



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:31 AM BST

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

This is a 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.

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

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

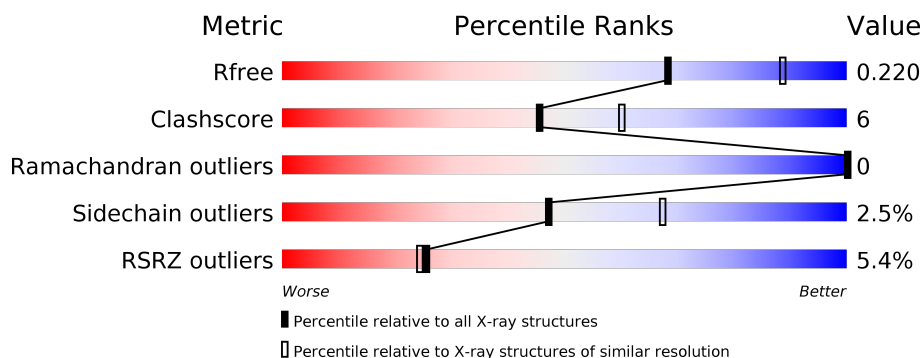
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	288	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	B	288	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>5%</div> </div> </div>
1	C	288	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	D	288	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>5%</div> </div> </div>
1	E	288	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</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	C	311	-	-	-	X
2	OLC	C	314	-	-	-	X
3	LFA	C	322	-	-	-	X
3	LFA	D	308	-	-	-	X
3	LFA	E	302	-	-	-	X
5	BOG	A	310	-	-	-	X
5	BOG	B	308	-	-	-	X
5	BOG	E	310	-	-	-	X

## 2 Entry composition

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

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

- Molecule 1 is a protein called Sodium pumping rhodopsin.

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

There are 45 discrepancies between the modelled and reference sequences:

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

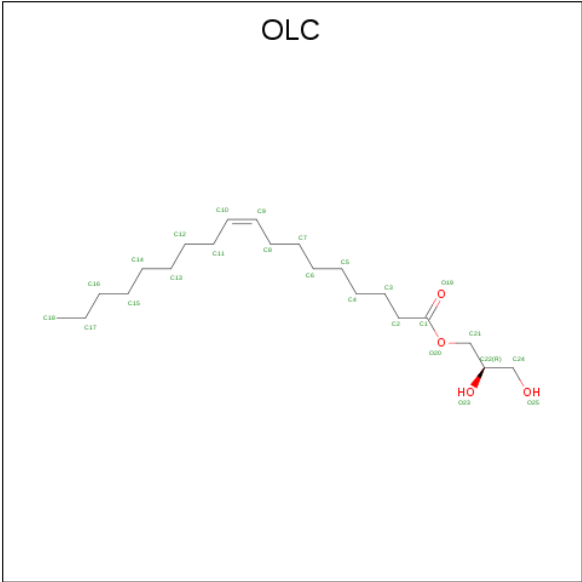
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Chain	Residue	Modelled	Actual	Comment	Reference
C	281	LEU	-	expression tag	UNP N0DKS8
C	282	GLU	-	expression tag	UNP N0DKS8
C	283	HIS	-	expression tag	UNP N0DKS8
C	284	HIS	-	expression tag	UNP N0DKS8
C	285	HIS	-	expression tag	UNP N0DKS8
C	286	HIS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

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



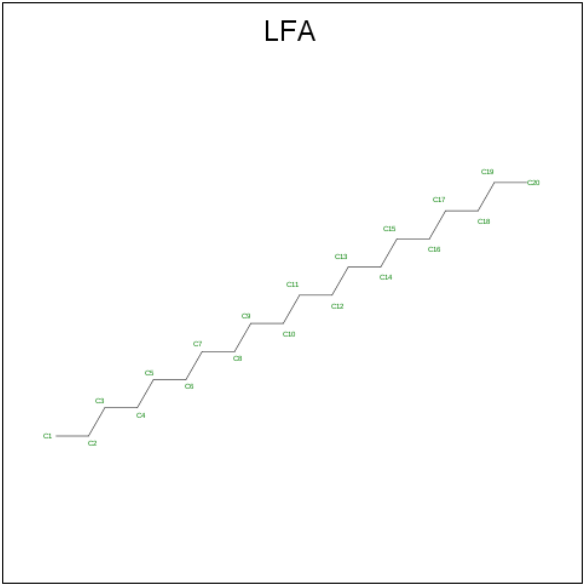
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 14 14	0	0
2	A	1	Total C O 13 9 4	0	0
2	A	1	Total C O 15 11 4	0	0
2	A	1	Total C 14 14	0	0
2	B	1	Total C O 22 18 4	0	0
2	B	1	Total C O 20 16 4	0	0
2	B	1	Total C O 16 12 4	0	0
2	C	1	Total C O 21 17 4	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 14 10 4	0	0
2	C	1	Total C O 21 17 4	0	0
2	C	1	Total C O 23 19 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0

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

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



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

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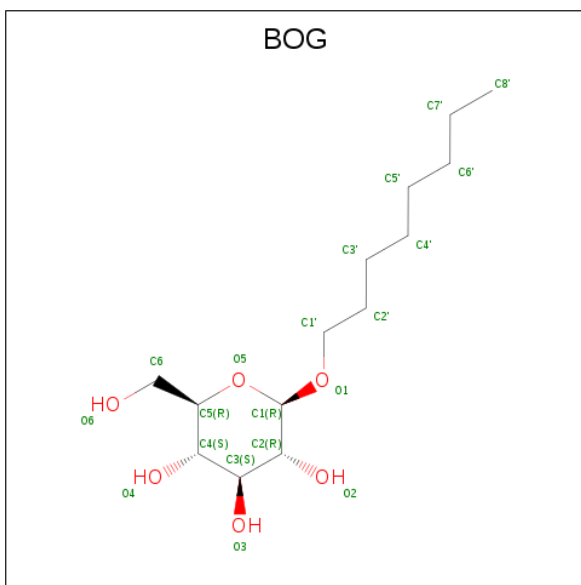
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C 6 6	0	0
3	E	1	Total C 20 20	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 14 14	0	0
3	E	1	Total C 4 4	0	0
3	E	1	Total C 5 5	0	0
3	E	1	Total C 14 14	0	0

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

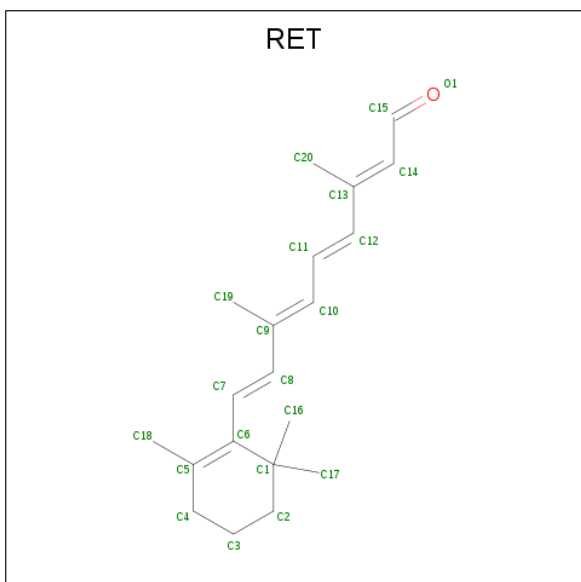
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

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



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

- Molecule 6 is 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	62	Total O 62 62	0	0
7	B	69	Total O 69 69	0	0
7	C	75	Total O 75 75	0	0
7	D	59	Total O 59 59	0	0
7	E	63	Total O 63 63	0	0

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 ( $\text{RSRZ} > 2$ ). 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.

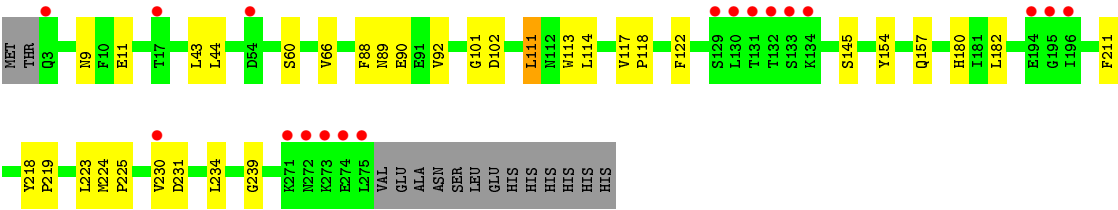
- Chain A:
- 
- Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows amino acid positions. A horizontal bar at the top indicates the percentage of sequences with a mutation at each position: 7% (red), 83% (green), 11% (yellow), and 5% (grey).
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1        | THR        | 0.00                       |
| 2        | Q3         | 0.00                       |
| 3        | V38        | 0.00                       |
| 4        | A41        | 0.00                       |
| 5        | L44        | 0.00                       |
| 6        | D54        | 0.00                       |
| 7        | K55        | 0.00                       |
| 8        | A56        | 0.00                       |
| 9        | F57        | 0.00                       |
| 10       | V66        | 0.00                       |
| 11       | M89        | 0.00                       |
| 12       | E90        | 0.00                       |
| 13       | E91        | 0.00                       |
| 14       | V92        | 0.00                       |
| 15       | G101       | 0.00                       |
| 16       | D102       | 0.00                       |
| 17       | L111       | 0.00                       |
| 18       | L114       | 0.00                       |
| 19       | V117       | 0.00                       |
| 20       | P118       | 0.00                       |
| 21       | T132       | 0.00                       |
| 22       | Y154       | 0.00                       |
| 23       | Q157       | 0.00                       |
| 24       | L164       | 0.00                       |
| 25       | L182       | 0.00                       |
| 26       | W183       | 0.00                       |
| 27       | E194       | 0.00                       |
| 28       | G195       | 0.00                       |
| 29       | I196       | 0.00                       |
| 30       | S197       | 0.00                       |
| 31       | P198       | 0.00                       |
| 32       | A199       | 0.00                       |
| 33       | F211       | 0.00                       |
| 34       | Y218       | 0.00                       |
| 35       | P219       | 0.00                       |
| 36       | L223       | 0.00                       |
| 37       | M224       | 0.00                       |
| 38       | P225       | 0.00                       |
| 39       | V230       | 0.00                       |
| 40       | F233       | 0.00                       |
| 41       | L234       | 0.00                       |
| 42       | G239       | 0.00                       |
| 43       | R243       | 0.00                       |
| 44       | V252       | 0.00                       |
| 45       | L269       | 0.00                       |
| 46       | S270       | 0.00                       |
| 47       | E271       | 0.00                       |
| 48       | N272       | 0.00                       |
| 49       | K273       | 0.00                       |
| 50       | E274       | 0.00                       |
| 51       | L275       | 0.00                       |
| 52       | VAL        | 0.00                       |
| 53       | GLU        | 0.00                       |
| 54       | ALA        | 0.00                       |
| 55       | ALA        | 0.00                       |
| 56       | ASN        | 0.00                       |
| 57       | SER        | 0.00                       |
| 58       | LEU        | 0.00                       |
| 59       | GLU        | 0.00                       |
| 60       | HIS        | 0.00                       |
| 61       | HIS        | 0.00                       |
| 62       | HIS        | 0.00                       |
| 63       | HIS        | 0.00                       |
| 64       | HIS        | 0.00                       |
| 65       | HIS        | 0.00                       |

- Chain B:
- 
- Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. A red dot above a position indicates a mutation. A bar chart at the top shows the distribution of mutations: 3% (red), 82% (green), 13% (yellow), and 5% (grey).
- | Position | Amino Acid | Information Content (bits) | Mutation |
|----------|------------|----------------------------|----------|
| 1        | THR        | 0.00                       | Yes      |
| 2        | THR        | 0.00                       | Yes      |
| 3        | THR        | 0.00                       | Yes      |
| 4        | THR        | 0.00                       | Yes      |
| 5        | THR        | 0.00                       | Yes      |
| 6        | THR        | 0.00                       | Yes      |
| 7        | THR        | 0.00                       | Yes      |
| 8        | THR        | 0.00                       | Yes      |
| 9        | THR        | 0.00                       | Yes      |
| 10       | THR        | 0.00                       | Yes      |
| 11       | THR        | 0.00                       | Yes      |
| 12       | THR        | 0.00                       | Yes      |
| 13       | THR        | 0.00                       | Yes      |
| 14       | THR        | 0.00                       | Yes      |
| 15       | THR        | 0.00                       | Yes      |
| 16       | THR        | 0.00                       | Yes      |
| 17       | THR        | 0.00                       | Yes      |
| 18       | THR        | 0.00                       | Yes      |
| 19       | THR        | 0.00                       | Yes      |
| 20       | THR        | 0.00                       | Yes      |
| 21       | THR        | 0.00                       | Yes      |
| 22       | THR        | 0.00                       | Yes      |
| 23       | THR        | 0.00                       | Yes      |
| 24       | THR        | 0.00                       | Yes      |
| 25       | THR        | 0.00                       | Yes      |
| 26       | THR        | 0.00                       | Yes      |
| 27       | THR        | 0.00                       | Yes      |
| 28       | THR        | 0.00                       | Yes      |
| 29       | THR        | 0.00                       | Yes      |
| 30       | THR        | 0.00                       | Yes      |
| 31       | THR        | 0.00                       | Yes      |
| 32       | THR        | 0.00                       | Yes      |
| 33       | THR        | 0.00                       | Yes      |
| 34       | THR        | 0.00                       | Yes      |
| 35       | THR        | 0.00                       | Yes      |
| 36       | THR        | 0.00                       | Yes      |
| 37       | THR        | 0.00                       | Yes      |
| 38       | THR        | 0.00                       | Yes      |
| 39       | THR        | 0.00                       | Yes      |
| 40       | THR        | 0.00                       | Yes      |
| 41       | THR        | 0.00                       | Yes      |
| 42       | THR        | 0.00                       | Yes      |
| 43       | THR        | 0.00                       | Yes      |
| 44       | THR        | 0.00                       | Yes      |
| 45       | THR        | 0.00                       | Yes      |
| 46       | THR        | 0.00                       | Yes      |
| 47       | THR        | 0.00                       | Yes      |
| 48       | THR        | 0.00                       | Yes      |
| 49       | THR        | 0.00                       | Yes      |
| 50       | THR        | 0.00                       | Yes      |
| 51       | THR        | 0.00                       | Yes      |
| 52       | THR        | 0.00                       | Yes      |
| 53       | THR        | 0.00                       | Yes      |
| 54       | THR        | 0.00                       | Yes      |
| 55       | THR        | 0.00                       | Yes      |
| 56       | THR        | 0.00                       | Yes      |
| 57       | THR        | 0.00                       | Yes      |
| 58       | THR        | 0.00                       | Yes      |
| 59       | THR        | 0.00                       | Yes      |
| 60       | THR        | 0.00                       | Yes      |
| 61       | THR        | 0.00                       | Yes      |
| 62       | THR        | 0.00                       | Yes      |
| 63       | THR        | 0.00                       | Yes      |
| 64       | THR        | 0.00                       | Yes      |
| 65       | THR        | 0.00                       | Yes      |
| 66       | THR        | 0.00                       | Yes      |
| 67       | THR        | 0.00                       | Yes      |
| 68       | THR        | 0.00                       | Yes      |
| 69       | THR        | 0.00                       | Yes      |
| 70       | THR        | 0.00                       | Yes      |
| 71       | THR        | 0.00                       | Yes      |
| 72       | THR        | 0.00                       | Yes      |
| 73       | THR        | 0.00                       | Yes      |
| 74       | THR        | 0.00                       | Yes      |
| 75       | THR        | 0.00                       | Yes      |
| 76       | THR        | 0.00                       | Yes      |
| 77       | THR        | 0.00                       | Yes      |
| 78       | THR        | 0.00                       | Yes      |
| 79       | THR        | 0.00                       | Yes      |
| 80       | THR        | 0.00                       | Yes      |
| 81       | THR        | 0.00                       | Yes      |
| 82       | THR        | 0.00                       | Yes      |
| 83       | THR        | 0.00                       | Yes      |
| 84       | THR        | 0.00                       | Yes      |
| 85       | THR        | 0.00                       | Yes      |
| 86       | THR        | 0.00                       | Yes      |
| 87       | THR        | 0.00                       | Yes      |
| 88       | THR        | 0.00                       | Yes      |
| 89       | THR        | 0.00                       | Yes      |
| 90       | THR        | 0.00                       | Yes      |
| 91       | THR        | 0.00                       | Yes      |
| 92       | THR        | 0.00                       | Yes      |
| 93       | THR        | 0.00                       | Yes      |
| 94       | THR        | 0.00                       | Yes      |
| 95       | THR        | 0.00                       | Yes      |
| 96       | THR        | 0.00                       | Yes      |
| 97       | THR        | 0.00                       | Yes      |
| 98       | THR        | 0.00                       | Yes      |
| 99       | THR        | 0.00                       | Yes      |
| 100      | THR        | 0.00                       | Yes      |
| 101      | THR        | 0.00                       | Yes      |
| 102      | THR        | 0.00                       | Yes      |
| 103      | THR        | 0.00                       | Yes      |
| 104      | THR        | 0.00                       | Yes      |
| 105      | THR        | 0.00                       | Yes      |
| 106      | THR        | 0.00                       | Yes      |
| 107      | THR        | 0.00                       | Yes      |
| 108      | THR        | 0.00                       | Yes      |
| 109      | THR        | 0.00                       | Yes      |
| 110      | THR        | 0.00                       | Yes      |
| 111      | THR        | 0.00                       | Yes      |
| 112      | THR        | 0.00                       | Yes      |
| 113      | THR        | 0.00                       | Yes      |
| 114      | THR        | 0.00                       | Yes      |
| 115      | THR        | 0.00                       | Yes      |
| 116      | THR        | 0.00                       | Yes      |
| 117      | THR        | 0.00                       | Yes      |
| 118      | THR        | 0.00                       | Yes      |
| 119      | THR        | 0.00                       | Yes      |
| 120      | THR        | 0.00                       | Yes      |
| 121      |            |                            |          |

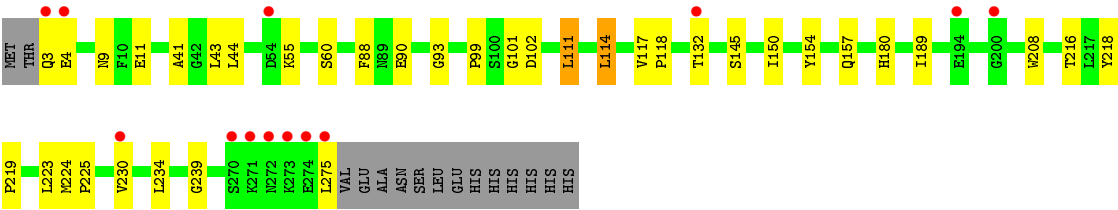
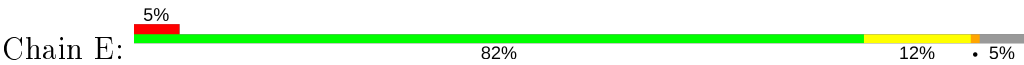
- [illegible]

- Chain D:  6% 83% 11% 5%





• 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, $\alpha$ , $\beta$ , $\gamma$	131.40Å 240.04Å 135.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.91 – 2.40 44.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.91-2.40) 99.8 (44.87-2.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.181 , 0.212 0.190 , 0.220	Depositor DCC
$R_{free}$ test set	4222 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

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

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.27	0/2236	0.41	0/3040
1	B	0.28	0/2230	0.41	0/3033
1	C	0.27	0/2235	0.41	0/3039
1	D	0.27	0/2227	0.41	0/3028
1	E	0.27	0/2229	0.41	0/3031
All	All	0.27	0/11157	0.41	0/15171

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2178	0	2154	24	0
1	B	2172	0	2149	33	0
1	C	2177	0	2152	34	0
1	D	2169	0	2142	24	0
1	E	2171	0	2149	24	0
2	A	56	0	78	0	0
2	B	58	0	79	4	0
2	C	260	0	370	9	0
2	D	32	0	40	0	0
2	E	53	0	84	1	0
3	A	61	0	119	1	0
3	B	37	0	74	1	0
3	C	74	0	147	5	0
3	D	98	0	198	0	0
3	E	65	0	127	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	20	0	28	1	0
5	B	20	0	28	2	0
5	C	20	0	28	2	0
5	D	20	0	28	1	0
5	E	20	0	28	0	0
6	A	20	0	27	6	0
6	B	20	0	27	5	0
6	C	20	0	27	5	0
6	D	20	0	27	6	0
6	E	20	0	27	5	0
7	A	62	0	0	0	0
7	B	69	0	0	2	0
7	C	75	0	0	2	0
7	D	59	0	0	2	0
7	E	63	0	0	1	0
All	All	12194	0	12337	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (156) 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	1.69	0.87
1:A:272:ASN:HD22	1:A:272:ASN:N	1.71	0.87
6:D:312:RET:H161	6:D:312:RET:H8	1.60	0.83
6:B:309:RET:H8	6:B:309:RET:H161	1.59	0.82
6:A:313:RET:H161	6:A:313:RET:H8	1.62	0.82
6:E:312:RET:H161	6:E:312:RET:H8	1.64	0.80
6:C:323:RET:H161	6:C:323:RET:H8	1.63	0.79
1:D:231:ASP:N	5:D:311:BOG:O6	2.21	0.70
1:E:60:SER:OG	7:E:401:HOH:O	2.10	0.69
1:A:164:LEU:HD21	5:A:310:BOG:H2'1	1.74	0.69
1:D:145:SER:OG	1:D:180:HIS:HD2	1.76	0.69
1:C:145:SER:OG	1:C:180:HIS:HD2	1.77	0.68
1:E:145:SER:OG	1:E:180:HIS:HD2	1.76	0.68
1:B:145:SER:OG	1:B:180:HIS:HD2	1.76	0.68
1:B:272:ASN:N	1:B:272:ASN:ND2	2.41	0.67
1:A:272:ASN:ND2	1:A:272:ASN:N	2.43	0.66
1:D:60:SER:OG	7:D:401:HOH:O	2.15	0.63
1:E:114:LEU:HD13	1:E:150:ILE:HG21	1.80	0.63
6:D:312:RET:H161	6:D:312:RET:C8	2.29	0.62
6:B:309:RET:H161	6:B:309:RET:C8	2.29	0.61
6:E:312:RET:H161	6:E:312:RET:C8	2.31	0.61
1:B:231:ASP:H	5:B:308:BOG:HO6	1.44	0.60
1:C:189:ILE:HD12	1:C:208:TRP:HB2	1.83	0.60
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.84	0.60
1:C:229:GLY:HA3	2:C:310:OLC:H22	1.83	0.59
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.83	0.59
1:A:234:LEU:O	1:A:239:GLY:HA3	2.03	0.59
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.85	0.59
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.85	0.59
1:D:234:LEU:O	1:D:239:GLY:HA3	2.03	0.59
1:A:224:MET:N	1:A:225:PRO:HD2	2.18	0.59
6:C:323:RET:H161	6:C:323:RET:C8	2.32	0.58
1:C:224:MET:N	1:C:225:PRO:HD2	2.18	0.58
1:E:234:LEU:O	1:E:239:GLY:HA3	2.03	0.58
1:E:189:ILE:HD12	1:E:208:TRP:HB2	1.86	0.57
1:C:234:LEU:O	1:C:239:GLY:HA3	2.04	0.57
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:MET:N	1:E:225:PRO:HD2	2.19	0.57
1:D:224:MET:N	1:D:225:PRO:HD2	2.19	0.57
1:B:234:LEU:O	1:B:239:GLY:HA3	2.04	0.56
1:B:224:MET:N	1:B:225:PRO:HD2	2.20	0.56
1:C:51:LYS:HD3	7:C:459:HOH:O	2.03	0.56
1:B:231:ASP:N	5:B:308:BOG:O6	2.22	0.56
1:B:41:ALA:HB1	1:C:66:VAL:HG13	1.88	0.56
3:E:306:LFA:H152	3:E:307:LFA:H201	1.86	0.55
1:C:164:LEU:HD21	5:C:321:BOG:H2'1	1.87	0.55
1:E:101:GLY:O	1:E:102:ASP:HB2	2.06	0.55
6:A:313:RET:C8	6:A:313:RET:H161	2.30	0.55
1:A:183:TRP:HE3	3:A:304:LFA:H162	1.72	0.54
1:C:231:ASP:N	5:C:321:BOG:O6	2.31	0.54
6:C:323:RET:H171	6:C:323:RET:H8	1.90	0.54
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.90	0.53
1:A:101:GLY:O	1:A:102:ASP:HB2	2.09	0.52
1:C:101:GLY:O	1:C:102:ASP:HB2	2.09	0.52
1:E:111:LEU:O	1:E:114:LEU:HB2	2.10	0.52
1:B:139:ARG:NH1	2:B:301:OLC:H24A	2.25	0.52
6:D:312:RET:H171	6:D:312:RET:H8	1.92	0.52
6:B:309:RET:H8	6:B:309:RET:H171	1.92	0.52
1:B:101:GLY:O	1:B:102:ASP:HB2	2.11	0.51
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.92	0.51
6:E:312:RET:H171	6:E:312:RET:H8	1.91	0.51
6:A:313:RET:H8	6:A:313:RET:H171	1.93	0.51
1:C:183:TRP:CE3	3:C:315:LFA:H41	2.45	0.51
1:A:3:GLN:NE2	1:E:90:GLU:OE1	2.44	0.50
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.93	0.50
1:B:139:ARG:HH11	2:B:301:OLC:H24A	1.77	0.49
1:D:101:GLY:O	1:D:102:ASP:HB2	2.14	0.48
1:A:44:LEU:HD21	1:B:43:LEU:HD11	1.95	0.48
2:C:313:OLC:H2	2:C:313:OLC:O23	2.14	0.47
1:B:186:LYS:HG2	3:B:305:LFA:H192	1.96	0.47
1:D:60:SER:CB	7:D:401:HOH:O	2.63	0.47
6:C:323:RET:H171	6:C:323:RET:C8	2.45	0.47
1:C:223:LEU:C	1:C:225:PRO:HD2	2.35	0.47
1:B:60:SER:HB3	7:B:409:HOH:O	2.14	0.46
1:E:223:LEU:C	1:E:225:PRO:HD2	2.36	0.46
1:A:223:LEU:C	1:A:225:PRO:HD2	2.35	0.46
1:B:223:LEU:C	1:B:225:PRO:HD2	2.36	0.46
1:C:180:HIS:CD2	2:C:307:OLC:H7A	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:312:RET:H171	6:D:312:RET:C8	2.46	0.46
3:E:306:LFA:H141	3:E:307:LFA:C20	2.46	0.46
1:D:44:LEU:HD21	1:E:43:LEU:HD11	1.97	0.45
1:C:216:THR:HG22	3:C:319:LFA:H201	1.98	0.45
1:D:223:LEU:C	1:D:225:PRO:HD2	2.37	0.45
6:B:309:RET:H171	6:B:309:RET:C8	2.46	0.45
1:C:163:ASN:HD22	2:C:312:OLC:C24	2.30	0.45
6:A:313:RET:C8	6:A:313:RET:H171	2.46	0.45
6:E:312:RET:H171	6:E:312:RET:C8	2.45	0.45
1:C:170:TRP:CH2	2:C:308:OLC:H9	2.52	0.45
1:D:90:GLU:OE2	1:E:3:GLN:NE2	2.50	0.45
1:C:55:LYS:NZ	7:C:408:HOH:O	2.49	0.44
1:B:38:VAL:HG11	1:B:252:VAL:HG22	2.00	0.43
2:C:304:OLC:H24	3:C:316:LFA:C13	2.49	0.43
1:C:216:THR:HG22	3:C:319:LFA:C20	2.49	0.43
1:B:145:SER:OG	1:B:180:HIS:CD2	2.65	0.43
1:B:139:ARG:HH11	2:B:301:OLC:C24	2.32	0.43
2:C:305:OLC:H3A	2:C:305:OLC:H6	1.79	0.43
1:A:90:GLU:HG2	1:B:99:PRO:HG3	2.01	0.43
1:B:154:TYR:O	1:B:157:GLN:HG3	2.18	0.43
1:D:114:LEU:O	1:D:118:PRO:HG2	2.19	0.43
1:B:114:LEU:O	1:B:118:PRO:HG2	2.19	0.43
1:C:114:LEU:O	1:C:118:PRO:HG2	2.19	0.43
1:D:154:TYR:O	1:D:157:GLN:HG3	2.19	0.42
1:A:114:LEU:O	1:A:118:PRO:HG2	2.19	0.42
1:C:186:LYS:HG2	3:C:315:LFA:H51	2.00	0.42
1:B:139:ARG:NH1	2:B:301:OLC:C24	2.83	0.42
1:D:88:PHE:CD2	1:E:99:PRO:HB3	2.55	0.42
1:A:224:MET:N	1:A:225:PRO:CD	2.83	0.42
1:E:224:MET:N	1:E:225:PRO:CD	2.83	0.42
6:E:312:RET:H181	6:E:312:RET:H7	1.72	0.42
1:E:101:GLY:O	1:E:102:ASP:CB	2.67	0.42
1:E:114:LEU:O	1:E:118:PRO:HG2	2.19	0.42
1:A:182:LEU:HD23	1:A:211:PHE:HE2	1.84	0.42
1:C:267:ILE:HG21	1:C:275:LEU:HB3	2.02	0.42
6:A:313:RET:H11	6:A:313:RET:H191	1.95	0.42
1:A:154:TYR:O	1:A:157:GLN:HG3	2.19	0.41
1:A:38:VAL:HG11	1:A:252:VAL:HG22	2.02	0.41
1:B:113:TRP:CD1	6:B:309:RET:H14	2.55	0.41
1:B:182:LEU:HD23	1:B:211:PHE:HE2	1.84	0.41
1:C:89:ASN:OD1	1:C:92:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLU:HG2	1:C:99:PRO:HG3	2.03	0.41
1:C:245:LEU:HD11	2:C:314:OLC:H5A	2.02	0.41
6:C:323:RET:H7	6:C:323:RET:H181	1.72	0.41
1:E:114:LEU:HD12	1:E:114:LEU:HA	1.81	0.41
1:E:9:ASN:HB3	1:E:11:GLU:OE1	2.20	0.41
1:C:264:ASN:HD22	2:C:305:OLC:H24	1.85	0.41
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.55	0.41
1:A:101:GLY:O	1:A:102:ASP:CB	2.68	0.41
1:C:224:MET:N	1:C:225:PRO:CD	2.82	0.41
1:D:182:LEU:HD23	1:D:211:PHE:HE2	1.85	0.41
1:D:118:PRO:O	1:D:122:PHE:HB2	2.21	0.41
1:E:154:TYR:O	1:E:157:GLN:HG3	2.21	0.41
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.20	0.41
1:B:218:TYR:N	1:B:219:PRO:HD2	2.35	0.41
1:D:111:LEU:O	1:D:114:LEU:HB2	2.21	0.41
1:E:218:TYR:N	1:E:219:PRO:HD2	2.36	0.41
1:A:218:TYR:N	1:A:219:PRO:HD2	2.36	0.41
6:A:313:RET:H181	6:A:313:RET:H7	1.71	0.41
1:C:182:LEU:HD23	1:C:211:PHE:HE2	1.85	0.41
6:D:312:RET:H11	6:D:312:RET:H191	1.92	0.41
1:D:218:TYR:N	1:D:219:PRO:HD2	2.35	0.41
1:B:224:MET:N	1:B:225:PRO:CD	2.84	0.40
1:C:111:LEU:O	1:C:114:LEU:HB2	2.21	0.40
1:D:224:MET:N	1:D:225:PRO:CD	2.84	0.40
1:A:90:GLU:CG	1:B:99:PRO:HG3	2.51	0.40
1:A:89:ASN:OD1	1:A:92:VAL:HG13	2.21	0.40
1:C:44:LEU:HD11	1:D:43:LEU:HD11	2.04	0.40
1:C:218:TYR:N	1:C:219:PRO:HD2	2.36	0.40
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.21	0.40
1:C:74:LEU:HA	1:C:74:LEU:HD22	1.95	0.40
1:B:90:GLU:CG	1:C:99:PRO:HG3	2.51	0.40
1:D:89:ASN:OD1	1:D:92:VAL:HG13	2.21	0.40
1:E:216:THR:O	1:E:219:PRO:HG2	2.22	0.40
1:A:111:LEU:O	1:A:114:LEU:HB2	2.21	0.40
1:B:244:GLN:HG2	7:B:405:HOH:O	2.21	0.40
1:D:113:TRP:CD1	6:D:312:RET:H14	2.57	0.40
2:E:303:OLC:H11A	2:E:303:OLC:H8	1.66	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
1	B	272/288 (94%)	265 (97%)	7 (3%)	0	100	100
1	C	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
1	D	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
1	E	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
All	All	1360/1440 (94%)	1329 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/247 (93%)	224 (97%)	6 (3%)	46	66
1	B	230/247 (93%)	226 (98%)	4 (2%)	60	78
1	C	230/247 (93%)	222 (96%)	8 (4%)	36	55
1	D	228/247 (92%)	226 (99%)	2 (1%)	78	90
1	E	229/247 (93%)	221 (96%)	8 (4%)	36	55
All	All	1147/1235 (93%)	1119 (98%)	28 (2%)	47	68

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	111	LEU
1	A	230	VAL
1	A	272	ASN
1	A	273	LYS
1	A	274	GLU
1	B	111	LEU
1	B	164	LEU
1	B	230	VAL
1	B	272	ASN
1	C	3	GLN
1	C	44	LEU
1	C	51	LYS
1	C	111	LEU
1	C	230	VAL
1	C	273	LYS
1	C	274	GLU
1	C	275	LEU
1	D	111	LEU
1	D	230	VAL
1	E	4	GLU
1	E	44	LEU
1	E	55	LYS
1	E	111	LEU
1	E	114	LEU
1	E	132	THR
1	E	230	VAL
1	E	275	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	ASN
1	B	141	GLN
1	B	180	HIS
1	B	272	ASN
1	C	3	GLN
1	C	180	HIS
1	D	141	GLN
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 69 ligands modelled in this entry, 5 are monoatomic - leaving 64 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	RET	A	313	1	20,20,21	0.73	0	27,27,28	1.61	5 (18%)
5	BOG	E	310	-	20,20,20	0.54	0	25,25,25	0.57	0
2	OLC	B	304	-	15,15,24	1.11	1 (6%)	16,16,25	0.98	2 (12%)
2	OLC	C	302	-	19,19,24	1.06	1 (5%)	20,20,25	0.91	2 (10%)
2	OLC	A	301	-	13,13,24	0.32	0	12,12,25	0.34	0
2	OLC	B	301	-	21,21,24	1.00	1 (4%)	22,22,25	0.92	1 (4%)
3	LFA	A	306	-	7,7,19	0.29	0	6,6,18	0.42	0
6	RET	C	323	1	20,20,21	0.68	0	27,27,28	1.61	4 (14%)
3	LFA	D	306	-	7,7,19	0.30	0	6,6,18	0.35	0
3	LFA	A	308	-	5,5,19	0.29	0	4,4,18	0.32	0
5	BOG	D	311	-	20,20,20	0.52	0	25,25,25	0.64	0
5	BOG	B	308	-	20,20,20	0.57	1 (5%)	25,25,25	0.54	0
2	OLC	E	304	-	24,24,24	0.91	1 (4%)	25,25,25	0.90	2 (8%)
2	OLC	A	303	-	14,14,24	1.21	1 (7%)	15,15,25	1.12	2 (13%)
3	LFA	C	322	-	3,3,19	0.39	0	2,2,18	0.56	0
2	OLC	C	307	-	24,24,24	0.97	1 (4%)	25,25,25	0.86	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	B	303	-	19,19,24	1.06	1 (5%)	20,20,25	0.87	1 (5%)
3	LFA	C	319	-	3,3,19	0.36	0	2,2,18	0.62	0
2	OLC	A	302	-	12,12,24	1.31	1 (8%)	13,13,25	1.20	2 (15%)
2	OLC	C	301	-	20,20,24	1.01	1 (5%)	21,21,25	0.98	1 (4%)
2	OLC	E	301	-	11,11,24	0.27	0	10,10,25	0.51	0
2	OLC	C	308	-	24,24,24	0.96	1 (4%)	25,25,25	0.84	1 (4%)
2	OLC	C	305	-	20,20,24	1.04	1 (5%)	21,21,25	0.87	1 (4%)
3	LFA	B	302	-	19,19,19	0.35	0	18,18,18	0.39	0
3	LFA	A	307	-	11,11,19	0.30	0	10,10,18	0.40	0
2	OLC	D	303	-	13,13,24	1.21	1 (7%)	14,14,25	0.96	1 (7%)
2	OLC	E	303	-	15,15,24	0.30	0	14,14,25	0.46	0
2	OLC	C	309	-	21,21,24	1.03	1 (4%)	22,22,25	0.89	1 (4%)
3	LFA	D	308	-	6,6,19	0.31	0	5,5,18	0.39	0
3	LFA	D	309	-	5,5,19	0.31	0	4,4,18	0.28	0
3	LFA	D	307	-	16,16,19	0.30	0	15,15,18	0.48	0
3	LFA	A	312	-	19,19,19	0.37	0	18,18,18	0.34	0
6	RET	E	312	1	20,20,21	0.79	0	27,27,28	1.54	5 (18%)
2	OLC	C	306	-	22,22,24	0.97	1 (4%)	23,23,25	0.87	2 (8%)
6	RET	B	309	1	20,20,21	0.67	0	27,27,28	1.58	6 (22%)
3	LFA	E	307	-	3,3,19	0.35	0	2,2,18	0.61	0
3	LFA	C	303	-	19,19,19	0.37	0	18,18,18	0.33	0
2	OLC	C	310	-	15,15,24	1.21	1 (6%)	16,16,25	1.05	1 (6%)
3	LFA	C	317	-	19,19,19	0.28	0	18,18,18	0.51	0
6	RET	D	312	1	20,20,21	0.68	0	27,27,28	1.62	5 (18%)
2	OLC	C	314	-	15,15,24	1.21	1 (6%)	16,16,25	1.00	1 (6%)
3	LFA	E	308	-	4,4,19	0.29	0	3,3,18	0.36	0
2	OLC	A	311	-	13,13,24	0.35	0	12,12,25	0.45	0
3	LFA	A	305	-	7,7,19	0.30	0	6,6,18	0.42	0
3	LFA	A	304	-	6,6,19	0.29	0	5,5,18	0.38	0
5	BOG	A	310	-	20,20,20	0.55	0	25,25,25	0.58	0
3	LFA	E	305	-	7,7,19	0.29	0	6,6,18	0.43	0
3	LFA	D	302	-	19,19,19	0.36	0	18,18,18	0.38	0
2	OLC	C	312	-	15,15,24	1.19	1 (6%)	16,16,25	0.93	1 (6%)
3	LFA	E	302	-	19,19,19	0.37	0	18,18,18	0.37	0
3	LFA	E	306	-	13,13,19	0.30	0	12,12,18	0.48	0
3	LFA	C	318	-	10,10,19	0.29	0	9,9,18	0.49	0
3	LFA	D	305	-	19,19,19	0.26	0	18,18,18	0.57	0
2	OLC	C	313	-	15,15,24	1.22	1 (6%)	16,16,25	1.02	1 (6%)
3	LFA	B	305	-	8,8,19	0.29	0	7,7,18	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	D	301	-	17,17,24	1.12	1 (5%)	18,18,25	0.99	1 (5%)
3	LFA	C	315	-	6,6,19	0.31	0	5,5,18	0.37	0
2	OLC	C	304	-	13,13,24	1.29	1 (7%)	14,14,25	1.03	1 (7%)
2	OLC	C	311	-	24,24,24	0.95	1 (4%)	25,25,25	0.82	1 (4%)
3	LFA	B	306	-	7,7,19	0.30	0	6,6,18	0.40	0
3	LFA	E	311	-	13,13,19	0.27	0	12,12,18	0.51	0
3	LFA	D	304	-	19,19,19	0.28	0	18,18,18	0.54	0
5	BOG	C	321	-	20,20,20	0.56	0	25,25,25	0.71	0
3	LFA	C	316	-	7,7,19	0.28	0	6,6,18	0.38	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
6	RET	A	313	1	-	0/13/30/31	0/1/1/1
5	BOG	E	310	-	-	9/11/31/31	0/1/1/1
2	OLC	B	304	-	-	2/15/15/24	-
2	OLC	C	302	-	-	12/19/19/24	-
2	OLC	A	301	-	-	6/11/11/24	-
2	OLC	B	301	-	-	7/21/21/24	-
3	LFA	A	306	-	-	3/5/5/17	-
6	RET	C	323	1	-	0/13/30/31	0/1/1/1
3	LFA	D	306	-	-	4/5/5/17	-
3	LFA	A	308	-	-	1/3/3/17	-
5	BOG	D	311	-	-	2/11/31/31	0/1/1/1
5	BOG	B	308	-	-	6/11/31/31	0/1/1/1
2	OLC	E	304	-	-	15/24/24/24	-
2	OLC	A	303	-	-	7/14/14/24	-
3	LFA	C	322	-	-	0/1/1/17	-
2	OLC	C	307	-	-	13/24/24/24	-
2	OLC	B	303	-	-	7/19/19/24	-
3	LFA	C	319	-	-	1/1/1/17	-
2	OLC	A	302	-	-	1/12/12/24	-
2	OLC	C	301	-	-	10/20/20/24	-
2	OLC	E	301	-	-	4/9/9/24	-
2	OLC	C	308	-	-	6/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	305	-	-	12/20/20/24	-
3	LFA	B	302	-	-	7/17/17/17	-
3	LFA	A	307	-	-	5/9/9/17	-
2	OLC	D	303	-	-	5/13/13/24	-
2	OLC	E	303	-	-	6/13/13/24	-
2	OLC	C	309	-	-	13/21/21/24	-
3	LFA	D	308	-	-	4/4/4/17	-
3	LFA	D	309	-	-	0/3/3/17	-
3	LFA	D	307	-	-	7/14/14/17	-
3	LFA	A	312	-	-	10/17/17/17	-
6	RET	E	312	1	-	0/13/30/31	0/1/1/1
2	OLC	C	306	-	-	12/22/22/24	-
6	RET	B	309	1	-	0/13/30/31	0/1/1/1
3	LFA	E	307	-	-	1/1/1/17	-
3	LFA	C	303	-	-	11/17/17/17	-
2	OLC	C	310	-	-	6/15/15/24	-
3	LFA	C	317	-	-	13/17/17/17	-
6	RET	D	312	1	-	0/13/30/31	0/1/1/1
2	OLC	C	314	-	-	10/15/15/24	-
3	LFA	E	308	-	-	1/2/2/17	-
2	OLC	A	311	-	-	6/11/11/24	-
3	LFA	A	305	-	-	3/5/5/17	-
3	LFA	A	304	-	-	1/4/4/17	-
5	BOG	A	310	-	-	5/11/31/31	0/1/1/1
3	LFA	E	305	-	-	1/5/5/17	-
3	LFA	D	302	-	-	7/17/17/17	-
2	OLC	C	312	-	-	7/15/15/24	-
3	LFA	E	302	-	-	7/17/17/17	-
3	LFA	E	306	-	-	5/11/11/17	-
3	LFA	C	318	-	-	4/8/8/17	-
3	LFA	D	305	-	-	9/17/17/17	-
2	OLC	C	313	-	-	10/15/15/24	-
3	LFA	B	305	-	-	3/6/6/17	-
2	OLC	D	301	-	-	7/17/17/24	-
3	LFA	C	315	-	-	4/4/4/17	-
2	OLC	C	304	-	-	8/13/13/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	311	-	-	14/24/24/24	-
3	LFA	B	306	-	-	2/5/5/17	-
3	LFA	E	311	-	-	3/11/11/17	-
3	LFA	D	304	-	-	9/17/17/17	-
5	BOG	C	321	-	-	4/11/31/31	0/1/1/1
3	LFA	C	316	-	-	4/5/5/17	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	310	OLC	O20-C1	4.50	1.46	1.33
2	C	313	OLC	O20-C1	4.48	1.46	1.33
2	C	314	OLC	O20-C1	4.47	1.46	1.33
2	C	307	OLC	O20-C1	4.45	1.46	1.33
2	C	309	OLC	O20-C1	4.44	1.46	1.33
2	C	304	OLC	O20-C1	4.42	1.46	1.33
2	C	311	OLC	O20-C1	4.41	1.46	1.33
2	C	305	OLC	O20-C1	4.38	1.46	1.33
2	C	312	OLC	O20-C1	4.37	1.46	1.33
2	C	308	OLC	O20-C1	4.37	1.46	1.33
2	D	301	OLC	O20-C1	4.35	1.46	1.33
2	A	302	OLC	O20-C1	4.35	1.46	1.33
2	B	303	OLC	O20-C1	4.34	1.46	1.33
2	C	301	OLC	O20-C1	4.32	1.46	1.33
2	C	302	OLC	O20-C1	4.31	1.45	1.33
2	B	301	OLC	O20-C1	4.29	1.45	1.33
2	A	303	OLC	O20-C1	4.28	1.45	1.33
2	C	306	OLC	O20-C1	4.25	1.45	1.33
2	D	303	OLC	O20-C1	4.15	1.45	1.33
2	B	304	OLC	O20-C1	4.06	1.45	1.33
2	E	304	OLC	O20-C1	4.06	1.45	1.33
5	B	308	BOG	O1-C1	2.08	1.43	1.40

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	313	RET	C18-C5-C6	-4.29	119.72	124.53
6	C	323	RET	C18-C5-C6	-4.20	119.82	124.53
6	D	312	RET	C18-C5-C6	-4.07	119.96	124.53
6	E	312	RET	C18-C5-C6	-3.99	120.05	124.53
6	B	309	RET	C18-C5-C6	-3.88	120.17	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	312	RET	C7-C8-C9	-3.22	121.37	126.23
6	C	323	RET	C7-C8-C9	-3.11	121.53	126.23
2	A	302	OLC	O20-C1-C2	3.11	121.67	111.91
2	A	303	OLC	O20-C1-C2	3.09	121.61	111.91
2	C	301	OLC	O20-C1-C2	3.09	121.59	111.91
6	A	313	RET	C7-C8-C9	-3.08	121.58	126.23
6	B	309	RET	C7-C8-C9	-2.98	121.72	126.23
6	E	312	RET	C7-C8-C9	-2.91	121.84	126.23
2	C	310	OLC	O20-C1-C2	2.90	121.00	111.91
2	E	304	OLC	O20-C1-C2	2.89	120.99	111.91
2	B	301	OLC	O20-C1-C2	2.86	120.89	111.91
2	C	302	OLC	O20-C1-C2	2.80	120.68	111.91
2	C	307	OLC	O20-C1-C2	2.78	120.63	111.91
2	C	308	OLC	O20-C1-C2	2.77	120.61	111.91
2	C	309	OLC	O20-C1-C2	2.75	120.53	111.91
2	C	314	OLC	O20-C1-C2	2.73	120.48	111.91
2	C	313	OLC	O20-C1-C2	2.72	120.44	111.91
2	D	301	OLC	O20-C1-C2	2.71	120.42	111.91
2	C	304	OLC	O20-C1-C2	2.69	120.36	111.91
2	C	306	OLC	O20-C1-C2	2.68	120.31	111.91
6	D	312	RET	C11-C10-C9	-2.67	123.50	127.31
6	B	309	RET	C11-C10-C9	-2.66	123.52	127.31
2	C	311	OLC	O20-C1-C2	2.59	120.04	111.91
2	B	304	OLC	O20-C1-C2	2.57	119.99	111.91
2	C	305	OLC	O20-C1-C2	2.52	119.82	111.91
2	E	304	OLC	O20-C1-O19	-2.52	117.23	123.59
2	B	303	OLC	O20-C1-C2	2.50	119.77	111.91
2	D	303	OLC	O20-C1-C2	2.50	119.76	111.91
2	A	302	OLC	O20-C1-O19	-2.47	117.35	123.59
2	C	312	OLC	O20-C1-C2	2.46	119.63	111.91
6	C	323	RET	C11-C10-C9	-2.46	123.80	127.31
6	D	312	RET	C20-C13-C12	2.43	121.91	118.08
2	A	303	OLC	O20-C1-O19	-2.33	117.70	123.59
6	A	313	RET	C10-C11-C12	-2.32	115.98	123.22
6	B	309	RET	C10-C11-C12	-2.32	115.99	123.22
6	E	312	RET	C10-C11-C12	-2.26	116.15	123.22
6	A	313	RET	C11-C10-C9	-2.26	124.09	127.31
6	D	312	RET	C10-C11-C12	-2.25	116.21	123.22
2	C	302	OLC	O20-C1-O19	-2.23	117.95	123.59
2	C	306	OLC	O20-C1-O19	-2.16	118.14	123.59
6	E	312	RET	C11-C10-C9	-2.16	124.22	127.31
6	B	309	RET	C19-C9-C8	2.14	121.45	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	323	RET	C10-C11-C12	-2.11	116.64	123.22
6	B	309	RET	C20-C13-C12	2.08	121.36	118.08
6	A	313	RET	C20-C13-C12	2.07	121.35	118.08
2	B	304	OLC	O20-C1-O19	-2.02	118.49	123.59
6	E	312	RET	C19-C9-C8	2.00	121.23	118.08

There are no chirality outliers.

All (362) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	310	BOG	C2-C1-O1-C1'
5	E	310	BOG	O5-C1-O1-C1'
5	E	310	BOG	C2'-C1'-O1-C1
2	E	304	OLC	O20-C21-C22-C24
2	E	304	OLC	O20-C21-C22-O23
2	A	303	OLC	O20-C21-C22-C24
2	C	307	OLC	O20-C21-C22-C24
2	C	307	OLC	O20-C21-C22-O23
3	C	319	LFA	C17-C18-C19-C20
2	C	301	OLC	C21-C22-C24-O25
2	C	308	OLC	C21-C22-C24-O25
2	C	308	OLC	O23-C22-C24-O25
2	C	305	OLC	C21-C22-C24-O25
2	C	305	OLC	O20-C21-C22-O23
2	D	303	OLC	C21-C22-C24-O25
2	C	306	OLC	O20-C21-C22-C24
2	C	306	OLC	O20-C21-C22-O23
3	E	307	LFA	C17-C18-C19-C20
2	C	314	OLC	O20-C21-C22-O23
5	A	310	BOG	C2'-C1'-O1-C1
2	C	313	OLC	C21-C22-C24-O25
2	C	313	OLC	C2-C1-O20-C21
2	C	313	OLC	O19-C1-O20-C21
2	C	304	OLC	C21-C22-C24-O25
2	C	306	OLC	O19-C1-O20-C21
2	C	306	OLC	C2-C1-O20-C21
2	E	304	OLC	O19-C1-O20-C21
2	C	305	OLC	C2-C1-O20-C21
2	E	304	OLC	C2-C1-O20-C21
2	A	303	OLC	C2-C1-O20-C21
2	A	303	OLC	O19-C1-O20-C21
2	C	305	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	A	303	OLC	O20-C21-C22-O23
2	C	312	OLC	O20-C21-C22-O23
2	B	304	OLC	C2-C1-O20-C21
2	B	301	OLC	C2-C1-O20-C21
2	B	303	OLC	C2-C1-O20-C21
2	C	310	OLC	C2-C1-O20-C21
2	C	312	OLC	C2-C1-O20-C21
2	D	301	OLC	C2-C1-O20-C21
2	C	304	OLC	C2-C1-O20-C21
2	B	304	OLC	O19-C1-O20-C21
2	C	302	OLC	O20-C21-C22-C24
2	C	305	OLC	O20-C21-C22-C24
2	C	312	OLC	O20-C21-C22-C24
2	B	301	OLC	O19-C1-O20-C21
5	E	310	BOG	O5-C5-C6-O6
2	C	314	OLC	C2-C1-O20-C21
2	D	303	OLC	O23-C22-C24-O25
2	C	313	OLC	O23-C22-C24-O25
2	C	304	OLC	O23-C22-C24-O25
2	C	302	OLC	C1-C2-C3-C4
2	D	303	OLC	C1-C2-C3-C4
2	C	311	OLC	C1-C2-C3-C4
2	D	301	OLC	C1-C2-C3-C4
2	B	303	OLC	O19-C1-O20-C21
2	C	310	OLC	O19-C1-O20-C21
2	C	304	OLC	O19-C1-O20-C21
2	C	312	OLC	O19-C1-O20-C21
2	D	301	OLC	O19-C1-O20-C21
5	E	310	BOG	C4-C5-C6-O6
3	A	307	LFA	C7-C8-C9-C10
2	C	314	OLC	O19-C1-O20-C21
2	C	302	OLC	O20-C21-C22-O23
2	C	309	OLC	O20-C21-C22-O23
2	C	301	OLC	C5-C6-C7-C8
2	C	314	OLC	O20-C21-C22-C24
5	E	310	BOG	C2'-C3'-C4'-C5'
3	B	306	LFA	C3-C4-C5-C6
2	A	301	OLC	C3-C4-C5-C6
2	C	307	OLC	C12-C13-C14-C15
3	C	303	LFA	C7-C8-C9-C10
3	E	311	LFA	C2-C3-C4-C5
3	D	304	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	A	311	OLC	C5-C6-C7-C8
3	D	302	LFA	C11-C10-C9-C8
3	D	307	LFA	C5-C6-C7-C8
3	B	305	LFA	C14-C15-C16-C17
2	C	302	OLC	C5-C6-C7-C8
2	C	302	OLC	C3-C4-C5-C6
2	A	301	OLC	C4-C5-C6-C7
2	C	307	OLC	C3-C4-C5-C6
2	E	303	OLC	C11-C12-C13-C14
2	C	311	OLC	C5-C6-C7-C8
2	C	311	OLC	C2-C3-C4-C5
2	C	306	OLC	C4-C5-C6-C7
3	E	306	LFA	C14-C15-C16-C17
3	E	306	LFA	C15-C16-C17-C18
2	E	304	OLC	C21-C22-C24-O25
2	C	309	OLC	C21-C22-C24-O25
2	C	306	OLC	C21-C22-C24-O25
3	A	307	LFA	C11-C10-C9-C8
3	C	317	LFA	C12-C13-C14-C15
3	C	316	LFA	C15-C16-C17-C18
2	E	301	OLC	C10-C11-C12-C13
2	C	311	OLC	C6-C7-C8-C9
2	C	307	OLC	C1-C2-C3-C4
3	A	306	LFA	C15-C16-C17-C18
3	B	302	LFA	C16-C17-C18-C19
3	D	302	LFA	C9-C10-C11-C12
3	D	302	LFA	C12-C13-C14-C15
2	C	313	OLC	C5-C6-C7-C8
2	C	301	OLC	C4-C5-C6-C7
3	B	305	LFA	C16-C17-C18-C19
3	D	305	LFA	C14-C15-C16-C17
3	D	308	LFA	C16-C17-C18-C19
2	C	306	OLC	C3-C4-C5-C6
2	C	307	OLC	C14-C15-C16-C17
2	B	303	OLC	C10-C11-C12-C13
2	E	301	OLC	C5-C6-C7-C8
5	B	308	BOG	O5-C5-C6-O6
3	E	311	LFA	C3-C4-C5-C6
3	C	316	LFA	C16-C17-C18-C19
3	D	306	LFA	C4-C5-C6-C7
3	A	312	LFA	C13-C14-C15-C16
2	C	313	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	D	311	BOG	C1'-C2'-C3'-C4'
5	E	310	BOG	O1-C1'-C2'-C3'
3	C	318	LFA	C3-C4-C5-C6
3	D	305	LFA	C11-C12-C13-C14
2	C	309	OLC	C2-C3-C4-C5
5	B	308	BOG	C4-C5-C6-O6
2	E	304	OLC	O23-C22-C24-O25
2	C	301	OLC	O23-C22-C24-O25
2	C	309	OLC	O23-C22-C24-O25
2	C	312	OLC	C3-C4-C5-C6
3	E	306	LFA	C9-C10-C11-C12
3	B	305	LFA	C15-C16-C17-C18
2	B	301	OLC	C10-C11-C12-C13
2	C	305	OLC	C10-C11-C12-C13
2	C	311	OLC	C10-C11-C12-C13
3	D	306	LFA	C2-C3-C4-C5
3	C	318	LFA	C4-C5-C6-C7
3	A	312	LFA	C16-C17-C18-C19
5	B	308	BOG	C1'-C2'-C3'-C4'
3	A	308	LFA	C2-C3-C4-C5
3	E	302	LFA	C11-C10-C9-C8
5	B	308	BOG	C3'-C4'-C5'-C6'
3	D	307	LFA	C7-C8-C9-C10
3	D	307	LFA	C11-C12-C13-C14
3	D	304	LFA	C3-C4-C5-C6
3	B	306	LFA	C2-C3-C4-C5
2	C	313	OLC	O20-C21-C22-O23
2	D	301	OLC	O20-C21-C22-O23
2	A	311	OLC	C11-C12-C13-C14
3	C	303	LFA	C16-C17-C18-C19
3	A	305	LFA	C4-C5-C6-C7
2	A	301	OLC	C10-C11-C12-C13
2	A	301	OLC	C6-C7-C8-C9
2	E	304	OLC	C6-C7-C8-C9
2	C	308	OLC	C6-C7-C8-C9
2	D	301	OLC	C6-C7-C8-C9
3	C	303	LFA	C2-C3-C4-C5
2	C	304	OLC	C2-C3-C4-C5
2	D	301	OLC	O20-C21-C22-C24
2	C	310	OLC	C2-C3-C4-C5
2	C	312	OLC	C4-C5-C6-C7
2	D	303	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	D	301	OLC	C2-C3-C4-C5
2	C	302	OLC	C4-C5-C6-C7
2	C	306	OLC	C5-C6-C7-C8
3	E	302	LFA	C7-C8-C9-C10
3	D	302	LFA	C10-C11-C12-C13
2	E	303	OLC	C6-C7-C8-C9
2	C	309	OLC	C6-C7-C8-C9
3	A	312	LFA	C7-C8-C9-C10
5	E	310	BOG	C1'-C2'-C3'-C4'
5	C	321	BOG	C1'-C2'-C3'-C4'
3	D	307	LFA	C2-C3-C4-C5
3	C	303	LFA	C9-C10-C11-C12
3	D	304	LFA	C9-C10-C11-C12
3	D	304	LFA	C4-C5-C6-C7
3	A	312	LFA	C6-C7-C8-C9
3	E	311	LFA	C4-C5-C6-C7
2	E	304	OLC	C2-C3-C4-C5
3	C	303	LFA	C15-C16-C17-C18
2	C	307	OLC	C5-C6-C7-C8
3	C	303	LFA	C13-C14-C15-C16
3	C	317	LFA	C13-C14-C15-C16
3	D	304	LFA	C11-C12-C13-C14
3	C	317	LFA	C15-C16-C17-C18
3	B	302	LFA	C6-C7-C8-C9
5	B	308	BOG	C5'-C6'-C7'-C8'
2	B	303	OLC	C4-C5-C6-C7
3	C	303	LFA	C3-C4-C5-C6
3	D	305	LFA	C1-C2-C3-C4
2	C	305	OLC	O23-C22-C24-O25
5	E	310	BOG	C5'-C6'-C7'-C8'
2	C	302	OLC	C6-C7-C8-C9
2	B	301	OLC	C6-C7-C8-C9
2	C	304	OLC	C1-C2-C3-C4
3	D	307	LFA	C13-C14-C15-C16
2	C	302	OLC	C2-C1-O20-C21
3	D	306	LFA	C1-C2-C3-C4
3	E	306	LFA	C13-C14-C15-C16
2	E	304	OLC	C3-C4-C5-C6
3	A	312	LFA	C14-C15-C16-C17
2	C	313	OLC	C6-C7-C8-C9
3	D	306	LFA	C5-C6-C7-C8
3	B	302	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	C	311	OLC	C2-C1-O20-C21
2	C	311	OLC	C4-C5-C6-C7
3	A	306	LFA	C14-C15-C16-C17
3	D	304	LFA	C14-C15-C16-C17
2	C	301	OLC	C10-C11-C12-C13
5	C	321	BOG	C5'-C6'-C7'-C8'
3	A	307	LFA	C1-C2-C3-C4
2	B	301	OLC	C5-C6-C7-C8
2	C	304	OLC	C4-C5-C6-C7
3	C	316	LFA	C17-C18-C19-C20
2	C	302	OLC	O19-C1-O20-C21
2	C	310	OLC	C1-C2-C3-C4
2	C	307	OLC	C15-C16-C17-C18
2	C	304	OLC	C3-C4-C5-C6
2	E	304	OLC	C11-C12-C13-C14
2	C	309	OLC	C4-C5-C6-C7
3	E	306	LFA	C7-C8-C9-C10
2	E	301	OLC	C4-C5-C6-C7
3	C	317	LFA	C16-C17-C18-C19
2	C	311	OLC	C3-C4-C5-C6
3	A	306	LFA	C16-C17-C18-C19
2	C	311	OLC	O19-C1-O20-C21
3	A	312	LFA	C12-C13-C14-C15
2	C	313	OLC	O20-C21-C22-C24
2	C	314	OLC	C2-C3-C4-C5
5	A	310	BOG	C5'-C6'-C7'-C8'
3	A	305	LFA	C1-C2-C3-C4
2	C	314	OLC	C4-C5-C6-C7
3	C	318	LFA	C1-C2-C3-C4
3	C	317	LFA	C9-C10-C11-C12
3	A	307	LFA	C9-C10-C11-C12
5	A	310	BOG	C1'-C2'-C3'-C4'
2	C	306	OLC	C12-C13-C14-C15
2	C	307	OLC	C4-C5-C6-C7
2	E	304	OLC	C12-C13-C14-C15
3	C	317	LFA	C3-C4-C5-C6
5	A	310	BOG	O1-C1'-C2'-C3'
3	D	302	LFA	C4-C5-C6-C7
2	C	305	OLC	C4-C5-C6-C7
2	E	303	OLC	C10-C11-C12-C13
2	C	308	OLC	C5-C6-C7-C8
3	C	303	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	C	315	LFA	C2-C3-C4-C5
3	A	305	LFA	C5-C6-C7-C8
2	C	311	OLC	O23-C22-C24-O25
2	C	306	OLC	O23-C22-C24-O25
2	C	314	OLC	O23-C22-C24-O25
2	C	306	OLC	C10-C11-C12-C13
2	A	311	OLC	C10-C11-C12-C13
2	B	301	OLC	C12-C13-C14-C15
3	C	316	LFA	C13-C14-C15-C16
2	C	314	OLC	C6-C7-C8-C9
2	C	309	OLC	C1-C2-C3-C4
2	C	301	OLC	C11-C12-C13-C14
3	C	315	LFA	C4-C5-C6-C7
2	C	309	OLC	C12-C13-C14-C15
3	C	318	LFA	C2-C3-C4-C5
2	C	309	OLC	C11-C12-C13-C14
2	A	303	OLC	C3-C4-C5-C6
3	D	304	LFA	C7-C8-C9-C10
3	D	308	LFA	C14-C15-C16-C17
3	E	305	LFA	C16-C17-C18-C19
2	E	304	OLC	C10-C11-C12-C13
2	A	301	OLC	C2-C3-C4-C5
3	A	307	LFA	C2-C3-C4-C5
3	D	308	LFA	C15-C16-C17-C18
3	A	304	LFA	C16-C17-C18-C19
3	D	305	LFA	C3-C4-C5-C6
3	A	312	LFA	C11-C12-C13-C14
2	A	303	OLC	C2-C3-C4-C5
3	E	308	LFA	C17-C18-C19-C20
2	A	311	OLC	C4-C5-C6-C7
2	C	308	OLC	C2-C3-C4-C5
3	D	305	LFA	C13-C14-C15-C16
2	E	304	OLC	C14-C15-C16-C17
3	D	302	LFA	C7-C8-C9-C10
2	E	303	OLC	C13-C14-C15-C16
3	D	305	LFA	C5-C6-C7-C8
3	D	305	LFA	C10-C11-C12-C13
3	D	304	LFA	C11-C10-C9-C8
2	C	308	OLC	C12-C13-C14-C15
2	B	303	OLC	C9-C10-C11-C12
2	A	311	OLC	C7-C8-C9-C10
3	B	302	LFA	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
2	C	314	OLC	C3-C4-C5-C6
3	E	302	LFA	C4-C5-C6-C7
3	C	317	LFA	C11-C10-C9-C8
2	C	306	OLC	C9-C10-C11-C12
3	C	317	LFA	C14-C15-C16-C17
2	A	303	OLC	C5-C6-C7-C8
3	C	317	LFA	C10-C11-C12-C13
3	E	302	LFA	C10-C11-C12-C13
3	A	312	LFA	C2-C3-C4-C5
5	D	311	BOG	C4'-C5'-C6'-C7'
2	C	302	OLC	C10-C11-C12-C13
2	E	304	OLC	C13-C14-C15-C16
2	C	301	OLC	C2-C1-O20-C21
3	B	302	LFA	C5-C6-C7-C8
2	C	305	OLC	C6-C7-C8-C9
3	C	317	LFA	C6-C7-C8-C9
2	C	307	OLC	C13-C14-C15-C16
2	C	311	OLC	C15-C16-C17-C18
2	C	309	OLC	O20-C21-C22-C24
2	C	310	OLC	O20-C21-C22-C24
2	C	301	OLC	C6-C7-C8-C9
2	C	310	OLC	C3-C4-C5-C6
3	D	305	LFA	C16-C17-C18-C19
3	D	307	LFA	C14-C15-C16-C17
2	C	301	OLC	C7-C8-C9-C10
3	D	304	LFA	C15-C16-C17-C18
2	C	309	OLC	C3-C4-C5-C6
3	C	303	LFA	C1-C2-C3-C4
3	D	302	LFA	C3-C4-C5-C6
2	C	301	OLC	O19-C1-O20-C21
3	D	307	LFA	C3-C4-C5-C6
3	C	303	LFA	C12-C13-C14-C15
3	C	317	LFA	C11-C12-C13-C14
2	C	307	OLC	C21-C22-C24-O25
2	C	314	OLC	C21-C22-C24-O25
3	E	302	LFA	C5-C6-C7-C8
3	B	302	LFA	C11-C10-C9-C8
3	C	317	LFA	C4-C5-C6-C7
3	A	312	LFA	C9-C10-C11-C12
5	C	321	BOG	C3'-C4'-C5'-C6'
2	A	302	OLC	O20-C21-C22-O23
2	C	307	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	C	305	OLC	C3-C4-C5-C6
2	B	301	OLC	C7-C8-C9-C10
2	E	304	OLC	C9-C10-C11-C12
2	B	303	OLC	C7-C8-C9-C10
2	C	309	OLC	C7-C8-C9-C10
3	C	317	LFA	C7-C8-C9-C10
3	A	312	LFA	C17-C18-C19-C20
2	E	301	OLC	C7-C8-C9-C10
2	C	305	OLC	C7-C8-C9-C10
5	A	310	BOG	C4-C5-C6-O6
2	C	302	OLC	C7-C8-C9-C10
2	B	303	OLC	C5-C6-C7-C8
2	C	311	OLC	O20-C21-C22-C24
2	A	301	OLC	C9-C10-C11-C12
2	A	311	OLC	C9-C10-C11-C12
3	E	302	LFA	C15-C16-C17-C18
3	B	302	LFA	C10-C11-C12-C13
3	D	305	LFA	C2-C3-C4-C5
2	C	305	OLC	C11-C12-C13-C14
3	C	315	LFA	C1-C2-C3-C4
5	B	308	BOG	C4'-C5'-C6'-C7'
3	D	308	LFA	C17-C18-C19-C20
2	C	312	OLC	C6-C7-C8-C9
2	E	303	OLC	C3-C4-C5-C6
2	C	302	OLC	C9-C10-C11-C12
2	C	311	OLC	O20-C1-C2-C3
2	C	313	OLC	O20-C1-C2-C3
2	C	307	OLC	O19-C1-O20-C21
2	C	309	OLC	C5-C6-C7-C8
2	C	311	OLC	O19-C1-C2-C3
5	C	321	BOG	C2'-C1'-O1-C1
3	C	303	LFA	C17-C18-C19-C20
3	C	315	LFA	C3-C4-C5-C6
2	D	303	OLC	O20-C1-C2-C3
3	E	302	LFA	C14-C15-C16-C17
2	E	303	OLC	C14-C15-C16-C17

There are no ring outliers.

26 monomers are involved in 55 short contacts:

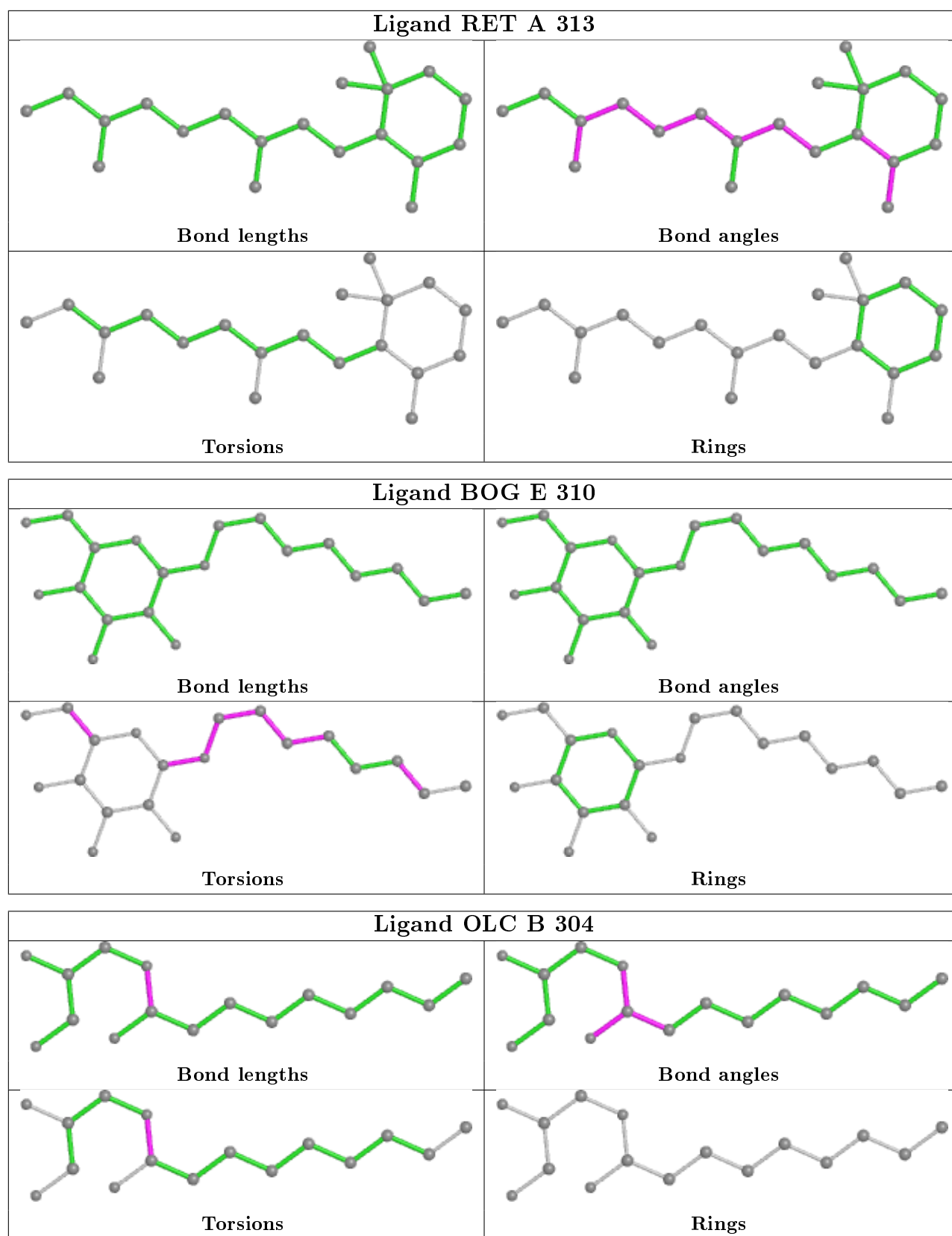
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	313	RET	6	0

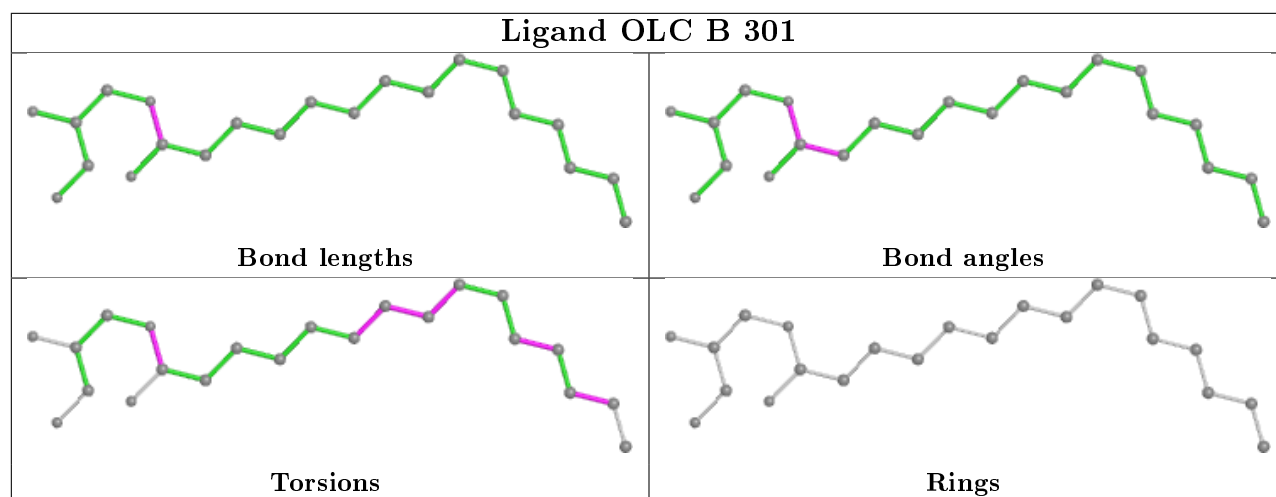
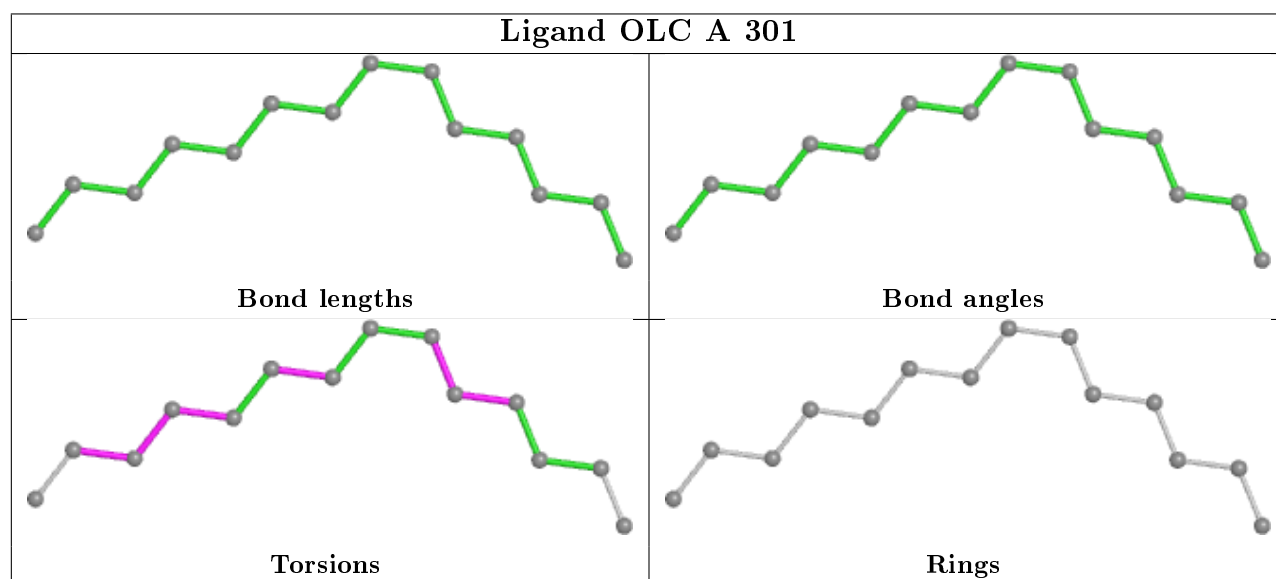
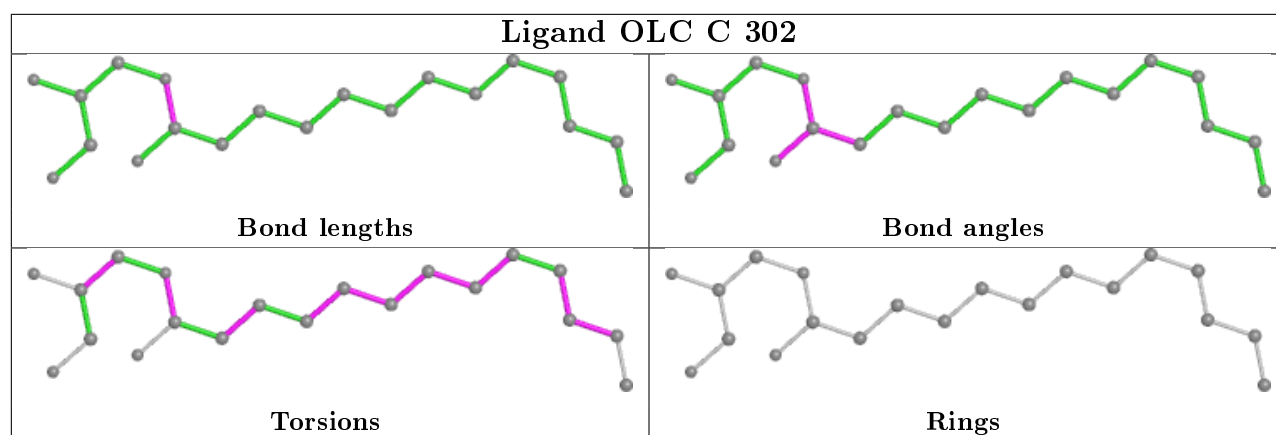
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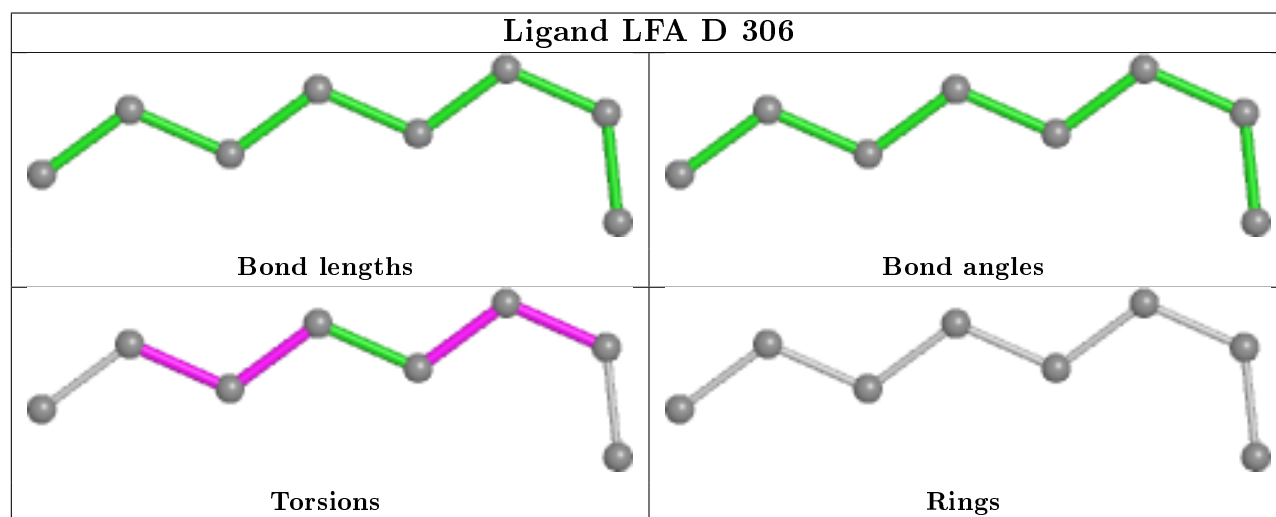
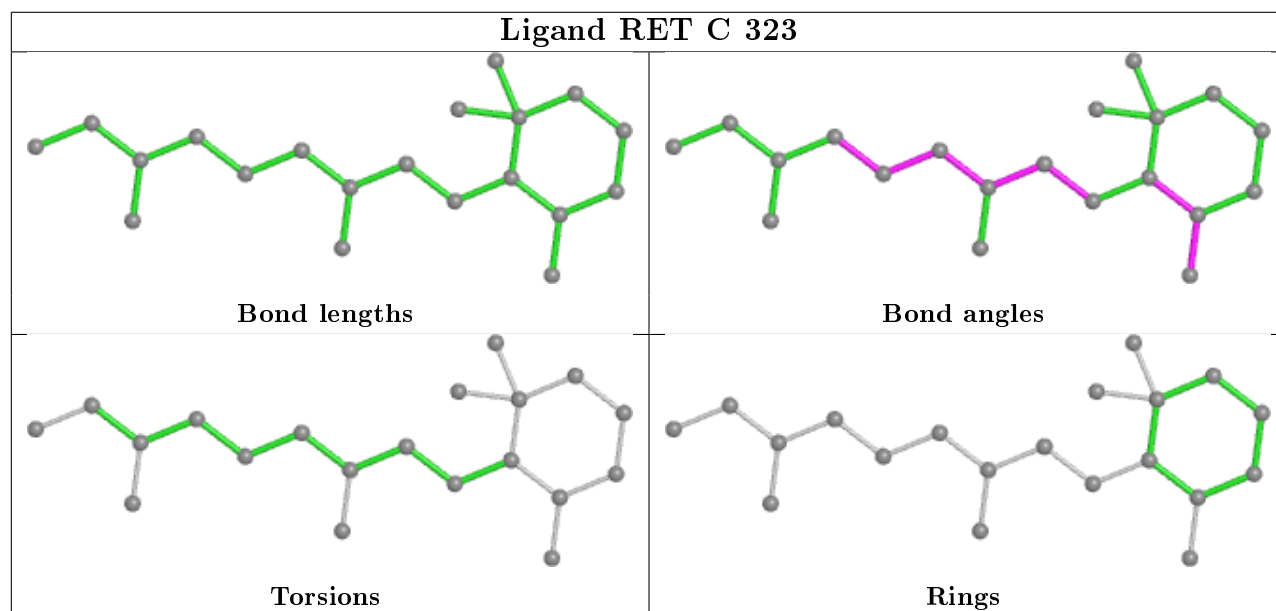
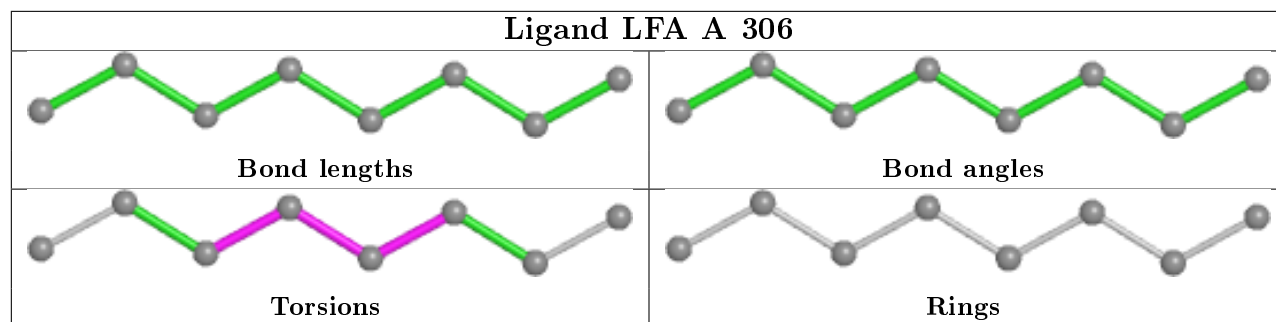
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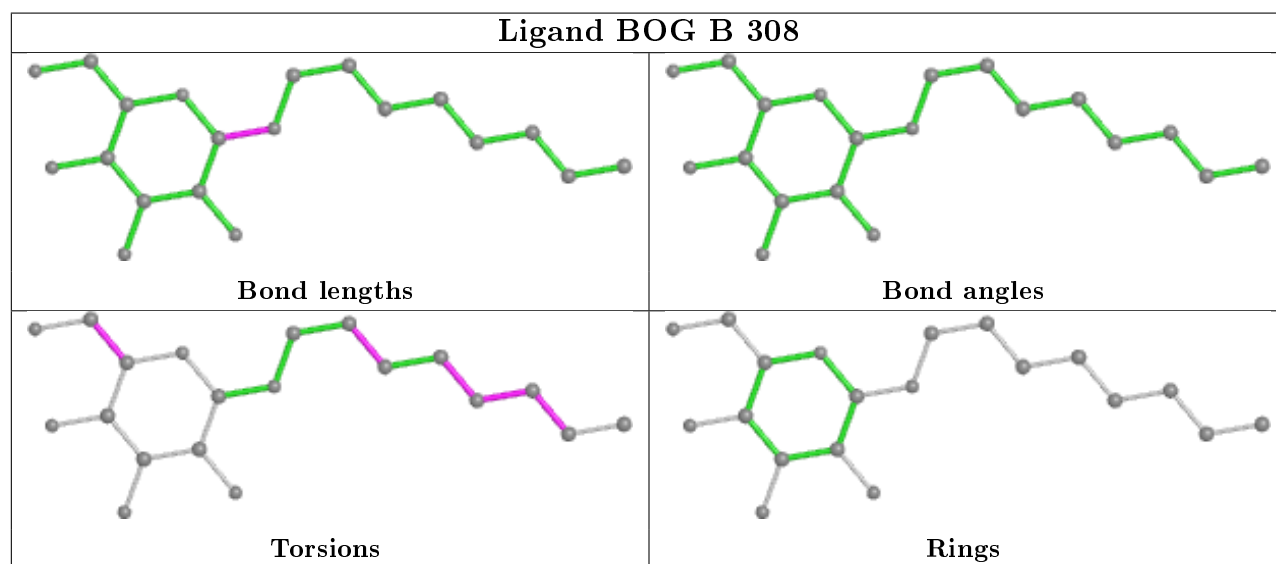
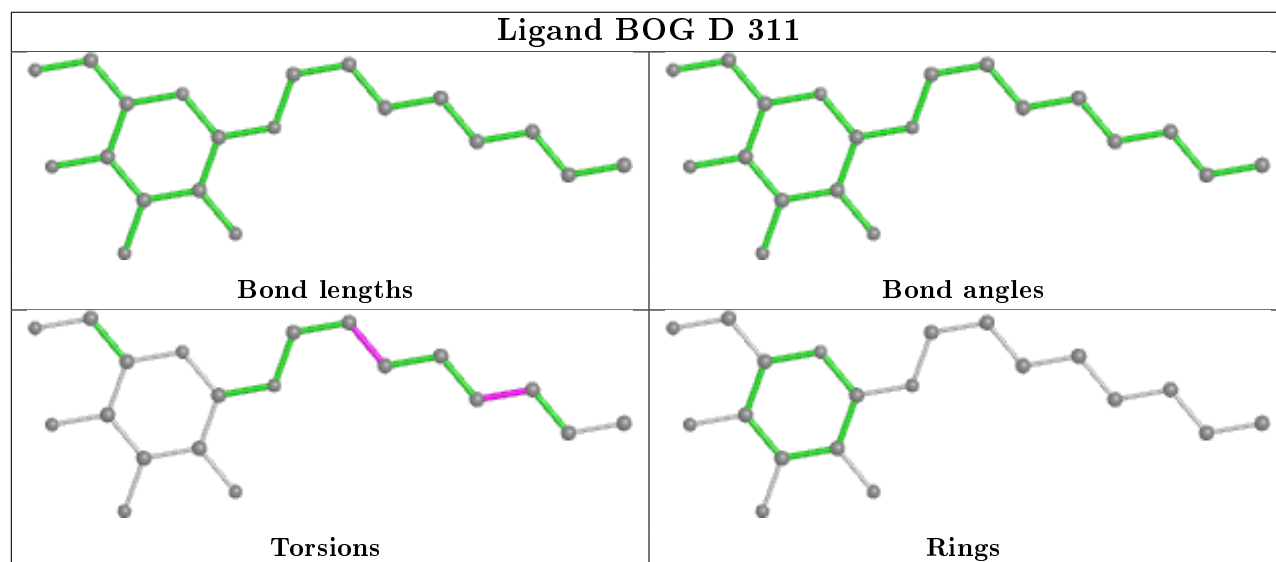
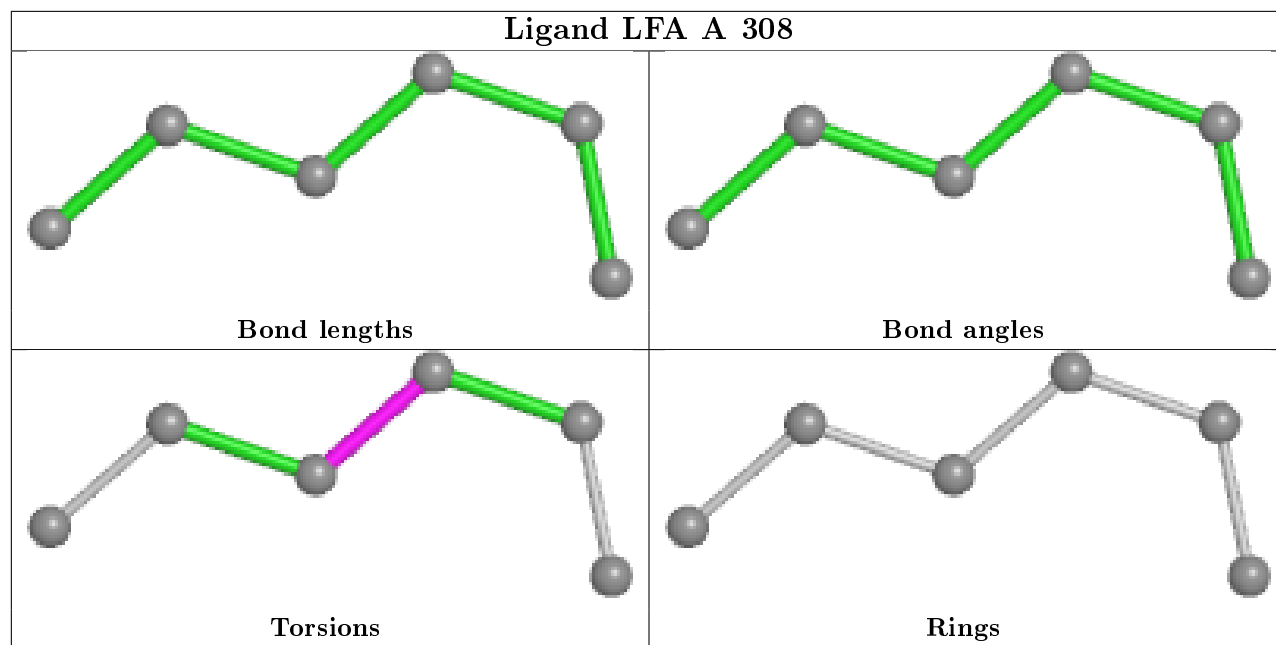
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	OLC	4	0
6	C	323	RET	5	0
5	D	311	BOG	1	0
5	B	308	BOG	2	0
2	C	307	OLC	1	0
3	C	319	LFA	2	0
2	C	308	OLC	1	0
2	C	305	OLC	2	0
2	E	303	OLC	1	0
6	E	312	RET	5	0
6	B	309	RET	5	0
3	E	307	LFA	2	0
2	C	310	OLC	1	0
6	D	312	RET	6	0
2	C	314	OLC	1	0
3	A	304	LFA	1	0
5	A	310	BOG	1	0
2	C	312	OLC	1	0
3	E	306	LFA	2	0
2	C	313	OLC	1	0
3	B	305	LFA	1	0
3	C	315	LFA	2	0
2	C	304	OLC	1	0
5	C	321	BOG	2	0
3	C	316	LFA	1	0

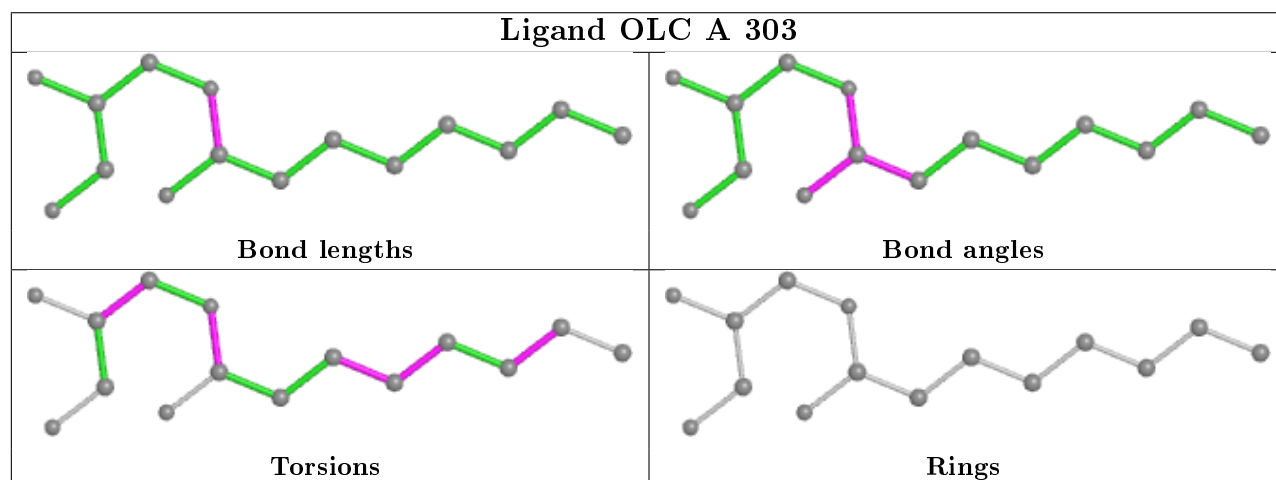
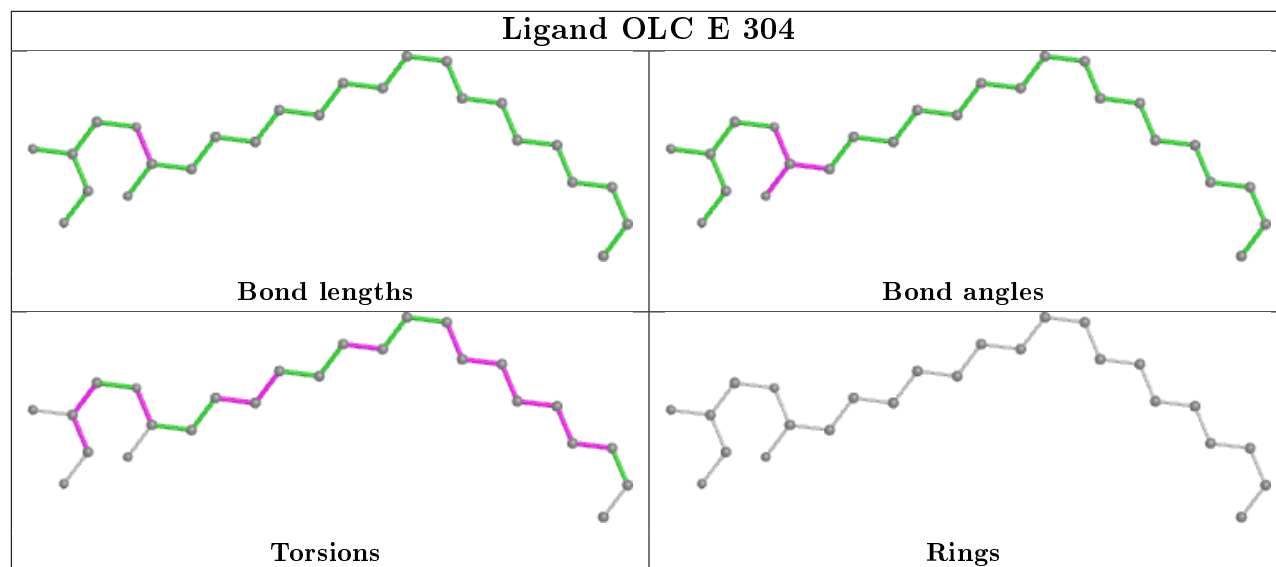
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

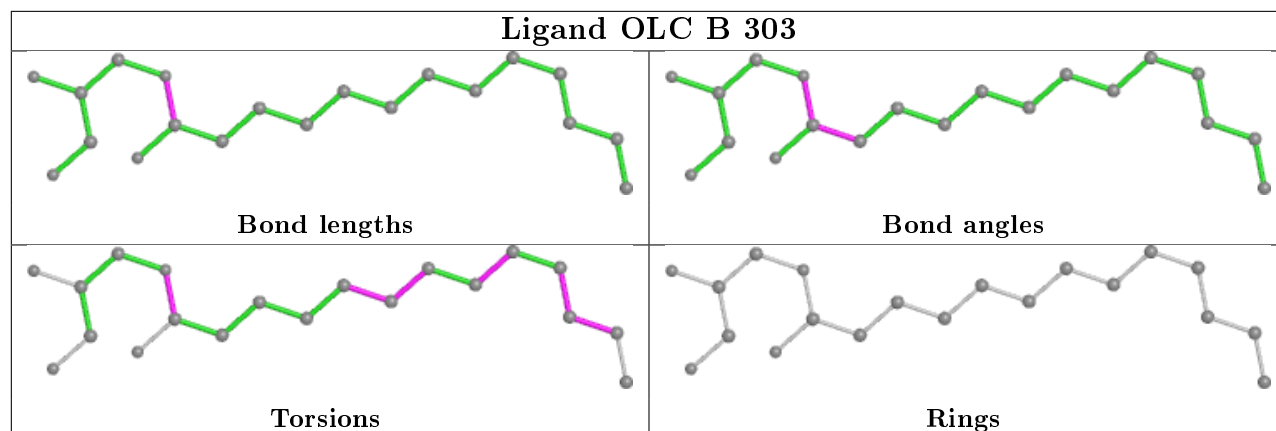
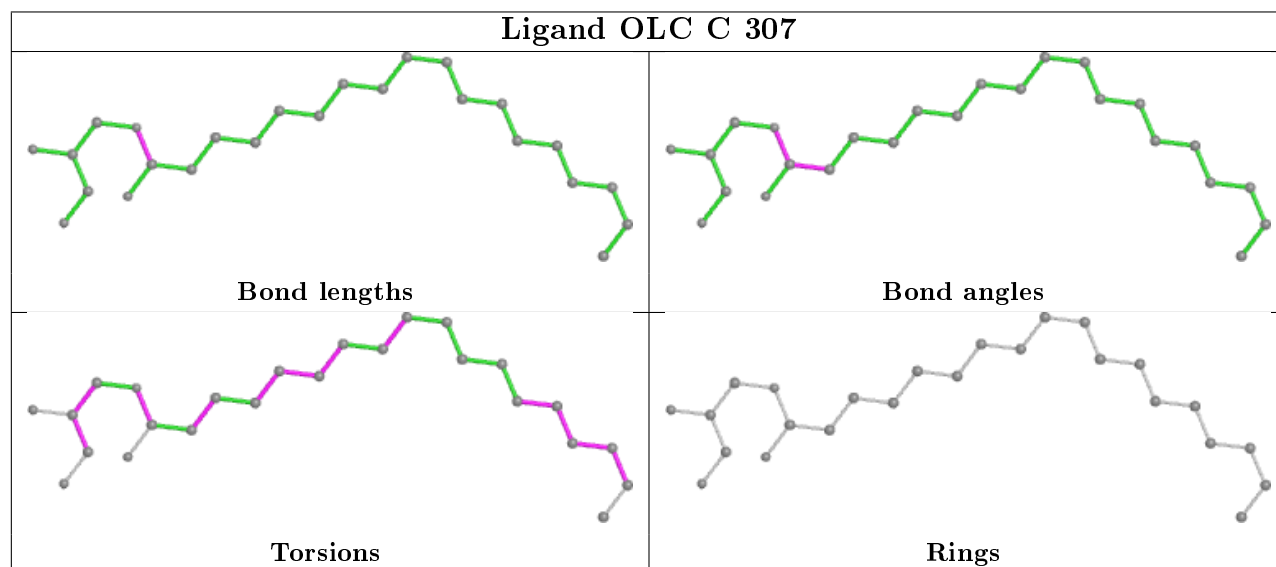
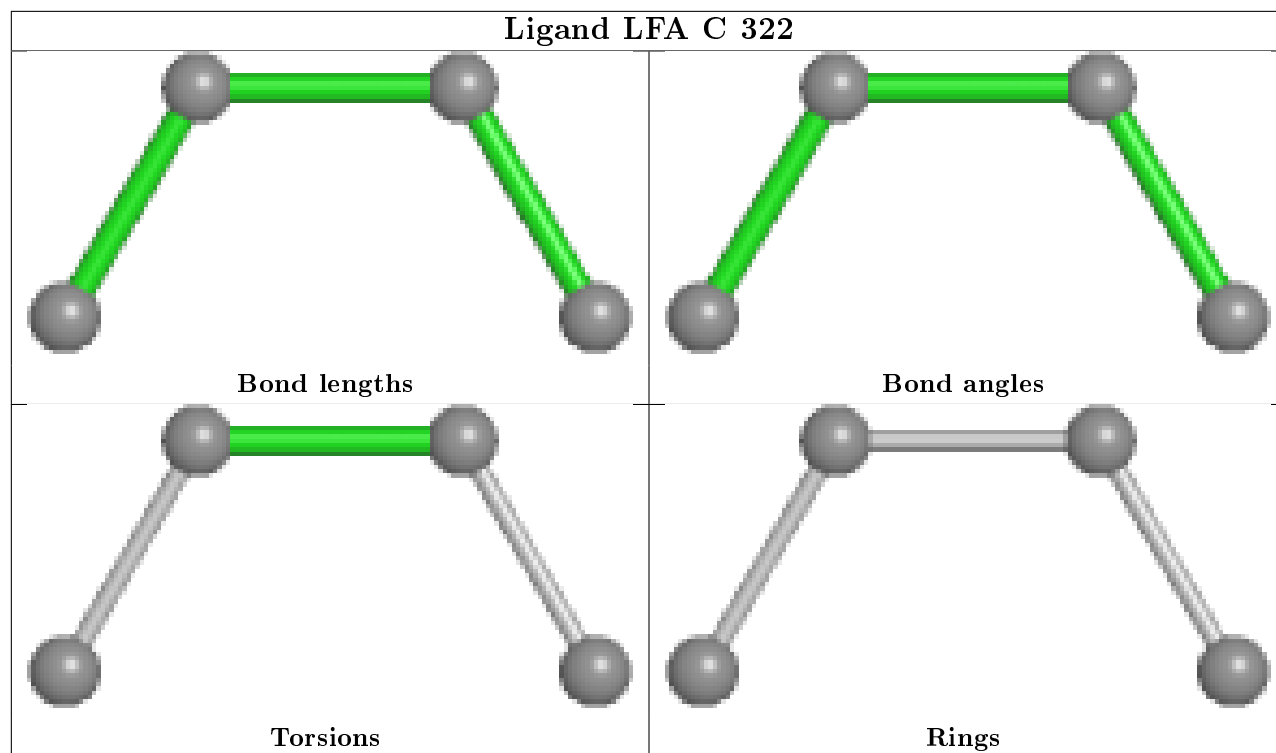




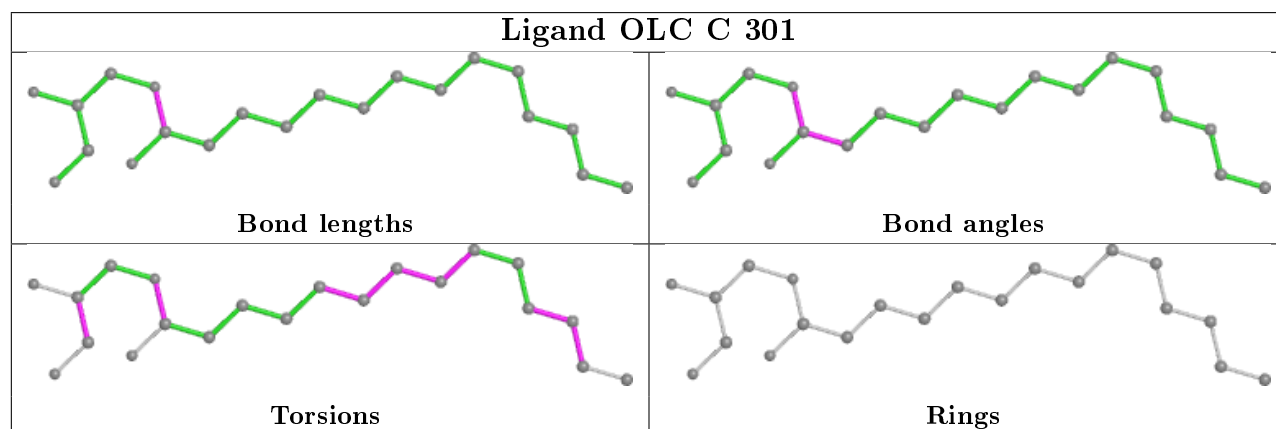
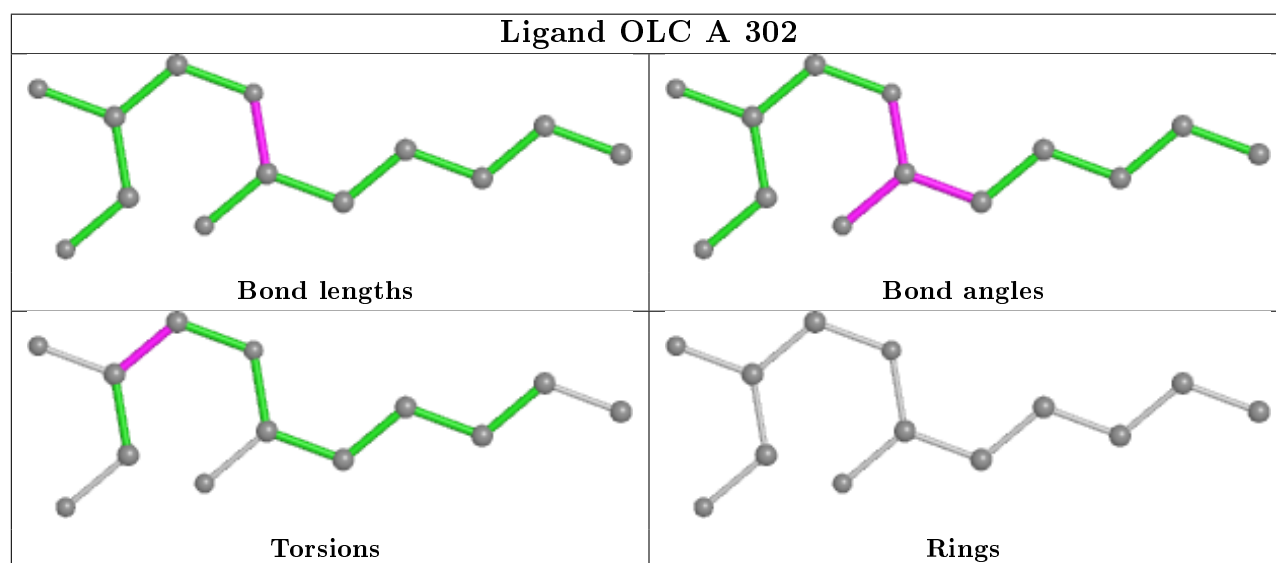
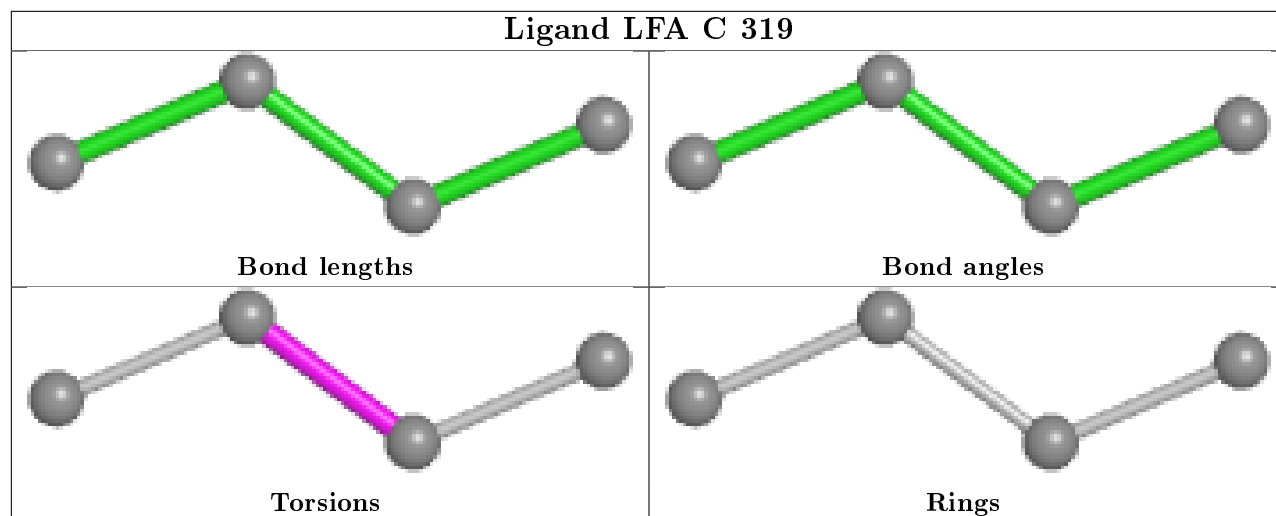


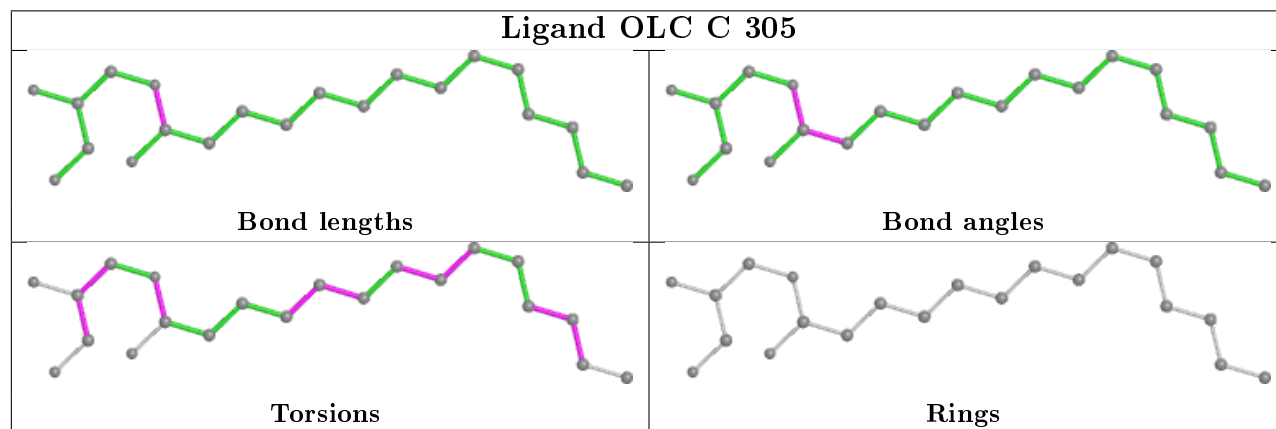
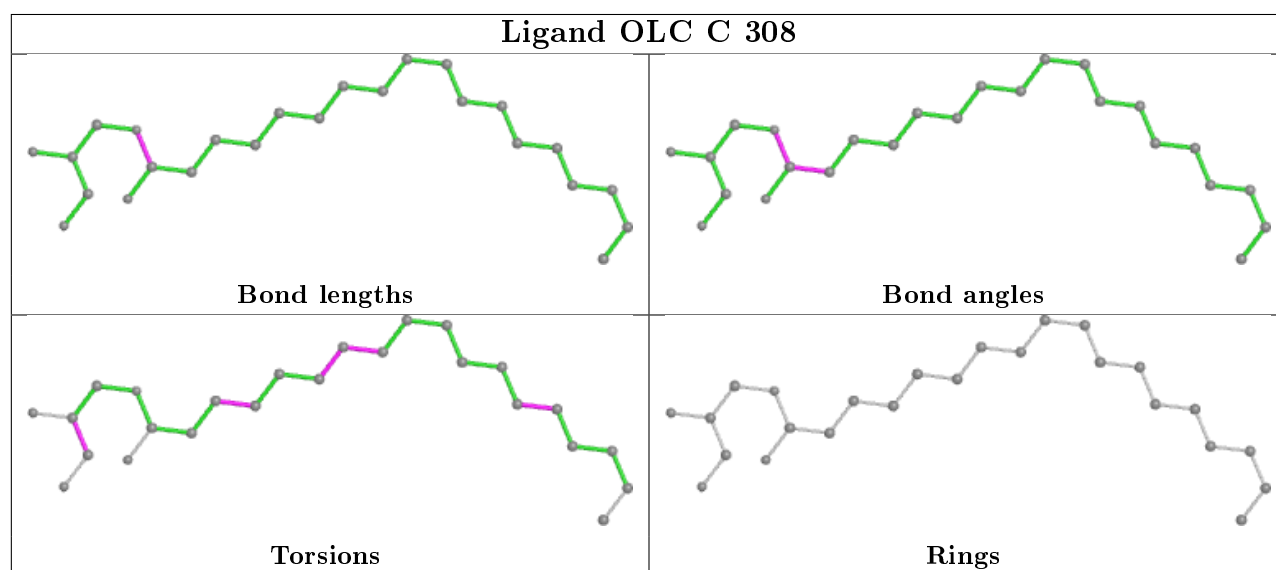
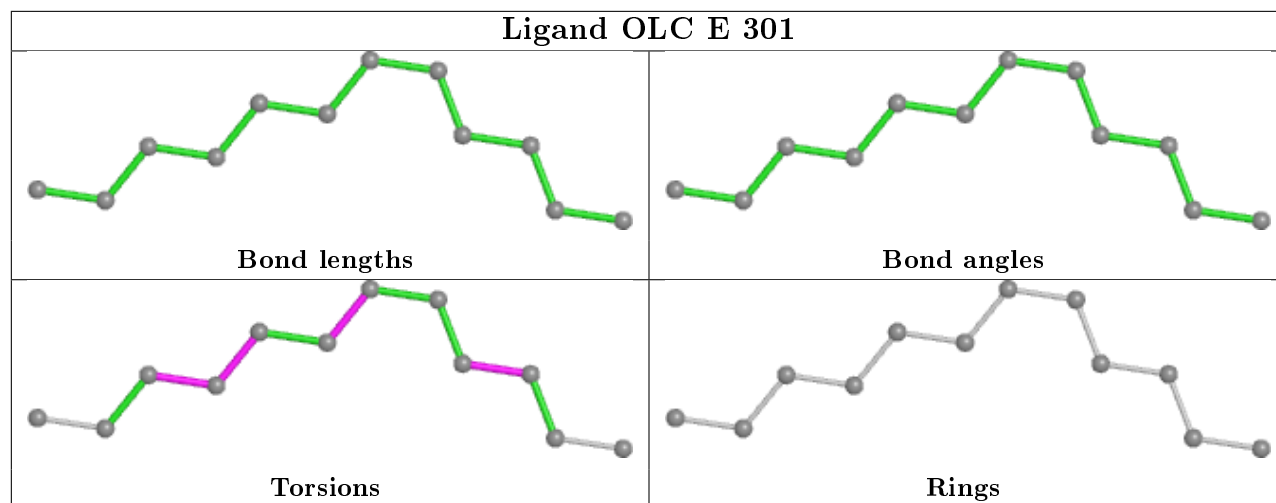


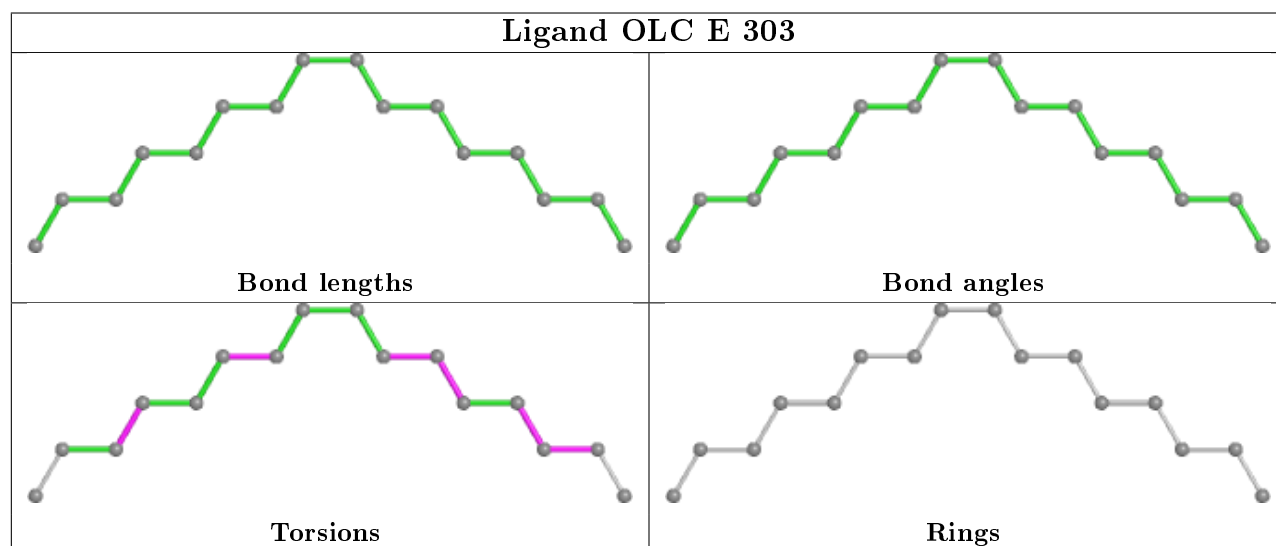
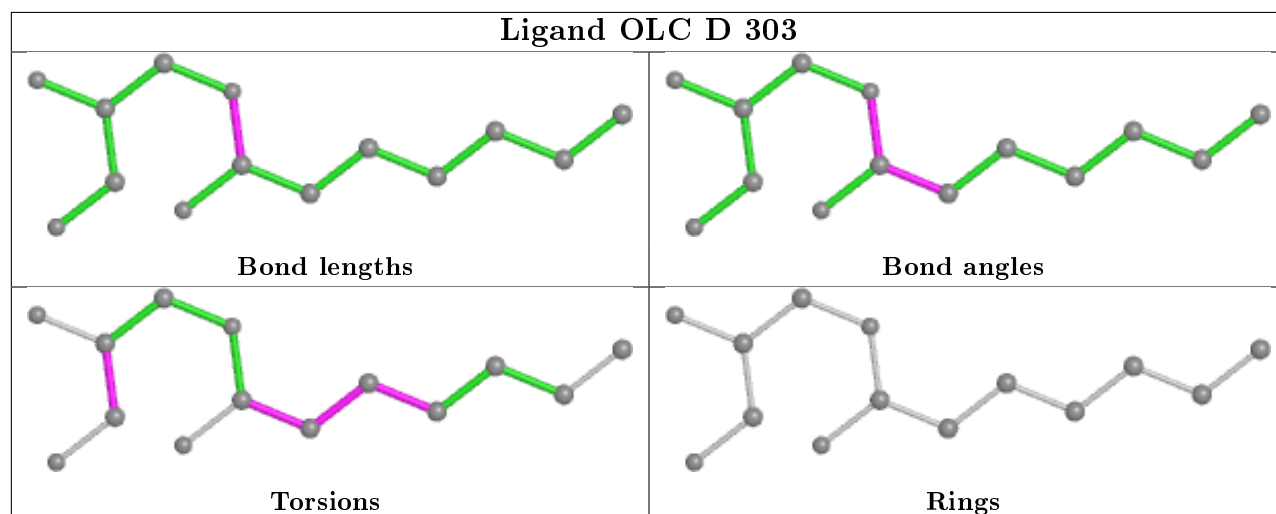
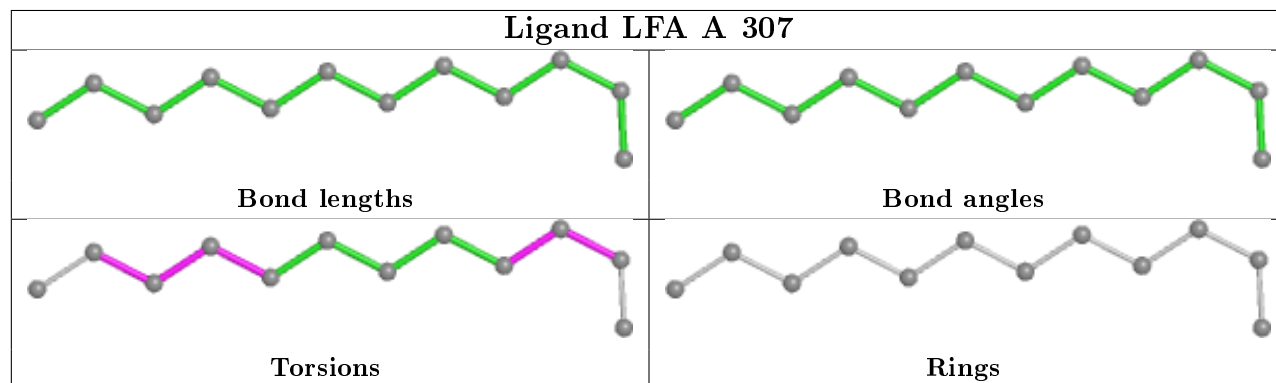
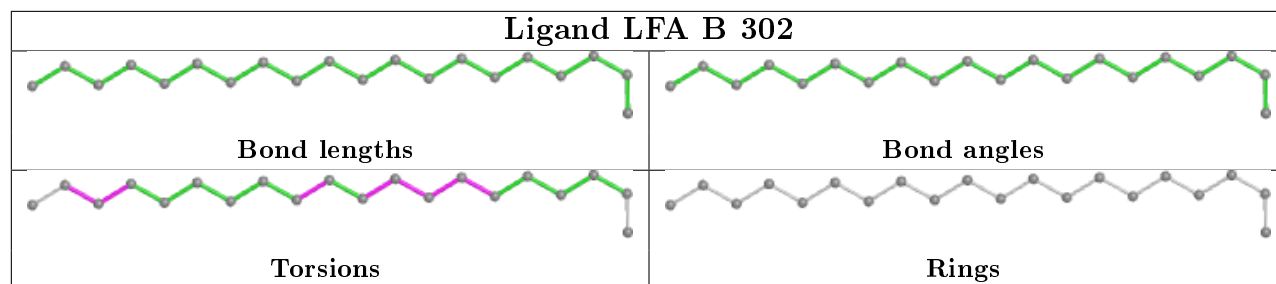


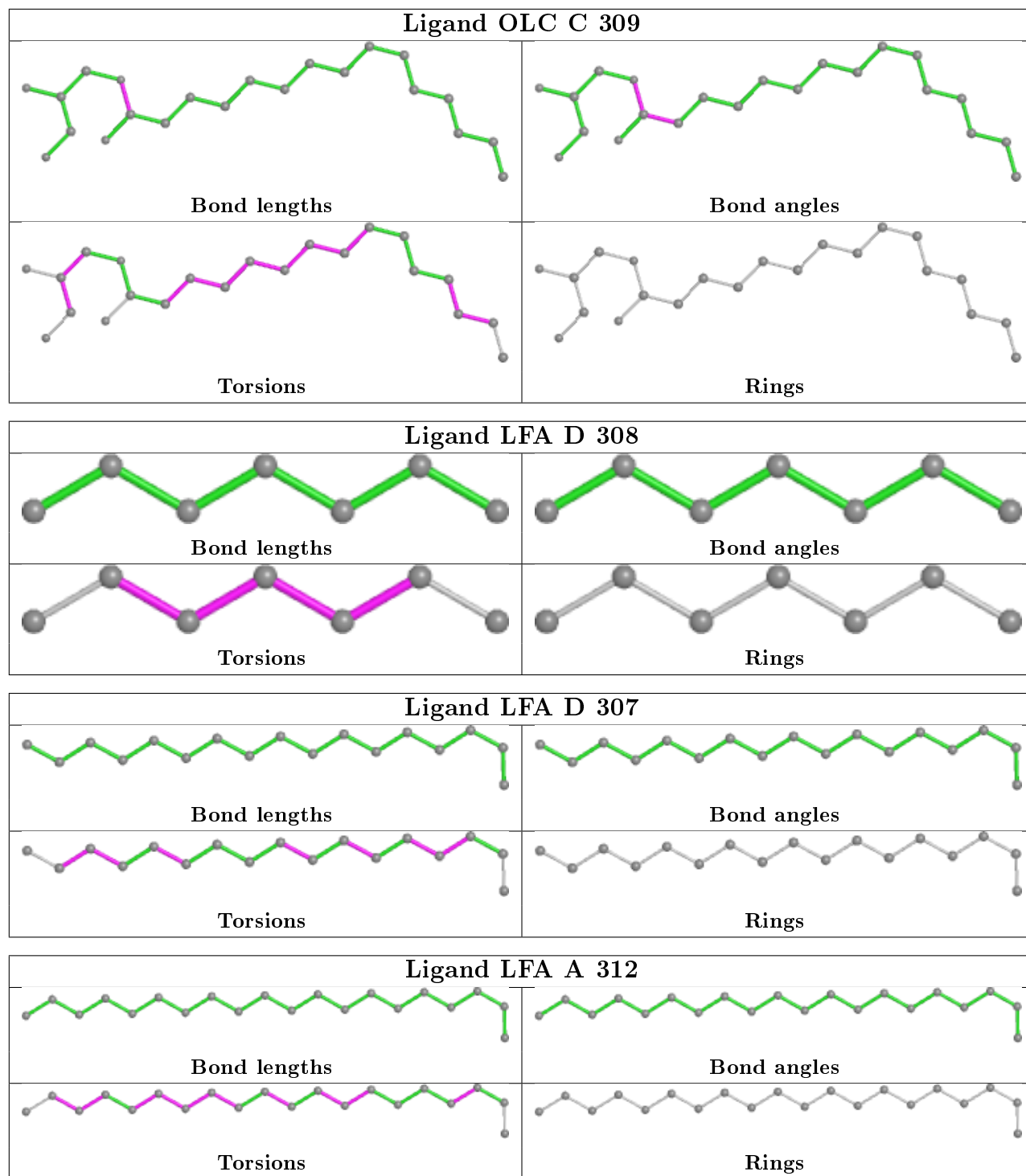


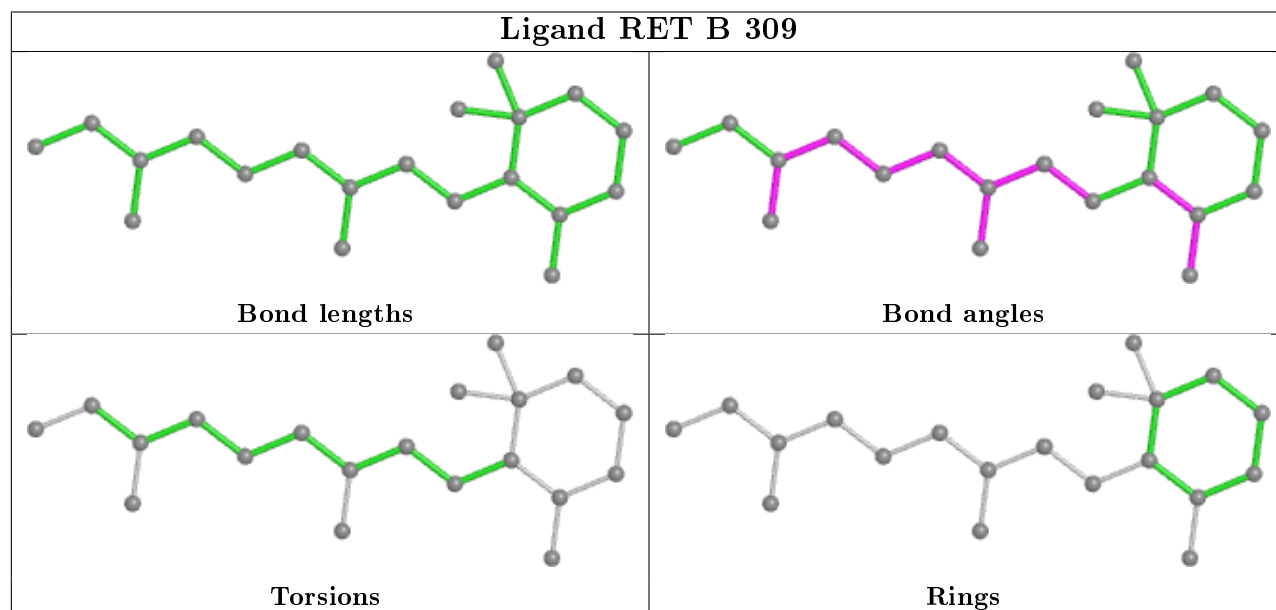
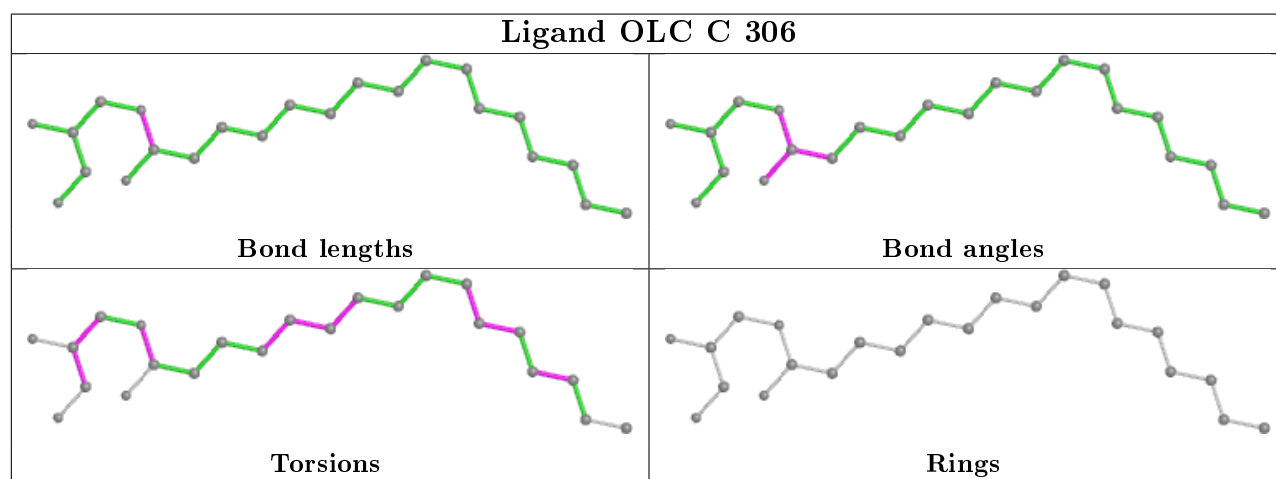
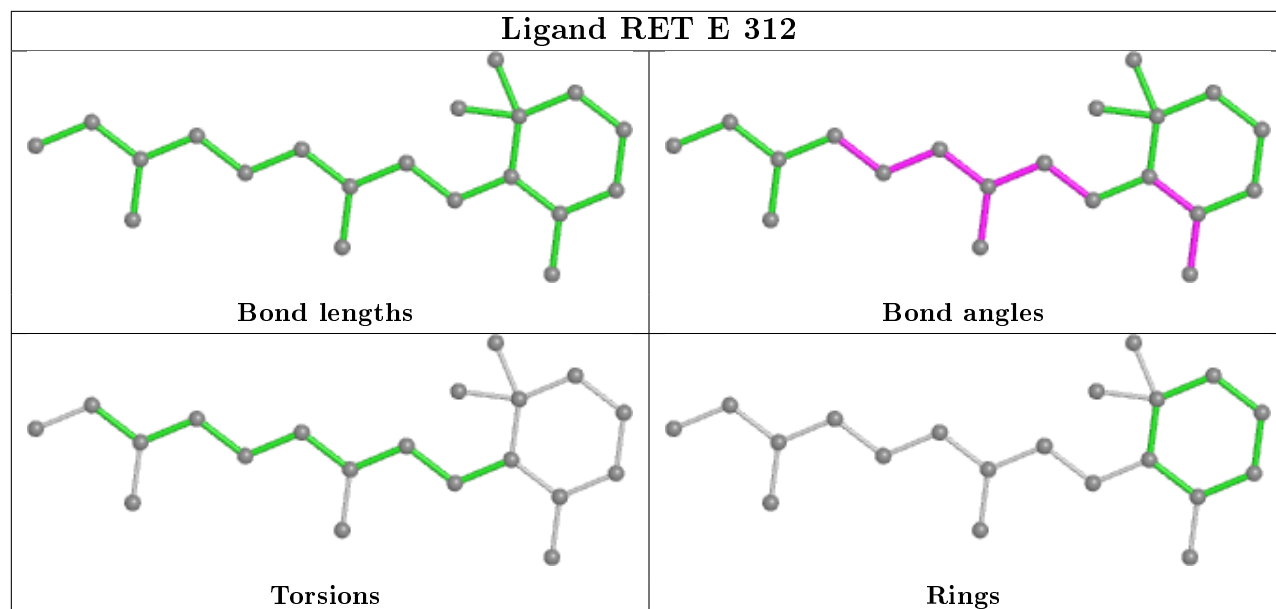


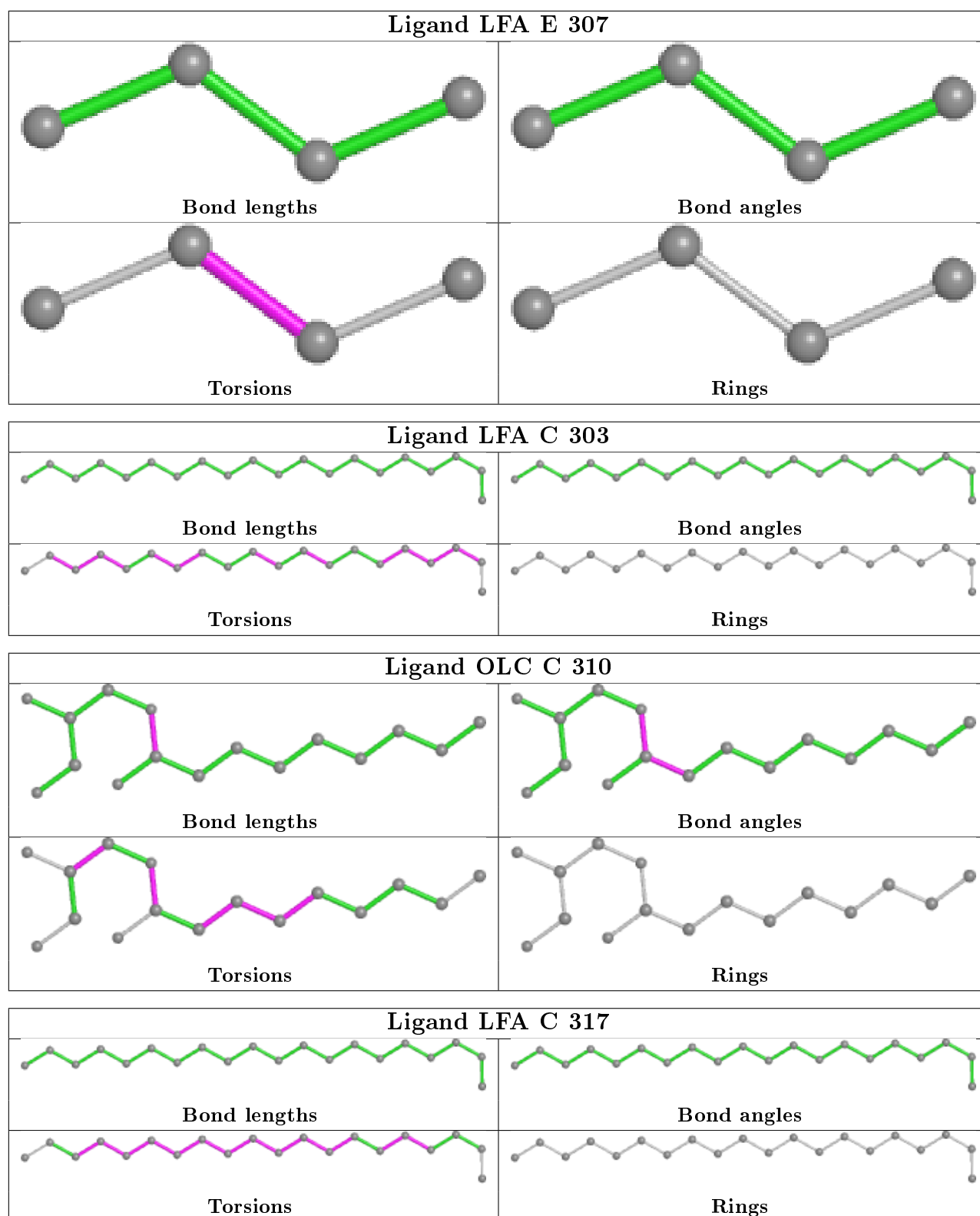


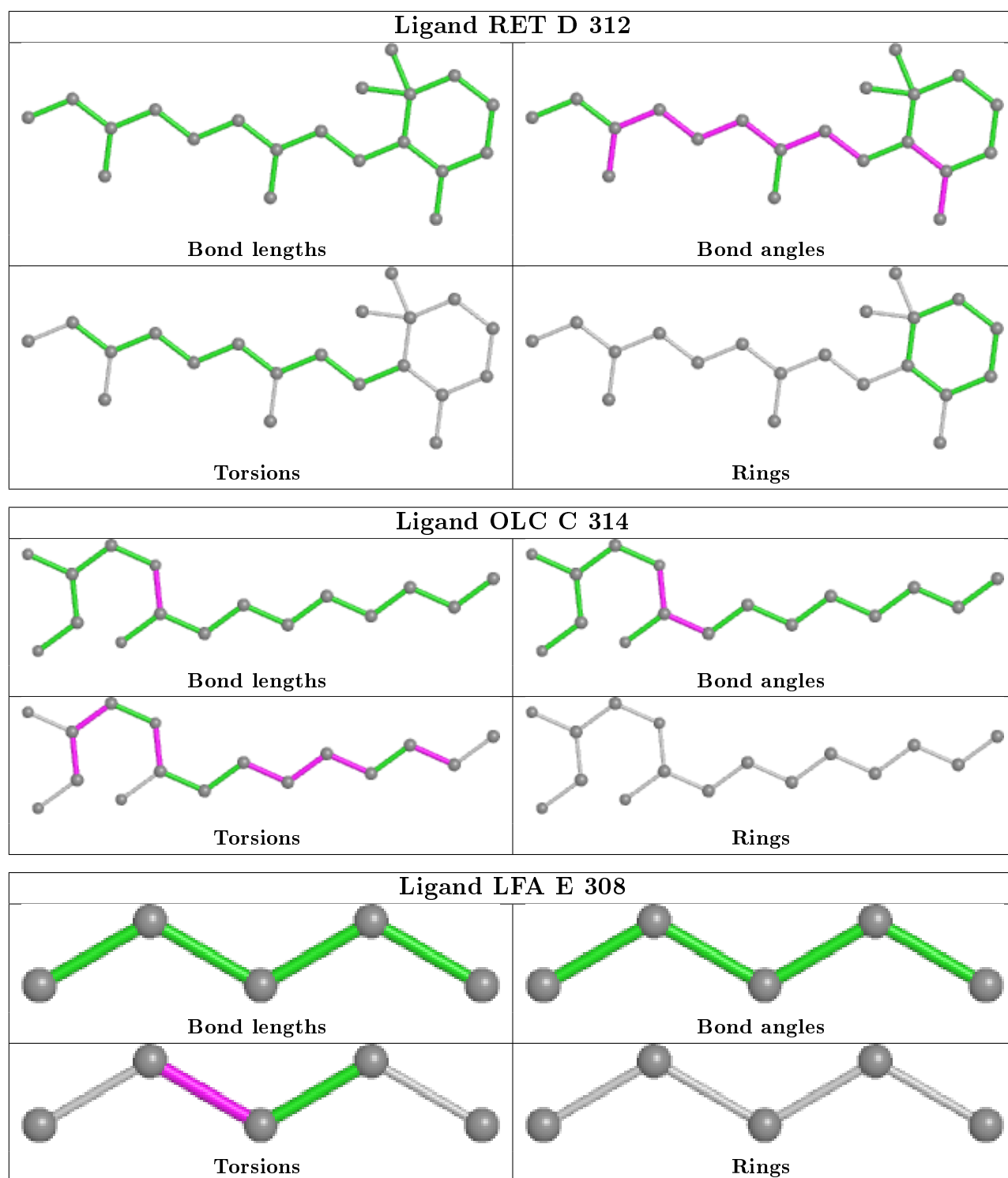


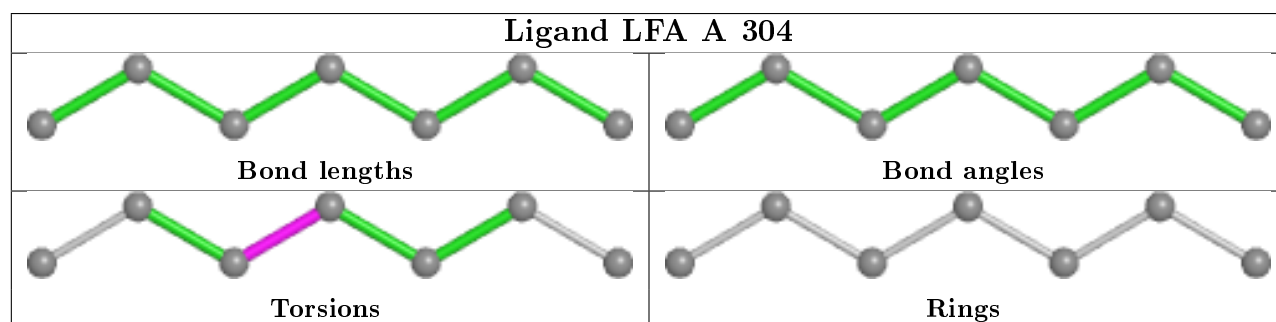
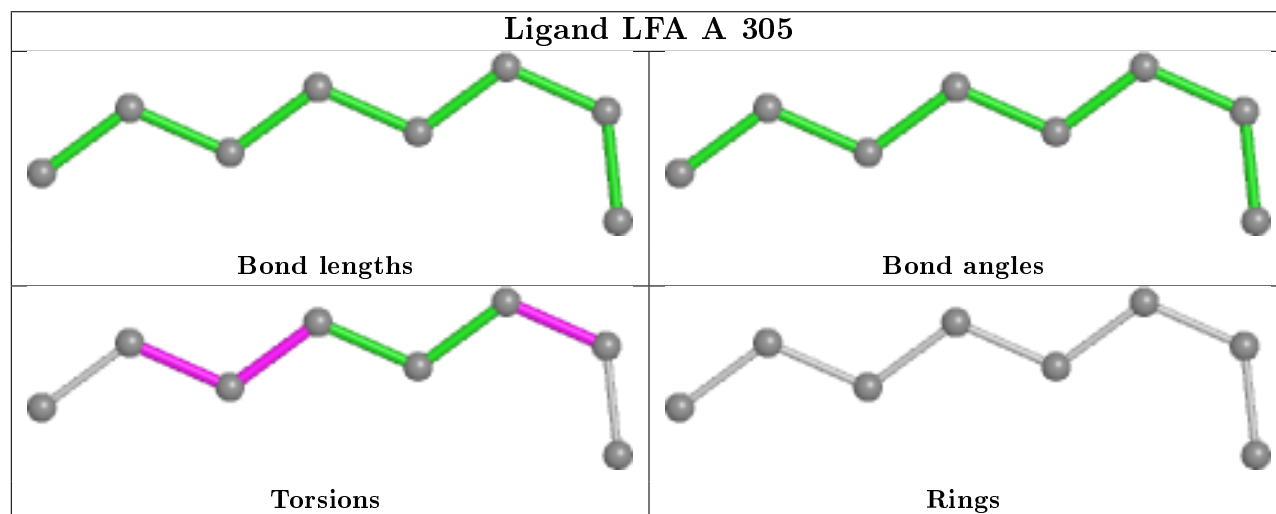
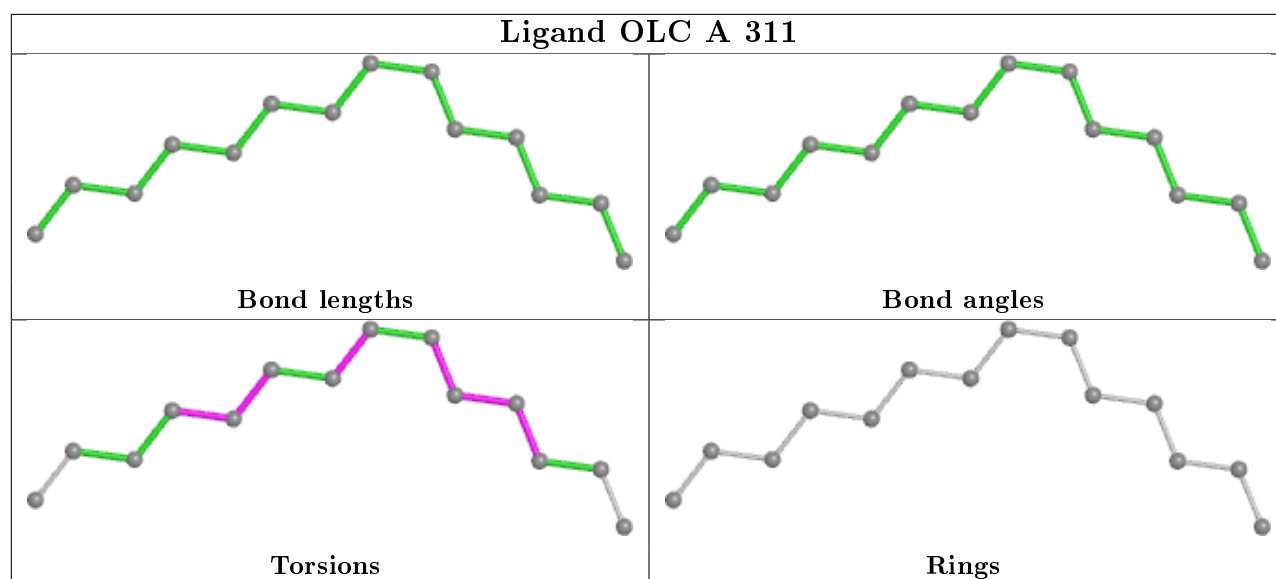




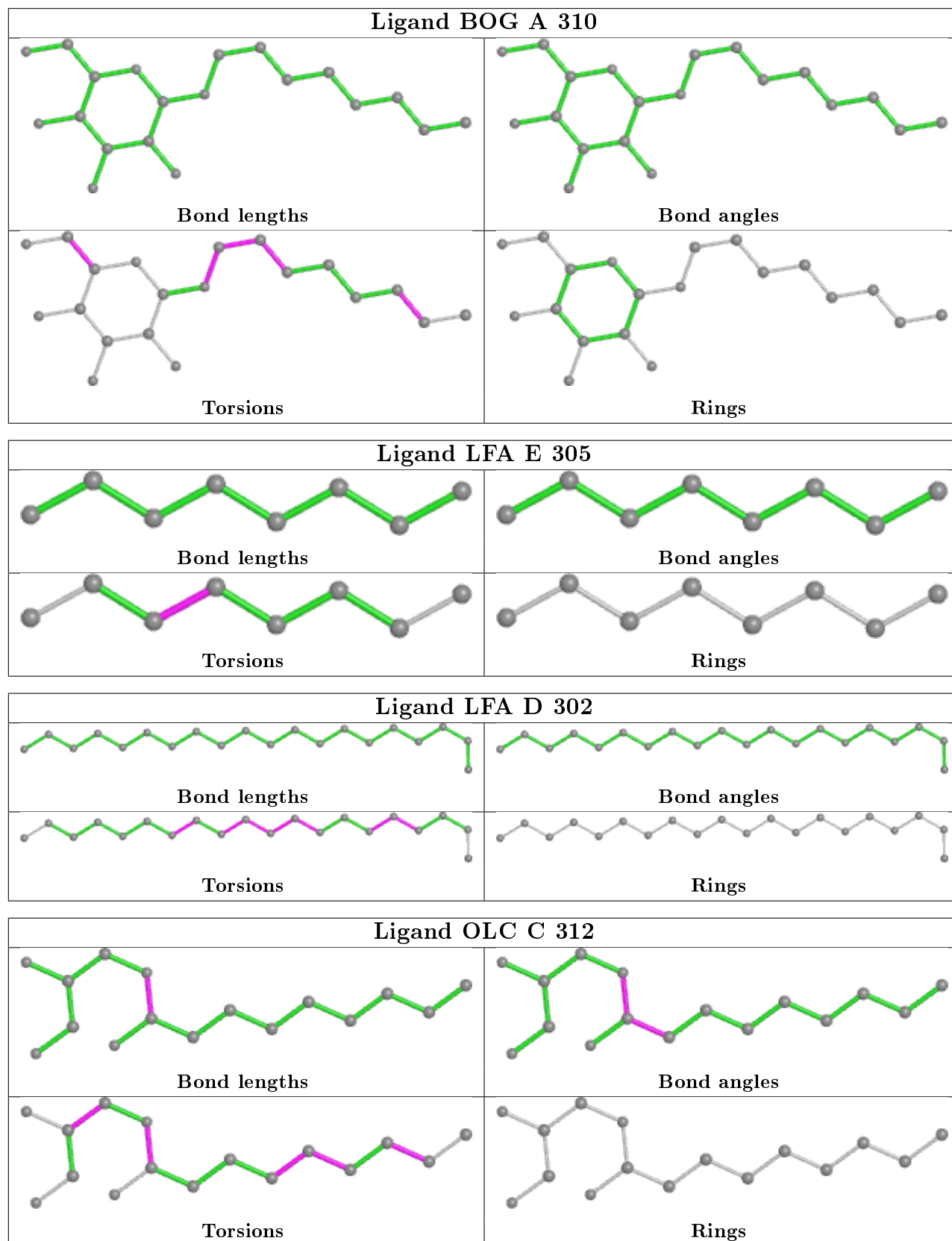


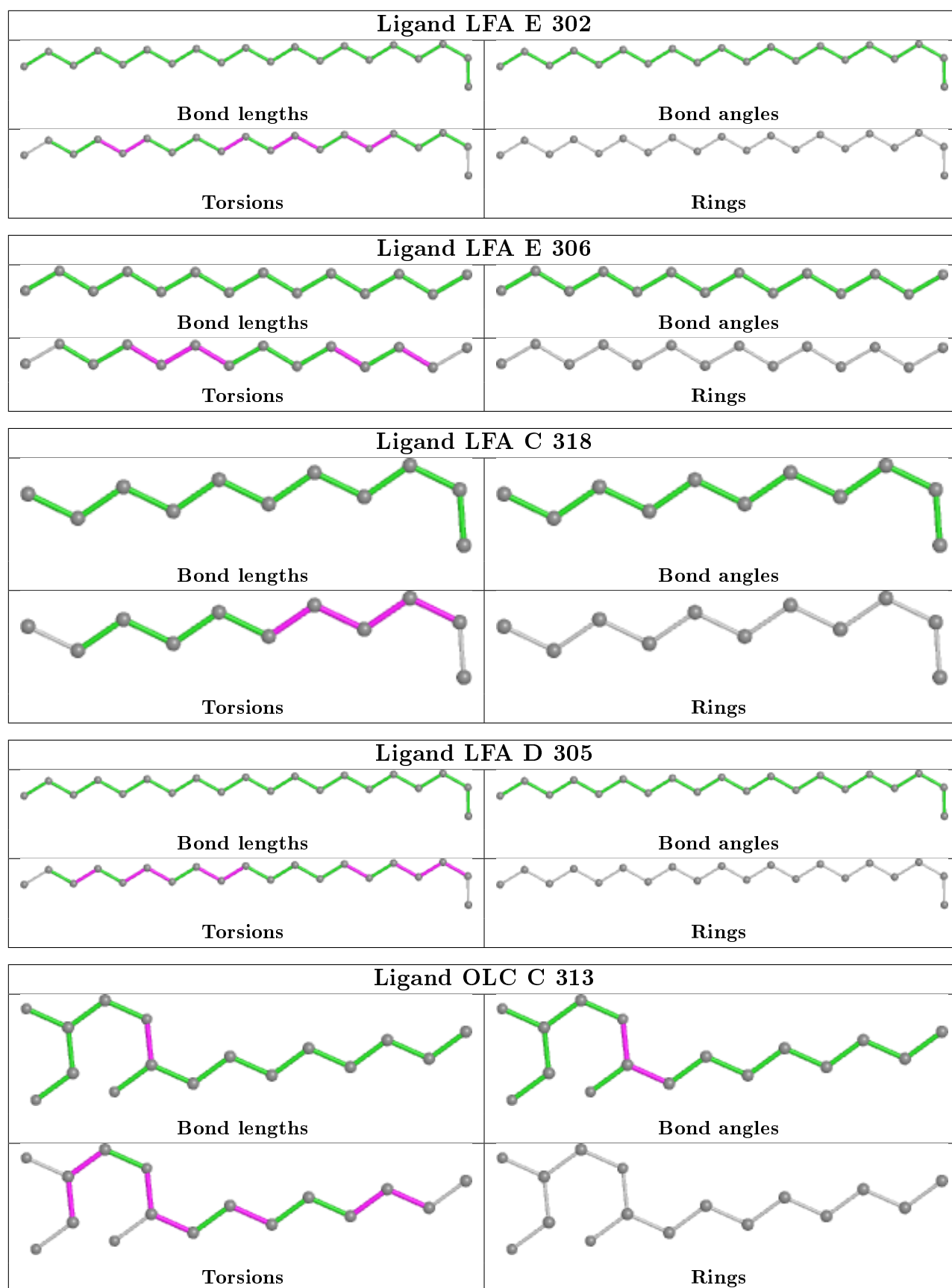


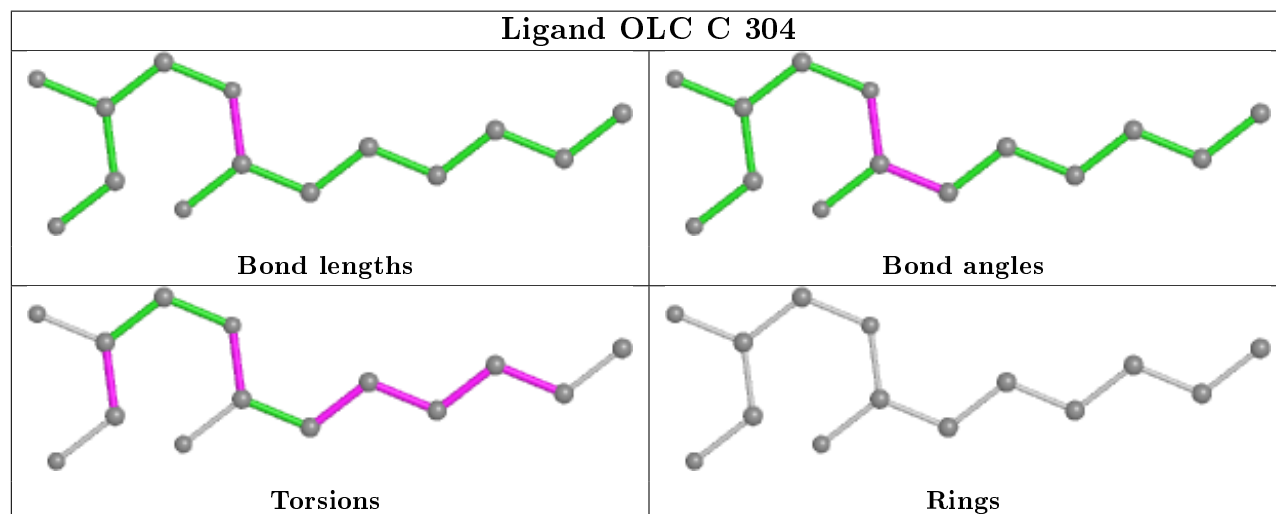
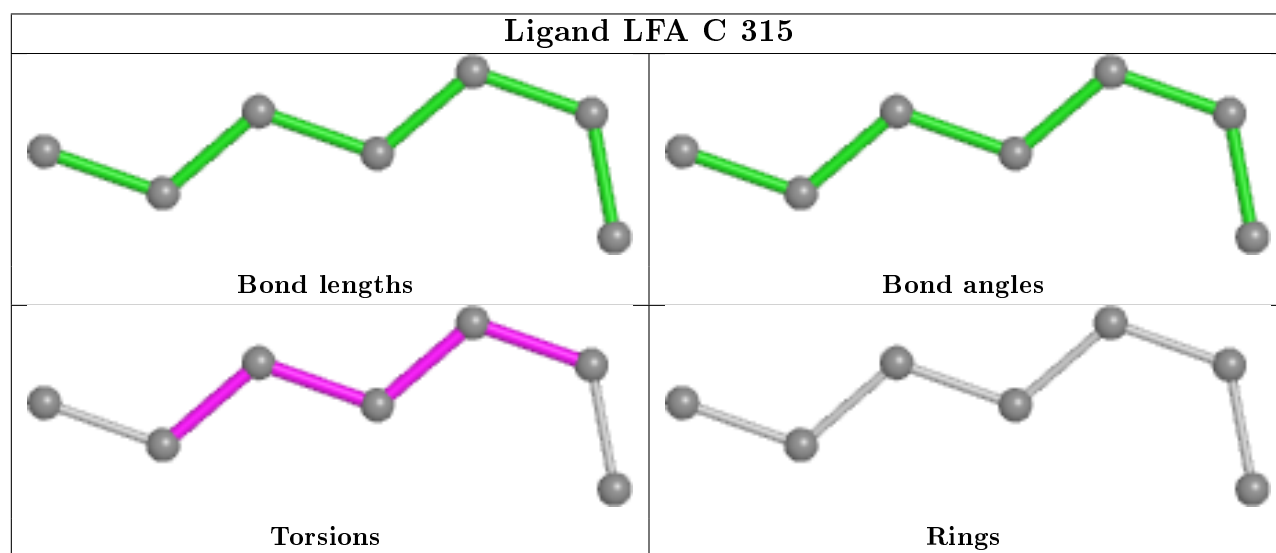
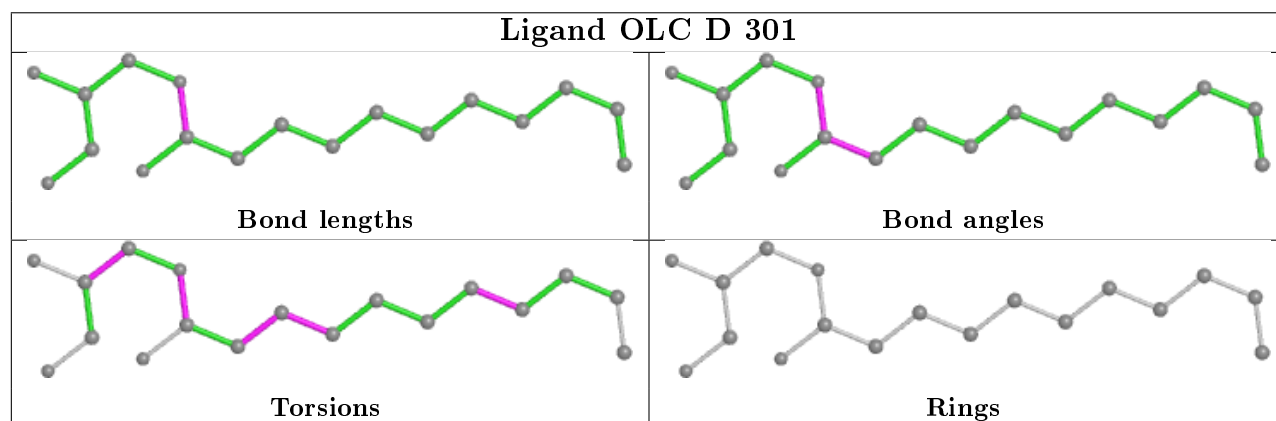
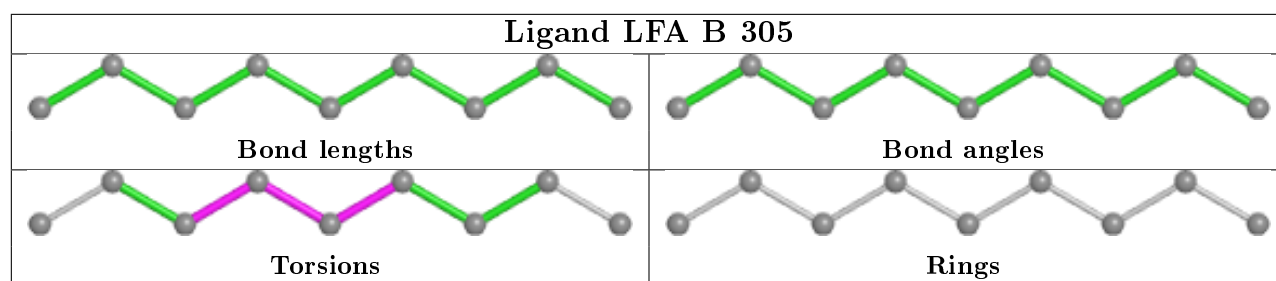


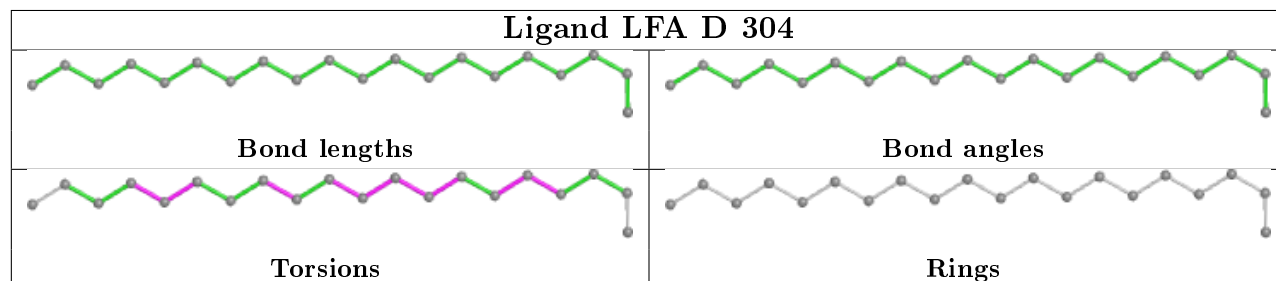
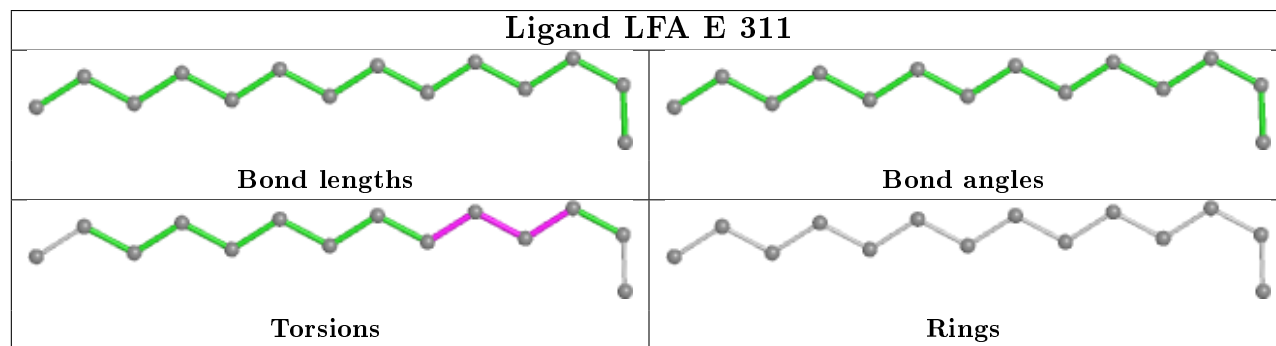
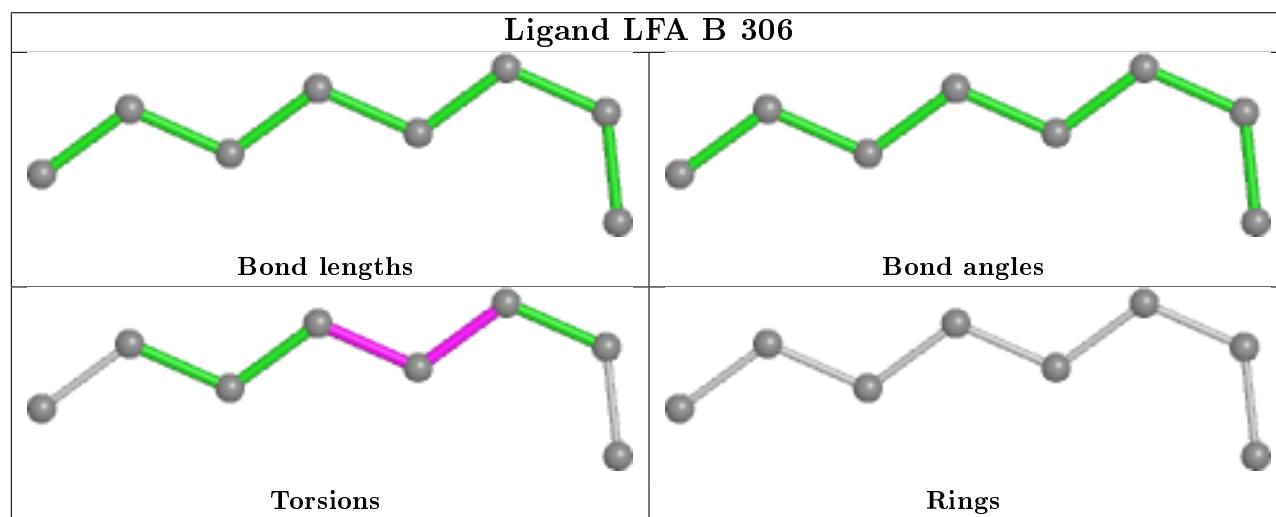
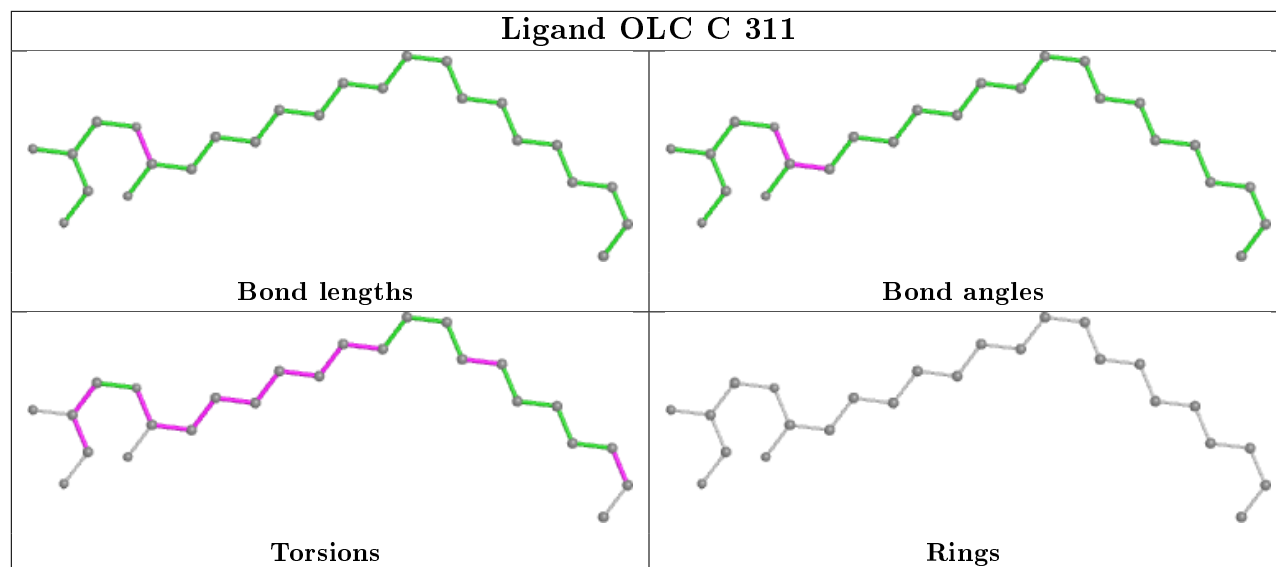


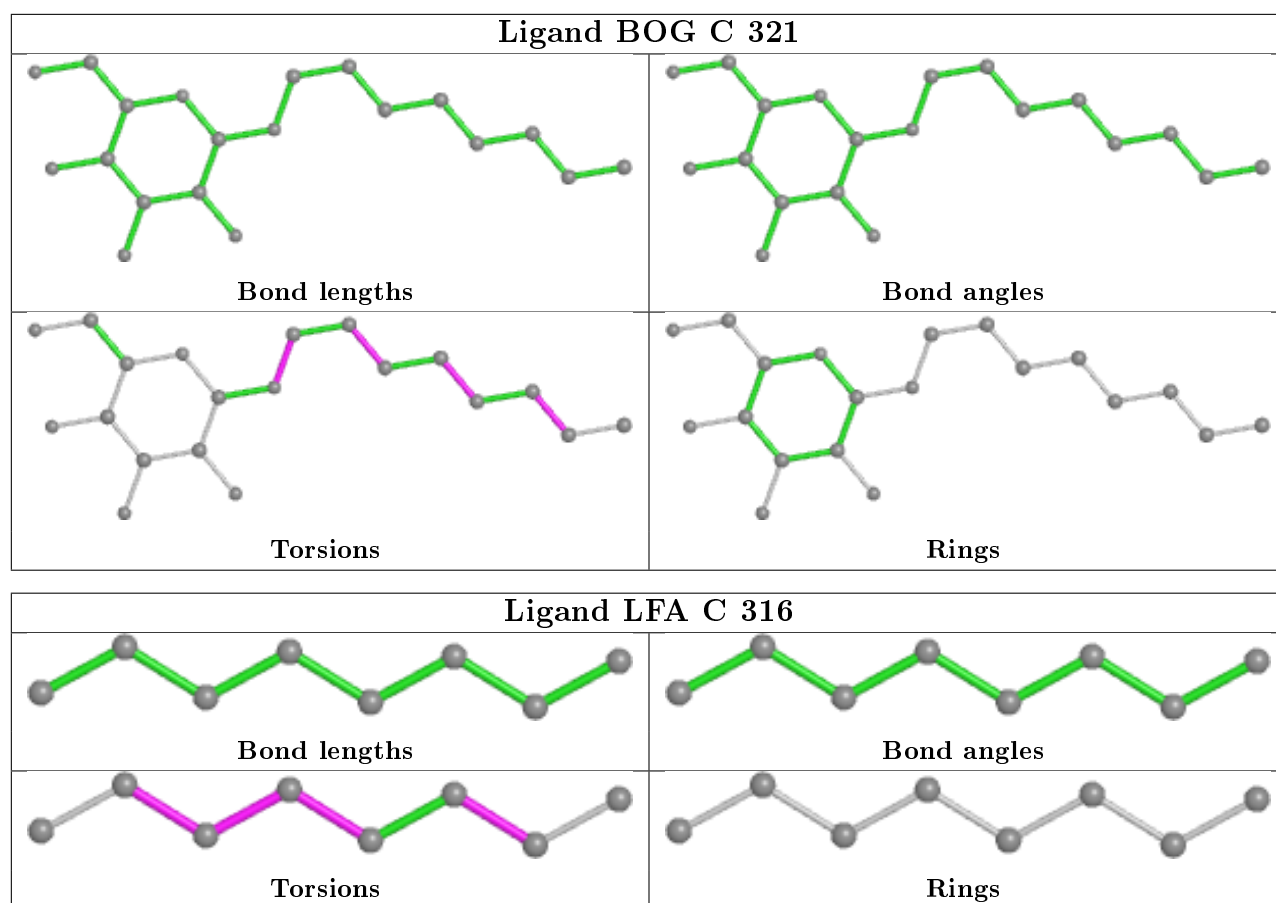












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	273/288 (94%)	-0.07	20 (7%) 15 13	37, 48, 73, 154	0
1	B	273/288 (94%)	-0.16	10 (3%) 41 41	36, 48, 69, 139	0
1	C	273/288 (94%)	-0.01	13 (4%) 30 29	36, 48, 71, 152	0
1	D	273/288 (94%)	0.10	18 (6%) 18 17	36, 50, 75, 164	0
1	E	273/288 (94%)	-0.08	13 (4%) 30 29	38, 48, 71, 169	0
All	All	1365/1440 (94%)	-0.04	74 (5%) 25 24	36, 48, 73, 169	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	274	GLU	16.1
1	E	275	LEU	10.4
1	D	275	LEU	9.7
1	A	275	LEU	8.3
1	E	273	LYS	7.6
1	A	274	GLU	6.9
1	B	275	LEU	6.9
1	B	273	LYS	6.8
1	D	273	LYS	6.5
1	A	272	ASN	6.5
1	C	274	GLU	5.9
1	C	273	LYS	5.8
1	B	272	ASN	5.6
1	C	275	LEU	5.5
1	A	273	LYS	5.3
1	B	274	GLU	5.3
1	B	3	GLN	5.1
1	D	272	ASN	4.8
1	D	131	THR	4.8
1	C	272	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	195	GLY	4.4
1	D	274	GLU	4.2
1	D	194	GLU	4.1
1	D	271	LYS	4.1
1	E	272	ASN	3.9
1	B	271	LYS	3.8
1	E	270	SER	3.8
1	C	230	VAL	3.8
1	D	130	LEU	3.7
1	D	230	VAL	3.6
1	A	271	LYS	3.6
1	E	194	GLU	3.5
1	B	230	VAL	3.5
1	D	132	THR	3.5
1	C	195	GLY	3.5
1	E	3	GLN	3.3
1	D	129	SER	3.2
1	C	196	ILE	3.1
1	A	270	SER	3.1
1	C	130	LEU	3.0
1	A	198	PRO	2.9
1	E	54	ASP	2.9
1	D	3	GLN	2.9
1	E	4	GLU	2.9
1	C	132	THR	2.8
1	D	54	ASP	2.8
1	B	54	ASP	2.6
1	C	271	LYS	2.6
1	A	57	PHE	2.5
1	C	3	GLN	2.5
1	A	233	PHE	2.5
1	E	230	VAL	2.4
1	A	55	LYS	2.4
1	A	194	GLU	2.4
1	D	133	SER	2.4
1	E	271	LYS	2.3
1	D	196	ILE	2.3
1	A	195	GLY	2.3
1	A	3	GLN	2.3
1	A	92	VAL	2.2
1	A	54	ASP	2.2
1	A	199	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	132	THR	2.2
1	B	270	SER	2.2
1	A	132	THR	2.2
1	C	270	SER	2.2
1	E	200	GLY	2.1
1	A	230	VAL	2.1
1	A	269	LEU	2.1
1	C	129	SER	2.1
1	D	17	THR	2.0
1	A	196	ILE	2.0
1	B	231	ASP	2.0
1	D	134	LYS	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	C	310	16/25	0.44	0.39	91,111,137,138	0
2	OLC	C	304	14/25	0.52	0.37	95,118,144,157	0
3	LFA	A	307	12/20	0.58	0.39	89,102,110,113	0
2	OLC	C	311	25/25	0.60	0.43	87,111,133,135	0
3	LFA	C	318	11/20	0.61	0.34	65,99,118,118	0
2	OLC	C	314	16/25	0.61	0.41	79,100,117,128	0
2	OLC	C	309	22/25	0.64	0.38	60,90,121,126	0
3	LFA	C	315	7/20	0.65	0.20	75,94,106,109	0
3	LFA	B	305	9/20	0.67	0.28	82,90,110,112	0
3	LFA	A	305	8/20	0.67	0.25	77,87,92,94	0
2	OLC	C	305	21/25	0.67	0.35	90,116,139,140	0

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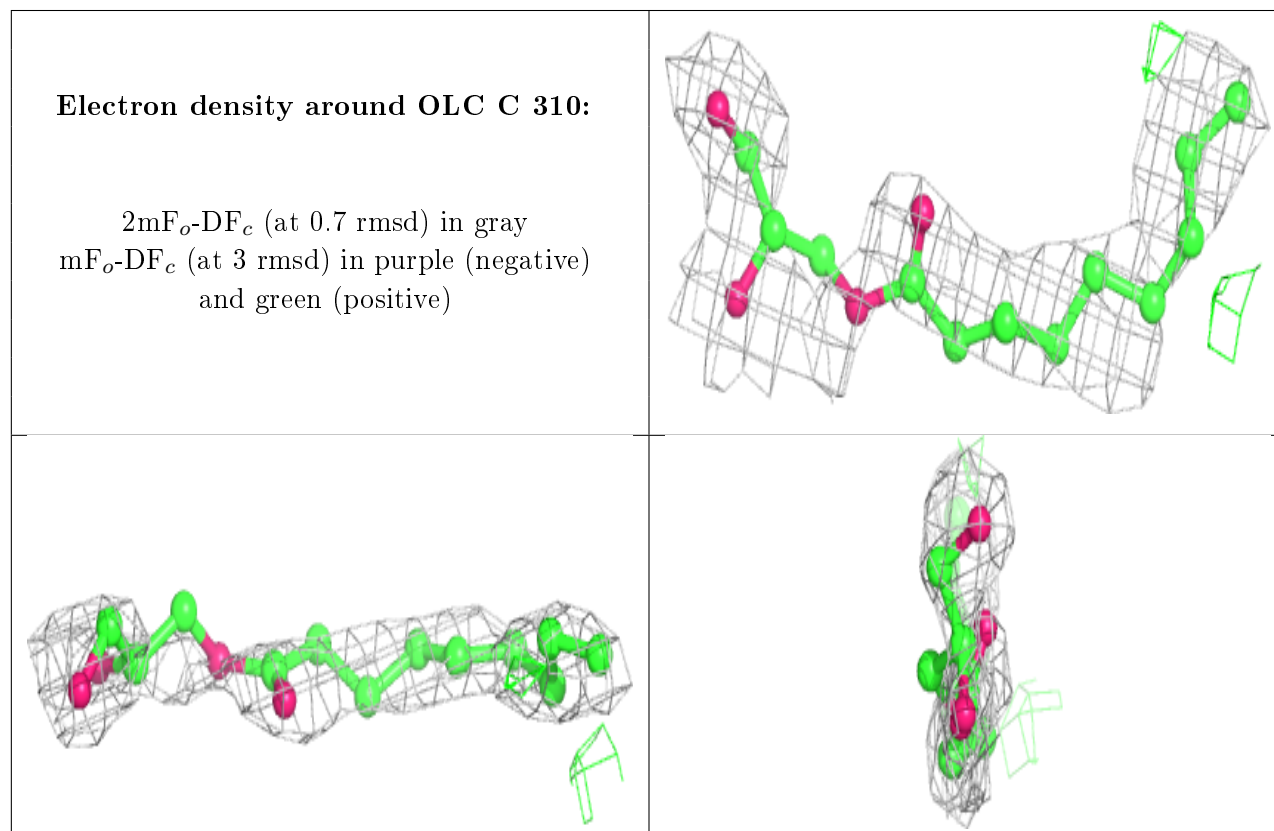
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LFA	D	308	7/20	0.71	0.44	74,89,98,102	0
3	LFA	C	322	4/20	0.72	1.23	72,76,78,80	0
3	LFA	C	316	8/20	0.73	0.37	76,89,94,97	0
3	LFA	E	305	8/20	0.74	0.23	80,86,90,92	0
5	BOG	B	308	20/20	0.74	0.43	80,101,109,114	0
3	LFA	D	304	20/20	0.74	0.24	81,102,113,115	0
5	BOG	A	310	20/20	0.74	0.46	81,101,112,115	0
3	LFA	E	302	20/20	0.75	0.74	61,81,101,101	0
2	OLC	C	307	25/25	0.75	0.33	74,104,118,129	0
2	OLC	C	313	16/25	0.76	0.21	58,99,118,123	0
5	BOG	E	310	20/20	0.76	0.47	71,98,112,112	0
3	LFA	D	309	6/20	0.77	0.34	80,90,93,94	0
3	LFA	D	305	20/20	0.78	0.25	83,103,113,115	0
3	LFA	E	306	14/20	0.78	0.25	73,95,106,109	0
3	LFA	A	306	8/20	0.78	0.29	70,93,119,125	0
3	LFA	C	317	20/20	0.79	0.21	73,92,103,108	0
2	OLC	B	303	20/25	0.80	0.19	69,87,106,107	0
3	LFA	B	306	8/20	0.80	0.30	76,86,100,105	0
3	LFA	A	312	20/20	0.80	0.68	64,80,91,95	0
3	LFA	D	306	8/20	0.81	0.27	81,95,117,120	0
2	OLC	C	308	25/25	0.82	0.26	67,101,124,139	0
3	LFA	D	302	20/20	0.82	0.63	54,69,89,89	0
3	LFA	E	307	4/20	0.82	0.13	67,72,78,78	0
3	LFA	C	303	20/20	0.82	0.62	59,77,86,88	0
3	LFA	A	304	7/20	0.82	0.32	79,84,94,99	0
5	BOG	D	311	20/20	0.82	0.45	75,96,104,105	0
3	LFA	B	302	20/20	0.83	0.65	60,77,100,103	0
2	OLC	C	306	23/25	0.83	0.35	59,73,107,144	0
5	BOG	C	321	20/20	0.83	0.43	71,88,104,105	0
3	LFA	E	308	5/20	0.83	0.34	78,90,101,103	0
2	OLC	A	311	14/25	0.84	0.46	67,82,92,92	0
2	OLC	A	302	13/25	0.86	0.22	67,74,85,88	0
2	OLC	C	302	20/25	0.87	0.20	71,91,100,101	0
3	LFA	A	308	6/20	0.87	0.22	68,71,79,86	0
2	OLC	E	304	25/25	0.88	0.21	55,96,127,129	0
3	LFA	C	319	4/20	0.89	0.27	78,78,78,87	0
2	OLC	A	303	15/25	0.89	0.17	64,83,106,117	0
2	OLC	B	301	22/25	0.89	0.16	76,85,104,111	0
2	OLC	C	312	16/25	0.90	0.25	62,83,96,101	0
2	OLC	C	301	21/25	0.90	0.25	55,72,89,104	0
2	OLC	A	301	14/25	0.90	0.28	54,64,73,73	0
2	OLC	E	303	16/25	0.90	0.42	56,64,80,83	0

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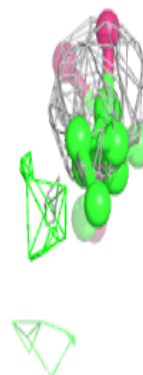
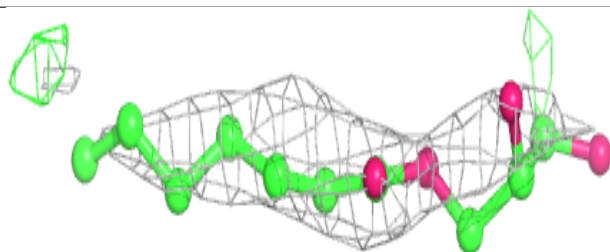
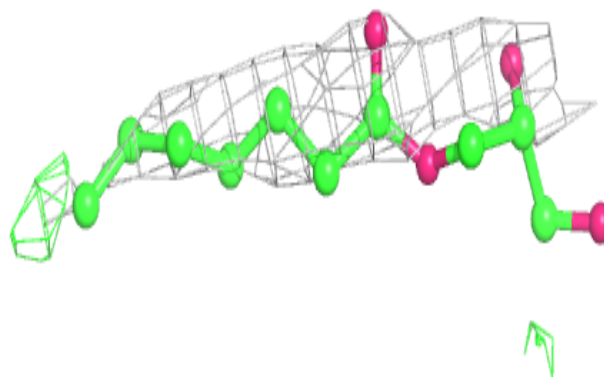
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLC	E	301	12/25	0.91	0.45	65,76,88,92	0
2	OLC	D	301	18/25	0.91	0.31	79,91,107,119	0
3	LFA	E	311	14/20	0.91	0.86	102,117,127,133	0
2	OLC	B	304	16/25	0.92	0.21	66,89,96,108	0
2	OLC	D	303	14/25	0.93	0.18	61,82,100,102	0
6	RET	B	309	20/21	0.94	0.14	40,45,50,52	0
6	RET	C	323	20/21	0.94	0.14	42,49,55,56	0
3	LFA	D	307	17/20	0.95	0.50	56,65,77,77	0
6	RET	D	312	20/21	0.95	0.14	44,52,59,64	0
6	RET	A	313	20/21	0.95	0.12	37,47,51,52	0
4	NA	E	309	1/1	0.96	0.04	38,38,38,38	0
4	NA	D	310	1/1	0.96	0.06	46,46,46,46	0
4	NA	A	309	1/1	0.97	0.09	47,47,47,47	0
6	RET	E	312	20/21	0.97	0.12	37,44,48,49	0
4	NA	C	320	1/1	0.99	0.04	40,40,40,40	0
4	NA	B	307	1/1	0.99	0.07	41,41,41,41	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.

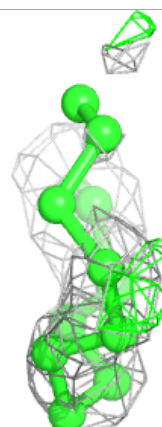
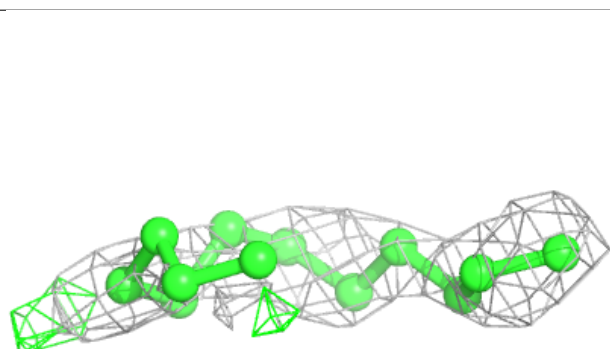
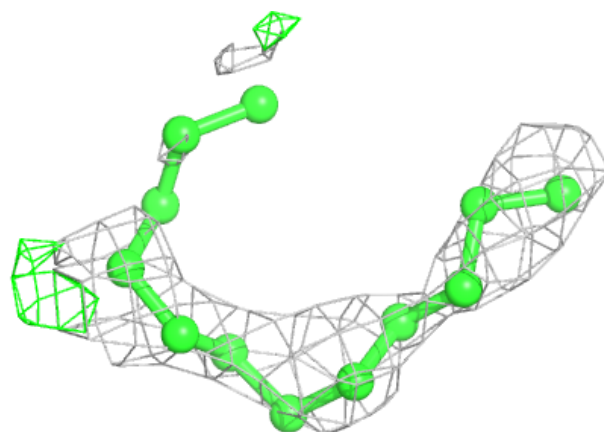


**Electron density around OLC C 304:**

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

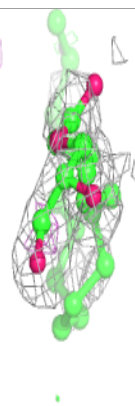
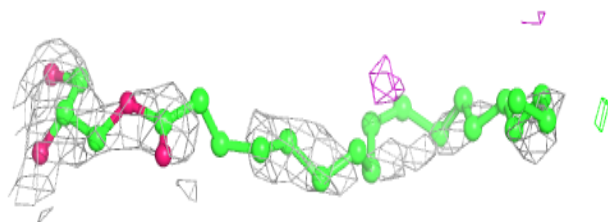
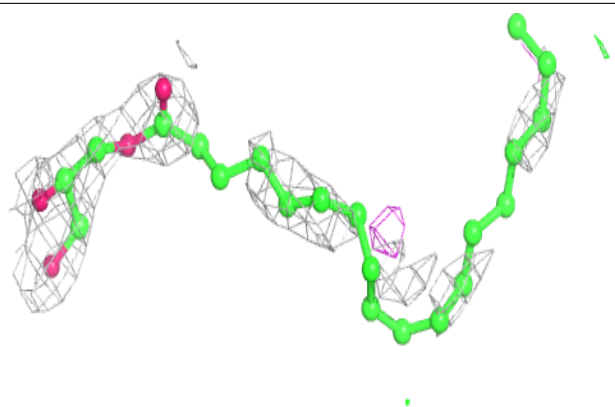
**Electron density around LFA A 307:**

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

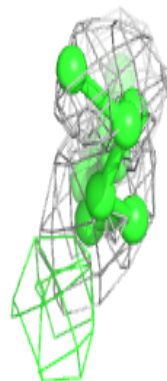
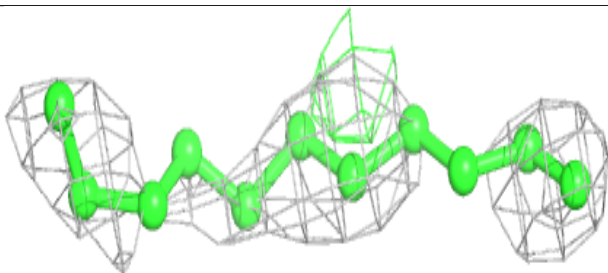
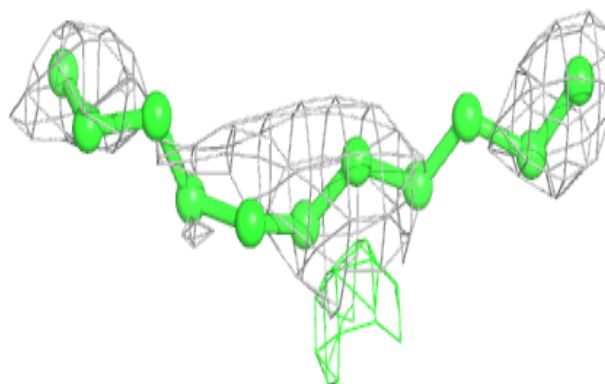


**Electron density around OLC C 311:**

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

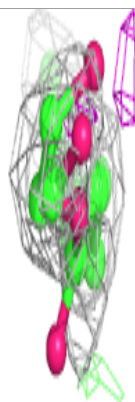
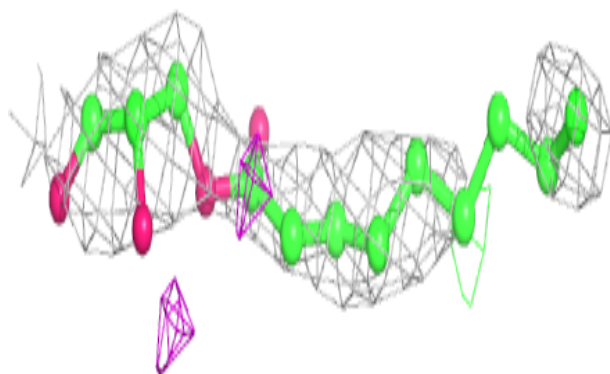
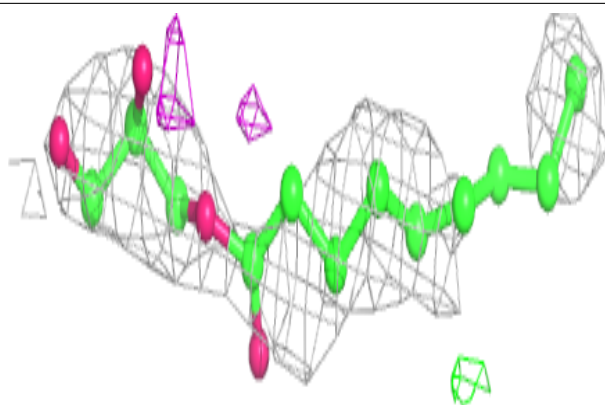
**Electron density around LFA C 318:**

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

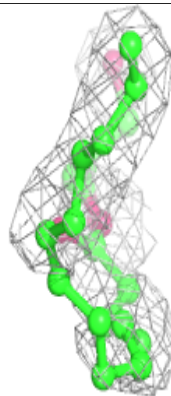
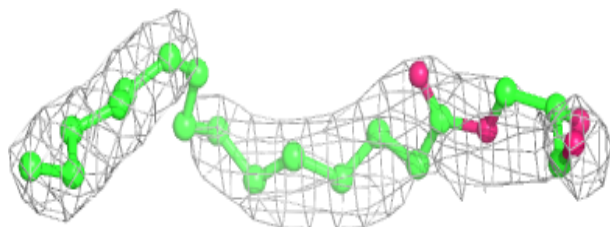
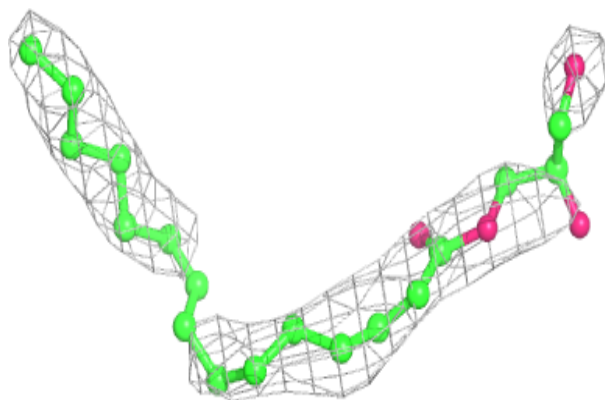


**Electron density around OLC C 314:**

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

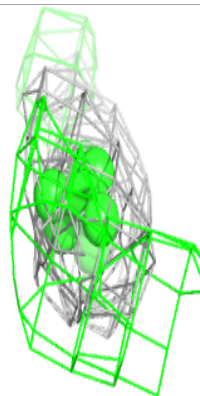
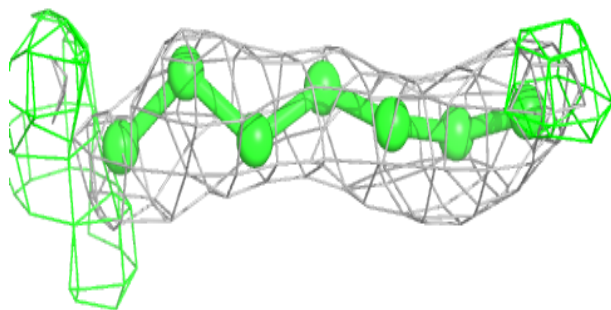
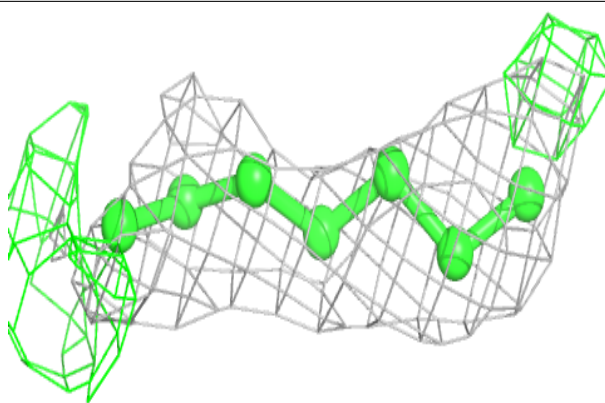
**Electron density around OLC C 309:**

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

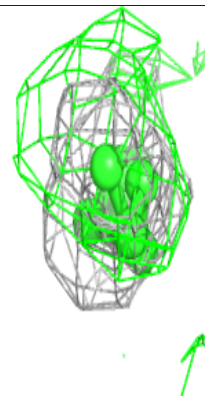
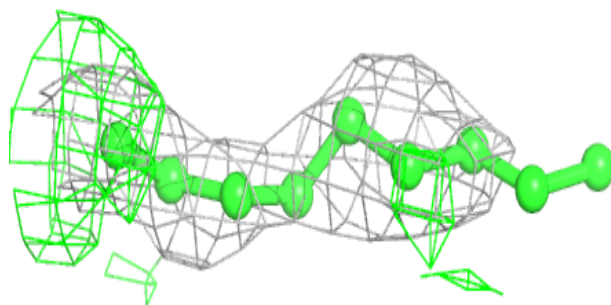
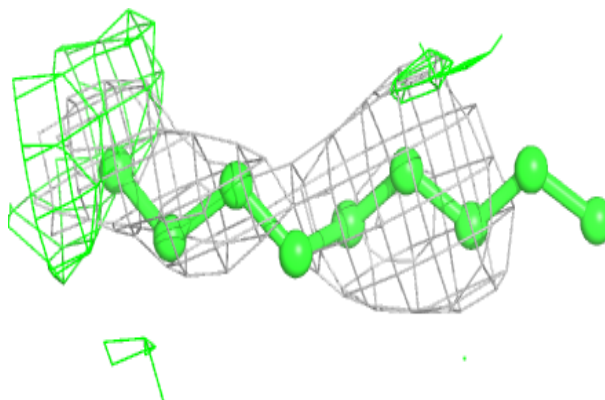


**Electron density around LFA C 315:**

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

**Electron density around LFA B 305:**

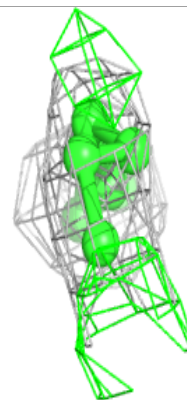
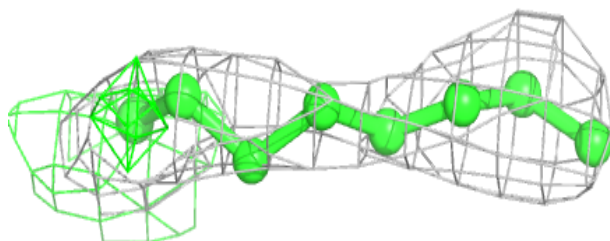
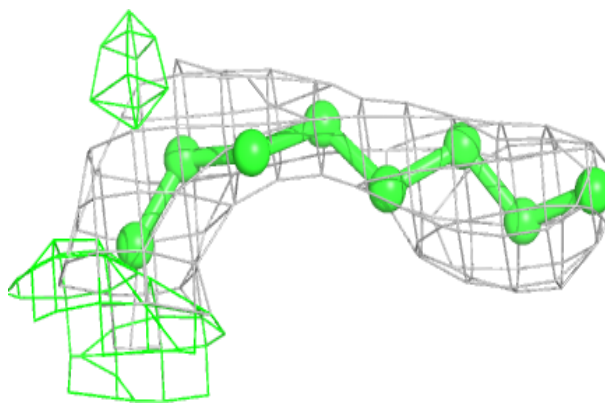
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



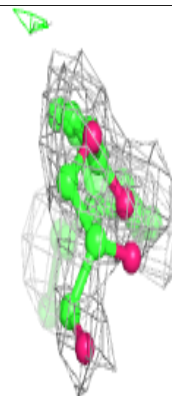
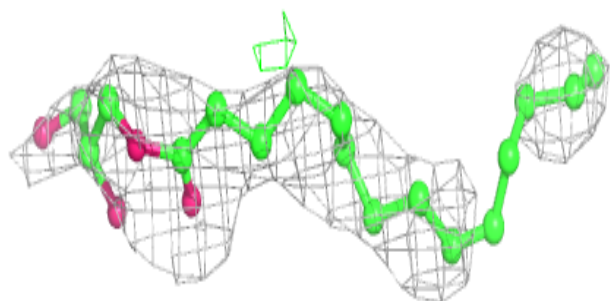
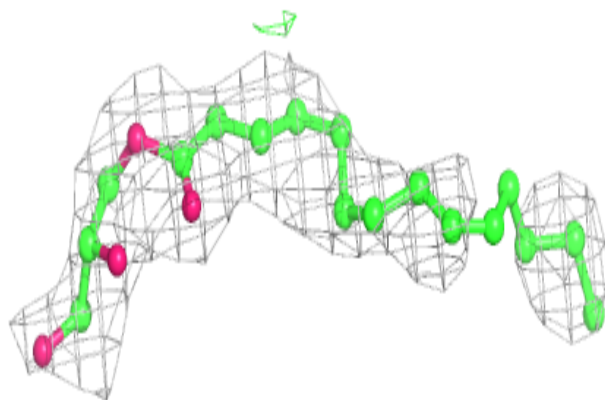


**Electron density around LFA A 305:**

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

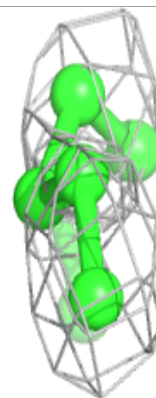
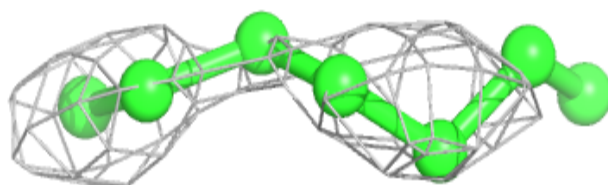
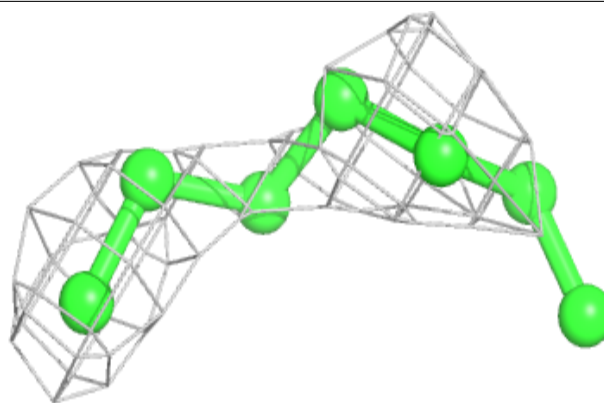
**Electron density around OLC C 305:**

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

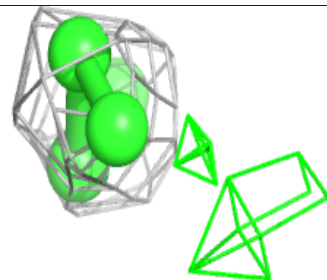
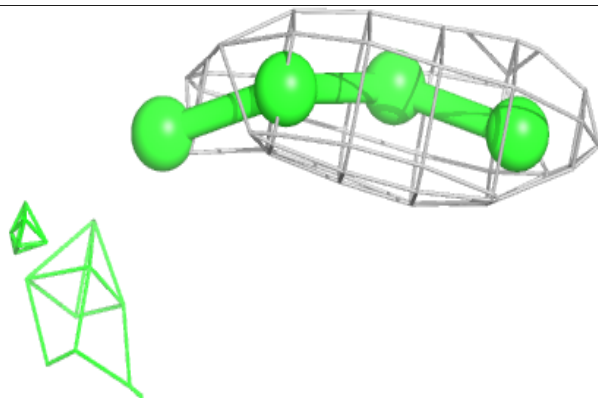
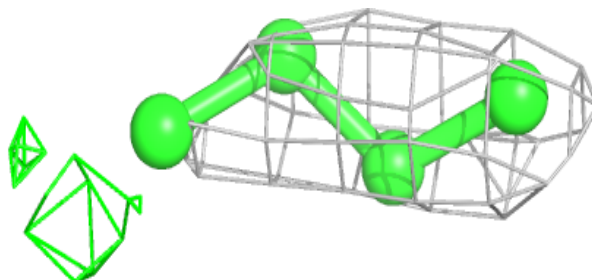


**Electron density around LFA D 308:**

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

**Electron density around LFA C 322:**

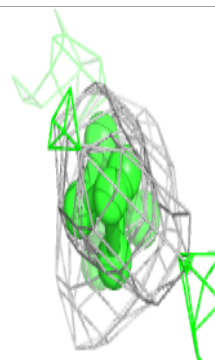
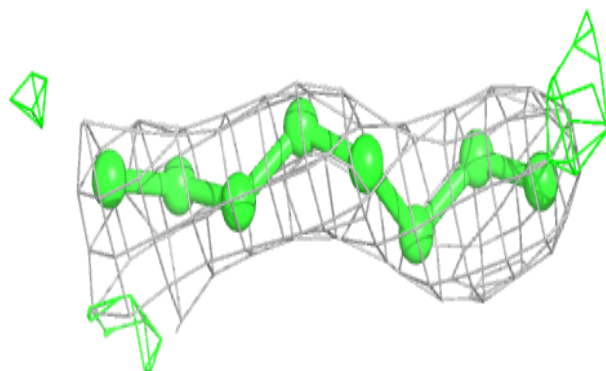
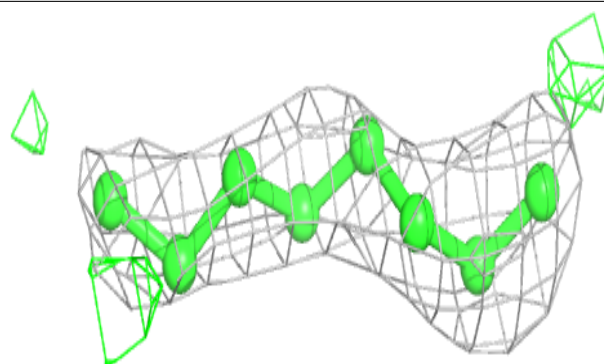
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



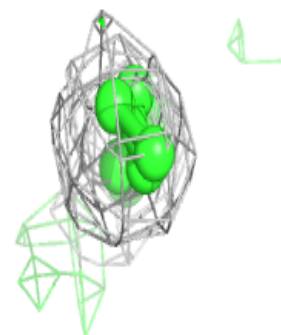
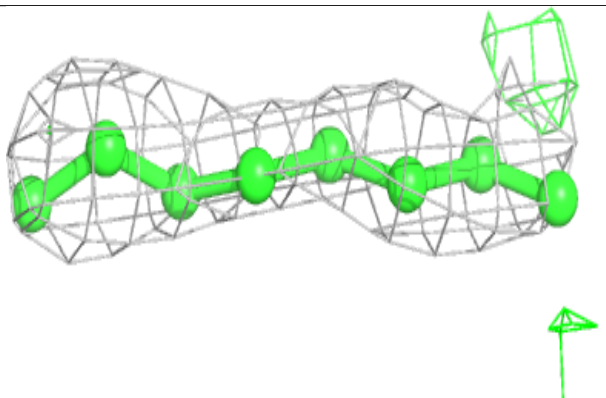
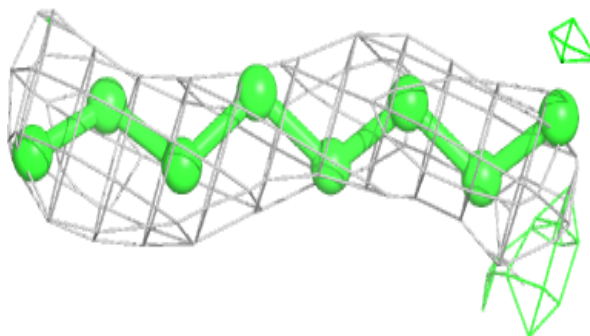


**Electron density around LFA C 316:**

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

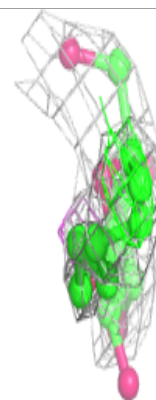
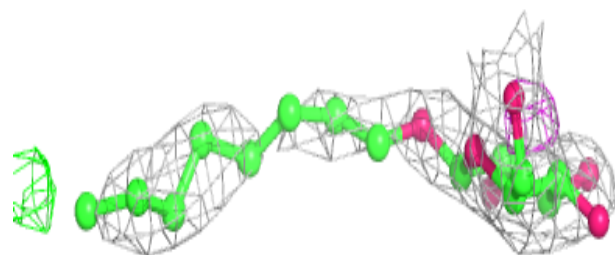
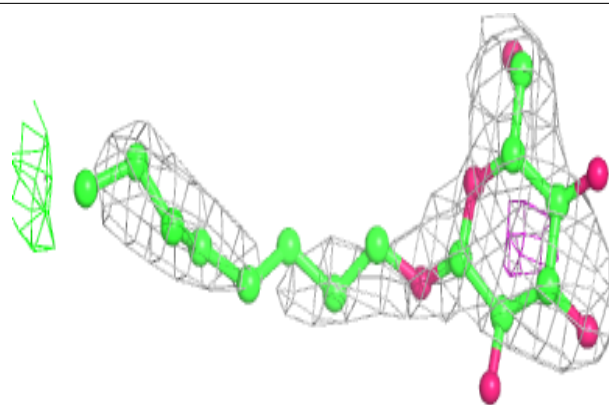
**Electron density around LFA E 305:**

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

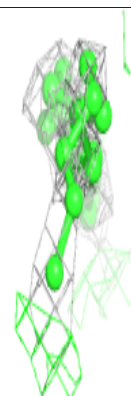
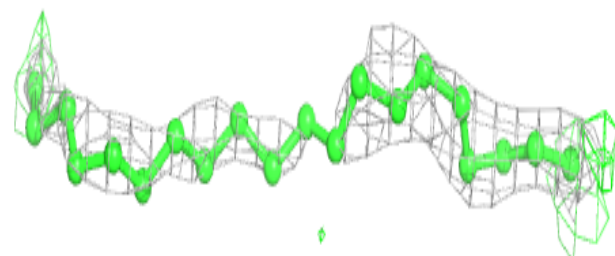
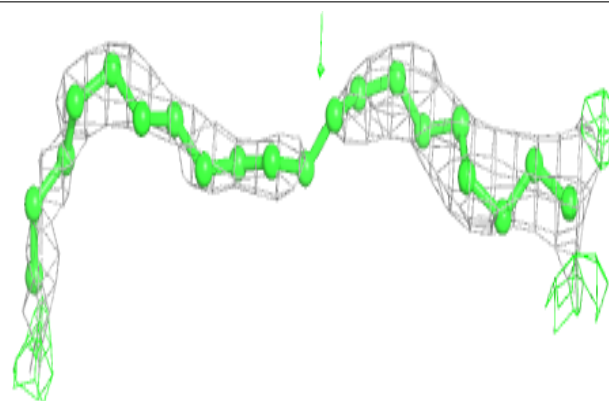


**Electron density around BOG B 308:**

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

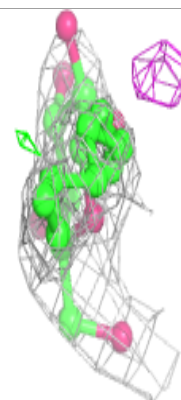
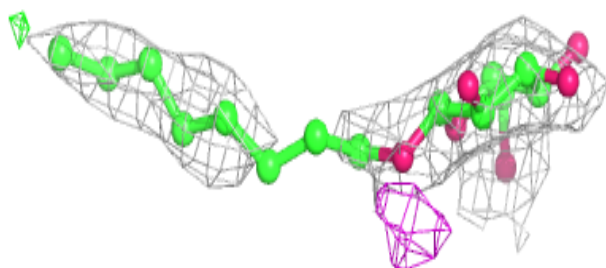
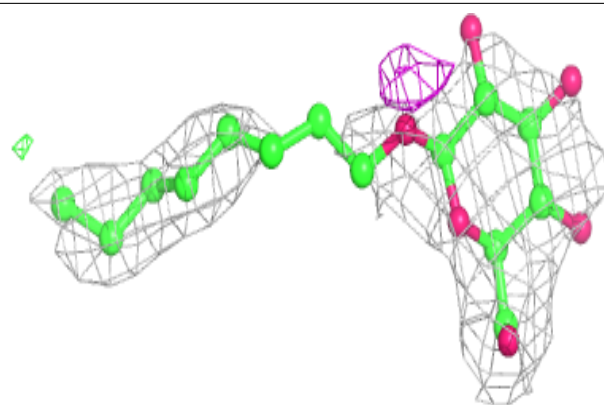
**Electron density around LFA D 304:**

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

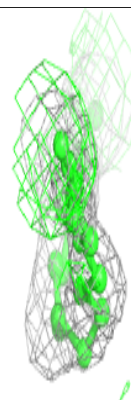
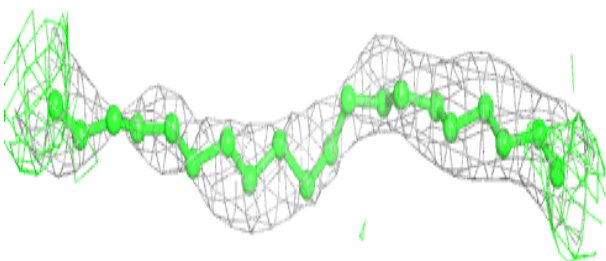
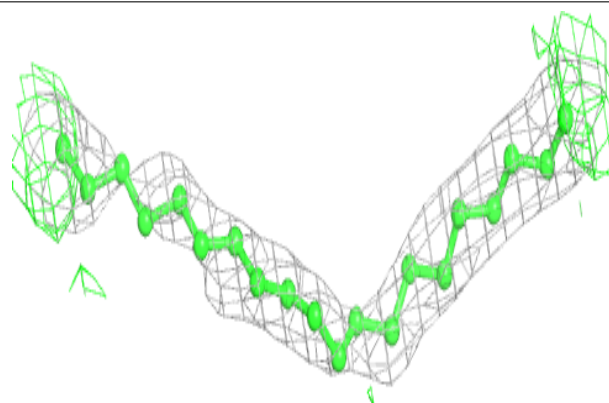


**Electron density around BOG A 310:**

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

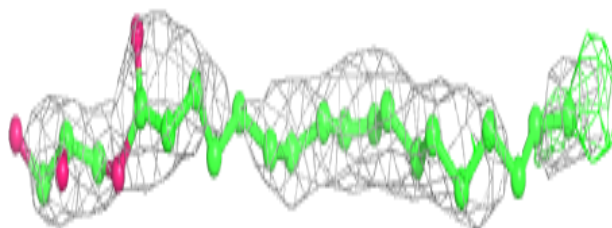
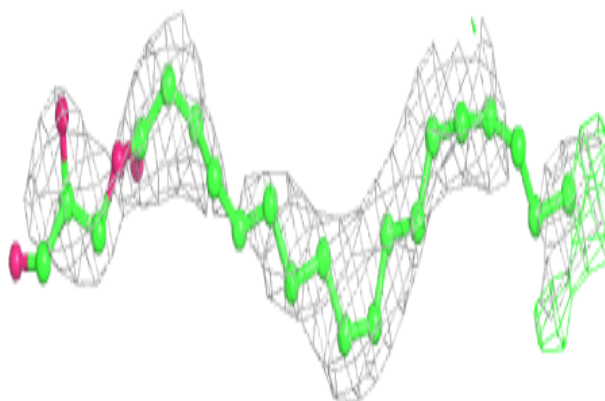
**Electron density around LFA E 302:**

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

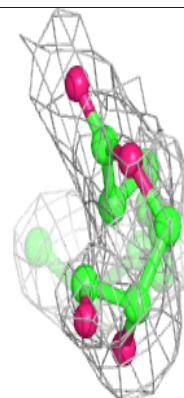
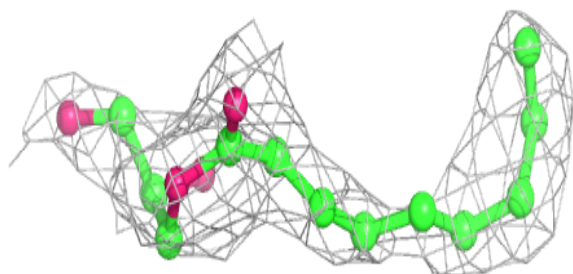
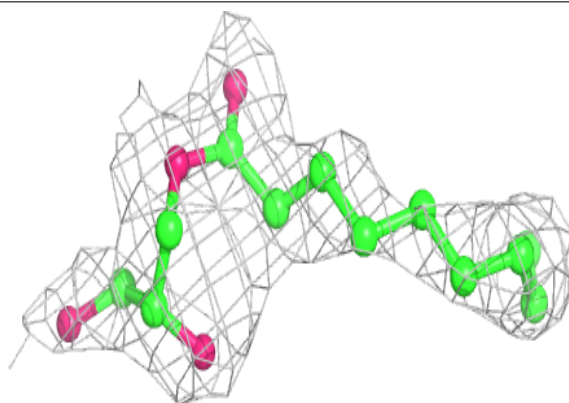


**Electron density around OLC C 307:**

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

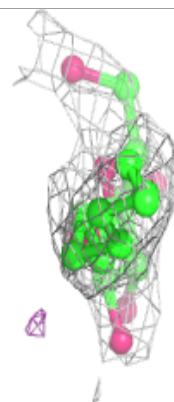
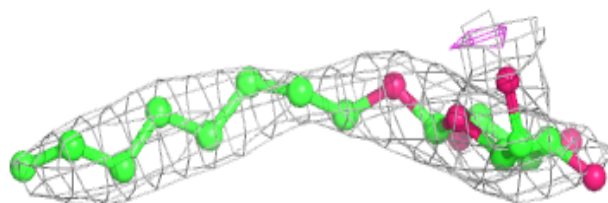
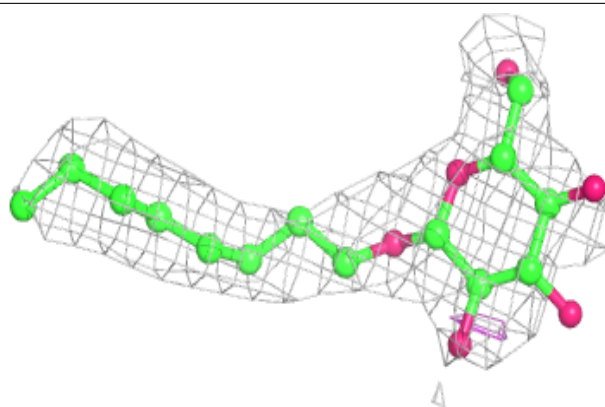
**Electron density around OLC C 313:**

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

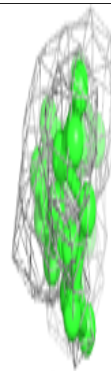
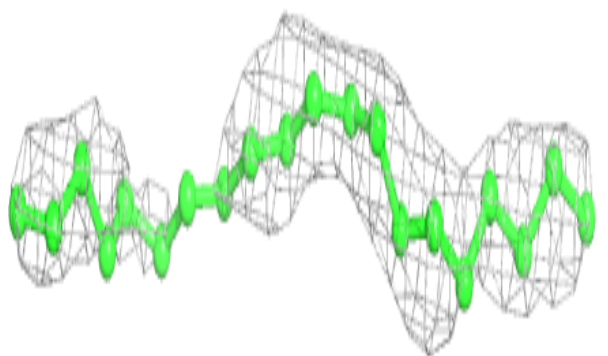
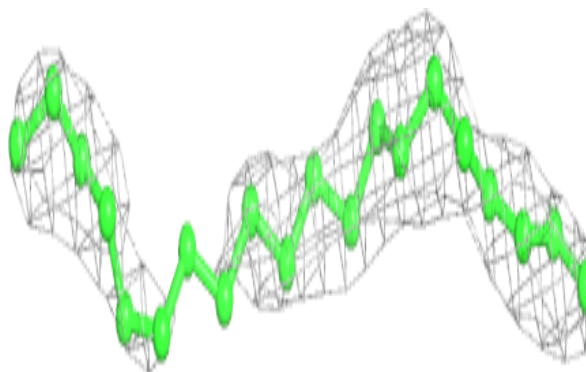


**Electron density around BOG E 310:**

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

**Electron density around LFA D 305:**

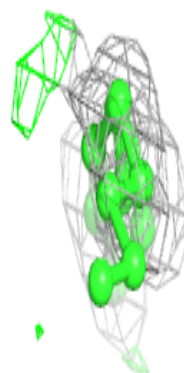
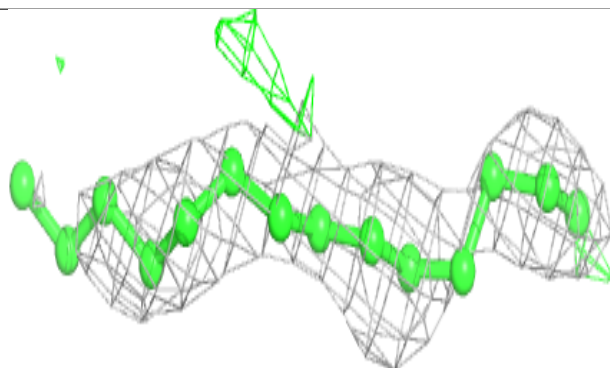
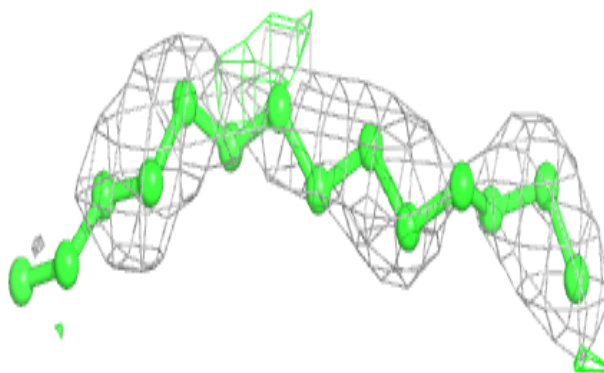
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



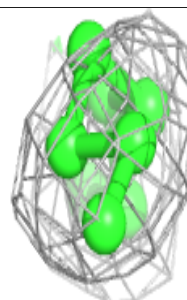
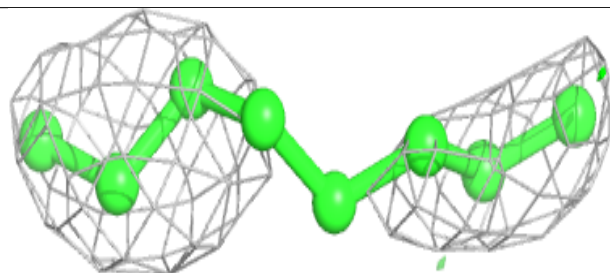
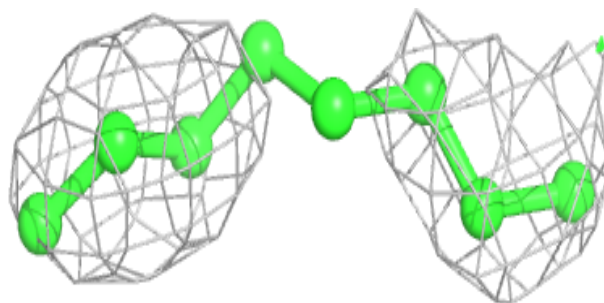


**Electron density around LFA E 306:**

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

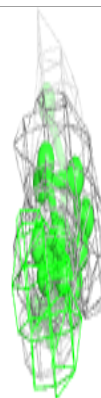
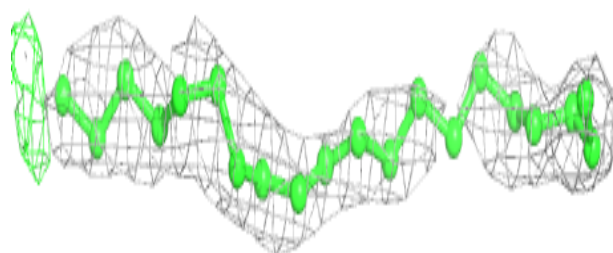
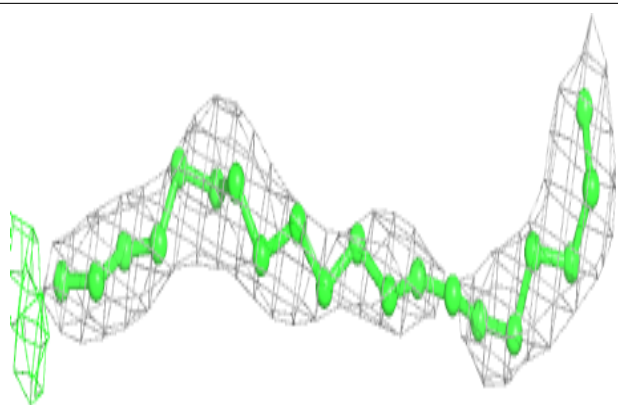
**Electron density around LFA A 306:**

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

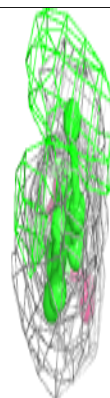
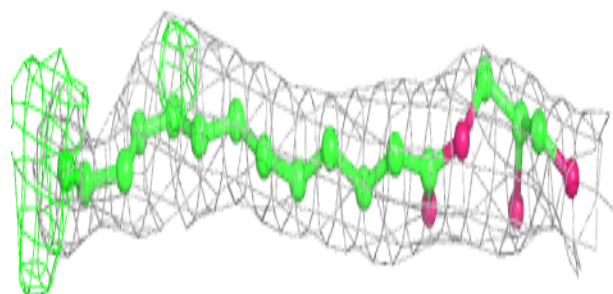
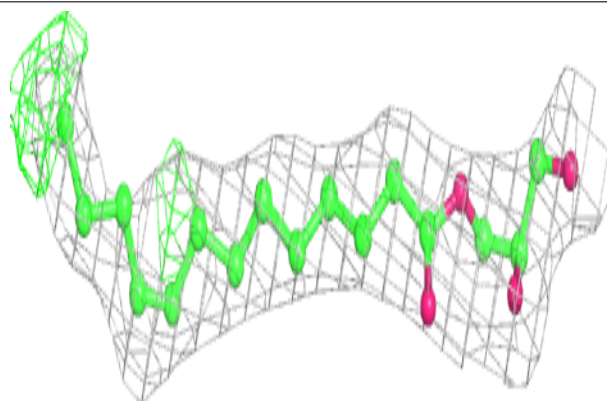


**Electron density around LFA C 317:**

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

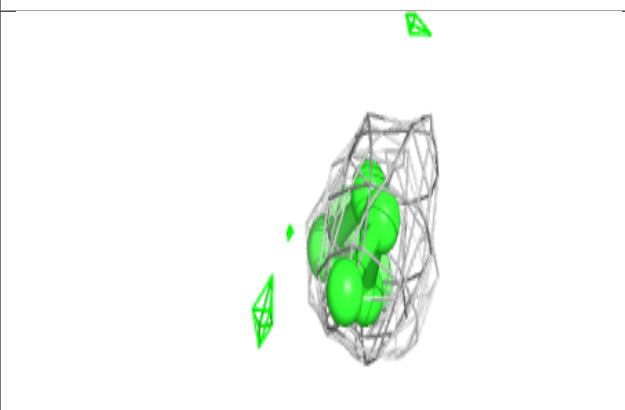
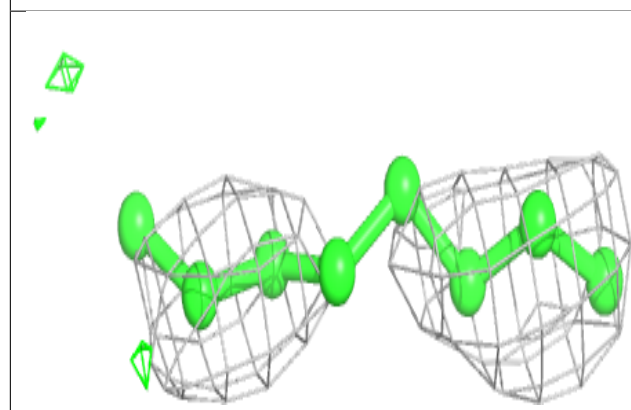
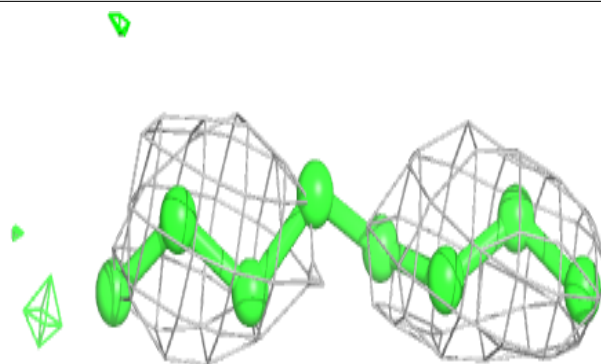
**Electron density around OLC B 303:**

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

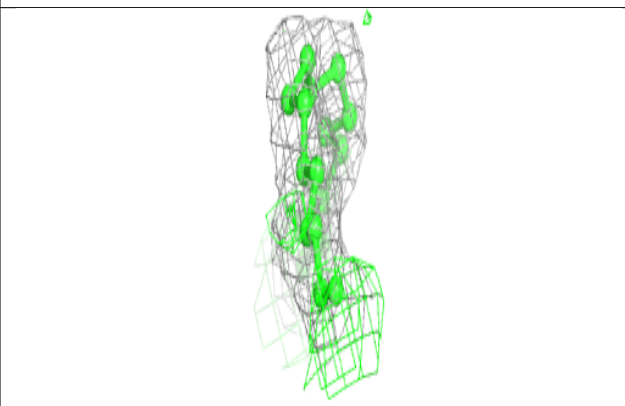
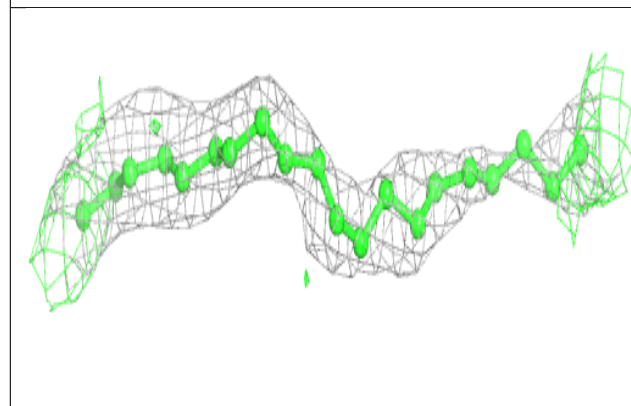
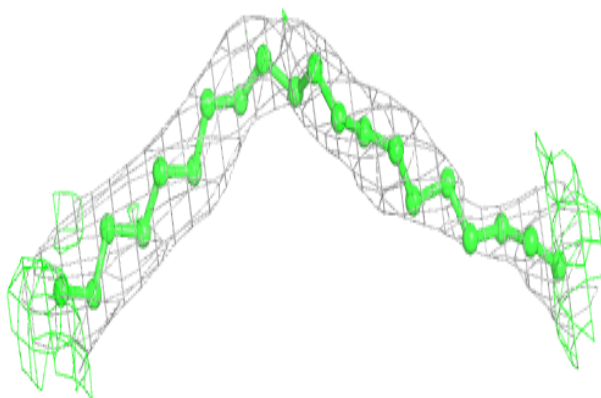


**Electron density around LFA B 306:**

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

**Electron density around LFA A 312:**

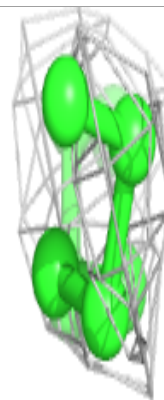
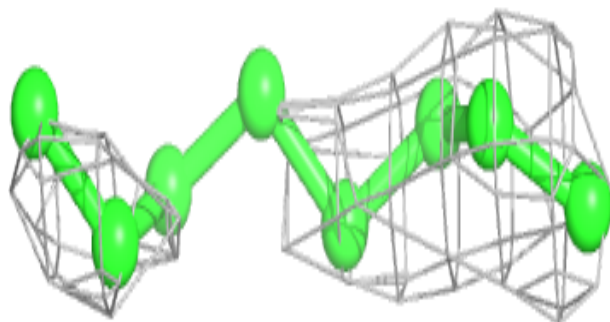
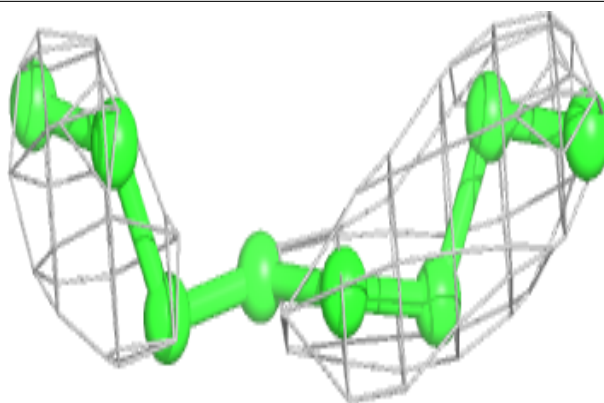
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



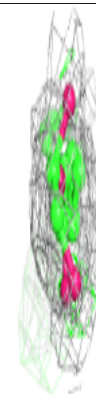
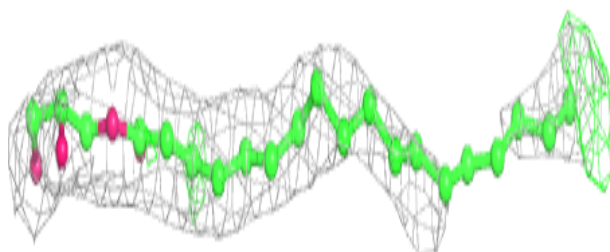
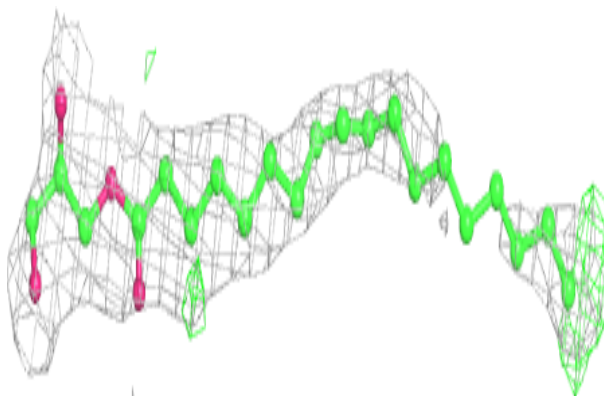


**Electron density around LFA D 306:**

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

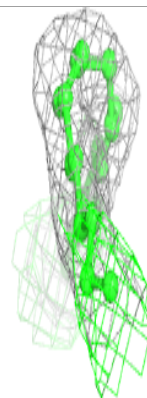
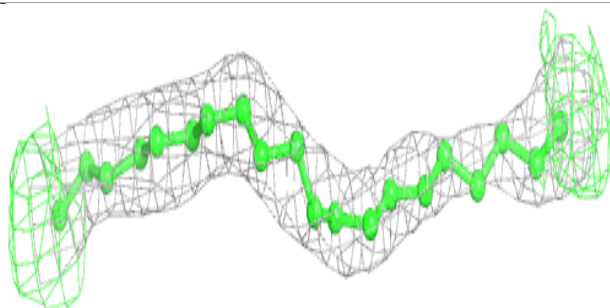
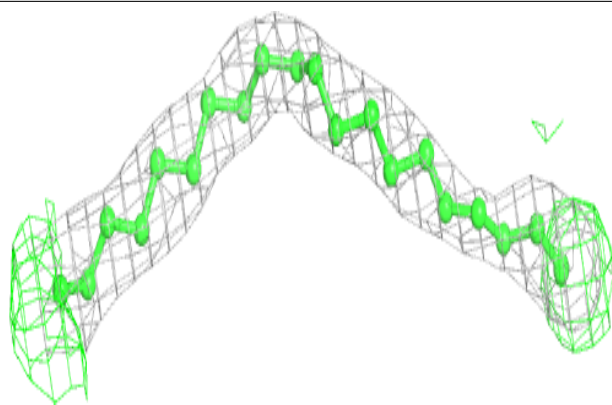
**Electron density around OLC C 308:**

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



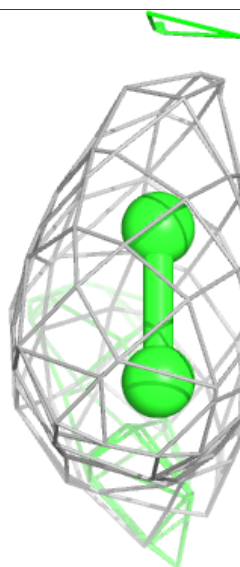
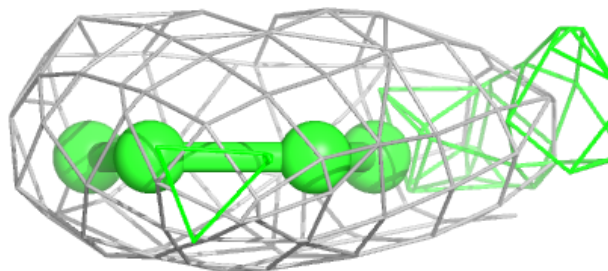
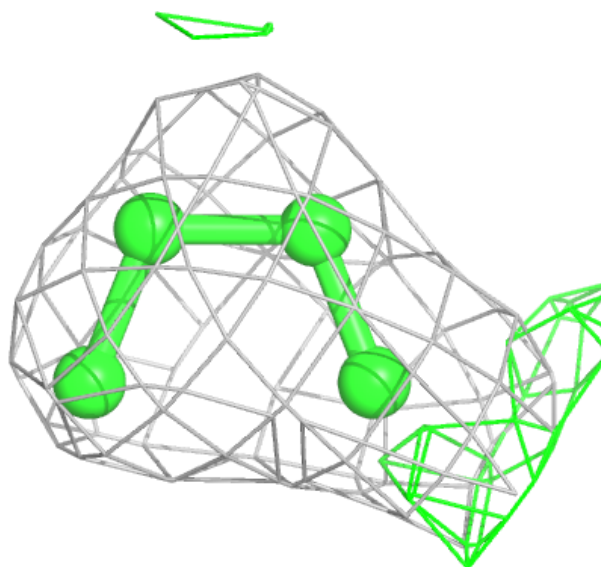
**Electron density around LFA D 302:**

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



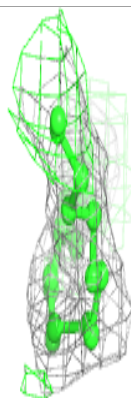
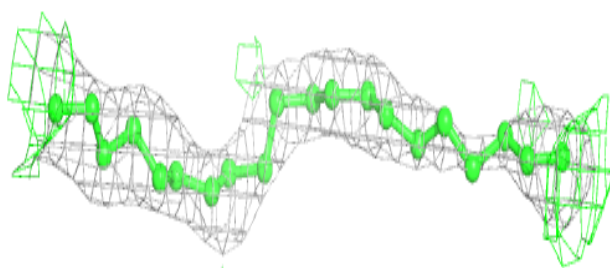
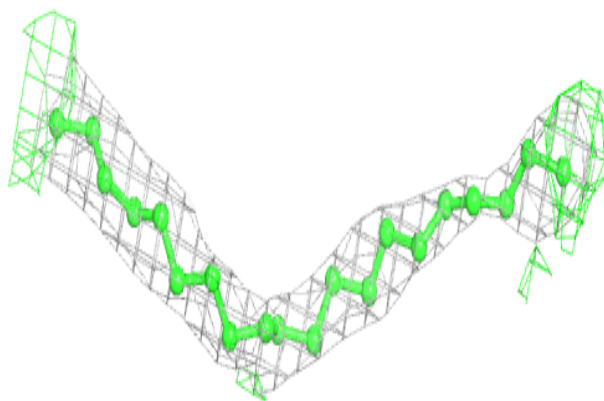
**Electron density around LFA E 307:**

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

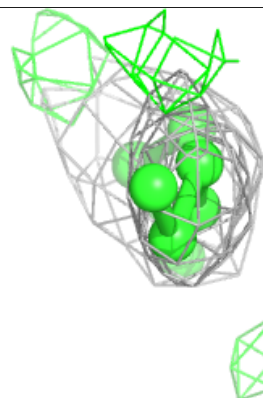
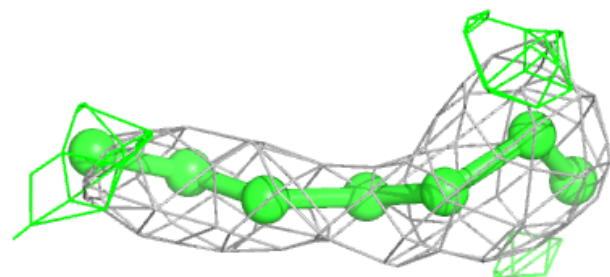
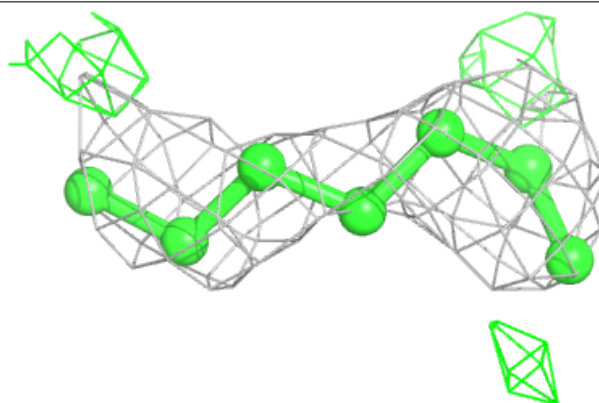


**Electron density around LFA C 303:**

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

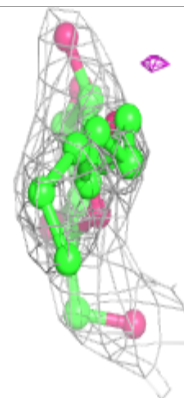
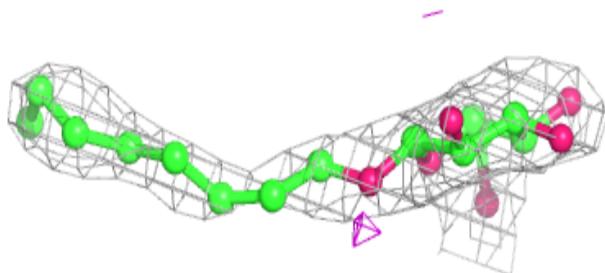
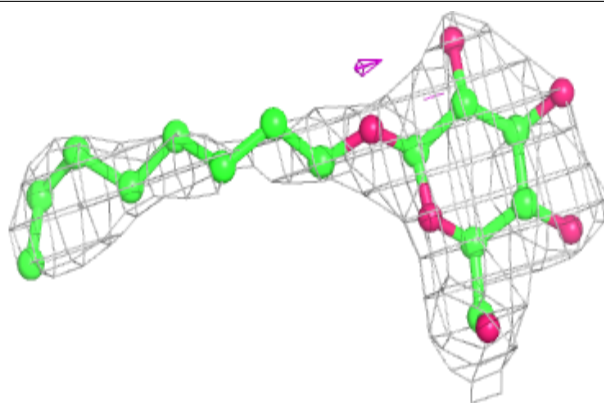
**Electron density around LFA A 304:**

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

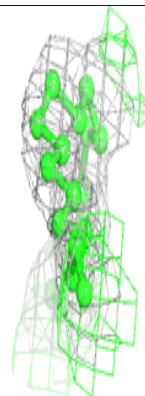
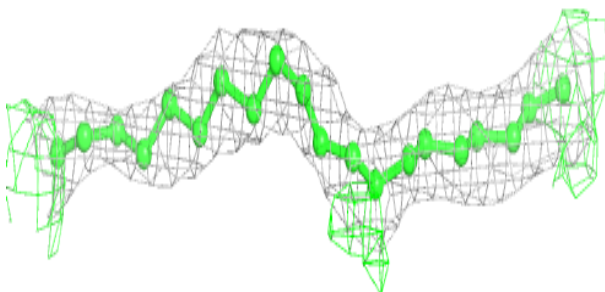
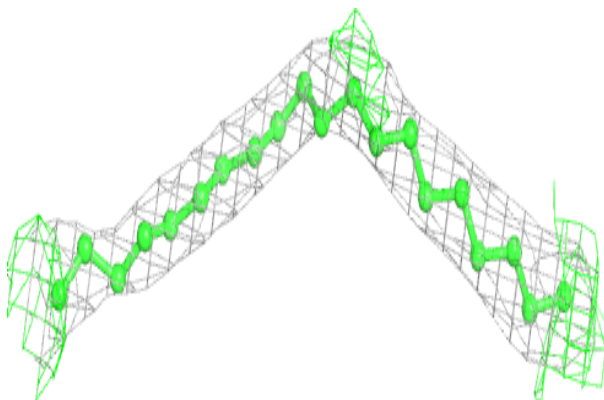


**Electron density around BOG D 311:**

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

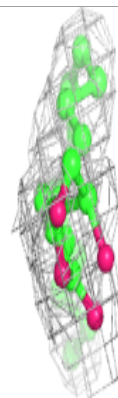
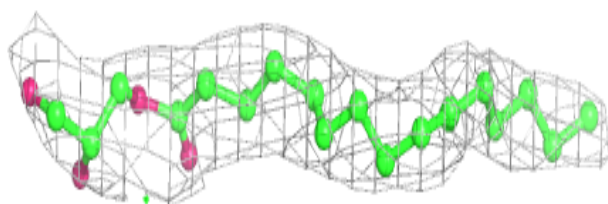
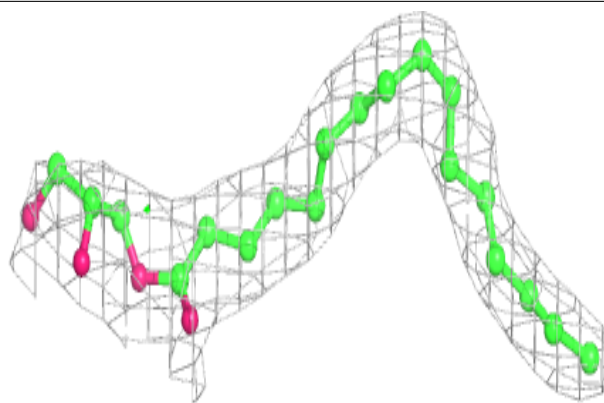
**Electron density around LFA B 302:**

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

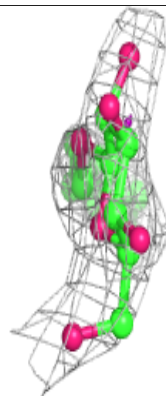
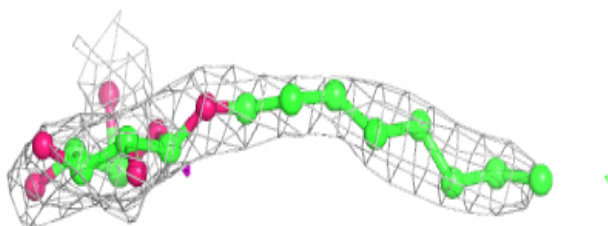
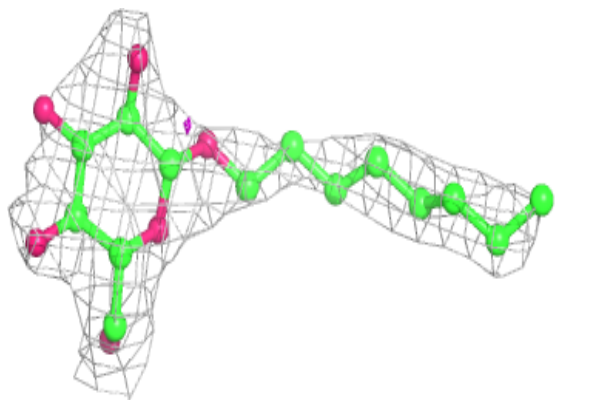


**Electron density around OLC C 306:**

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

**Electron density around BOG C 321:**

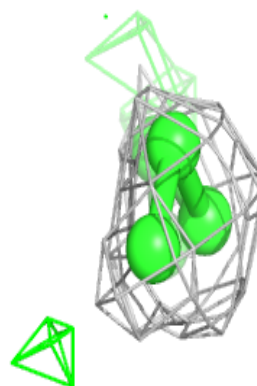
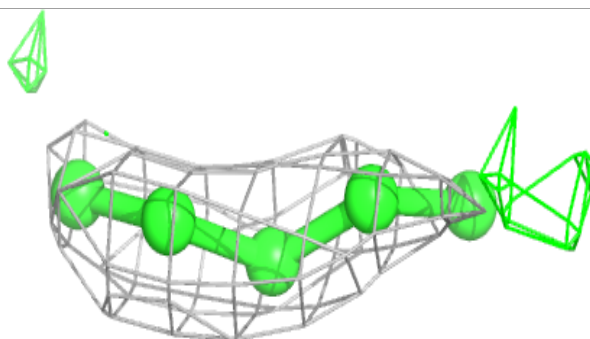
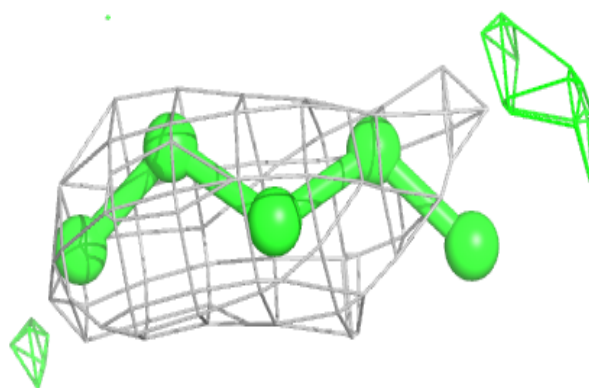
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



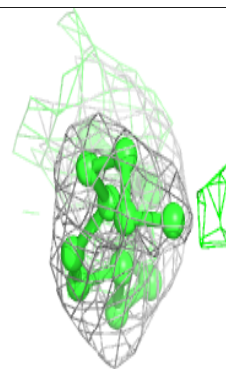
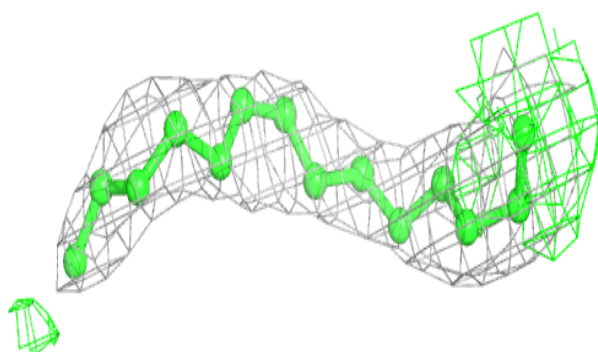
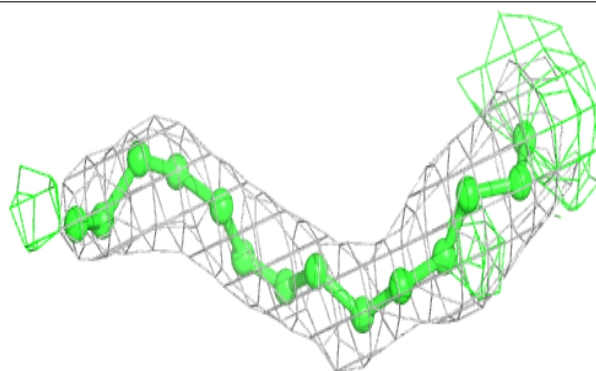


**Electron density around LFA E 308:**

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

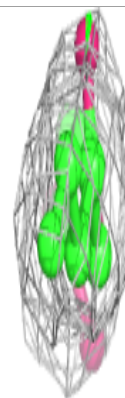
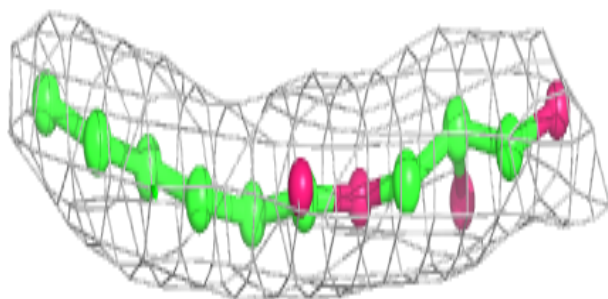
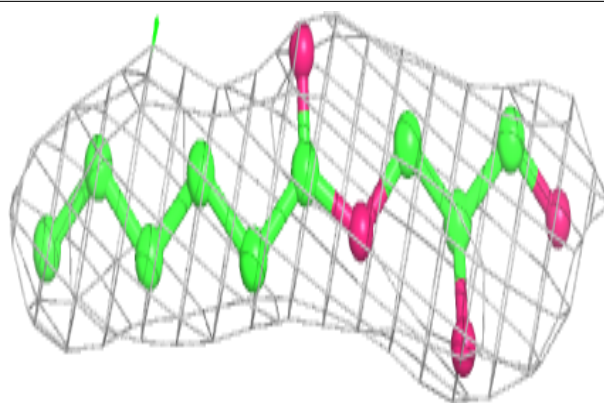
**Electron density around OLC A 311:**

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

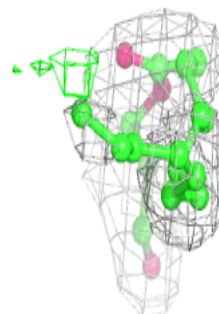
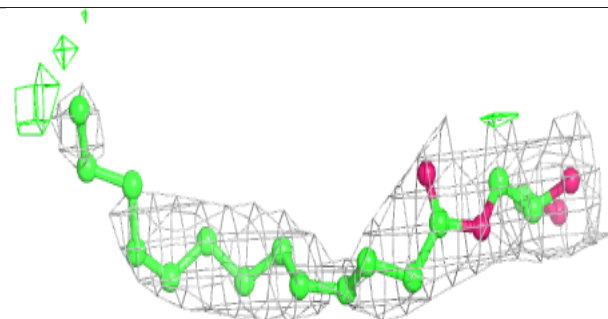
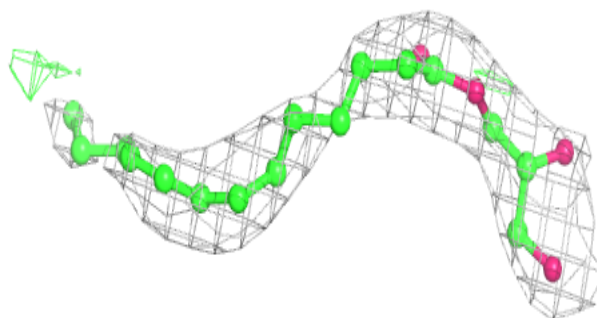


**Electron density around OLC A 302:**

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

**Electron density around OLC C 302:**

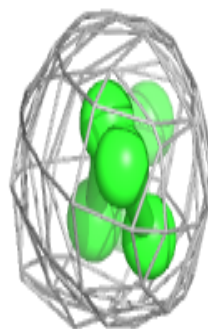
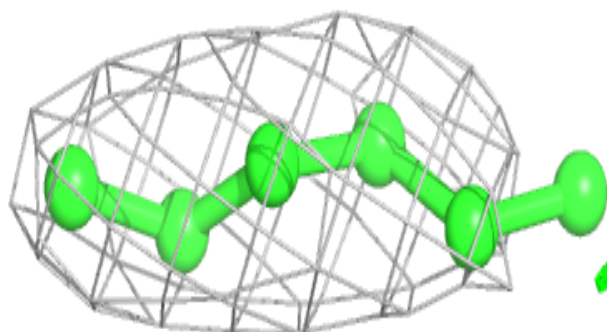
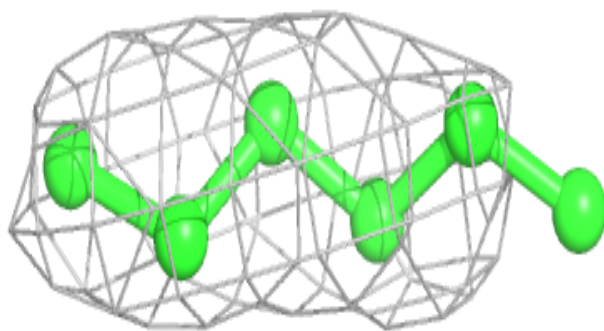
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



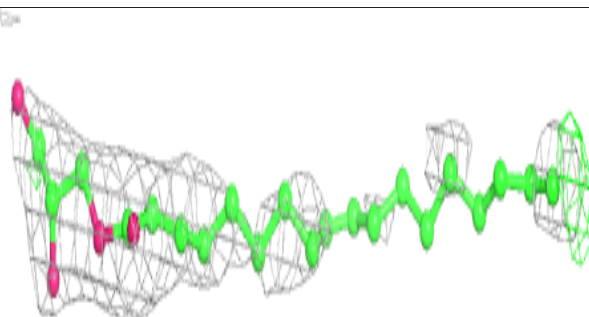
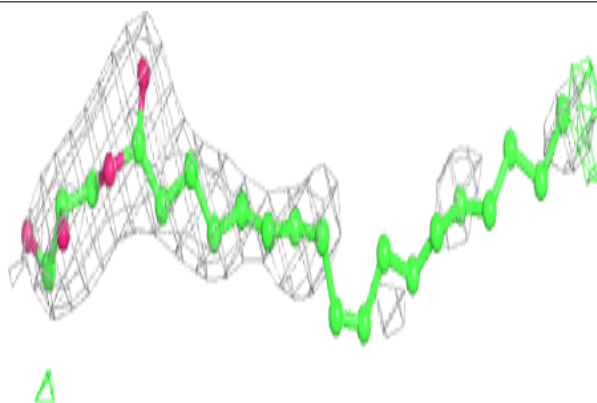


**Electron density around LFA A 308:**

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

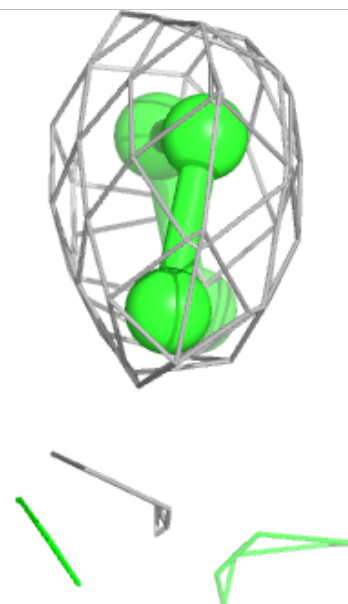
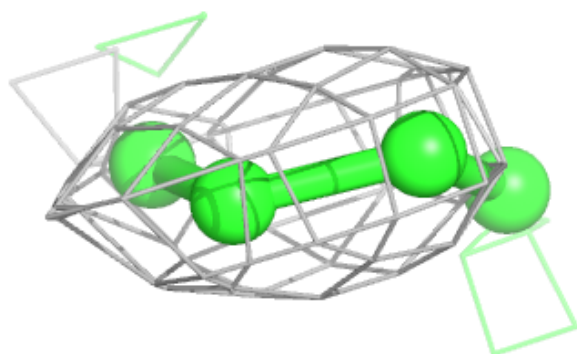
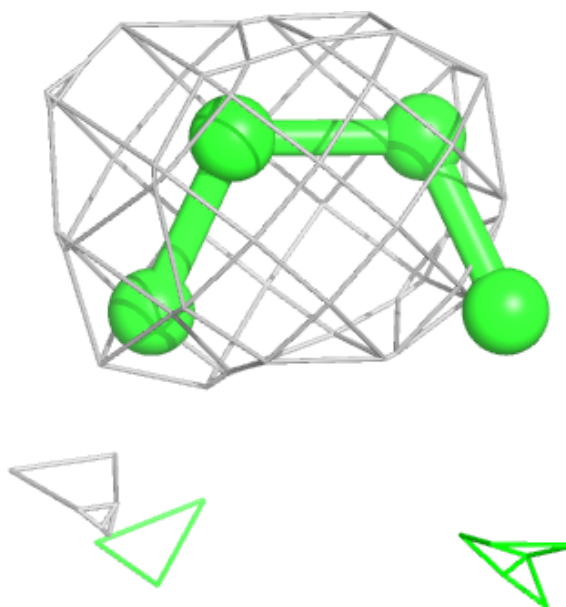
**Electron density around OLC E 304:**

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



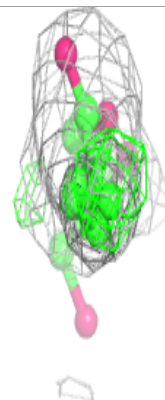
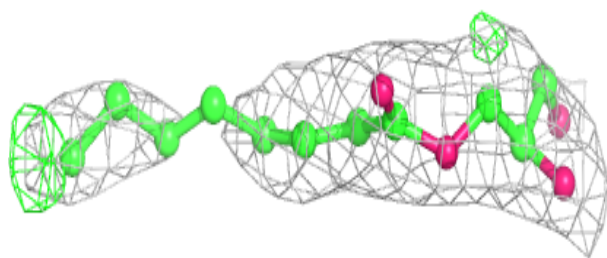
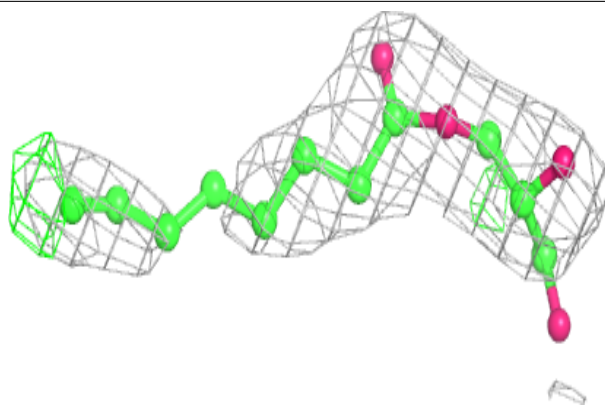
**Electron density around LFA C 319:**

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

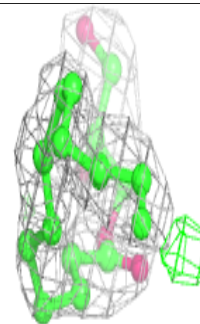
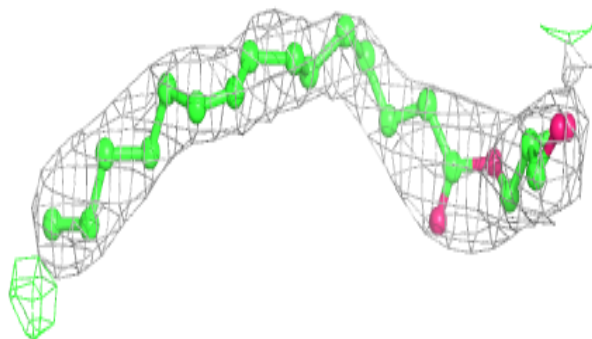
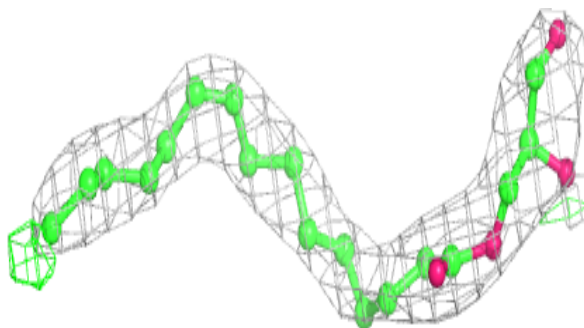


**Electron density around OLC A 303:**

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

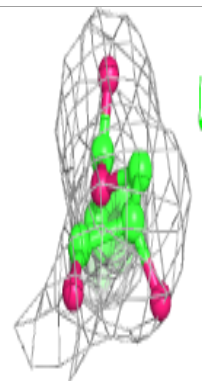
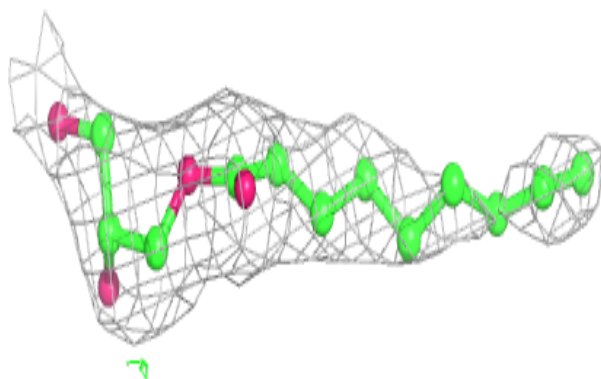
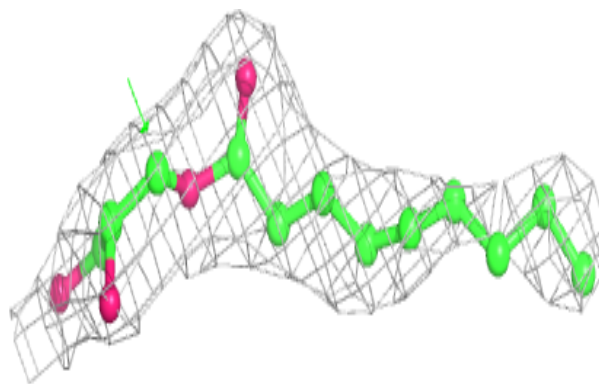
**Electron density around OLC B 301:**

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

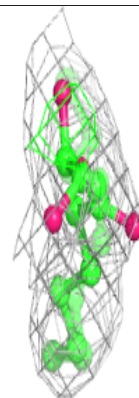
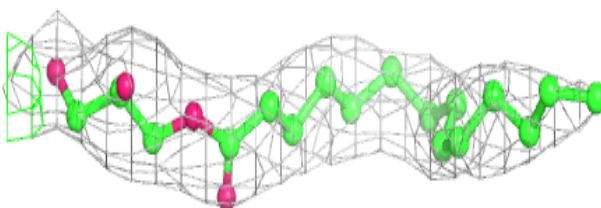
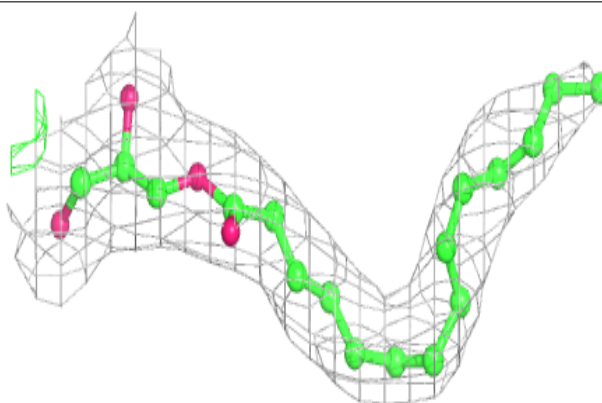


**Electron density around OLC C 312:**

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

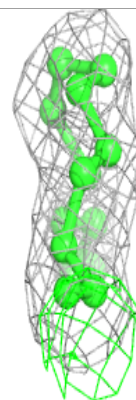
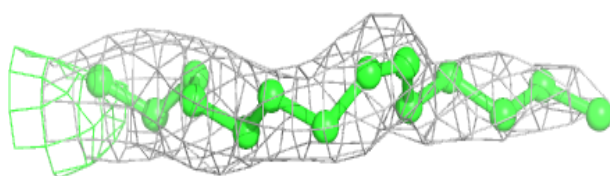
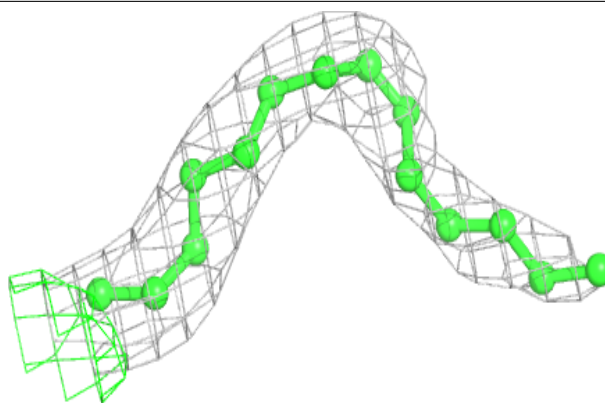
**Electron density around OLC C 301:**

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

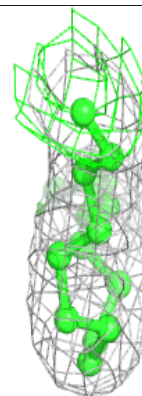
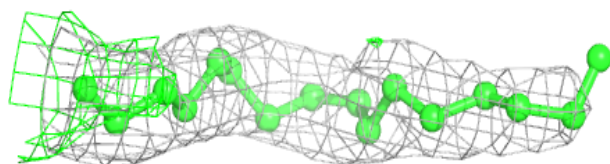
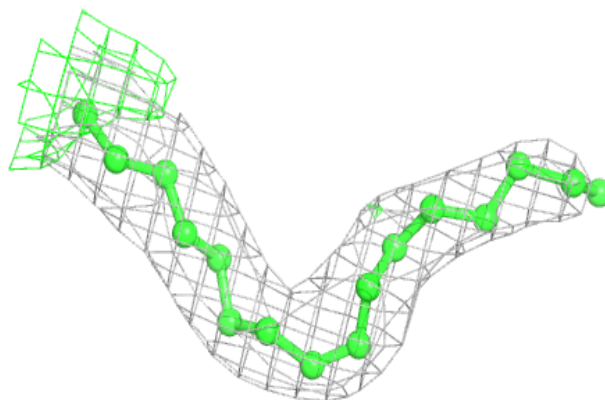


**Electron density around OLC A 301:**

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

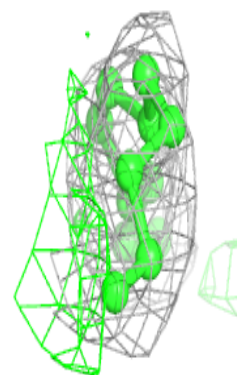
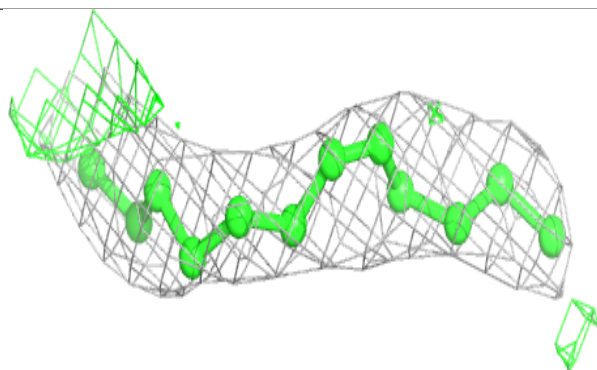
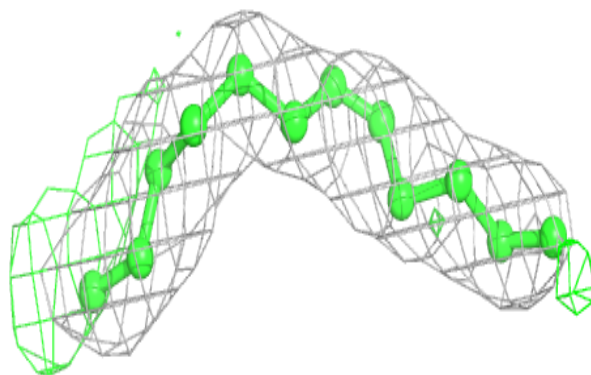
**Electron density around OLC E 303:**

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

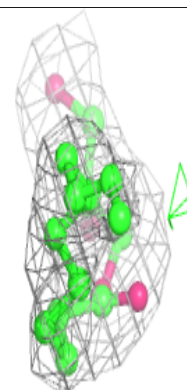
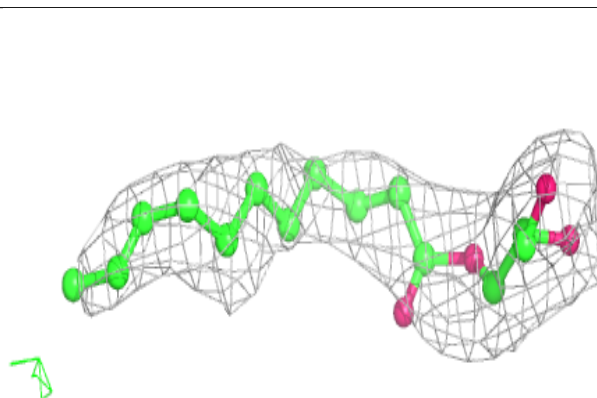
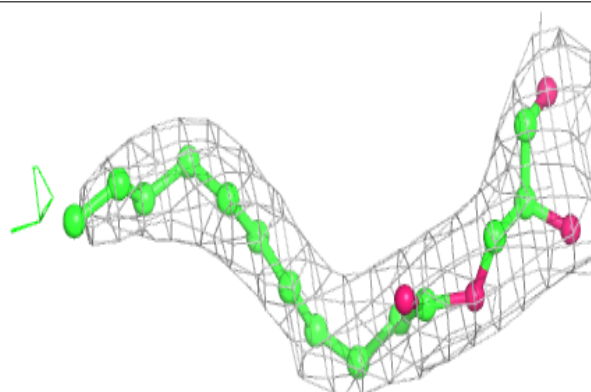


**Electron density around OLC E 301:**

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

**Electron density around OLC D 301:**

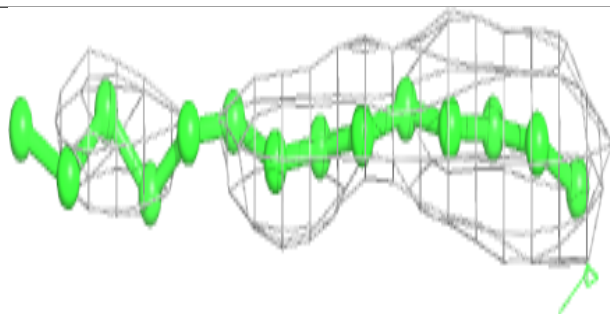
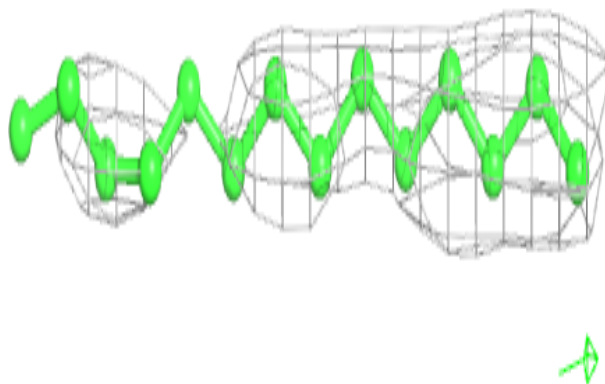
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



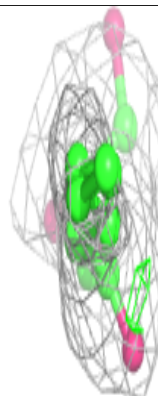
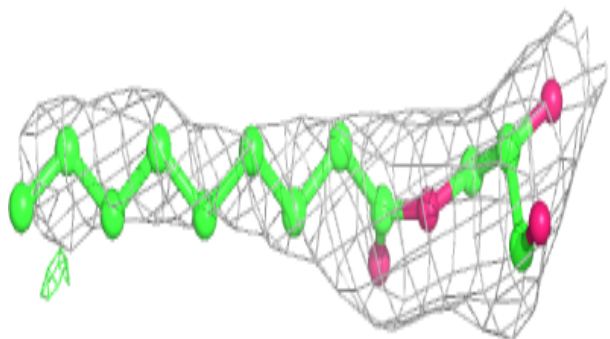
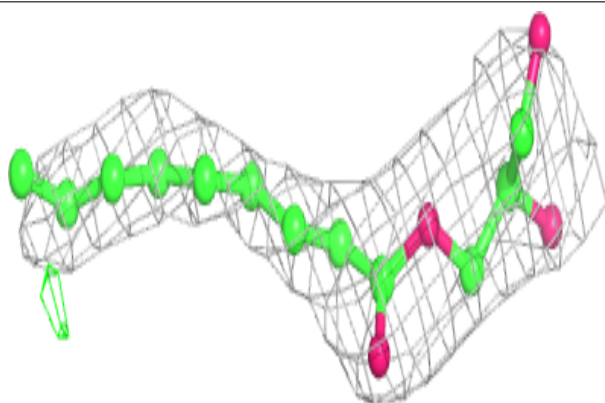


**Electron density around LFA E 311:**

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

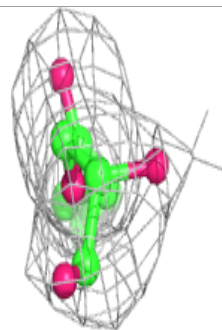
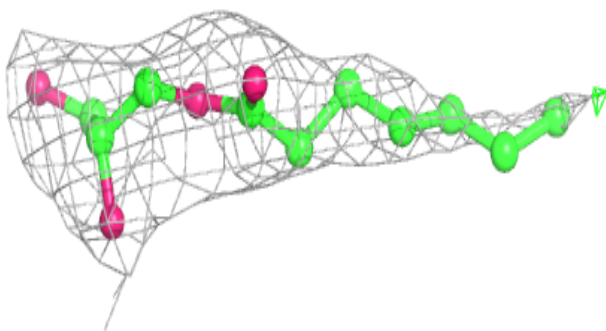
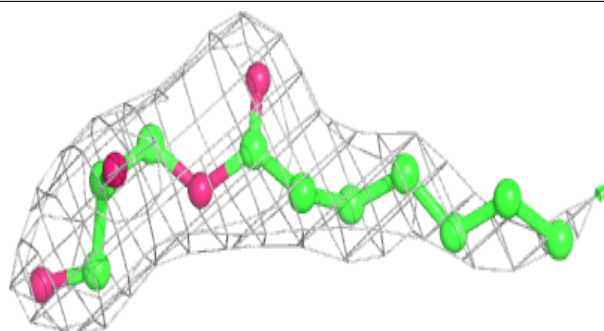
**Electron density around OLC B 304:**

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

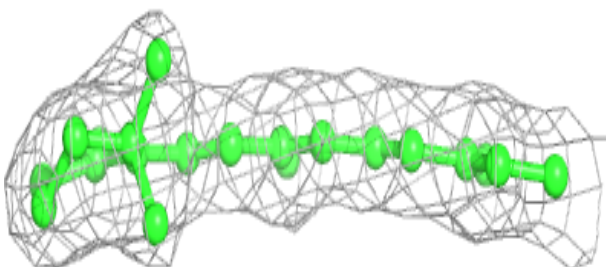
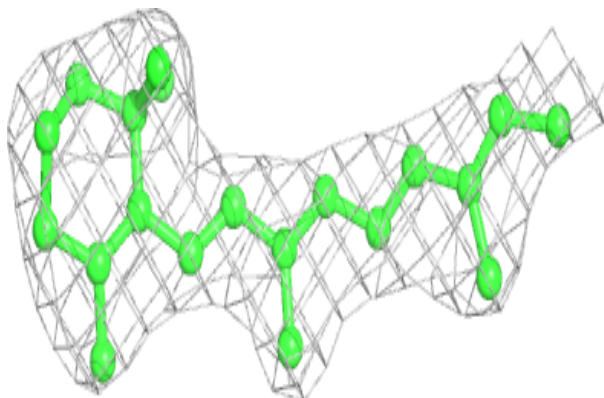


**Electron density around OLC D 303:**

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

**Electron density around RET B 309:**

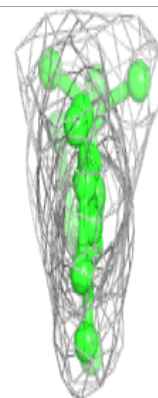
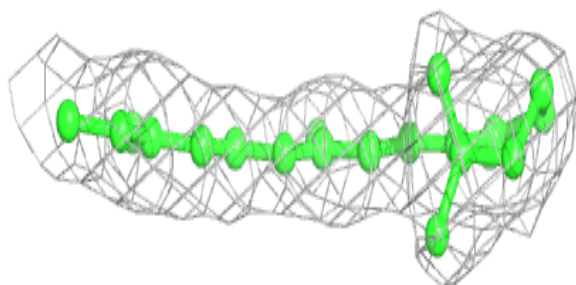
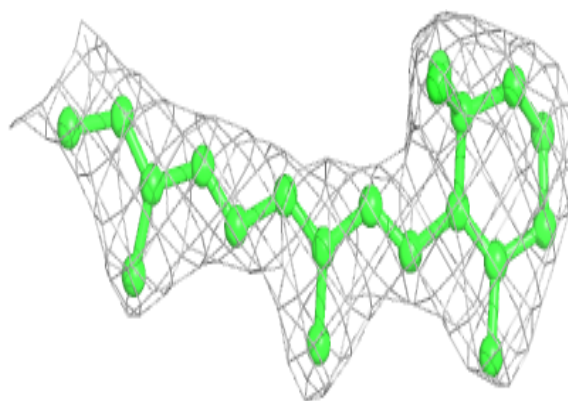
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



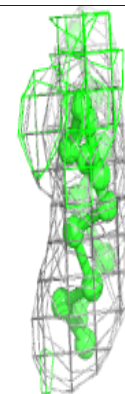
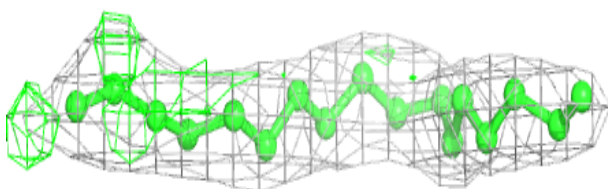
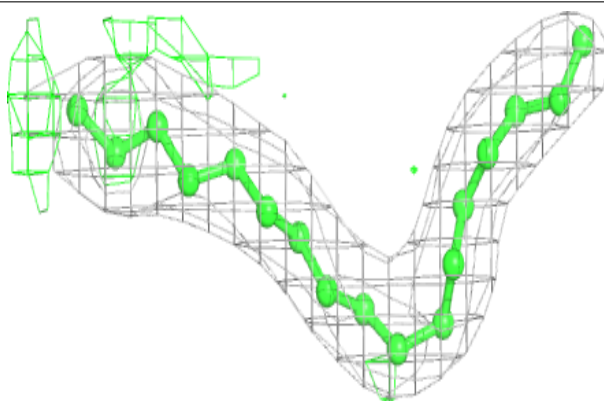


**Electron density around RET C 323:**

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

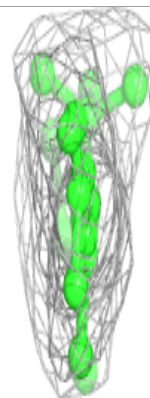
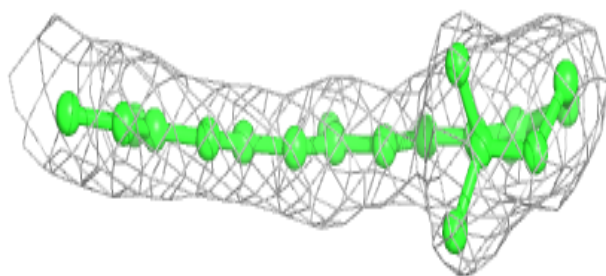
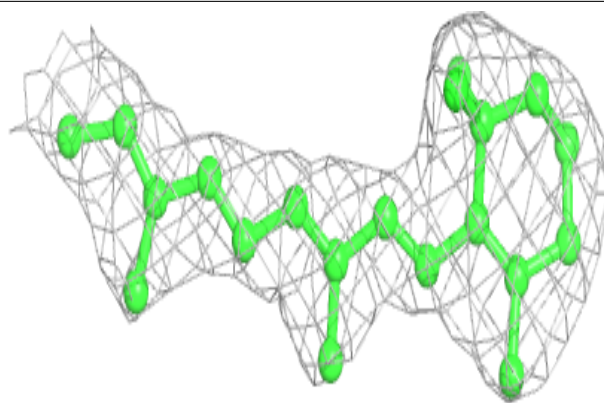
**Electron density around LFA D 307:**

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

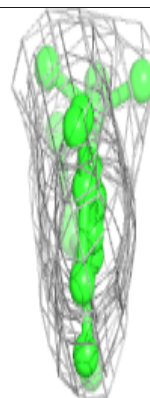
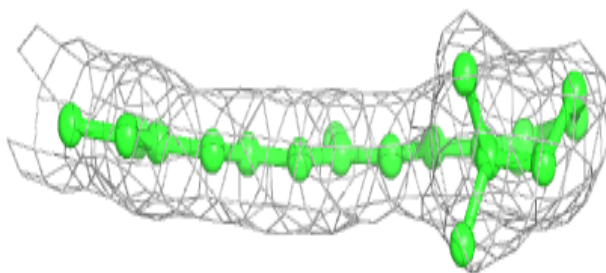
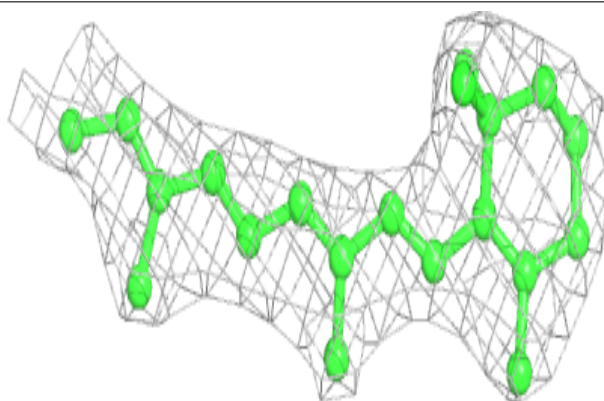


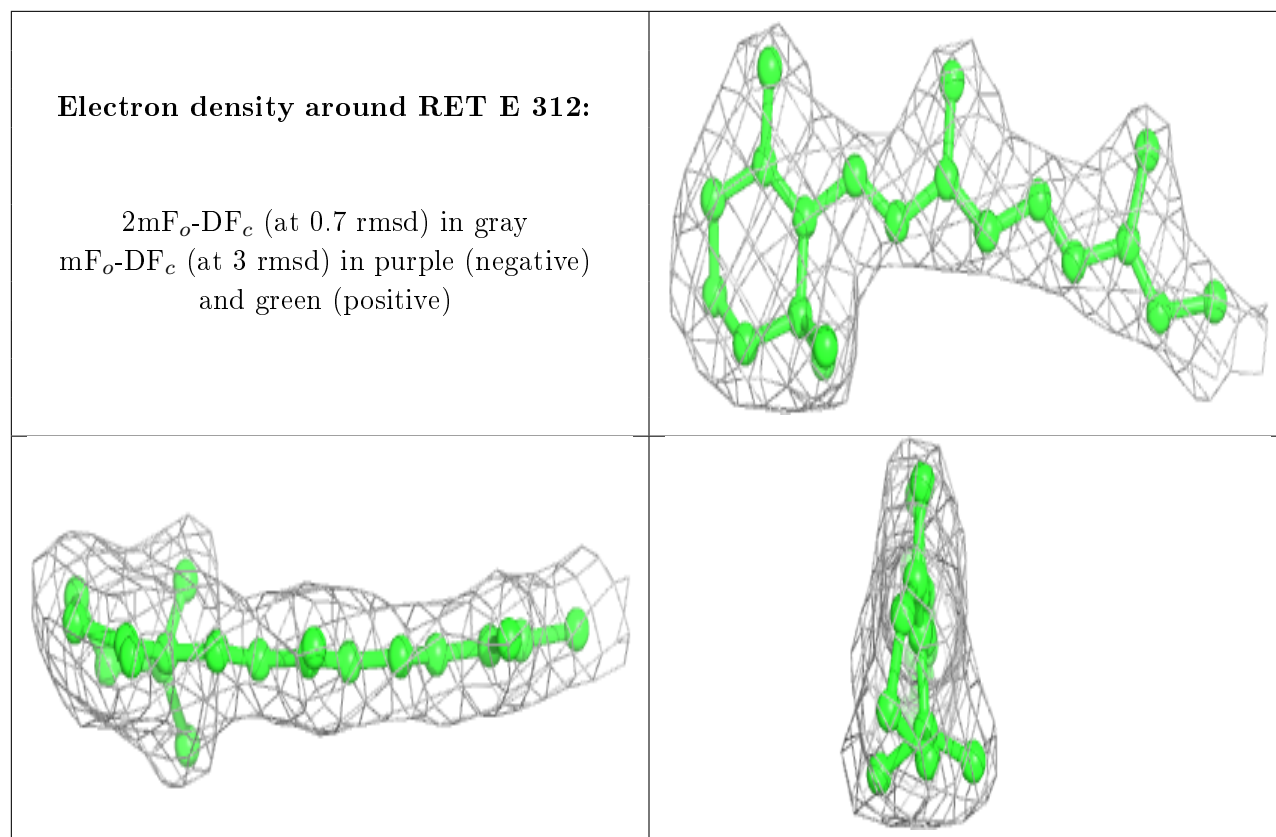
**Electron density around RET D 312:**

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

**Electron density around RET A 313:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.