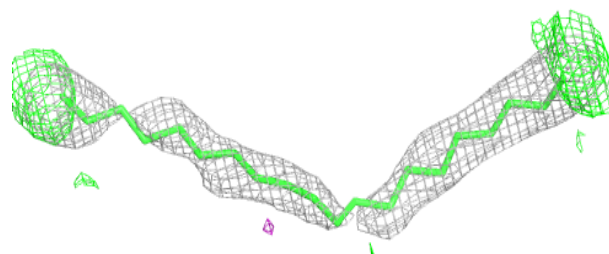


**Electron density around OLC C 304:**

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

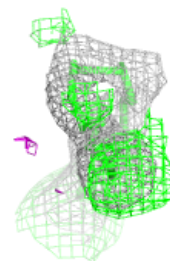
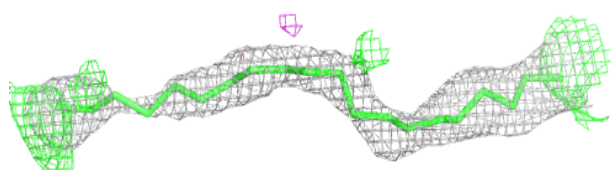
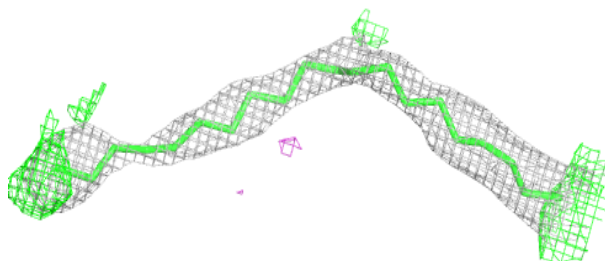
**Electron density around LFA E 302:**

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

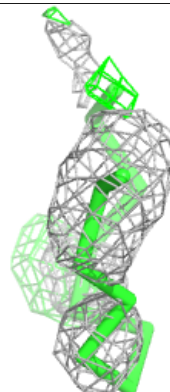
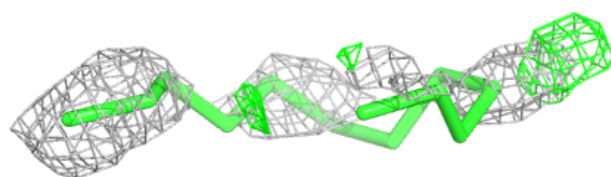


**Electron density around LFA C 303:**

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

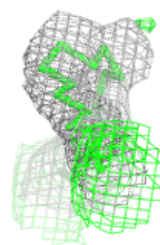
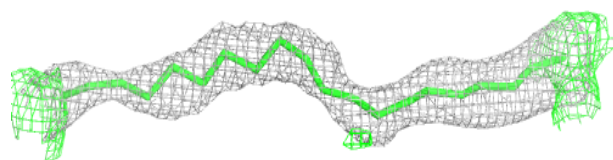
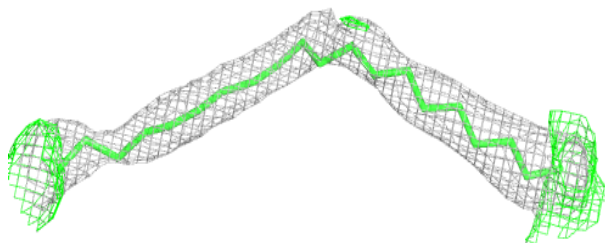
**Electron density around LFA A 307:**

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and green (positive)

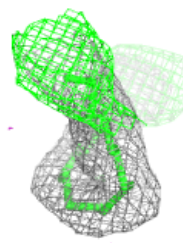
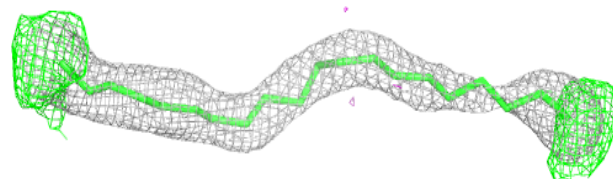
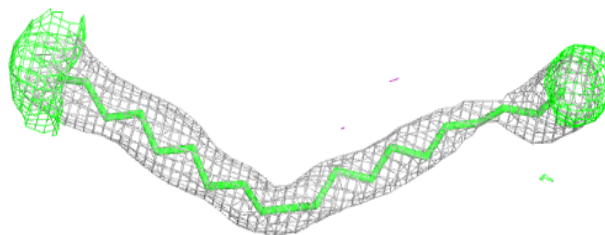


**Electron density around LFA B 302:**

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

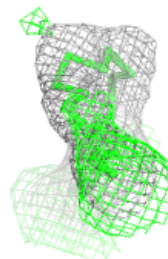
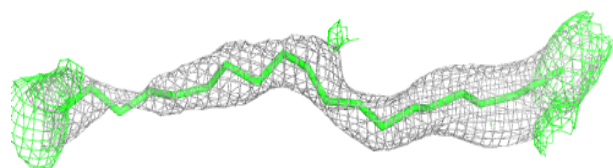
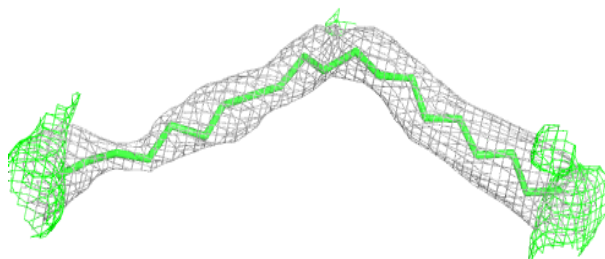
**Electron density around LFA D 302:**

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

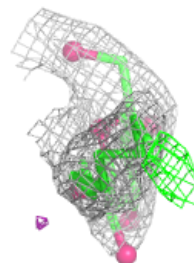
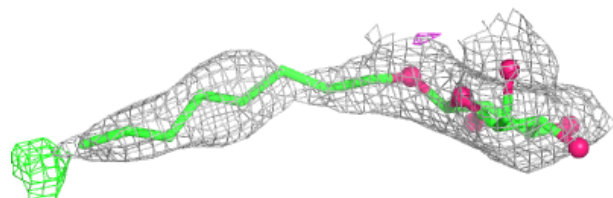
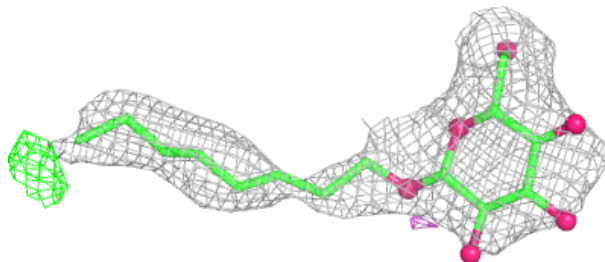


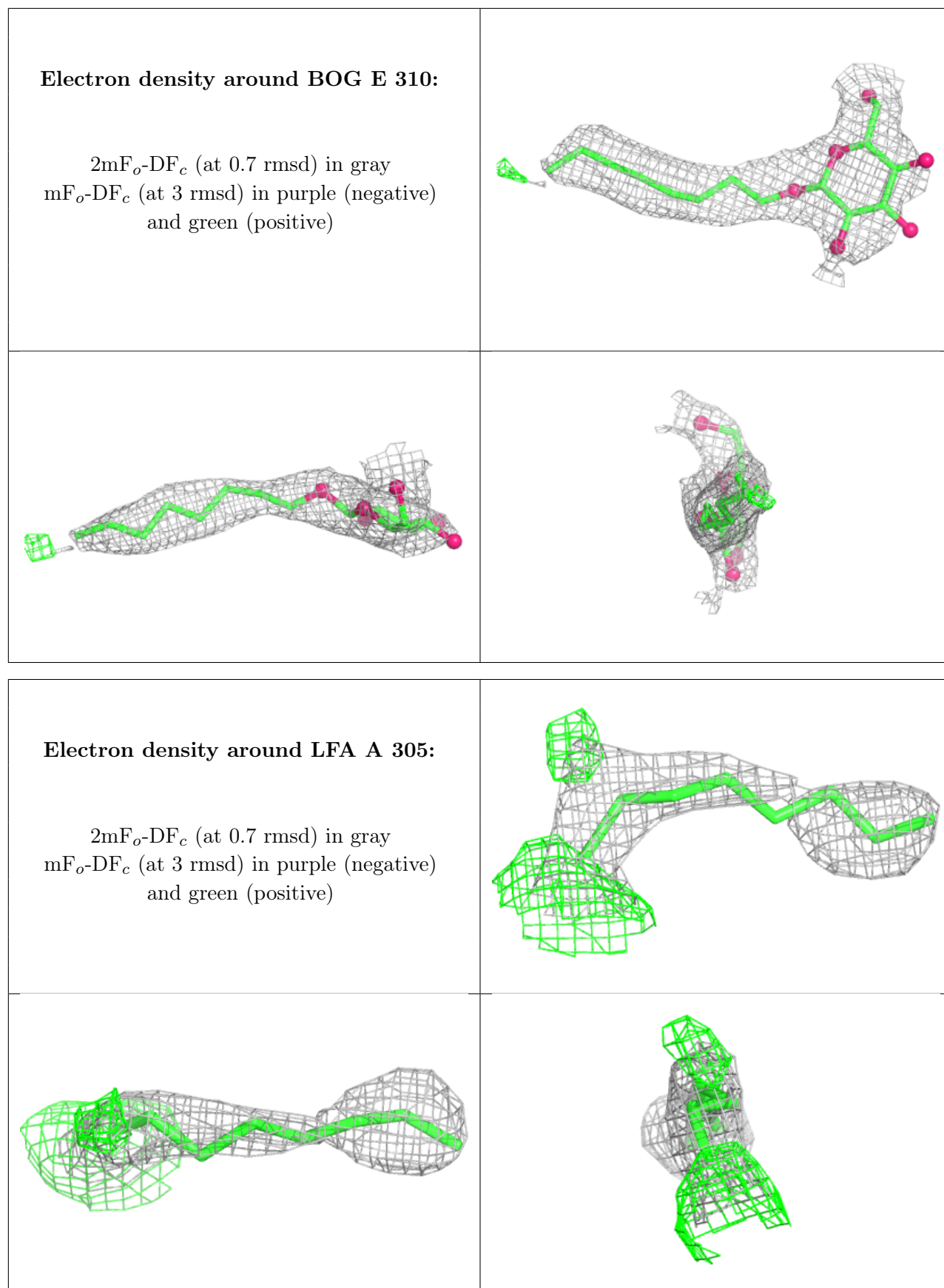
**Electron density around LFA A 312:**

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

**Electron density around BOG A 310:**

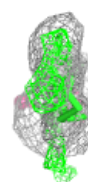
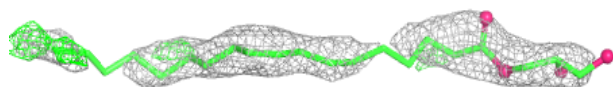
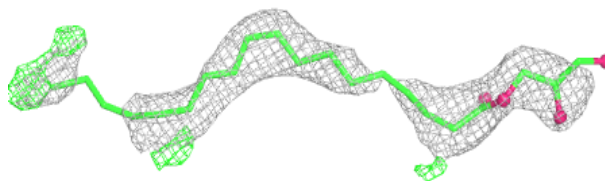
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



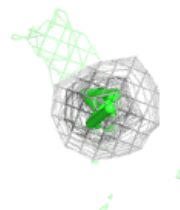
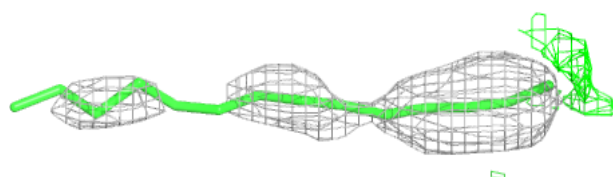
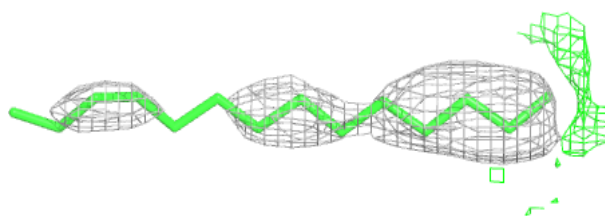


**Electron density around OLC C 307:**

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

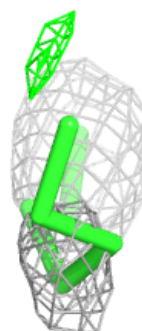
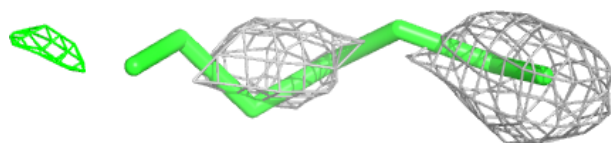
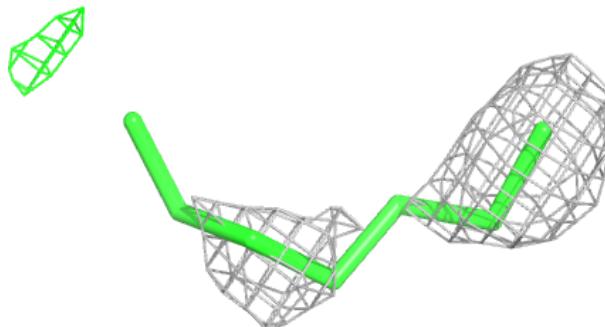
**Electron density around LFA E 311:**

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

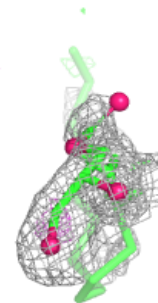
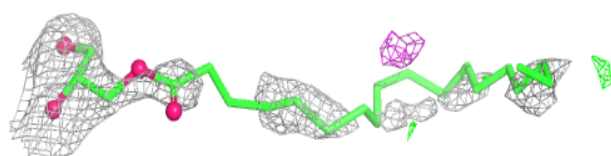
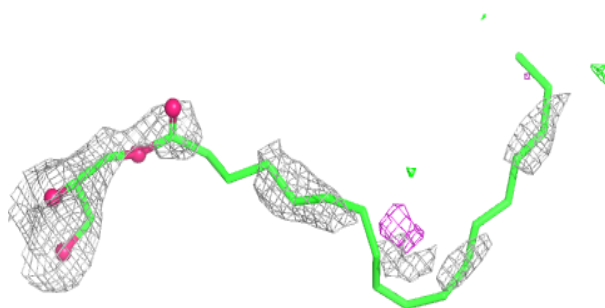


**Electron density around LFA D 308:**

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

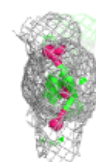
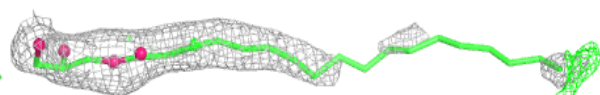
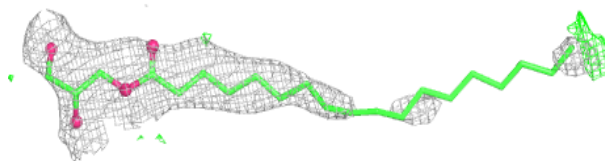
**Electron density around OLC C 311:**

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

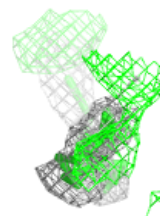
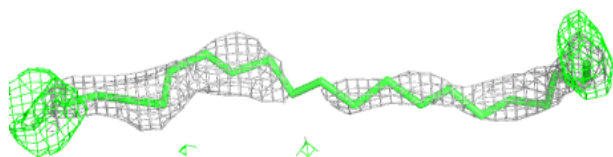
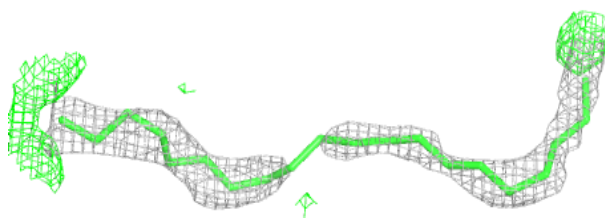


**Electron density around OLC C 308:**

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

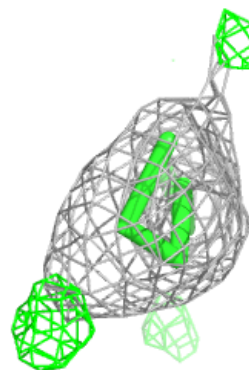
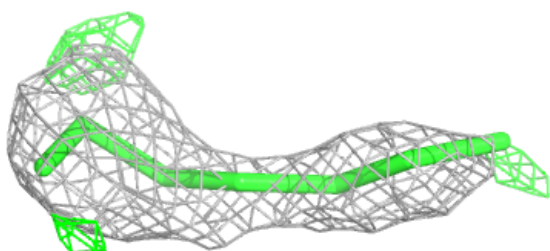
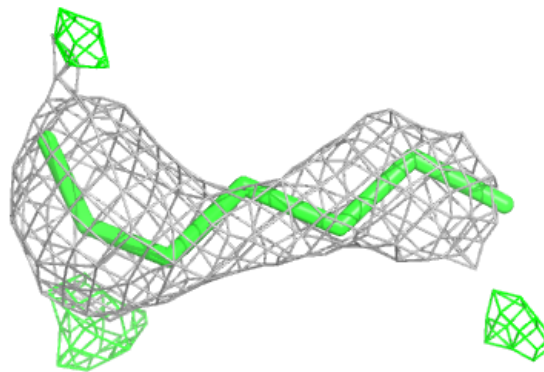
**Electron density around LFA D 304:**

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



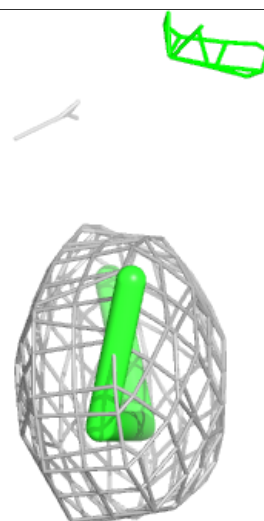
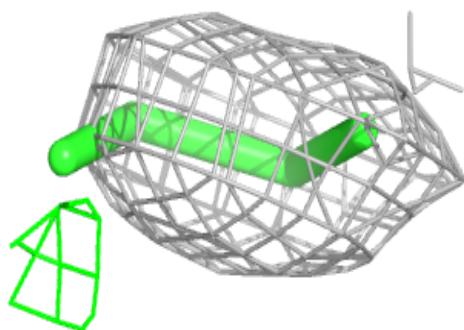
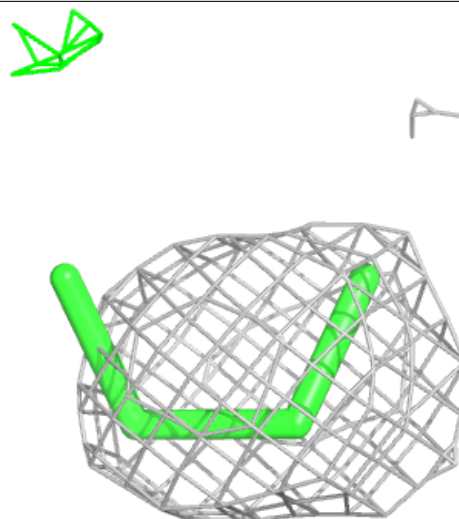
**Electron density around LFA A 304:**

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



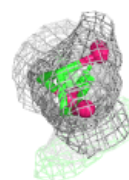
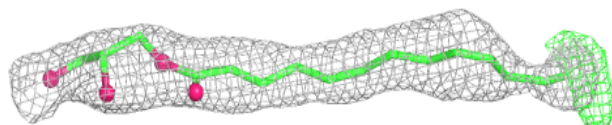
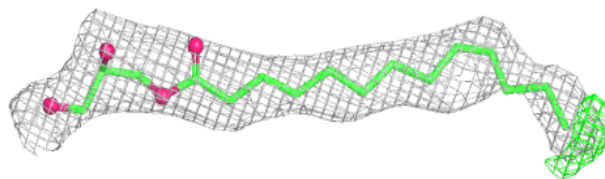
**Electron density around LFA C 319:**

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



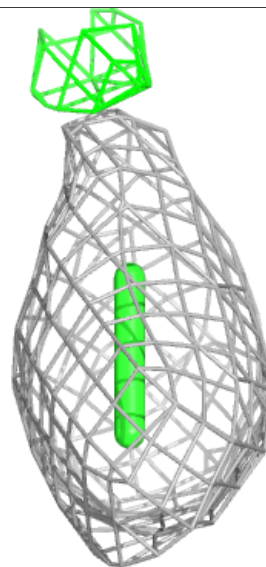
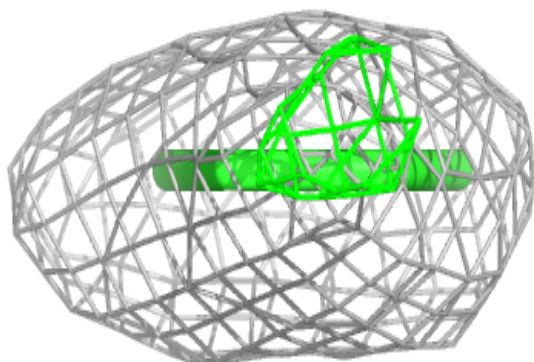
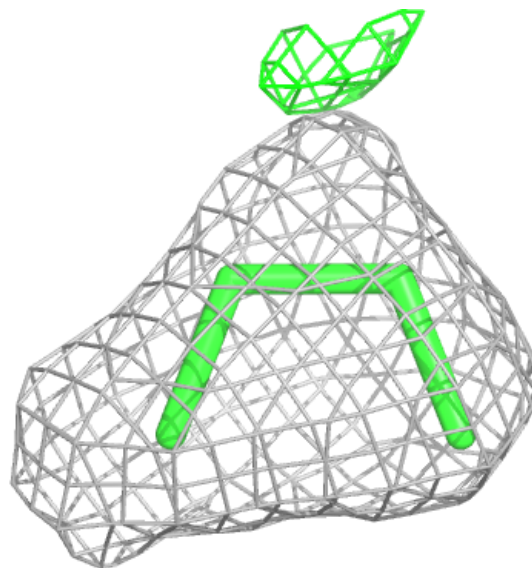
**Electron density around OLC B 303:**

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



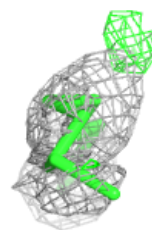
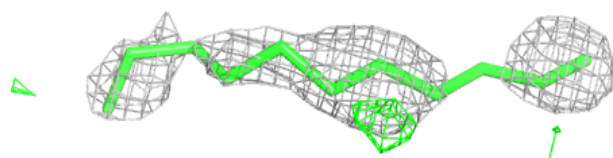
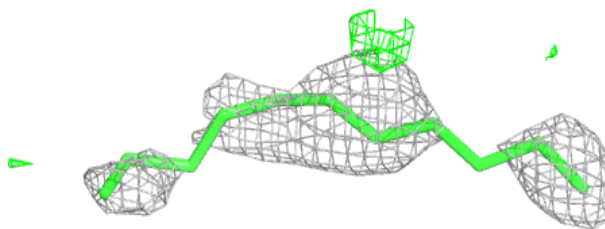
**Electron density around LFA E 307:**

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

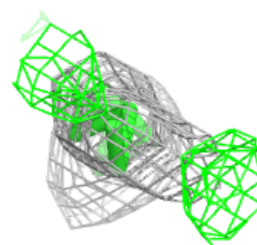
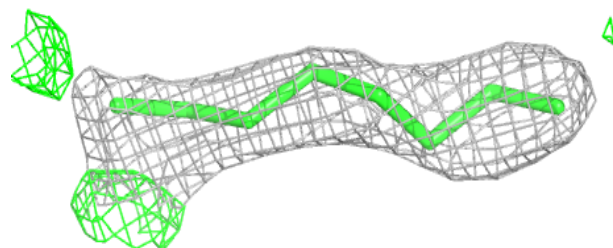
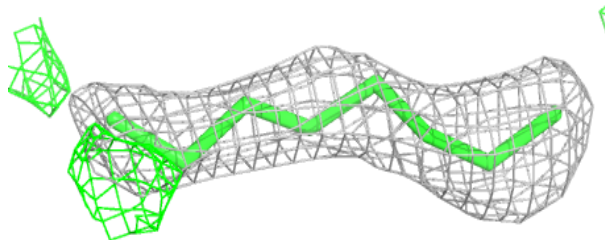


**Electron density around LFA C 318:**

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

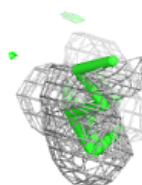
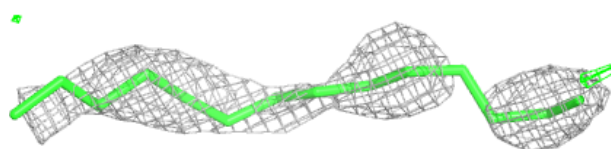
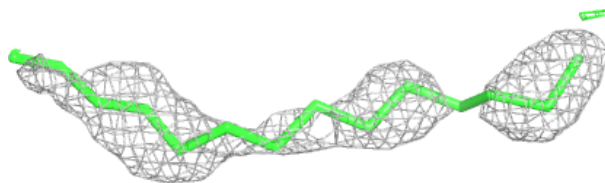
**Electron density around LFA C 316:**

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

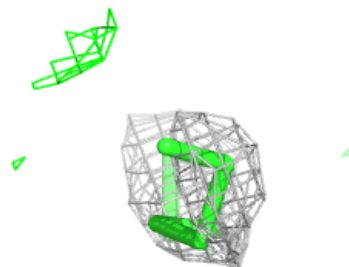
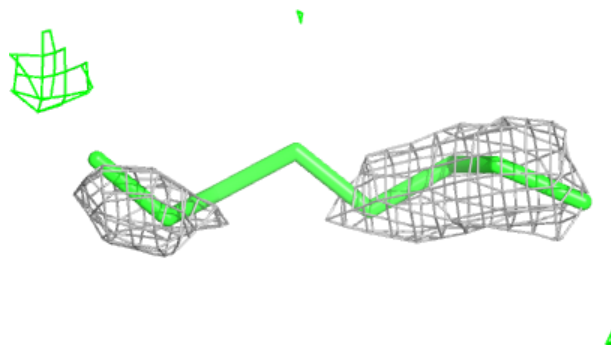
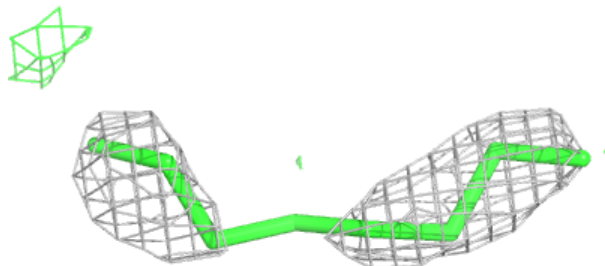


**Electron density around LFA E 306:**

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

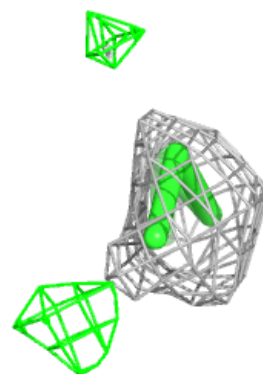
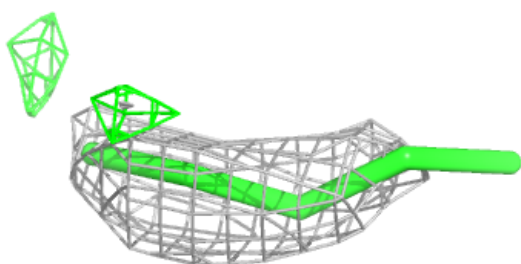
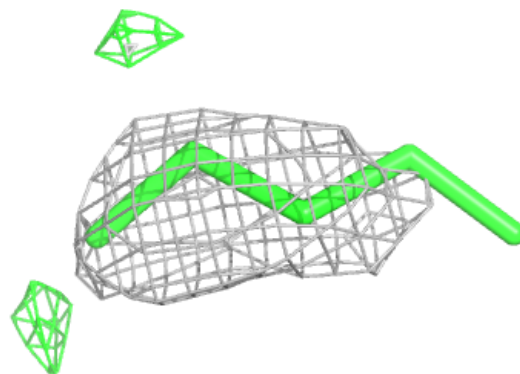
**Electron density around LFA D 306:**

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

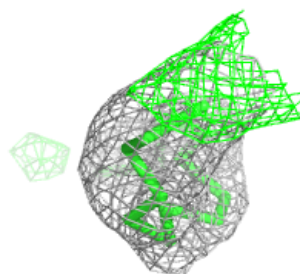
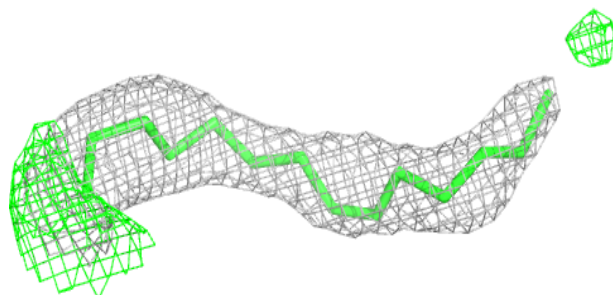
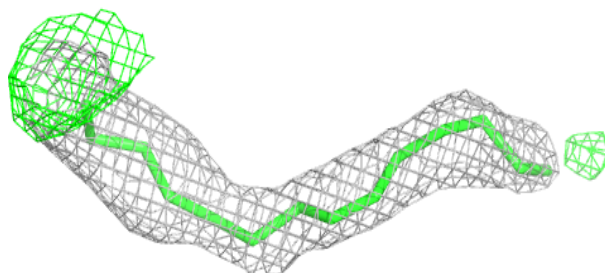


**Electron density around LFA E 308:**

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

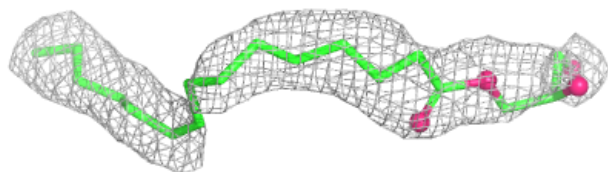
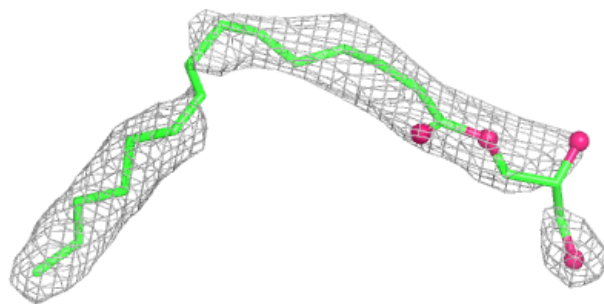
**Electron density around OLC A 311:**

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

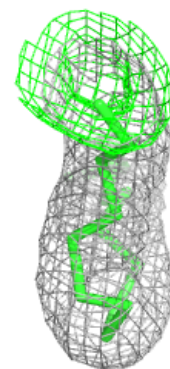
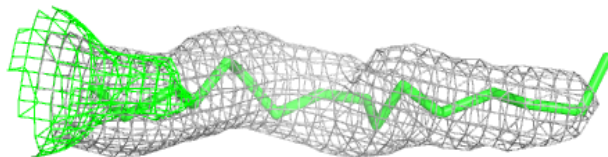
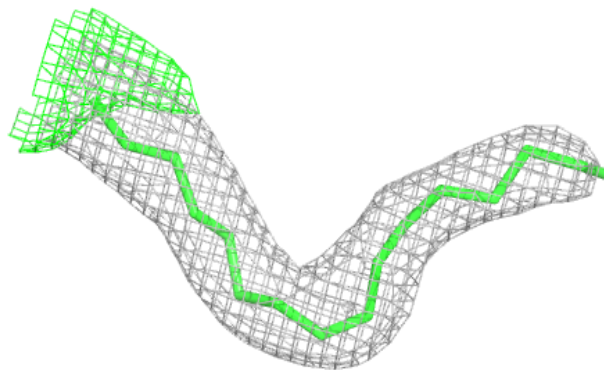


**Electron density around OLC C 309:**

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

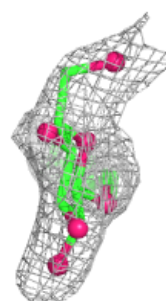
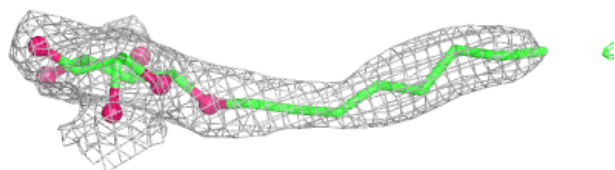
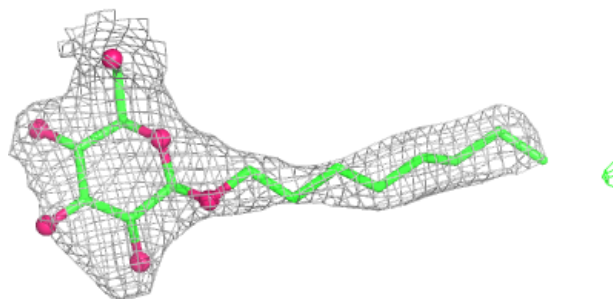
**Electron density around OLC E 303:**

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

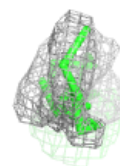
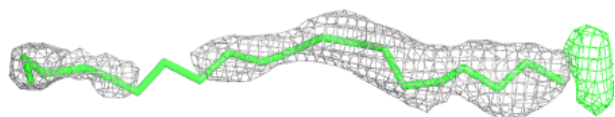
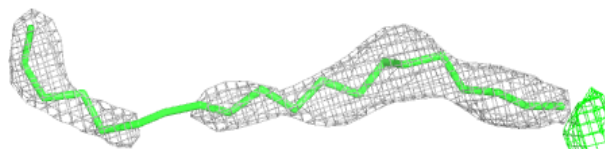


**Electron density around BOG C 321:**

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

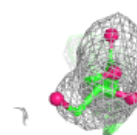
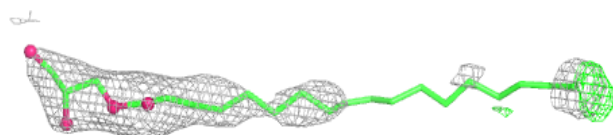
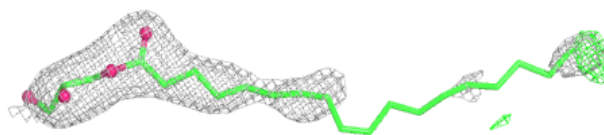
**Electron density around LFA C 317:**

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

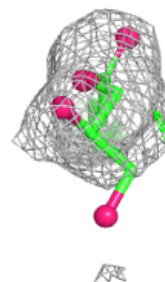
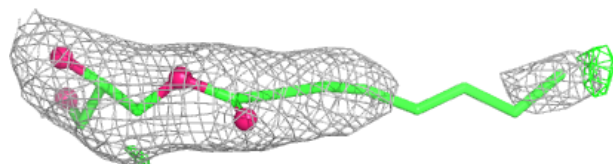
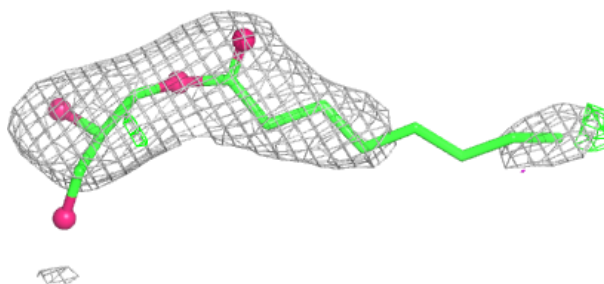


**Electron density around OLC E 304:**

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

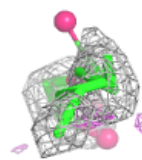
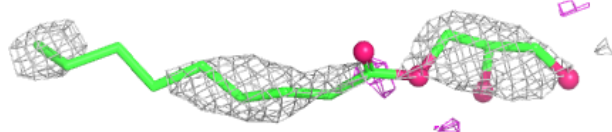
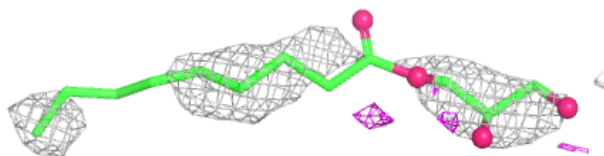
**Electron density around OLC A 303:**

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

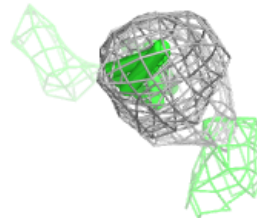
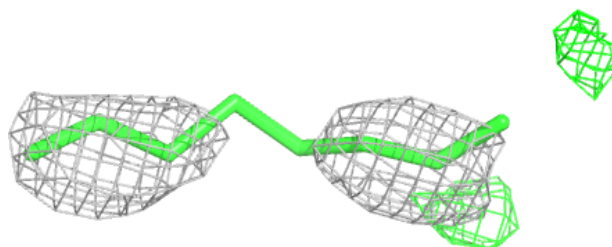
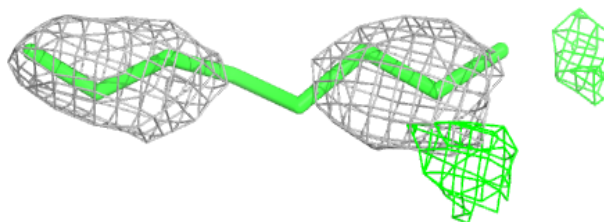


**Electron density around OLC C 314:**

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

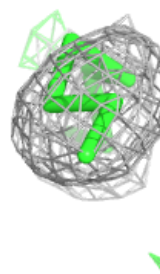
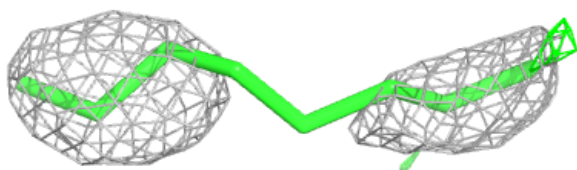
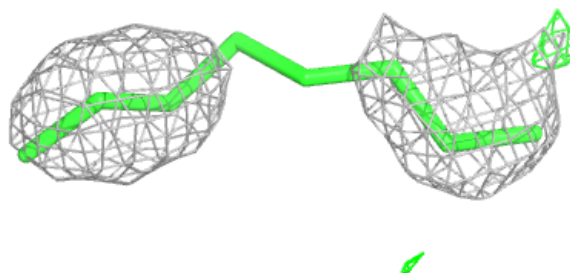
**Electron density around LFA B 306:**

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

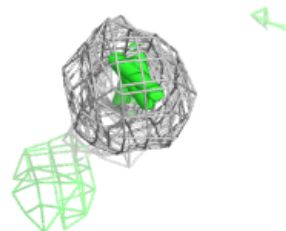
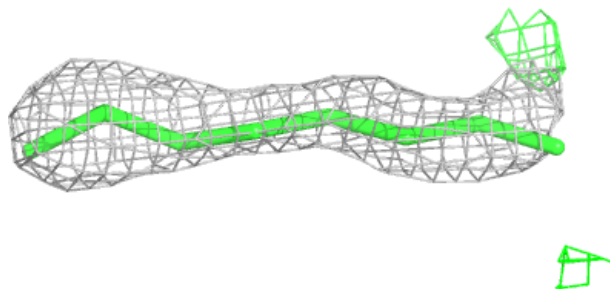
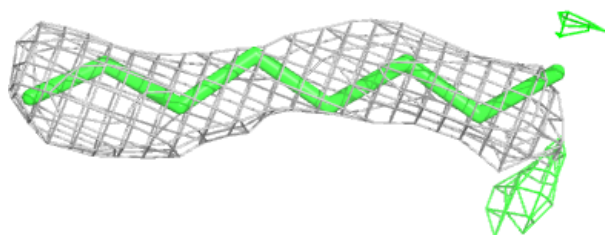


**Electron density around LFA A 306:**

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

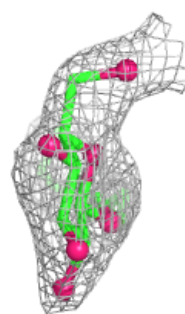
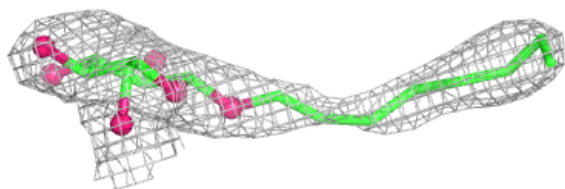
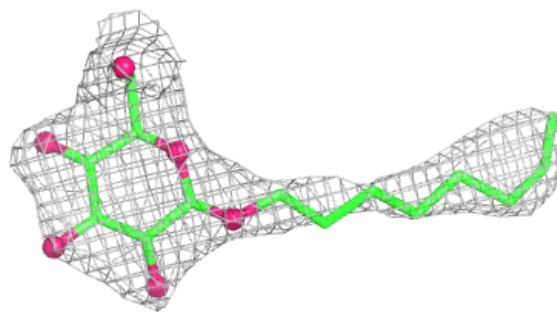
**Electron density around LFA E 305:**

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

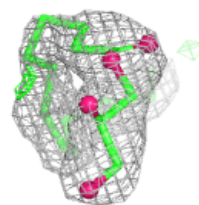
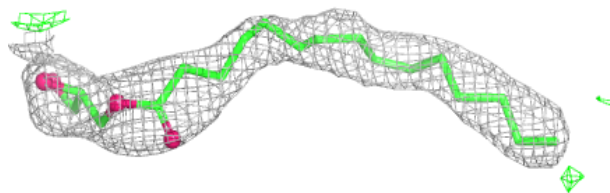
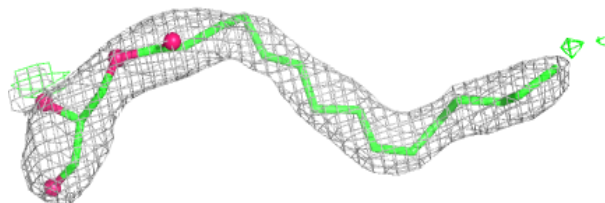


**Electron density around BOG D 311:**

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

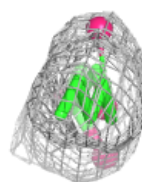
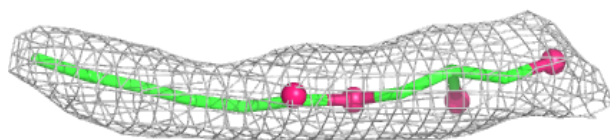
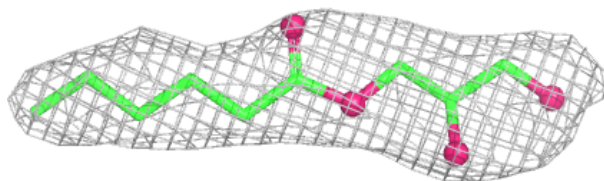
**Electron density around OLC B 301:**

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

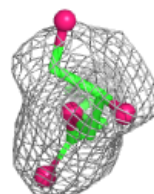
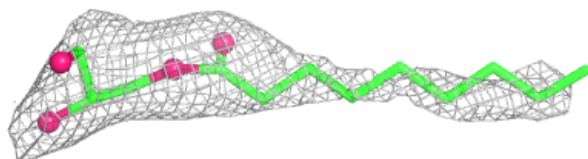
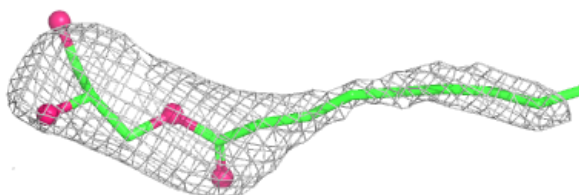


**Electron density around OLC A 302:**

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

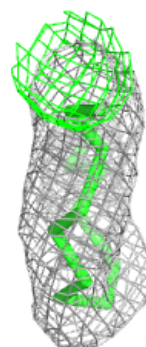
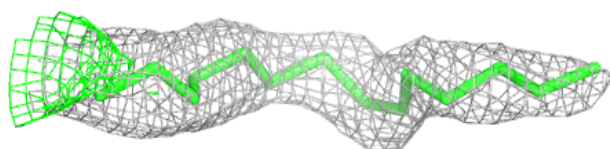
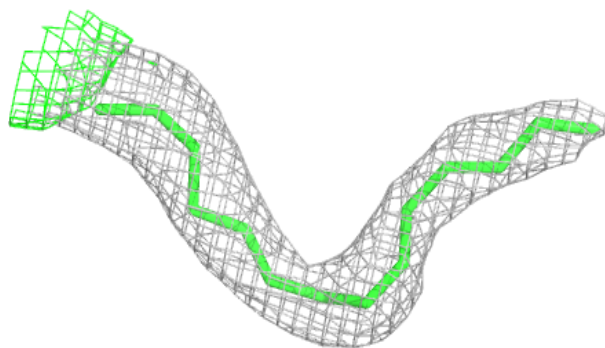
**Electron density around OLC B 304:**

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

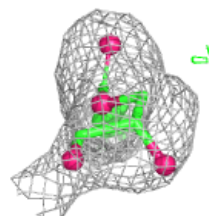
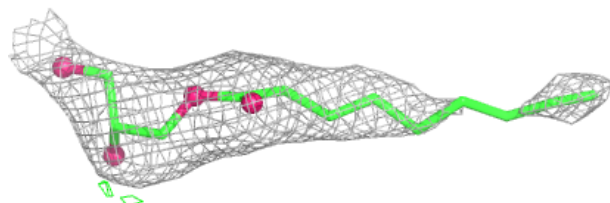
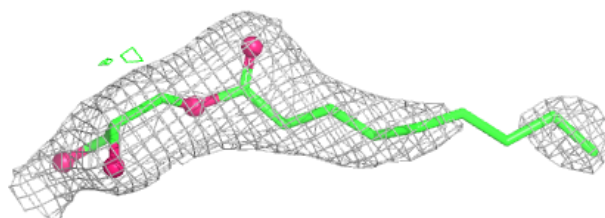


**Electron density around OLC A 301:**

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

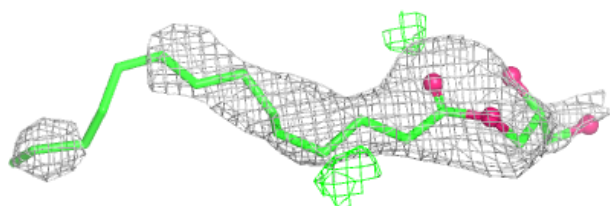
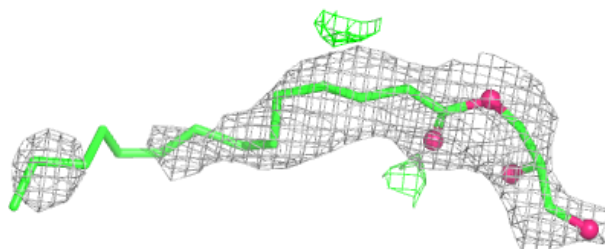
**Electron density around OLC C 312:**

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

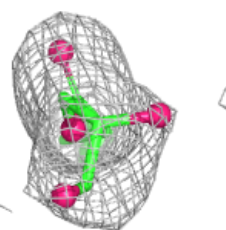
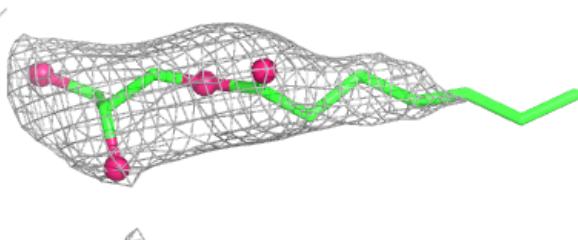
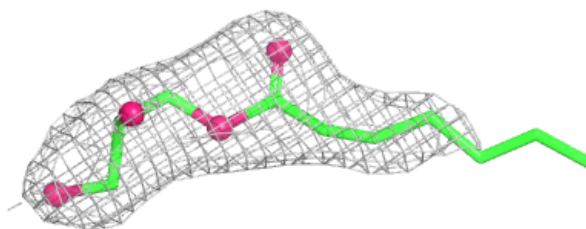


**Electron density around OLC C 305:**

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

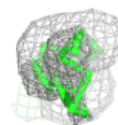
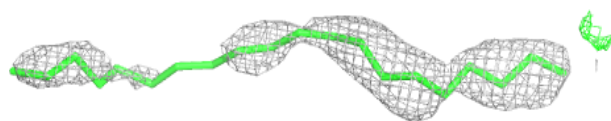
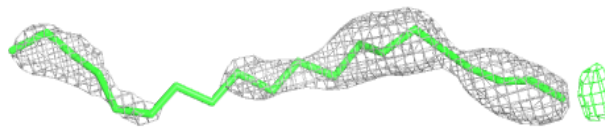
**Electron density around OLC D 303:**

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

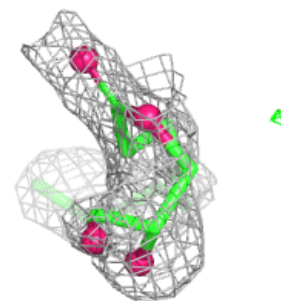
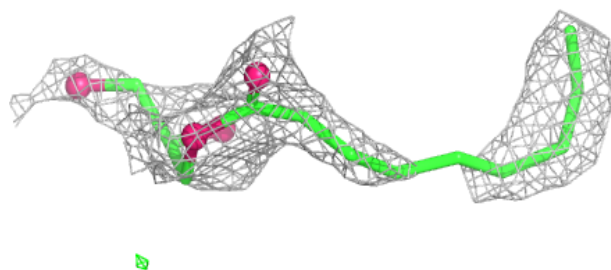
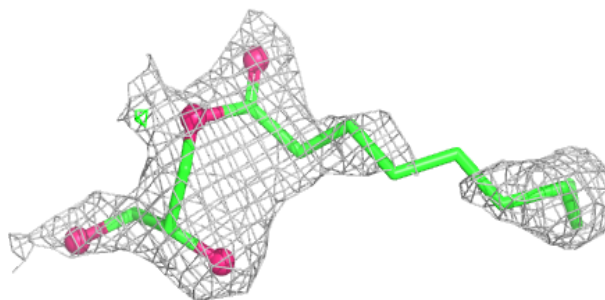


**Electron density around LFA D 305:**

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

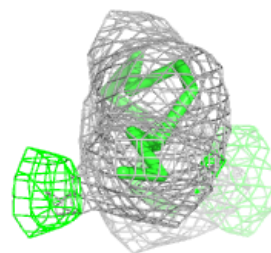
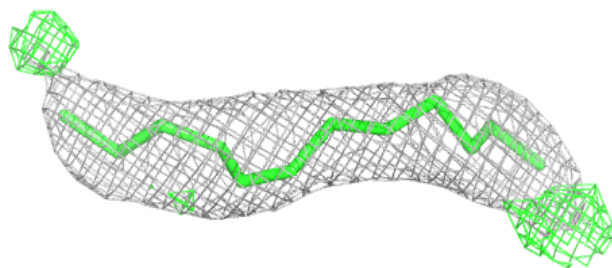
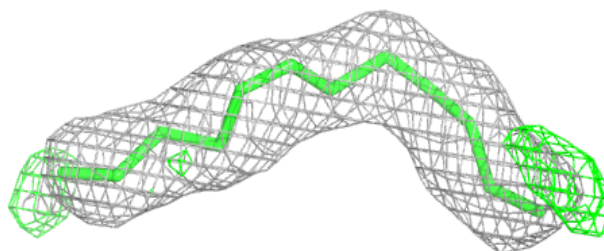
**Electron density around OLC C 313:**

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

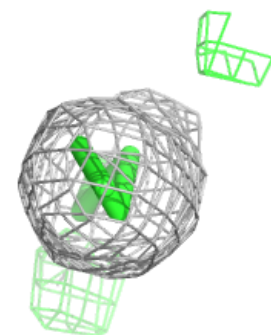
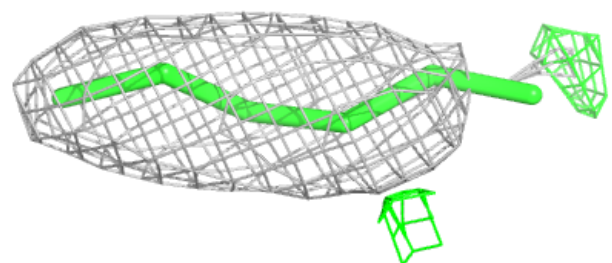
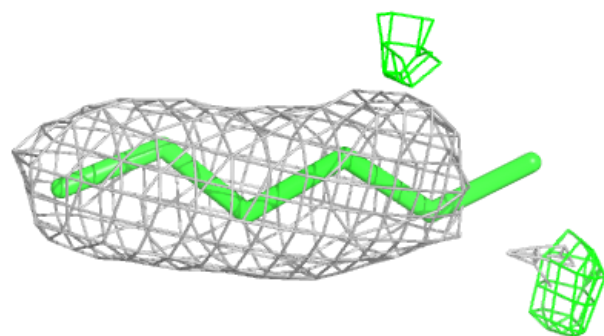


**Electron density around OLC E 301:**

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

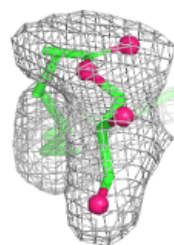
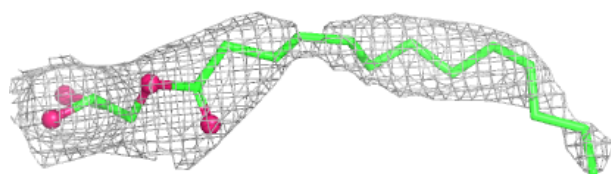
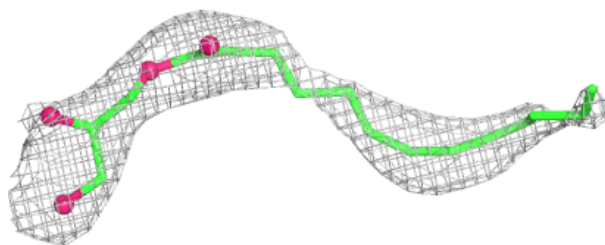
**Electron density around LFA A 308:**

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

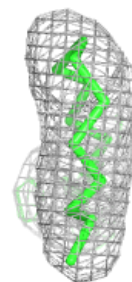
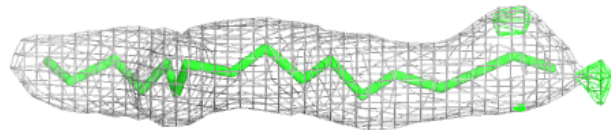
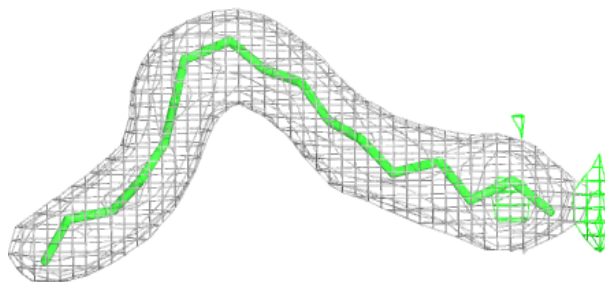


**Electron density around OLC C 302:**

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

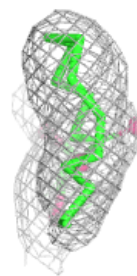
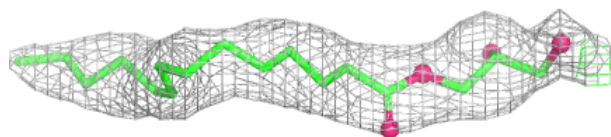
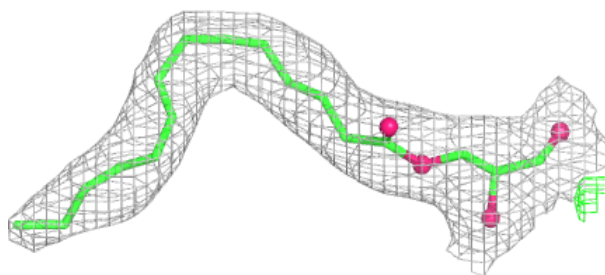
**Electron density around LFA D 307:**

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

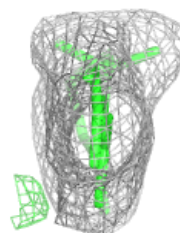
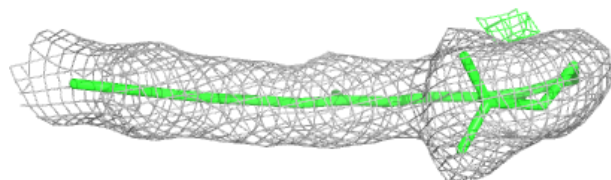
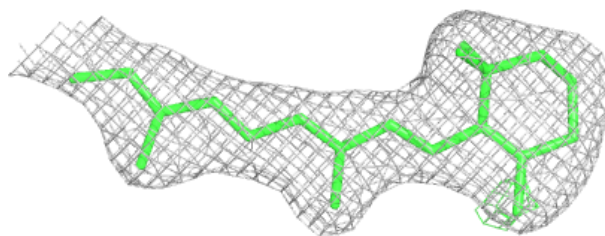


**Electron density around OLC C 301:**

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

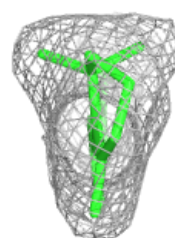
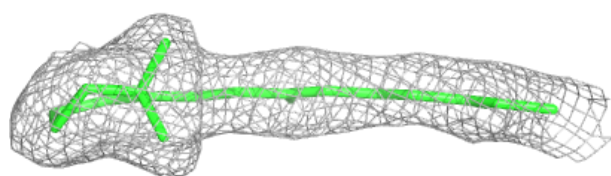
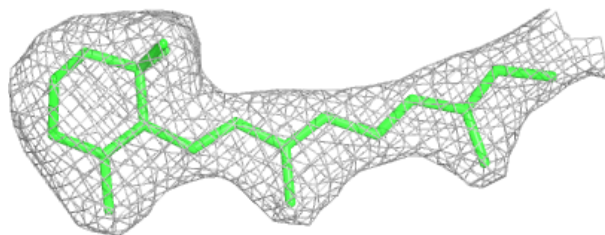
**Electron density around RET B 309:**

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

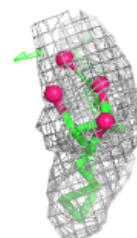
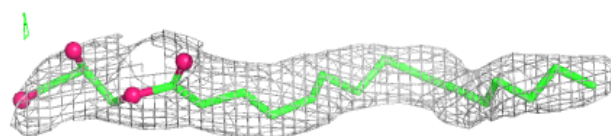
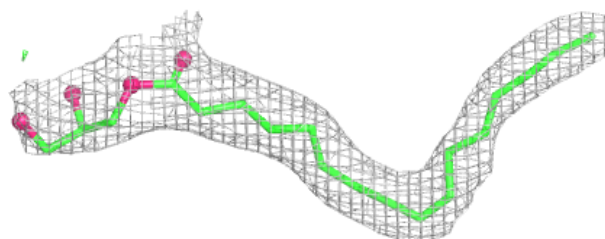


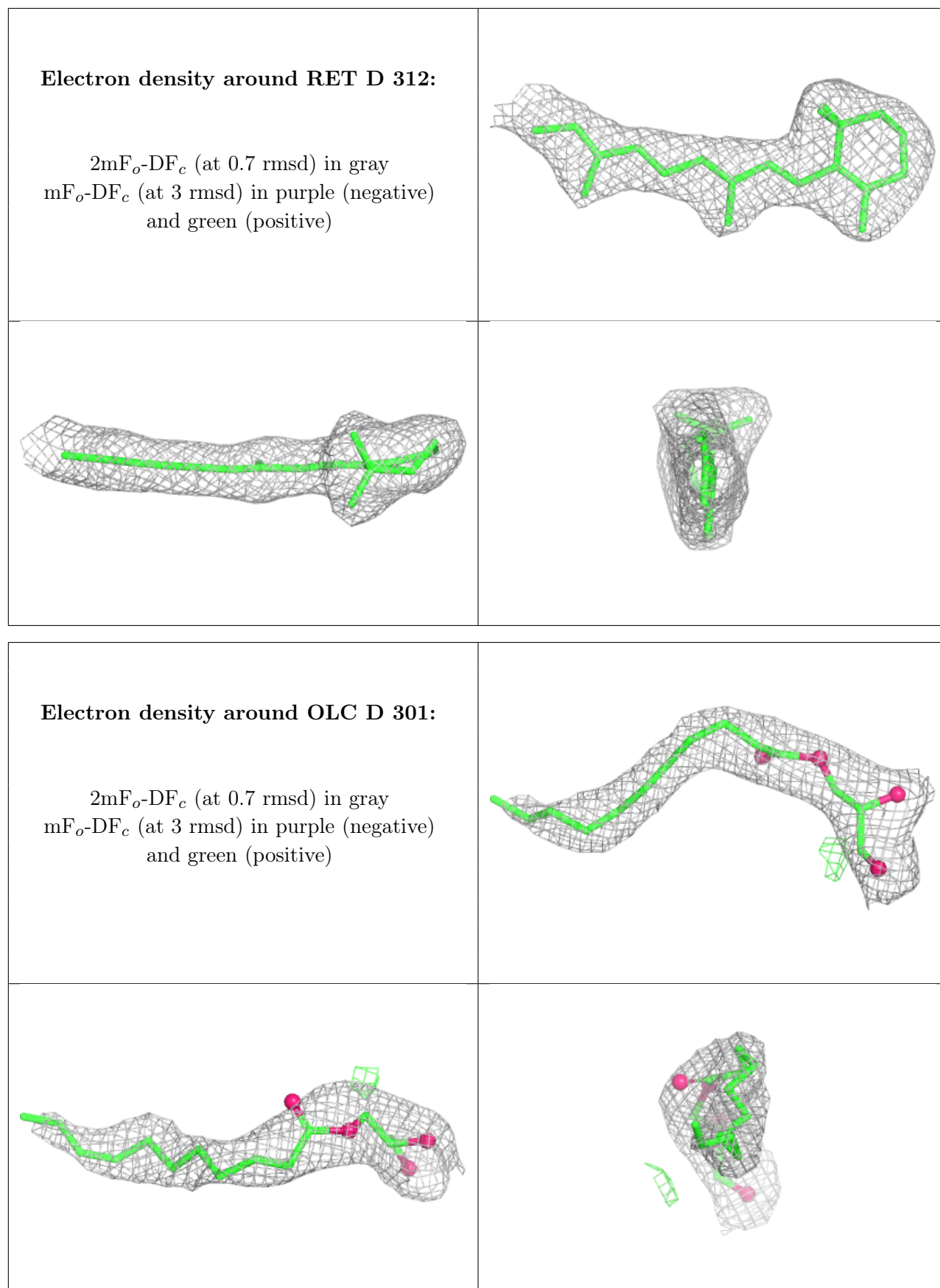
**Electron density around RET E 312:**

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

**Electron density around OLC C 306:**

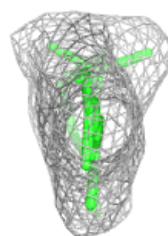
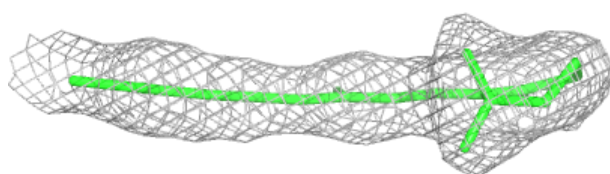
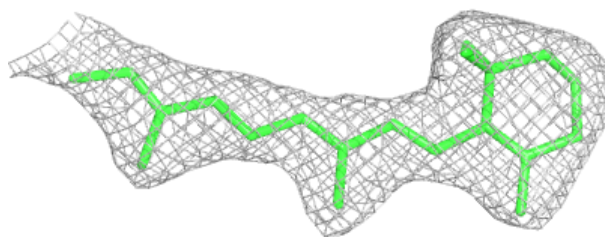
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



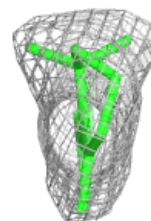
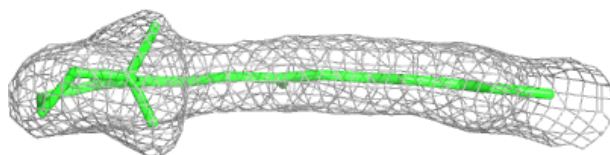
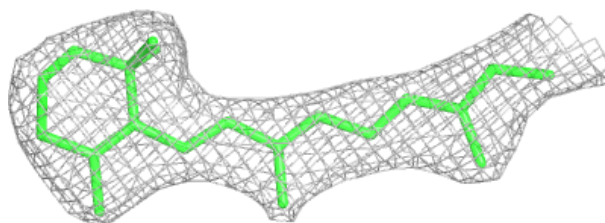


**Electron density around RET C 323:**

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

**Electron density around RET A 313:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.