



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:40 AM BST

PDB ID : 6YC1  
Title : Crystal structure of the H30A mutant of the light-driven sodium pump KR2 in the pentameric form, pH 8.0  
Authors : Kovalev, K.; Gushchin, I.; Gordeliy, V.  
Deposited on : 2020-03-18  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

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

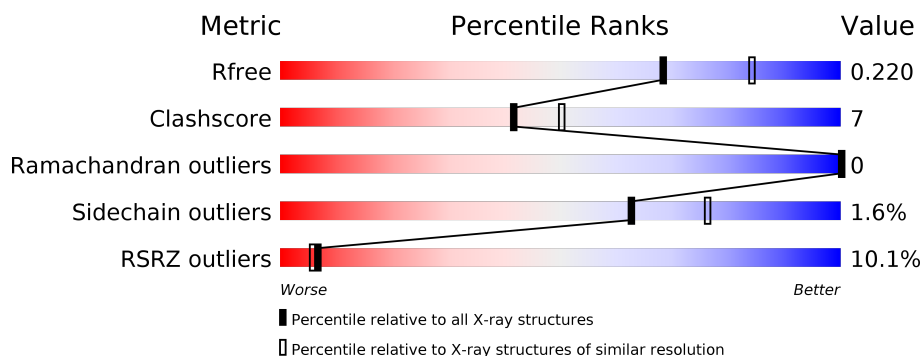
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	273	<div> <div>11%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>
1	B	273	<div> <div>9%</div> <div> <div></div> <div>84%</div> <div>15%</div> </div> </div>
1	C	273	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>17%</div> </div> </div>
1	D	273	<div> <div>13%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
1	E	273	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OLC	E	306	-	-	-	X
2	OLC	E	310	-	-	-	X
3	LFA	A	319	-	-	-	X
3	LFA	B	303	-	-	-	X
3	LFA	C	304	-	-	-	X
3	LFA	D	303	-	-	-	X
3	LFA	D	320	-	-	-	X
3	LFA	E	302	-	-	-	X
5	BOG	A	315	-	-	-	X
5	BOG	B	314	-	-	-	X
5	BOG	C	317	-	-	-	X
5	BOG	D	318	-	-	-	X
5	BOG	E	316	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Sodium pumping rhodopsin.

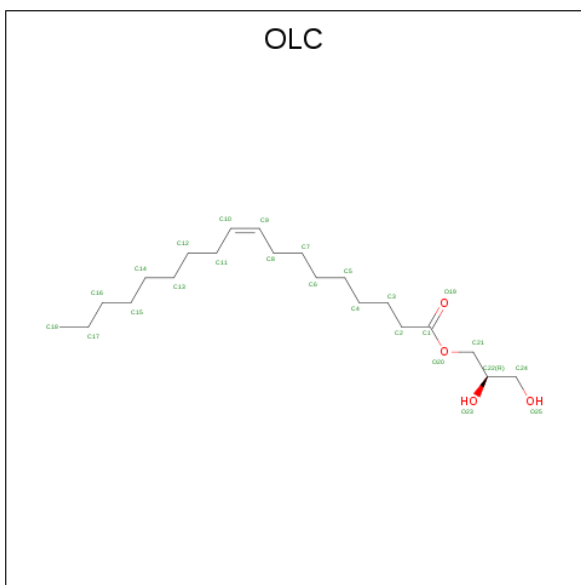
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	2	0
			2183	1456	328	390	9			
1	B	273	Total	C	N	O	S	0	2	0
			2180	1452	330	389	9			
1	C	273	Total	C	N	O	S	0	2	0
			2182	1455	328	390	9			
1	D	273	Total	C	N	O	S	0	2	0
			2177	1451	329	388	9			
1	E	273	Total	C	N	O	S	0	2	0
			2179	1453	329	388	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	HIS	conflict	UNP N0DKS8
B	30	ALA	HIS	conflict	UNP N0DKS8
C	30	ALA	HIS	conflict	UNP N0DKS8
D	30	ALA	HIS	conflict	UNP N0DKS8
E	30	ALA	HIS	conflict	UNP N0DKS8

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





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

*Continued on next page...*

*Continued from previous page...*

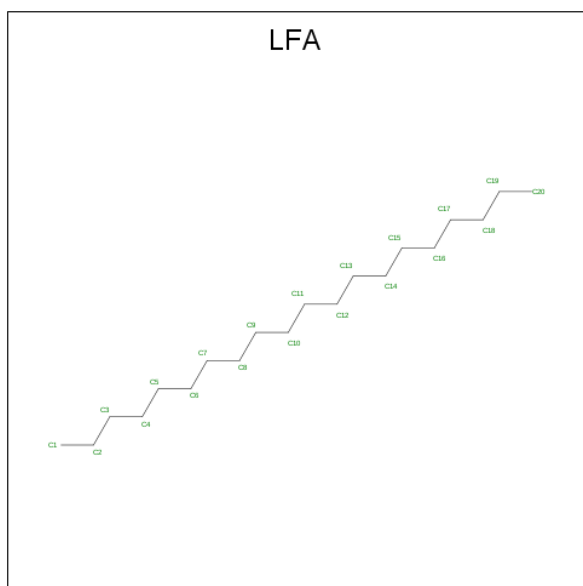
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 16 12 4	0	0
2	B	1	Total C 7 7	0	0
2	C	1	Total C O 21 17 4	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 12 8 4	0	0
2	C	1	Total C O 23 19 4	0	0
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C 7 7	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C O 16 12 4	0	0
2	D	1	Total C O 13 9 4	0	0
2	D	1	Total C O 25 21 4	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C O 18 16 2	0	0
2	D	1	Total C O 14 10 4	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C O 25 21 4	0	0
2	E	1	Total C O 25 21 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C 8 8	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 20 16 4	0	0
2	E	1	Total C O 15 11 4	0	0
2	E	1	Total C O 15 11 4	0	0
2	E	1	Total C 6 6	0	0
2	E	1	Total C O 22 18 4	0	0
2	E	1	Total C O 20 16 4	0	0

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



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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

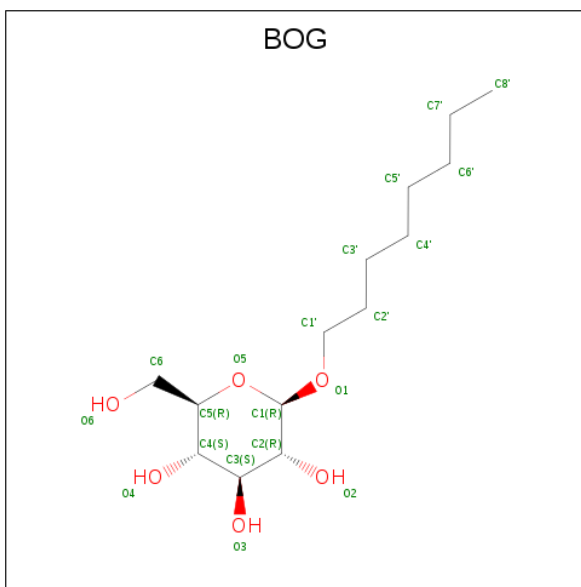
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C 17 17	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 14 14	0	0
3	E	1	Total C 20 20	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 14 14	0	0
3	E	1	Total C 4 4	0	0
3	E	1	Total C 5 5	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by author).

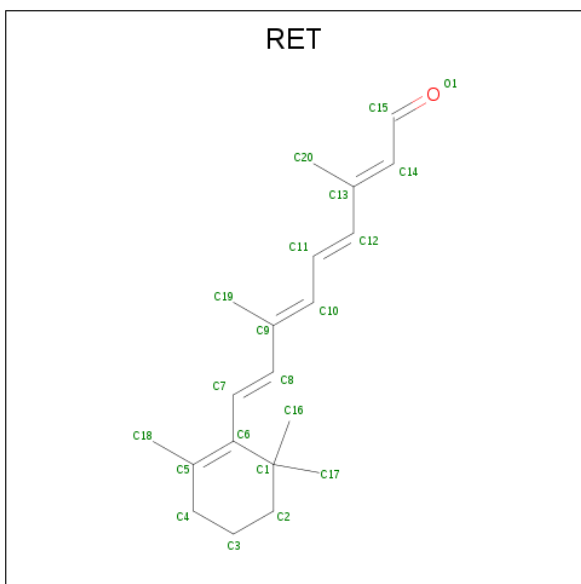
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

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



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

- Molecule 6 is RETINAL (three-letter code: 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

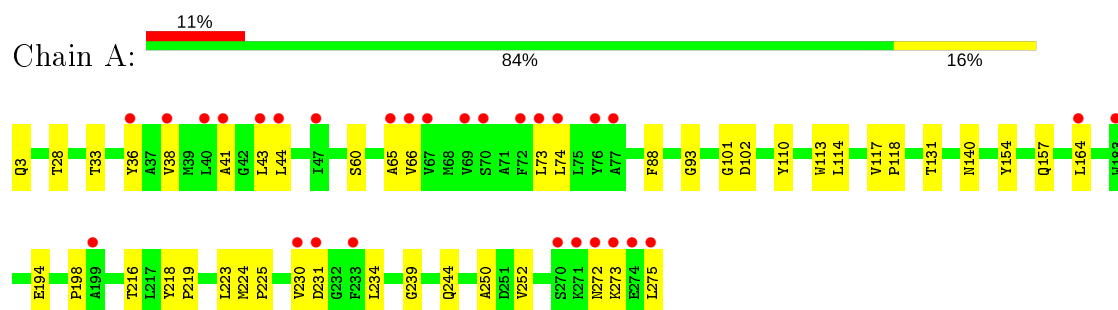
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	121	Total O 121 121	0	0
7	B	113	Total O 113 113	0	0
7	C	115	Total O 115 115	0	0
7	D	104	Total O 104 104	0	0
7	E	114	Total O 114 114	0	0

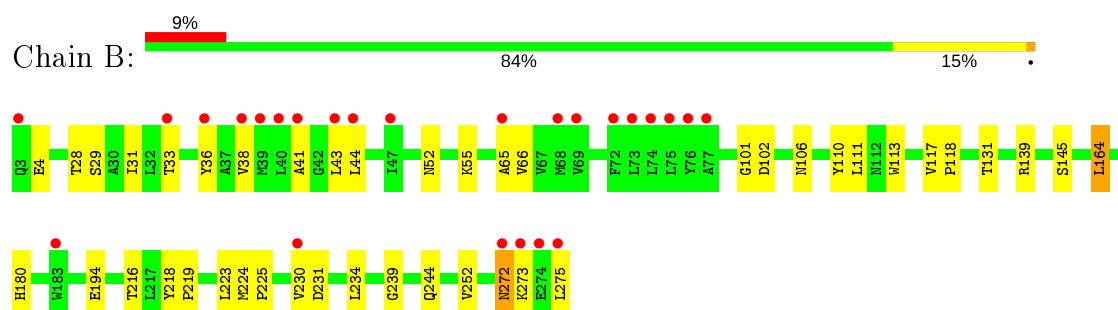
### 3 Residue-property plots [i](#)

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.

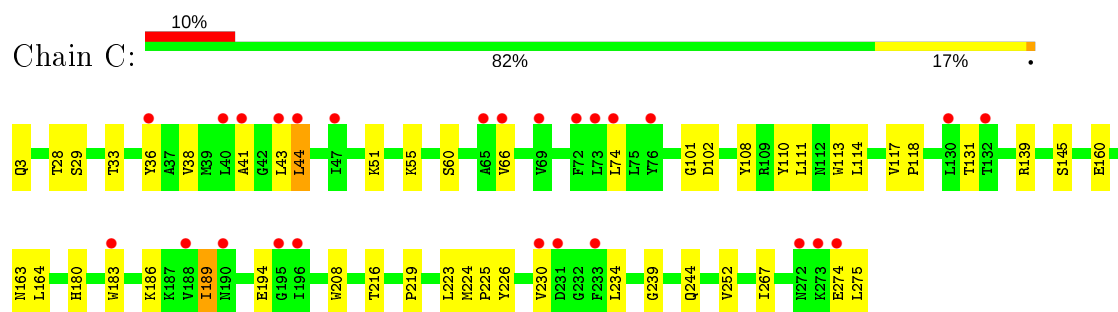
- Molecule 1: Sodium pumping rhodopsin



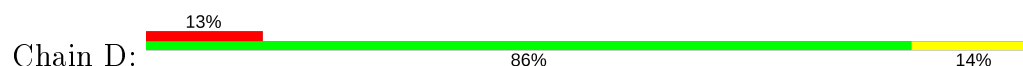
- Molecule 1: Sodium pumping rhodopsin



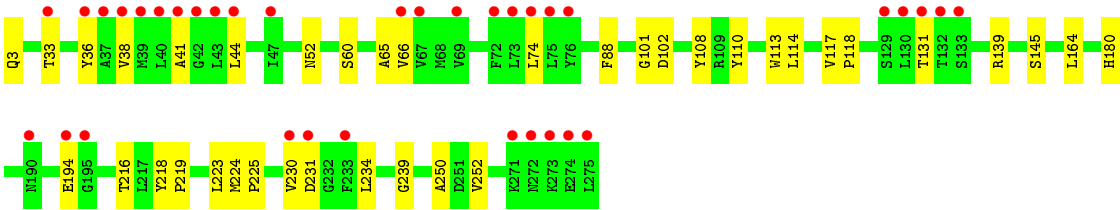
- Molecule 1: Sodium pumping rhodopsin



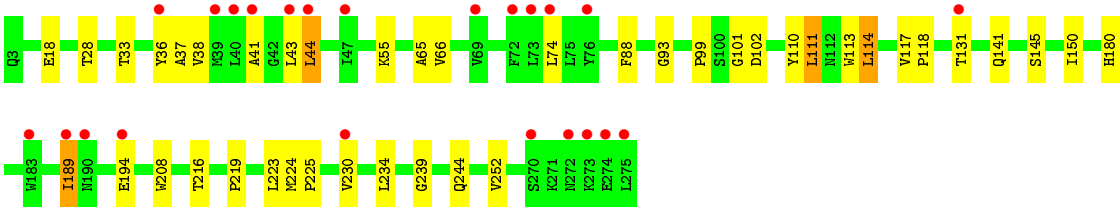
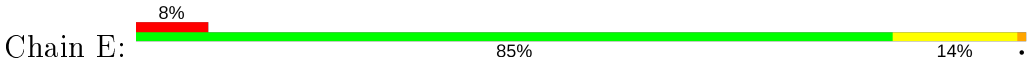
- Molecule 1: Sodium pumping rhodopsin







● Molecule 1: Sodium pumping rhodopsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.09Å 239.73Å 135.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 48.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.20) 98.8 (48.01-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.181 , 0.209 0.196 , 0.220	Depositor DCC
$R_{free}$ test set	5272 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.63	0/2241	0.62	0/3047
1	B	0.63	0/2238	0.62	0/3044
1	C	0.63	0/2240	0.62	0/3046
1	D	0.63	0/2235	0.63	0/3039
1	E	0.63	0/2237	0.62	0/3042
All	All	0.63	0/11191	0.62	0/15218

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2183	0	2156	33	0
1	B	2180	0	2155	38	0
1	C	2182	0	2154	43	0
1	D	2177	0	2148	31	0
1	E	2179	0	2155	32	0
2	A	155	0	228	5	0
2	B	127	0	178	5	0
2	C	163	0	222	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	154	0	215	3	0
2	E	147	0	209	3	0
3	A	78	0	151	0	0
3	B	58	0	113	0	0
3	C	65	0	127	8	0
3	D	112	0	225	3	0
3	E	51	0	100	0	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	1	0
5	D	20	0	28	3	0
5	E	20	0	28	0	0
6	A	20	0	27	4	0
6	B	20	0	27	3	0
6	C	20	0	27	2	0
6	D	20	0	27	2	0
6	E	20	0	27	3	0
7	A	121	0	0	3	0
7	B	113	0	0	2	0
7	C	115	0	0	3	0
7	D	104	0	0	5	0
7	E	114	0	0	2	0
All	All	12783	0	12811	176	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.

All (176) 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:N	1:B:272:ASN:HD22	1.64	0.94
6:D:319:RET:H161	6:D:319:RET:H8	1.61	0.82
6:B:315:RET:H8	6:B:315:RET:H161	1.62	0.82
6:C:318:RET:H8	6:C:318:RET:H161	1.62	0.81
6:A:316:RET:H8	6:A:316:RET:H161	1.63	0.80
6:E:317:RET:H8	6:E:317:RET:H161	1.63	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:GLN:HG2	7:D:434:HOH:O	1.84	0.77
1:B:145:SER:OG	1:B:180:HIS:HD2	1.69	0.75
2:D:310:OLC:H11A	3:D:314:LFA:H12	1.68	0.75
1:A:3:GLN:HG2	7:E:412:HOH:O	1.87	0.74
1:B:272:ASN:N	1:B:272:ASN:ND2	2.35	0.73
1:C:55:LYS:NZ	7:C:402:HOH:O	2.12	0.72
1:E:145:SER:OG	1:E:180:HIS:HD2	1.73	0.71
1:C:145:SER:OG	1:C:180:HIS:HD2	1.72	0.70
1:D:231:ASP:N	5:D:318:BOG:O6	2.15	0.70
1:D:145:SER:OG	1:D:180:HIS:HD2	1.73	0.70
1:D:52:ASN:OD1	7:D:403:HOH:O	2.13	0.66
1:B:272:ASN:H	1:B:272:ASN:HD22	1.42	0.65
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.79	0.64
1:E:234:LEU:O	1:E:239:GLY:HA3	1.97	0.64
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.80	0.64
1:A:234:LEU:O	1:A:239:GLY:HA3	1.98	0.64
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.80	0.64
1:B:44:LEU:HD21	1:C:43:LEU:HD11	1.80	0.63
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.78	0.63
1:D:234:LEU:O	1:D:239:GLY:HA3	1.99	0.63
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.80	0.63
1:B:234:LEU:O	1:B:239:GLY:HA3	1.98	0.62
1:C:164:LEU:HD21	5:C:317:BOG:H2'1	1.81	0.62
1:B:272:ASN:H	1:B:272:ASN:ND2	1.95	0.62
1:E:114:LEU:HD13	1:E:150:ILE:HG21	1.81	0.62
1:A:44:LEU:HD21	1:B:43:LEU:HD11	1.81	0.61
1:C:234:LEU:O	1:C:239:GLY:HA3	2.01	0.61
1:E:141:GLN:HG2	2:E:304:OLC:H5A	1.82	0.60
6:D:319:RET:H161	6:D:319:RET:C8	2.32	0.60
1:C:186:LYS:HG2	3:C:311:LFA:C5	2.34	0.57
1:B:231:ASP:N	5:B:314:BOG:O6	2.24	0.57
2:C:305:OLC:H13	2:D:301:OLC:H4A	1.86	0.57
7:B:420:HOH:O	1:C:3:GLN:HB2	2.05	0.57
1:C:189:ILE:HD12	1:C:208:TRP:HB2	1.86	0.57
1:C:131:THR:HG21	1:C:194:GLU:OE1	2.06	0.56
1:A:272:ASN:CB	1:A:273:LYS:HE3	2.37	0.55
1:C:183:TRP:CE3	3:C:311:LFA:H41	2.41	0.55
1:E:141:GLN:HG2	2:E:304:OLC:C5	2.37	0.55
1:B:139:ARG:NH1	2:B:301:OLC:H24A	2.22	0.55
1:C:183:TRP:CZ3	3:C:311:LFA:H61	2.43	0.54
1:C:186:LYS:HG2	3:C:311:LFA:H51	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:GLU:OE1	7:E:403:HOH:O	2.19	0.53
1:B:41:ALA:HB1	1:C:66:VAL:HG13	1.90	0.53
6:A:316:RET:C8	6:A:316:RET:H161	2.33	0.53
1:C:139:ARG:NH2	3:C:313:LFA:H203	2.22	0.53
1:C:275:LEU:CD2	2:C:305:OLC:O23	2.56	0.53
1:B:131:THR:HG21	1:B:194:GLU:OE1	2.09	0.53
6:E:317:RET:C8	6:E:317:RET:H161	2.33	0.53
1:B:139:ARG:NH2	2:B:304:OLC:H21A	2.25	0.52
1:B:139:ARG:HH11	2:B:301:OLC:H24A	1.75	0.52
1:C:44:LEU:CD1	1:D:65:ALA:HB1	2.40	0.52
1:E:111:LEU:O	1:E:114:LEU:HB2	2.10	0.52
1:E:189:ILE:HD12	1:E:208:TRP:HB2	1.92	0.51
1:A:275:LEU:HD21	2:A:302:OLC:H24A	1.93	0.51
1:A:131:THR:HG21	1:A:194:GLU:OE1	2.11	0.51
1:A:110:TYR:O	1:A:113:TRP:HB2	2.11	0.51
1:A:275:LEU:CD2	2:A:302:OLC:H24A	2.41	0.51
6:B:315:RET:C8	6:B:315:RET:H161	2.32	0.51
1:A:231:ASP:H	5:A:315:BOG:HO6	1.52	0.50
1:D:131:THR:HG21	1:D:194:GLU:OE1	2.10	0.50
1:A:224:MET:N	1:A:225:PRO:HD2	2.26	0.50
1:B:139:ARG:HH11	2:B:301:OLC:C24	2.25	0.50
3:C:304:LFA:H172	3:D:303:LFA:H61	1.94	0.50
1:B:139:ARG:NH1	2:B:301:OLC:C24	2.74	0.49
1:B:224:MET:N	1:B:225:PRO:HD2	2.27	0.49
1:C:110:TYR:O	1:C:113:TRP:HB2	2.12	0.49
1:B:110:TYR:O	1:B:113:TRP:HB2	2.12	0.49
1:E:110:TYR:O	1:E:113:TRP:HB2	2.12	0.49
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.93	0.49
1:E:101:GLY:O	1:E:102:ASP:HB2	2.12	0.49
1:C:224:MET:N	1:C:225:PRO:HD2	2.27	0.49
1:B:44:LEU:CD2	1:C:43:LEU:HD11	2.43	0.48
1:D:224:MET:N	1:D:225:PRO:HD2	2.28	0.48
1:A:164:LEU:HD21	5:A:315:BOG:H2'1	1.95	0.48
1:E:131:THR:HG21	1:E:194:GLU:OE1	2.13	0.48
1:C:101:GLY:O	1:C:102:ASP:HB2	2.13	0.48
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.95	0.48
1:D:110:TYR:O	1:D:113:TRP:HB2	2.13	0.48
1:D:231:ASP:H	5:D:318:BOG:HO6	1.54	0.48
6:C:318:RET:H161	6:C:318:RET:C8	2.33	0.48
1:A:101:GLY:O	1:A:102:ASP:HB2	2.15	0.47
1:D:101:GLY:O	1:D:102:ASP:HB2	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:LEU:C	1:E:225:PRO:HD2	2.35	0.47
1:D:60:SER:CB	7:D:404:HOH:O	2.61	0.47
1:E:224:MET:N	1:E:225:PRO:HD2	2.28	0.47
1:B:101:GLY:O	1:B:102:ASP:HB2	2.15	0.47
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.96	0.47
1:D:38:VAL:HG11	1:D:252:VAL:HG22	1.97	0.47
1:B:216:THR:O	1:B:219:PRO:HG2	2.15	0.47
1:C:163:ASN:HD22	2:C:309:OLC:C24	2.28	0.47
1:C:114:LEU:HD22	2:C:302:OLC:H10	1.96	0.46
1:A:140:ASN:HB3	2:A:303:OLC:H2A	1.96	0.46
1:C:216:THR:O	1:C:219:PRO:HG2	2.15	0.46
1:D:44:LEU:HD21	1:E:43:LEU:HD11	1.97	0.46
1:A:223:LEU:C	1:A:225:PRO:HD2	2.34	0.46
1:E:216:THR:O	1:E:219:PRO:HG2	2.16	0.46
1:C:223:LEU:C	1:C:225:PRO:HD2	2.35	0.46
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.81	0.46
1:C:275:LEU:HD21	2:C:305:OLC:O23	2.16	0.46
1:B:223:LEU:C	1:B:225:PRO:HD2	2.37	0.46
1:C:38:VAL:HG11	1:C:252:VAL:HG22	1.97	0.45
1:D:41:ALA:HB1	1:E:66:VAL:HG13	1.97	0.45
1:E:44:LEU:HA	1:E:44:LEU:HD23	1.81	0.45
1:A:216:THR:O	1:A:219:PRO:HG2	2.16	0.45
1:D:60:SER:HB3	7:D:404:HOH:O	2.14	0.45
1:C:44:LEU:HD11	1:D:65:ALA:HB1	1.97	0.45
1:C:33:THR:HG21	1:D:108[A]:TYR:CZ	2.52	0.45
1:A:198:PRO:HD2	7:A:488:HOH:O	2.16	0.45
1:C:186:LYS:HG2	3:C:311:LFA:H52	1.98	0.45
1:A:65:ALA:HB1	1:E:44:LEU:CD1	2.46	0.45
1:B:33:THR:HA	1:B:36:TYR:CE2	2.52	0.45
1:D:216:THR:O	1:D:219:PRO:HG2	2.15	0.45
1:B:52:ASN:O	1:B:273:LYS:HG3	2.17	0.45
1:D:223:LEU:C	1:D:225:PRO:HD2	2.37	0.45
1:A:33:THR:HA	1:A:36:TYR:CE2	2.52	0.45
1:B:29:SER:CB	1:C:108[B]:TYR:HH	2.21	0.44
1:C:51:LYS:HD3	7:C:470:HOH:O	2.17	0.44
1:D:88:PHE:CD2	1:E:99:PRO:HB3	2.52	0.44
1:B:38:VAL:HG11	1:B:252:VAL:HG22	1.98	0.44
2:A:317:OLC:H11A	2:A:317:OLC:H8	1.82	0.44
1:C:28:THR:HG23	1:C:244:GLN:HG3	1.98	0.44
1:D:33:THR:HA	1:D:36:TYR:CE2	2.52	0.44
1:A:38:VAL:HG11	1:A:252:VAL:HG22	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HA	1:B:164:LEU:HD23	1.80	0.43
1:A:44:LEU:CD2	1:B:43:LEU:HD11	2.46	0.43
6:B:315:RET:H7	6:B:315:RET:H181	1.81	0.43
1:D:139:ARG:NH1	2:D:301:OLC:H24	2.33	0.43
2:A:317:OLC:C17	2:E:309:OLC:C10	2.97	0.43
1:B:33:THR:HG21	1:C:108[A]:TYR:CZ	2.53	0.43
1:C:33:THR:HA	1:C:36:TYR:CE2	2.53	0.43
1:D:164:LEU:HD21	5:D:318:BOG:H2'1	2.01	0.43
1:C:160:GLU:O	1:C:226:TYR:OH	2.32	0.43
1:E:33:THR:HA	1:E:36:TYR:CE2	2.53	0.43
1:A:44:LEU:HD21	1:B:65:ALA:HB1	2.02	0.42
1:B:28:THR:HG23	1:B:244:GLN:HG3	2.01	0.42
1:A:114:LEU:O	1:A:118:PRO:HG2	2.19	0.42
1:A:154:TYR:O	1:A:157:GLN:HG3	2.19	0.42
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.55	0.42
6:A:316:RET:H7	6:A:316:RET:H181	1.78	0.42
1:C:267:ILE:HG21	1:C:275:LEU:HG	2.02	0.42
1:D:114:LEU:O	1:D:118:PRO:HG2	2.20	0.42
1:E:74:LEU:HA	1:E:74:LEU:HD22	1.92	0.42
1:B:231:ASP:H	5:B:314:BOG:HO6	1.60	0.41
1:D:74:LEU:HA	1:D:74:LEU:HD22	1.91	0.41
1:C:114:LEU:O	1:C:118:PRO:HG2	2.20	0.41
1:D:44:LEU:HD21	1:E:65:ALA:HB1	2.02	0.41
1:B:31:ILE:HD12	1:B:31:ILE:HA	1.90	0.41
1:C:74:LEU:HA	1:C:74:LEU:HD22	1.92	0.41
1:A:73:LEU:CD1	1:E:37:ALA:HA	2.50	0.41
1:A:218:TYR:CE2	1:A:250:ALA:HB1	2.56	0.41
7:A:470:HOH:O	1:B:55:LYS:HE3	2.19	0.41
2:C:305:OLC:H7	2:C:305:OLC:H11	2.02	0.41
1:E:114:LEU:HD12	1:E:114:LEU:HA	1.84	0.41
1:A:43:LEU:HD11	1:E:44:LEU:HD11	2.03	0.41
1:C:60:SER:CB	7:C:403:HOH:O	2.69	0.41
1:A:60:SER:CB	7:A:402:HOH:O	2.68	0.41
3:C:304:LFA:H32	3:D:320:LFA:H102	2.03	0.41
1:C:29:SER:OG	1:D:108[B]:TYR:OH	2.07	0.41
1:E:114:LEU:O	1:E:118:PRO:HG2	2.21	0.41
7:D:403:HOH:O	1:E:55:LYS:CE	2.68	0.41
6:E:317:RET:H191	6:E:317:RET:H11	1.95	0.41
1:A:28:THR:HG23	1:A:244:GLN:HG3	2.03	0.40
1:E:28:THR:HG23	1:E:244:GLN:HG3	2.04	0.40
1:A:88:PHE:CZ	1:A:93:GLY:HA2	2.56	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ASN:HB2	7:B:477:HOH:O	2.21	0.40
1:A:74:LEU:HD22	1:A:74:LEU:HA	1.93	0.40
1:B:218:TYR:N	1:B:219:PRO:HD2	2.36	0.40
6:A:316:RET:H191	6:A:316:RET:H11	1.96	0.40
1:D:218:TYR:CE2	1:D:250:ALA:HB1	2.57	0.40
1:E:38:VAL:HG11	1:E:252:VAL:HG22	2.04	0.40

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	273/273 (100%)	267 (98%)	6 (2%)	0	100	100
1	B	273/273 (100%)	267 (98%)	6 (2%)	0	100	100
1	C	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
1	D	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
1	E	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
All	All	1365/1365 (100%)	1338 (98%)	27 (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	230/233 (99%)	229 (100%)	1 (0%)	91	96
1	B	231/233 (99%)	225 (97%)	6 (3%)	46	58
1	C	230/233 (99%)	225 (98%)	5 (2%)	52	65
1	D	229/233 (98%)	228 (100%)	1 (0%)	91	96
1	E	230/233 (99%)	225 (98%)	5 (2%)	52	65
All	All	1150/1165 (99%)	1132 (98%)	18 (2%)	62	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	VAL
1	B	4	GLU
1	B	111	LEU
1	B	164	LEU
1	B	230	VAL
1	B	272	ASN
1	B	275	LEU
1	C	44	LEU
1	C	111	LEU
1	C	189	ILE
1	C	230	VAL
1	C	274	GLU
1	D	230	VAL
1	E	44	LEU
1	E	111	LEU
1	E	114	LEU
1	E	189	ILE
1	E	230	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 91 ligands modelled in this entry, 5 are monoatomic - leaving 86 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	OLC	C	310	-	6,6,24	0.30	0	5,5,25	0.37	0
6	RET	A	316	1	20,20,21	1.72	3 (15%)	27,27,28	1.12	1 (3%)
2	OLC	B	308	-	6,6,24	0.47	0	5,5,25	0.54	0
2	OLC	C	306	-	21,21,24	1.02	1 (4%)	22,22,25	0.89	1 (4%)
2	OLC	B	304	-	24,24,24	0.95	1 (4%)	25,25,25	0.84	1 (4%)
2	OLC	E	305	-	19,19,24	1.07	1 (5%)	20,20,25	0.98	1 (5%)
6	RET	B	315	1	20,20,21	1.66	3 (15%)	27,27,28	1.13	2 (7%)
2	OLC	A	303	-	24,24,24	0.96	1 (4%)	25,25,25	0.83	1 (4%)
3	LFA	A	310	-	7,7,19	0.10	0	6,6,18	0.07	0
3	LFA	A	308	-	6,6,19	0.12	0	5,5,18	0.07	0
3	LFA	D	315	-	6,6,19	0.11	0	5,5,18	0.07	0
3	LFA	B	309	-	8,8,19	0.11	0	7,7,18	0.08	0
3	LFA	E	312	-	13,13,19	0.08	0	12,12,18	0.05	0
2	OLC	A	306	-	14,14,24	1.21	1 (7%)	15,15,25	1.09	2 (13%)
3	LFA	B	310	-	7,7,19	0.12	0	6,6,18	0.07	0
3	LFA	B	311	-	9,9,19	0.10	0	8,8,18	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	RET	D	319	1	20,20,21	1.64	3 (15%)	27,27,28	1.14	2 (7%)
3	LFA	C	304	-	19,19,19	0.12	0	18,18,18	0.10	0
2	OLC	D	309	-	6,6,24	0.34	0	5,5,25	0.29	0
3	LFA	B	312	-	6,6,19	0.11	0	5,5,18	0.06	0
3	LFA	E	314	-	4,4,19	0.15	0	3,3,18	0.23	0
2	OLC	A	305	-	24,24,24	0.99	1 (4%)	25,25,25	0.88	2 (8%)
2	OLC	A	301	-	8,8,24	0.36	0	6,7,25	0.44	0
2	OLC	E	306	-	14,14,24	1.22	1 (7%)	15,15,25	1.03	1 (6%)
3	LFA	C	313	-	19,19,19	0.08	0	18,18,18	0.04	0
2	OLC	E	308	-	5,5,24	0.33	0	4,4,25	0.28	0
2	OLC	A	307	-	6,6,24	0.27	0	5,5,25	0.43	0
3	LFA	D	316	-	5,5,19	0.15	0	4,4,18	0.11	0
3	LFA	E	302	-	19,19,19	0.14	0	18,18,18	0.11	0
2	OLC	E	303	-	7,7,24	0.29	0	6,6,25	0.39	0
2	OLC	A	318	-	16,19,24	0.24	0	15,19,25	0.56	0
3	LFA	D	312	-	19,19,19	0.07	0	18,18,18	0.05	0
3	LFA	A	319	-	19,19,19	0.13	0	18,18,18	0.10	0
6	RET	E	317	1	20,20,21	1.72	3 (15%)	27,27,28	1.13	1 (3%)
5	BOG	C	317	-	20,20,20	0.56	0	25,25,25	0.54	0
3	LFA	B	316	-	3,3,19	0.25	0	2,2,18	0.43	0
3	LFA	D	314	-	16,16,19	0.07	0	15,15,18	0.08	0
2	OLC	E	310	-	19,19,24	1.07	1 (5%)	20,20,25	0.94	1 (5%)
2	OLC	D	304	-	12,12,24	1.35	1 (8%)	13,13,25	1.07	1 (7%)
6	RET	C	318	1	20,20,21	1.74	3 (15%)	27,27,28	1.09	1 (3%)
2	OLC	A	317	-	15,18,24	0.26	0	14,18,25	0.51	0
2	OLC	E	304	-	15,15,24	0.28	0	14,14,25	0.48	0
2	OLC	D	301	-	17,17,24	1.10	1 (5%)	18,18,25	0.98	1 (5%)
2	OLC	C	308	-	21,21,24	1.03	1 (4%)	22,22,25	0.92	1 (4%)
2	OLC	E	301	-	24,24,24	0.93	1 (4%)	25,25,25	0.86	1 (4%)
3	LFA	B	303	-	19,19,19	0.13	0	18,18,18	0.11	0
3	LFA	D	320	-	13,13,19	0.09	0	12,12,18	0.06	0
2	OLC	D	306	-	17,17,24	1.12	1 (5%)	18,18,25	1.10	1 (5%)
5	BOG	A	315	-	20,20,20	0.54	0	25,25,25	0.66	0
2	OLC	C	302	-	19,19,24	1.05	1 (5%)	20,20,25	0.92	2 (10%)
2	OLC	E	309	-	21,21,24	1.03	1 (4%)	22,22,25	0.84	1 (4%)
3	LFA	D	313	-	7,7,19	0.10	0	6,6,18	0.06	0
3	LFA	A	313	-	15,15,19	0.08	0	14,14,18	0.06	0
5	BOG	D	318	-	20,20,20	0.51	0	25,25,25	0.58	0
3	LFA	D	311	-	19,19,19	0.08	0	18,18,18	0.03	0
3	LFA	C	315	-	3,3,19	0.26	0	2,2,18	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	D	307	-	14,17,24	0.26	0	13,17,25	0.55	0
2	OLC	B	306	-	20,20,24	1.03	1 (5%)	21,21,25	0.92	1 (4%)
3	LFA	D	303	-	19,19,19	0.13	0	18,18,18	0.09	0
2	OLC	C	307	-	19,19,24	1.05	1 (5%)	20,20,25	0.94	1 (5%)
5	BOG	B	314	-	20,20,20	0.59	1 (5%)	25,25,25	0.60	0
2	OLC	B	305	-	19,19,24	1.05	1 (5%)	20,20,25	0.95	2 (10%)
3	LFA	C	311	-	6,6,19	0.12	0	5,5,18	0.08	0
2	OLC	C	301	-	20,20,24	1.02	1 (5%)	21,21,25	0.98	1 (4%)
2	OLC	B	301	-	21,21,24	0.98	1 (4%)	22,22,25	0.89	1 (4%)
2	OLC	D	308	-	13,13,24	1.23	1 (7%)	14,14,25	0.98	2 (14%)
3	LFA	C	312	-	7,7,19	0.11	0	6,6,18	0.07	0
3	LFA	A	312	-	5,5,19	0.14	0	4,4,18	0.10	0
5	BOG	E	316	-	20,20,20	0.53	0	25,25,25	0.49	0
2	OLC	D	302	-	15,15,24	1.22	1 (6%)	16,16,25	1.04	1 (6%)
3	LFA	A	311	-	3,3,19	0.26	0	2,2,18	0.43	0
2	OLC	B	302	-	15,15,24	1.20	1 (6%)	16,16,25	0.96	1 (6%)
2	OLC	A	304	-	12,12,24	1.31	1 (8%)	13,13,25	1.18	2 (15%)
2	OLC	C	303	-	11,11,24	1.41	1 (9%)	12,12,25	1.06	1 (8%)
3	LFA	A	309	-	7,7,19	0.13	0	6,6,18	0.07	0
2	OLC	D	305	-	24,24,24	0.94	1 (4%)	25,25,25	0.85	1 (4%)
2	OLC	C	309	-	15,15,24	1.18	1 (6%)	16,16,25	0.94	2 (12%)
2	OLC	A	302	-	21,21,24	0.99	1 (4%)	22,22,25	0.93	2 (9%)
2	OLC	D	310	-	24,24,24	0.93	1 (4%)	25,25,25	0.77	1 (4%)
2	OLC	E	307	-	14,14,24	1.19	1 (7%)	15,15,25	1.03	2 (13%)
3	LFA	E	313	-	3,3,19	0.24	0	2,2,18	0.43	0
2	OLC	C	305	-	22,22,24	0.94	1 (4%)	23,23,25	0.81	2 (8%)
3	LFA	E	311	-	7,7,19	0.11	0	6,6,18	0.07	0
2	OLC	B	307	-	15,15,24	1.15	1 (6%)	16,16,25	0.96	2 (12%)
3	LFA	C	314	-	5,5,19	0.14	0	4,4,18	0.11	0
3	LFA	A	320	-	8,8,19	0.11	0	7,7,18	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	310	-	-	2/4/4/24	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	RET	A	316	1	-	0/13/30/31	0/1/1/1
2	OLC	B	308	-	-	3/4/4/24	-
2	OLC	C	306	-	-	8/21/21/24	-
2	OLC	B	304	-	-	13/24/24/24	-
2	OLC	E	305	-	-	6/19/19/24	-
6	RET	B	315	1	-	0/13/30/31	0/1/1/1
2	OLC	A	303	-	-	12/24/24/24	-
3	LFA	A	310	-	-	3/5/5/17	-
3	LFA	A	308	-	-	1/4/4/17	-
3	LFA	D	315	-	-	4/4/4/17	-
3	LFA	B	309	-	-	3/6/6/17	-
3	LFA	E	312	-	-	5/11/11/17	-
2	OLC	A	306	-	-	6/14/14/24	-
3	LFA	B	310	-	-	4/5/5/17	-
3	LFA	B	311	-	-	4/7/7/17	-
6	RET	D	319	1	-	0/13/30/31	0/1/1/1
3	LFA	C	304	-	-	12/17/17/17	-
2	OLC	D	309	-	-	3/4/4/24	-
3	LFA	B	312	-	-	2/4/4/17	-
3	LFA	E	314	-	-	1/2/2/17	-
2	OLC	A	305	-	-	13/24/24/24	-
2	OLC	A	301	-	-	3/6/6/24	-
2	OLC	E	306	-	-	10/14/14/24	-
3	LFA	C	313	-	-	12/17/17/17	-
2	OLC	E	308	-	-	0/3/3/24	-
2	OLC	A	307	-	-	3/4/4/24	-
3	LFA	D	316	-	-	0/3/3/17	-
3	LFA	E	302	-	-	8/17/17/17	-
2	OLC	E	303	-	-	1/5/5/24	-
2	OLC	A	318	-	-	9/15/17/24	-
3	LFA	D	312	-	-	9/17/17/17	-
3	LFA	A	319	-	-	8/17/17/17	-
6	RET	E	317	1	-	0/13/30/31	0/1/1/1
5	BOG	C	317	-	-	3/11/31/31	0/1/1/1
3	LFA	B	316	-	-	0/1/1/17	-
3	LFA	D	314	-	-	9/14/14/17	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	E	310	-	-	12/19/19/24	-
2	OLC	D	304	-	-	3/12/12/24	-
6	RET	C	318	1	-	0/13/30/31	0/1/1/1
2	OLC	A	317	-	-	9/14/16/24	-
2	OLC	E	304	-	-	8/13/13/24	-
2	OLC	D	301	-	-	9/17/17/24	-
2	OLC	C	308	-	-	9/21/21/24	-
2	OLC	E	301	-	-	10/24/24/24	-
3	LFA	B	303	-	-	8/17/17/17	-
3	LFA	D	320	-	-	5/11/11/17	-
2	OLC	D	306	-	-	3/17/17/24	-
5	BOG	A	315	-	-	5/11/31/31	0/1/1/1
2	OLC	C	302	-	-	8/19/19/24	-
2	OLC	E	309	-	-	7/21/21/24	-
3	LFA	D	313	-	-	4/5/5/17	-
3	LFA	A	313	-	-	8/13/13/17	-
5	BOG	D	318	-	-	3/11/31/31	0/1/1/1
3	LFA	D	311	-	-	8/17/17/17	-
3	LFA	C	315	-	-	1/1/1/17	-
2	OLC	D	307	-	-	5/13/15/24	-
2	OLC	B	306	-	-	12/20/20/24	-
3	LFA	D	303	-	-	7/17/17/17	-
2	OLC	C	307	-	-	5/19/19/24	-
5	BOG	B	314	-	-	5/11/31/31	0/1/1/1
2	OLC	B	305	-	-	5/19/19/24	-
3	LFA	C	311	-	-	2/4/4/17	-
2	OLC	C	301	-	-	9/20/20/24	-
2	OLC	B	301	-	-	7/21/21/24	-
2	OLC	D	308	-	-	5/13/13/24	-
3	LFA	C	312	-	-	5/5/5/17	-
3	LFA	A	312	-	-	1/3/3/17	-
5	BOG	E	316	-	-	9/11/31/31	0/1/1/1
2	OLC	D	302	-	-	7/15/15/24	-
3	LFA	A	311	-	-	0/1/1/17	-
2	OLC	B	302	-	-	5/15/15/24	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	304	-	-	2/12/12/24	-
2	OLC	C	303	-	-	3/11/11/24	-
3	LFA	A	309	-	-	3/5/5/17	-
2	OLC	D	305	-	-	12/24/24/24	-
2	OLC	C	309	-	-	5/15/15/24	-
2	OLC	A	302	-	-	12/21/21/24	-
2	OLC	D	310	-	-	15/24/24/24	-
2	OLC	E	307	-	-	8/14/14/24	-
3	LFA	E	313	-	-	1/1/1/17	-
2	OLC	C	305	-	-	11/22/22/24	-
3	LFA	E	311	-	-	2/5/5/17	-
2	OLC	B	307	-	-	4/15/15/24	-
3	LFA	C	314	-	-	1/3/3/17	-
3	LFA	A	320	-	-	3/6/6/17	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	305	OLC	O20-C1	4.52	1.46	1.33
2	D	304	OLC	O20-C1	4.51	1.46	1.33
2	D	302	OLC	O20-C1	4.50	1.46	1.33
2	C	303	OLC	O20-C1	4.50	1.46	1.33
6	C	318	RET	C14-C13	4.47	1.37	1.33
2	C	308	OLC	O20-C1	4.46	1.46	1.33
2	C	306	OLC	O20-C1	4.45	1.46	1.33
2	E	305	OLC	O20-C1	4.44	1.46	1.33
2	B	302	OLC	O20-C1	4.43	1.46	1.33
2	E	309	OLC	O20-C1	4.43	1.46	1.33
2	A	303	OLC	O20-C1	4.43	1.46	1.33
2	D	306	OLC	O20-C1	4.41	1.46	1.33
2	E	310	OLC	O20-C1	4.41	1.46	1.33
2	E	306	OLC	O20-C1	4.39	1.46	1.33
2	B	306	OLC	O20-C1	4.37	1.46	1.33
2	C	309	OLC	O20-C1	4.36	1.46	1.33
2	A	304	OLC	O20-C1	4.35	1.46	1.33
2	C	301	OLC	O20-C1	4.35	1.46	1.33
2	C	307	OLC	O20-C1	4.34	1.46	1.33
2	D	305	OLC	O20-C1	4.33	1.46	1.33
2	B	304	OLC	O20-C1	4.32	1.46	1.33
2	E	301	OLC	O20-C1	4.32	1.46	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	305	OLC	O20-C1	4.31	1.45	1.33
2	C	302	OLC	O20-C1	4.29	1.45	1.33
2	A	306	OLC	O20-C1	4.29	1.45	1.33
2	D	301	OLC	O20-C1	4.27	1.45	1.33
6	E	317	RET	C14-C13	4.26	1.37	1.33
2	D	310	OLC	O20-C1	4.26	1.45	1.33
6	A	316	RET	C14-C13	4.23	1.37	1.33
2	B	301	OLC	O20-C1	4.22	1.45	1.33
2	B	307	OLC	O20-C1	4.21	1.45	1.33
2	D	308	OLC	O20-C1	4.21	1.45	1.33
6	C	318	RET	C10-C9	4.19	1.41	1.35
2	A	302	OLC	O20-C1	4.18	1.45	1.33
2	E	307	OLC	O20-C1	4.17	1.45	1.33
6	A	316	RET	C10-C9	4.16	1.41	1.35
6	B	315	RET	C10-C9	4.15	1.41	1.35
6	E	317	RET	C10-C9	4.14	1.41	1.35
2	C	305	OLC	O20-C1	4.10	1.45	1.33
6	D	319	RET	C10-C9	4.04	1.41	1.35
6	D	319	RET	C14-C13	3.80	1.36	1.33
6	B	315	RET	C14-C13	3.68	1.36	1.33
6	B	315	RET	C8-C9	-2.70	1.40	1.45
6	E	317	RET	C8-C9	-2.56	1.40	1.45
6	A	316	RET	C8-C9	-2.56	1.40	1.45
6	C	318	RET	C8-C9	-2.54	1.40	1.45
6	D	319	RET	C8-C9	-2.51	1.40	1.45
5	B	314	BOG	O1-C1	2.16	1.43	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	319	RET	C19-C9-C10	-4.07	117.22	122.92
6	B	315	RET	C19-C9-C10	-4.03	117.28	122.92
6	E	317	RET	C19-C9-C10	-3.94	117.40	122.92
6	A	316	RET	C19-C9-C10	-3.79	117.61	122.92
6	C	318	RET	C19-C9-C10	-3.76	117.66	122.92
2	A	304	OLC	O20-C1-C2	3.06	121.50	111.91
2	D	306	OLC	O20-C1-C2	3.05	121.48	111.91
2	C	301	OLC	O20-C1-C2	3.04	121.44	111.91
2	E	305	OLC	O20-C1-C2	3.02	121.38	111.91
2	A	302	OLC	O20-C1-C2	2.99	121.28	111.91
2	A	306	OLC	O20-C1-C2	2.95	121.16	111.91
2	D	302	OLC	O20-C1-C2	2.92	121.07	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	308	OLC	O20-C1-C2	2.92	121.06	111.91
2	A	305	OLC	O20-C1-C2	2.89	120.98	111.91
2	E	310	OLC	O20-C1-C2	2.85	120.86	111.91
2	C	307	OLC	O20-C1-C2	2.85	120.84	111.91
2	B	304	OLC	O20-C1-C2	2.84	120.83	111.91
2	B	305	OLC	O20-C1-C2	2.82	120.77	111.91
2	C	302	OLC	O20-C1-C2	2.79	120.68	111.91
2	E	306	OLC	O20-C1-C2	2.79	120.65	111.91
2	B	306	OLC	O20-C1-C2	2.77	120.60	111.91
2	D	304	OLC	O20-C1-C2	2.76	120.56	111.91
2	C	306	OLC	O20-C1-C2	2.71	120.42	111.91
2	B	301	OLC	O20-C1-C2	2.70	120.37	111.91
2	E	307	OLC	O20-C1-C2	2.69	120.36	111.91
2	A	303	OLC	O20-C1-C2	2.68	120.31	111.91
2	E	301	OLC	O20-C1-C2	2.63	120.17	111.91
2	B	302	OLC	O20-C1-C2	2.62	120.14	111.91
2	D	305	OLC	O20-C1-C2	2.61	120.11	111.91
2	B	307	OLC	O20-C1-C2	2.60	120.07	111.91
2	D	301	OLC	O20-C1-C2	2.59	120.03	111.91
2	C	303	OLC	O20-C1-C2	2.59	120.02	111.91
2	D	308	OLC	O20-C1-C2	2.58	120.01	111.91
2	E	309	OLC	O20-C1-C2	2.55	119.92	111.91
2	D	310	OLC	O20-C1-C2	2.48	119.69	111.91
2	C	309	OLC	O20-C1-C2	2.47	119.66	111.91
2	C	305	OLC	O20-C1-C2	2.45	119.60	111.91
2	E	307	OLC	O20-C1-O19	-2.38	117.58	123.59
6	D	319	RET	C8-C9-C10	2.34	122.53	118.94
2	A	302	OLC	O20-C1-O19	-2.31	117.77	123.59
2	A	306	OLC	O20-C1-O19	-2.29	117.83	123.59
6	B	315	RET	C8-C9-C10	2.27	122.43	118.94
2	A	304	OLC	O20-C1-O19	-2.26	117.89	123.59
2	C	305	OLC	O20-C1-O19	-2.22	117.99	123.59
2	B	305	OLC	O20-C1-O19	-2.03	118.46	123.59
2	C	302	OLC	O20-C1-O19	-2.03	118.47	123.59
2	D	308	OLC	O20-C1-O19	-2.03	118.48	123.59
2	A	305	OLC	O20-C1-O19	-2.01	118.53	123.59
2	C	309	OLC	O20-C1-O19	-2.00	118.53	123.59
2	B	307	OLC	O20-C1-O19	-2.00	118.54	123.59

There are no chirality outliers.

All (471) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	306	OLC	O20-C21-C22-C24
2	C	306	OLC	O20-C21-C22-O23
2	B	304	OLC	C21-C22-C24-O25
2	A	303	OLC	C6-C7-C8-C9
2	A	306	OLC	O20-C21-C22-C24
2	A	305	OLC	O20-C21-C22-C24
2	A	305	OLC	O20-C21-C22-O23
2	A	305	OLC	O19-C1-O20-C21
2	E	306	OLC	C21-C22-C24-O25
2	E	306	OLC	O20-C21-C22-O23
2	C	308	OLC	C21-C22-C24-O25
2	C	308	OLC	O23-C22-C24-O25
2	E	301	OLC	C21-C22-C24-O25
2	E	301	OLC	O23-C22-C24-O25
3	C	315	LFA	C17-C18-C19-C20
2	B	306	OLC	C21-C22-C24-O25
2	B	306	OLC	O20-C21-C22-C24
2	C	307	OLC	C21-C22-C24-O25
2	C	307	OLC	O23-C22-C24-O25
2	B	305	OLC	C10-C11-C12-C13
2	C	301	OLC	C21-C22-C24-O25
2	D	308	OLC	C21-C22-C24-O25
2	D	308	OLC	O23-C22-C24-O25
5	E	316	BOG	C2-C1-O1-C1'
5	E	316	BOG	O5-C1-O1-C1'
5	E	316	BOG	C2'-C1'-O1-C1
2	D	302	OLC	O20-C21-C22-O23
2	B	302	OLC	C21-C22-C24-O25
2	C	303	OLC	C21-C22-C24-O25
2	D	305	OLC	C21-C22-C24-O25
2	D	310	OLC	C21-C22-C24-O25
2	D	310	OLC	O23-C22-C24-O25
2	D	310	OLC	O19-C1-O20-C21
2	E	307	OLC	O20-C21-C22-C24
2	E	307	OLC	O20-C21-C22-O23
3	E	313	LFA	C17-C18-C19-C20
2	B	307	OLC	C21-C22-C24-O25
2	B	307	OLC	O23-C22-C24-O25
2	A	305	OLC	C2-C1-O20-C21
2	A	306	OLC	O19-C1-O20-C21
2	D	305	OLC	O19-C1-O20-C21
2	C	305	OLC	O19-C1-O20-C21
2	D	305	OLC	C2-C1-O20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	310	OLC	C2-C1-O20-C21
2	C	305	OLC	C2-C1-O20-C21
2	A	306	OLC	C2-C1-O20-C21
2	D	301	OLC	C2-C1-O20-C21
2	E	307	OLC	O19-C1-O20-C21
2	E	307	OLC	C2-C1-O20-C21
5	E	316	BOG	O5-C5-C6-O6
2	A	306	OLC	O20-C21-C22-O23
2	B	306	OLC	O20-C21-C22-O23
2	A	304	OLC	O20-C21-C22-O23
2	D	301	OLC	O19-C1-O20-C21
5	E	316	BOG	C4-C5-C6-O6
2	A	303	OLC	C2-C1-O20-C21
2	D	306	OLC	C2-C1-O20-C21
2	B	305	OLC	C2-C1-O20-C21
2	B	301	OLC	C2-C1-O20-C21
2	D	302	OLC	C2-C1-O20-C21
2	B	304	OLC	O20-C21-C22-C24
2	A	303	OLC	O19-C1-O20-C21
5	A	315	BOG	O5-C5-C6-O6
2	E	310	OLC	C1-C2-C3-C4
2	D	304	OLC	C1-C2-C3-C4
2	E	309	OLC	C1-C2-C3-C4
2	D	306	OLC	O19-C1-O20-C21
2	B	301	OLC	O19-C1-O20-C21
2	B	307	OLC	C2-C1-O20-C21
2	B	302	OLC	O23-C22-C24-O25
2	B	305	OLC	O19-C1-O20-C21
2	B	304	OLC	C1-C2-C3-C4
2	C	302	OLC	C1-C2-C3-C4
2	D	308	OLC	C1-C2-C3-C4
2	B	302	OLC	C1-C2-C3-C4
2	E	304	OLC	C4-C5-C6-C7
5	B	314	BOG	O5-C5-C6-O6
2	D	302	OLC	O19-C1-O20-C21
5	A	315	BOG	C4-C5-C6-O6
5	B	314	BOG	C4-C5-C6-O6
2	B	307	OLC	O19-C1-O20-C21
2	B	304	OLC	O20-C21-C22-O23
2	E	305	OLC	O20-C21-C22-O23
2	E	310	OLC	O20-C21-C22-O23
2	D	304	OLC	O20-C21-C22-O23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	E	309	OLC	O20-C21-C22-O23
2	A	303	OLC	C1-C2-C3-C4
2	E	306	OLC	C2-C1-O20-C21
2	B	306	OLC	C2-C1-O20-C21
5	E	316	BOG	O1-C1'-C2'-C3'
2	A	305	OLC	C13-C14-C15-C16
2	A	305	OLC	C4-C5-C6-C7
3	D	314	LFA	C5-C6-C7-C8
2	B	306	OLC	C2-C3-C4-C5
5	E	316	BOG	C2'-C3'-C4'-C5'
2	E	306	OLC	O20-C21-C22-C24
2	E	310	OLC	O20-C21-C22-C24
2	D	304	OLC	O20-C21-C22-C24
2	E	309	OLC	O20-C21-C22-C24
2	D	302	OLC	O20-C21-C22-C24
3	D	313	LFA	C2-C3-C4-C5
5	B	314	BOG	C3'-C4'-C5'-C6'
3	C	312	LFA	C15-C16-C17-C18
2	D	310	OLC	C11-C12-C13-C14
3	D	312	LFA	C14-C15-C16-C17
2	C	302	OLC	C3-C4-C5-C6
2	C	310	OLC	C5-C6-C7-C8
2	E	305	OLC	C5-C6-C7-C8
3	A	310	LFA	C16-C17-C18-C19
3	E	312	LFA	C13-C14-C15-C16
2	A	318	OLC	C13-C14-C15-C16
3	D	320	LFA	C2-C3-C4-C5
2	E	309	OLC	C11-C12-C13-C14
3	C	312	LFA	C16-C17-C18-C19
2	C	305	OLC	C4-C5-C6-C7
2	C	306	OLC	C3-C4-C5-C6
3	B	310	LFA	C3-C4-C5-C6
3	D	303	LFA	C11-C10-C9-C8
2	A	302	OLC	C3-C4-C5-C6
2	C	306	OLC	C1-C2-C3-C4
2	C	301	OLC	C5-C6-C7-C8
2	D	310	OLC	C4-C5-C6-C7
2	E	305	OLC	C3-C4-C5-C6
3	E	312	LFA	C9-C10-C11-C12
3	B	310	LFA	C2-C3-C4-C5
2	A	307	OLC	C4-C5-C6-C7
2	D	307	OLC	C2-C3-C4-C5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	312	LFA	C2-C3-C4-C5
3	A	309	LFA	C4-C5-C6-C7
2	A	318	OLC	C5-C6-C7-C8
2	C	302	OLC	C5-C6-C7-C8
2	A	318	OLC	C12-C13-C14-C15
3	D	314	LFA	C11-C12-C13-C14
3	A	313	LFA	C3-C4-C5-C6
3	A	313	LFA	C4-C5-C6-C7
2	A	302	OLC	C21-C22-C24-O25
2	E	307	OLC	C21-C22-C24-O25
2	C	305	OLC	C21-C22-C24-O25
2	D	301	OLC	O20-C21-C22-O23
3	E	312	LFA	C14-C15-C16-C17
3	B	303	LFA	C16-C17-C18-C19
2	C	309	OLC	C3-C4-C5-C6
2	A	305	OLC	C10-C11-C12-C13
2	D	301	OLC	C6-C7-C8-C9
2	D	307	OLC	C10-C11-C12-C13
3	B	309	LFA	C14-C15-C16-C17
2	E	306	OLC	C4-C5-C6-C7
3	D	314	LFA	C7-C8-C9-C10
3	D	311	LFA	C6-C7-C8-C9
3	D	311	LFA	C9-C10-C11-C12
3	D	303	LFA	C9-C10-C11-C12
2	D	310	OLC	C13-C14-C15-C16
3	D	312	LFA	C11-C12-C13-C14
3	D	320	LFA	C3-C4-C5-C6
3	D	303	LFA	C12-C13-C14-C15
2	A	305	OLC	C3-C4-C5-C6
2	C	301	OLC	C4-C5-C6-C7
2	E	305	OLC	C10-C11-C12-C13
2	C	308	OLC	C2-C3-C4-C5
2	A	302	OLC	C4-C5-C6-C7
2	C	309	OLC	C2-C1-O20-C21
3	A	313	LFA	C10-C11-C12-C13
2	C	305	OLC	C3-C4-C5-C6
3	C	313	LFA	C13-C14-C15-C16
2	A	318	OLC	C11-C12-C13-C14
3	D	311	LFA	C3-C4-C5-C6
3	D	315	LFA	C15-C16-C17-C18
2	C	301	OLC	O23-C22-C24-O25
2	D	305	OLC	O23-C22-C24-O25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	E	307	OLC	O23-C22-C24-O25
3	E	302	LFA	C7-C8-C9-C10
3	D	312	LFA	C13-C14-C15-C16
3	D	314	LFA	C13-C14-C15-C16
2	E	301	OLC	C10-C11-C12-C13
2	E	306	OLC	O19-C1-O20-C21
2	B	306	OLC	O19-C1-O20-C21
5	A	315	BOG	C1'-C2'-C3'-C4'
5	D	318	BOG	C1'-C2'-C3'-C4'
3	A	319	LFA	C16-C17-C18-C19
2	A	305	OLC	C2-C3-C4-C5
2	D	310	OLC	C12-C13-C14-C15
3	D	312	LFA	C4-C5-C6-C7
5	C	317	BOG	C1'-C2'-C3'-C4'
3	B	309	LFA	C16-C17-C18-C19
2	B	306	OLC	C5-C6-C7-C8
2	D	305	OLC	C4-C5-C6-C7
3	C	311	LFA	C2-C3-C4-C5
5	B	314	BOG	C1'-C2'-C3'-C4'
3	E	312	LFA	C15-C16-C17-C18
3	C	304	LFA	C2-C3-C4-C5
3	C	304	LFA	C7-C8-C9-C10
2	C	308	OLC	C5-C6-C7-C8
2	C	309	OLC	O19-C1-O20-C21
2	A	303	OLC	C13-C14-C15-C16
2	B	304	OLC	C10-C11-C12-C13
2	A	301	OLC	C10-C11-C12-C13
2	E	310	OLC	C6-C7-C8-C9
2	A	317	OLC	C6-C7-C8-C9
2	D	301	OLC	C1-C2-C3-C4
3	D	311	LFA	C11-C10-C9-C8
2	B	304	OLC	C14-C15-C16-C17
3	C	304	LFA	C16-C17-C18-C19
2	E	301	OLC	C1-C2-C3-C4
2	D	301	OLC	O20-C21-C22-C24
2	B	304	OLC	C3-C4-C5-C6
2	A	305	OLC	C12-C13-C14-C15
3	C	313	LFA	C4-C5-C6-C7
3	E	302	LFA	C11-C10-C9-C8
2	B	304	OLC	C4-C5-C6-C7
2	E	305	OLC	C4-C5-C6-C7
3	A	319	LFA	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	315	BOG	C3'-C4'-C5'-C6'
2	C	305	OLC	C12-C13-C14-C15
3	C	304	LFA	C15-C16-C17-C18
3	A	319	LFA	C13-C14-C15-C16
2	E	310	OLC	C4-C5-C6-C7
3	B	311	LFA	C5-C6-C7-C8
3	C	313	LFA	C12-C13-C14-C15
2	E	310	OLC	C3-C4-C5-C6
3	D	320	LFA	C4-C5-C6-C7
3	D	303	LFA	C7-C8-C9-C10
2	A	305	OLC	C6-C7-C8-C9
2	B	306	OLC	C10-C11-C12-C13
2	C	307	OLC	C6-C7-C8-C9
2	A	302	OLC	C6-C7-C8-C9
3	A	313	LFA	C7-C8-C9-C10
2	E	304	OLC	C5-C6-C7-C8
3	A	313	LFA	C11-C12-C13-C14
3	D	315	LFA	C16-C17-C18-C19
3	D	311	LFA	C4-C5-C6-C7
3	D	311	LFA	C14-C15-C16-C17
2	D	308	OLC	C2-C3-C4-C5
3	A	320	LFA	C4-C5-C6-C7
2	A	302	OLC	C10-C11-C12-C13
2	C	308	OLC	C1-C2-C3-C4
3	C	304	LFA	C13-C14-C15-C16
2	C	302	OLC	C4-C5-C6-C7
2	B	308	OLC	C4-C5-C6-C7
2	A	303	OLC	C14-C15-C16-C17
5	E	316	BOG	C1'-C2'-C3'-C4'
3	B	312	LFA	C15-C16-C17-C18
3	B	303	LFA	C11-C10-C9-C8
3	A	309	LFA	C5-C6-C7-C8
5	A	315	BOG	C5'-C6'-C7'-C8'
5	B	314	BOG	C5'-C6'-C7'-C8'
3	D	312	LFA	C1-C2-C3-C4
5	C	317	BOG	C5'-C6'-C7'-C8'
2	A	307	OLC	C6-C7-C8-C9
2	A	317	OLC	C13-C14-C15-C16
2	C	310	OLC	C6-C7-C8-C9
3	D	312	LFA	C3-C4-C5-C6
3	D	313	LFA	C4-C5-C6-C7
2	E	306	OLC	O23-C22-C24-O25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	306	OLC	O23-C22-C24-O25
2	C	303	OLC	O23-C22-C24-O25
2	A	302	OLC	O23-C22-C24-O25
3	B	311	LFA	C7-C8-C9-C10
2	D	306	OLC	C5-C6-C7-C8
2	C	308	OLC	C6-C7-C8-C9
2	C	306	OLC	C5-C6-C7-C8
2	B	304	OLC	C5-C6-C7-C8
2	A	317	OLC	C14-C15-C16-C17
2	E	301	OLC	C14-C15-C16-C17
3	A	313	LFA	C5-C6-C7-C8
3	D	314	LFA	C3-C4-C5-C6
2	E	301	OLC	C4-C5-C6-C7
2	D	310	OLC	C2-C3-C4-C5
2	A	302	OLC	O20-C21-C22-C24
2	A	305	OLC	C11-C12-C13-C14
3	D	314	LFA	C14-C15-C16-C17
3	D	311	LFA	C11-C12-C13-C14
3	C	304	LFA	C4-C5-C6-C7
2	D	307	OLC	C5-C6-C7-C8
2	C	309	OLC	C4-C5-C6-C7
2	C	306	OLC	C2-C1-O20-C21
2	D	305	OLC	C6-C7-C8-C9
2	D	310	OLC	C10-C11-C12-C13
3	D	313	LFA	C5-C6-C7-C8
3	B	303	LFA	C6-C7-C8-C9
2	D	309	OLC	C2-C3-C4-C5
3	A	313	LFA	C13-C14-C15-C16
3	E	311	LFA	C16-C17-C18-C19
2	E	310	OLC	C2-C1-O20-C21
2	A	317	OLC	C11-C12-C13-C14
3	A	319	LFA	C6-C7-C8-C9
3	C	313	LFA	C15-C16-C17-C18
2	D	309	OLC	C4-C5-C6-C7
2	E	309	OLC	C4-C5-C6-C7
2	E	303	OLC	C4-C5-C6-C7
2	C	302	OLC	C10-C11-C12-C13
2	D	310	OLC	C5-C6-C7-C8
2	E	306	OLC	C3-C4-C5-C6
2	C	305	OLC	C5-C6-C7-C8
3	B	303	LFA	C10-C11-C12-C13
5	D	318	BOG	C3'-C4'-C5'-C6'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	C	313	LFA	C9-C10-C11-C12
2	C	306	OLC	O19-C1-O20-C21
3	C	313	LFA	C10-C11-C12-C13
2	E	306	OLC	C5-C6-C7-C8
3	D	303	LFA	C10-C11-C12-C13
2	B	308	OLC	C6-C7-C8-C9
2	C	305	OLC	C10-C11-C12-C13
2	A	317	OLC	C3-C4-C5-C6
2	E	310	OLC	O19-C1-O20-C21
3	C	312	LFA	C17-C18-C19-C20
3	D	315	LFA	C14-C15-C16-C17
2	D	302	OLC	C4-C5-C6-C7
2	D	305	OLC	C3-C4-C5-C6
5	E	316	BOG	C5'-C6'-C7'-C8'
3	C	311	LFA	C4-C5-C6-C7
3	A	313	LFA	C11-C10-C9-C8
3	A	320	LFA	C3-C4-C5-C6
2	E	307	OLC	C2-C3-C4-C5
2	E	304	OLC	C11-C12-C13-C14
3	C	304	LFA	C3-C4-C5-C6
2	C	303	OLC	O20-C21-C22-O23
2	D	309	OLC	C5-C6-C7-C8
3	A	309	LFA	C1-C2-C3-C4
3	A	310	LFA	C15-C16-C17-C18
3	C	313	LFA	C11-C12-C13-C14
2	D	301	OLC	C7-C8-C9-C10
2	E	310	OLC	C2-C3-C4-C5
3	D	320	LFA	C11-C12-C13-C14
2	B	302	OLC	C2-C1-O20-C21
2	A	302	OLC	O20-C21-C22-O23
2	D	301	OLC	C2-C3-C4-C5
2	B	308	OLC	C7-C8-C9-C10
2	B	304	OLC	O23-C22-C24-O25
2	E	304	OLC	C13-C14-C15-C16
2	B	301	OLC	C10-C11-C12-C13
3	D	312	LFA	C10-C11-C12-C13
2	A	317	OLC	C5-C6-C7-C8
2	A	302	OLC	C2-C3-C4-C5
3	A	308	LFA	C17-C18-C19-C20
3	D	313	LFA	C1-C2-C3-C4
2	D	302	OLC	C5-C6-C7-C8
2	B	302	OLC	O19-C1-O20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	302	OLC	C6-C7-C8-C9
3	C	304	LFA	C1-C2-C3-C4
3	D	312	LFA	C5-C6-C7-C8
3	B	311	LFA	C1-C2-C3-C4
2	A	317	OLC	C12-C13-C14-C15
2	A	317	OLC	C2-C3-C4-C5
2	C	308	OLC	C10-C11-C12-C13
3	C	313	LFA	C14-C15-C16-C17
3	C	304	LFA	C14-C15-C16-C17
3	C	304	LFA	C9-C10-C11-C12
3	B	303	LFA	C9-C10-C11-C12
2	A	318	OLC	C15-C16-C17-C18
2	E	307	OLC	C4-C5-C6-C7
3	D	312	LFA	C12-C13-C14-C15
3	C	312	LFA	C13-C14-C15-C16
3	C	313	LFA	C16-C17-C18-C19
2	B	305	OLC	C4-C5-C6-C7
3	E	302	LFA	C12-C13-C14-C15
2	B	301	OLC	O20-C21-C22-C24
2	D	310	OLC	C1-C2-C3-C4
3	E	312	LFA	C7-C8-C9-C10
3	E	302	LFA	C15-C16-C17-C18
3	D	314	LFA	C11-C10-C9-C8
3	B	310	LFA	C5-C6-C7-C8
3	D	311	LFA	C7-C8-C9-C10
3	C	304	LFA	C12-C13-C14-C15
2	A	306	OLC	C3-C4-C5-C6
2	E	310	OLC	C5-C6-C7-C8
3	E	311	LFA	C17-C18-C19-C20
2	E	301	OLC	C3-C4-C5-C6
2	B	306	OLC	C4-C5-C6-C7
3	D	303	LFA	C4-C5-C6-C7
3	C	312	LFA	C14-C15-C16-C17
2	C	308	OLC	C4-C5-C6-C7
2	A	318	OLC	C7-C8-C9-C10
2	E	304	OLC	C7-C8-C9-C10
2	D	305	OLC	C9-C10-C11-C12
2	E	301	OLC	C5-C6-C7-C8
2	D	305	OLC	C1-C2-C3-C4
2	A	318	OLC	C6-C7-C8-C9
2	C	307	OLC	C2-C3-C4-C5
2	E	301	OLC	C22-C21-O20-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	E	314	LFA	C17-C18-C19-C20
3	B	310	LFA	C1-C2-C3-C4
2	C	301	OLC	C10-C11-C12-C13
3	E	302	LFA	C17-C18-C19-C20
2	C	301	OLC	C11-C12-C13-C14
2	C	308	OLC	C7-C8-C9-C10
2	C	307	OLC	C5-C6-C7-C8
2	B	304	OLC	C13-C14-C15-C16
2	C	302	OLC	O20-C21-C22-C24
2	A	304	OLC	O20-C21-C22-C24
2	D	305	OLC	O20-C21-C22-C24
2	B	306	OLC	C3-C4-C5-C6
2	B	301	OLC	C5-C6-C7-C8
2	A	303	OLC	C9-C10-C11-C12
2	B	301	OLC	C7-C8-C9-C10
2	C	305	OLC	O23-C22-C24-O25
2	E	309	OLC	C7-C8-C9-C10
3	C	313	LFA	C6-C7-C8-C9
2	A	307	OLC	C5-C6-C7-C8
2	A	318	OLC	C14-C15-C16-C17
3	D	303	LFA	C17-C18-C19-C20
3	E	302	LFA	C5-C6-C7-C8
3	E	302	LFA	C4-C5-C6-C7
3	C	313	LFA	C11-C10-C9-C8
2	C	309	OLC	C6-C7-C8-C9
5	C	317	BOG	C4-C5-C6-O6
2	A	303	OLC	C15-C16-C17-C18
2	D	305	OLC	C12-C13-C14-C15
2	D	310	OLC	C3-C4-C5-C6
2	D	310	OLC	C15-C16-C17-C18
2	B	305	OLC	C9-C10-C11-C12
2	C	302	OLC	O20-C21-C22-O23
2	C	306	OLC	C9-C10-C11-C12
2	E	301	OLC	C7-C8-C9-C10
2	D	307	OLC	C7-C8-C9-C10
3	A	320	LFA	C1-C2-C3-C4
3	C	314	LFA	C6-C7-C8-C9
3	E	302	LFA	C11-C12-C13-C14
3	A	319	LFA	C12-C13-C14-C15
3	B	309	LFA	C15-C16-C17-C18
2	A	317	OLC	C10-C11-C12-C13
3	D	314	LFA	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	E	305	OLC	C9-C10-C11-C12
2	A	305	OLC	C9-C10-C11-C12
2	E	310	OLC	C9-C10-C11-C12
2	D	310	OLC	C7-C8-C9-C10
2	A	301	OLC	C11-C12-C13-C14
3	B	312	LFA	C17-C18-C19-C20
3	B	311	LFA	C2-C3-C4-C5
3	D	314	LFA	C2-C3-C4-C5
2	A	303	OLC	C7-C8-C9-C10
2	A	301	OLC	C9-C10-C11-C12
2	E	304	OLC	C9-C10-C11-C12
2	B	306	OLC	C7-C8-C9-C10
2	C	301	OLC	C7-C8-C9-C10
2	E	304	OLC	C3-C4-C5-C6
3	B	303	LFA	C17-C18-C19-C20
2	A	303	OLC	O20-C1-C2-C3
2	B	304	OLC	C9-C10-C11-C12
2	B	304	OLC	C7-C8-C9-C10
2	C	305	OLC	C9-C10-C11-C12
3	A	319	LFA	C14-C15-C16-C17
2	E	309	OLC	C9-C10-C11-C12
2	A	306	OLC	C5-C6-C7-C8
3	A	319	LFA	C2-C3-C4-C5
2	A	318	OLC	C9-C10-C11-C12
2	C	302	OLC	C9-C10-C11-C12
2	D	305	OLC	C14-C15-C16-C17
3	B	303	LFA	C7-C8-C9-C10
2	A	302	OLC	C9-C10-C11-C12
2	C	305	OLC	C7-C8-C9-C10
2	E	310	OLC	C21-C22-C24-O25
2	D	308	OLC	C2-C1-O20-C21
2	D	307	OLC	C1-C2-C3-C4
3	D	315	LFA	C17-C18-C19-C20
2	A	302	OLC	C2-C1-O20-C21
2	B	301	OLC	C3-C4-C5-C6
3	B	303	LFA	C5-C6-C7-C8
2	A	302	OLC	O19-C1-O20-C21
3	A	310	LFA	C14-C15-C16-C17
2	A	303	OLC	O19-C1-C2-C3
2	C	301	OLC	C2-C1-O20-C21
2	C	301	OLC	O19-C1-O20-C21
3	C	313	LFA	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	301	OLC	C4-C5-C6-C7
3	D	320	LFA	C1-C2-C3-C4
2	E	306	OLC	O20-C1-C2-C3
3	C	304	LFA	C17-C18-C19-C20
5	D	318	BOG	C2'-C3'-C4'-C5'
2	A	303	OLC	C12-C13-C14-C15
3	A	319	LFA	C9-C10-C11-C12
2	E	304	OLC	C12-C13-C14-C15

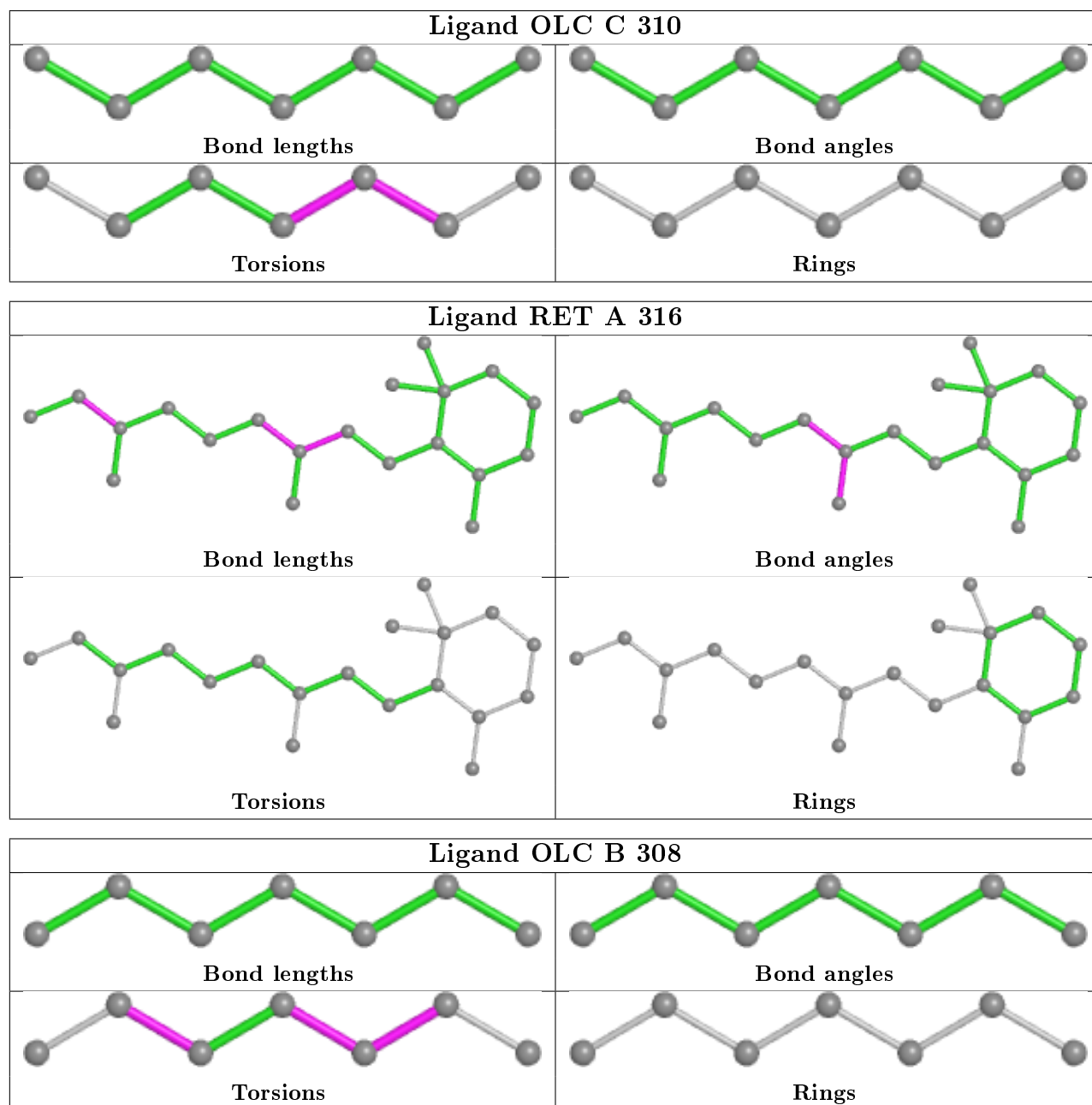
There are no ring outliers.

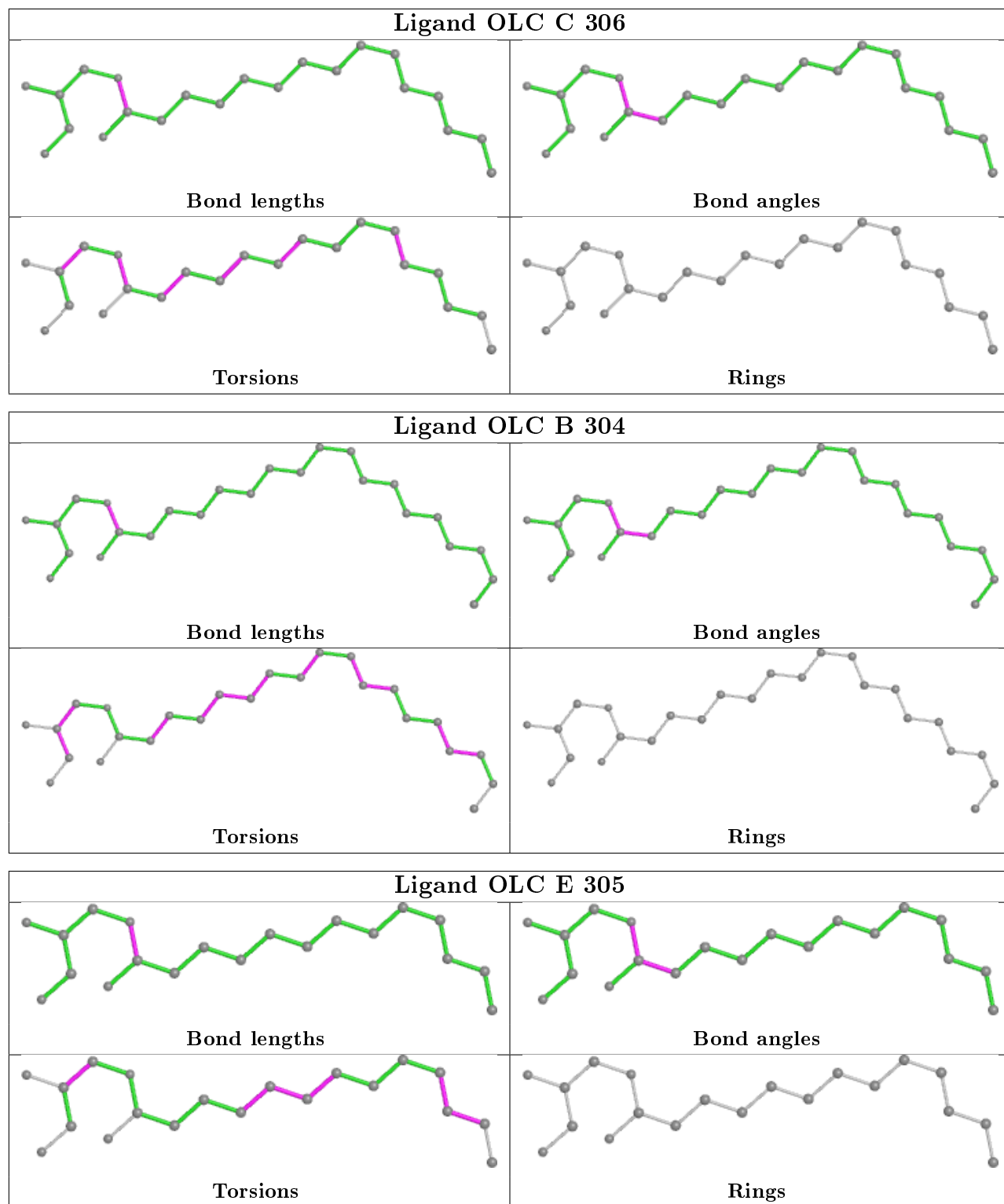
27 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	316	RET	4	0
2	B	304	OLC	1	0
6	B	315	RET	3	0
2	A	303	OLC	1	0
6	D	319	RET	2	0
3	C	304	LFA	2	0
3	C	313	LFA	1	0
6	E	317	RET	3	0
5	C	317	BOG	1	0
3	D	314	LFA	1	0
6	C	318	RET	2	0
2	A	317	OLC	2	0
2	E	304	OLC	2	0
2	D	301	OLC	2	0
3	D	320	LFA	1	0
5	A	315	BOG	2	0
2	C	302	OLC	1	0
2	E	309	OLC	1	0
5	D	318	BOG	3	0
3	D	303	LFA	1	0
5	B	314	BOG	2	0
3	C	311	LFA	5	0
2	B	301	OLC	4	0
2	C	309	OLC	1	0
2	A	302	OLC	2	0
2	D	310	OLC	1	0
2	C	305	OLC	4	0

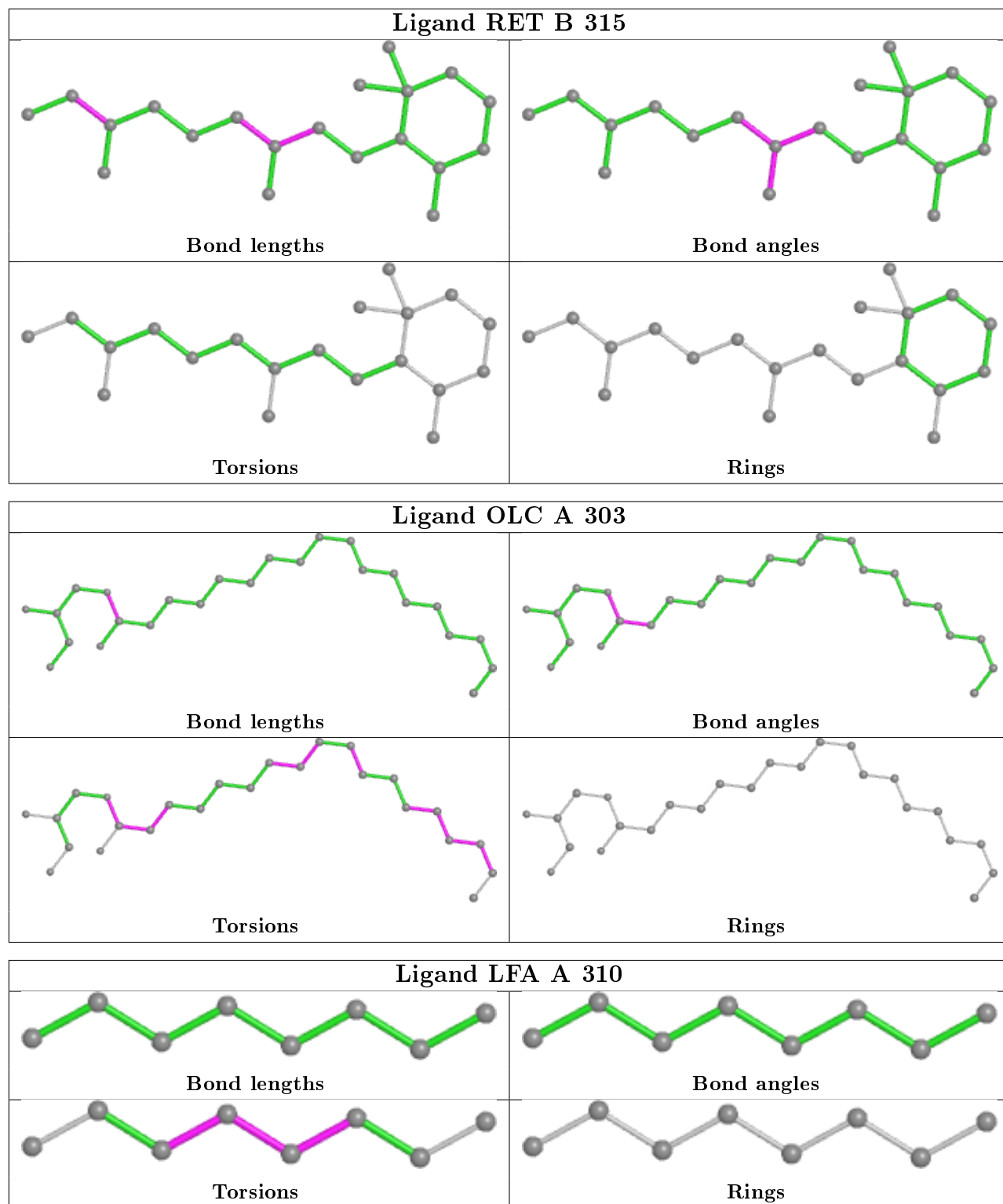
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

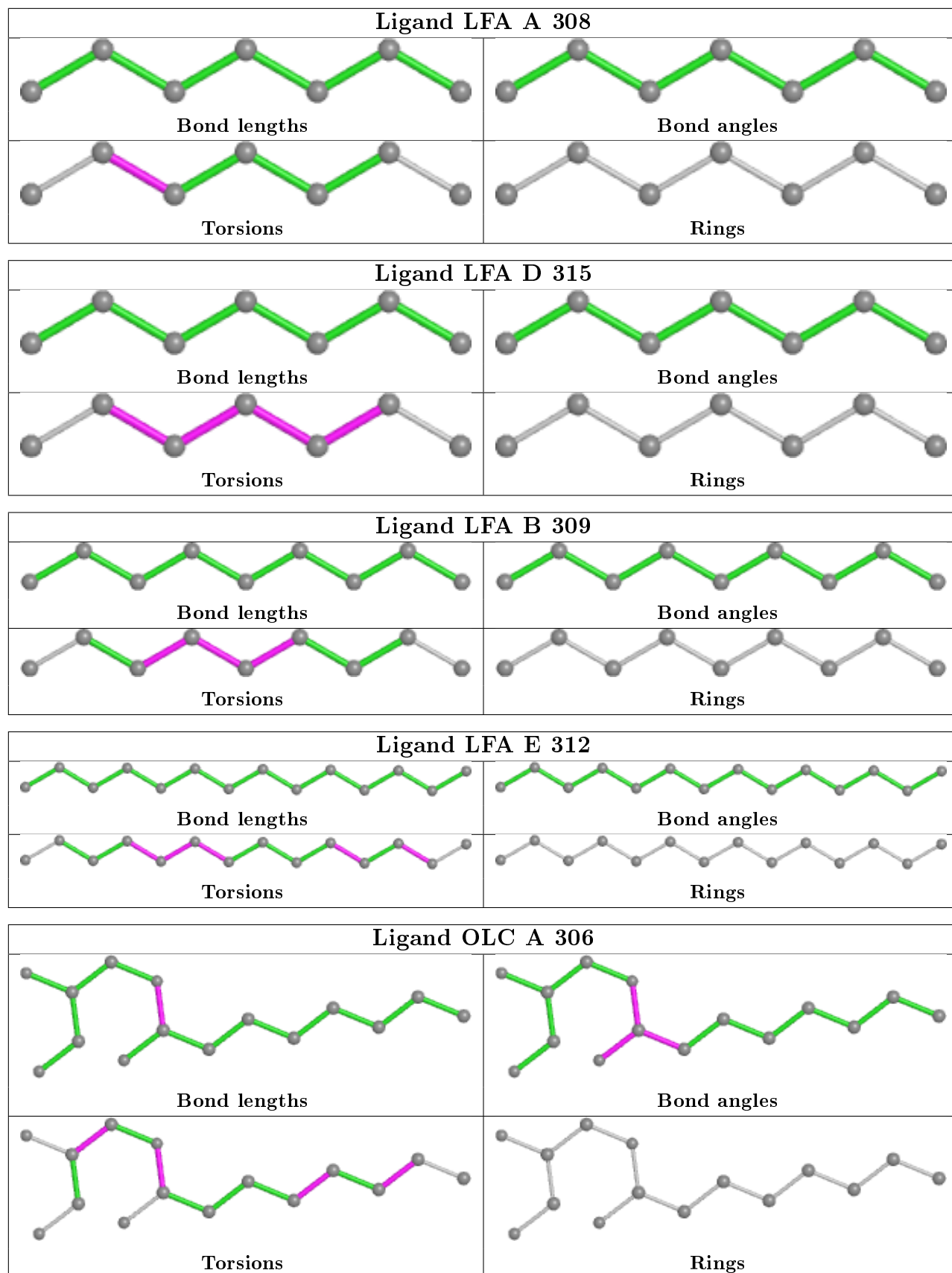
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

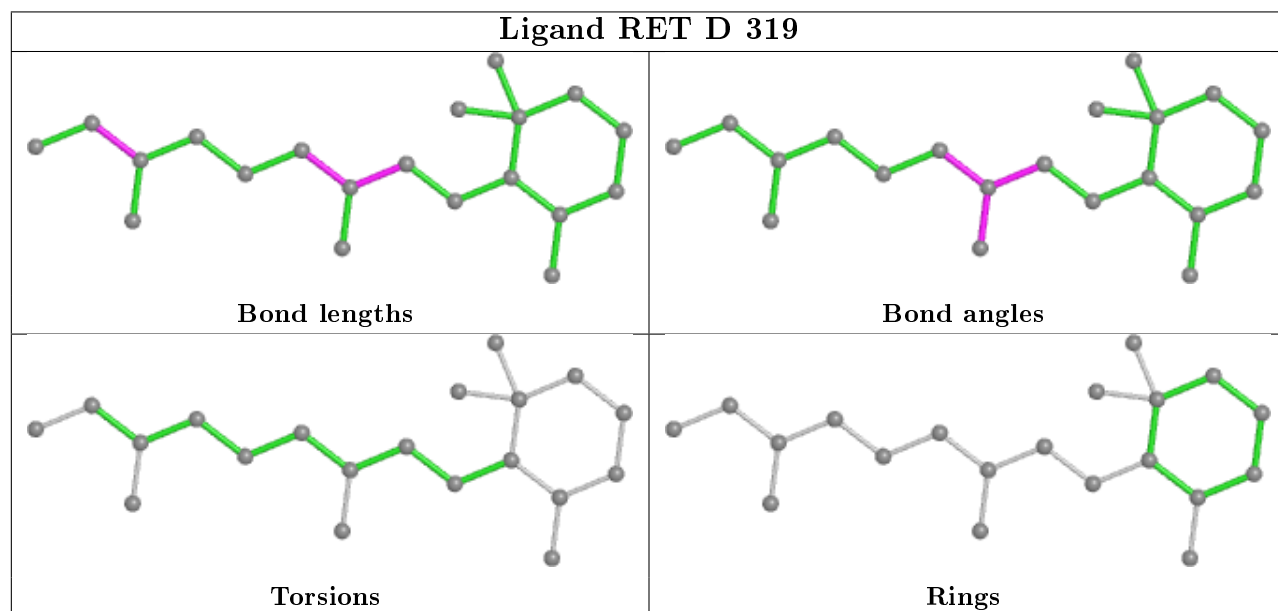
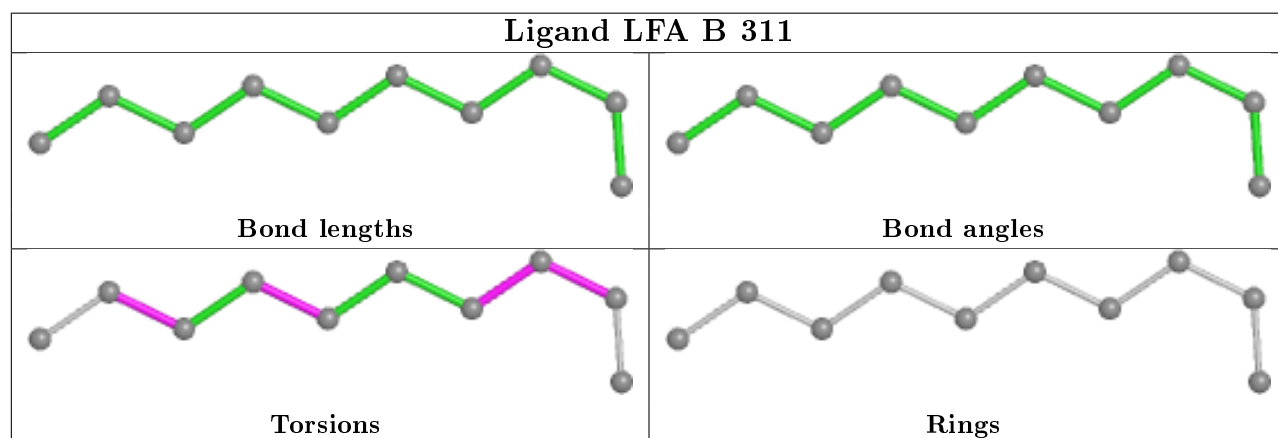
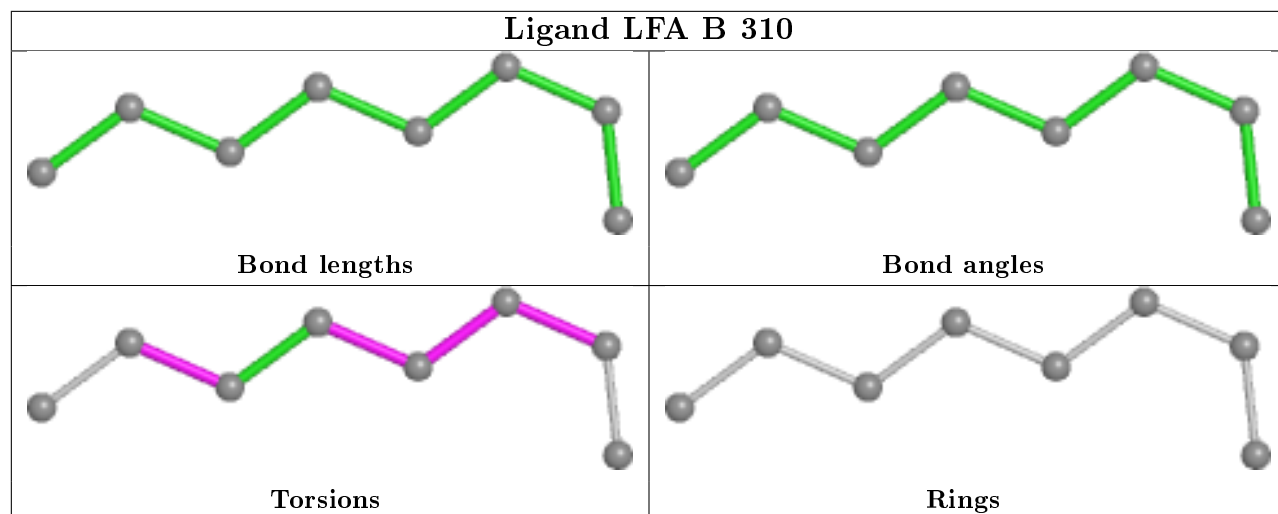


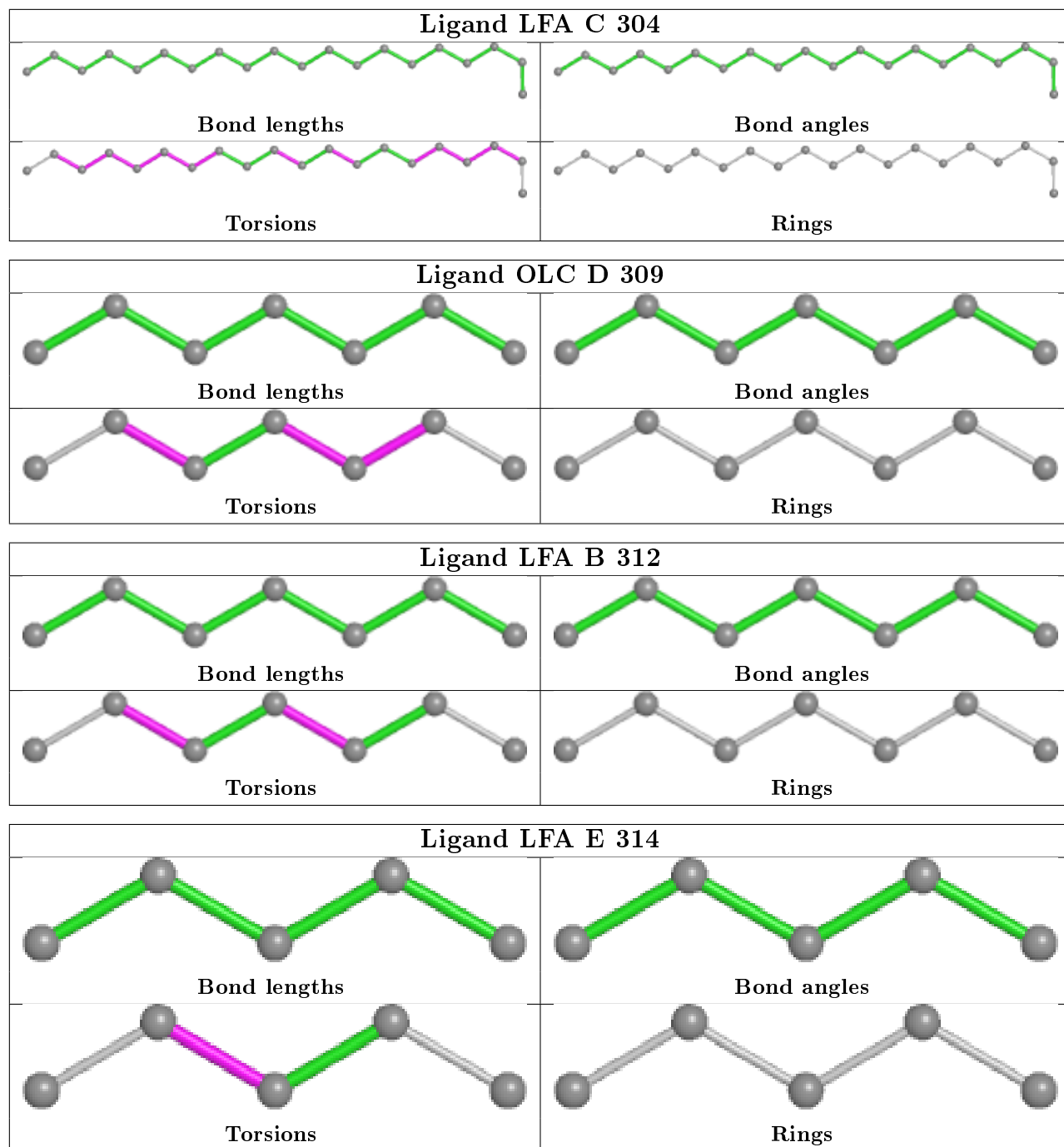


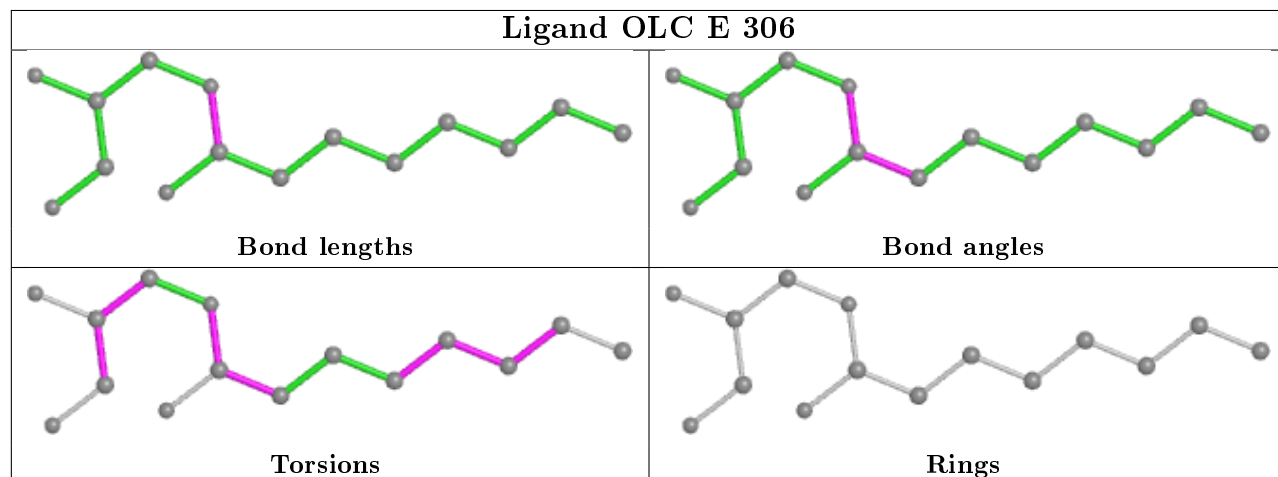
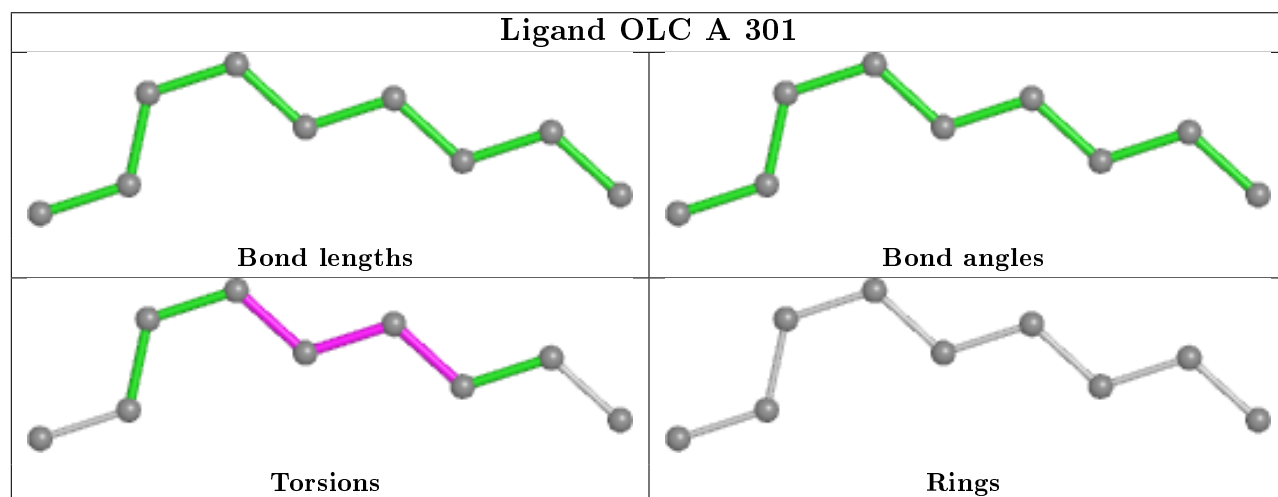
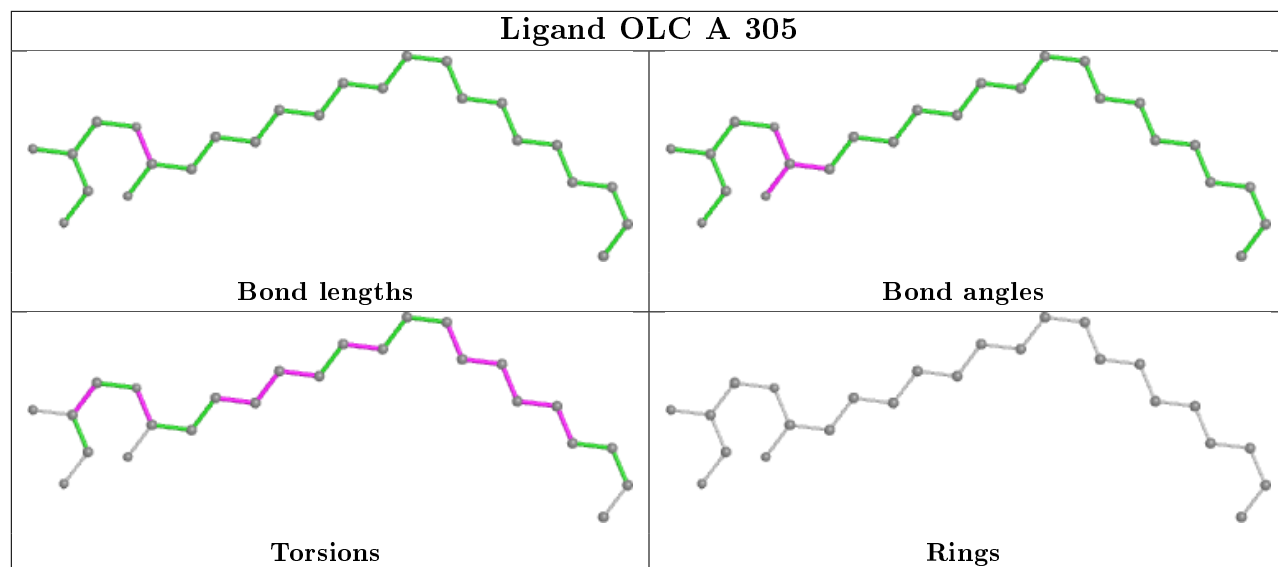


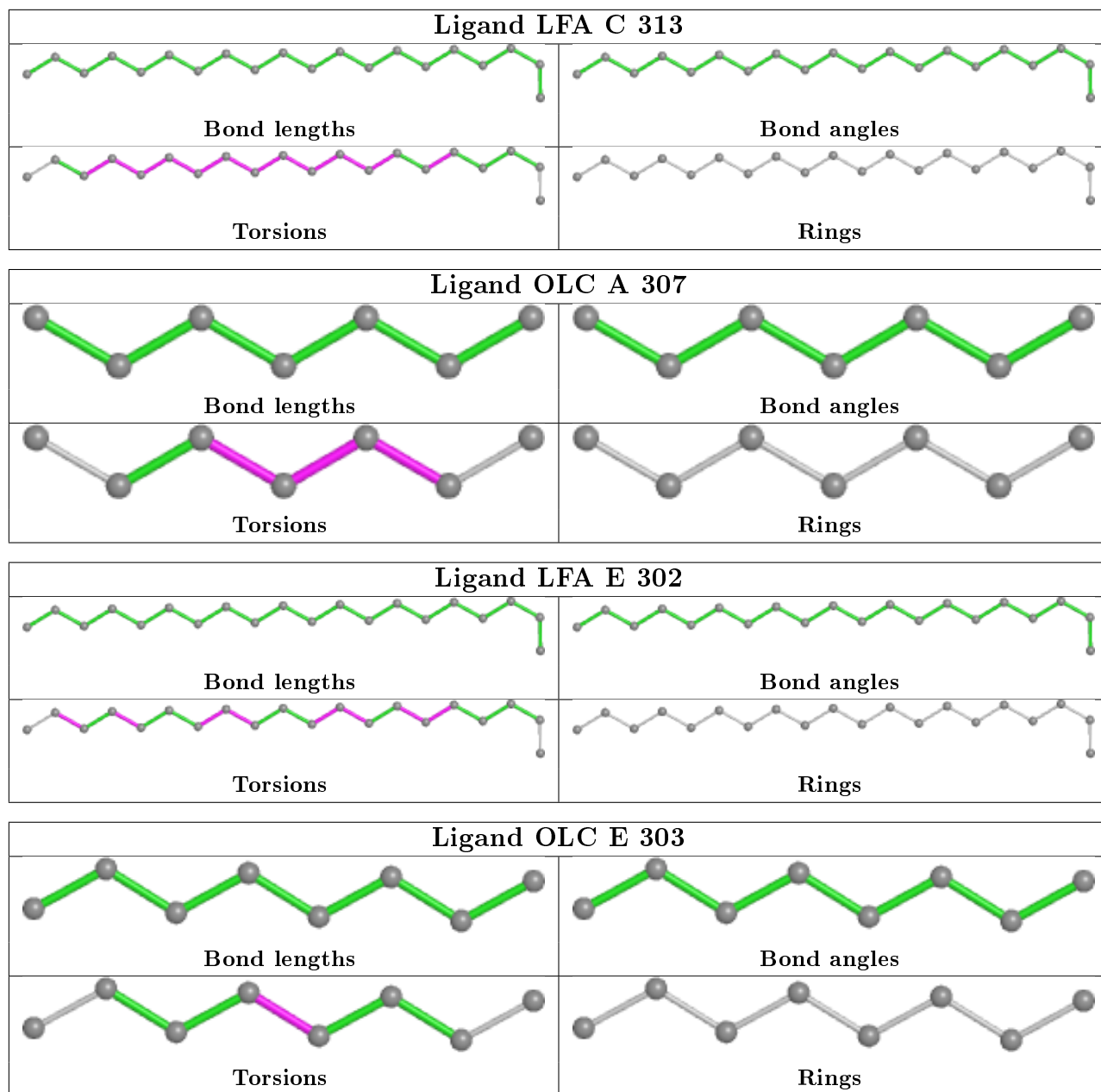


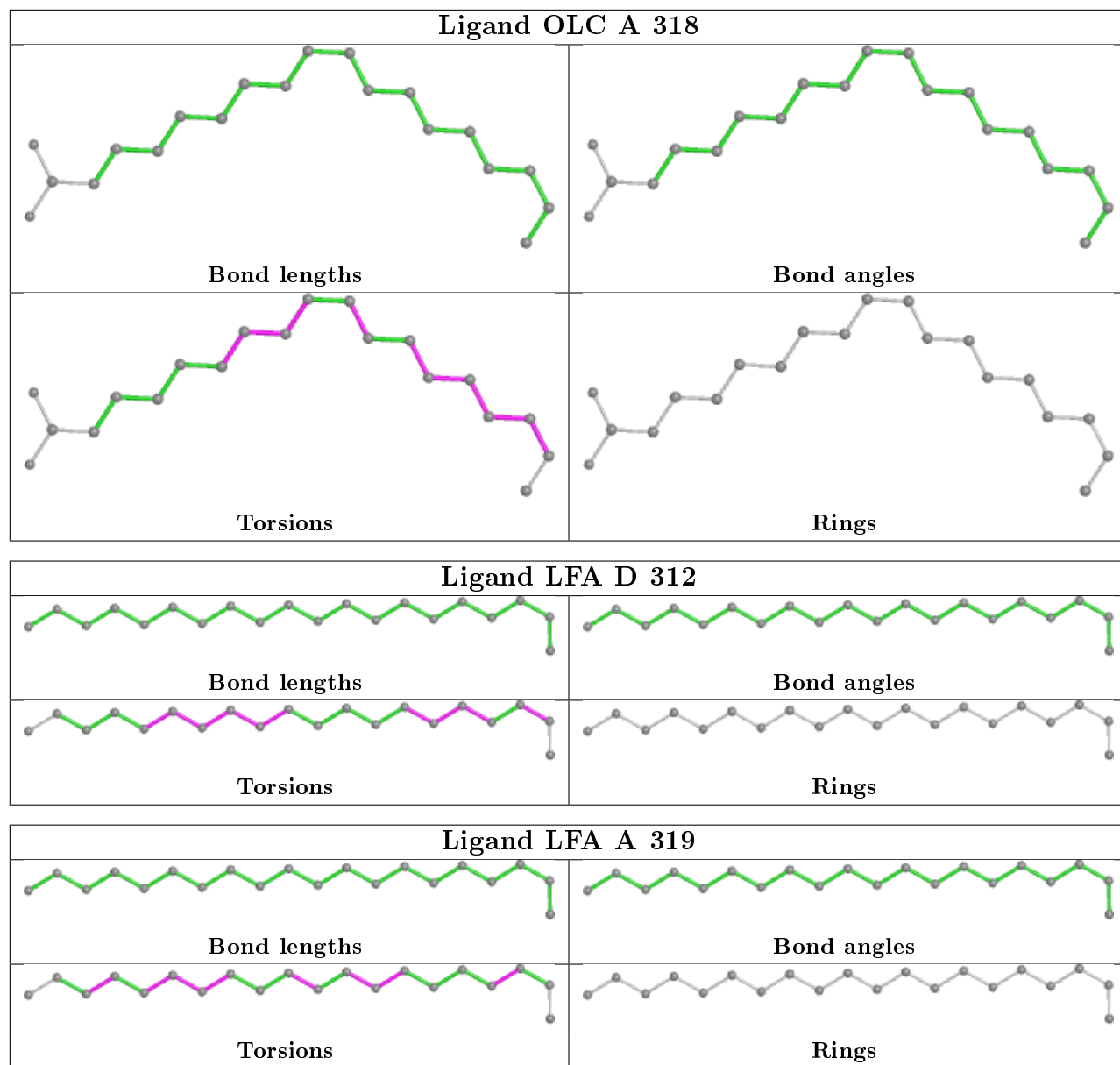


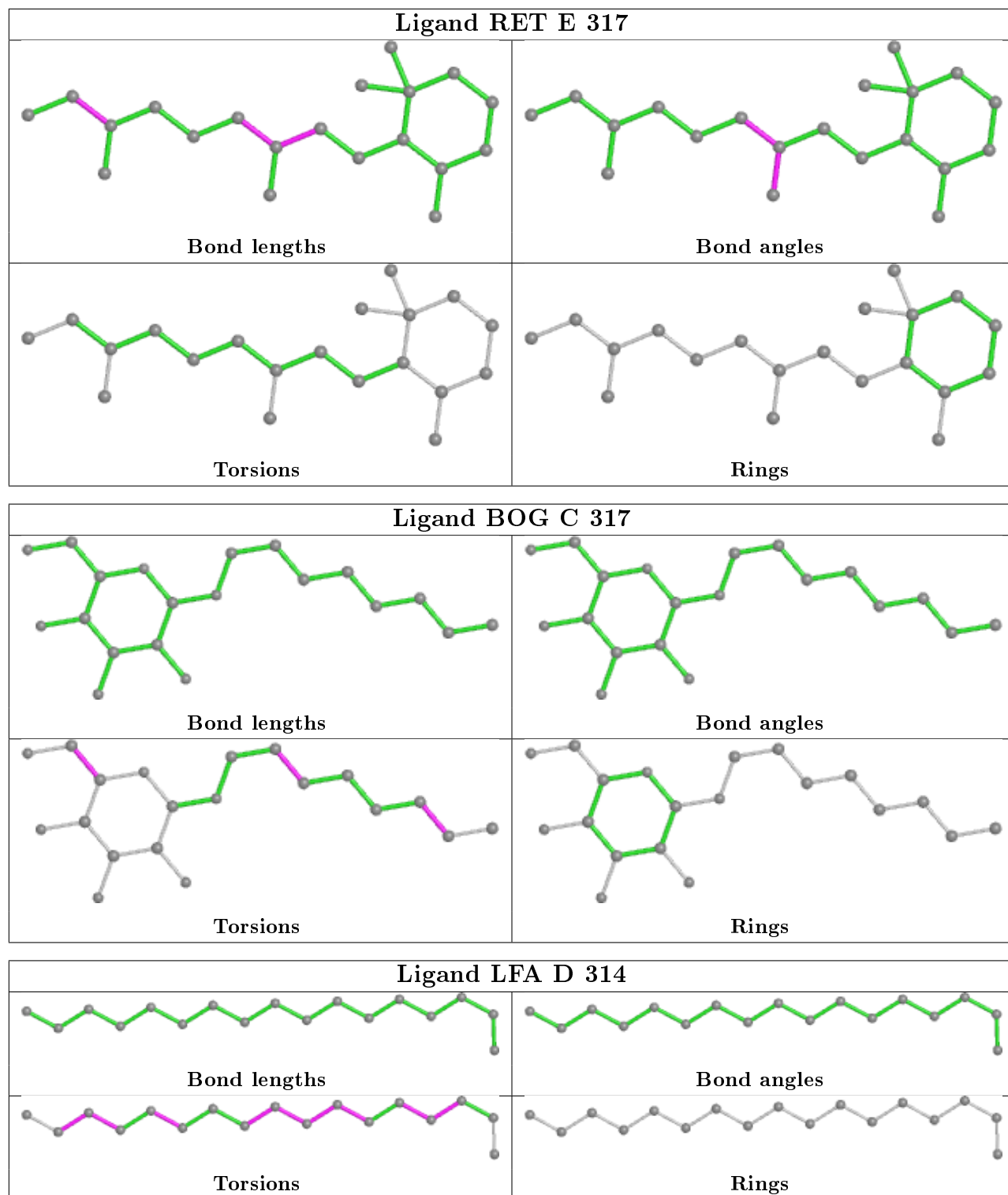




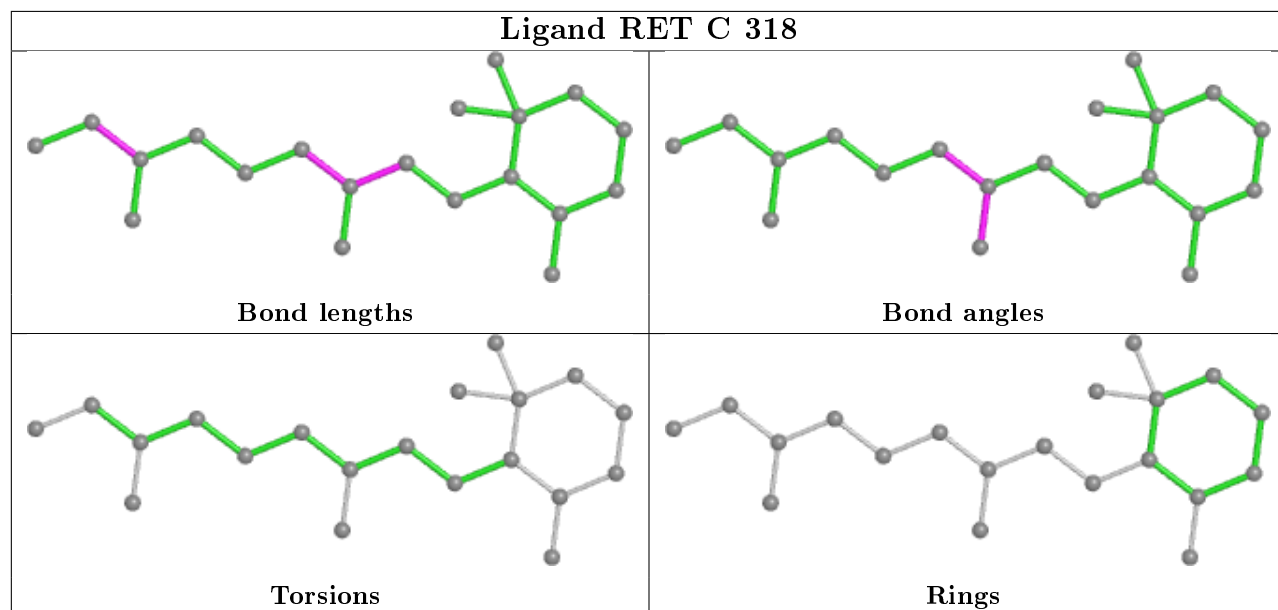
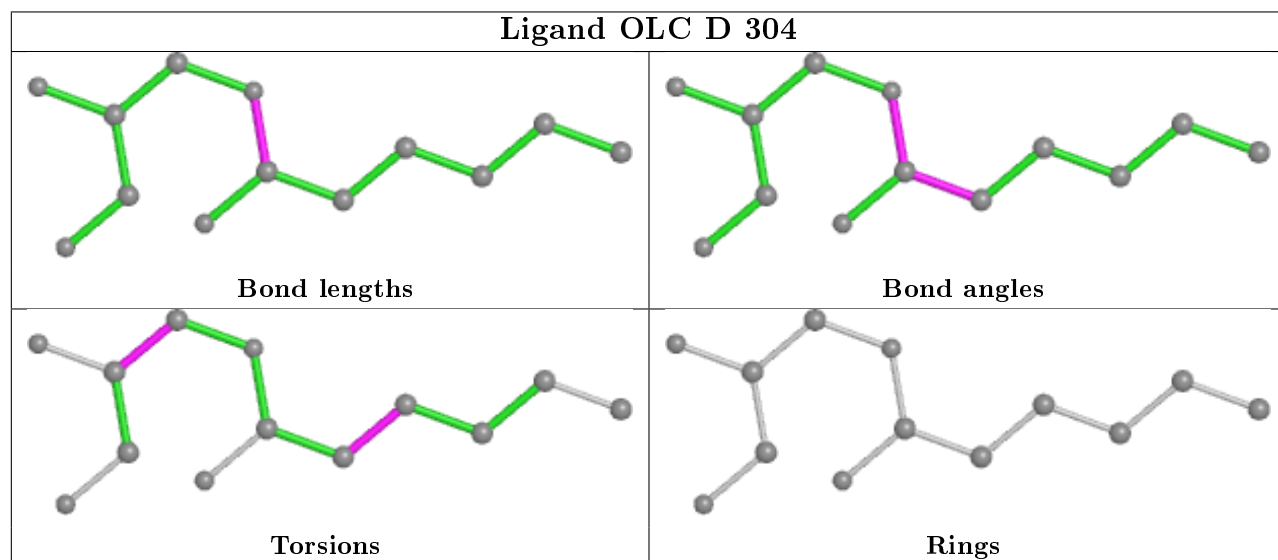
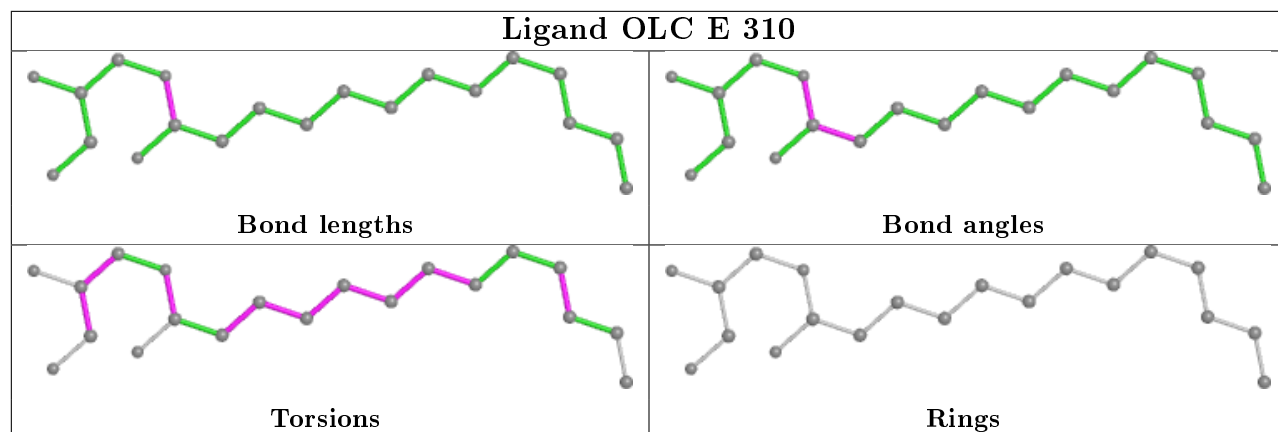


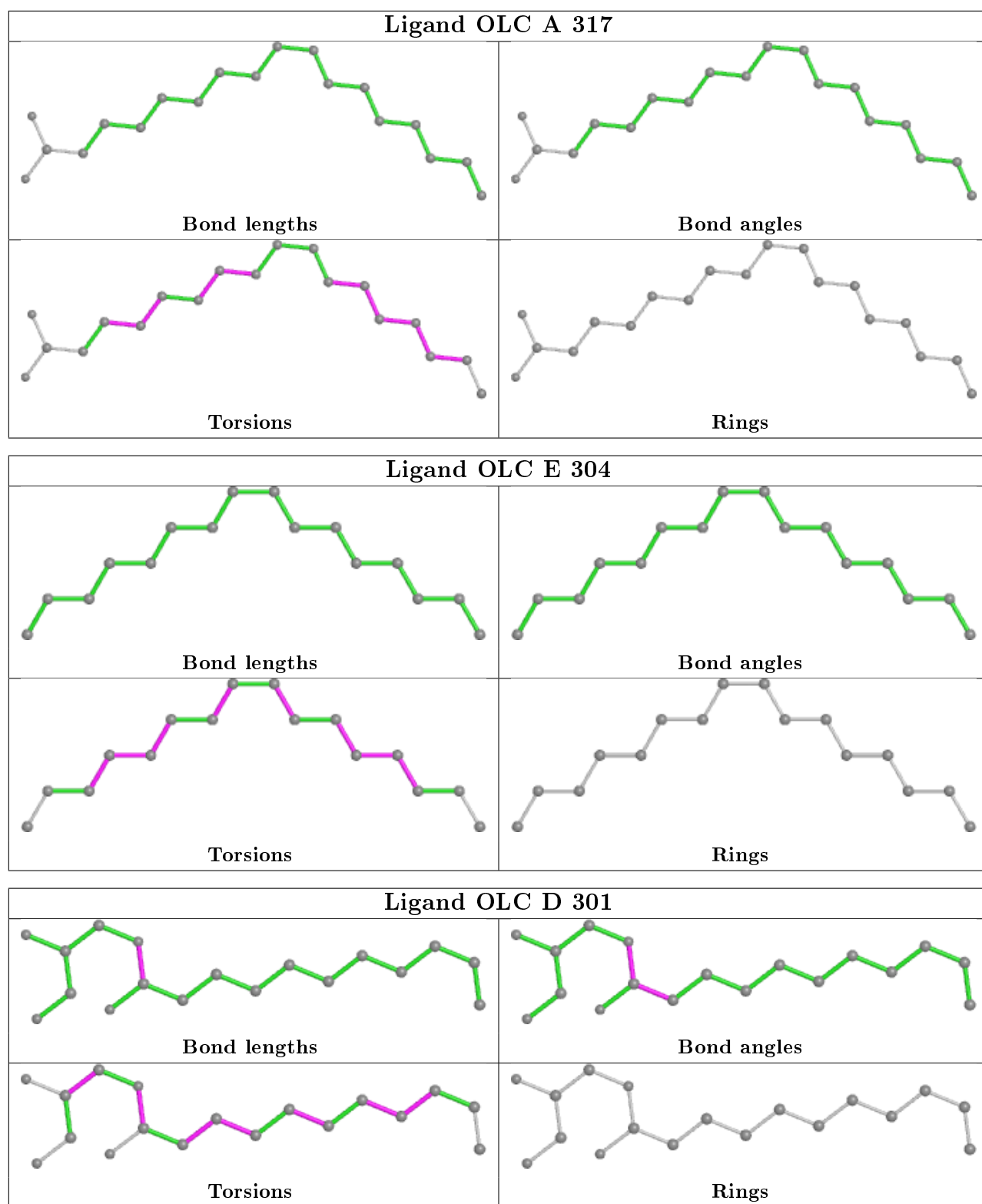


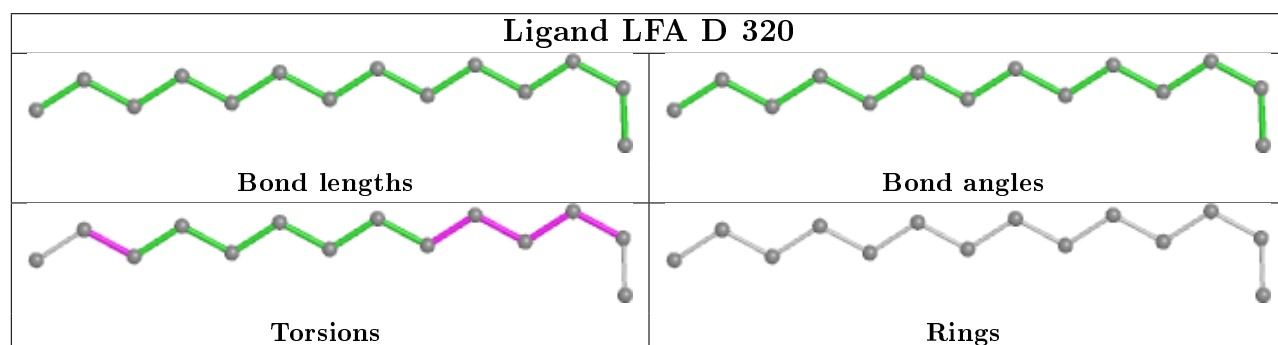
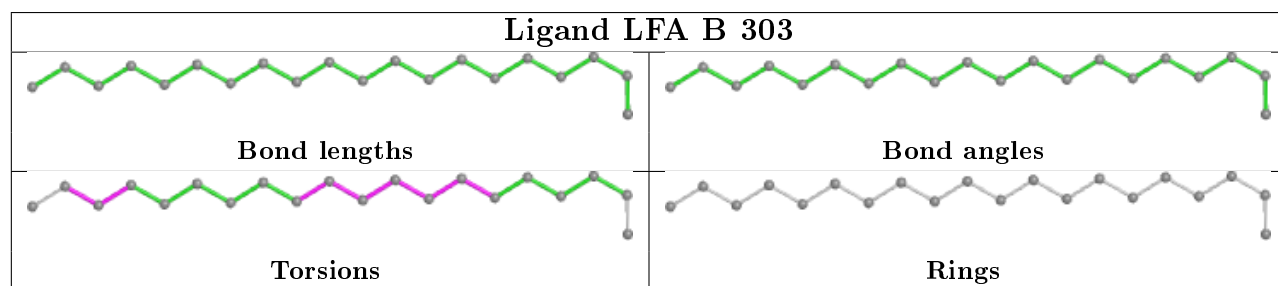
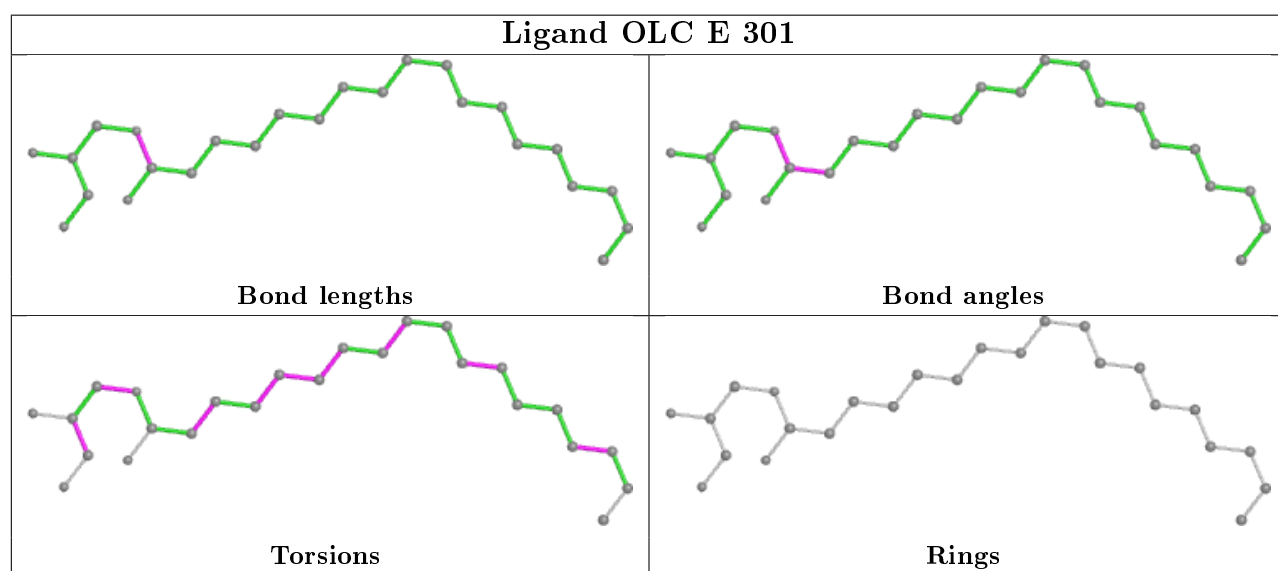
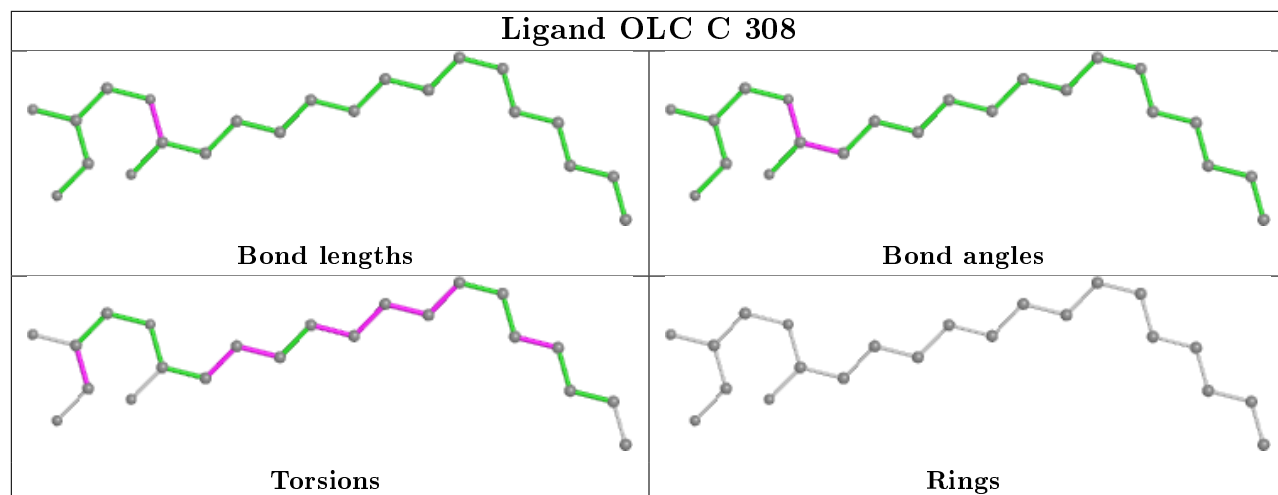


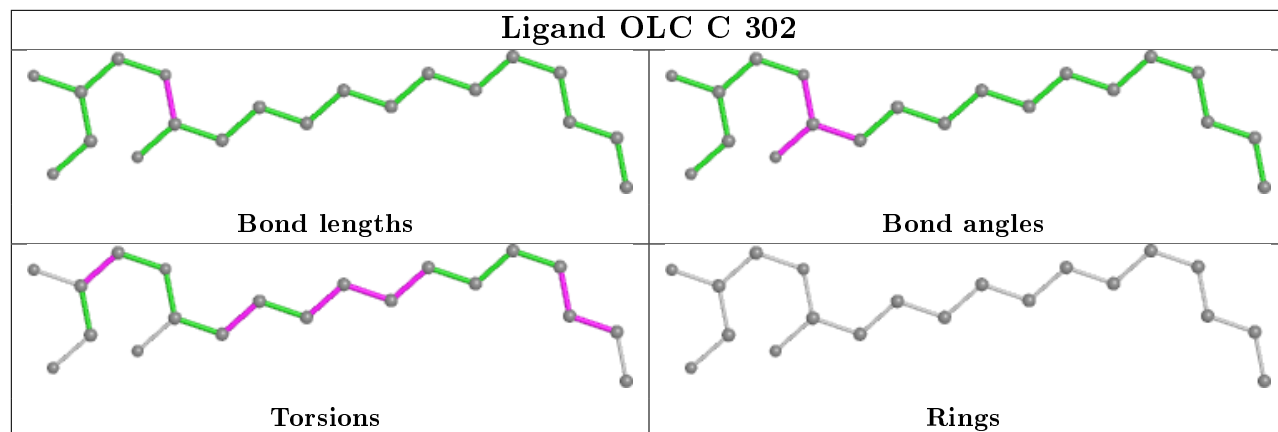
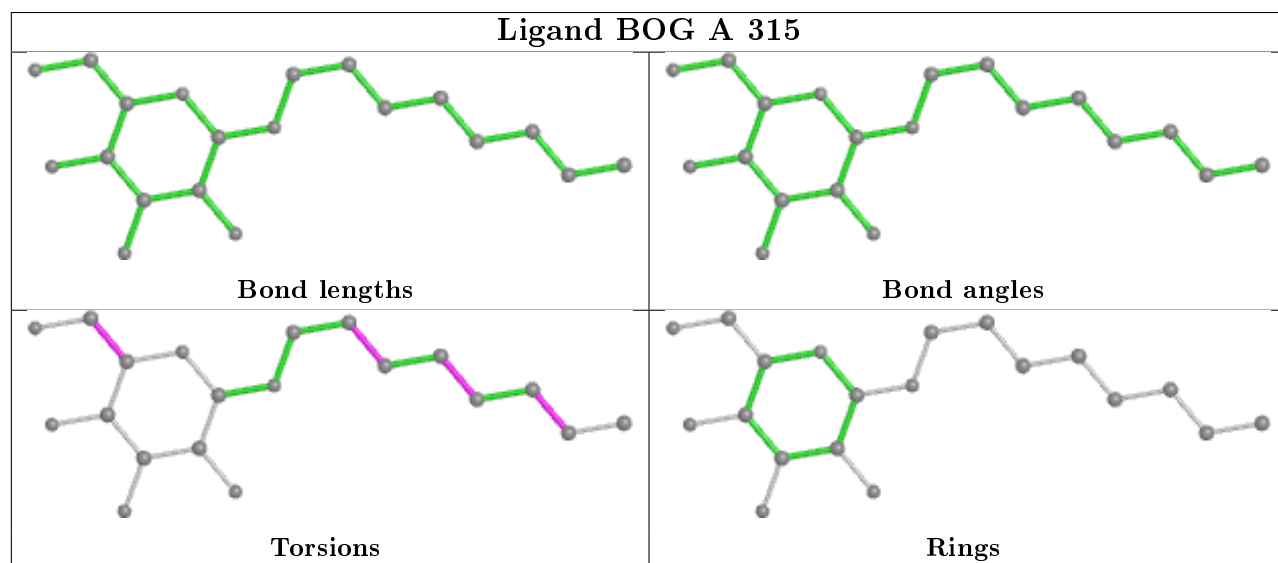
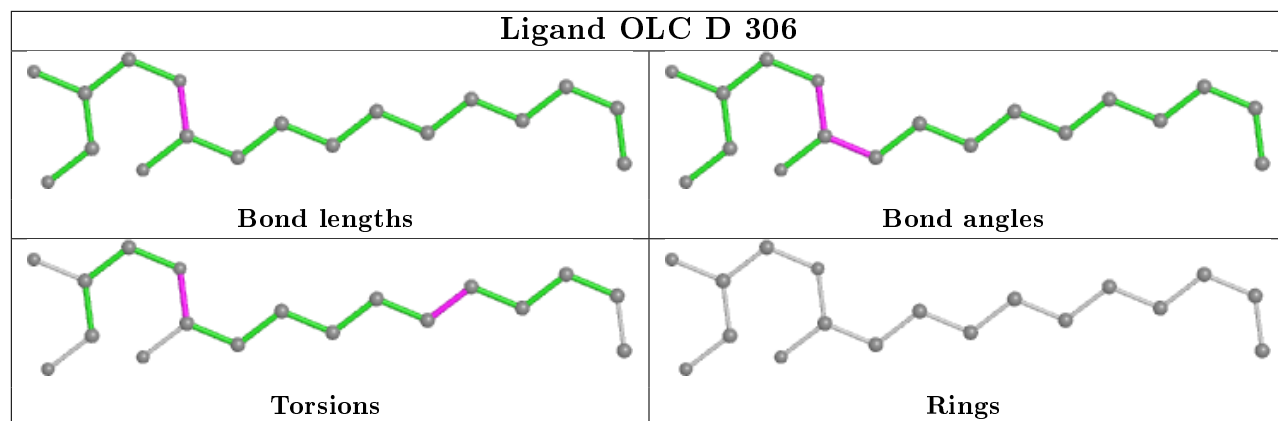




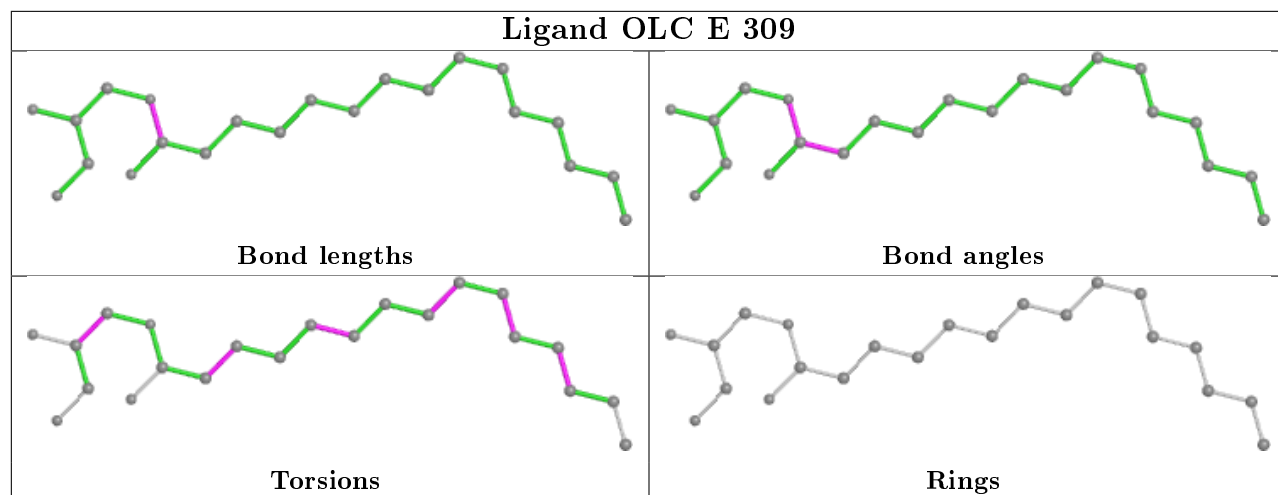




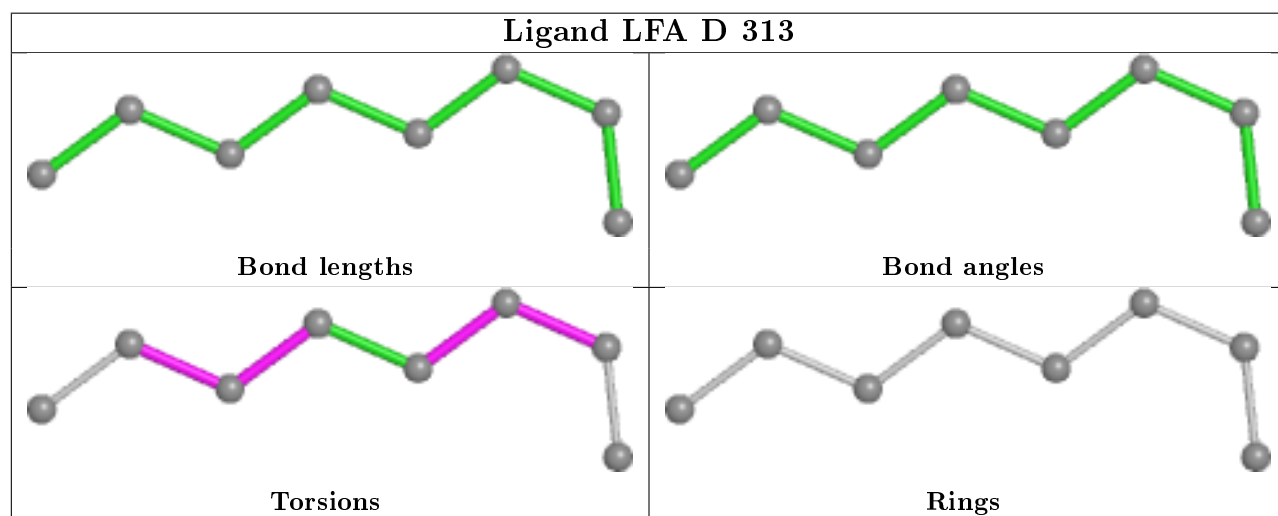




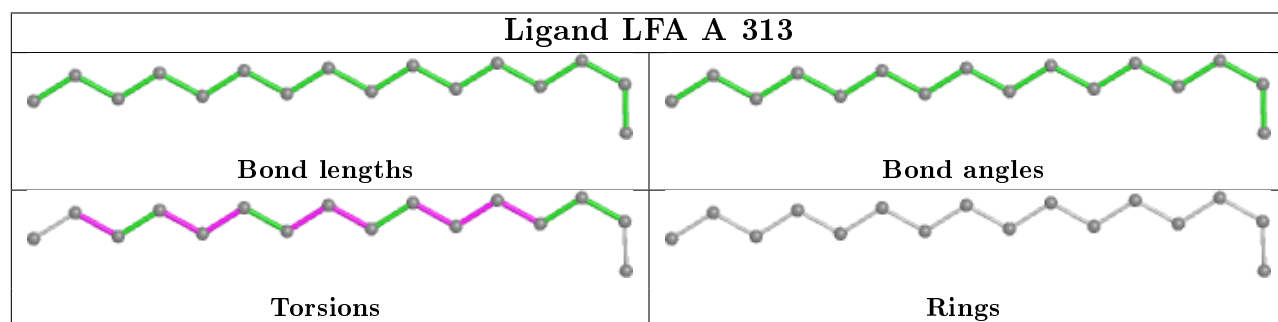
## Ligand OLC E 309

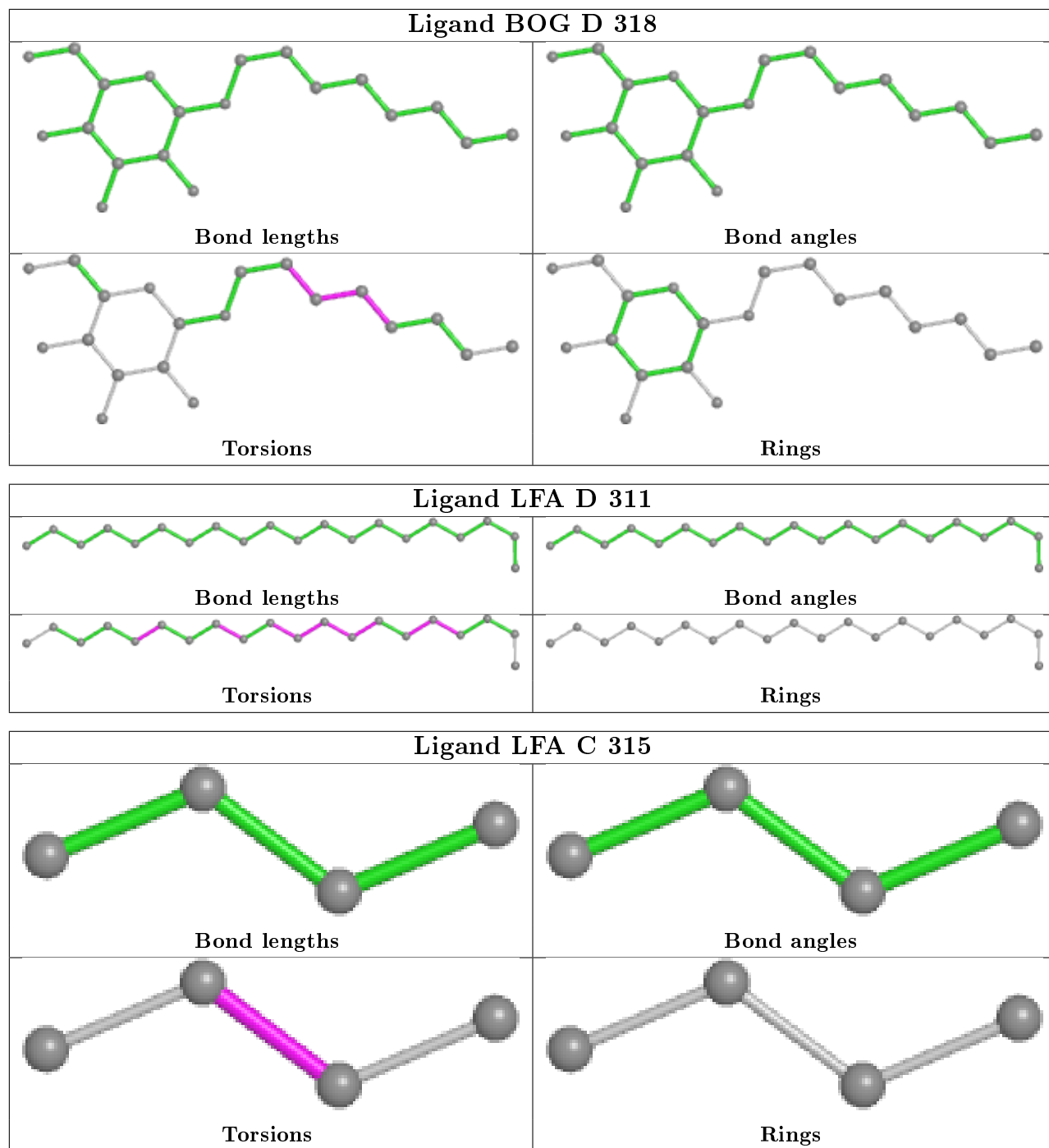


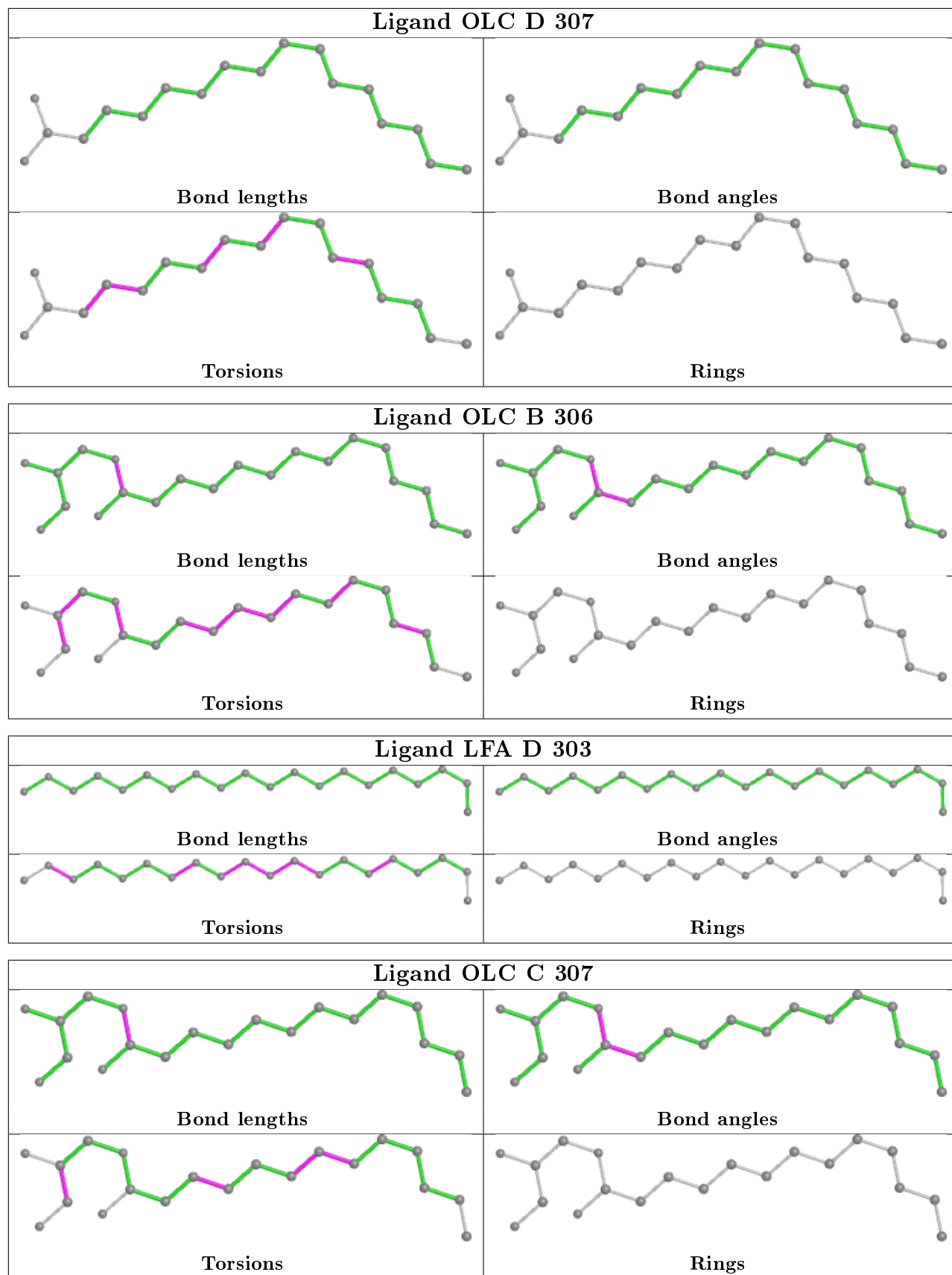
## Ligand LFA D 313

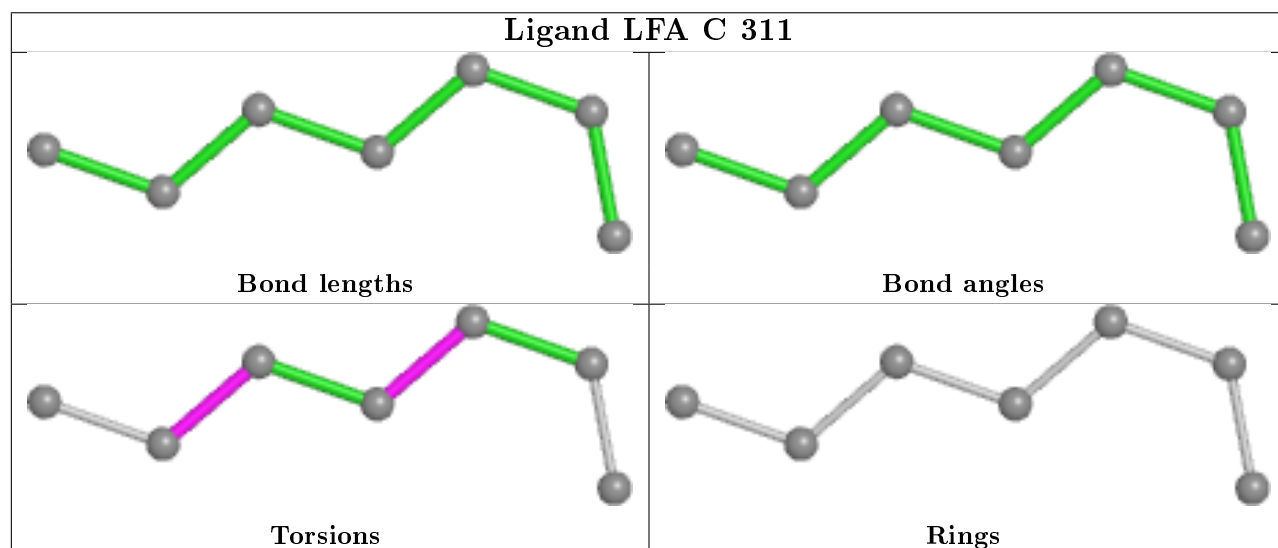
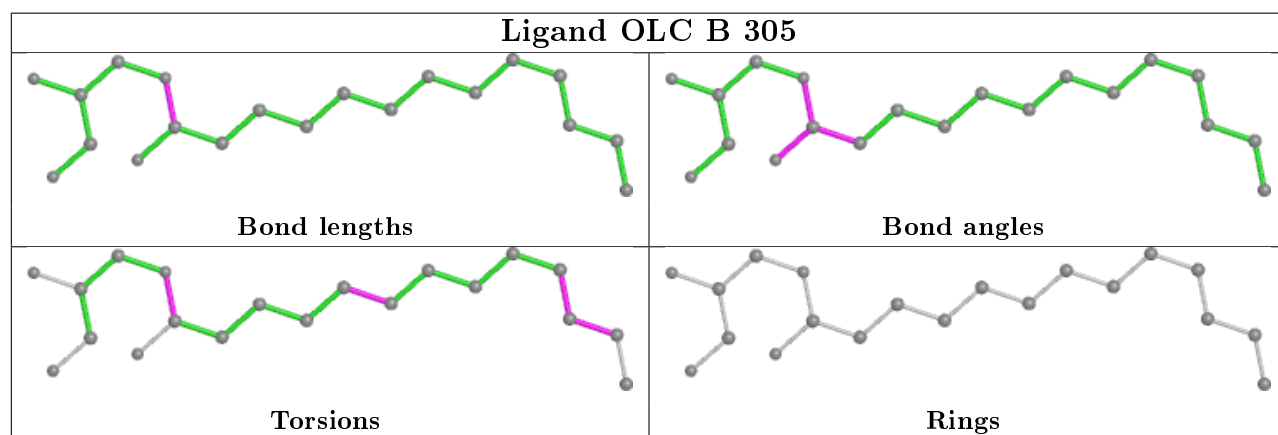
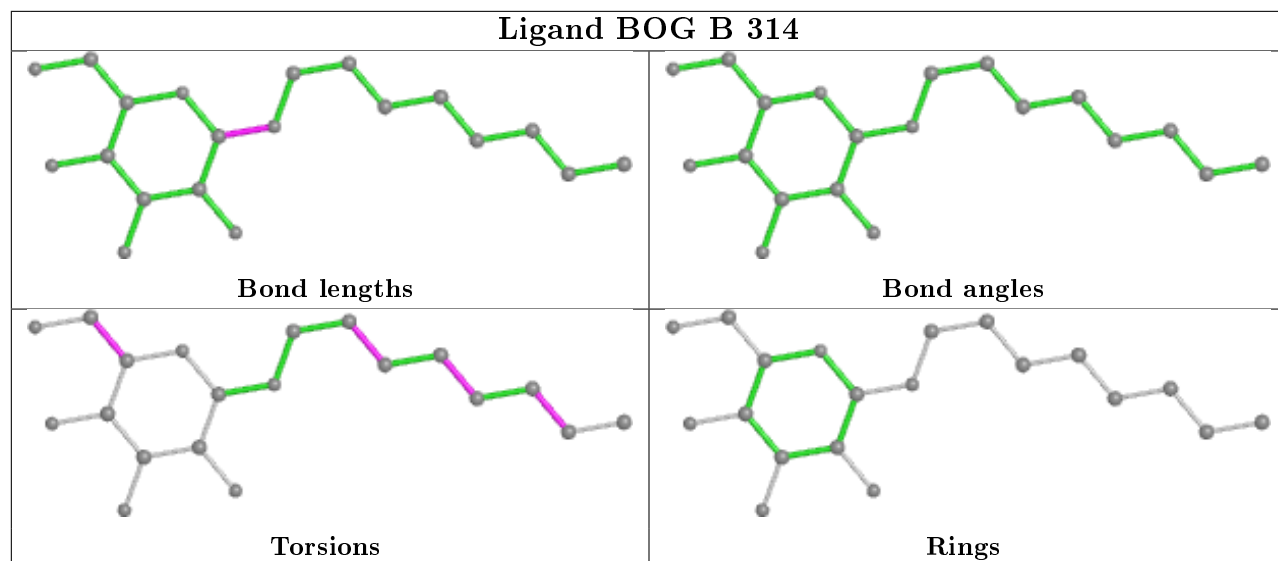


## Ligand LFA A 313

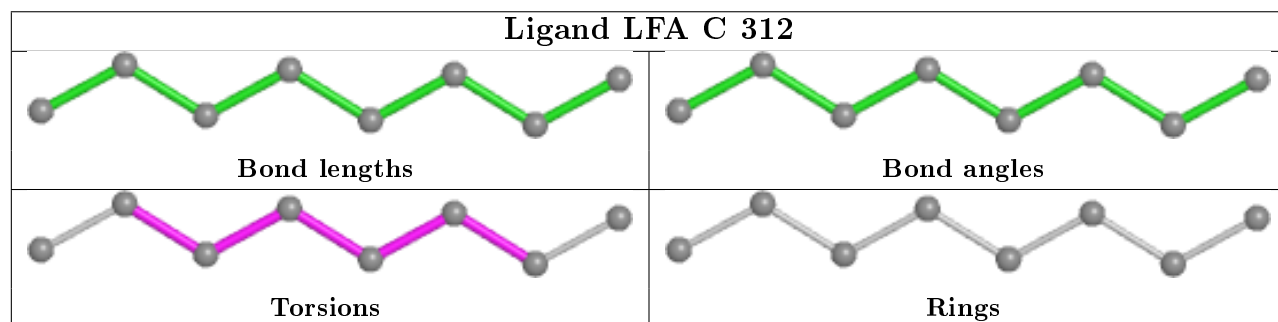
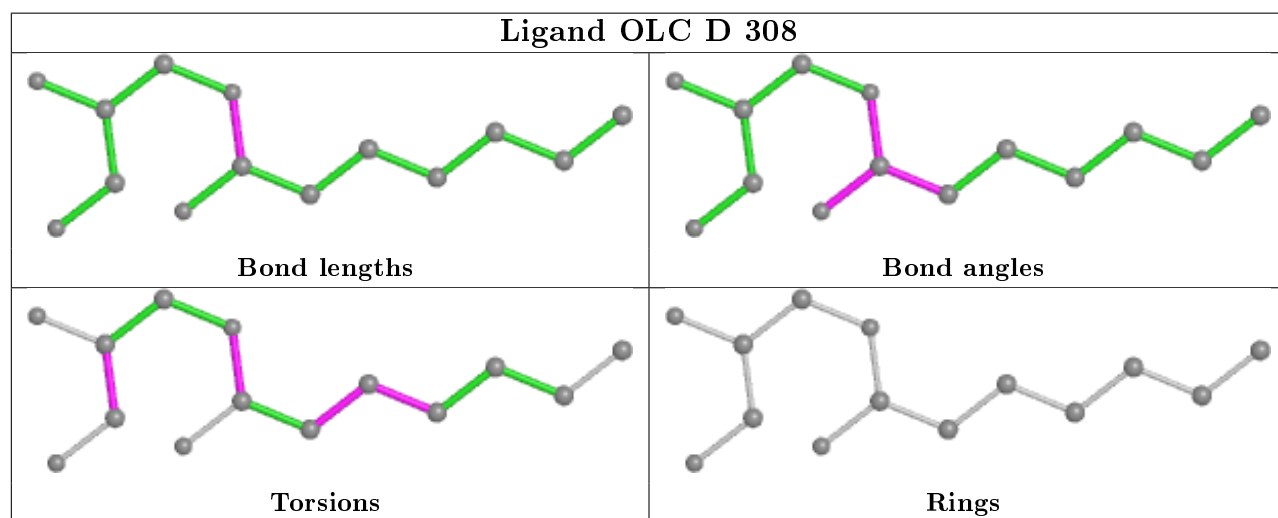
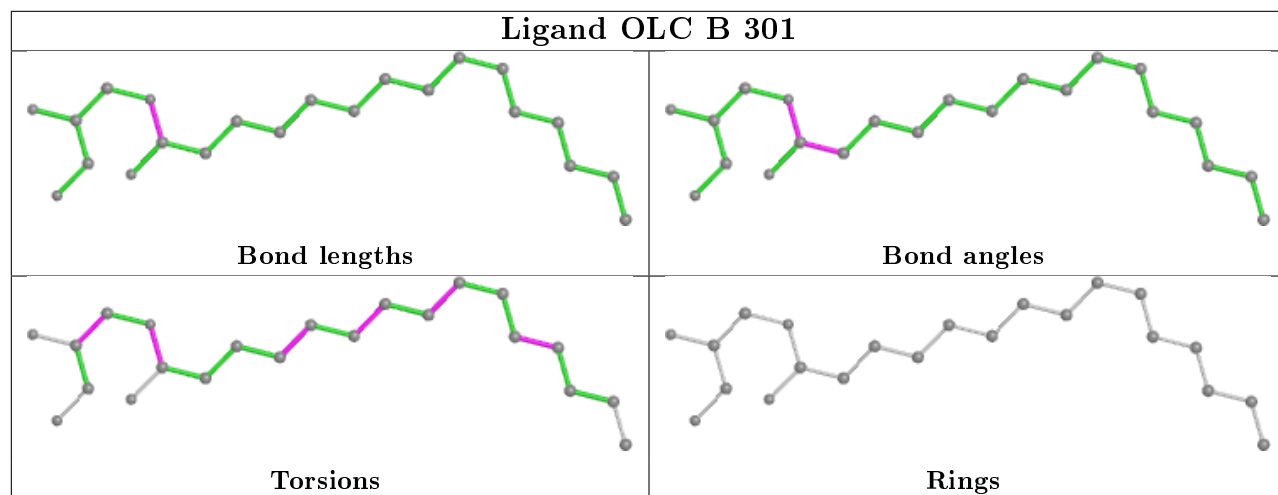
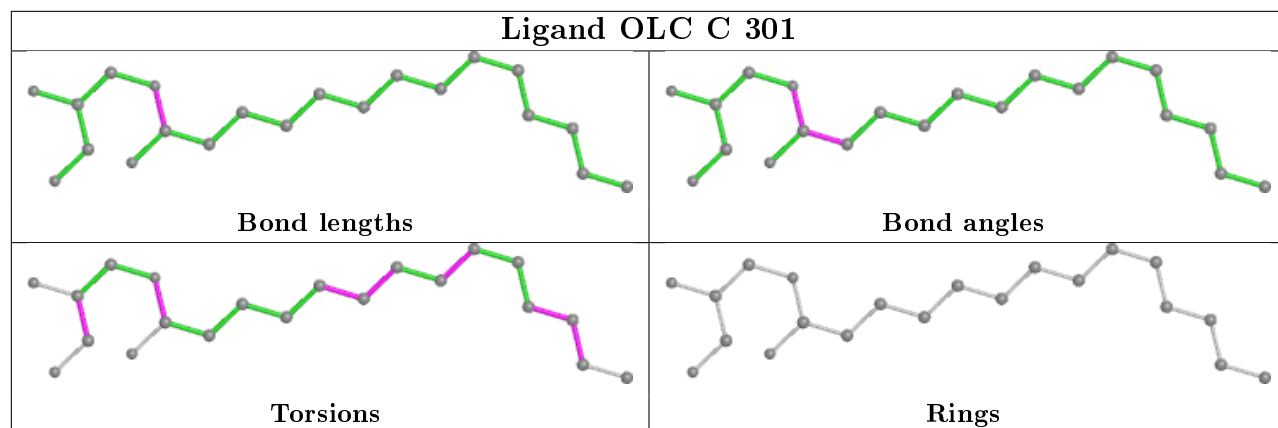


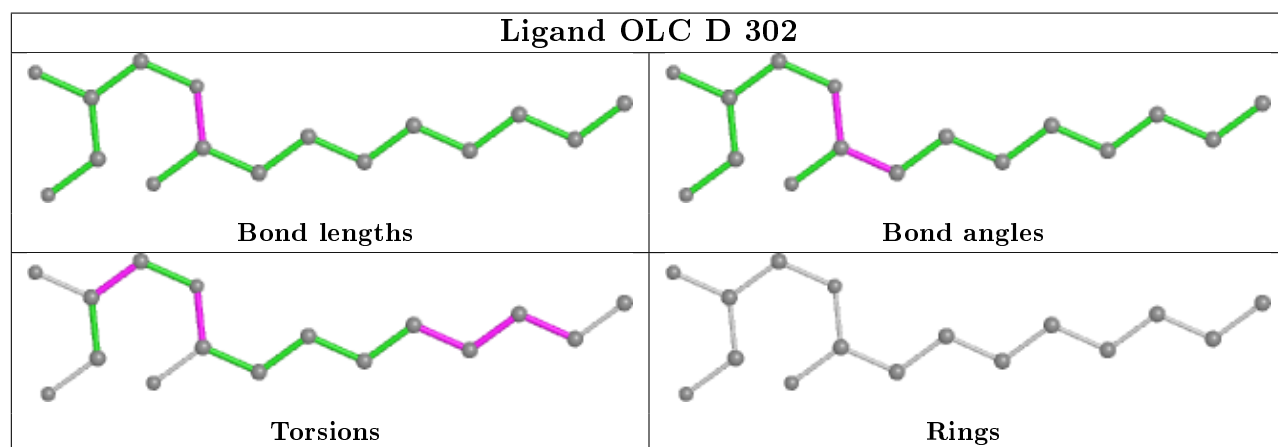
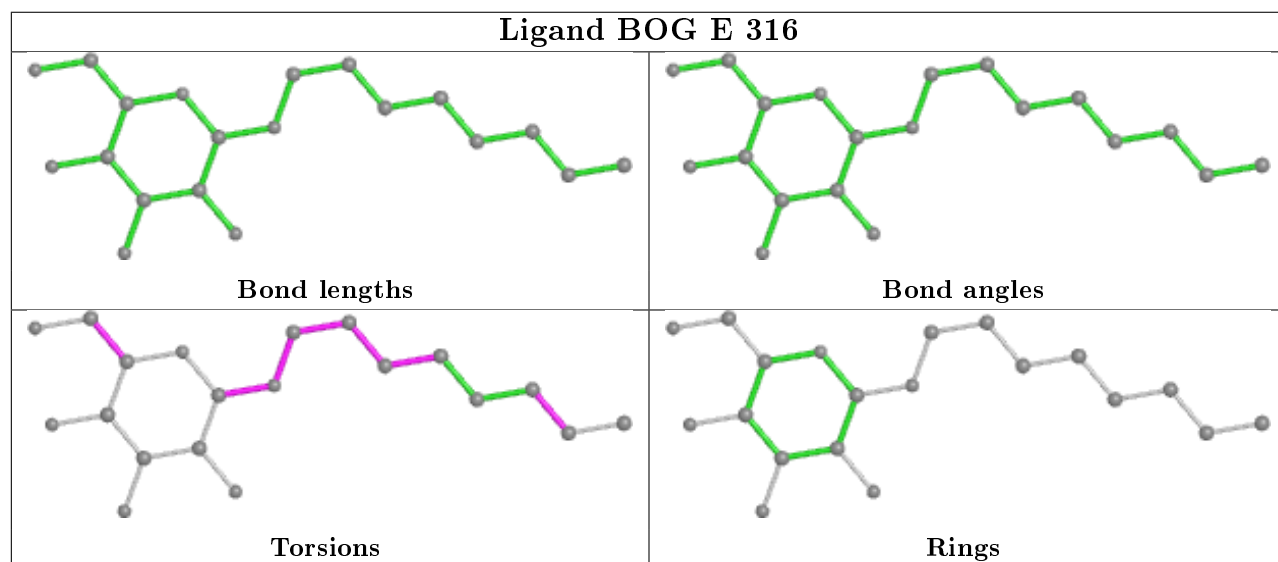
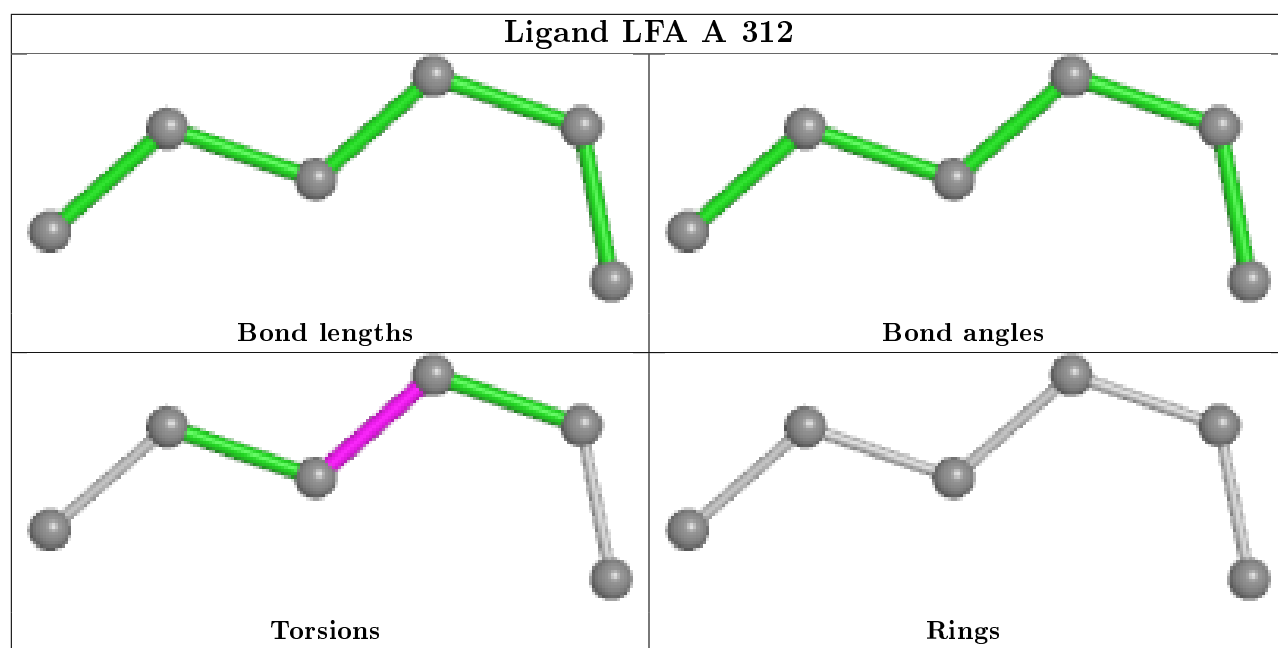


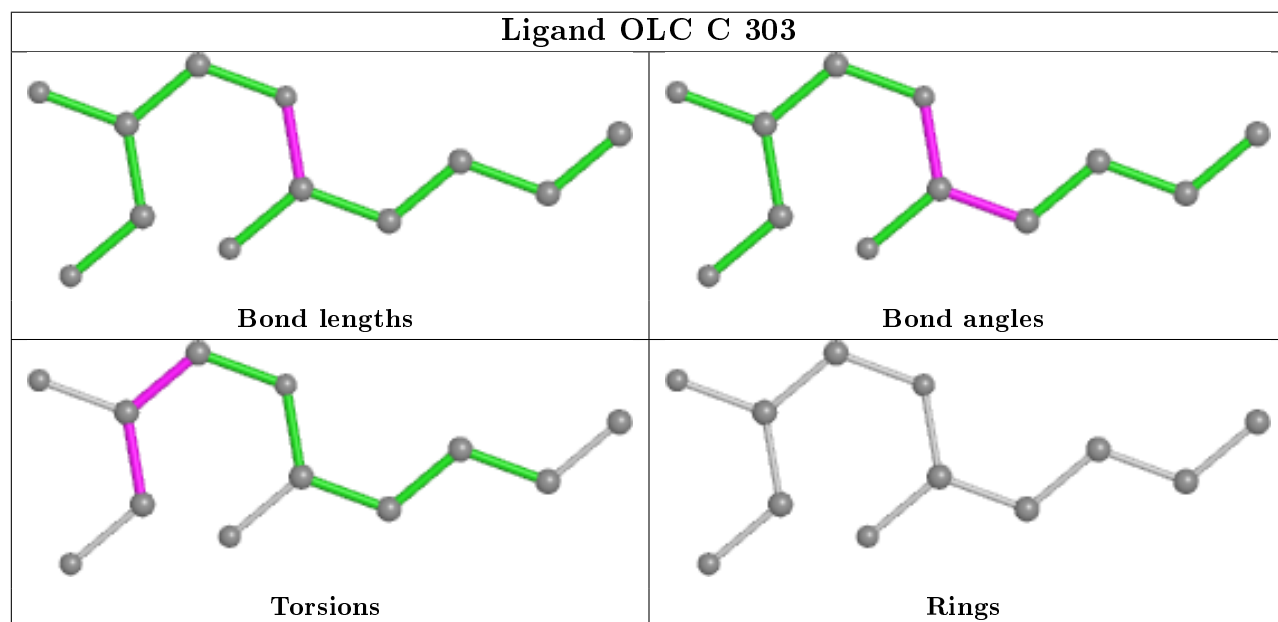
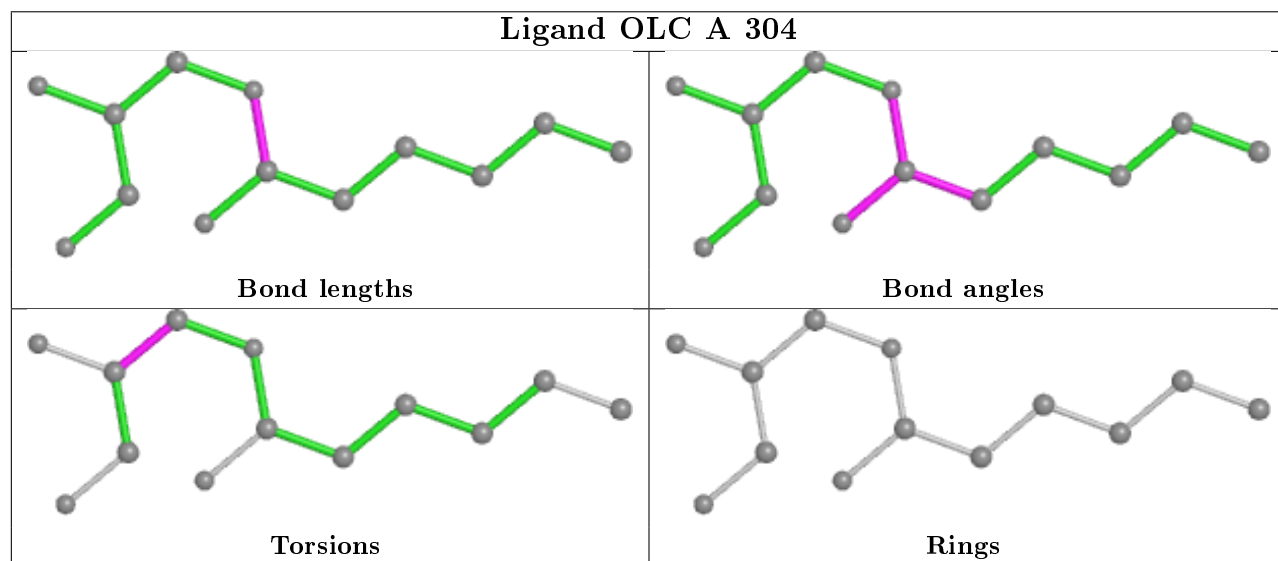
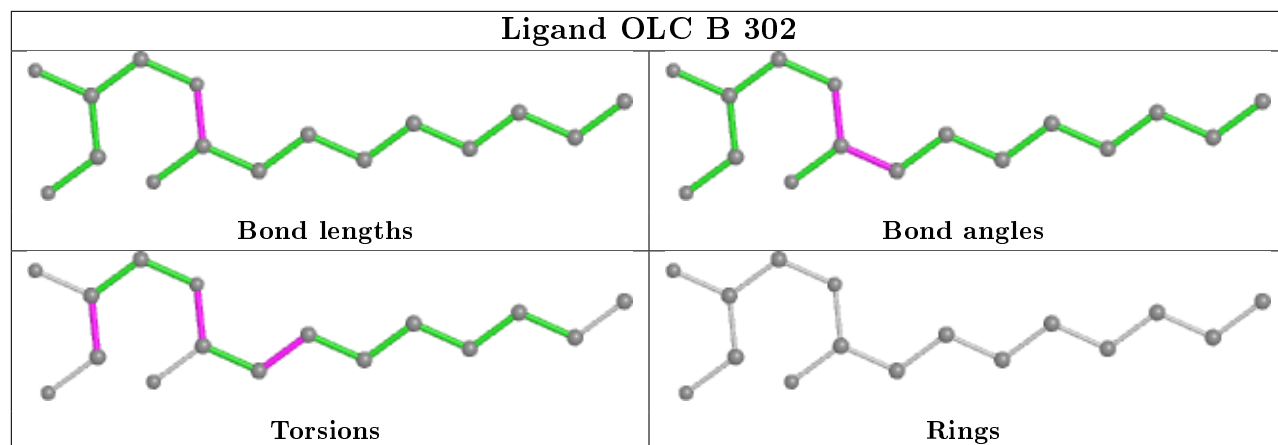


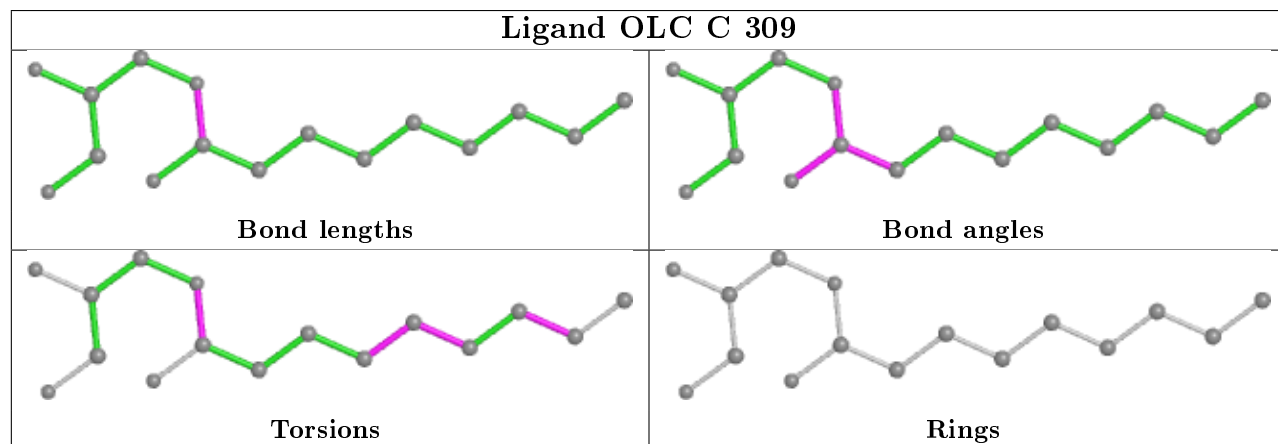
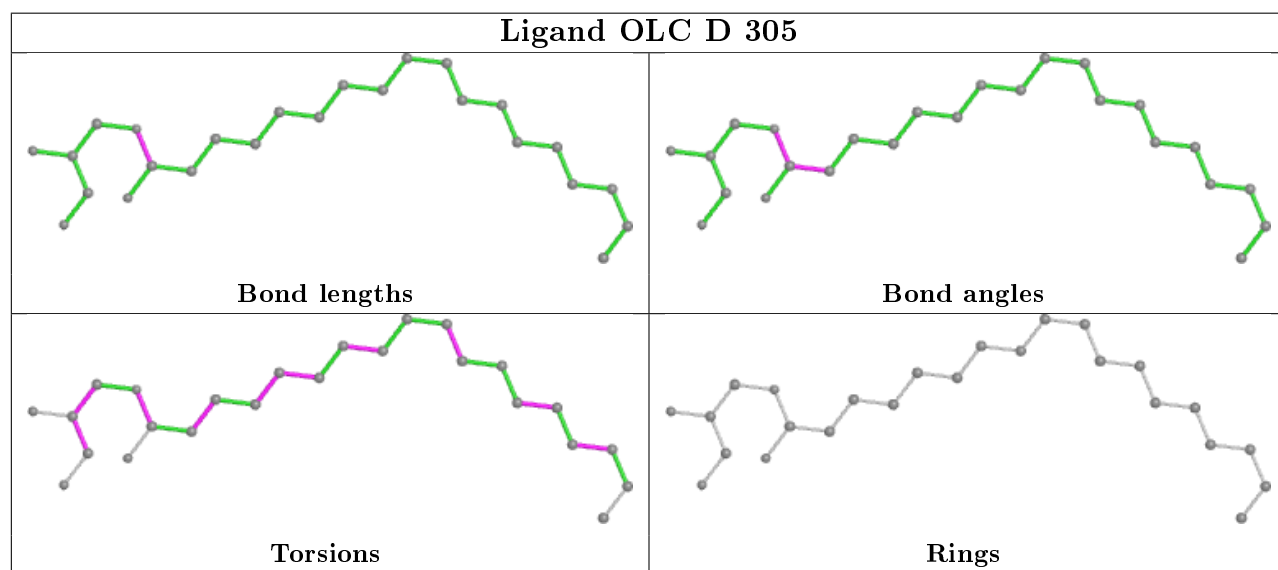
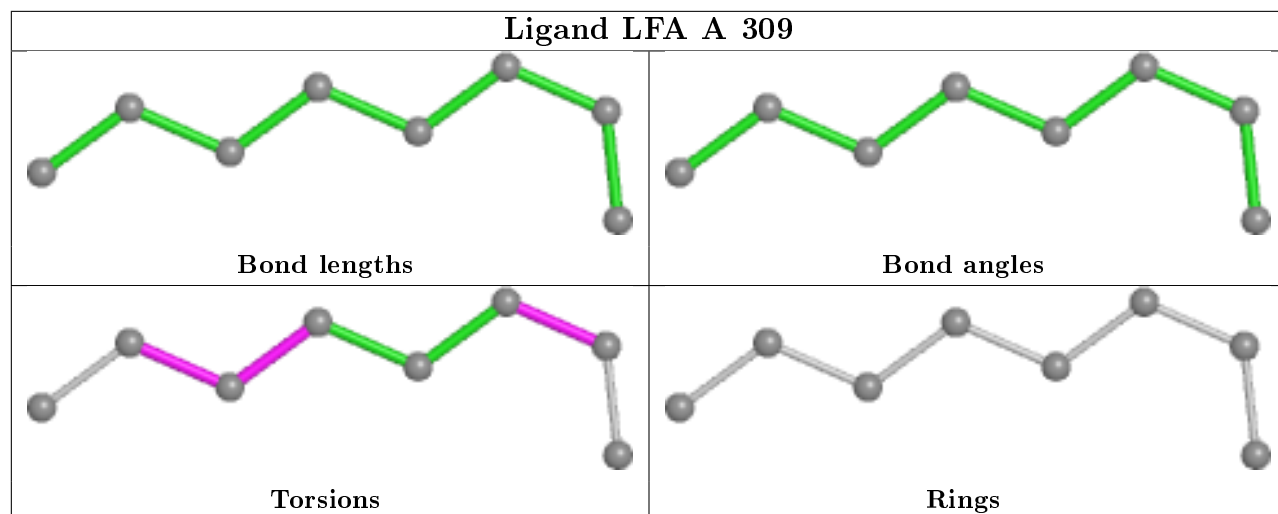


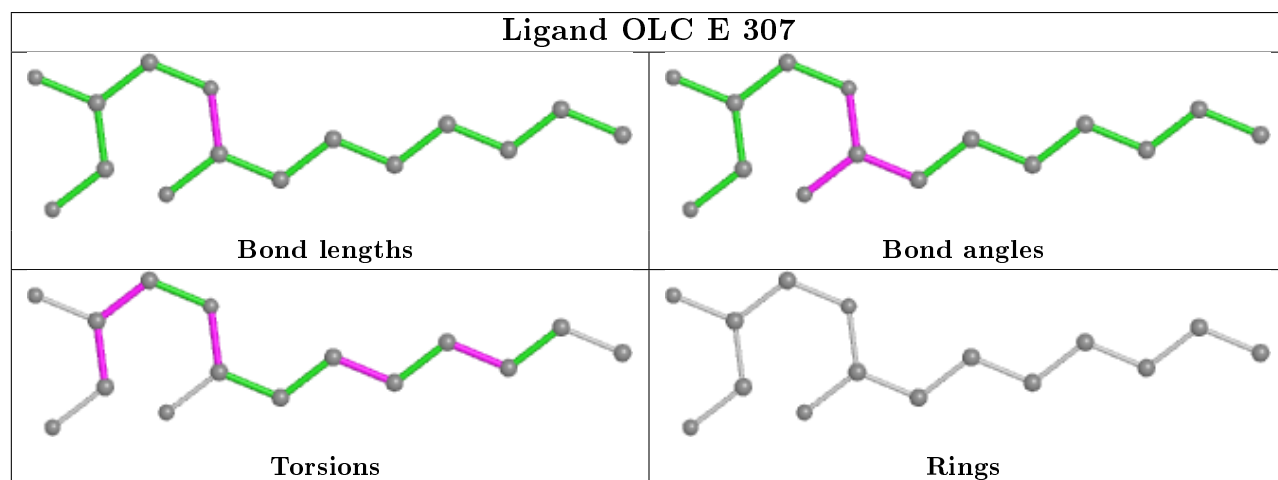
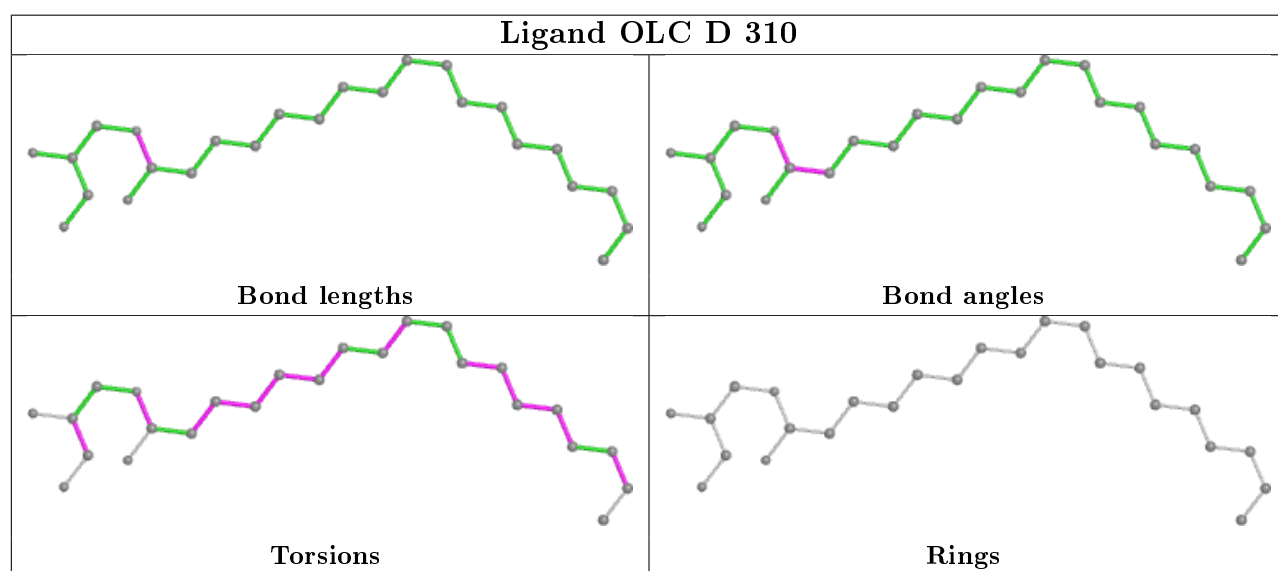
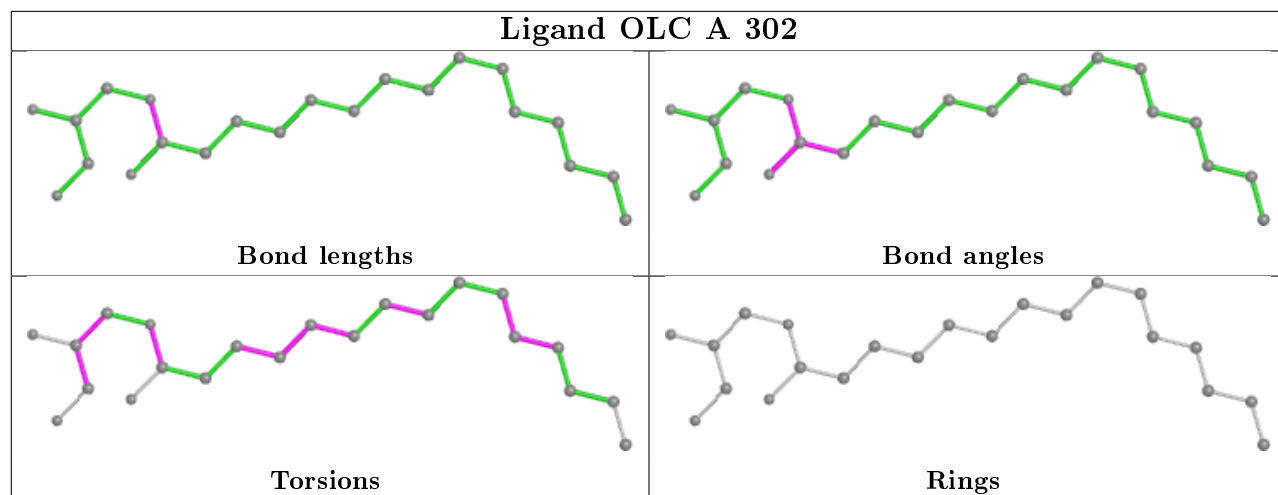


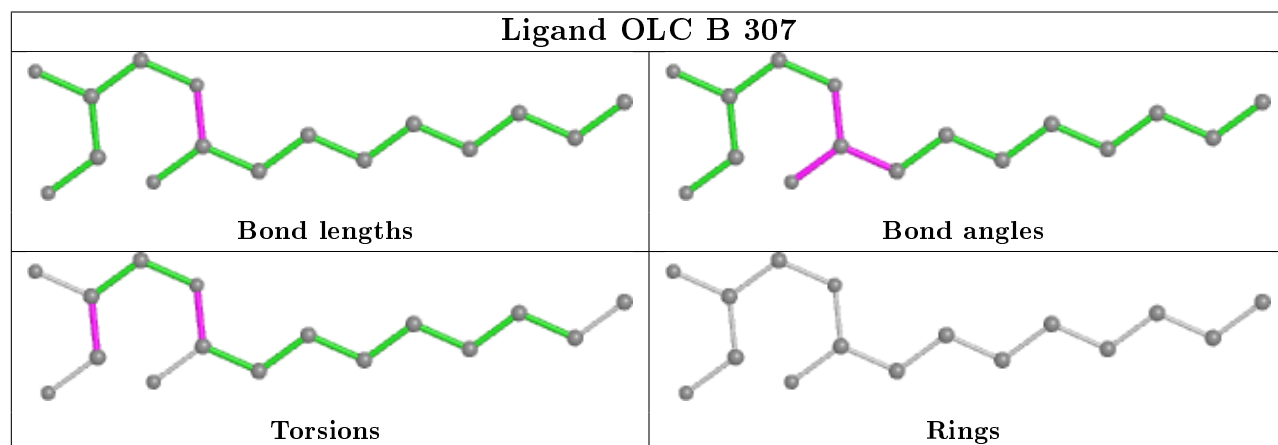
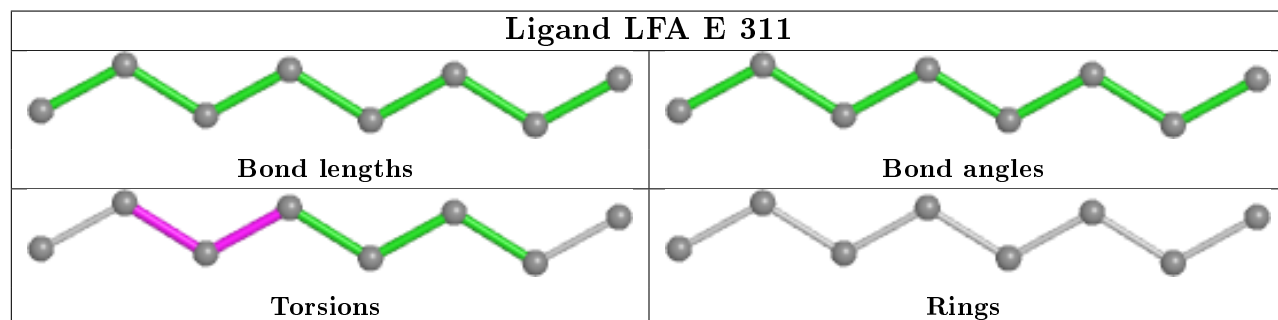
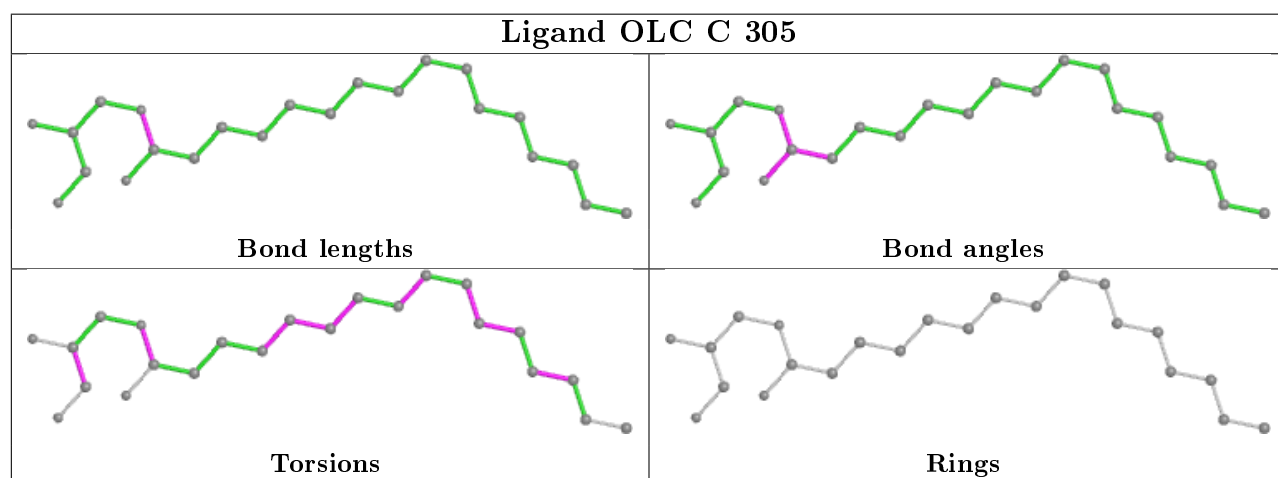
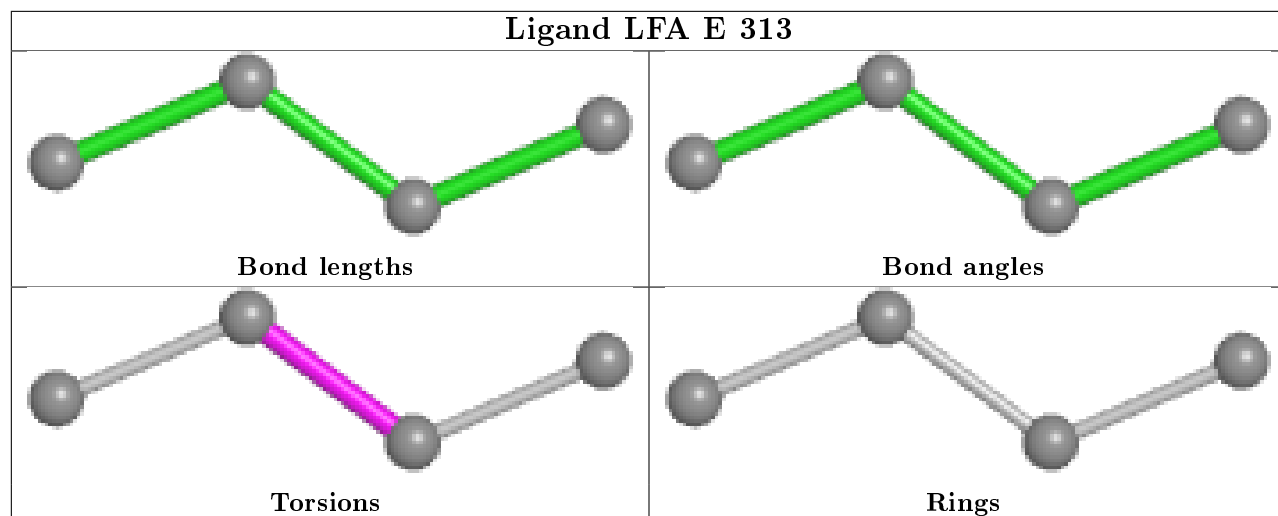


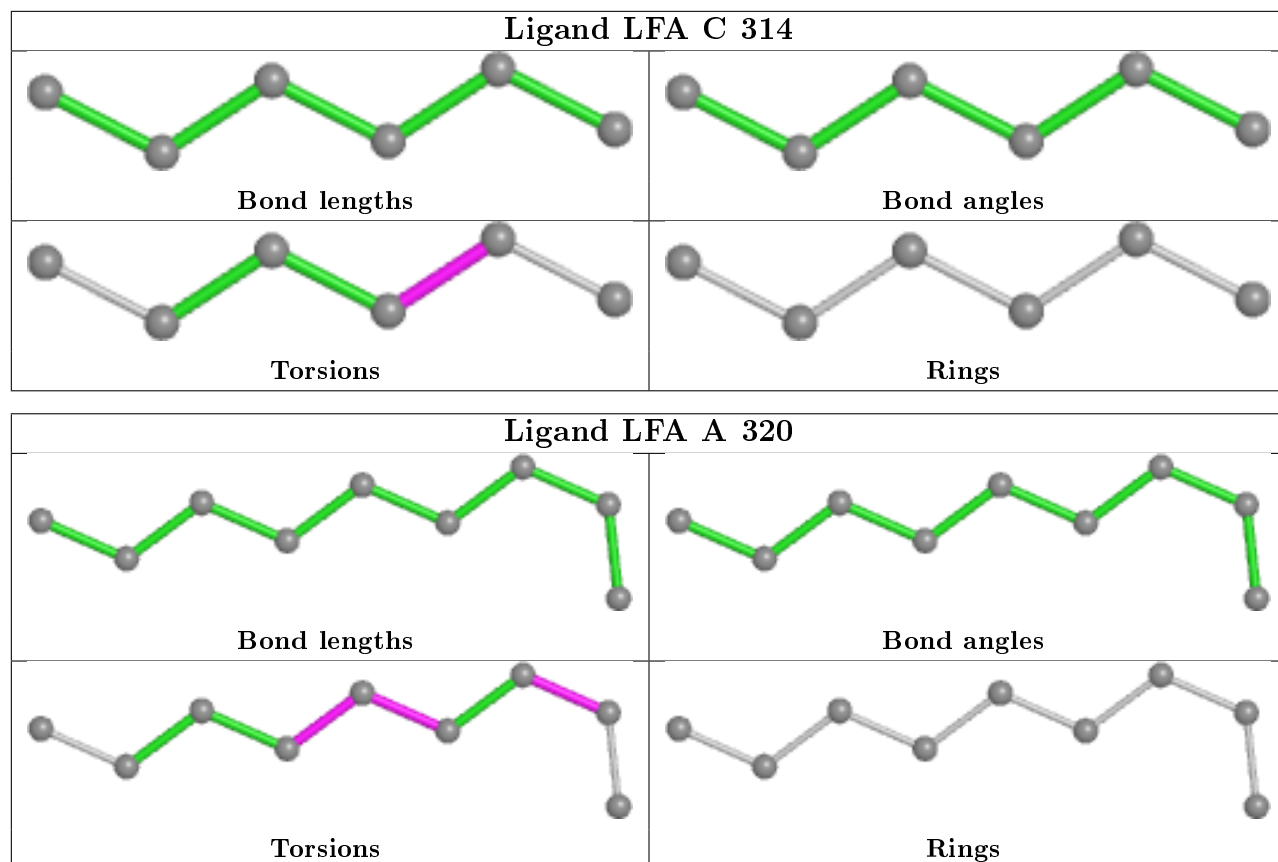












## 5.7 Other polymers [i](#)

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	273/273 (100%)	0.26	29 (10%) 6 5	34, 43, 66, 123	0
1	B	273/273 (100%)	0.15	25 (9%) 9 7	34, 45, 69, 124	0
1	C	273/273 (100%)	0.18	26 (9%) 8 7	35, 44, 66, 129	0
1	D	273/273 (100%)	0.40	35 (12%) 3 3	35, 46, 73, 138	0
1	E	273/273 (100%)	0.20	23 (8%) 11 9	35, 45, 67, 120	0
All	All	1365/1365 (100%)	0.24	138 (10%) 7 6	34, 44, 70, 138	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	230	VAL	6.7
1	A	272	ASN	5.8
1	D	275	LEU	5.4
1	D	40	LEU	5.3
1	A	73	LEU	4.9
1	B	272	ASN	4.8
1	B	40	LEU	4.8
1	E	40	LEU	4.8
1	D	230	VAL	4.7
1	A	43	LEU	4.6
1	B	73	LEU	4.5
1	C	40	LEU	4.5
1	A	40	LEU	4.5
1	A	69	VAL	4.4
1	D	131	THR	4.4
1	B	230	VAL	4.3
1	D	43	LEU	4.3
1	B	72	PHE	4.3
1	C	73	LEU	4.3
1	D	69	VAL	4.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	43	LEU	4.2
1	D	130	LEU	3.9
1	D	271	LYS	3.9
1	D	73	LEU	3.9
1	A	270	SER	3.9
1	E	72	PHE	3.8
1	A	230	VAL	3.8
1	D	273	LYS	3.8
1	D	129	SER	3.8
1	D	41	ALA	3.8
1	B	43	LEU	3.8
1	D	233	PHE	3.7
1	C	69	VAL	3.7
1	A	271	LYS	3.6
1	A	273	LYS	3.6
1	E	44	LEU	3.6
1	B	44	LEU	3.6
1	B	273	LYS	3.6
1	D	38	VAL	3.5
1	A	72	PHE	3.5
1	A	275	LEU	3.5
1	C	183	TRP	3.4
1	E	73	LEU	3.4
1	B	69	VAL	3.3
1	E	69	VAL	3.3
1	D	36	TYR	3.2
1	A	44	LEU	3.2
1	D	72	PHE	3.2
1	E	274	GLU	3.1
1	D	37	ALA	3.1
1	A	183	TRP	3.0
1	C	43	LEU	3.0
1	C	44	LEU	3.0
1	C	72	PHE	3.0
1	E	76	TYR	2.9
1	A	274	GLU	2.9
1	D	132	THR	2.9
1	C	76	TYR	2.9
1	E	273	LYS	2.9
1	A	76	TYR	2.9
1	E	41	ALA	2.9
1	B	275	LEU	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	41	ALA	2.8
1	D	194	GLU	2.8
1	E	270	SER	2.7
1	D	195	GLY	2.7
1	C	132	THR	2.7
1	B	36	TYR	2.7
1	C	66	VAL	2.7
1	D	39	MET	2.7
1	B	76	TYR	2.6
1	A	77	ALA	2.6
1	D	75	LEU	2.6
1	C	190	ASN	2.6
1	D	231	ASP	2.6
1	C	41	ALA	2.6
1	A	47	ILE	2.6
1	E	190	ASN	2.6
1	C	273	LYS	2.6
1	B	75	LEU	2.5
1	E	275	LEU	2.5
1	E	47	ILE	2.5
1	E	36	TYR	2.5
1	D	44	LEU	2.5
1	A	199	ALA	2.5
1	C	130	LEU	2.5
1	A	36	TYR	2.4
1	D	272	ASN	2.4
1	E	272	ASN	2.4
1	E	183	TRP	2.4
1	C	65	ALA	2.4
1	D	66	VAL	2.4
1	B	183	TRP	2.3
1	E	74	LEU	2.3
1	E	189	ILE	2.3
1	B	68	MET	2.3
1	C	231	ASP	2.3
1	D	76	TYR	2.3
1	D	42	GLY	2.3
1	B	38	VAL	2.3
1	B	41	ALA	2.3
1	B	77	ALA	2.3
1	B	3	GLN	2.3
1	B	39	MET	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	230	VAL	2.2
1	C	36	TYR	2.2
1	A	66	VAL	2.2
1	C	233	PHE	2.2
1	D	133	SER	2.2
1	A	74	LEU	2.2
1	C	272	ASN	2.2
1	A	164	LEU	2.2
1	C	196	ILE	2.2
1	B	274	GLU	2.2
1	A	70	SER	2.2
1	E	131	THR	2.1
1	B	74	LEU	2.1
1	E	39	MET	2.1
1	B	65	ALA	2.1
1	D	33	THR	2.1
1	B	47	ILE	2.1
1	D	67	VAL	2.1
1	E	194	GLU	2.1
1	C	47	ILE	2.1
1	C	74	LEU	2.1
1	D	74	LEU	2.1
1	A	65	ALA	2.1
1	D	190	ASN	2.1
1	C	195	GLY	2.1
1	A	38	VAL	2.1
1	D	47	ILE	2.0
1	C	274	GLU	2.0
1	A	67	VAL	2.0
1	A	231	ASP	2.0
1	C	188	VAL	2.0
1	A	233	PHE	2.0
1	D	274	GLU	2.0
1	B	33	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	OLC	A	305	25/25	0.33	0.30	74,97,112,116	0
3	LFA	D	316	6/20	0.56	0.32	85,101,111,117	0
2	OLC	E	309	22/25	0.57	0.37	77,92,116,119	0
5	BOG	E	316	20/20	0.59	0.45	69,102,118,125	0
3	LFA	A	310	8/20	0.61	0.25	69,93,107,114	0
2	OLC	D	304	13/25	0.62	0.23	100,119,160,162	0
5	BOG	C	317	20/20	0.63	0.45	65,88,109,110	0
2	OLC	E	304	16/25	0.65	0.26	73,88,101,106	0
2	OLC	A	303	25/25	0.65	0.34	76,101,116,141	0
3	LFA	A	319	20/20	0.65	1.05	59,71,83,86	0
3	LFA	C	314	6/20	0.66	0.17	64,70,78,84	0
3	LFA	A	320	9/20	0.66	0.23	72,78,96,99	0
3	LFA	C	311	7/20	0.67	0.33	77,92,106,109	0
2	OLC	E	310	20/25	0.67	0.46	58,106,126,127	0
5	BOG	A	315	20/20	0.67	0.55	72,96,118,132	0
2	OLC	E	308	6/25	0.67	0.22	65,78,83,84	0
5	BOG	B	314	20/20	0.68	0.49	73,94,108,109	0
2	OLC	E	306	15/25	0.68	0.47	85,104,129,131	0
2	OLC	C	308	22/25	0.68	0.32	51,89,123,128	0
3	LFA	E	311	8/20	0.68	0.26	67,91,98,99	0
3	LFA	E	302	20/20	0.68	1.07	59,71,84,92	0
2	OLC	B	304	25/25	0.68	0.21	66,94,105,112	0
2	OLC	B	308	7/25	0.69	0.23	67,74,84,85	0
3	LFA	B	311	10/20	0.69	0.20	76,91,95,97	0
2	OLC	D	305	25/25	0.69	0.22	71,101,116,120	0
3	LFA	C	312	8/20	0.70	0.18	69,81,87,91	0
3	LFA	A	308	7/20	0.70	0.31	80,85,92,93	0
2	OLC	D	302	16/25	0.70	0.28	70,90,108,120	0
2	OLC	C	303	12/25	0.70	0.24	74,86,123,131	0
3	LFA	B	303	20/20	0.71	1.13	61,76,90,100	0
2	OLC	D	310	25/25	0.72	0.28	69,90,112,138	0
2	OLC	B	306	21/25	0.72	0.30	58,81,114,116	0

Continued on next page...

*Continued from previous page...*

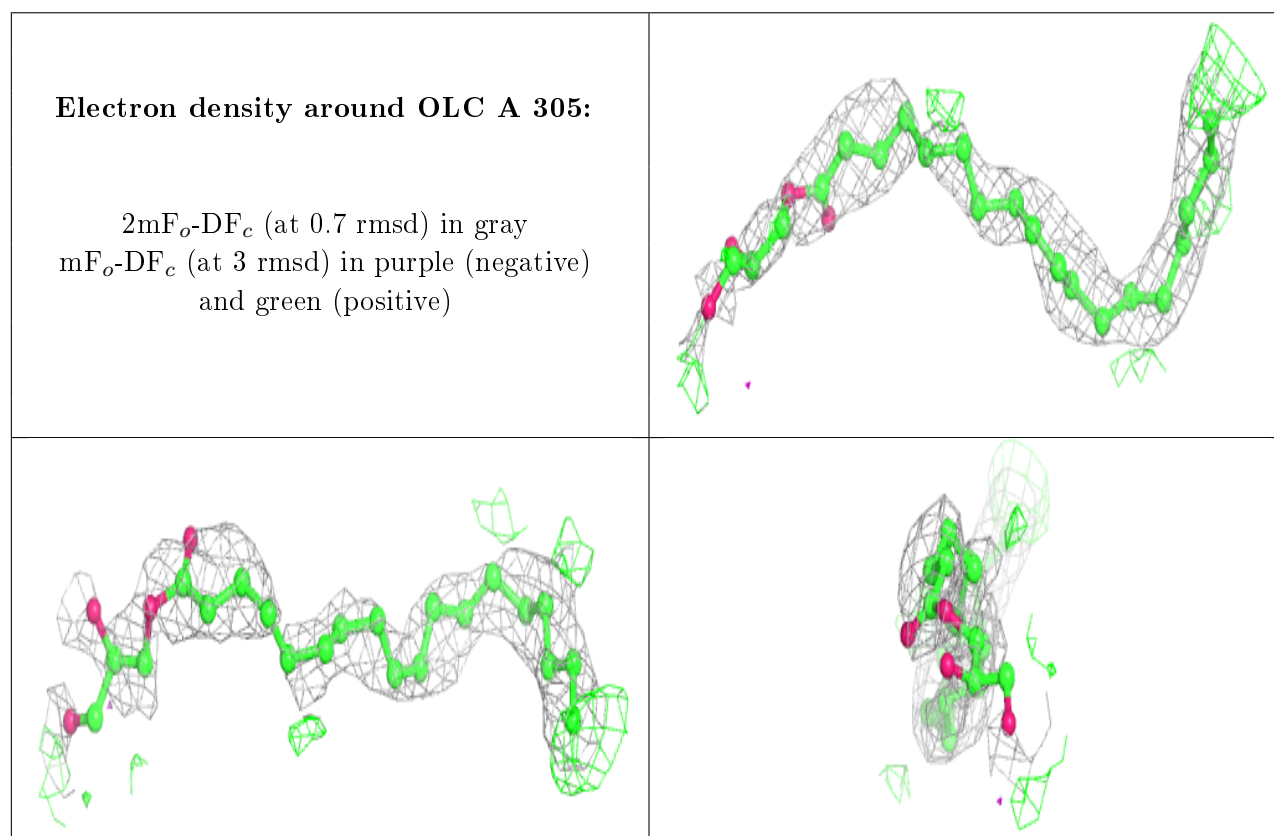
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LFA	C	315	4/20	0.72	0.21	78,80,88,89	0
2	OLC	B	305	20/25	0.72	0.23	61,83,97,106	0
3	LFA	B	309	9/20	0.73	0.29	75,88,108,117	0
3	LFA	D	311	20/20	0.73	0.20	83,91,106,109	0
3	LFA	D	303	20/20	0.73	1.01	55,73,91,91	0
3	LFA	E	312	14/20	0.74	0.22	77,86,98,98	0
2	OLC	D	309	7/25	0.74	0.20	74,76,81,85	0
2	OLC	C	307	20/25	0.74	0.27	65,93,123,125	0
3	LFA	B	312	7/20	0.75	0.20	72,79,90,101	0
2	OLC	A	302	22/25	0.75	0.27	43,64,96,102	0
3	LFA	D	313	8/20	0.75	0.21	69,83,101,103	0
2	OLC	C	306	22/25	0.76	0.22	69,95,112,117	0
2	OLC	E	301	25/25	0.76	0.27	62,89,127,140	0
5	BOG	D	318	20/20	0.76	0.56	84,99,116,125	0
2	OLC	D	307	18/25	0.77	0.23	55,93,113,117	0
3	LFA	C	304	20/20	0.77	0.97	53,67,80,82	0
3	LFA	D	312	20/20	0.77	0.20	76,89,100,101	0
3	LFA	A	309	8/20	0.77	0.26	70,75,79,80	0
2	OLC	D	306	18/25	0.77	0.23	69,88,116,126	0
2	OLC	A	304	13/25	0.78	0.20	60,71,80,82	0
2	OLC	C	302	20/25	0.78	0.23	65,82,96,104	0
3	LFA	D	315	7/20	0.78	0.20	72,74,97,101	0
3	LFA	A	313	16/20	0.80	0.25	77,98,114,116	0
3	LFA	D	320	14/20	0.80	1.16	78,93,109,110	0
2	OLC	B	302	16/25	0.80	0.30	68,85,125,142	0
2	OLC	A	306	15/25	0.81	0.19	60,72,102,112	0
3	LFA	B	310	8/20	0.82	0.26	69,84,85,94	0
2	OLC	C	301	21/25	0.82	0.26	49,55,82,91	0
2	OLC	C	305	23/25	0.82	0.30	46,70,115,119	0
2	OLC	A	301	9/25	0.83	0.16	63,71,81,87	0
2	OLC	C	309	16/25	0.83	0.18	57,76,83,84	0
2	OLC	A	318	20/25	0.84	0.26	65,76,96,100	0
2	OLC	E	305	20/25	0.84	0.30	76,86,95,98	0
2	OLC	B	301	22/25	0.84	0.18	65,82,92,98	0
2	OLC	C	310	7/25	0.85	0.18	65,79,91,98	0
2	OLC	A	307	7/25	0.85	0.22	72,76,87,89	0
2	OLC	D	301	18/25	0.85	0.22	62,77,93,102	0
3	LFA	C	313	20/20	0.85	0.22	65,84,115,119	0
2	OLC	E	303	8/25	0.86	0.18	66,70,90,96	0
2	OLC	B	307	16/25	0.88	0.23	60,80,97,101	0
3	LFA	B	316	4/20	0.89	1.42	72,74,78,81	0
2	OLC	A	317	19/25	0.89	0.30	55,60,71,74	0

*Continued on next page...*

Continued from previous page...

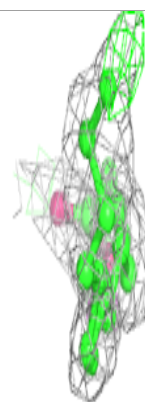
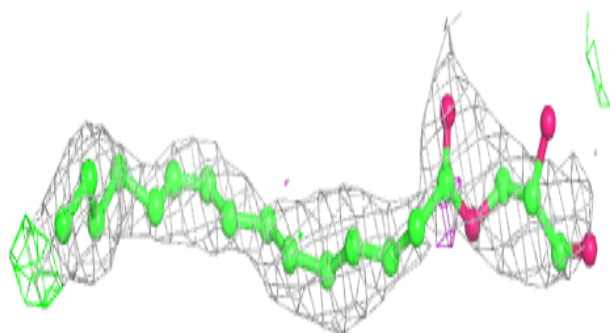
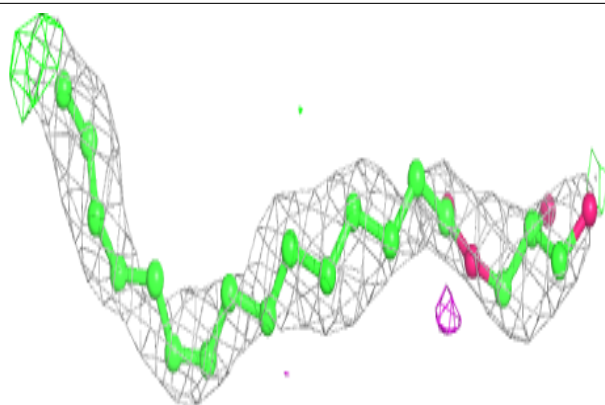
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	RET	A	316	20/21	0.89	0.14	35,42,47,48	0
3	LFA	A	311	4/20	0.90	0.11	77,78,78,84	0
2	OLC	E	307	15/25	0.91	0.22	62,73,90,97	0
3	LFA	D	314	17/20	0.92	0.45	51,60,79,79	0
6	RET	B	315	20/21	0.92	0.14	36,41,46,53	0
3	LFA	E	313	4/20	0.93	0.19	68,70,71,76	0
3	LFA	E	314	5/20	0.93	0.14	75,78,80,88	0
4	NA	A	314	1/1	0.94	0.05	41,41,41,41	0
3	LFA	A	312	6/20	0.94	0.15	56,59,72,82	0
6	RET	D	319	20/21	0.94	0.12	39,43,50,55	0
2	OLC	D	308	14/25	0.94	0.12	58,83,93,110	0
6	RET	E	317	20/21	0.95	0.13	36,41,45,46	0
6	RET	C	318	20/21	0.96	0.12	38,43,48,50	0
4	NA	D	317	1/1	0.96	0.05	39,39,39,39	0
4	NA	E	315	1/1	0.97	0.06	36,36,36,36	0
4	NA	C	316	1/1	0.98	0.04	38,38,38,38	0
4	NA	B	313	1/1	0.98	0.04	35,35,35,35	0

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

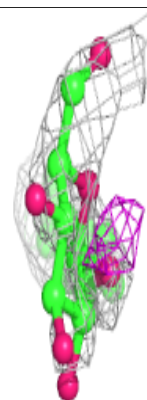
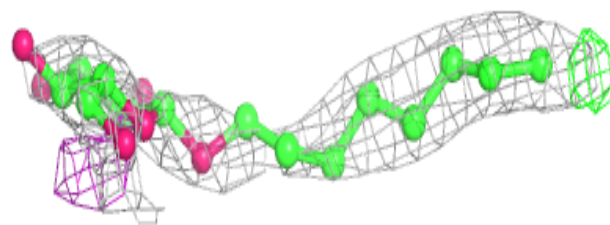
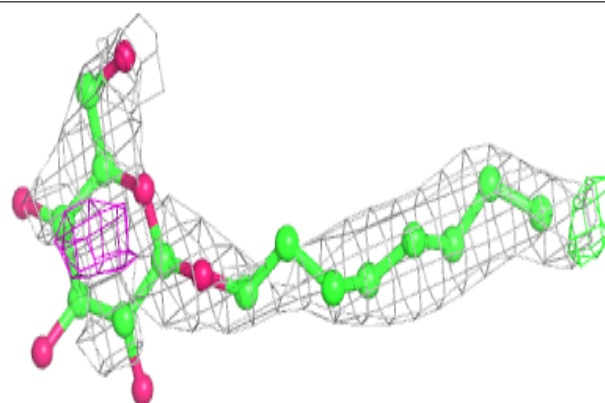


**Electron density around OLC E 309:**

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

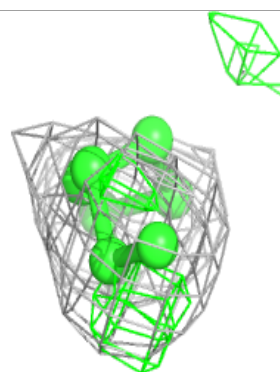
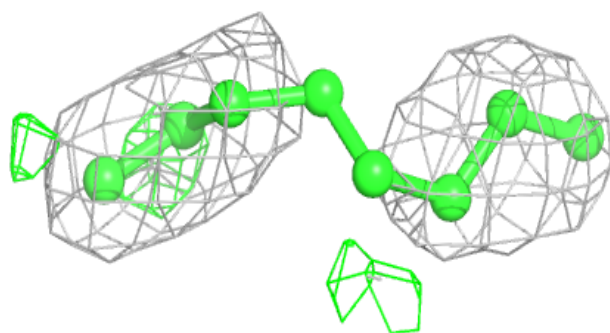
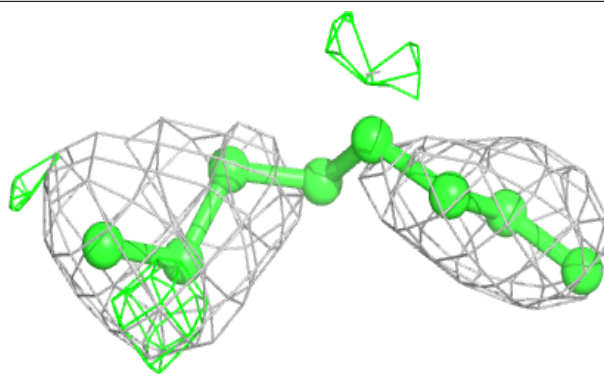
**Electron density around BOG E 316:**

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

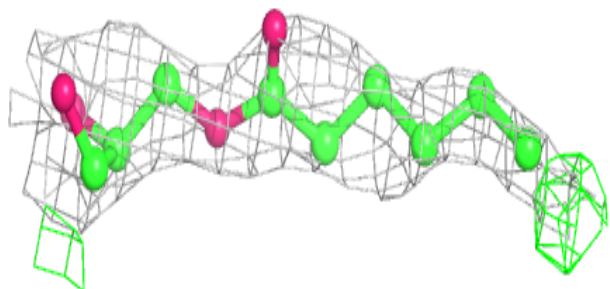
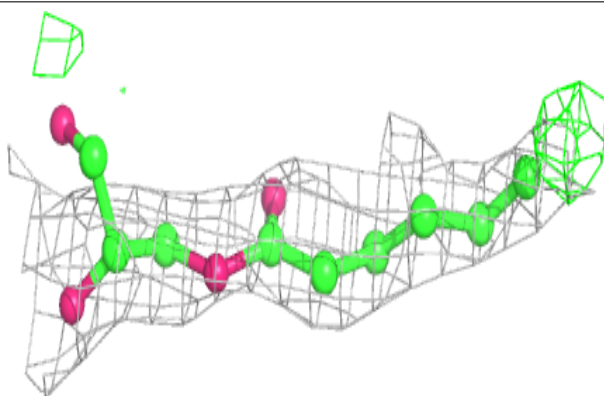


**Electron density around LFA A 310:**

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

**Electron density around OLC D 304:**

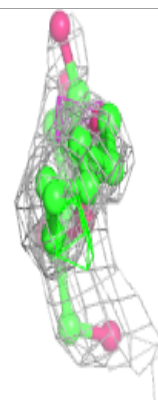
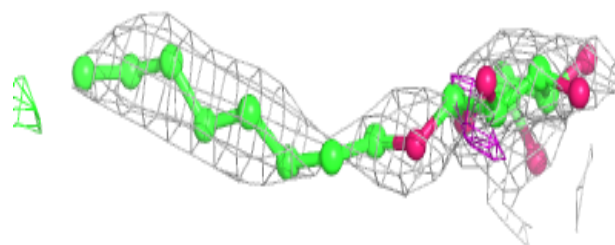
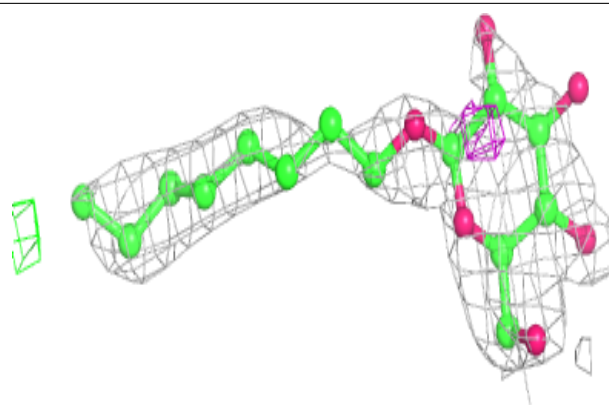
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



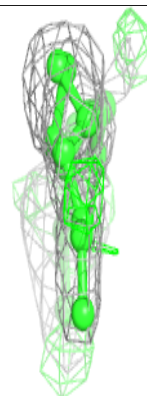
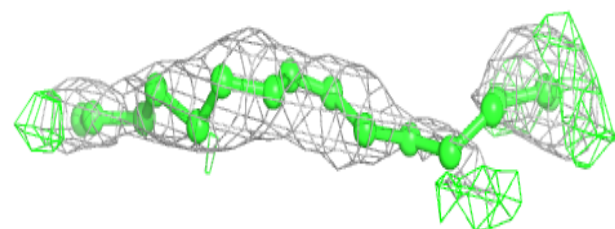
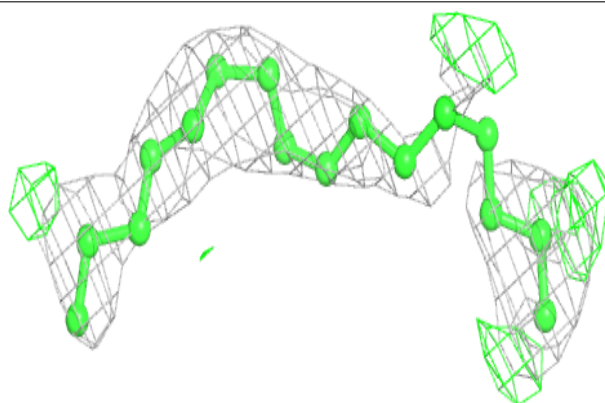


**Electron density around BOG C 317:**

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

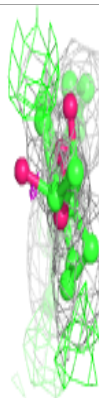
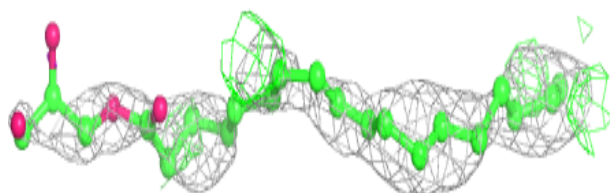
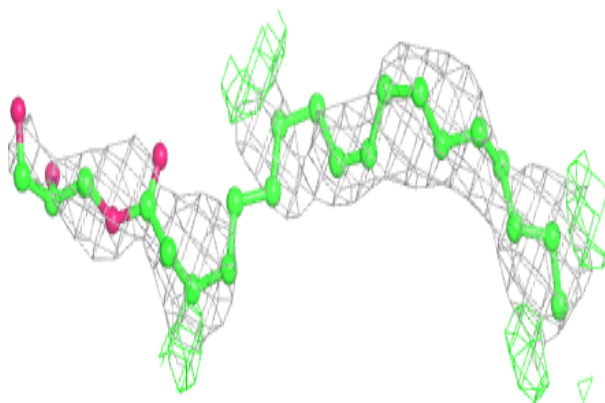
**Electron density around OLC E 304:**

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

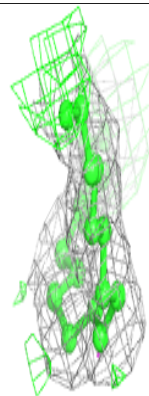
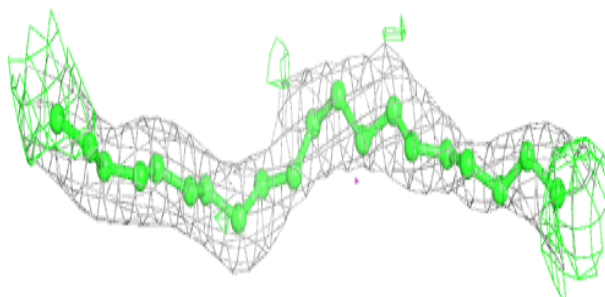
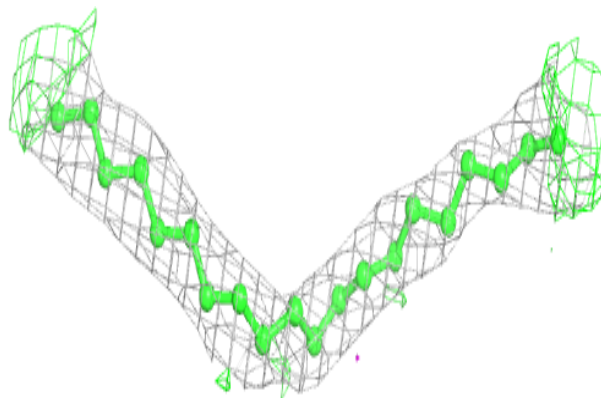


**Electron density around OLC A 303:**

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

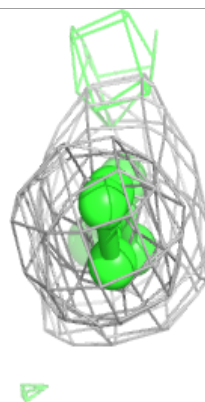
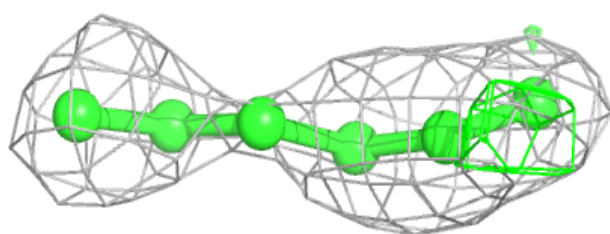
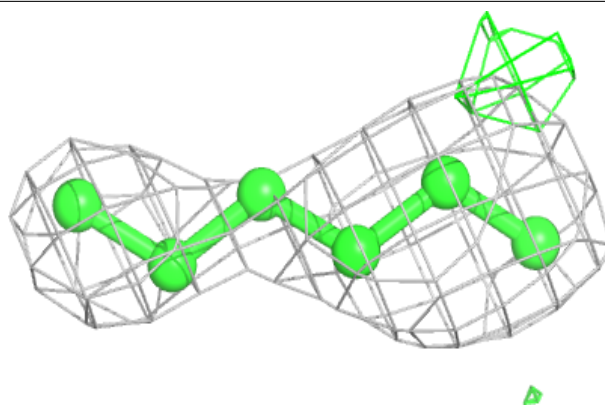
**Electron density around LFA A 319:**

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

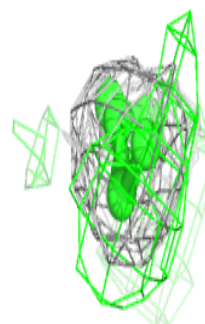
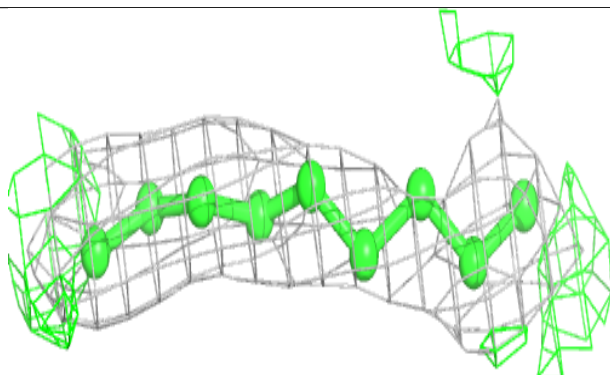
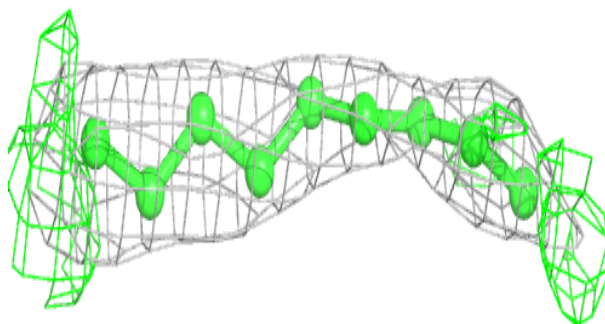


**Electron density around LFA C 314:**

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

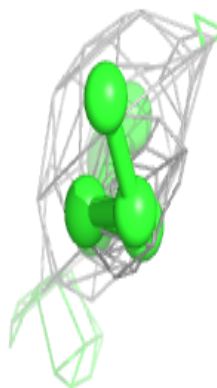
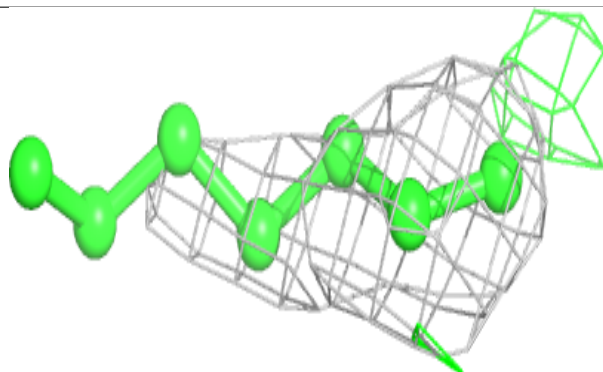
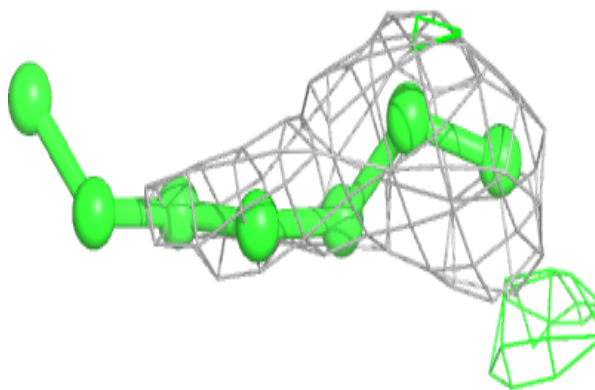
**Electron density around LFA A 320:**

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

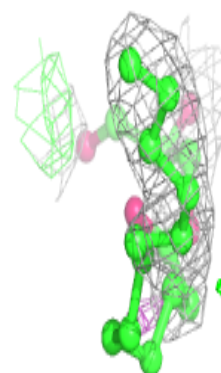
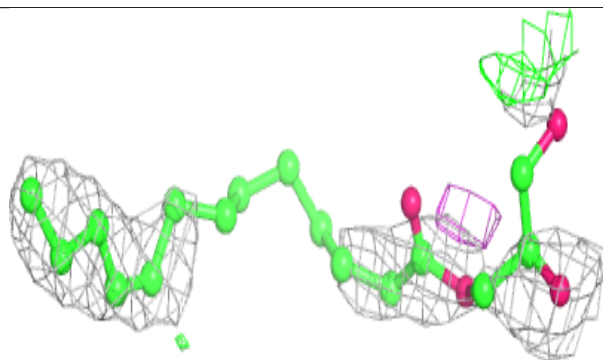
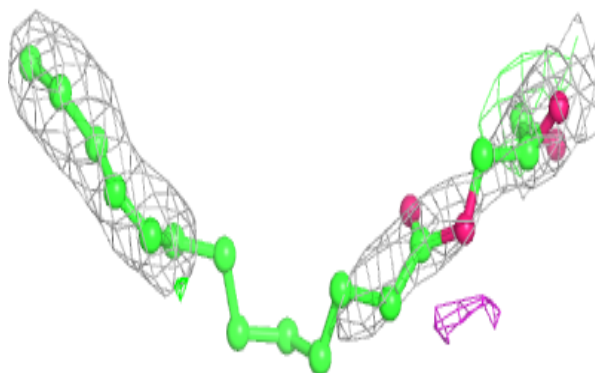


**Electron density around LFA C 311:**

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

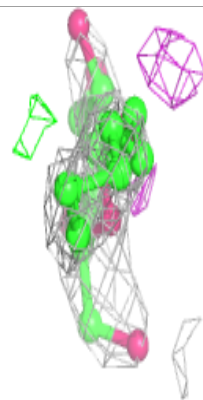
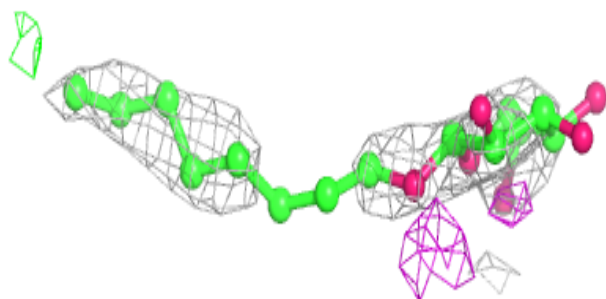
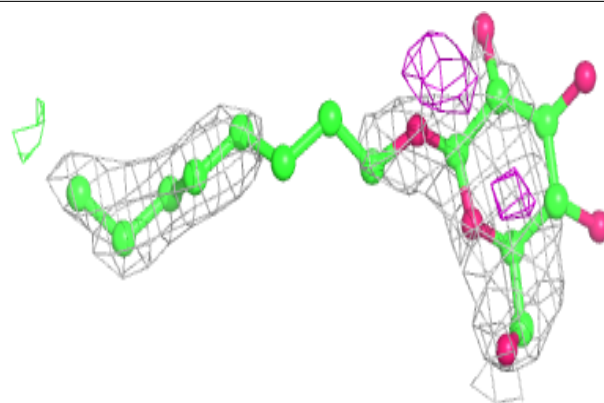
**Electron density around OLC E 310:**

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

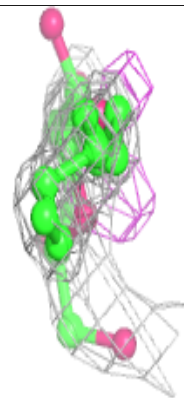
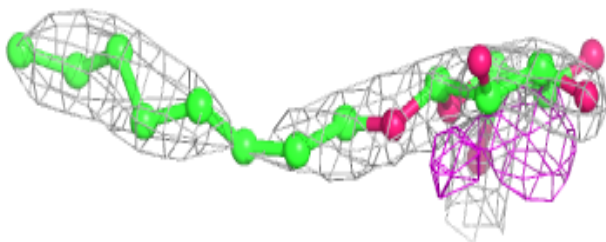
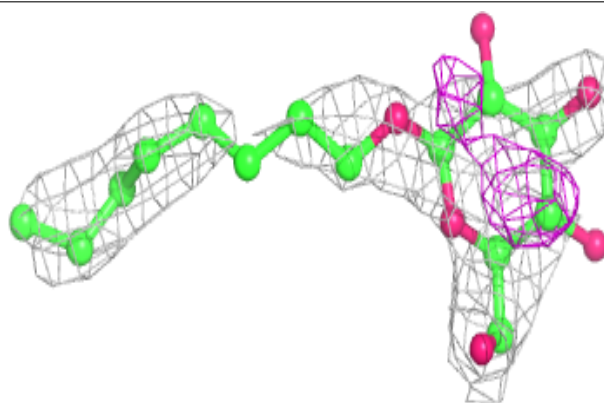


**Electron density around BOG A 315:**

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

**Electron density around BOG B 314:**

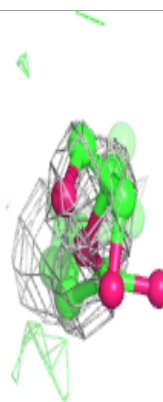
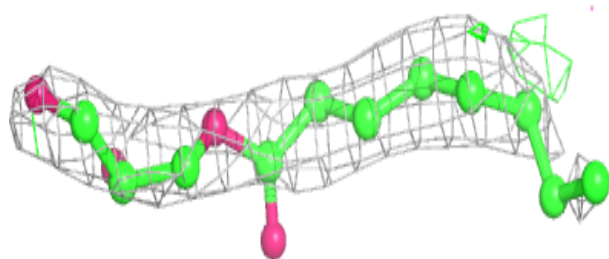
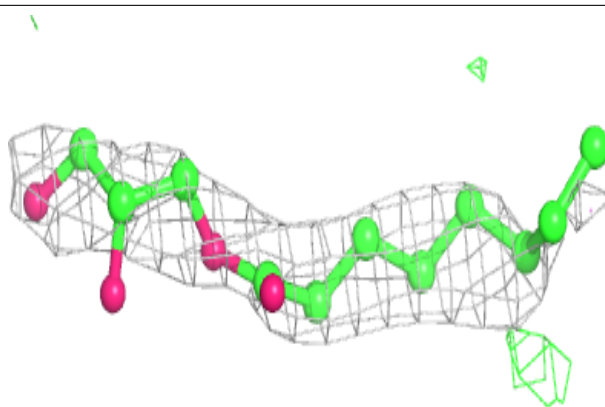
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



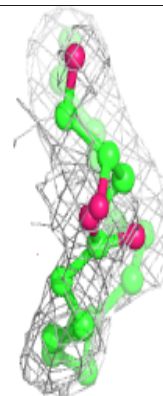
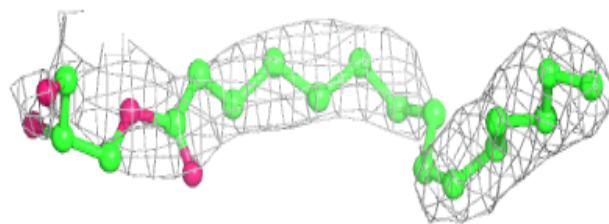
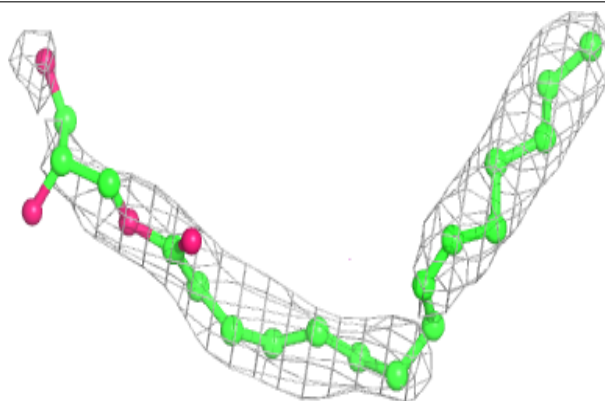


**Electron density around OLC E 306:**

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

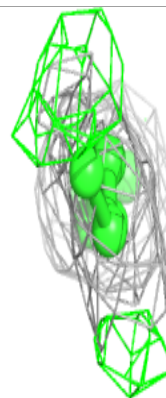
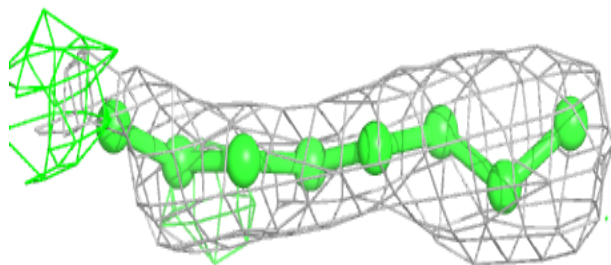
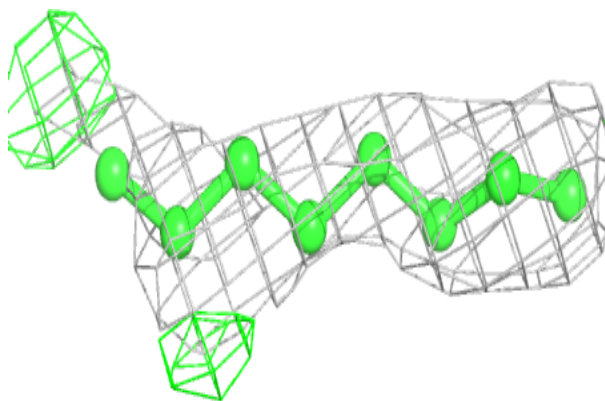
**Electron density around OLC C 308:**

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

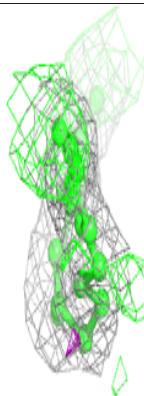
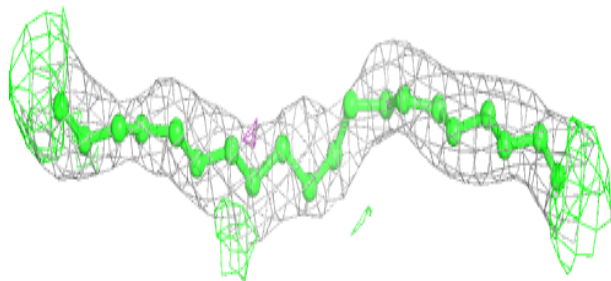
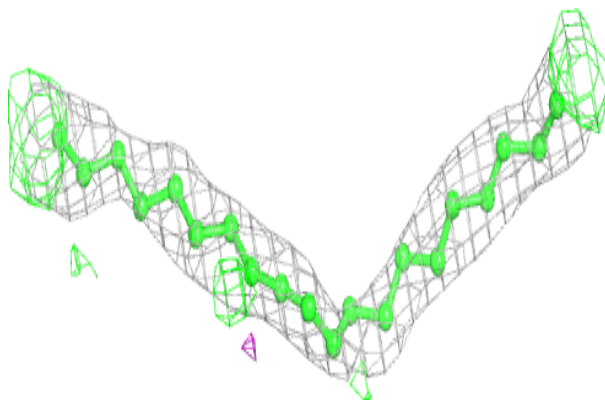


**Electron density around LFA E 311:**

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

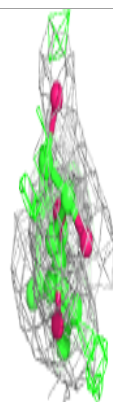
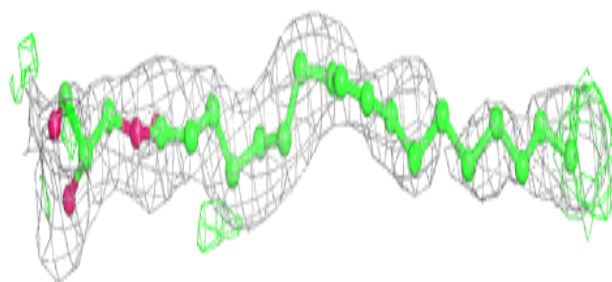
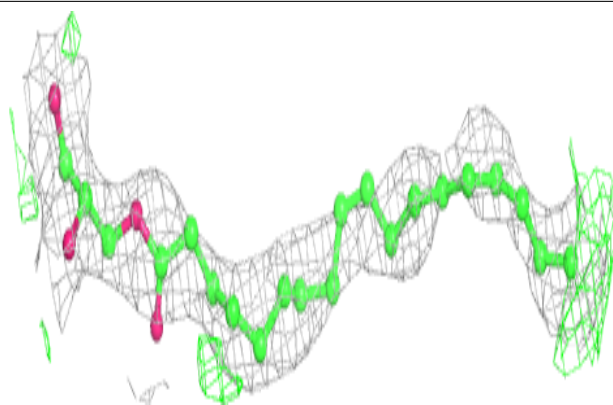
**Electron density around LFA E 302:**

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

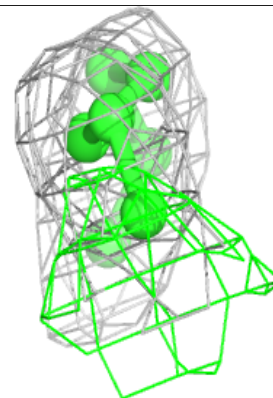
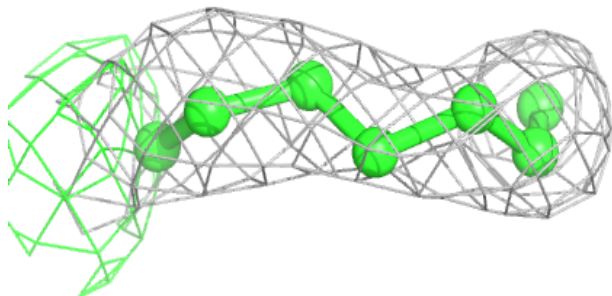
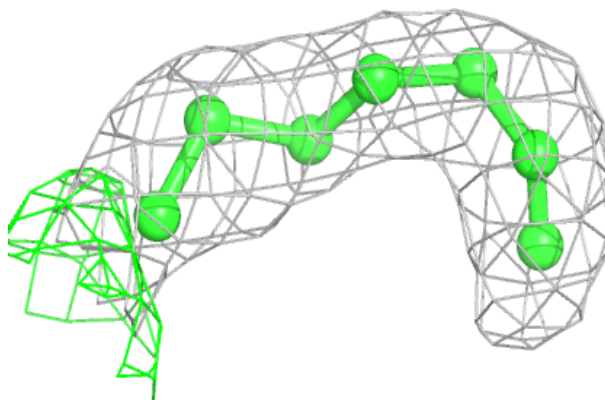


**Electron density around OLC B 304:**

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

**Electron density around OLC B 308:**

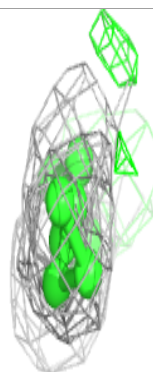
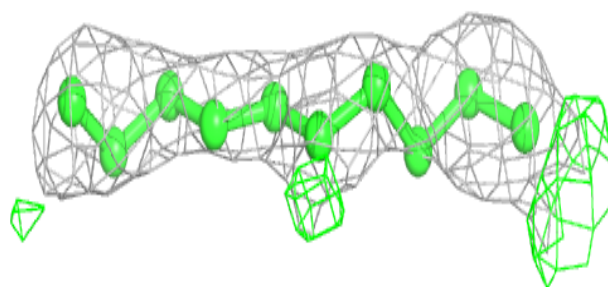
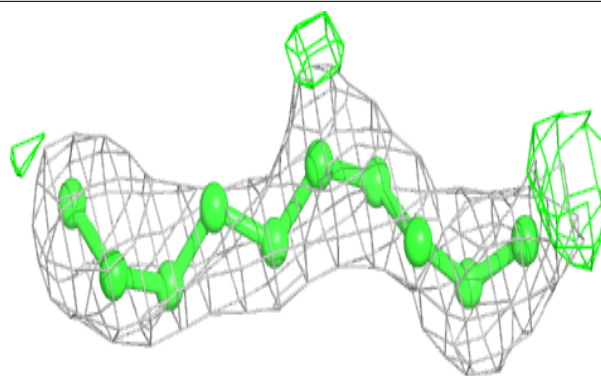
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



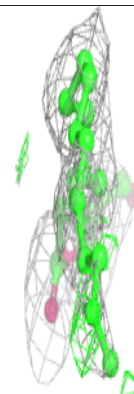
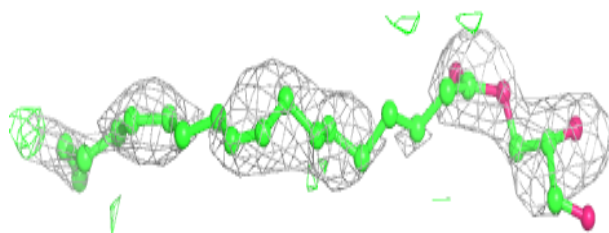
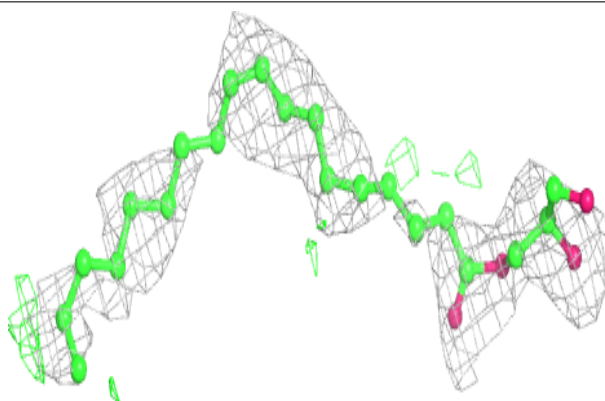


**Electron density around LFA B 311:**

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

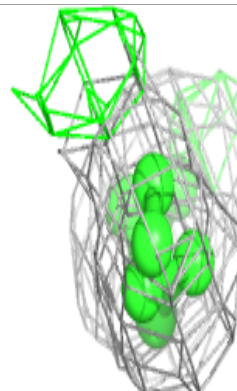
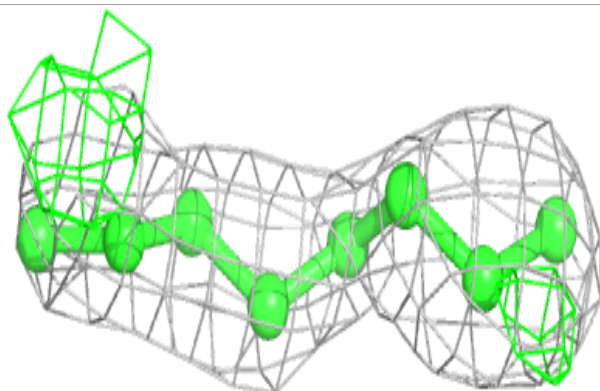
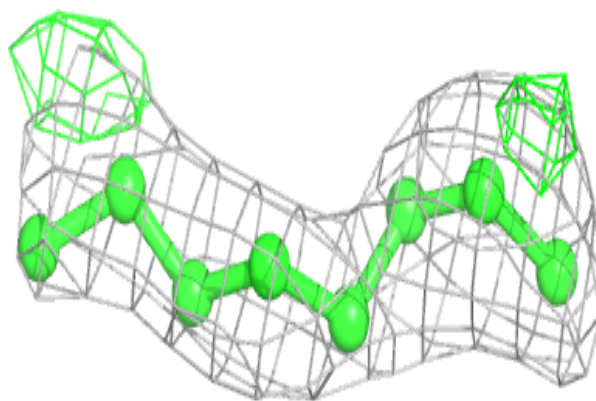
**Electron density around OLC D 305:**

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

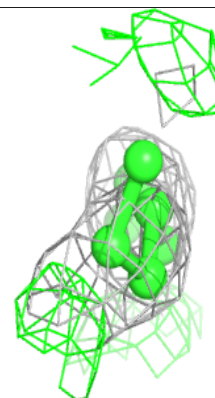
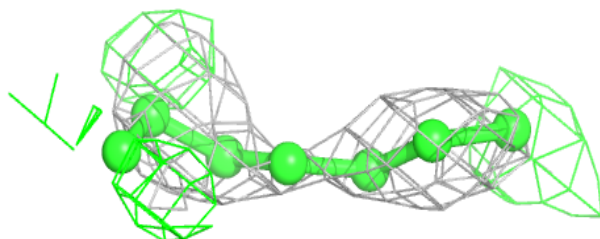
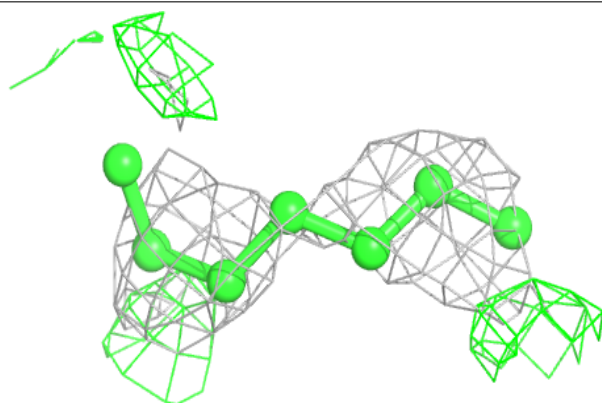


**Electron density around LFA C 312:**

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

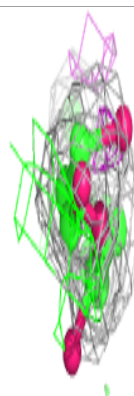
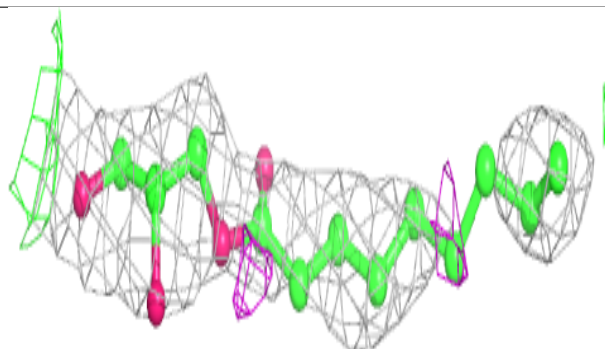
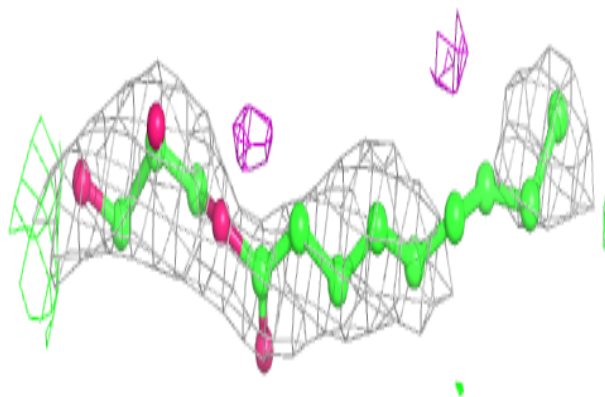
**Electron density around LFA A 308:**

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

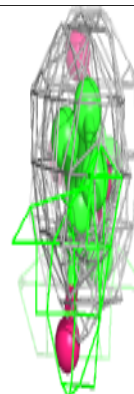
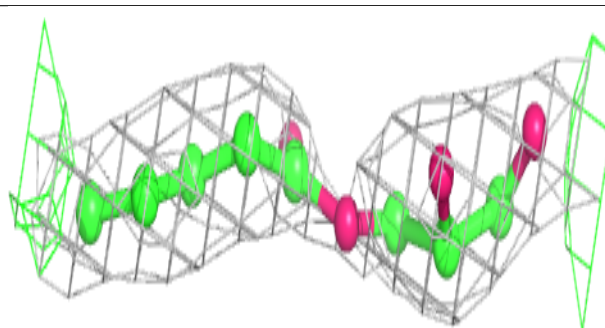
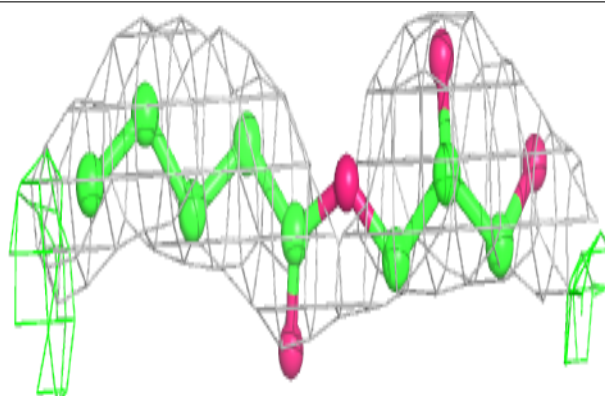


**Electron density around OLC D 302:**

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

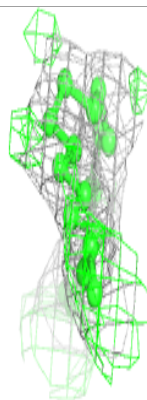
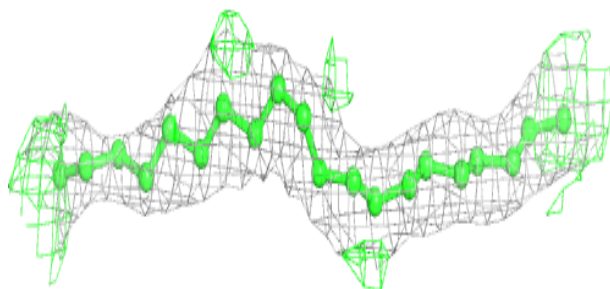
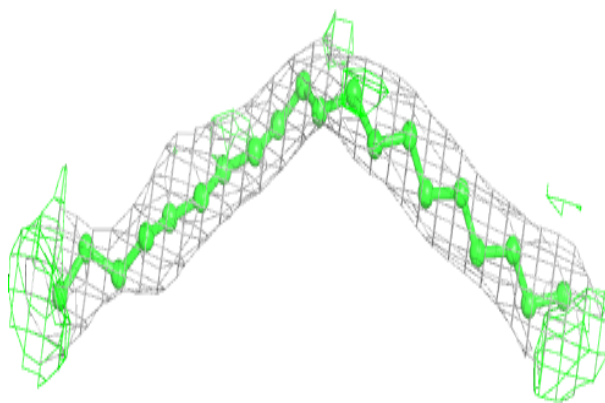
**Electron density around OLC C 303:**

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

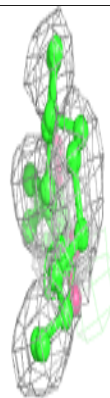
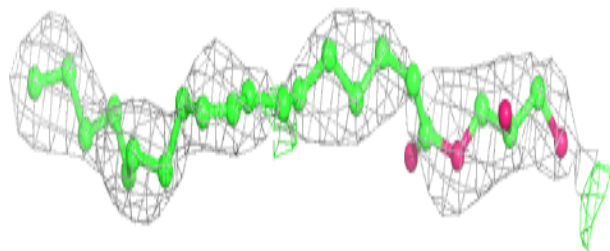
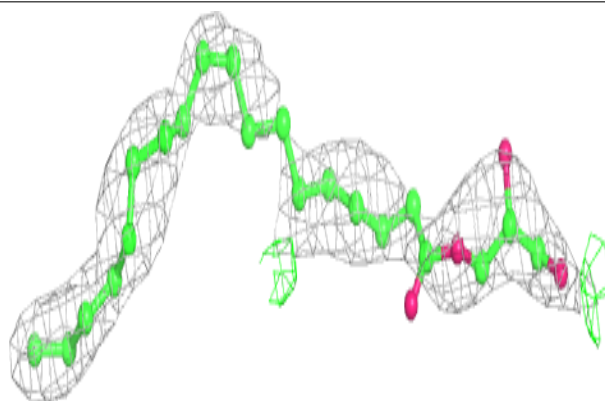


**Electron density around LFA B 303:**

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

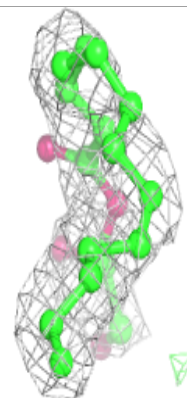
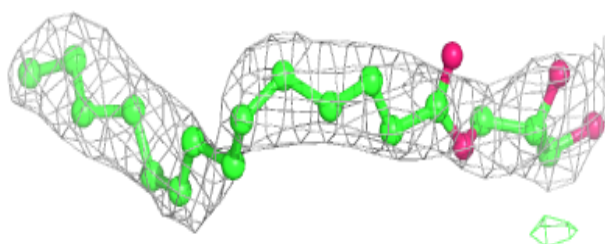
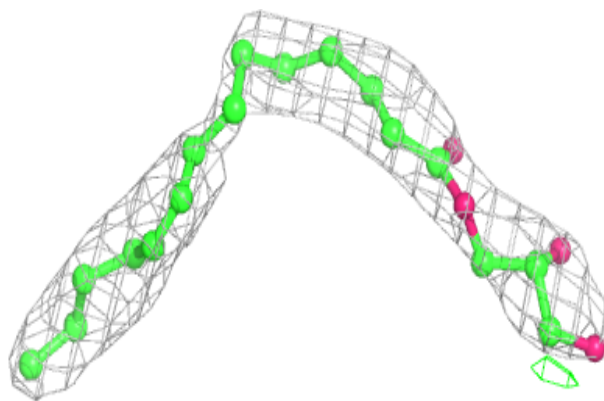
**Electron density around OLC D 310:**

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

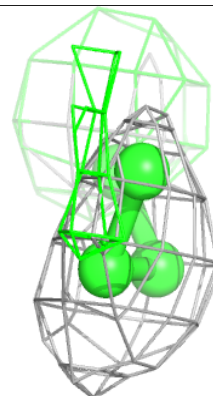
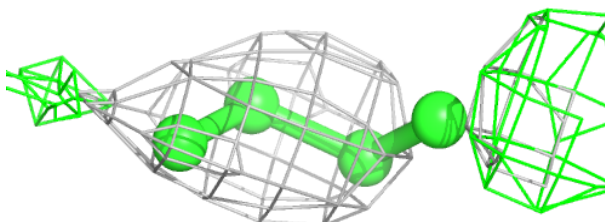
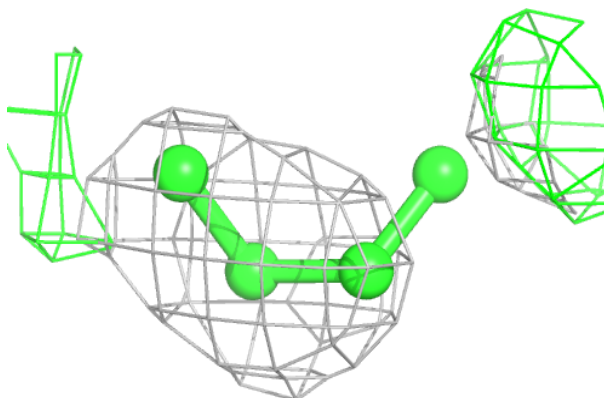


**Electron density around OLC B 306:**

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

**Electron density around LFA C 315:**

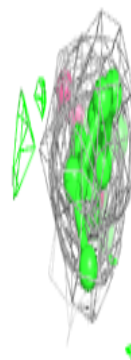
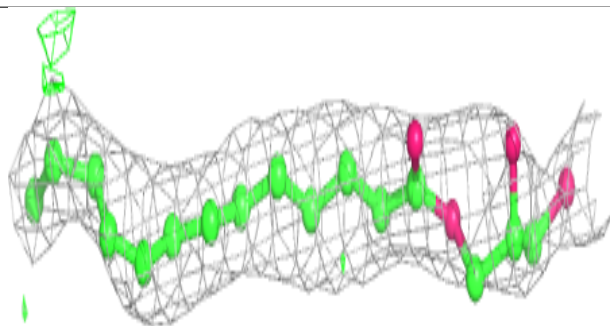
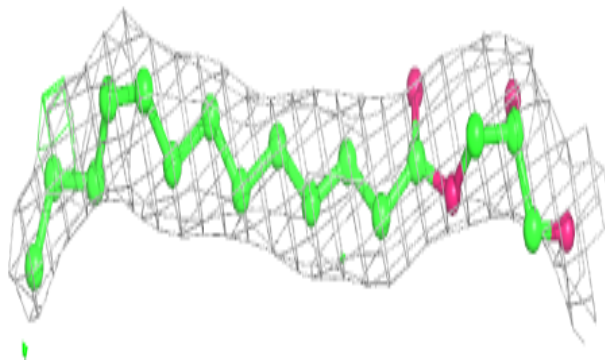
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



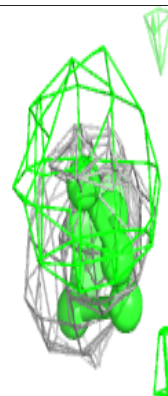
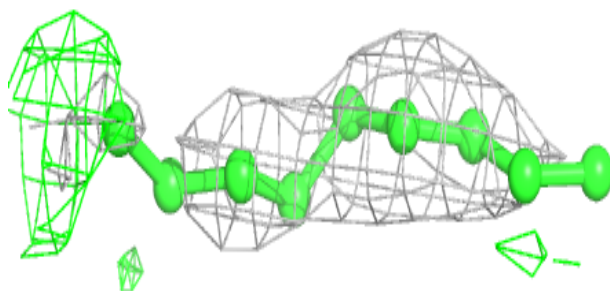
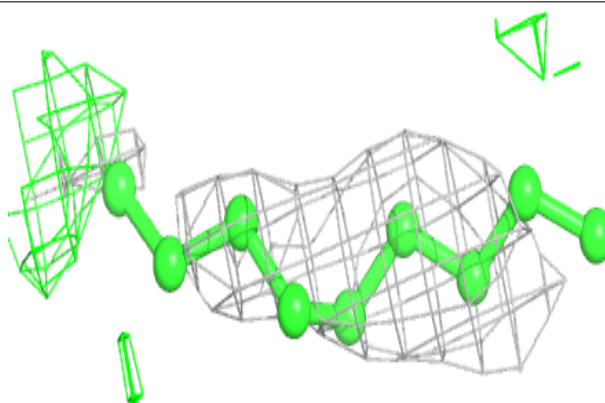


**Electron density around OLC B 305:**

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

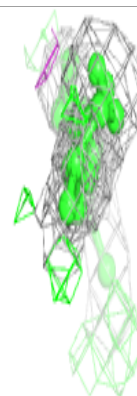
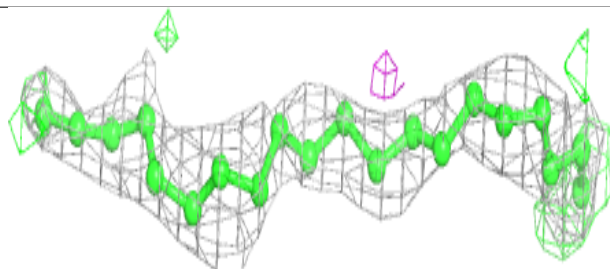
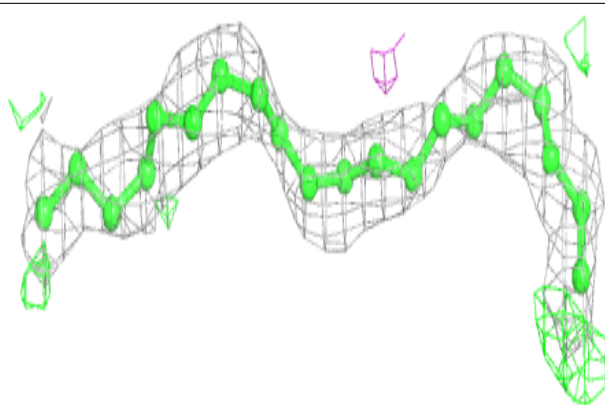
**Electron density around LFA B 309:**

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

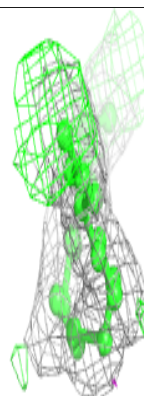
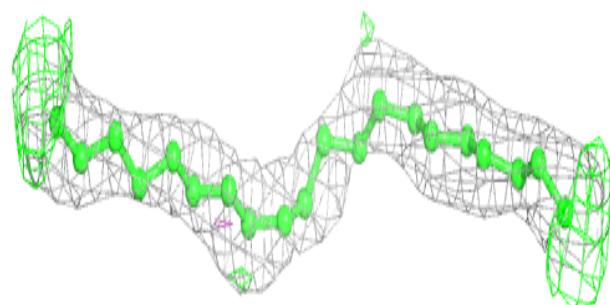
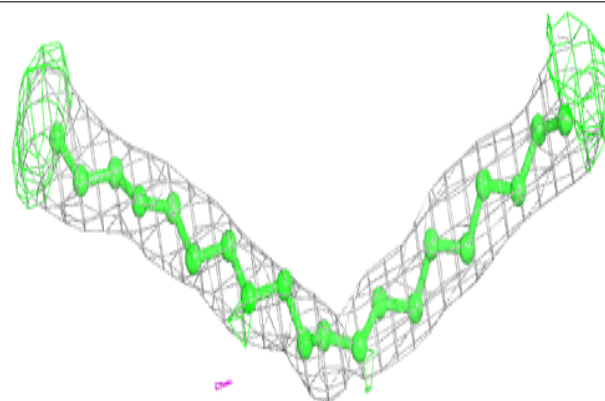


**Electron density around LFA D 311:**

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

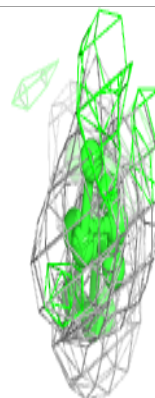
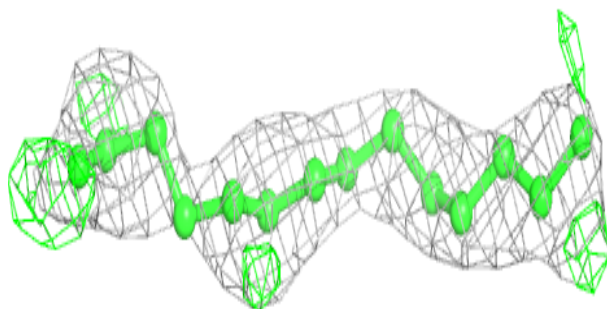
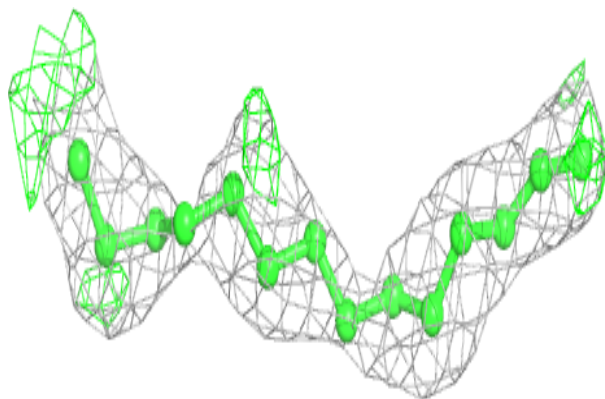
**Electron density around LFA D 303:**

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

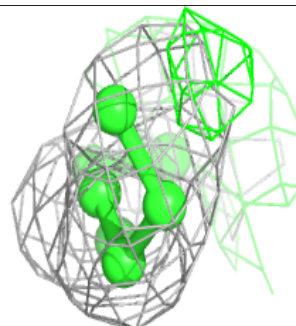
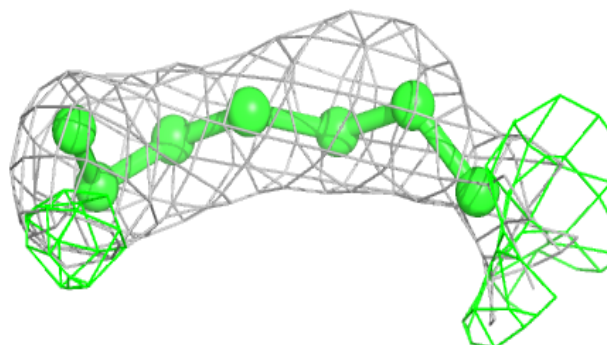
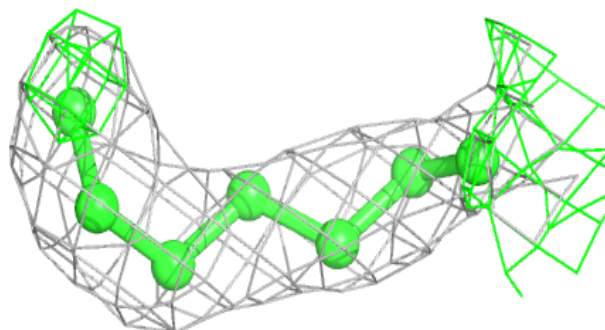


**Electron density around LFA E 312:**

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

**Electron density around OLC D 309:**

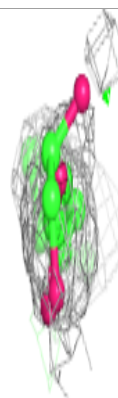
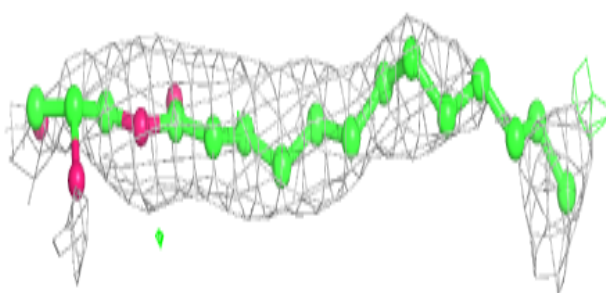
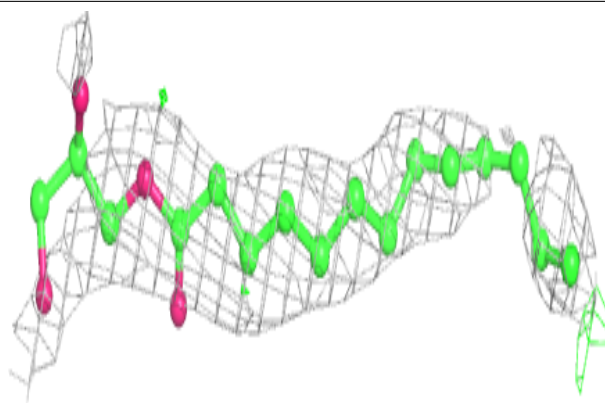
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



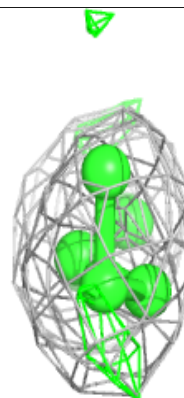
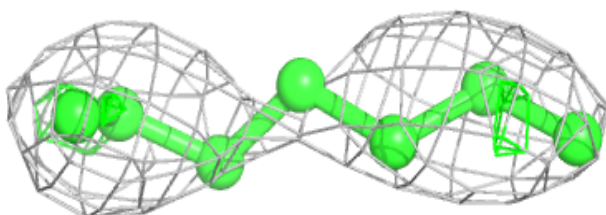
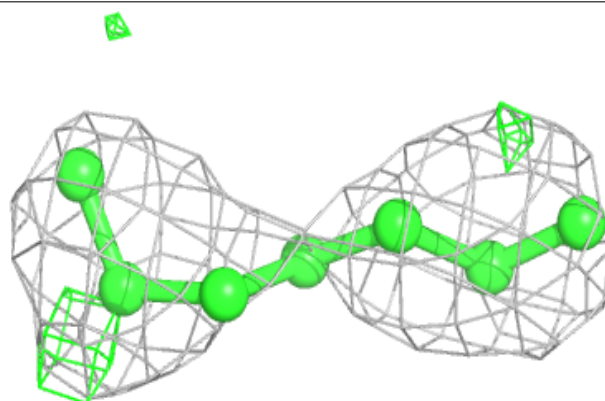


**Electron density around OLC C 307:**

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

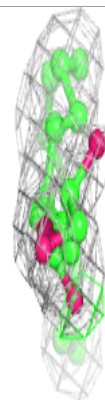
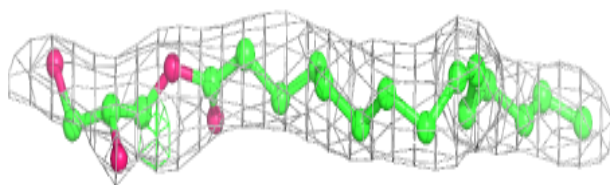
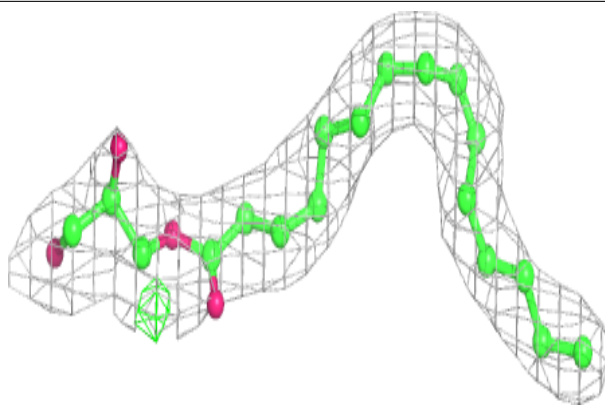
**Electron density around LFA B 312:**

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

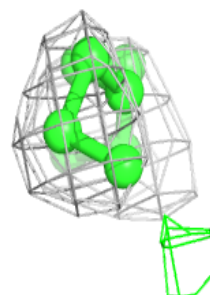
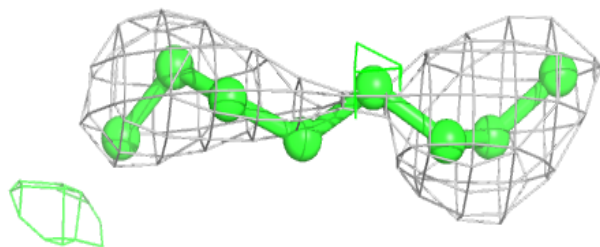
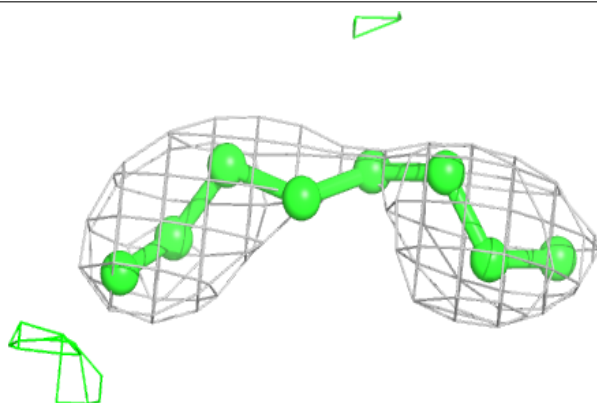


**Electron density around OLC A 302:**

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

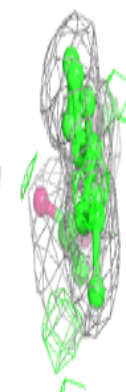
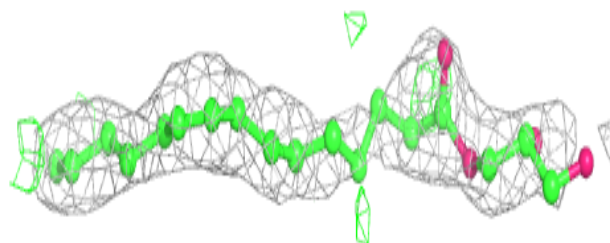
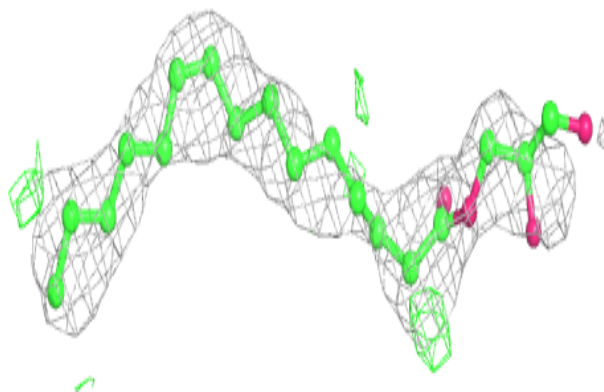
**Electron density around LFA D 313:**

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

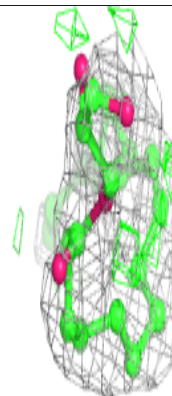
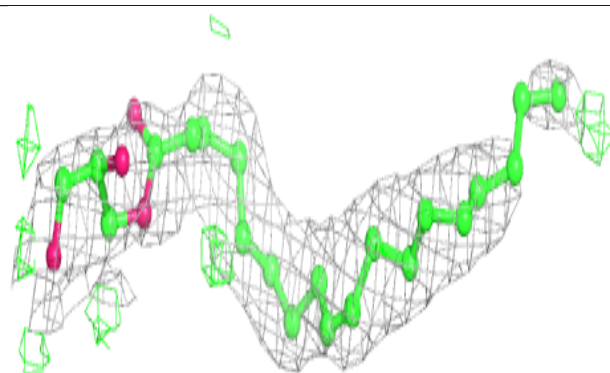
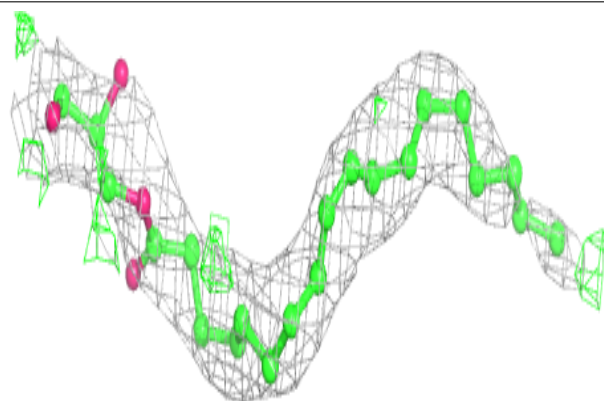


**Electron density around OLC C 306:**

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

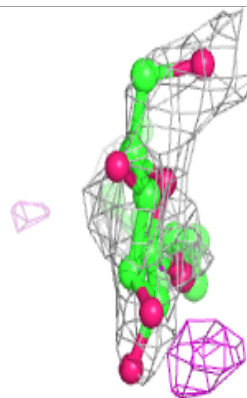
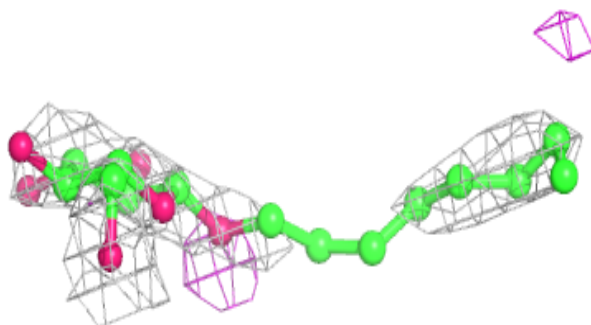
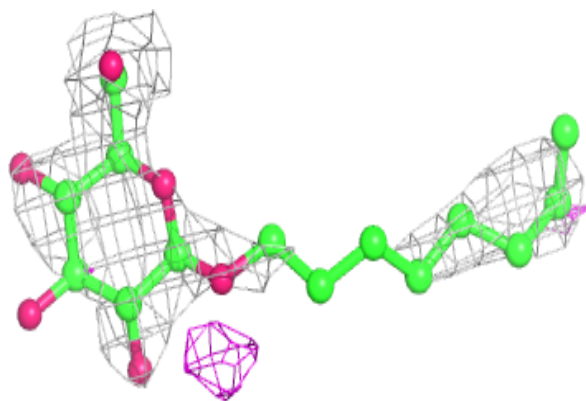
**Electron density around OLC E 301:**

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

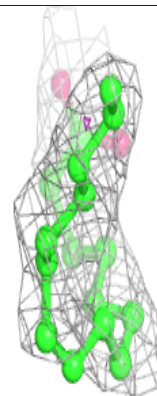
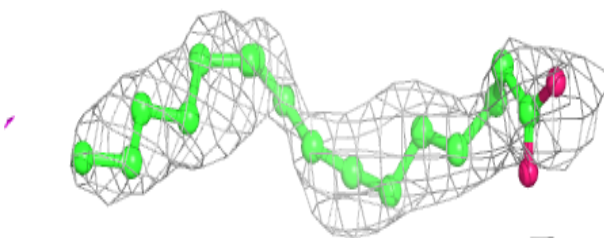
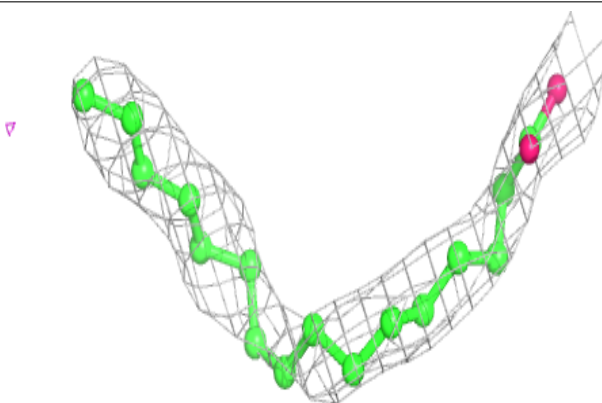


**Electron density around BOG D 318:**

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

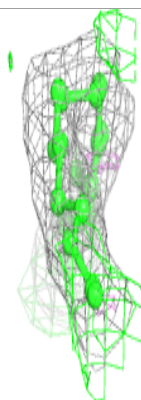
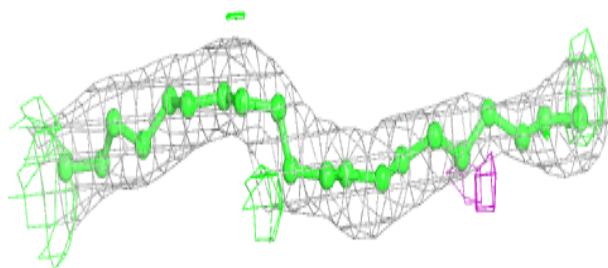
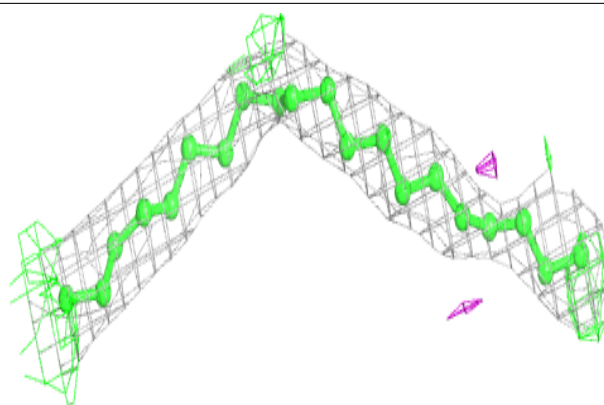
**Electron density around OLC D 307:**

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

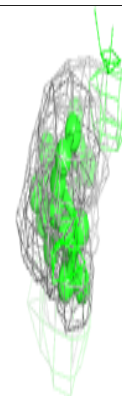
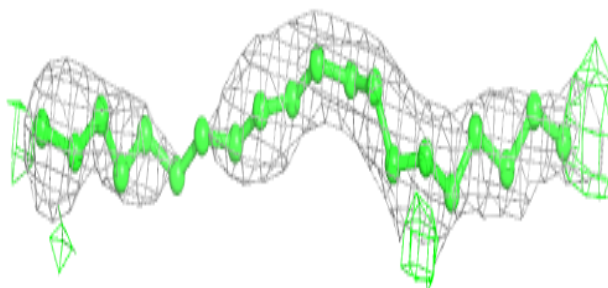
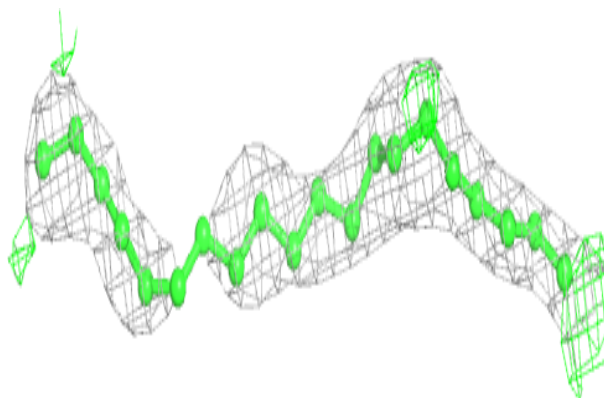


**Electron density around LFA C 304:**

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

**Electron density around LFA D 312:**

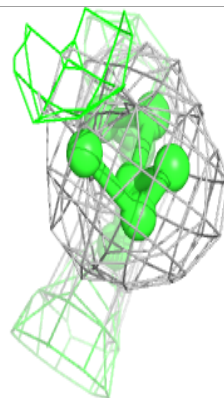
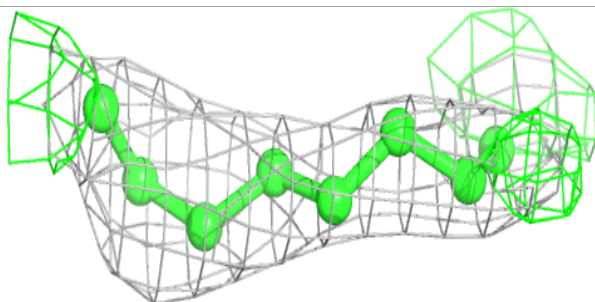
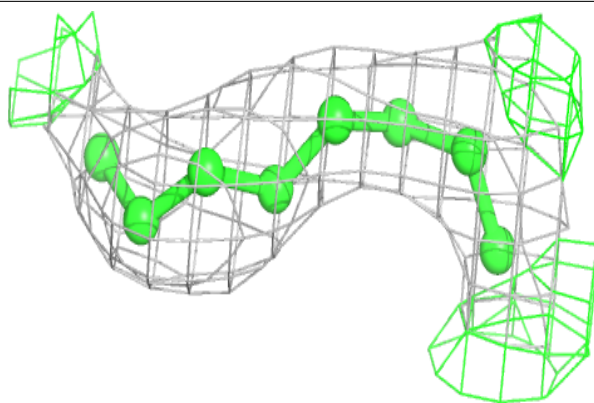
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



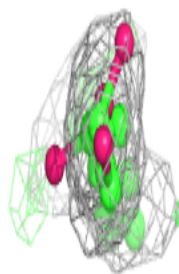
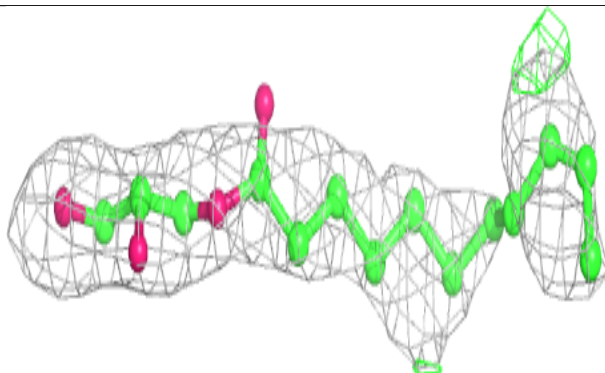
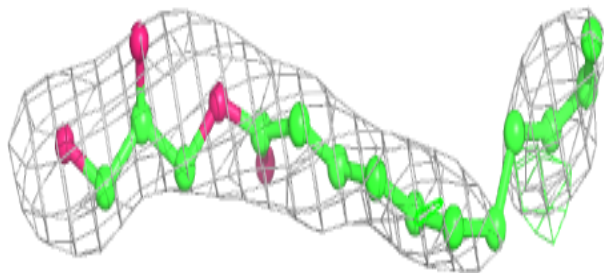


**Electron density around LFA A 309:**

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

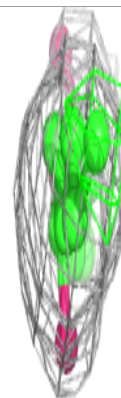
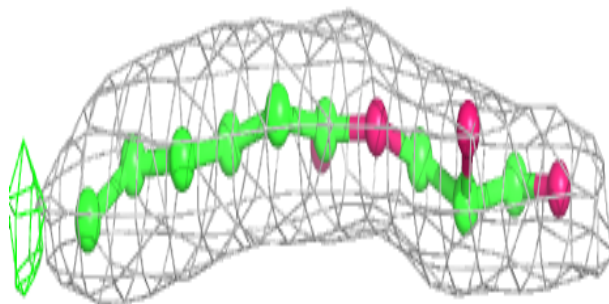
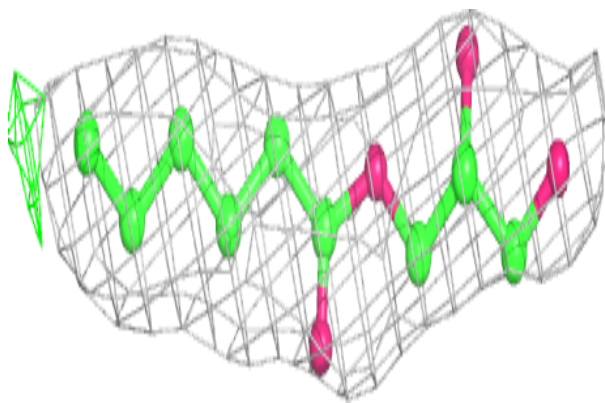
**Electron density around OLC D 306:**

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

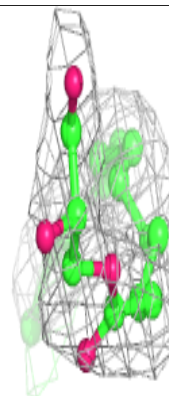
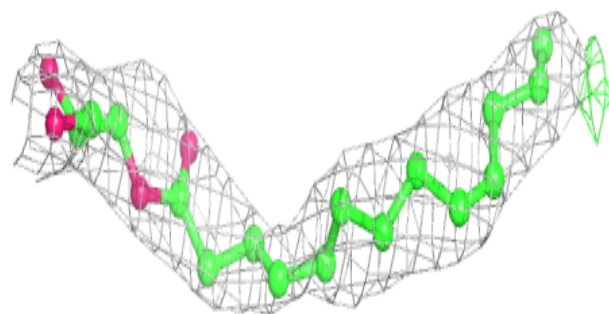
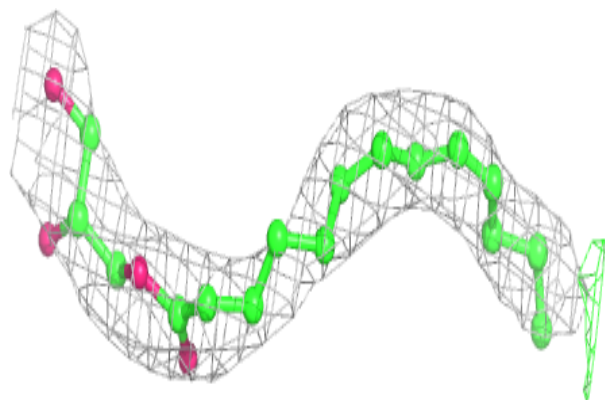


**Electron density around OLC A 304:**

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

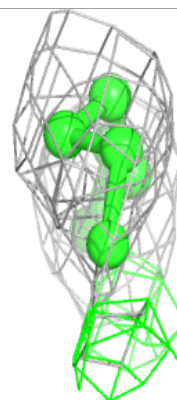
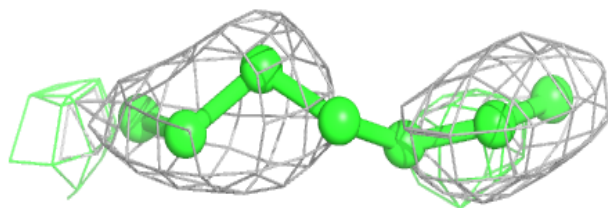
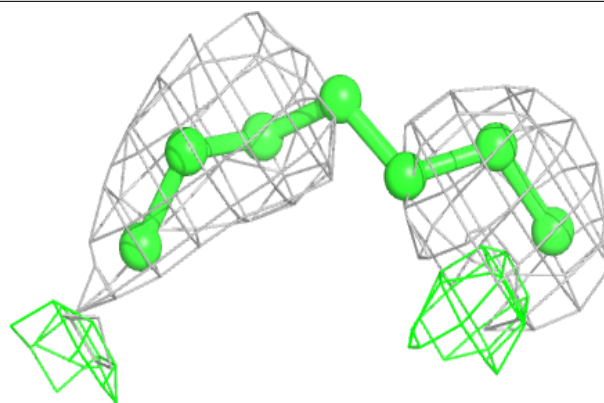
**Electron density around OLC C 302:**

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

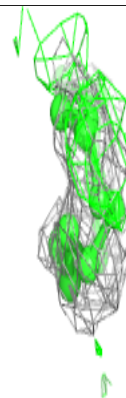
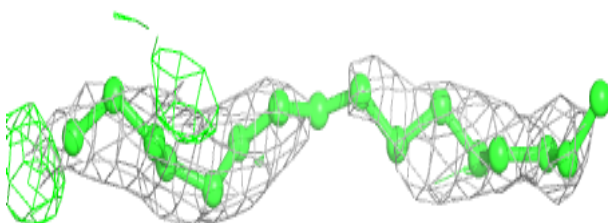
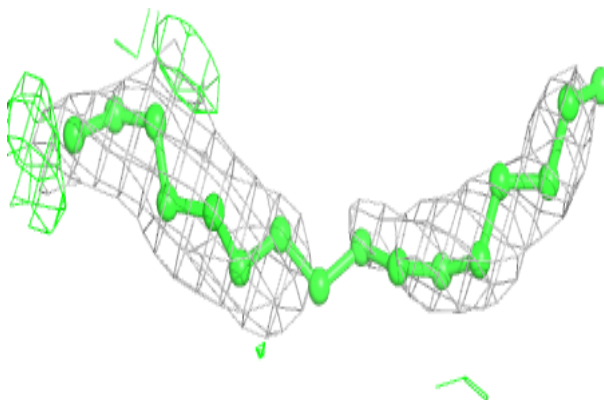


**Electron density around LFA D 315:**

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

**Electron density around LFA A 313:**

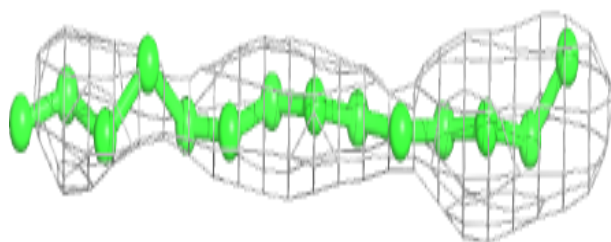
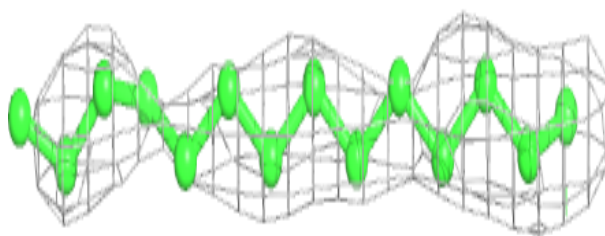
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



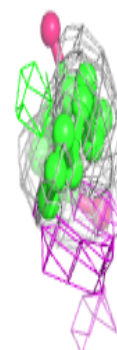
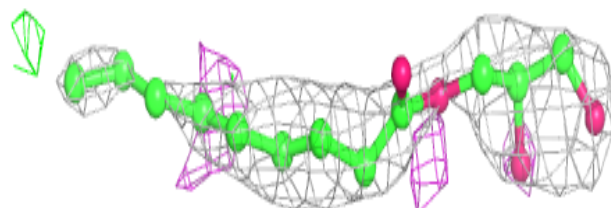
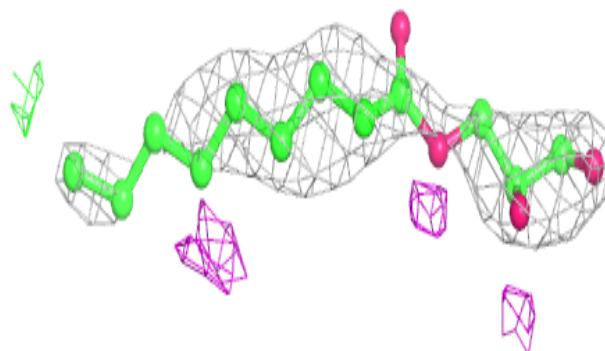


**Electron density around LFA D 320:**

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

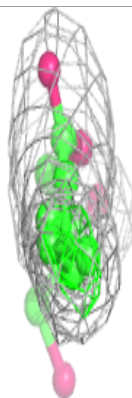
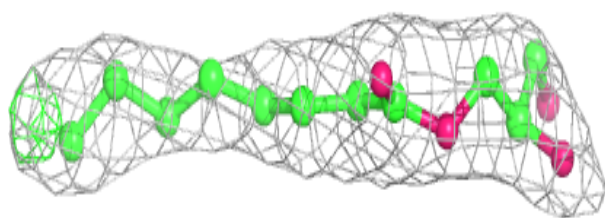
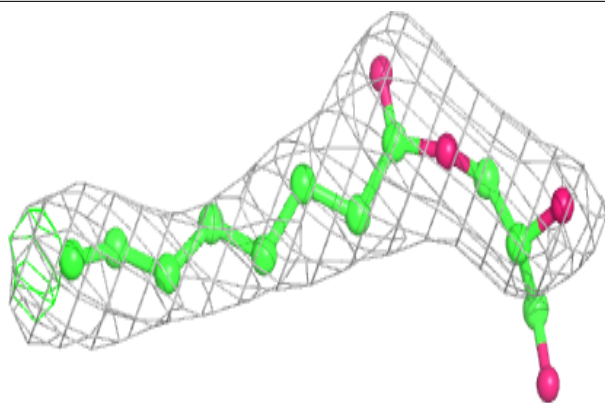
**Electron density around OLC B 302:**

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

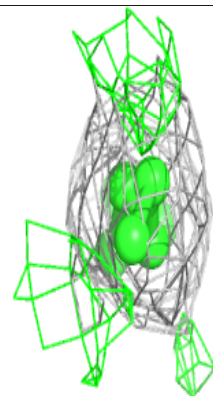
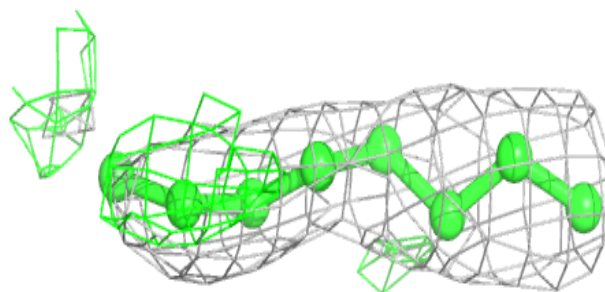
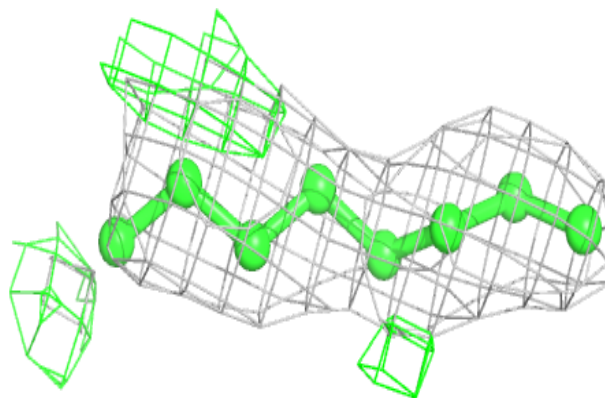


**Electron density around OLC A 306:**

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

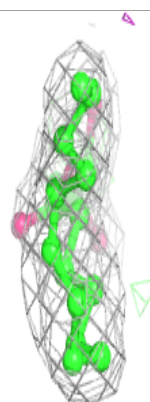
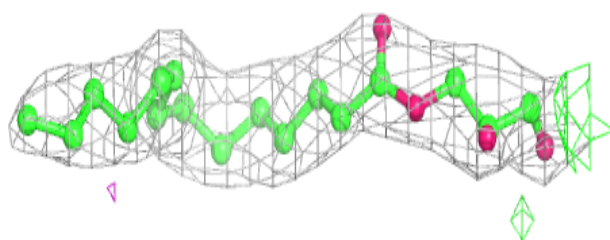
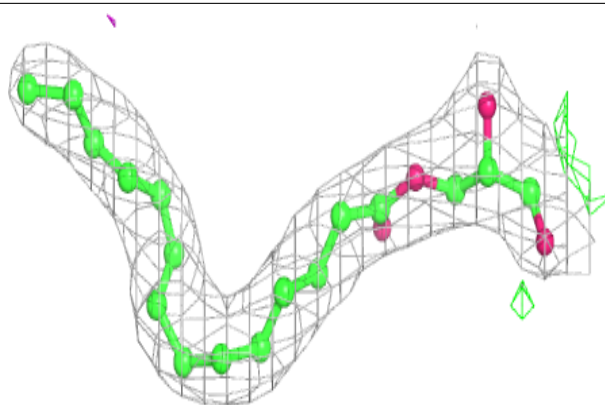
**Electron density around LFA B 310:**

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

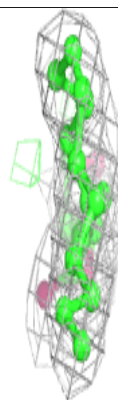
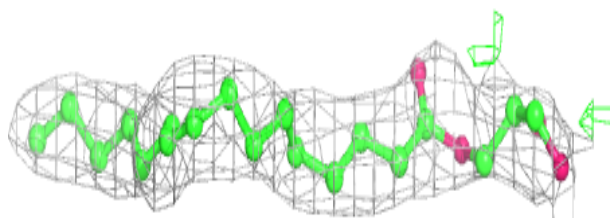
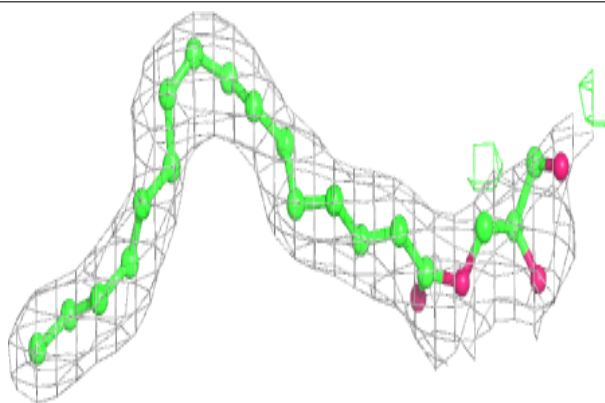


**Electron density around OLC C 301:**

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

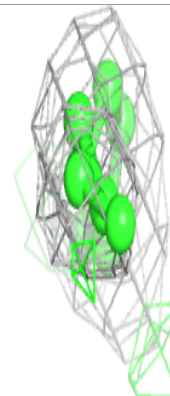
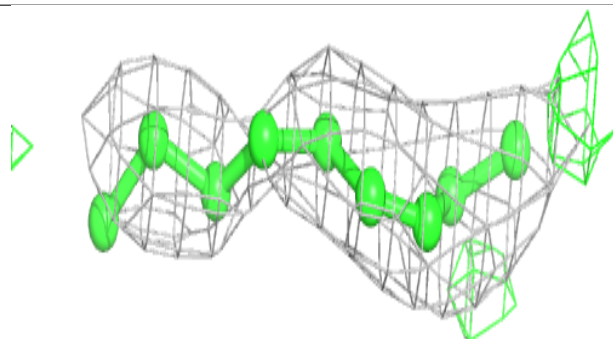
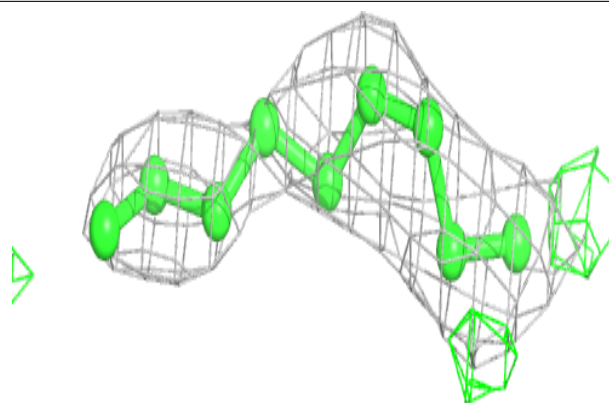
**Electron density around OLC C 305:**

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

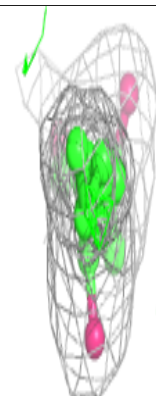
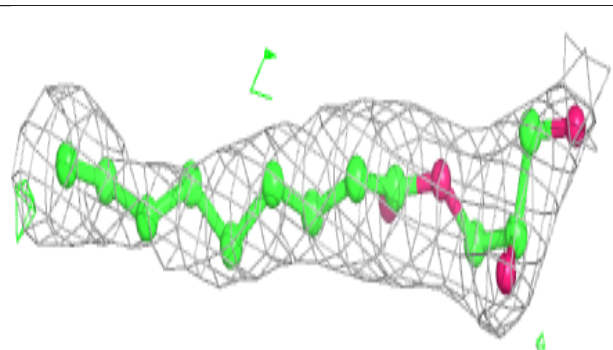
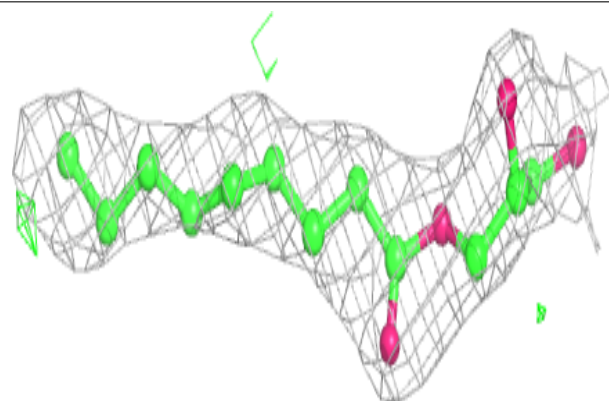


**Electron density around OLC A 301:**

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

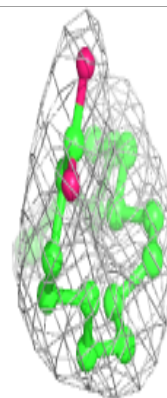
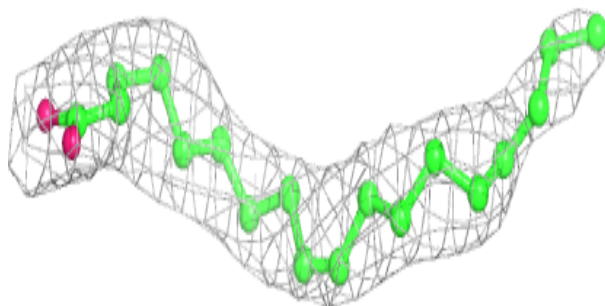
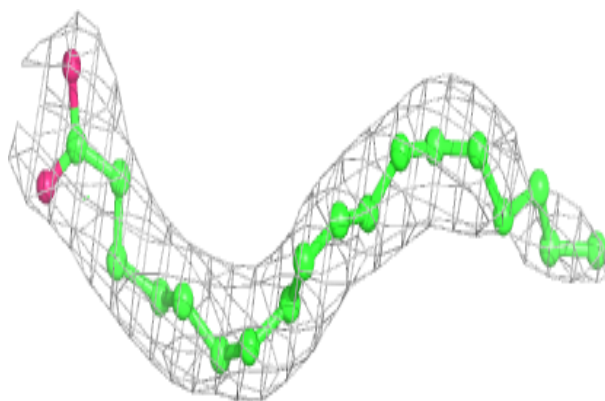
**Electron density around OLC C 309:**

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

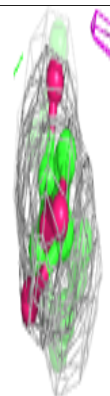
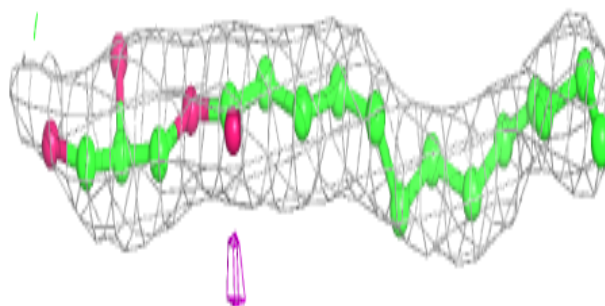
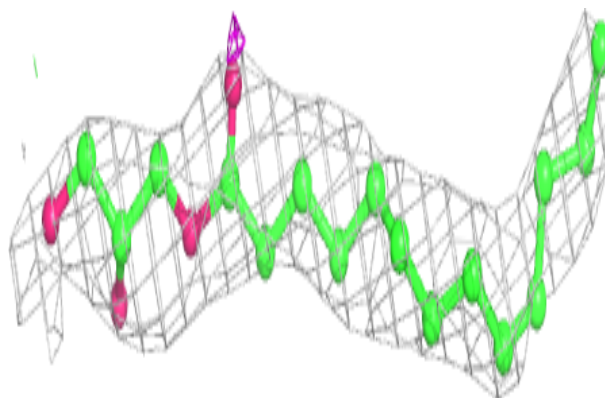


**Electron density around OLC A 318:**

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

**Electron density around OLC E 305:**

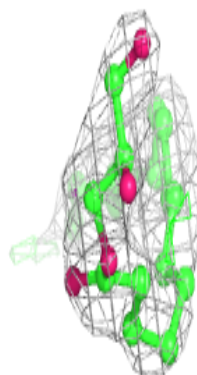
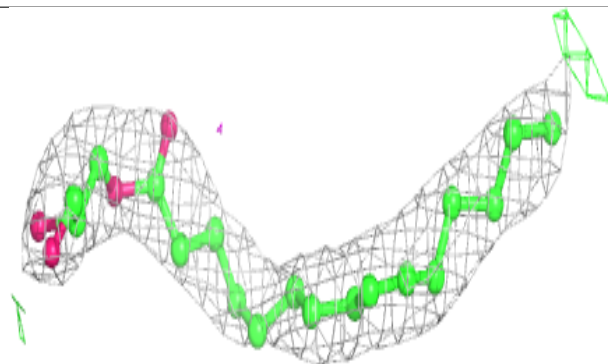
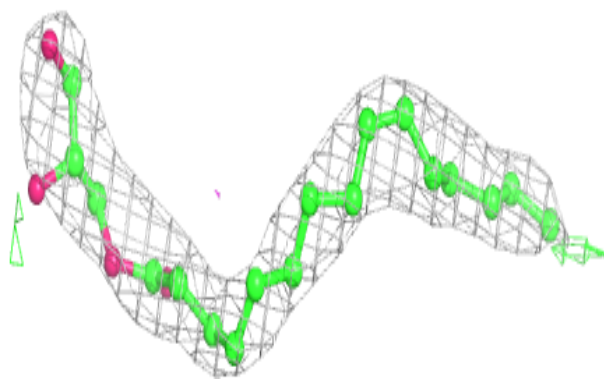
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



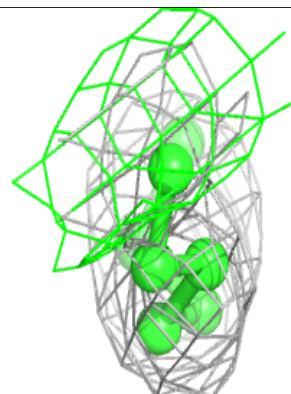
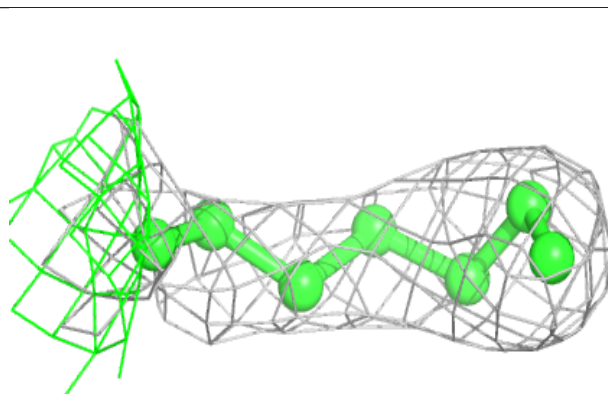
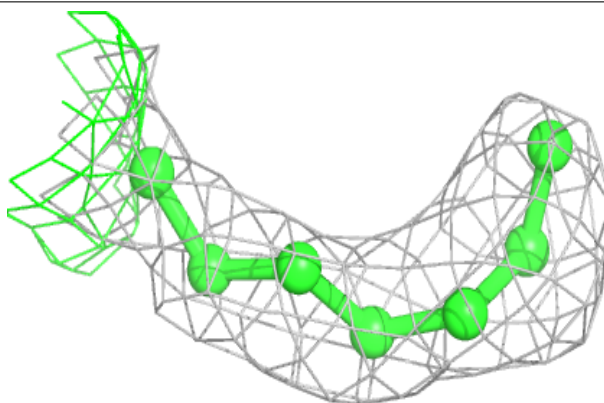


**Electron density around OLC B 301:**

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

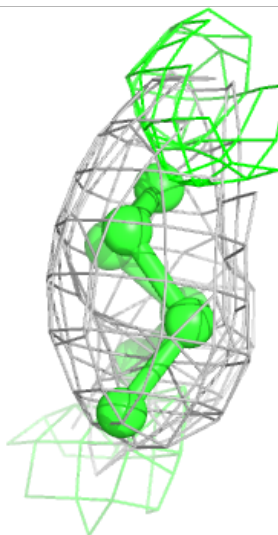
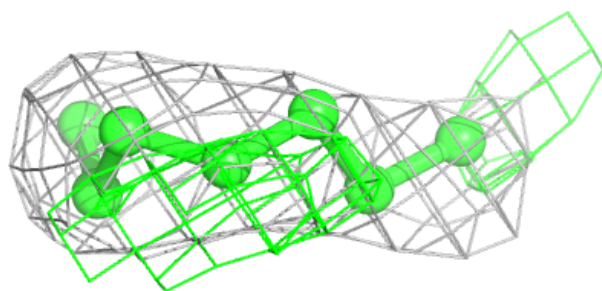
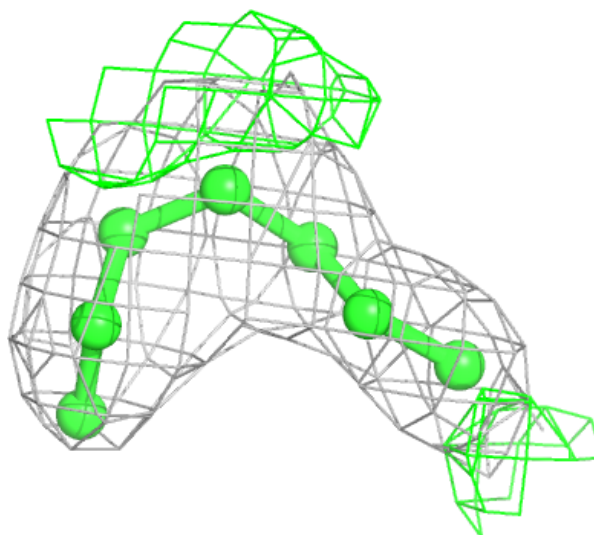
**Electron density around OLC C 310:**

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



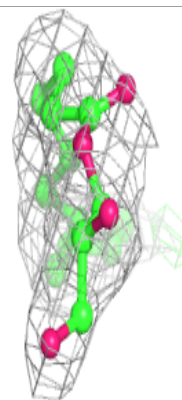
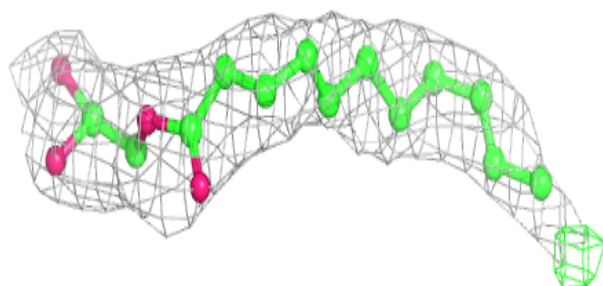
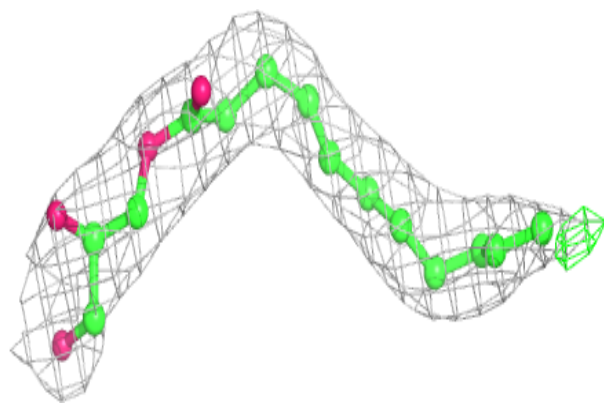
**Electron density around OLC A 307:**

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

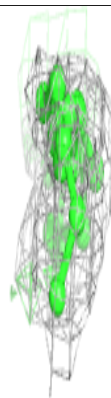
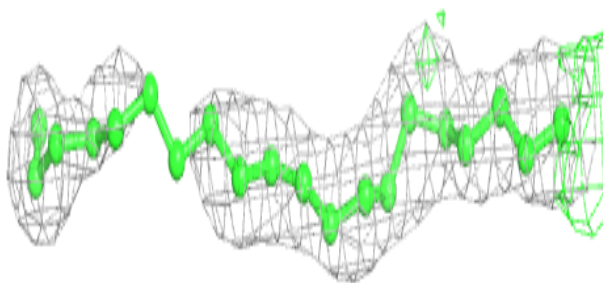
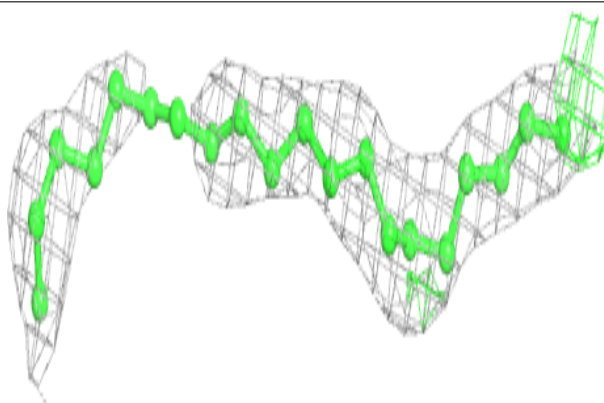


**Electron density around OLC D 301:**

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

**Electron density around LFA C 313:**

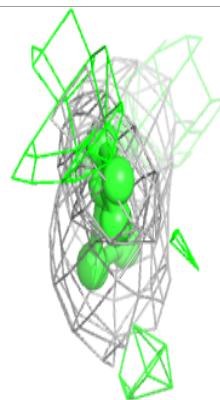
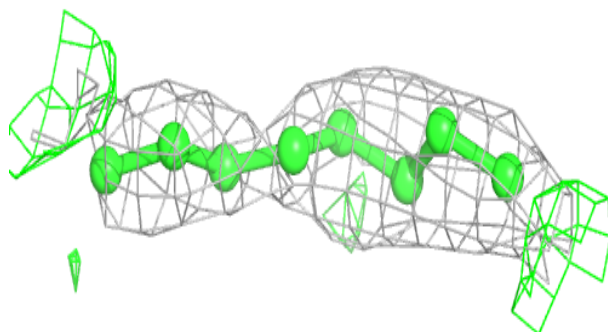
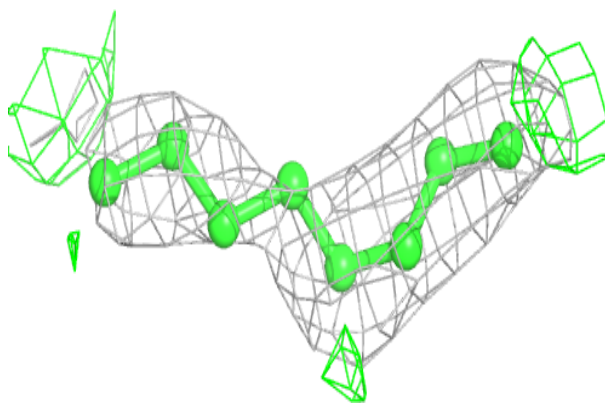
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



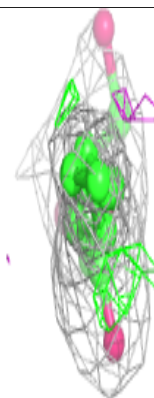
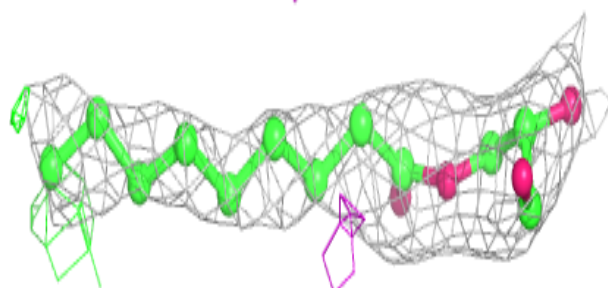
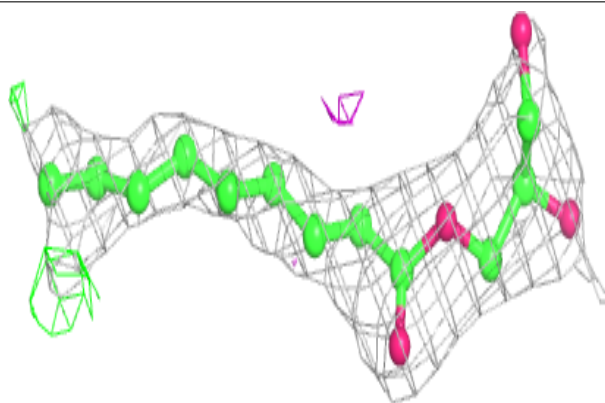


**Electron density around OLC E 303:**

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

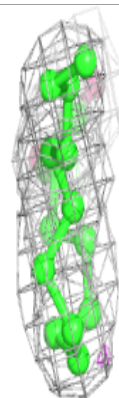
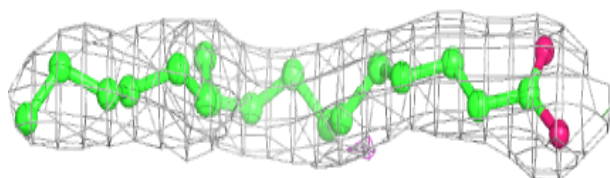
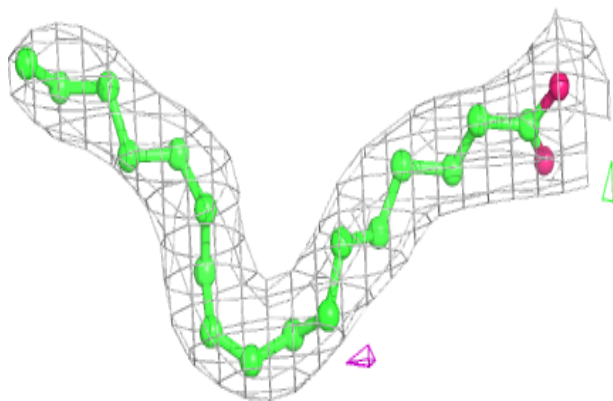
**Electron density around OLC B 307:**

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

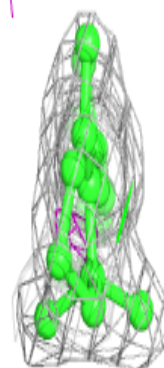
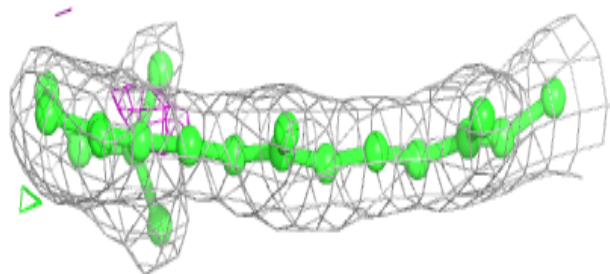
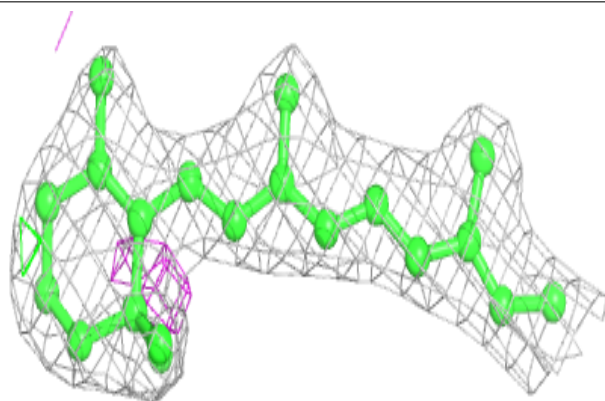


**Electron density around OLC A 317:**

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

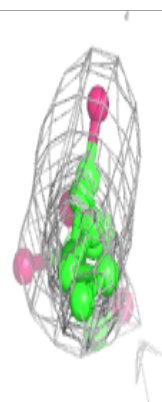
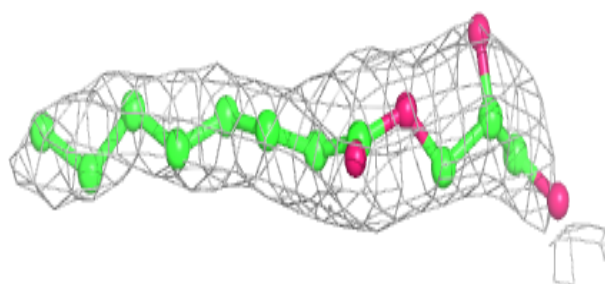
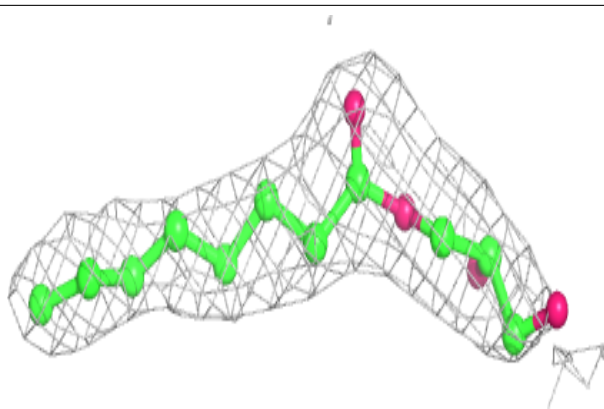
**Electron density around RET A 316:**

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

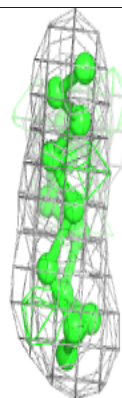
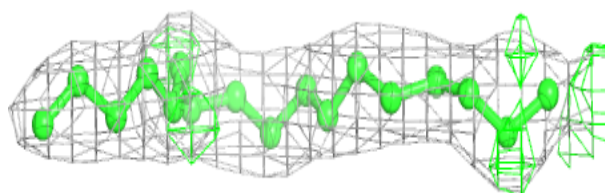
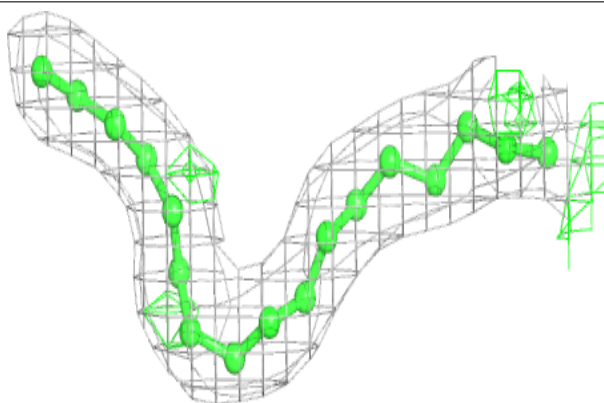


**Electron density around OLC E 307:**

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

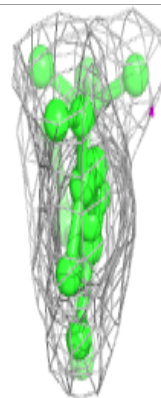
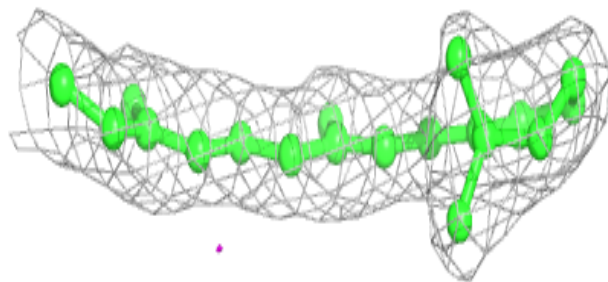
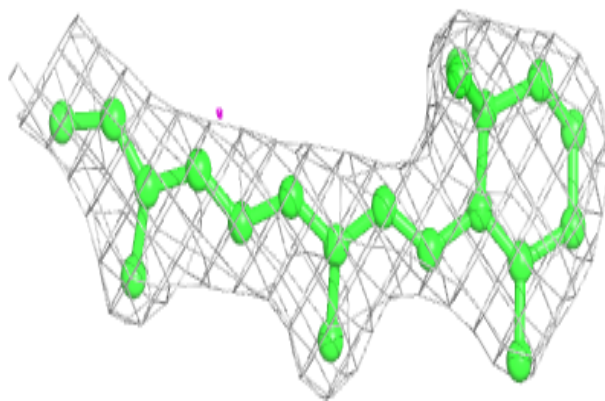
**Electron density around LFA D 314:**

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



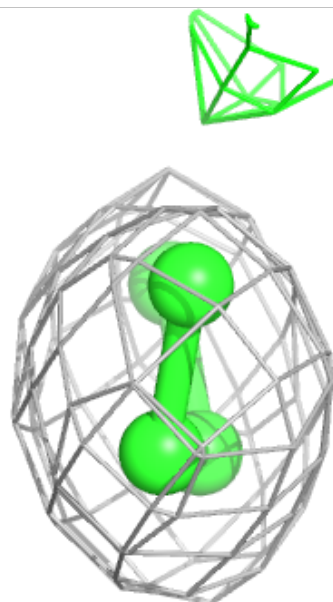
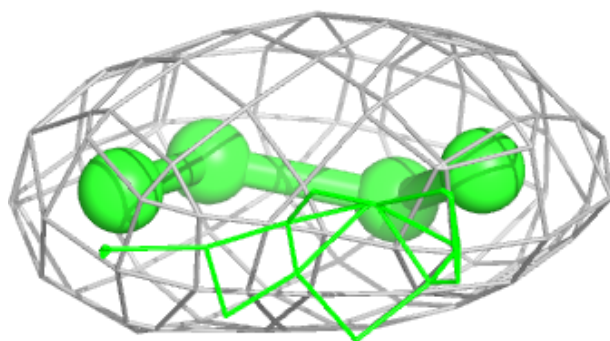
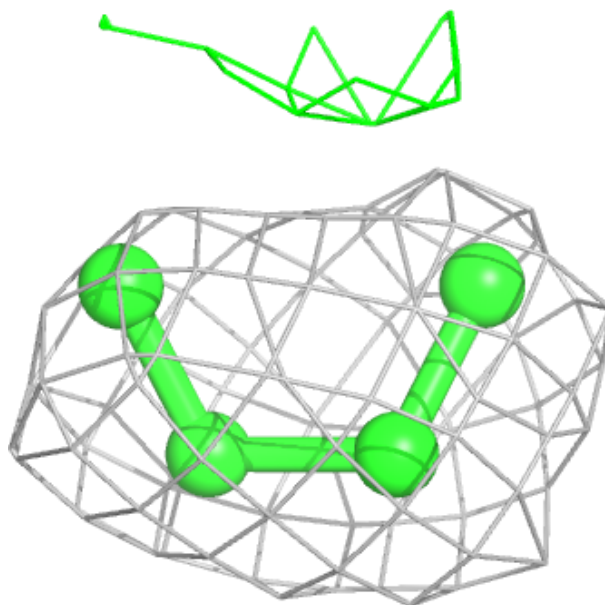
**Electron density around RET B 315:**

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



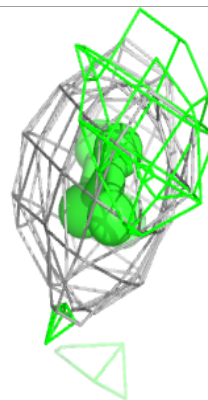
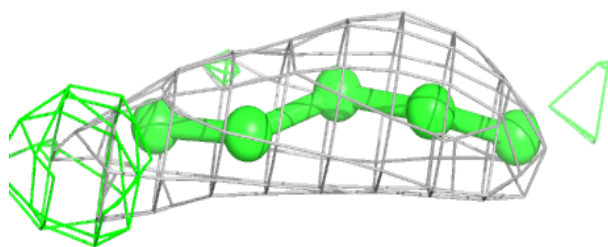
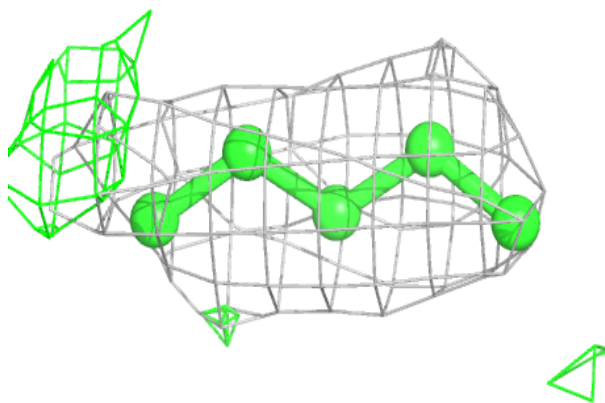
**Electron density around LFA E 313:**

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



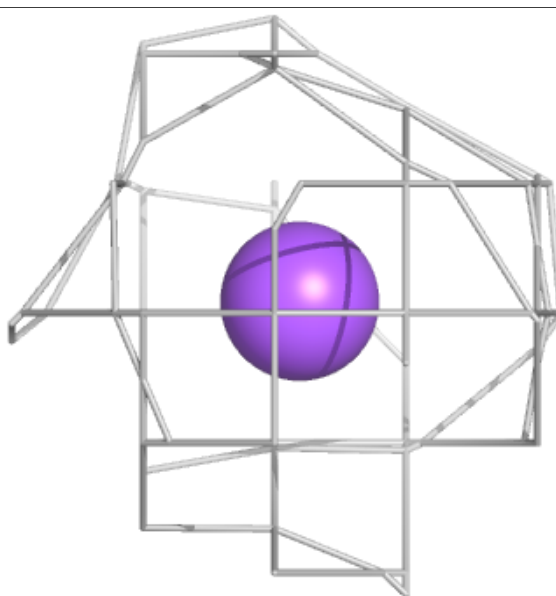
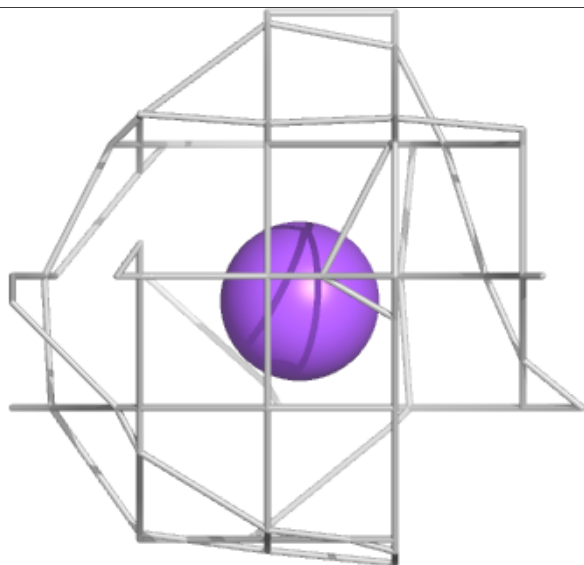
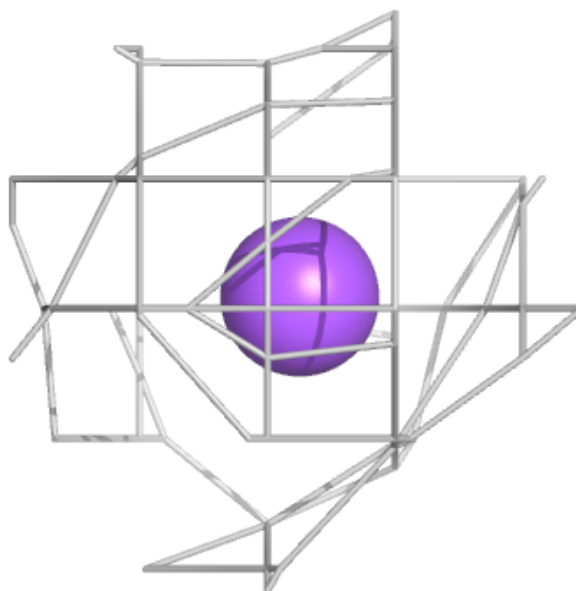
**Electron density around LFA E 314:**

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



**Electron density around NA A 314:**

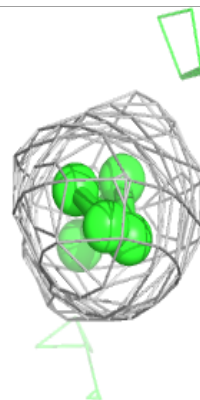
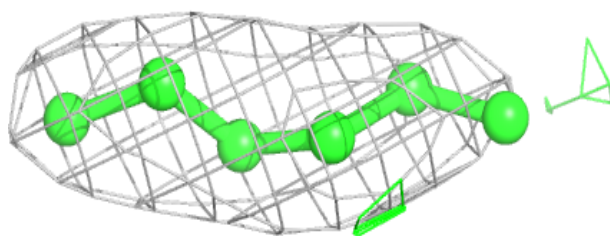
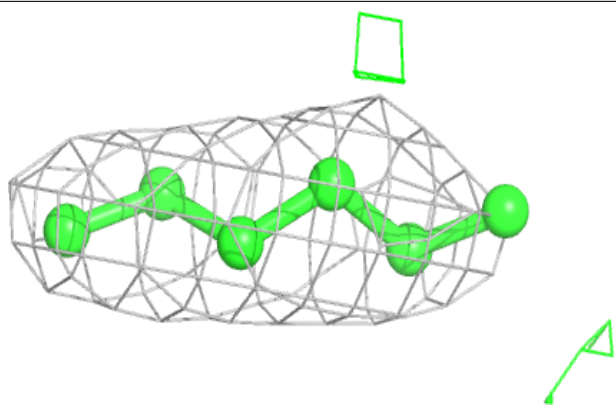
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



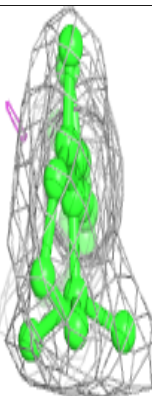
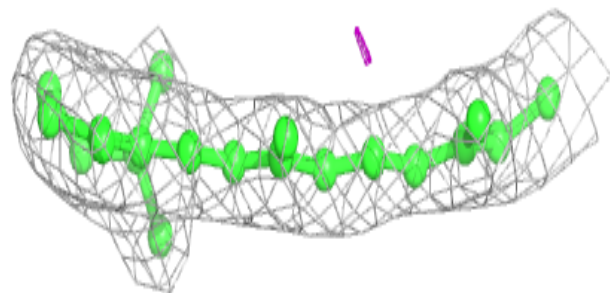
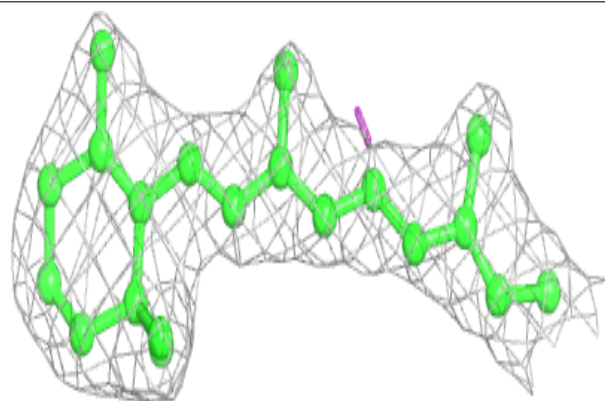


**Electron density around LFA A 312:**

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

**Electron density around RET D 319:**

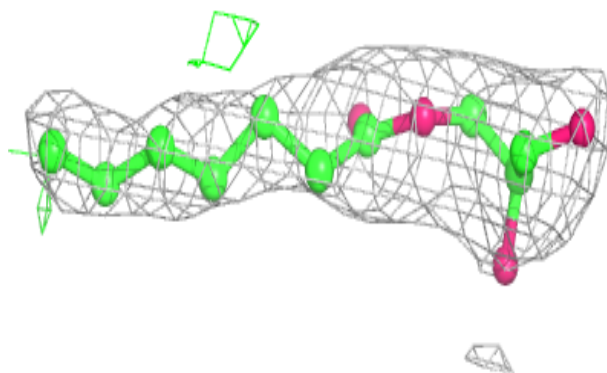
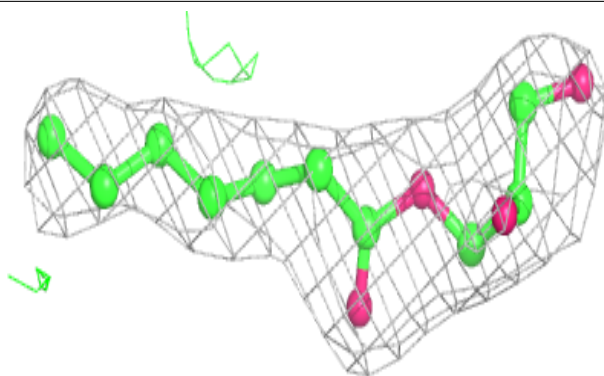
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



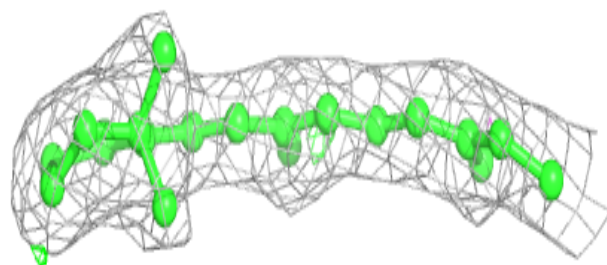
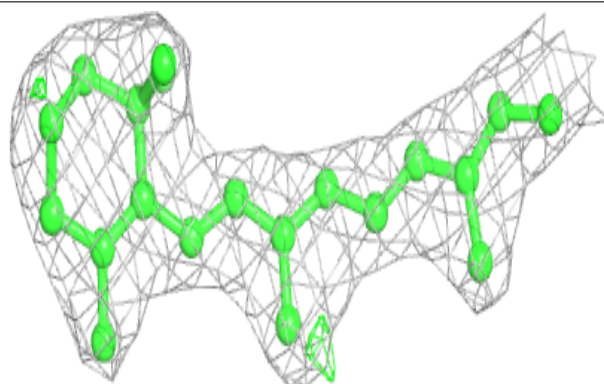


**Electron density around OLC D 308:**

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

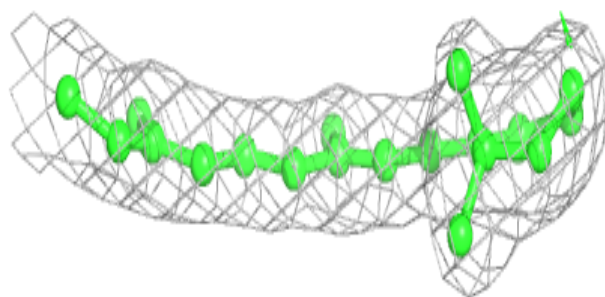
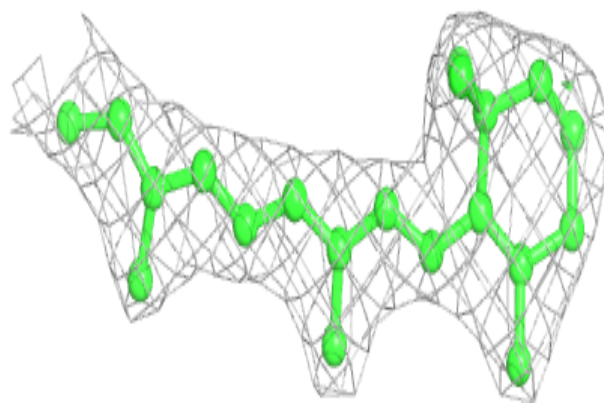
**Electron density around RET E 317:**

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



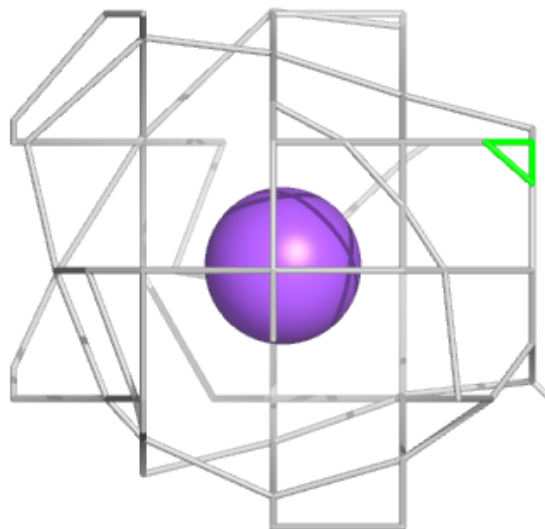
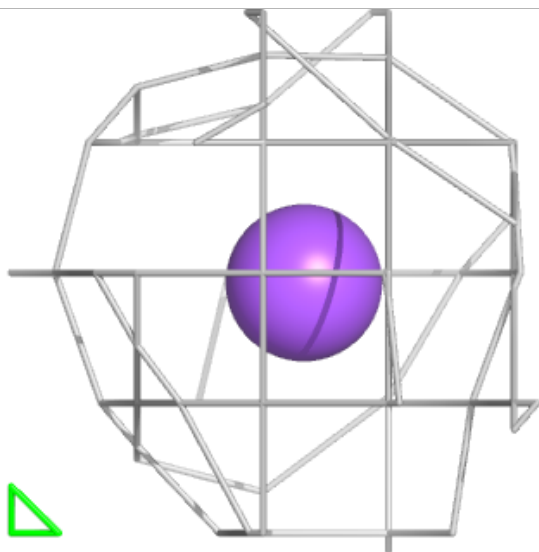
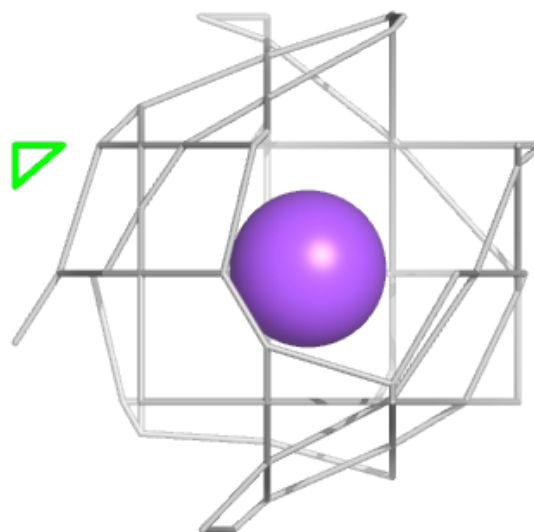
**Electron density around RET C 318:**

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



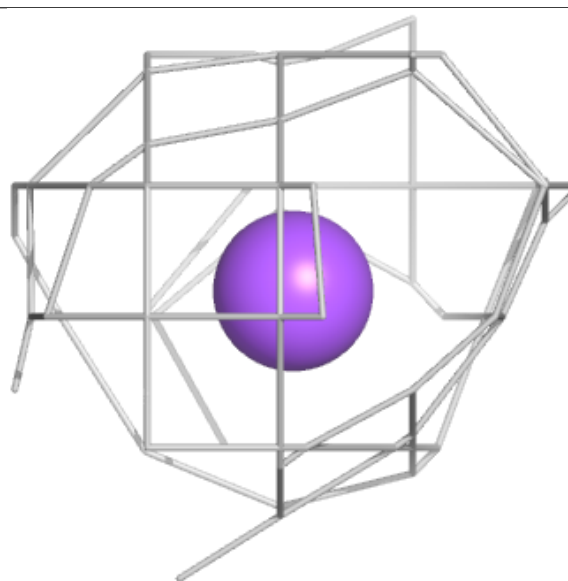
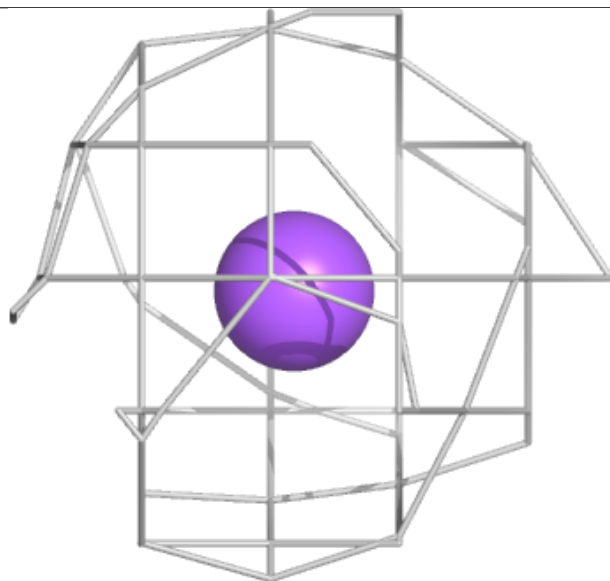
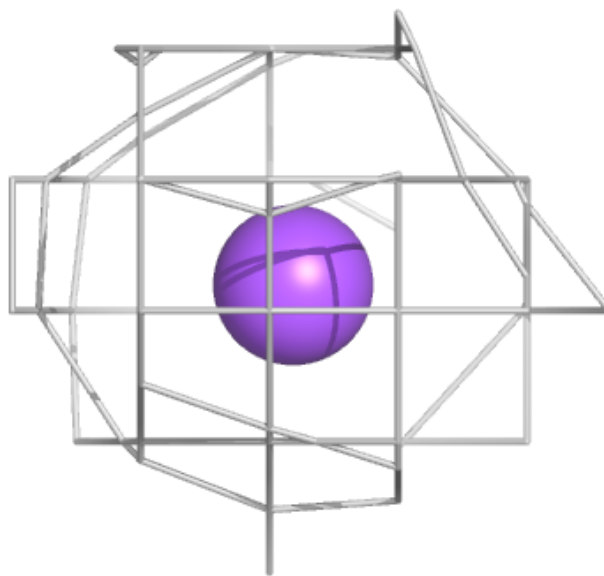
**Electron density around NA D 317:**

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



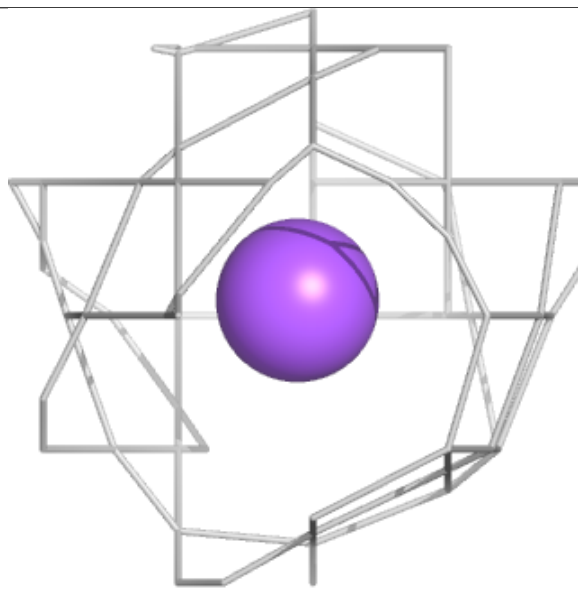
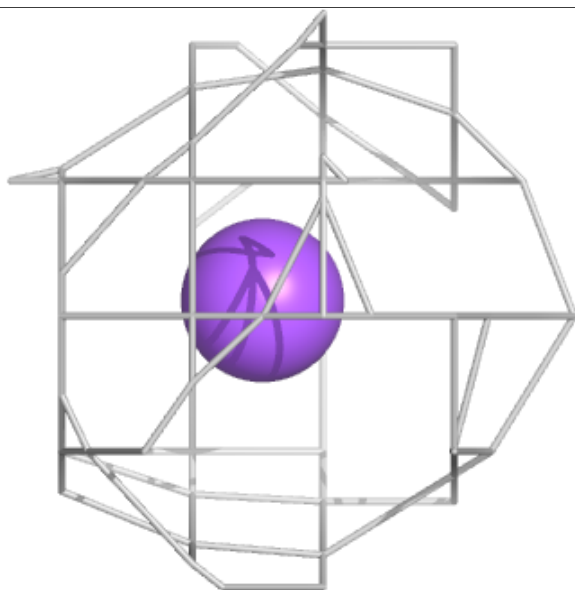
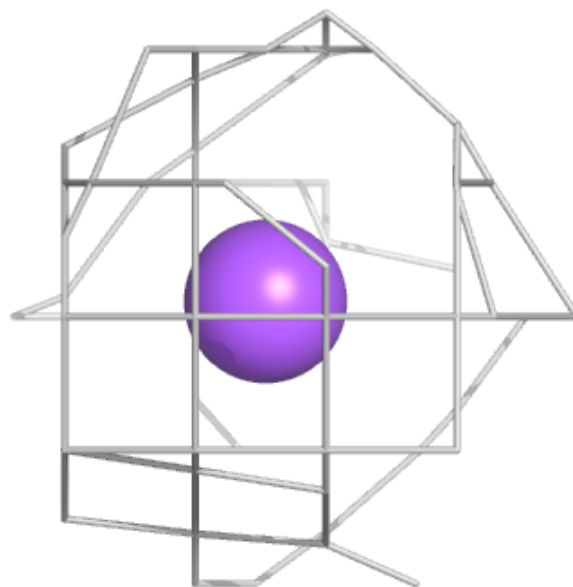
**Electron density around NA E 315:**

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



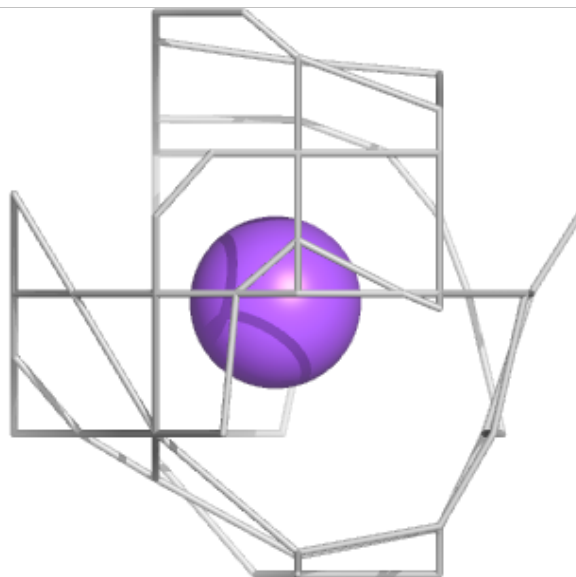
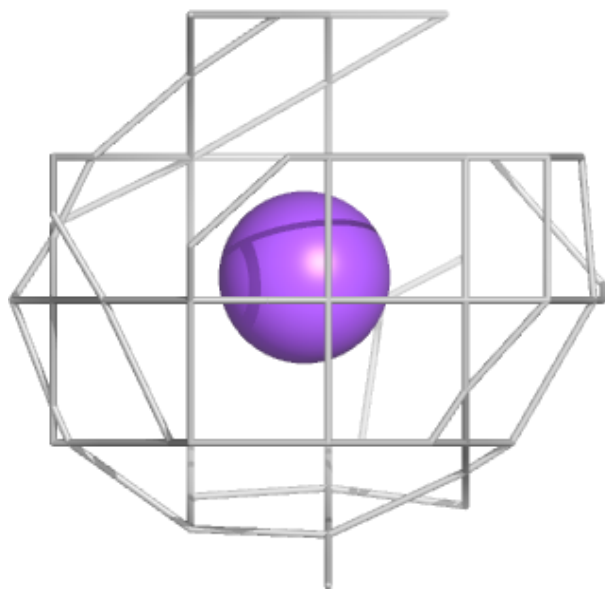
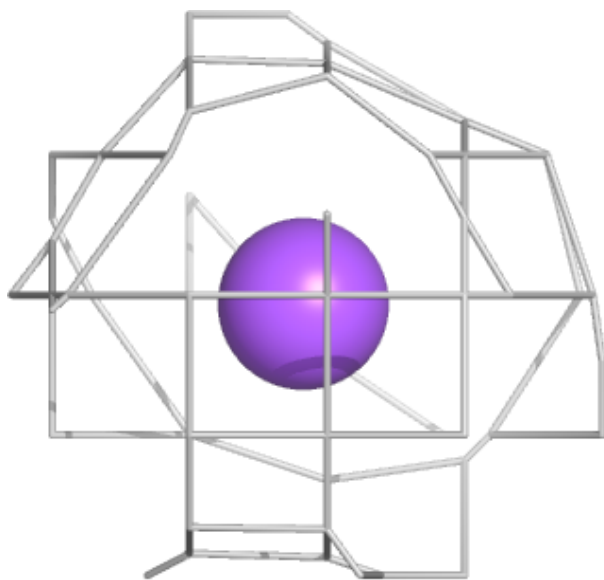
**Electron density around NA C 316:**

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



**Electron density around NA B 313:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.