



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:56 AM UTC

PDB ID : 6RF3 / pdb\_00006rf3  
Title : Crystal structure of the potassium-pumping G263F 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.

The types of validation reports are described at

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

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

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

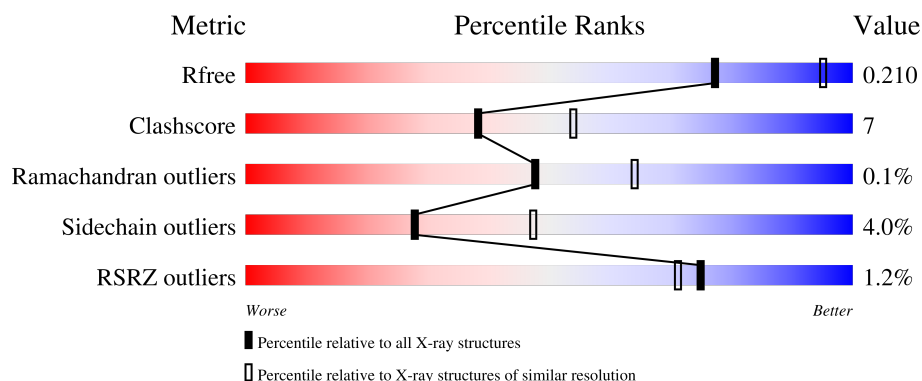
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



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

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

| Mol | Chain | Length | Quality of chain                                           |
|-----|-------|--------|------------------------------------------------------------|
| 1   | A     | 288    | <div> <div>80%</div> <div>15%</div> <div>• 5%</div> </div> |
| 1   | B     | 288    | <div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div> |
| 1   | C     | 288    | <div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div> |
| 1   | D     | 288    | <div> <div>82%</div> <div>12%</div> <div>5%</div> </div>   |
| 1   | E     | 288    | <div> <div>81%</div> <div>12%</div> <div>• 5%</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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | LFA  | E     | 322 | -         | -        | -       | X                |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13092 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       | 0       | 0     |
|     |       |          | 2200  | 1475 | 329 | 387 | 9 |         |         |       |
| 1   | B     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2194  | 1470 | 330 | 385 | 9 |         |         |       |
| 1   | C     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2199  | 1474 | 329 | 387 | 9 |         |         |       |
| 1   | D     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2191  | 1469 | 329 | 384 | 9 |         |         |       |
| 1   | E     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2193  | 1471 | 329 | 384 | 9 |         |         |       |

There are 45 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 263     | PHE      | GLY    | 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     | 263     | PHE      | GLY    | 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     | 263     | PHE      | GLY    | engineered mutation | UNP N0DKS8 |

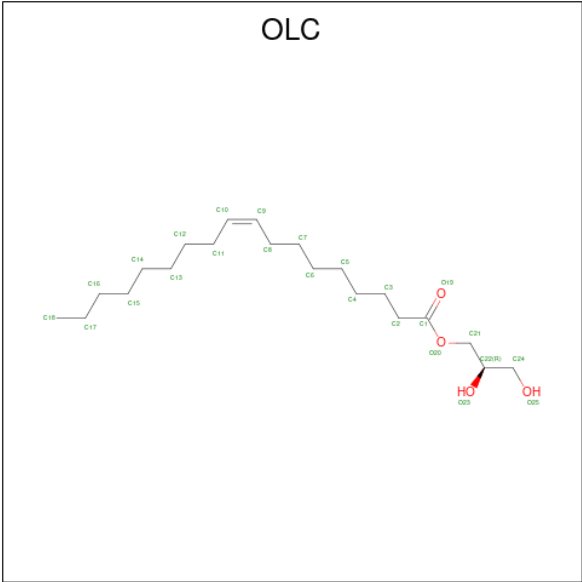
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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | 281     | LEU      | -      | expression tag      | UNP N0DKS8 |
| C     | 282     | GLU      | -      | 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     | 263     | PHE      | GLY    | 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     | 263     | PHE      | GLY    | engineered mutation | UNP N0DKS8 |
| E     | 281     | LEU      | -      | expression tag      | UNP N0DKS8 |
| E     | 282     | GLU      | -      | expression tag      | UNP N0DKS8 |
| E     | 283     | HIS      | -      | expression tag      | UNP N0DKS8 |
| E     | 284     | HIS      | -      | expression tag      | UNP N0DKS8 |
| E     | 285     | HIS      | -      | expression tag      | UNP N0DKS8 |
| E     | 286     | HIS      | -      | expression tag      | UNP N0DKS8 |
| E     | 287     | HIS      | -      | expression tag      | UNP N0DKS8 |
| E     | 288     | HIS      | -      | expression tag      | UNP N0DKS8 |

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula:  $C_{21}H_{40}O_4$ ).



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

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| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 15    | 11 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 16 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 24    | 20 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 16 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 21    | 17 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 12 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 12 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 17    | 13 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 15    | 11 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 12 | 4 |         |         |
| 2   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 21    | 17 | 4 |         |         |
| 2   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 14    | 10 | 4 |         |         |
| 2   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 21    | 17 | 4 |         |         |
| 2   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 23    | 19 | 4 |         |         |
| 2   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |
| 2   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |
| 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 |         |         |

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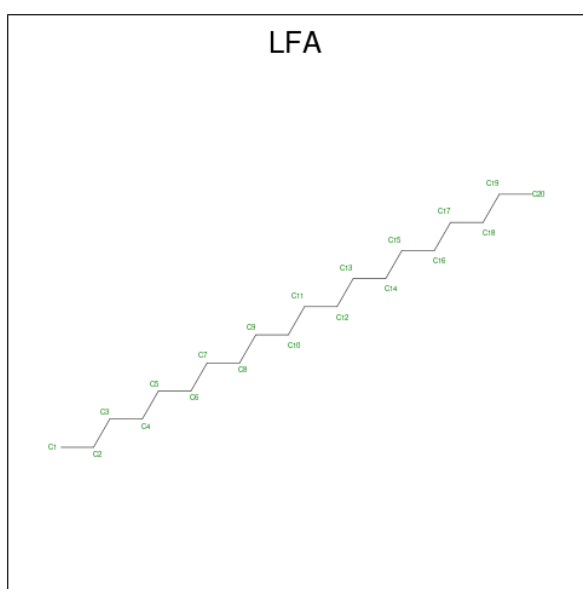
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 2   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 12 | 4 |         |         |
| 2   | C     | 1        | Total | C  | O | 0       | 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       |
|     |       |          | 13    | 9  | 4 |         |         |
| 2   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |
| 2   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 14 | 4 |         |         |
| 2   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 23    | 19 | 4 |         |         |
| 2   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |
| 2   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 14    | 10 | 4 |         |         |
| 2   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 15    | 11 | 4 |         |         |
| 2   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 14    | 10 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 12 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 24    | 20 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 24    | 20 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 16 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 15    | 11 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 15    | 11 | 4 |         |         |

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| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 11    | 7  | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 16 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 25    | 21 | 4 |         |         |

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



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 3   | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 8     | 8  |         |         |
| 3   | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 8     | 8  |         |         |
| 3   | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |
| 3   | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 3   | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 3   | A     | 1        | Total | C  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 3   | B     | 1        | Total C<br>20 20 | 0       | 0       |
| 3   | B     | 1        | Total C<br>9 9   | 0       | 0       |
| 3   | B     | 1        | Total C<br>8 8   | 0       | 0       |
| 3   | B     | 1        | Total C<br>10 10 | 0       | 0       |
| 3   | B     | 1        | Total C<br>7 7   | 0       | 0       |
| 3   | C     | 1        | Total C<br>20 20 | 0       | 0       |
| 3   | C     | 1        | Total C<br>7 7   | 0       | 0       |
| 3   | C     | 1        | Total C<br>8 8   | 0       | 0       |
| 3   | C     | 1        | Total C<br>20 20 | 0       | 0       |
| 3   | C     | 1        | Total C<br>11 11 | 0       | 0       |
| 3   | C     | 1        | Total C<br>4 4   | 0       | 0       |
| 3   | C     | 1        | Total C<br>20 20 | 0       | 0       |
| 3   | D     | 1        | Total C<br>20 20 | 0       | 0       |
| 3   | D     | 1        | Total C<br>20 20 | 0       | 0       |
| 3   | D     | 1        | Total C<br>8 8   | 0       | 0       |
| 3   | D     | 1        | Total C<br>17 17 | 0       | 0       |
| 3   | D     | 1        | Total C<br>7 7   | 0       | 0       |
| 3   | D     | 1        | Total C<br>6 6   | 0       | 0       |
| 3   | E     | 1        | Total C<br>20 20 | 0       | 0       |
| 3   | E     | 1        | Total C<br>8 8   | 0       | 0       |
| 3   | E     | 1        | Total C<br>14 14 | 0       | 0       |

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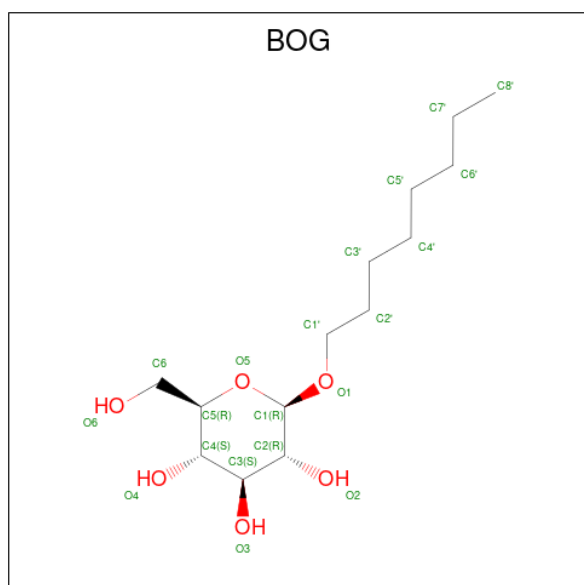
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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 3   | E     | 1        | Total C<br>4 4   | 0       | 0       |
| 3   | E     | 1        | Total C<br>5 5   | 0       | 0       |
| 3   | E     | 1        | Total C<br>20 20 | 0       | 0       |
| 3   | E     | 1        | Total C<br>4 4   | 0       | 0       |
| 3   | E     | 1        | Total C<br>14 14 | 0       | 0       |

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

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | A     | 1        | Total Na<br>1 1 | 0       | 0       |
| 4   | B     | 1        | Total Na<br>1 1 | 0       | 0       |
| 4   | C     | 1        | Total Na<br>1 1 | 0       | 0       |
| 4   | D     | 1        | Total Na<br>1 1 | 0       | 0       |
| 4   | E     | 1        | Total Na<br>1 1 | 0       | 0       |

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



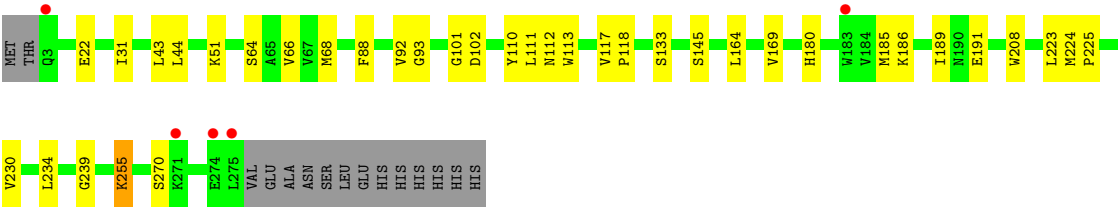
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 5   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 14 | 6 |         |         |
| 5   | B     | 1        | Total | C  | O | 0       | 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 water.

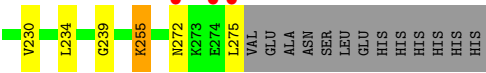
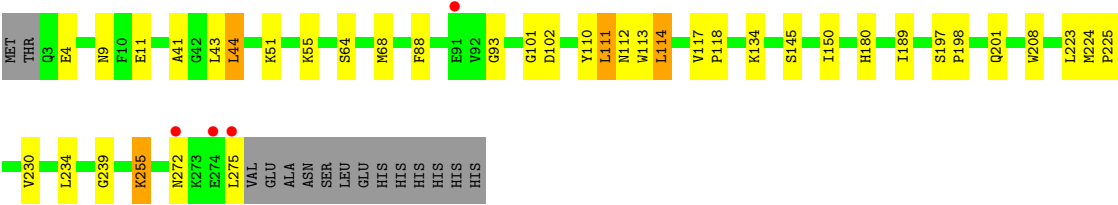
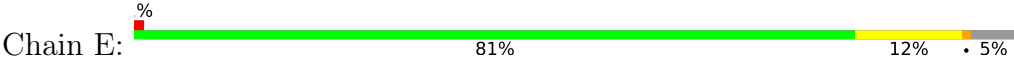
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 97       | Total | O  | 0       | 0       |
|     |       |          | 97    | 97 |         |         |
| 6   | B     | 86       | Total | O  | 0       | 0       |
|     |       |          | 86    | 86 |         |         |
| 6   | C     | 94       | Total | O  | 0       | 0       |
|     |       |          | 94    | 94 |         |         |
| 6   | D     | 89       | Total | O  | 0       | 0       |
|     |       |          | 89    | 89 |         |         |
| 6   | E     | 96       | Total | O  | 0       | 0       |
|     |       |          | 96    | 96 |         |         |







● Molecule 1: Sodium pumping rhodopsin



## 4 Data and refinement statistics

| Property                                                                | Value                                                                         | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 131.68Å 239.69Å 134.58Å<br>90.00° 90.00° 90.00°                               | Depositor        |
| Resolution (Å)                                                          | 47.97 – 2.40<br>47.97 – 2.40                                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (47.97-2.40)<br>99.9 (47.97-2.40)                                        | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                                          | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                               | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.85 (at 2.39Å)                                                               | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0230                                                               | Depositor        |
| R, $R_{free}$                                                           | 0.172 , 0.205<br>0.184 , 0.210                                                | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4195 reflections (5.04%)                                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 45.7                                                                          | Xtriage          |
| Anisotropy                                                              | 0.596                                                                         | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 52.7                                                                   | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$                   | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l<br>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                                                   | 13092                                                                         | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 56.0                                                                          | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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: LYR, NA, LFA, BOG, OLC

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     | 0.48         | 0/2229  | 0.91        | 0/3030  |
| 1   | B     | 0.49         | 0/2223  | 0.91        | 0/3023  |
| 1   | C     | 0.48         | 0/2228  | 0.91        | 0/3029  |
| 1   | D     | 0.48         | 0/2220  | 0.92        | 0/3018  |
| 1   | E     | 0.48         | 0/2222  | 0.91        | 0/3021  |
| All | All   | 0.48         | 0/11122 | 0.91        | 0/15121 |

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                   | 2                   |
| 1   | C     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 243 | ARG  | Sidechain |
| 1   | B     | 243 | ARG  | Sidechain |
| 1   | B     | 273 | LYS  | Peptide   |
| 1   | C     | 270 | SER  | 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     | 2200  | 0        | 2184     | 34      | 0            |
| 1   | B     | 2194  | 0        | 2179     | 37      | 0            |
| 1   | C     | 2199  | 0        | 2182     | 39      | 0            |
| 1   | D     | 2191  | 0        | 2172     | 28      | 0            |
| 1   | E     | 2193  | 0        | 2179     | 27      | 0            |
| 2   | A     | 228   | 0        | 326      | 7       | 0            |
| 2   | B     | 269   | 0        | 378      | 7       | 0            |
| 2   | C     | 240   | 0        | 343      | 5       | 0            |
| 2   | D     | 176   | 0        | 250      | 2       | 0            |
| 2   | E     | 259   | 0        | 371      | 13      | 0            |
| 3   | A     | 65    | 0        | 126      | 1       | 0            |
| 3   | B     | 54    | 0        | 106      | 1       | 0            |
| 3   | C     | 90    | 0        | 182      | 6       | 0            |
| 3   | D     | 78    | 0        | 153      | 3       | 0            |
| 3   | E     | 89    | 0        | 176      | 6       | 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       | 3       | 0            |
| 5   | B     | 20    | 0        | 28       | 4       | 0            |
| 5   | C     | 20    | 0        | 28       | 1       | 0            |
| 5   | D     | 20    | 0        | 28       | 1       | 0            |
| 5   | E     | 20    | 0        | 28       | 0       | 0            |
| 6   | A     | 97    | 0        | 0        | 4       | 0            |
| 6   | B     | 86    | 0        | 0        | 1       | 0            |
| 6   | C     | 94    | 0        | 0        | 3       | 0            |
| 6   | D     | 89    | 0        | 0        | 2       | 0            |
| 6   | E     | 96    | 0        | 0        | 4       | 0            |
| All | All   | 13092 | 0        | 13447    | 180     | 0            |

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

All (180) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:316:LFA:H141 | 3:E:317:LFA:H201 | 1.51                     | 0.89              |
| 1:C:267:ILE:HG21 | 1:C:275:LEU:HB3  | 1.57                     | 0.85              |
| 3:E:316:LFA:C14  | 3:E:317:LFA:H201 | 2.05                     | 0.84              |
| 1:B:255:LYR:H9   | 1:B:255:LYR:H183 | 1.60                     | 0.82              |
| 1:A:164:LEU:HD21 | 5:A:320:BOG:H2'1 | 1.61                     | 0.80              |
| 1:A:255:LYR:H9   | 1:A:255:LYR:H183 | 1.62                     | 0.80              |
| 1:D:255:LYR:H183 | 1:D:255:LYR:H9   | 1.62                     | 0.80              |
| 1:C:255:LYR:H183 | 1:C:255:LYR:H9   | 1.62                     | 0.79              |
| 1:E:255:LYR:H9   | 1:E:255:LYR:H183 | 1.64                     | 0.79              |
| 1:A:272:ASN:HD22 | 1:A:272:ASN:N    | 1.84                     | 0.76              |
| 1:B:272:ASN:HD22 | 1:B:272:ASN:N    | 1.84                     | 0.76              |
| 1:C:51:LYS:HD3   | 6:C:447:HOH:O    | 1.86                     | 0.75              |
| 1:B:231:ASP:H    | 5:B:321:BOG:HO6  | 1.34                     | 0.73              |
| 2:A:307:OLC:O19  | 2:A:308:OLC:H21A | 1.88                     | 0.72              |
| 2:A:301:OLC:C8   | 2:B:304:OLC:H10  | 2.21                     | 0.70              |
| 1:E:114:LEU:HD13 | 1:E:150:ILE:HG21 | 1.74                     | 0.70              |
| 1:E:145:SER:OG   | 1:E:180:HIS:HD2  | 1.75                     | 0.69              |
| 1:C:145:SER:OG   | 1:C:180:HIS:HD2  | 1.76                     | 0.68              |
| 2:E:303:OLC:C24  | 3:E:315:LFA:C13  | 2.72                     | 0.68              |
| 1:B:145:SER:OG   | 1:B:180:HIS:HD2  | 1.75                     | 0.68              |
| 1:C:183:TRP:CZ3  | 3:C:314:LFA:H61  | 2.29                     | 0.68              |
| 1:D:145:SER:OG   | 1:D:180:HIS:HD2  | 1.76                     | 0.68              |
| 2:E:303:OLC:H24  | 3:E:315:LFA:C13  | 2.26                     | 0.66              |
| 3:D:313:LFA:C17  | 2:E:301:OLC:H21A | 2.25                     | 0.65              |
| 2:B:313:OLC:H2   | 2:B:315:OLC:H24A | 1.79                     | 0.64              |
| 1:A:139:ARG:HH22 | 2:A:302:OLC:H24A | 1.63                     | 0.63              |
| 1:C:224:MET:N    | 1:C:225:PRO:HD2  | 2.16                     | 0.60              |
| 1:A:224:MET:N    | 1:A:225:PRO:HD2  | 2.16                     | 0.60              |
| 1:D:234:LEU:O    | 1:D:239:GLY:HA3  | 2.02                     | 0.60              |
| 1:A:52:ASN:OD1   | 6:A:401:HOH:O    | 2.17                     | 0.59              |
| 1:E:234:LEU:O    | 1:E:239:GLY:HA3  | 2.02                     | 0.59              |
| 1:D:224:MET:N    | 1:D:225:PRO:HD2  | 2.17                     | 0.59              |
| 3:D:313:LFA:H172 | 2:E:301:OLC:H21A | 1.84                     | 0.59              |
| 6:A:418:HOH:O    | 1:B:3:GLN:HG3    | 2.02                     | 0.59              |
| 1:B:255:LYR:H183 | 1:B:255:LYR:C9   | 2.32                     | 0.59              |
| 1:E:224:MET:N    | 1:E:225:PRO:HD2  | 2.17                     | 0.58              |
| 1:C:164:LEU:HD21 | 5:C:321:BOG:H2'1 | 1.86                     | 0.58              |
| 1:E:55:LYS:HE3   | 6:E:480:HOH:O    | 2.04                     | 0.58              |
| 1:B:224:MET:N    | 1:B:225:PRO:HD2  | 2.17                     | 0.58              |
| 1:C:216:THR:CG2  | 3:C:318:LFA:H201 | 2.34                     | 0.58              |
| 1:A:255:LYR:H183 | 1:A:255:LYR:C9   | 2.33                     | 0.57              |
| 1:A:140:ASN:HB3  | 2:A:304:OLC:H2A  | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:117:VAL:HB   | 1:B:118:PRO:HD3  | 1.87                     | 0.57              |
| 1:C:255:LYR:H183 | 1:C:255:LYR:C9   | 2.33                     | 0.57              |
| 1:A:234:LEU:O    | 1:A:239:GLY:HA3  | 2.05                     | 0.56              |
| 2:E:305:OLC:C17  | 2:E:312:OLC:H11A | 2.36                     | 0.56              |
| 1:C:234:LEU:O    | 1:C:239:GLY:HA3  | 2.05                     | 0.56              |
| 1:A:117:VAL:HB   | 1:A:118:PRO:HD3  | 1.88                     | 0.56              |
| 1:C:117:VAL:HB   | 1:C:118:PRO:HD3  | 1.88                     | 0.56              |
| 2:E:304:OLC:H4   | 2:E:304:OLC:O19  | 2.05                     | 0.55              |
| 1:E:117:VAL:HB   | 1:E:118:PRO:HD3  | 1.88                     | 0.55              |
| 1:B:234:LEU:O    | 1:B:239:GLY:HA3  | 2.05                     | 0.55              |
| 1:C:189:ILE:HD12 | 1:C:208:TRP:HB2  | 1.89                     | 0.55              |
| 1:D:117:VAL:HB   | 1:D:118:PRO:HD3  | 1.88                     | 0.54              |
| 1:E:198:PRO:HG2  | 6:E:485:HOH:O    | 2.07                     | 0.54              |
| 1:A:272:ASN:N    | 1:A:272:ASN:ND2  | 2.55                     | 0.54              |
| 1:E:111:LEU:O    | 1:E:114:LEU:HB2  | 2.09                     | 0.53              |
| 1:C:55:LYS:NZ    | 6:C:404:HOH:O    | 2.42                     | 0.52              |
| 1:C:267:ILE:CG2  | 1:C:275:LEU:HB3  | 2.34                     | 0.52              |
| 1:D:255:LYR:H183 | 1:D:255:LYR:C9   | 2.33                     | 0.52              |
| 1:B:139:ARG:HH11 | 2:B:301:OLC:C24  | 2.23                     | 0.52              |
| 1:B:223:LEU:C    | 1:B:225:PRO:HD2  | 2.35                     | 0.52              |
| 2:E:303:OLC:H24A | 3:E:315:LFA:C13  | 2.39                     | 0.51              |
| 1:B:139:ARG:NH1  | 2:B:301:OLC:C24  | 2.73                     | 0.51              |
| 1:C:216:THR:HG22 | 3:C:318:LFA:H201 | 1.91                     | 0.51              |
| 3:C:302:LFA:H32  | 3:E:323:LFA:H102 | 1.92                     | 0.51              |
| 1:B:183:TRP:CZ3  | 3:B:316:LFA:H182 | 2.45                     | 0.51              |
| 2:B:306:OLC:H10  | 1:C:114:LEU:HD22 | 1.93                     | 0.51              |
| 1:C:223:LEU:C    | 1:C:225:PRO:HD2  | 2.35                     | 0.51              |
| 1:A:223:LEU:C    | 1:A:225:PRO:HD2  | 2.34                     | 0.51              |
| 1:D:44:LEU:HD21  | 1:E:43:LEU:HD11  | 1.92                     | 0.51              |
| 1:B:164:LEU:HD11 | 5:B:321:BOG:H2'1 | 1.93                     | 0.50              |
| 2:E:305:OLC:C17  | 2:E:312:OLC:C11  | 2.90                     | 0.50              |
| 1:B:231:ASP:N    | 5:B:321:BOG:O6   | 2.22                     | 0.50              |
| 1:C:163:ASN:HD22 | 2:C:311:OLC:C24  | 2.25                     | 0.50              |
| 1:E:223:LEU:C    | 1:E:225:PRO:HD2  | 2.37                     | 0.50              |
| 1:E:255:LYR:H183 | 1:E:255:LYR:C9   | 2.35                     | 0.50              |
| 2:E:310:OLC:O19  | 2:E:312:OLC:O25  | 2.25                     | 0.49              |
| 1:B:41:ALA:HB1   | 1:C:66:VAL:HG13  | 1.94                     | 0.49              |
| 1:C:183:TRP:CE3  | 3:C:314:LFA:H41  | 2.46                     | 0.49              |
| 1:D:223:LEU:C    | 1:D:225:PRO:HD2  | 2.38                     | 0.49              |
| 1:D:164:LEU:HD21 | 5:D:317:BOG:H2'1 | 1.94                     | 0.49              |
| 6:B:409:HOH:O    | 1:C:3:GLN:HB2    | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:255:LYR:H9   | 1:D:255:LYR:H192 | 1.95                     | 0.49              |
| 1:C:255:LYR:H9   | 1:C:255:LYR:H192 | 1.95                     | 0.49              |
| 1:B:271:LYS:C    | 1:B:272:ASN:HD22 | 2.22                     | 0.48              |
| 1:C:41:ALA:HB1   | 1:D:66:VAL:HG13  | 1.94                     | 0.48              |
| 1:A:164:LEU:HD21 | 5:A:320:BOG:C2'  | 2.38                     | 0.48              |
| 1:A:40:LEU:HD23  | 1:B:73:LEU:HD11  | 1.96                     | 0.48              |
| 1:D:169:VAL:HG11 | 2:D:304:OLC:H2   | 1.96                     | 0.48              |
| 1:C:101:GLY:O    | 1:C:102:ASP:HB2  | 2.13                     | 0.48              |
| 1:A:66:VAL:HG13  | 1:E:41:ALA:HB1   | 1.94                     | 0.48              |
| 2:E:306:OLC:H2   | 2:E:306:OLC:H5   | 1.64                     | 0.48              |
| 1:A:164:LEU:CD2  | 5:A:320:BOG:H2'1 | 2.40                     | 0.47              |
| 1:B:255:LYR:H9   | 1:B:255:LYR:H192 | 1.96                     | 0.47              |
| 1:B:101:GLY:O    | 1:B:102:ASP:HB2  | 2.15                     | 0.47              |
| 1:D:51:LYS:HG2   | 6:D:460:HOH:O    | 2.13                     | 0.47              |
| 1:C:229:GLY:HA3  | 2:C:309:OLC:H22  | 1.95                     | 0.47              |
| 1:A:271:LYS:C    | 1:A:272:ASN:HD22 | 2.23                     | 0.47              |
| 1:E:255:LYR:H9   | 1:E:255:LYR:H192 | 1.96                     | 0.47              |
| 1:E:51:LYS:HD3   | 6:E:407:HOH:O    | 2.14                     | 0.47              |
| 1:C:44:LEU:HD11  | 1:D:43:LEU:HD11  | 1.98                     | 0.46              |
| 1:A:244:GLN:HG2  | 6:A:425:HOH:O    | 2.16                     | 0.46              |
| 1:E:88:PHE:CZ    | 1:E:93:GLY:HA2   | 2.51                     | 0.46              |
| 1:A:101:GLY:O    | 1:A:102:ASP:HB2  | 2.15                     | 0.46              |
| 1:A:255:LYR:H9   | 1:A:255:LYR:H192 | 1.98                     | 0.46              |
| 1:B:185:MET:O    | 1:B:189:ILE:HG12 | 2.15                     | 0.46              |
| 2:E:304:OLC:O19  | 2:E:304:OLC:C4   | 2.64                     | 0.46              |
| 3:A:315:LFA:H72  | 3:A:315:LFA:H102 | 1.80                     | 0.45              |
| 1:E:101:GLY:O    | 1:E:102:ASP:HB2  | 2.16                     | 0.45              |
| 2:A:311:OLC:H5A  | 2:B:301:OLC:H17  | 1.97                     | 0.45              |
| 1:D:51:LYS:HE2   | 6:D:460:HOH:O    | 2.16                     | 0.45              |
| 1:D:255:LYR:C9   | 1:D:255:LYR:H192 | 2.47                     | 0.45              |
| 1:B:272:ASN:N    | 1:B:272:ASN:ND2  | 2.56                     | 0.45              |
| 2:C:304:OLC:H8   | 2:C:304:OLC:H11A | 1.79                     | 0.44              |
| 1:D:186:LYS:HD3  | 1:D:208:TRP:CZ2  | 2.52                     | 0.44              |
| 1:A:164:LEU:HD23 | 2:A:306:OLC:H24  | 1.98                     | 0.44              |
| 1:A:185:MET:O    | 1:A:189:ILE:HG12 | 2.18                     | 0.44              |
| 1:A:224:MET:N    | 1:A:225:PRO:CD   | 2.81                     | 0.44              |
| 1:C:110:TYR:O    | 1:C:113:TRP:HB2  | 2.17                     | 0.44              |
| 1:A:88:PHE:CZ    | 1:A:93:GLY:HA2   | 2.53                     | 0.44              |
| 1:C:56:LYS:HG2   | 6:C:484:HOH:O    | 2.18                     | 0.44              |
| 1:A:44:LEU:HD21  | 1:B:65:ALA:HB1   | 2.00                     | 0.44              |
| 1:C:216:THR:HG21 | 3:C:318:LFA:H201 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:305:OLC:H7   | 2:C:305:OLC:H11  | 2.00                     | 0.44              |
| 1:B:255:LYR:C9   | 1:B:255:LYR:H192 | 2.48                     | 0.43              |
| 1:D:185:MET:O    | 1:D:189:ILE:HG12 | 2.18                     | 0.43              |
| 1:B:224:MET:N    | 1:B:225:PRO:CD   | 2.81                     | 0.43              |
| 1:C:131:THR:HG21 | 1:C:194:GLU:OE1  | 2.19                     | 0.43              |
| 1:C:255:LYR:C9   | 1:C:255:LYR:H192 | 2.48                     | 0.43              |
| 1:E:197:SER:O    | 1:E:201:GLN:HG3  | 2.19                     | 0.43              |
| 1:A:41:ALA:HB1   | 1:B:66:VAL:HG13  | 1.99                     | 0.43              |
| 1:E:224:MET:N    | 1:E:225:PRO:CD   | 2.82                     | 0.43              |
| 1:C:224:MET:N    | 1:C:225:PRO:CD   | 2.81                     | 0.43              |
| 1:D:64:SER:O     | 1:D:68:MET:HG2   | 2.19                     | 0.43              |
| 1:A:110:TYR:HA   | 1:A:113:TRP:CE3  | 2.54                     | 0.43              |
| 1:D:133:SER:OG   | 1:D:191:GLU:OE2  | 2.36                     | 0.43              |
| 2:C:304:OLC:H3   | 3:D:311:LFA:H202 | 2.01                     | 0.43              |
| 1:B:110:TYR:O    | 1:B:113:TRP:HB2  | 2.19                     | 0.42              |
| 1:A:114:LEU:O    | 1:A:118:PRO:HG2  | 2.18                     | 0.42              |
| 2:E:305:OLC:C17  | 2:E:312:OLC:C10  | 2.97                     | 0.42              |
| 1:A:255:LYR:C9   | 1:A:255:LYR:H192 | 2.49                     | 0.42              |
| 1:B:88:PHE:CZ    | 1:B:93:GLY:HA2   | 2.53                     | 0.42              |
| 1:C:89:ASN:OD1   | 1:C:92:VAL:HG13  | 2.19                     | 0.42              |
| 1:E:9:ASN:HB3    | 1:E:11:GLU:OE1   | 2.20                     | 0.42              |
| 1:E:189:ILE:CD1  | 1:E:208:TRP:HB2  | 2.49                     | 0.42              |
| 1:E:255:LYR:C9   | 1:E:255:LYR:H192 | 2.48                     | 0.42              |
| 1:E:64:SER:O     | 1:E:68:MET:HG2   | 2.20                     | 0.42              |
| 1:A:110:TYR:O    | 1:A:113:TRP:HB2  | 2.19                     | 0.42              |
| 1:D:224:MET:N    | 1:D:225:PRO:CD   | 2.83                     | 0.42              |
| 1:E:114:LEU:HD12 | 1:E:114:LEU:HA   | 1.87                     | 0.41              |
| 1:D:110:TYR:HA   | 1:D:113:TRP:CE3  | 2.55                     | 0.41              |
| 2:D:302:OLC:C6   | 2:E:309:OLC:C18  | 2.98                     | 0.41              |
| 1:E:110:TYR:O    | 1:E:113:TRP:HB2  | 2.20                     | 0.41              |
| 1:A:198:PRO:HD2  | 6:A:426:HOH:O    | 2.19                     | 0.41              |
| 1:D:22:GLU:HB2   | 6:E:412:HOH:O    | 2.21                     | 0.41              |
| 1:D:88:PHE:CZ    | 1:D:93:GLY:HA2   | 2.55                     | 0.41              |
| 1:B:9:ASN:HB3    | 1:B:11:GLU:OE1   | 2.20                     | 0.41              |
| 1:C:110:TYR:HA   | 1:C:113:TRP:CE3  | 2.56                     | 0.41              |
| 1:D:110:TYR:O    | 1:D:113:TRP:HB2  | 2.20                     | 0.41              |
| 1:D:255:LYR:H81  | 1:D:255:LYR:H10  | 1.88                     | 0.41              |
| 1:E:44:LEU:HD23  | 1:E:44:LEU:HA    | 1.82                     | 0.41              |
| 1:B:44:LEU:HD21  | 1:C:65:ALA:HB1   | 2.03                     | 0.41              |
| 1:B:110:TYR:HA   | 1:B:113:TRP:CE3  | 2.55                     | 0.41              |
| 1:B:154:TYR:O    | 1:B:157:GLN:HG3  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:114:LEU:O    | 1:C:118:PRO:HG2  | 2.21                     | 0.41              |
| 1:D:101:GLY:O    | 1:D:102:ASP:HB2  | 2.21                     | 0.41              |
| 1:E:114:LEU:O    | 1:E:118:PRO:HG2  | 2.21                     | 0.41              |
| 1:B:235:TYR:CD1  | 5:B:321:BOG:H62  | 2.56                     | 0.41              |
| 1:C:44:LEU:HD23  | 1:C:44:LEU:HA    | 1.81                     | 0.41              |
| 1:C:56:LYS:HD3   | 1:C:57:PHE:CE1   | 2.56                     | 0.41              |
| 1:C:255:LYR:H81  | 1:C:255:LYR:H10  | 1.90                     | 0.40              |
| 2:A:310:OLC:C9   | 2:A:311:OLC:H21  | 2.52                     | 0.40              |
| 1:B:64:SER:O     | 1:B:68:MET:HG2   | 2.21                     | 0.40              |
| 1:A:64:SER:O     | 1:A:68:MET:HG2   | 2.21                     | 0.40              |
| 1:A:154:TYR:O    | 1:A:157:GLN:HG3  | 2.20                     | 0.40              |
| 1:B:255:LYR:H81  | 1:B:255:LYR:H10  | 1.89                     | 0.40              |
| 1:A:90:GLU:CD    | 1:B:99:PRO:HG3   | 2.46                     | 0.40              |
| 1:B:139:ARG:HH11 | 2:B:301:OLC:H24A | 1.86                     | 0.40              |
| 1:D:31:ILE:HD12  | 1:D:31:ILE:HA    | 1.99                     | 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     | 270/288 (94%)   | 265 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | B     | 270/288 (94%)   | 264 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 1   | C     | 270/288 (94%)   | 265 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | D     | 270/288 (94%)   | 265 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | E     | 270/288 (94%)   | 265 (98%)  | 4 (2%)  | 1 (0%)   | 30          | 43  |
| All | All   | 1350/1440 (94%) | 1324 (98%) | 25 (2%) | 1 (0%)   | 48          | 64  |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 272 | ASN  |

### 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     | 230/248 (93%)   | 220 (96%)  | 10 (4%)  | 26          | 44 |
| 1   | B     | 230/248 (93%)   | 221 (96%)  | 9 (4%)   | 28          | 48 |
| 1   | C     | 230/248 (93%)   | 216 (94%)  | 14 (6%)  | 17          | 30 |
| 1   | D     | 228/248 (92%)   | 223 (98%)  | 5 (2%)   | 45          | 67 |
| 1   | E     | 229/248 (92%)   | 221 (96%)  | 8 (4%)   | 32          | 53 |
| All | All   | 1147/1240 (92%) | 1101 (96%) | 46 (4%)  | 28          | 47 |

All (46) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | GLU  |
| 1   | A     | 55  | LYS  |
| 1   | A     | 91  | GLU  |
| 1   | A     | 92  | VAL  |
| 1   | A     | 111 | LEU  |
| 1   | A     | 112 | ASN  |
| 1   | A     | 230 | VAL  |
| 1   | A     | 270 | SER  |
| 1   | A     | 272 | ASN  |
| 1   | A     | 273 | LYS  |
| 1   | B     | 92  | VAL  |
| 1   | B     | 103 | LEU  |
| 1   | B     | 111 | LEU  |
| 1   | B     | 112 | ASN  |
| 1   | B     | 137 | SER  |
| 1   | B     | 164 | LEU  |
| 1   | B     | 230 | VAL  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 275 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 3   | GLN  |
| 1   | C     | 44  | LEU  |
| 1   | C     | 51  | LYS  |
| 1   | C     | 56  | LYS  |
| 1   | C     | 91  | GLU  |
| 1   | C     | 92  | VAL  |
| 1   | C     | 111 | LEU  |
| 1   | C     | 112 | ASN  |
| 1   | C     | 132 | THR  |
| 1   | C     | 189 | ILE  |
| 1   | C     | 230 | VAL  |
| 1   | C     | 272 | ASN  |
| 1   | C     | 273 | LYS  |
| 1   | C     | 274 | GLU  |
| 1   | D     | 92  | VAL  |
| 1   | D     | 111 | LEU  |
| 1   | D     | 112 | ASN  |
| 1   | D     | 230 | VAL  |
| 1   | D     | 270 | SER  |
| 1   | E     | 4   | GLU  |
| 1   | E     | 44  | LEU  |
| 1   | E     | 111 | LEU  |
| 1   | E     | 112 | ASN  |
| 1   | E     | 114 | LEU  |
| 1   | E     | 134 | LYS  |
| 1   | E     | 230 | VAL  |
| 1   | E     | 275 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 141 | GLN  |
| 1   | A     | 244 | GLN  |
| 1   | A     | 272 | ASN  |
| 1   | B     | 180 | HIS  |
| 1   | B     | 244 | GLN  |
| 1   | B     | 272 | ASN  |
| 1   | C     | 3   | GLN  |
| 1   | C     | 7   | ASN  |
| 1   | C     | 141 | GLN  |
| 1   | C     | 180 | HIS  |
| 1   | D     | 3   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 141 | GLN  |
| 1   | D     | 180 | HIS  |
| 1   | E     | 141 | GLN  |
| 1   | E     | 180 | HIS  |
| 1   | E     | 244 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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 | $\# Z  > 2$ |
| 1   | LYR  | D     | 255 | 1    | 27,29,30     | 0.63 | 0           | 30,37,39    | 1.77 | 7 (23%)     |
| 1   | LYR  | E     | 255 | 1    | 27,29,30     | 0.67 | 0           | 30,37,39    | 1.76 | 7 (23%)     |
| 1   | LYR  | C     | 255 | 1    | 27,29,30     | 0.63 | 0           | 30,37,39    | 1.75 | 7 (23%)     |
| 1   | LYR  | B     | 255 | 1    | 27,29,30     | 0.62 | 0           | 30,37,39    | 1.76 | 7 (23%)     |
| 1   | LYR  | A     | 255 | 1    | 27,29,30     | 0.64 | 0           | 30,37,39    | 1.74 | 7 (23%)     |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 1   | LYR  | D     | 255 | 1    | -       | 3/22/40/42 | 0/1/1/1 |
| 1   | LYR  | E     | 255 | 1    | -       | 3/22/40/42 | 0/1/1/1 |
| 1   | LYR  | C     | 255 | 1    | -       | 2/22/40/42 | 0/1/1/1 |
| 1   | LYR  | B     | 255 | 1    | -       | 3/22/40/42 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 1   | LYR  | A     | 255 | 1    | -       | 4/22/40/42 | 0/1/1/1 |

There are no bond length outliers.

All (35) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | E     | 255 | LYR  | C1-NZ-CE    | 4.44  | 121.84      | 112.85   |
| 1   | E     | 255 | LYR  | C13-C12-C11 | -4.42 | 119.66      | 124.48   |
| 1   | D     | 255 | LYR  | C1-NZ-CE    | 4.40  | 121.78      | 112.85   |
| 1   | C     | 255 | LYR  | C1-NZ-CE    | 4.39  | 121.75      | 112.85   |
| 1   | A     | 255 | LYR  | C13-C12-C11 | -4.38 | 119.70      | 124.48   |
| 1   | C     | 255 | LYR  | C13-C12-C11 | -4.35 | 119.73      | 124.48   |
| 1   | B     | 255 | LYR  | C13-C12-C11 | -4.22 | 119.88      | 124.48   |
| 1   | D     | 255 | LYR  | C13-C12-C11 | -4.17 | 119.94      | 124.48   |
| 1   | B     | 255 | LYR  | C1-NZ-CE    | 4.16  | 121.28      | 112.85   |
| 1   | A     | 255 | LYR  | C1-NZ-CE    | 3.78  | 120.52      | 112.85   |
| 1   | A     | 255 | LYR  | C10-C9-C80  | -3.11 | 121.63      | 126.23   |
| 1   | D     | 255 | LYR  | C10-C9-C80  | -3.07 | 121.70      | 126.23   |
| 1   | B     | 255 | LYR  | C10-C9-C80  | -2.98 | 121.83      | 126.23   |
| 1   | C     | 255 | LYR  | C10-C9-C80  | -2.82 | 122.06      | 126.23   |
| 1   | B     | 255 | LYR  | C7-C6-C5    | -2.61 | 115.63      | 123.20   |
| 1   | E     | 255 | LYR  | C10-C9-C80  | -2.58 | 122.42      | 126.23   |
| 1   | A     | 255 | LYR  | C7-C6-C5    | -2.53 | 115.87      | 123.20   |
| 1   | D     | 255 | LYR  | C7-C6-C5    | -2.42 | 116.18      | 123.20   |
| 1   | E     | 255 | LYR  | C7-C6-C5    | -2.39 | 116.28      | 123.20   |
| 1   | E     | 255 | LYR  | C8-C80-C9   | 2.38  | 121.72      | 118.09   |
| 1   | D     | 255 | LYR  | C4-C3-C5    | 2.37  | 121.70      | 118.09   |
| 1   | B     | 255 | LYR  | C8-C80-C9   | 2.35  | 121.68      | 118.09   |
| 1   | D     | 255 | LYR  | C6-C7-C80   | -2.33 | 124.01      | 127.28   |
| 1   | C     | 255 | LYR  | C6-C7-C80   | -2.28 | 124.09      | 127.28   |
| 1   | B     | 255 | LYR  | C4-C3-C5    | 2.27  | 121.55      | 118.09   |
| 1   | C     | 255 | LYR  | C4-C3-C5    | 2.26  | 121.55      | 118.09   |
| 1   | A     | 255 | LYR  | C8-C80-C9   | 2.26  | 121.53      | 118.09   |
| 1   | C     | 255 | LYR  | C7-C6-C5    | -2.24 | 116.70      | 123.20   |
| 1   | A     | 255 | LYR  | C6-C7-C80   | -2.24 | 124.14      | 127.28   |
| 1   | D     | 255 | LYR  | C8-C80-C9   | 2.24  | 121.50      | 118.09   |
| 1   | C     | 255 | LYR  | C8-C80-C9   | 2.21  | 121.46      | 118.09   |
| 1   | B     | 255 | LYR  | C6-C7-C80   | -2.20 | 124.19      | 127.28   |
| 1   | E     | 255 | LYR  | C6-C7-C80   | -2.15 | 124.27      | 127.28   |
| 1   | A     | 255 | LYR  | C4-C3-C5    | 2.13  | 121.35      | 118.09   |
| 1   | E     | 255 | LYR  | C4-C3-C5    | 2.10  | 121.30      | 118.09   |

There are no chirality outliers.

All (15) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | E     | 255 | LYR  | C2-C1-NZ-CE |
| 1   | A     | 255 | LYR  | C2-C1-NZ-CE |
| 1   | C     | 255 | LYR  | C2-C1-NZ-CE |
| 1   | B     | 255 | LYR  | C2-C1-NZ-CE |
| 1   | D     | 255 | LYR  | C2-C1-NZ-CE |
| 1   | D     | 255 | LYR  | CE-CD-CG-CB |
| 1   | A     | 255 | LYR  | CE-CD-CG-CB |
| 1   | C     | 255 | LYR  | CE-CD-CG-CB |
| 1   | B     | 255 | LYR  | CE-CD-CG-CB |
| 1   | E     | 255 | LYR  | CE-CD-CG-CB |
| 1   | B     | 255 | LYR  | CG-CD-CE-NZ |
| 1   | A     | 255 | LYR  | CG-CD-CE-NZ |
| 1   | D     | 255 | LYR  | CG-CD-CE-NZ |
| 1   | A     | 255 | LYR  | CD-CE-NZ-C1 |
| 1   | E     | 255 | LYR  | CD-CE-NZ-C1 |

There are no ring outliers.

5 monomers are involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | D     | 255 | LYR  | 5       | 0            |
| 1   | E     | 255 | LYR  | 4       | 0            |
| 1   | C     | 255 | LYR  | 5       | 0            |
| 1   | B     | 255 | LYR  | 5       | 0            |
| 1   | A     | 255 | LYR  | 4       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 103 ligands modelled in this entry, 5 are monoatomic - leaving 98 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | OLC  | E     | 304 | -    | 15,15,24     | 1.18 | 1 (6%)      | 16,16,25    | 1.06 | 2 (12%)     |
| 3   | LFA  | E     | 315 | -    | 7,7,19       | 0.27 | 0           | 6,6,18      | 0.49 | 0           |
| 2   | OLC  | C     | 305 | -    | 22,22,24     | 0.99 | 1 (4%)      | 23,23,25    | 0.91 | 2 (8%)      |
| 2   | OLC  | E     | 305 | -    | 23,23,24     | 0.95 | 1 (4%)      | 24,24,25    | 0.97 | 2 (8%)      |
| 2   | OLC  | D     | 303 | -    | 24,24,24     | 0.97 | 1 (4%)      | 25,25,25    | 0.93 | 1 (4%)      |
| 3   | LFA  | B     | 319 | -    | 6,6,19       | 0.32 | 0           | 5,5,18      | 0.37 | 0           |
| 2   | OLC  | E     | 303 | -    | 13,13,24     | 1.30 | 1 (7%)      | 14,14,25    | 1.08 | 1 (7%)      |
| 3   | LFA  | C     | 302 | -    | 19,19,19     | 0.40 | 0           | 18,18,18    | 0.28 | 0           |
| 2   | OLC  | C     | 312 | -    | 15,15,24     | 1.22 | 1 (6%)      | 16,16,25    | 1.03 | 1 (6%)      |
| 2   | OLC  | B     | 309 | -    | 20,20,24     | 1.05 | 1 (5%)      | 21,21,25    | 1.01 | 1 (4%)      |
| 2   | OLC  | C     | 313 | -    | 15,15,24     | 1.26 | 1 (6%)      | 16,16,25    | 1.10 | 1 (6%)      |
| 5   | BOG  | A     | 320 | -    | 20,20,20     | 0.56 | 0           | 25,25,25    | 0.64 | 0           |
| 2   | OLC  | B     | 306 | -    | 19,19,24     | 1.07 | 1 (5%)      | 20,20,25    | 0.91 | 1 (5%)      |
| 3   | LFA  | E     | 319 | -    | 19,19,19     | 0.41 | 0           | 18,18,18    | 0.31 | 0           |
| 2   | OLC  | E     | 307 | -    | 19,19,24     | 1.06 | 1 (5%)      | 20,20,25    | 0.96 | 1 (5%)      |
| 2   | OLC  | A     | 303 | -    | 21,21,24     | 0.99 | 1 (4%)      | 22,22,25    | 0.88 | 2 (9%)      |
| 2   | OLC  | A     | 304 | -    | 24,24,24     | 0.98 | 1 (4%)      | 25,25,25    | 0.85 | 1 (4%)      |
| 3   | LFA  | C     | 317 | -    | 10,10,19     | 0.31 | 0           | 9,9,18      | 0.48 | 0           |
| 2   | OLC  | A     | 301 | -    | 14,14,24     | 1.22 | 1 (7%)      | 15,15,25    | 1.03 | 1 (6%)      |
| 3   | LFA  | C     | 316 | -    | 19,19,19     | 0.28 | 0           | 18,18,18    | 0.49 | 0           |
| 3   | LFA  | C     | 318 | -    | 3,3,19       | 0.32 | 0           | 2,2,18      | 0.67 | 0           |
| 3   | LFA  | D     | 315 | -    | 5,5,19       | 0.35 | 0           | 4,4,18      | 0.29 | 0           |
| 3   | LFA  | A     | 314 | -    | 7,7,19       | 0.27 | 0           | 6,6,18      | 0.45 | 0           |
| 2   | OLC  | A     | 302 | -    | 24,24,24     | 0.97 | 1 (4%)      | 25,25,25    | 0.84 | 1 (4%)      |
| 2   | OLC  | D     | 301 | -    | 17,17,24     | 1.13 | 1 (5%)      | 18,18,25    | 1.02 | 1 (5%)      |
| 2   | OLC  | B     | 308 | -    | 19,19,24     | 1.08 | 1 (5%)      | 20,20,25    | 0.97 | 2 (10%)     |
| 2   | OLC  | A     | 311 | -    | 15,15,24     | 1.25 | 1 (6%)      | 16,16,25    | 1.03 | 1 (6%)      |
| 2   | OLC  | E     | 312 | -    | 24,24,24     | 0.98 | 1 (4%)      | 25,25,25    | 0.86 | 1 (4%)      |
| 2   | OLC  | D     | 307 | -    | 13,13,24     | 1.25 | 1 (7%)      | 14,14,25    | 1.08 | 2 (14%)     |
| 3   | LFA  | C     | 315 | -    | 7,7,19       | 0.29 | 0           | 6,6,18      | 0.36 | 0           |
| 2   | OLC  | E     | 306 | -    | 23,23,24     | 1.00 | 1 (4%)      | 24,24,25    | 0.86 | 2 (8%)      |
| 3   | LFA  | D     | 314 | -    | 6,6,19       | 0.31 | 0           | 5,5,18      | 0.38 | 0           |
| 2   | OLC  | A     | 321 | -    | 24,24,24     | 0.96 | 1 (4%)      | 25,25,25    | 0.87 | 1 (4%)      |
| 2   | OLC  | E     | 310 | -    | 14,14,24     | 1.22 | 1 (7%)      | 15,15,25    | 0.96 | 1 (6%)      |
| 2   | OLC  | D     | 305 | -    | 22,22,24     | 1.00 | 1 (4%)      | 23,23,25    | 0.83 | 1 (4%)      |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | OLC  | C     | 307 | -    | 24,24,24     | 0.97 | 1 (4%)   | 25,25,25    | 0.91 | 1 (4%)   |
| 2   | OLC  | D     | 308 | -    | 14,14,24     | 1.24 | 1 (7%)   | 15,15,25    | 0.93 | 1 (6%)   |
| 3   | LFA  | B     | 302 | -    | 19,19,19     | 0.38 | 0        | 18,18,18    | 0.39 | 0        |
| 2   | OLC  | B     | 304 | -    | 24,24,24     | 0.98 | 1 (4%)   | 25,25,25    | 0.88 | 1 (4%)   |
| 2   | OLC  | B     | 313 | -    | 16,16,24     | 1.17 | 1 (6%)   | 17,17,25    | 0.97 | 1 (5%)   |
| 2   | OLC  | C     | 303 | -    | 13,13,24     | 1.27 | 1 (7%)   | 14,14,25    | 1.06 | 1 (7%)   |
| 2   | OLC  | E     | 309 | -    | 24,24,24     | 0.93 | 1 (4%)   | 25,25,25    | 0.89 | 2 (8%)   |
| 3   | LFA  | D     | 311 | -    | 19,19,19     | 0.26 | 0        | 18,18,18    | 0.55 | 0        |
| 2   | OLC  | A     | 310 | -    | 15,15,24     | 1.18 | 1 (6%)   | 16,16,25    | 0.95 | 1 (6%)   |
| 2   | OLC  | C     | 310 | -    | 24,24,24     | 0.96 | 1 (4%)   | 25,25,25    | 0.84 | 1 (4%)   |
| 2   | OLC  | B     | 303 | -    | 13,13,24     | 1.26 | 1 (7%)   | 14,14,25    | 1.11 | 1 (7%)   |
| 2   | OLC  | A     | 305 | -    | 12,12,24     | 1.32 | 1 (8%)   | 13,13,25    | 1.20 | 2 (15%)  |
| 3   | LFA  | A     | 318 | -    | 19,19,19     | 0.28 | 0        | 18,18,18    | 0.51 | 0        |
| 2   | OLC  | C     | 311 | -    | 15,15,24     | 1.19 | 1 (6%)   | 16,16,25    | 0.99 | 2 (12%)  |
| 3   | LFA  | C     | 319 | -    | 19,19,19     | 0.37 | 0        | 18,18,18    | 0.41 | 0        |
| 3   | LFA  | B     | 316 | -    | 8,8,19       | 0.31 | 0        | 7,7,18      | 0.44 | 0        |
| 2   | OLC  | B     | 305 | -    | 14,14,24     | 1.24 | 1 (7%)   | 15,15,25    | 0.99 | 1 (6%)   |
| 3   | LFA  | D     | 310 | -    | 19,19,19     | 0.29 | 0        | 18,18,18    | 0.53 | 0        |
| 2   | OLC  | D     | 302 | -    | 12,12,24     | 1.34 | 1 (8%)   | 13,13,25    | 1.13 | 1 (7%)   |
| 3   | LFA  | A     | 312 | -    | 6,6,19       | 0.30 | 0        | 5,5,18      | 0.40 | 0        |
| 2   | OLC  | B     | 314 | -    | 14,14,24     | 1.27 | 1 (7%)   | 15,15,25    | 1.01 | 1 (6%)   |
| 2   | OLC  | E     | 313 | -    | 19,19,24     | 1.10 | 1 (5%)   | 20,20,25    | 1.01 | 1 (5%)   |
| 3   | LFA  | E     | 302 | -    | 19,19,19     | 0.40 | 0        | 18,18,18    | 0.35 | 0        |
| 2   | OLC  | D     | 306 | -    | 24,24,24     | 1.01 | 1 (4%)   | 25,25,25    | 0.92 | 1 (4%)   |
| 3   | LFA  | A     | 317 | -    | 5,5,19       | 0.28 | 0        | 4,4,18      | 0.37 | 0        |
| 3   | LFA  | A     | 315 | -    | 11,11,19     | 0.31 | 0        | 10,10,18    | 0.46 | 0        |
| 2   | OLC  | C     | 301 | -    | 20,20,24     | 0.97 | 1 (5%)   | 21,21,25    | 0.97 | 1 (4%)   |
| 2   | OLC  | C     | 309 | -    | 15,15,24     | 1.24 | 1 (6%)   | 16,16,25    | 1.11 | 1 (6%)   |
| 5   | BOG  | B     | 321 | -    | 20,20,20     | 0.60 | 1 (5%)   | 25,25,25    | 0.61 | 0        |
| 2   | OLC  | C     | 306 | -    | 24,24,24     | 0.97 | 1 (4%)   | 25,25,25    | 0.91 | 1 (4%)   |
| 3   | LFA  | E     | 317 | -    | 3,3,19       | 0.33 | 0        | 2,2,18      | 0.66 | 0        |
| 2   | OLC  | E     | 311 | -    | 10,10,24     | 1.48 | 1 (10%)  | 11,11,25    | 1.22 | 2 (18%)  |
| 2   | OLC  | B     | 307 | -    | 23,23,24     | 0.98 | 1 (4%)   | 24,24,25    | 0.87 | 1 (4%)   |
| 3   | LFA  | A     | 316 | -    | 3,3,19       | 0.37 | 0        | 2,2,18      | 0.61 | 0        |
| 2   | OLC  | B     | 315 | -    | 15,15,24     | 1.27 | 1 (6%)   | 16,16,25    | 0.98 | 1 (6%)   |
| 3   | LFA  | C     | 314 | -    | 6,6,19       | 0.34 | 0        | 5,5,18      | 0.35 | 0        |
| 3   | LFA  | A     | 313 | -    | 7,7,19       | 0.30 | 0        | 6,6,18      | 0.45 | 0        |
| 3   | LFA  | E     | 318 | -    | 4,4,19       | 0.30 | 0        | 3,3,18      | 0.38 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | LFA  | D     | 312 | -    | 7,7,19       | 0.29 | 0        | 6,6,18      | 0.41 | 0        |
| 3   | LFA  | E     | 323 | -    | 13,13,19     | 0.30 | 0        | 12,12,18    | 0.47 | 0        |
| 2   | OLC  | E     | 308 | -    | 14,14,24     | 1.25 | 1 (7%)   | 15,15,25    | 1.08 | 1 (6%)   |
| 3   | LFA  | B     | 317 | -    | 7,7,19       | 0.27 | 0        | 6,6,18      | 0.47 | 0        |
| 2   | OLC  | B     | 312 | -    | 15,15,24     | 1.13 | 1 (6%)   | 16,16,25    | 0.95 | 2 (12%)  |
| 2   | OLC  | B     | 311 | -    | 24,24,24     | 0.98 | 1 (4%)   | 25,25,25    | 0.87 | 2 (8%)   |
| 2   | OLC  | C     | 308 | -    | 21,21,24     | 1.02 | 1 (4%)   | 22,22,25    | 0.96 | 2 (9%)   |
| 2   | OLC  | C     | 304 | -    | 20,20,24     | 1.07 | 1 (5%)   | 21,21,25    | 0.91 | 1 (4%)   |
| 2   | OLC  | A     | 309 | -    | 14,14,24     | 1.24 | 1 (7%)   | 15,15,25    | 1.15 | 2 (13%)  |
| 2   | OLC  | D     | 309 | -    | 24,24,24     | 0.96 | 1 (4%)   | 25,25,25    | 0.79 | 1 (4%)   |
| 3   | LFA  | B     | 318 | -    | 9,9,19       | 0.32 | 0        | 8,8,18      | 0.49 | 0        |
| 2   | OLC  | E     | 314 | -    | 24,24,24     | 0.96 | 1 (4%)   | 25,25,25    | 0.87 | 1 (4%)   |
| 5   | BOG  | C     | 321 | -    | 20,20,20     | 0.56 | 1 (5%)   | 25,25,25    | 0.61 | 0        |
| 2   | OLC  | E     | 301 | -    | 24,24,24     | 0.95 | 1 (4%)   | 25,25,25    | 0.88 | 1 (4%)   |
| 2   | OLC  | A     | 307 | -    | 15,15,24     | 1.21 | 1 (6%)   | 16,16,25    | 1.30 | 2 (12%)  |
| 5   | BOG  | E     | 321 | -    | 20,20,20     | 0.55 | 0        | 25,25,25    | 0.53 | 0        |
| 2   | OLC  | B     | 310 | -    | 15,15,24     | 1.22 | 1 (6%)   | 16,16,25    | 1.03 | 1 (6%)   |
| 3   | LFA  | D     | 313 | -    | 16,16,19     | 0.31 | 0        | 15,15,18    | 0.48 | 0        |
| 3   | LFA  | E     | 322 | -    | 3,3,19       | 0.35 | 0        | 2,2,18      | 0.61 | 0        |
| 2   | OLC  | A     | 308 | -    | 24,24,24     | 0.97 | 1 (4%)   | 25,25,25    | 0.89 | 1 (4%)   |
| 2   | OLC  | D     | 304 | -    | 17,17,24     | 1.13 | 1 (5%)   | 18,18,25    | 1.08 | 1 (5%)   |
| 5   | BOG  | D     | 317 | -    | 20,20,20     | 0.55 | 0        | 25,25,25    | 0.70 | 0        |
| 3   | LFA  | E     | 316 | -    | 13,13,19     | 0.28 | 0        | 12,12,18    | 0.50 | 0        |
| 2   | OLC  | B     | 301 | -    | 24,24,24     | 0.96 | 1 (4%)   | 25,25,25    | 0.91 | 1 (4%)   |
| 2   | OLC  | A     | 306 | -    | 14,14,24     | 1.23 | 1 (7%)   | 15,15,25    | 1.02 | 1 (6%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings |
|-----|------|-------|-----|------|---------|-------------|-------|
| 2   | OLC  | E     | 304 | -    | -       | 6/15/15/24  | -     |
| 3   | LFA  | E     | 315 | -    | -       | 1/5/5/17    | -     |
| 2   | OLC  | C     | 305 | -    | -       | 11/22/22/24 | -     |
| 2   | OLC  | E     | 305 | -    | -       | 12/23/23/24 | -     |
| 2   | OLC  | D     | 303 | -    | -       | 10/24/24/24 | -     |
| 3   | LFA  | B     | 319 | -    | -       | 2/4/4/17    | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | OLC  | E     | 303 | -    | -       | 5/13/13/24  | -       |
| 3   | LFA  | C     | 302 | -    | -       | 12/17/17/17 | -       |
| 2   | OLC  | C     | 312 | -    | -       | 11/15/15/24 | -       |
| 2   | OLC  | B     | 309 | -    | -       | 10/20/20/24 | -       |
| 2   | OLC  | C     | 313 | -    | -       | 8/15/15/24  | -       |
| 5   | BOG  | A     | 320 | -    | -       | 5/11/31/31  | 0/1/1/1 |
| 2   | OLC  | B     | 306 | -    | -       | 9/19/19/24  | -       |
| 3   | LFA  | E     | 319 | -    | -       | 10/17/17/17 | -       |
| 2   | OLC  | E     | 307 | -    | -       | 7/19/19/24  | -       |
| 2   | OLC  | A     | 303 | -    | -       | 6/21/21/24  | -       |
| 2   | OLC  | A     | 304 | -    | -       | 14/24/24/24 | -       |
| 3   | LFA  | C     | 317 | -    | -       | 3/8/8/17    | -       |
| 2   | OLC  | A     | 301 | -    | -       | 6/14/14/24  | -       |
| 3   | LFA  | C     | 316 | -    | -       | 11/17/17/17 | -       |
| 3   | LFA  | C     | 318 | -    | -       | 1/1/1/17    | -       |
| 3   | LFA  | D     | 315 | -    | -       | 0/3/3/17    | -       |
| 3   | LFA  | A     | 314 | -    | -       | 3/5/5/17    | -       |
| 2   | OLC  | A     | 302 | -    | -       | 15/24/24/24 | -       |
| 2   | OLC  | D     | 301 | -    | -       | 9/17/17/24  | -       |
| 2   | OLC  | B     | 308 | -    | -       | 6/19/19/24  | -       |
| 2   | OLC  | A     | 311 | -    | -       | 7/15/15/24  | -       |
| 2   | OLC  | E     | 312 | -    | -       | 10/24/24/24 | -       |
| 2   | OLC  | D     | 307 | -    | -       | 7/13/13/24  | -       |
| 3   | LFA  | C     | 315 | -    | -       | 4/5/5/17    | -       |
| 2   | OLC  | E     | 306 | -    | -       | 14/23/23/24 | -       |
| 3   | LFA  | D     | 314 | -    | -       | 3/4/4/17    | -       |
| 2   | OLC  | A     | 321 | -    | -       | 10/24/24/24 | -       |
| 2   | OLC  | E     | 310 | -    | -       | 8/14/14/24  | -       |
| 2   | OLC  | D     | 305 | -    | -       | 7/22/22/24  | -       |
| 2   | OLC  | C     | 307 | -    | -       | 6/24/24/24  | -       |
| 2   | OLC  | D     | 308 | -    | -       | 11/14/14/24 | -       |
| 3   | LFA  | B     | 302 | -    | -       | 6/17/17/17  | -       |
| 2   | OLC  | B     | 304 | -    | -       | 9/24/24/24  | -       |
| 2   | OLC  | B     | 313 | -    | -       | 10/16/16/24 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | OLC  | C     | 303 | -    | -       | 9/13/13/24  | -       |
| 2   | OLC  | E     | 309 | -    | -       | 17/24/24/24 | -       |
| 3   | LFA  | D     | 311 | -    | -       | 8/17/17/17  | -       |
| 2   | OLC  | A     | 310 | -    | -       | 8/15/15/24  | -       |
| 2   | OLC  | C     | 310 | -    | -       | 13/24/24/24 | -       |
| 2   | OLC  | B     | 303 | -    | -       | 8/13/13/24  | -       |
| 2   | OLC  | A     | 305 | -    | -       | 1/12/12/24  | -       |
| 3   | LFA  | A     | 318 | -    | -       | 8/17/17/17  | -       |
| 2   | OLC  | C     | 311 | -    | -       | 7/15/15/24  | -       |
| 3   | LFA  | C     | 319 | -    | -       | 9/17/17/17  | -       |
| 3   | LFA  | B     | 316 | -    | -       | 3/6/6/17    | -       |
| 2   | OLC  | B     | 305 | -    | -       | 4/14/14/24  | -       |
| 3   | LFA  | D     | 310 | -    | -       | 11/17/17/17 | -       |
| 2   | OLC  | D     | 302 | -    | -       | 7/12/12/24  | -       |
| 3   | LFA  | A     | 312 | -    | -       | 3/4/4/17    | -       |
| 2   | OLC  | B     | 314 | -    | -       | 8/14/14/24  | -       |
| 2   | OLC  | E     | 313 | -    | -       | 12/19/19/24 | -       |
| 3   | LFA  | E     | 302 | -    | -       | 8/17/17/17  | -       |
| 2   | OLC  | D     | 306 | -    | -       | 12/24/24/24 | -       |
| 3   | LFA  | A     | 317 | -    | -       | 2/3/3/17    | -       |
| 3   | LFA  | A     | 315 | -    | -       | 4/9/9/17    | -       |
| 2   | OLC  | C     | 301 | -    | -       | 11/20/20/24 | -       |
| 2   | OLC  | C     | 309 | -    | -       | 8/15/15/24  | -       |
| 5   | BOG  | B     | 321 | -    | -       | 5/11/31/31  | 0/1/1/1 |
| 2   | OLC  | C     | 306 | -    | -       | 10/24/24/24 | -       |
| 3   | LFA  | E     | 317 | -    | -       | 1/1/1/17    | -       |
| 2   | OLC  | E     | 311 | -    | -       | 6/10/10/24  | -       |
| 2   | OLC  | B     | 307 | -    | -       | 8/23/23/24  | -       |
| 3   | LFA  | A     | 316 | -    | -       | 0/1/1/17    | -       |
| 2   | OLC  | B     | 315 | -    | -       | 7/15/15/24  | -       |
| 3   | LFA  | C     | 314 | -    | -       | 3/4/4/17    | -       |
| 3   | LFA  | A     | 313 | -    | -       | 1/5/5/17    | -       |
| 3   | LFA  | E     | 318 | -    | -       | 1/2/2/17    | -       |
| 3   | LFA  | D     | 312 | -    | -       | 4/5/5/17    | -       |
| 3   | LFA  | E     | 323 | -    | -       | 4/11/11/17  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | OLC  | E     | 308 | -    | -       | 9/14/14/24  | -       |
| 3   | LFA  | B     | 317 | -    | -       | 4/5/5/17    | -       |
| 2   | OLC  | B     | 312 | -    | -       | 5/15/15/24  | -       |
| 2   | OLC  | B     | 311 | -    | -       | 15/24/24/24 | -       |
| 2   | OLC  | C     | 308 | -    | -       | 8/21/21/24  | -       |
| 2   | OLC  | C     | 304 | -    | -       | 9/20/20/24  | -       |
| 2   | OLC  | A     | 309 | -    | -       | 8/14/14/24  | -       |
| 2   | OLC  | D     | 309 | -    | -       | 13/24/24/24 | -       |
| 3   | LFA  | B     | 318 | -    | -       | 5/7/7/17    | -       |
| 2   | OLC  | E     | 314 | -    | -       | 10/24/24/24 | -       |
| 5   | BOG  | C     | 321 | -    | -       | 3/11/31/31  | 0/1/1/1 |
| 2   | OLC  | E     | 301 | -    | -       | 13/24/24/24 | -       |
| 2   | OLC  | A     | 307 | -    | -       | 4/15/15/24  | -       |
| 5   | BOG  | E     | 321 | -    | -       | 9/11/31/31  | 0/1/1/1 |
| 2   | OLC  | B     | 310 | -    | -       | 9/15/15/24  | -       |
| 3   | LFA  | D     | 313 | -    | -       | 9/14/14/17  | -       |
| 3   | LFA  | E     | 322 | -    | -       | 0/1/1/17    | -       |
| 2   | OLC  | A     | 308 | -    | -       | 15/24/24/24 | -       |
| 2   | OLC  | D     | 304 | -    | -       | 5/17/17/24  | -       |
| 5   | BOG  | D     | 317 | -    | -       | 2/11/31/31  | 0/1/1/1 |
| 3   | LFA  | E     | 316 | -    | -       | 5/11/11/17  | -       |
| 2   | OLC  | B     | 301 | -    | -       | 9/24/24/24  | -       |
| 2   | OLC  | A     | 306 | -    | -       | 5/14/14/24  | -       |

All (62) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | B     | 315 | OLC  | O20-C1 | 4.67 | 1.47        | 1.33     |
| 2   | A     | 311 | OLC  | O20-C1 | 4.63 | 1.46        | 1.33     |
| 2   | D     | 306 | OLC  | O20-C1 | 4.63 | 1.46        | 1.33     |
| 2   | C     | 313 | OLC  | O20-C1 | 4.61 | 1.46        | 1.33     |
| 2   | C     | 309 | OLC  | O20-C1 | 4.58 | 1.46        | 1.33     |
| 2   | E     | 312 | OLC  | O20-C1 | 4.57 | 1.46        | 1.33     |
| 2   | E     | 313 | OLC  | O20-C1 | 4.51 | 1.46        | 1.33     |
| 2   | C     | 304 | OLC  | O20-C1 | 4.51 | 1.46        | 1.33     |
| 2   | B     | 310 | OLC  | O20-C1 | 4.49 | 1.46        | 1.33     |
| 2   | A     | 307 | OLC  | O20-C1 | 4.49 | 1.46        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | D     | 303 | OLC  | O20-C1 | 4.49 | 1.46        | 1.33     |
| 2   | C     | 306 | OLC  | O20-C1 | 4.48 | 1.46        | 1.33     |
| 2   | E     | 303 | OLC  | O20-C1 | 4.48 | 1.46        | 1.33     |
| 2   | A     | 304 | OLC  | O20-C1 | 4.48 | 1.46        | 1.33     |
| 2   | D     | 302 | OLC  | O20-C1 | 4.48 | 1.46        | 1.33     |
| 2   | B     | 309 | OLC  | O20-C1 | 4.48 | 1.46        | 1.33     |
| 2   | A     | 302 | OLC  | O20-C1 | 4.47 | 1.46        | 1.33     |
| 2   | B     | 314 | OLC  | O20-C1 | 4.47 | 1.46        | 1.33     |
| 2   | E     | 308 | OLC  | O20-C1 | 4.47 | 1.46        | 1.33     |
| 2   | C     | 312 | OLC  | O20-C1 | 4.47 | 1.46        | 1.33     |
| 2   | A     | 308 | OLC  | O20-C1 | 4.47 | 1.46        | 1.33     |
| 2   | E     | 306 | OLC  | O20-C1 | 4.46 | 1.46        | 1.33     |
| 2   | B     | 311 | OLC  | O20-C1 | 4.46 | 1.46        | 1.33     |
| 2   | B     | 305 | OLC  | O20-C1 | 4.45 | 1.46        | 1.33     |
| 2   | E     | 311 | OLC  | O20-C1 | 4.44 | 1.46        | 1.33     |
| 2   | A     | 321 | OLC  | O20-C1 | 4.43 | 1.46        | 1.33     |
| 2   | C     | 307 | OLC  | O20-C1 | 4.43 | 1.46        | 1.33     |
| 2   | E     | 301 | OLC  | O20-C1 | 4.43 | 1.46        | 1.33     |
| 2   | B     | 307 | OLC  | O20-C1 | 4.43 | 1.46        | 1.33     |
| 2   | B     | 304 | OLC  | O20-C1 | 4.43 | 1.46        | 1.33     |
| 2   | E     | 314 | OLC  | O20-C1 | 4.42 | 1.46        | 1.33     |
| 2   | D     | 304 | OLC  | O20-C1 | 4.41 | 1.46        | 1.33     |
| 2   | B     | 301 | OLC  | O20-C1 | 4.41 | 1.46        | 1.33     |
| 2   | D     | 309 | OLC  | O20-C1 | 4.40 | 1.46        | 1.33     |
| 2   | A     | 309 | OLC  | O20-C1 | 4.40 | 1.46        | 1.33     |
| 2   | A     | 301 | OLC  | O20-C1 | 4.40 | 1.46        | 1.33     |
| 2   | D     | 305 | OLC  | O20-C1 | 4.39 | 1.46        | 1.33     |
| 2   | C     | 310 | OLC  | O20-C1 | 4.39 | 1.46        | 1.33     |
| 2   | B     | 308 | OLC  | O20-C1 | 4.39 | 1.46        | 1.33     |
| 2   | E     | 307 | OLC  | O20-C1 | 4.39 | 1.46        | 1.33     |
| 2   | C     | 308 | OLC  | O20-C1 | 4.38 | 1.46        | 1.33     |
| 2   | C     | 303 | OLC  | O20-C1 | 4.38 | 1.46        | 1.33     |
| 2   | D     | 308 | OLC  | O20-C1 | 4.37 | 1.46        | 1.33     |
| 2   | A     | 305 | OLC  | O20-C1 | 4.37 | 1.46        | 1.33     |
| 2   | B     | 313 | OLC  | O20-C1 | 4.37 | 1.46        | 1.33     |
| 2   | E     | 304 | OLC  | O20-C1 | 4.36 | 1.46        | 1.33     |
| 2   | D     | 301 | OLC  | O20-C1 | 4.36 | 1.46        | 1.33     |
| 2   | B     | 306 | OLC  | O20-C1 | 4.35 | 1.46        | 1.33     |
| 2   | B     | 303 | OLC  | O20-C1 | 4.33 | 1.46        | 1.33     |
| 2   | C     | 311 | OLC  | O20-C1 | 4.33 | 1.46        | 1.33     |
| 2   | A     | 306 | OLC  | O20-C1 | 4.33 | 1.46        | 1.33     |
| 2   | A     | 310 | OLC  | O20-C1 | 4.33 | 1.46        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | E     | 310 | OLC  | O20-C1 | 4.31 | 1.45        | 1.33     |
| 2   | C     | 305 | OLC  | O20-C1 | 4.31 | 1.45        | 1.33     |
| 2   | E     | 305 | OLC  | O20-C1 | 4.27 | 1.45        | 1.33     |
| 2   | D     | 307 | OLC  | O20-C1 | 4.25 | 1.45        | 1.33     |
| 2   | A     | 303 | OLC  | O20-C1 | 4.22 | 1.45        | 1.33     |
| 2   | E     | 309 | OLC  | O20-C1 | 4.20 | 1.45        | 1.33     |
| 2   | C     | 301 | OLC  | O20-C1 | 4.14 | 1.45        | 1.33     |
| 2   | B     | 312 | OLC  | O20-C1 | 4.12 | 1.45        | 1.33     |
| 5   | B     | 321 | BOG  | O1-C1  | 2.27 | 1.44        | 1.40     |
| 5   | C     | 321 | BOG  | O1-C1  | 2.01 | 1.43        | 1.40     |

All (76) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2   | A     | 307 | OLC  | O20-C1-C2 | 3.59 | 122.77      | 111.83   |
| 2   | A     | 305 | OLC  | O20-C1-C2 | 3.20 | 121.58      | 111.83   |
| 2   | E     | 313 | OLC  | O20-C1-C2 | 3.18 | 121.54      | 111.83   |
| 2   | A     | 309 | OLC  | O20-C1-C2 | 3.17 | 121.51      | 111.83   |
| 2   | C     | 307 | OLC  | O20-C1-C2 | 3.15 | 121.45      | 111.83   |
| 2   | C     | 313 | OLC  | O20-C1-C2 | 3.13 | 121.38      | 111.83   |
| 2   | B     | 309 | OLC  | O20-C1-C2 | 3.13 | 121.37      | 111.83   |
| 2   | C     | 309 | OLC  | O20-C1-C2 | 3.12 | 121.33      | 111.83   |
| 2   | C     | 308 | OLC  | O20-C1-C2 | 3.07 | 121.19      | 111.83   |
| 2   | D     | 304 | OLC  | O20-C1-C2 | 3.06 | 121.16      | 111.83   |
| 2   | E     | 304 | OLC  | O20-C1-C2 | 3.02 | 121.05      | 111.83   |
| 2   | C     | 306 | OLC  | O20-C1-C2 | 3.01 | 121.02      | 111.83   |
| 2   | D     | 303 | OLC  | O20-C1-C2 | 2.99 | 120.96      | 111.83   |
| 2   | C     | 301 | OLC  | O20-C1-C2 | 2.98 | 120.93      | 111.83   |
| 2   | D     | 306 | OLC  | O20-C1-C2 | 2.98 | 120.93      | 111.83   |
| 2   | B     | 304 | OLC  | O20-C1-C2 | 2.97 | 120.90      | 111.83   |
| 2   | E     | 305 | OLC  | O20-C1-C2 | 2.97 | 120.90      | 111.83   |
| 2   | D     | 302 | OLC  | O20-C1-C2 | 2.96 | 120.88      | 111.83   |
| 2   | B     | 303 | OLC  | O20-C1-C2 | 2.95 | 120.84      | 111.83   |
| 2   | E     | 307 | OLC  | O20-C1-C2 | 2.95 | 120.84      | 111.83   |
| 2   | D     | 307 | OLC  | O20-C1-C2 | 2.94 | 120.81      | 111.83   |
| 2   | E     | 311 | OLC  | O20-C1-C2 | 2.94 | 120.80      | 111.83   |
| 2   | E     | 308 | OLC  | O20-C1-C2 | 2.93 | 120.78      | 111.83   |
| 2   | B     | 311 | OLC  | O20-C1-C2 | 2.92 | 120.73      | 111.83   |
| 2   | C     | 305 | OLC  | O20-C1-C2 | 2.92 | 120.73      | 111.83   |
| 2   | B     | 301 | OLC  | O20-C1-C2 | 2.90 | 120.68      | 111.83   |
| 2   | E     | 303 | OLC  | O20-C1-C2 | 2.90 | 120.67      | 111.83   |
| 2   | B     | 308 | OLC  | O20-C1-C2 | 2.90 | 120.67      | 111.83   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | E     | 309 | OLC  | O20-C1-C2  | 2.88  | 120.61      | 111.83   |
| 2   | A     | 311 | OLC  | O20-C1-C2  | 2.86  | 120.56      | 111.83   |
| 2   | B     | 310 | OLC  | O20-C1-C2  | 2.86  | 120.55      | 111.83   |
| 2   | C     | 312 | OLC  | O20-C1-C2  | 2.85  | 120.52      | 111.83   |
| 2   | A     | 308 | OLC  | O20-C1-C2  | 2.84  | 120.50      | 111.83   |
| 2   | E     | 306 | OLC  | O20-C1-C2  | 2.83  | 120.45      | 111.83   |
| 2   | A     | 304 | OLC  | O20-C1-C2  | 2.82  | 120.45      | 111.83   |
| 2   | A     | 301 | OLC  | O20-C1-C2  | 2.82  | 120.44      | 111.83   |
| 2   | A     | 302 | OLC  | O20-C1-C2  | 2.81  | 120.41      | 111.83   |
| 2   | B     | 307 | OLC  | O20-C1-C2  | 2.81  | 120.41      | 111.83   |
| 2   | C     | 303 | OLC  | O20-C1-C2  | 2.81  | 120.41      | 111.83   |
| 2   | A     | 303 | OLC  | O20-C1-C2  | 2.81  | 120.39      | 111.83   |
| 2   | E     | 312 | OLC  | O20-C1-C2  | 2.80  | 120.36      | 111.83   |
| 2   | E     | 314 | OLC  | O20-C1-C2  | 2.79  | 120.35      | 111.83   |
| 2   | D     | 301 | OLC  | O20-C1-C2  | 2.79  | 120.33      | 111.83   |
| 2   | A     | 306 | OLC  | O20-C1-C2  | 2.77  | 120.28      | 111.83   |
| 2   | C     | 304 | OLC  | O20-C1-C2  | 2.76  | 120.27      | 111.83   |
| 2   | C     | 311 | OLC  | O20-C1-C2  | 2.73  | 120.16      | 111.83   |
| 2   | B     | 306 | OLC  | O20-C1-C2  | 2.72  | 120.13      | 111.83   |
| 2   | A     | 321 | OLC  | O20-C1-C2  | 2.71  | 120.11      | 111.83   |
| 2   | B     | 305 | OLC  | O20-C1-C2  | 2.71  | 120.10      | 111.83   |
| 2   | E     | 301 | OLC  | O20-C1-C2  | 2.71  | 120.09      | 111.83   |
| 2   | B     | 314 | OLC  | O20-C1-C2  | 2.69  | 120.03      | 111.83   |
| 2   | C     | 310 | OLC  | O20-C1-C2  | 2.68  | 120.00      | 111.83   |
| 2   | B     | 315 | OLC  | O20-C1-C2  | 2.67  | 119.98      | 111.83   |
| 2   | B     | 313 | OLC  | O20-C1-C2  | 2.67  | 119.98      | 111.83   |
| 2   | E     | 310 | OLC  | O20-C1-C2  | 2.59  | 119.74      | 111.83   |
| 2   | D     | 309 | OLC  | O20-C1-C2  | 2.55  | 119.60      | 111.83   |
| 2   | A     | 310 | OLC  | O20-C1-C2  | 2.52  | 119.51      | 111.83   |
| 2   | D     | 308 | OLC  | O20-C1-C2  | 2.51  | 119.49      | 111.83   |
| 2   | D     | 305 | OLC  | O20-C1-C2  | 2.51  | 119.48      | 111.83   |
| 2   | B     | 312 | OLC  | O20-C1-C2  | 2.47  | 119.38      | 111.83   |
| 2   | A     | 309 | OLC  | O20-C1-O19 | -2.34 | 117.79      | 123.63   |
| 2   | E     | 309 | OLC  | O20-C1-O19 | -2.32 | 117.81      | 123.63   |
| 2   | A     | 305 | OLC  | O20-C1-O19 | -2.29 | 117.90      | 123.63   |
| 2   | E     | 304 | OLC  | O20-C1-O19 | -2.25 | 118.00      | 123.63   |
| 2   | A     | 307 | OLC  | O20-C1-O19 | -2.18 | 118.19      | 123.63   |
| 2   | B     | 311 | OLC  | O20-C1-O19 | -2.17 | 118.21      | 123.63   |
| 2   | C     | 311 | OLC  | O20-C1-O19 | -2.14 | 118.27      | 123.63   |
| 2   | E     | 311 | OLC  | O20-C1-O19 | -2.14 | 118.28      | 123.63   |
| 2   | C     | 305 | OLC  | O20-C1-O19 | -2.13 | 118.29      | 123.63   |
| 2   | B     | 308 | OLC  | O20-C1-O19 | -2.11 | 118.35      | 123.63   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | D     | 307 | OLC  | O20-C1-O19 | -2.11 | 118.35      | 123.63   |
| 2   | A     | 303 | OLC  | O20-C1-O19 | -2.07 | 118.44      | 123.63   |
| 2   | E     | 305 | OLC  | O20-C1-O19 | -2.07 | 118.45      | 123.63   |
| 2   | C     | 308 | OLC  | O20-C1-O19 | -2.05 | 118.50      | 123.63   |
| 2   | E     | 306 | OLC  | O20-C1-O19 | -2.03 | 118.55      | 123.63   |
| 2   | B     | 312 | OLC  | O20-C1-O19 | -2.01 | 118.59      | 123.63   |

There are no chirality outliers.

All (710) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 301 | OLC  | O20-C21-C22-O23 |
| 2   | A     | 307 | OLC  | O20-C21-C22-C24 |
| 2   | A     | 307 | OLC  | O20-C21-C22-O23 |
| 2   | A     | 308 | OLC  | C21-C22-C24-O25 |
| 2   | A     | 308 | OLC  | O20-C21-C22-O23 |
| 2   | A     | 309 | OLC  | C21-C22-C24-O25 |
| 2   | A     | 310 | OLC  | C21-C22-C24-O25 |
| 2   | A     | 310 | OLC  | O20-C21-C22-C24 |
| 2   | A     | 310 | OLC  | O20-C21-C22-O23 |
| 2   | A     | 311 | OLC  | C21-C22-C24-O25 |
| 2   | B     | 303 | OLC  | C21-C22-C24-O25 |
| 2   | B     | 308 | OLC  | C10-C11-C12-C13 |
| 2   | B     | 311 | OLC  | O20-C21-C22-C24 |
| 2   | B     | 313 | OLC  | O20-C21-C22-C24 |
| 2   | B     | 313 | OLC  | O20-C21-C22-O23 |
| 2   | B     | 314 | OLC  | O20-C21-C22-C24 |
| 2   | B     | 314 | OLC  | O20-C21-C22-O23 |
| 2   | B     | 315 | OLC  | C21-C22-C24-O25 |
| 2   | B     | 315 | OLC  | O20-C21-C22-O23 |
| 2   | C     | 301 | OLC  | C21-C22-C24-O25 |
| 2   | C     | 303 | OLC  | C21-C22-C24-O25 |
| 2   | C     | 303 | OLC  | O20-C21-C22-O23 |
| 2   | C     | 307 | OLC  | C21-C22-C24-O25 |
| 2   | C     | 308 | OLC  | C21-C22-C24-O25 |
| 2   | C     | 309 | OLC  | C21-C22-C24-O25 |
| 2   | C     | 310 | OLC  | C21-C22-C24-O25 |
| 2   | C     | 312 | OLC  | C21-C22-C24-O25 |
| 2   | C     | 312 | OLC  | O23-C22-C24-O25 |
| 2   | C     | 312 | OLC  | O20-C21-C22-C24 |
| 2   | C     | 312 | OLC  | C2-C1-O20-C21   |
| 2   | C     | 312 | OLC  | O19-C1-O20-C21  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 313 | OLC  | O20-C21-C22-O23 |
| 2   | D     | 302 | OLC  | C21-C22-C24-O25 |
| 2   | D     | 302 | OLC  | O20-C21-C22-C24 |
| 2   | D     | 303 | OLC  | O20-C21-C22-O23 |
| 2   | D     | 307 | OLC  | C21-C22-C24-O25 |
| 2   | D     | 308 | OLC  | O20-C21-C22-C24 |
| 2   | D     | 308 | OLC  | O20-C21-C22-O23 |
| 2   | D     | 309 | OLC  | C21-C22-C24-O25 |
| 2   | E     | 304 | OLC  | C21-C22-C24-O25 |
| 2   | E     | 305 | OLC  | C21-C22-C24-O25 |
| 2   | E     | 305 | OLC  | O20-C21-C22-C24 |
| 2   | E     | 306 | OLC  | C21-C22-C24-O25 |
| 2   | E     | 307 | OLC  | C10-C11-C12-C13 |
| 2   | E     | 308 | OLC  | O20-C21-C22-O23 |
| 2   | E     | 309 | OLC  | O20-C21-C22-C24 |
| 2   | E     | 309 | OLC  | O20-C21-C22-O23 |
| 2   | E     | 310 | OLC  | C21-C22-C24-O25 |
| 2   | E     | 310 | OLC  | O20-C21-C22-O23 |
| 2   | E     | 311 | OLC  | C21-C22-C24-O25 |
| 2   | E     | 313 | OLC  | C21-C22-C24-O25 |
| 5   | A     | 320 | BOG  | C2'-C1'-O1-C1   |
| 2   | A     | 302 | OLC  | O19-C1-O20-C21  |
| 2   | A     | 309 | OLC  | O19-C1-O20-C21  |
| 2   | C     | 305 | OLC  | O19-C1-O20-C21  |
| 2   | C     | 305 | OLC  | C2-C1-O20-C21   |
| 2   | A     | 302 | OLC  | C2-C1-O20-C21   |
| 2   | A     | 309 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 314 | OLC  | C2-C1-O20-C21   |
| 2   | C     | 304 | OLC  | C2-C1-O20-C21   |
| 2   | D     | 309 | OLC  | O19-C1-O20-C21  |
| 2   | A     | 306 | OLC  | C2-C1-O20-C21   |
| 2   | A     | 321 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 301 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 308 | OLC  | C2-C1-O20-C21   |
| 2   | D     | 309 | OLC  | C2-C1-O20-C21   |
| 2   | A     | 306 | OLC  | O19-C1-O20-C21  |
| 2   | A     | 321 | OLC  | O19-C1-O20-C21  |
| 2   | B     | 314 | OLC  | O19-C1-O20-C21  |
| 2   | C     | 304 | OLC  | O19-C1-O20-C21  |
| 2   | E     | 309 | OLC  | O19-C1-O20-C21  |
| 2   | A     | 304 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 312 | OLC  | C2-C1-O20-C21   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 311 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 311 | OLC  | O20-C21-C22-O23 |
| 2   | C     | 311 | OLC  | O20-C21-C22-O23 |
| 2   | C     | 312 | OLC  | O20-C21-C22-O23 |
| 2   | B     | 301 | OLC  | O19-C1-O20-C21  |
| 2   | E     | 309 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 308 | OLC  | O19-C1-O20-C21  |
| 2   | C     | 311 | OLC  | O19-C1-O20-C21  |
| 2   | A     | 304 | OLC  | O19-C1-O20-C21  |
| 2   | B     | 312 | OLC  | O19-C1-O20-C21  |
| 2   | D     | 301 | OLC  | C2-C1-O20-C21   |
| 2   | D     | 301 | OLC  | O19-C1-O20-C21  |
| 2   | A     | 308 | OLC  | C2-C1-O20-C21   |
| 2   | C     | 303 | OLC  | C2-C1-O20-C21   |
| 2   | C     | 309 | OLC  | C2-C1-O20-C21   |
| 2   | D     | 303 | OLC  | C2-C1-O20-C21   |
| 2   | D     | 304 | OLC  | C2-C1-O20-C21   |
| 2   | E     | 311 | OLC  | C2-C1-O20-C21   |
| 2   | E     | 306 | OLC  | C2-C3-C4-C5     |
| 2   | A     | 301 | OLC  | O20-C21-C22-C24 |
| 2   | C     | 311 | OLC  | O20-C21-C22-C24 |
| 2   | E     | 310 | OLC  | O20-C21-C22-C24 |
| 2   | E     | 311 | OLC  | O20-C21-C22-C24 |
| 5   | E     | 321 | BOG  | C2-C1-O1-C1'    |
| 2   | E     | 311 | OLC  | O19-C1-O20-C21  |
| 2   | D     | 302 | OLC  | O20-C21-C22-O23 |
| 2   | E     | 305 | OLC  | O20-C21-C22-O23 |
| 2   | E     | 311 | OLC  | O20-C21-C22-O23 |
| 2   | C     | 309 | OLC  | O19-C1-O20-C21  |
| 2   | D     | 303 | OLC  | O19-C1-O20-C21  |
| 2   | B     | 311 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 305 | OLC  | O23-C22-C24-O25 |
| 2   | C     | 301 | OLC  | O23-C22-C24-O25 |
| 2   | D     | 308 | OLC  | O23-C22-C24-O25 |
| 2   | D     | 309 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 304 | OLC  | O23-C22-C24-O25 |
| 2   | C     | 310 | OLC  | C1-C2-C3-C4     |
| 2   | B     | 313 | OLC  | C1-C2-C3-C4     |
| 2   | D     | 307 | OLC  | C1-C2-C3-C4     |
| 2   | A     | 304 | OLC  | C1-C2-C3-C4     |
| 2   | A     | 306 | OLC  | C1-C2-C3-C4     |
| 2   | E     | 301 | OLC  | C1-C2-C3-C4     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 303 | OLC  | O19-C1-O20-C21  |
| 2   | A     | 302 | OLC  | C1-C2-C3-C4     |
| 2   | E     | 313 | OLC  | C1-C2-C3-C4     |
| 2   | D     | 304 | OLC  | O19-C1-O20-C21  |
| 5   | E     | 321 | BOG  | O5-C1-O1-C1'    |
| 2   | C     | 301 | OLC  | C2-C1-O20-C21   |
| 2   | E     | 303 | OLC  | C2-C1-O20-C21   |
| 2   | A     | 308 | OLC  | O19-C1-O20-C21  |
| 2   | B     | 306 | OLC  | C1-C2-C3-C4     |
| 5   | B     | 321 | BOG  | O5-C5-C6-O6     |
| 5   | E     | 321 | BOG  | O5-C5-C6-O6     |
| 5   | E     | 321 | BOG  | C4-C5-C6-O6     |
| 2   | B     | 311 | OLC  | O19-C1-O20-C21  |
| 2   | B     | 306 | OLC  | O20-C21-C22-O23 |
| 2   | C     | 301 | OLC  | O20-C21-C22-O23 |
| 2   | D     | 301 | OLC  | O20-C21-C22-O23 |
| 2   | E     | 303 | OLC  | O20-C21-C22-O23 |
| 2   | E     | 313 | OLC  | O20-C21-C22-O23 |
| 5   | B     | 321 | BOG  | C4-C5-C6-O6     |
| 2   | D     | 304 | OLC  | C1-C2-C3-C4     |
| 2   | E     | 305 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 304 | OLC  | C1-C2-C3-C4     |
| 2   | A     | 321 | OLC  | C2-C3-C4-C5     |
| 5   | E     | 321 | BOG  | O1-C1'-C2'-C3'  |
| 2   | B     | 314 | OLC  | C1-C2-C3-C4     |
| 2   | C     | 310 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 306 | OLC  | O20-C21-C22-C24 |
| 2   | C     | 303 | OLC  | O20-C21-C22-C24 |
| 2   | C     | 313 | OLC  | O20-C21-C22-C24 |
| 2   | D     | 301 | OLC  | O20-C21-C22-C24 |
| 2   | E     | 303 | OLC  | O20-C21-C22-C24 |
| 2   | E     | 308 | OLC  | O20-C21-C22-C24 |
| 2   | E     | 313 | OLC  | O20-C21-C22-C24 |
| 2   | E     | 305 | OLC  | O19-C1-O20-C21  |
| 2   | B     | 310 | OLC  | O20-C21-C22-O23 |
| 2   | C     | 306 | OLC  | O20-C21-C22-O23 |
| 2   | A     | 302 | OLC  | C21-C22-C24-O25 |
| 2   | A     | 304 | OLC  | C21-C22-C24-O25 |
| 2   | B     | 305 | OLC  | C21-C22-C24-O25 |
| 2   | B     | 310 | OLC  | C21-C22-C24-O25 |
| 2   | B     | 314 | OLC  | C21-C22-C24-O25 |
| 2   | C     | 305 | OLC  | C21-C22-C24-O25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | D     | 306 | OLC  | C21-C22-C24-O25 |
| 2   | D     | 308 | OLC  | C21-C22-C24-O25 |
| 2   | E     | 301 | OLC  | C21-C22-C24-O25 |
| 2   | E     | 309 | OLC  | C21-C22-C24-O25 |
| 2   | C     | 301 | OLC  | O19-C1-O20-C21  |
| 5   | B     | 321 | BOG  | C1'-C2'-C3'-C4' |
| 2   | B     | 313 | OLC  | C5-C6-C7-C8     |
| 2   | D     | 303 | OLC  | C5-C6-C7-C8     |
| 3   | C     | 319 | LFA  | C12-C13-C14-C15 |
| 2   | E     | 303 | OLC  | O19-C1-O20-C21  |
| 2   | A     | 302 | OLC  | C4-C5-C6-C7     |
| 2   | B     | 305 | OLC  | C4-C5-C6-C7     |
| 2   | B     | 307 | OLC  | C3-C4-C5-C6     |
| 2   | C     | 305 | OLC  | C3-C4-C5-C6     |
| 3   | B     | 302 | LFA  | C16-C17-C18-C19 |
| 2   | A     | 302 | OLC  | O23-C22-C24-O25 |
| 2   | A     | 308 | OLC  | O23-C22-C24-O25 |
| 2   | A     | 309 | OLC  | O23-C22-C24-O25 |
| 2   | A     | 311 | OLC  | O23-C22-C24-O25 |
| 2   | B     | 303 | OLC  | O23-C22-C24-O25 |
| 2   | B     | 310 | OLC  | O23-C22-C24-O25 |
| 2   | C     | 303 | OLC  | O23-C22-C24-O25 |
| 2   | C     | 307 | OLC  | O23-C22-C24-O25 |
| 2   | C     | 308 | OLC  | O23-C22-C24-O25 |
| 2   | C     | 309 | OLC  | O23-C22-C24-O25 |
| 2   | C     | 310 | OLC  | O23-C22-C24-O25 |
| 2   | D     | 302 | OLC  | O23-C22-C24-O25 |
| 2   | D     | 307 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 306 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 309 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 310 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 313 | OLC  | O23-C22-C24-O25 |
| 5   | E     | 321 | BOG  | C2'-C1'-O1-C1   |
| 2   | A     | 308 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 305 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 301 | OLC  | C5-C6-C7-C8     |
| 2   | D     | 309 | OLC  | C2-C3-C4-C5     |
| 2   | C     | 310 | OLC  | C10-C11-C12-C13 |
| 3   | B     | 316 | LFA  | C16-C17-C18-C19 |
| 3   | D     | 313 | LFA  | C7-C8-C9-C10    |
| 2   | B     | 306 | OLC  | C5-C6-C7-C8     |
| 3   | B     | 317 | LFA  | C3-C4-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | B     | 314 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 310 | OLC  | C2-C3-C4-C5     |
| 2   | D     | 305 | OLC  | C5-C6-C7-C8     |
| 3   | A     | 315 | LFA  | C11-C10-C9-C8   |
| 2   | B     | 313 | OLC  | C4-C5-C6-C7     |
| 3   | D     | 310 | LFA  | C6-C7-C8-C9     |
| 2   | C     | 310 | OLC  | O19-C1-O20-C21  |
| 2   | B     | 304 | OLC  | C14-C15-C16-C17 |
| 2   | B     | 304 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 310 | OLC  | C5-C6-C7-C8     |
| 2   | E     | 306 | OLC  | C5-C6-C7-C8     |
| 3   | D     | 314 | LFA  | C15-C16-C17-C18 |
| 2   | B     | 309 | OLC  | C2-C3-C4-C5     |
| 3   | B     | 317 | LFA  | C2-C3-C4-C5     |
| 3   | B     | 318 | LFA  | C5-C6-C7-C8     |
| 3   | C     | 315 | LFA  | C16-C17-C18-C19 |
| 3   | C     | 316 | LFA  | C12-C13-C14-C15 |
| 3   | D     | 312 | LFA  | C2-C3-C4-C5     |
| 3   | D     | 314 | LFA  | C16-C17-C18-C19 |
| 2   | D     | 302 | OLC  | C1-C2-C3-C4     |
| 2   | A     | 303 | OLC  | C3-C4-C5-C6     |
| 2   | A     | 308 | OLC  | C13-C14-C15-C16 |
| 3   | C     | 319 | LFA  | C9-C10-C11-C12  |
| 2   | A     | 321 | OLC  | C5-C6-C7-C8     |
| 5   | E     | 321 | BOG  | C2'-C3'-C4'-C5' |
| 3   | A     | 318 | LFA  | C5-C6-C7-C8     |
| 2   | A     | 304 | OLC  | C6-C7-C8-C9     |
| 2   | A     | 321 | OLC  | C10-C11-C12-C13 |
| 2   | C     | 305 | OLC  | C10-C11-C12-C13 |
| 2   | D     | 305 | OLC  | C6-C7-C8-C9     |
| 2   | E     | 301 | OLC  | C10-C11-C12-C13 |
| 2   | C     | 311 | OLC  | C3-C4-C5-C6     |
| 2   | D     | 305 | OLC  | C3-C4-C5-C6     |
| 3   | E     | 319 | LFA  | C6-C7-C8-C9     |
| 2   | A     | 301 | OLC  | C1-C2-C3-C4     |
| 2   | A     | 302 | OLC  | C11-C12-C13-C14 |
| 2   | B     | 304 | OLC  | C3-C4-C5-C6     |
| 2   | B     | 310 | OLC  | C2-C3-C4-C5     |
| 2   | D     | 309 | OLC  | C11-C12-C13-C14 |
| 5   | D     | 317 | BOG  | C1'-C2'-C3'-C4' |
| 3   | D     | 312 | LFA  | C4-C5-C6-C7     |
| 2   | A     | 302 | OLC  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | D     | 304 | OLC  | C5-C6-C7-C8     |
| 3   | D     | 313 | LFA  | C15-C16-C17-C18 |
| 2   | B     | 303 | OLC  | C1-C2-C3-C4     |
| 2   | B     | 311 | OLC  | C1-C2-C3-C4     |
| 2   | E     | 304 | OLC  | C2-C1-O20-C21   |
| 2   | A     | 309 | OLC  | O20-C21-C22-C24 |
| 2   | E     | 312 | OLC  | O20-C21-C22-C24 |
| 2   | D     | 309 | OLC  | C13-C14-C15-C16 |
| 3   | A     | 318 | LFA  | C11-C12-C13-C14 |
| 3   | C     | 319 | LFA  | C10-C11-C12-C13 |
| 3   | A     | 314 | LFA  | C16-C17-C18-C19 |
| 2   | B     | 306 | OLC  | C3-C4-C5-C6     |
| 2   | D     | 309 | OLC  | C12-C13-C14-C15 |
| 2   | A     | 308 | OLC  | C11-C12-C13-C14 |
| 2   | B     | 311 | OLC  | C4-C5-C6-C7     |
| 2   | E     | 309 | OLC  | C2-C3-C4-C5     |
| 2   | A     | 321 | OLC  | C12-C13-C14-C15 |
| 2   | E     | 305 | OLC  | C3-C4-C5-C6     |
| 2   | E     | 312 | OLC  | C11-C12-C13-C14 |
| 2   | E     | 314 | OLC  | C2-C1-O20-C21   |
| 2   | E     | 305 | OLC  | C11-C12-C13-C14 |
| 2   | A     | 303 | OLC  | C6-C7-C8-C9     |
| 2   | A     | 308 | OLC  | C10-C11-C12-C13 |
| 2   | B     | 301 | OLC  | C10-C11-C12-C13 |
| 2   | C     | 304 | OLC  | C10-C11-C12-C13 |
| 2   | C     | 304 | OLC  | C6-C7-C8-C9     |
| 2   | C     | 310 | OLC  | C6-C7-C8-C9     |
| 2   | D     | 301 | OLC  | C6-C7-C8-C9     |
| 2   | E     | 306 | OLC  | C6-C7-C8-C9     |
| 2   | D     | 309 | OLC  | C1-C2-C3-C4     |
| 2   | B     | 311 | OLC  | C5-C6-C7-C8     |
| 2   | C     | 303 | OLC  | C2-C3-C4-C5     |
| 2   | D     | 305 | OLC  | C4-C5-C6-C7     |
| 2   | E     | 310 | OLC  | C3-C4-C5-C6     |
| 3   | E     | 323 | LFA  | C3-C4-C5-C6     |
| 3   | A     | 318 | LFA  | C6-C7-C8-C9     |
| 3   | A     | 318 | LFA  | C15-C16-C17-C18 |
| 3   | C     | 319 | LFA  | C11-C10-C9-C8   |
| 3   | C     | 302 | LFA  | C3-C4-C5-C6     |
| 5   | C     | 321 | BOG  | C1'-C2'-C3'-C4' |
| 2   | D     | 301 | OLC  | C1-C2-C3-C4     |
| 2   | D     | 306 | OLC  | C1-C2-C3-C4     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 306 | OLC  | C14-C15-C16-C17 |
| 2   | E     | 307 | OLC  | C4-C5-C6-C7     |
| 3   | D     | 310 | LFA  | C3-C4-C5-C6     |
| 3   | E     | 323 | LFA  | C4-C5-C6-C7     |
| 3   | E     | 319 | LFA  | C16-C17-C18-C19 |
| 2   | B     | 310 | OLC  | C1-C2-C3-C4     |
| 2   | D     | 307 | OLC  | C2-C3-C4-C5     |
| 3   | C     | 302 | LFA  | C7-C8-C9-C10    |
| 3   | D     | 310 | LFA  | C9-C10-C11-C12  |
| 3   | E     | 323 | LFA  | C2-C3-C4-C5     |
| 2   | E     | 313 | OLC  | C6-C7-C8-C9     |
| 3   | E     | 319 | LFA  | C13-C14-C15-C16 |
| 2   | D     | 305 | OLC  | C2-C1-O20-C21   |
| 2   | E     | 307 | OLC  | C5-C6-C7-C8     |
| 2   | E     | 307 | OLC  | C3-C4-C5-C6     |
| 2   | E     | 308 | OLC  | C4-C5-C6-C7     |
| 3   | E     | 302 | LFA  | C7-C8-C9-C10    |
| 2   | C     | 305 | OLC  | C12-C13-C14-C15 |
| 2   | C     | 308 | OLC  | C11-C12-C13-C14 |
| 3   | B     | 302 | LFA  | C7-C8-C9-C10    |
| 3   | B     | 316 | LFA  | C15-C16-C17-C18 |
| 3   | B     | 316 | LFA  | C14-C15-C16-C17 |
| 2   | C     | 311 | OLC  | C4-C5-C6-C7     |
| 2   | E     | 314 | OLC  | C12-C13-C14-C15 |
| 2   | A     | 310 | OLC  | C4-C5-C6-C7     |
| 2   | B     | 307 | OLC  | C4-C5-C6-C7     |
| 3   | C     | 302 | LFA  | C9-C10-C11-C12  |
| 2   | B     | 315 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 305 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 311 | OLC  | O23-C22-C24-O25 |
| 3   | A     | 318 | LFA  | C9-C10-C11-C12  |
| 2   | B     | 305 | OLC  | C2-C3-C4-C5     |
| 2   | C     | 306 | OLC  | C3-C4-C5-C6     |
| 2   | A     | 303 | OLC  | C10-C11-C12-C13 |
| 2   | B     | 307 | OLC  | C6-C7-C8-C9     |
| 2   | C     | 308 | OLC  | C6-C7-C8-C9     |
| 2   | D     | 306 | OLC  | C6-C7-C8-C9     |
| 2   | E     | 309 | OLC  | C10-C11-C12-C13 |
| 2   | E     | 309 | OLC  | C6-C7-C8-C9     |
| 2   | E     | 309 | OLC  | C3-C4-C5-C6     |
| 3   | B     | 319 | LFA  | C15-C16-C17-C18 |
| 3   | C     | 302 | LFA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | E     | 309 | OLC  | C1-C2-C3-C4     |
| 2   | B     | 310 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 301 | OLC  | C4-C5-C6-C7     |
| 5   | D     | 317 | BOG  | C4'-C5'-C6'-C7' |
| 2   | B     | 311 | OLC  | C11-C12-C13-C14 |
| 2   | A     | 302 | OLC  | C12-C13-C14-C15 |
| 2   | A     | 303 | OLC  | C4-C5-C6-C7     |
| 2   | E     | 304 | OLC  | O19-C1-O20-C21  |
| 2   | E     | 314 | OLC  | O19-C1-O20-C21  |
| 3   | E     | 316 | LFA  | C14-C15-C16-C17 |
| 2   | E     | 313 | OLC  | C3-C4-C5-C6     |
| 2   | C     | 312 | OLC  | C2-C3-C4-C5     |
| 2   | B     | 309 | OLC  | C10-C11-C12-C13 |
| 2   | B     | 311 | OLC  | C10-C11-C12-C13 |
| 2   | C     | 307 | OLC  | C6-C7-C8-C9     |
| 2   | E     | 305 | OLC  | C6-C7-C8-C9     |
| 2   | E     | 314 | OLC  | C6-C7-C8-C9     |
| 3   | B     | 302 | LFA  | C6-C7-C8-C9     |
| 2   | D     | 306 | OLC  | C2-C1-O20-C21   |
| 3   | C     | 316 | LFA  | C15-C16-C17-C18 |
| 3   | C     | 302 | LFA  | C16-C17-C18-C19 |
| 3   | C     | 317 | LFA  | C4-C5-C6-C7     |
| 3   | D     | 313 | LFA  | C9-C10-C11-C12  |
| 2   | D     | 305 | OLC  | O19-C1-O20-C21  |
| 3   | C     | 317 | LFA  | C3-C4-C5-C6     |
| 3   | E     | 319 | LFA  | C14-C15-C16-C17 |
| 2   | B     | 310 | OLC  | C5-C6-C7-C8     |
| 2   | E     | 314 | OLC  | C5-C6-C7-C8     |
| 2   | C     | 306 | OLC  | C12-C13-C14-C15 |
| 2   | E     | 312 | OLC  | O20-C21-C22-O23 |
| 2   | D     | 306 | OLC  | O19-C1-O20-C21  |
| 2   | C     | 309 | OLC  | C2-C3-C4-C5     |
| 2   | E     | 312 | OLC  | C4-C5-C6-C7     |
| 2   | A     | 308 | OLC  | C6-C7-C8-C9     |
| 2   | C     | 301 | OLC  | C10-C11-C12-C13 |
| 2   | A     | 302 | OLC  | C3-C4-C5-C6     |
| 2   | A     | 304 | OLC  | C13-C14-C15-C16 |
| 2   | E     | 301 | OLC  | C14-C15-C16-C17 |
| 3   | E     | 319 | LFA  | C12-C13-C14-C15 |
| 2   | E     | 301 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 313 | OLC  | C2-C1-O20-C21   |
| 2   | D     | 308 | OLC  | C2-C1-O20-C21   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | B     | 321 | BOG  | C5'-C6'-C7'-C8' |
| 2   | B     | 307 | OLC  | C11-C12-C13-C14 |
| 3   | D     | 313 | LFA  | C13-C14-C15-C16 |
| 2   | E     | 301 | OLC  | C5-C6-C7-C8     |
| 2   | E     | 313 | OLC  | C5-C6-C7-C8     |
| 2   | A     | 302 | OLC  | C2-C3-C4-C5     |
| 2   | C     | 306 | OLC  | C5-C6-C7-C8     |
| 3   | E     | 302 | LFA  | C11-C10-C9-C8   |
| 3   | D     | 311 | LFA  | C1-C2-C3-C4     |
| 3   | D     | 313 | LFA  | C16-C17-C18-C19 |
| 2   | E     | 309 | OLC  | C11-C12-C13-C14 |
| 3   | D     | 312 | LFA  | C5-C6-C7-C8     |
| 2   | E     | 312 | OLC  | C22-C21-O20-C1  |
| 3   | A     | 313 | LFA  | C1-C2-C3-C4     |
| 3   | C     | 317 | LFA  | C1-C2-C3-C4     |
| 2   | B     | 306 | OLC  | C4-C5-C6-C7     |
| 2   | E     | 314 | OLC  | C13-C14-C15-C16 |
| 3   | C     | 316 | LFA  | C16-C17-C18-C19 |
| 3   | D     | 310 | LFA  | C11-C10-C9-C8   |
| 3   | C     | 315 | LFA  | C13-C14-C15-C16 |
| 2   | D     | 309 | OLC  | C10-C11-C12-C13 |
| 3   | B     | 318 | LFA  | C7-C8-C9-C10    |
| 2   | B     | 301 | OLC  | C15-C16-C17-C18 |
| 3   | E     | 318 | LFA  | C17-C18-C19-C20 |
| 2   | B     | 315 | OLC  | C1-C2-C3-C4     |
| 2   | A     | 311 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 303 | OLC  | C2-C1-O20-C21   |
| 2   | B     | 303 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 312 | OLC  | C6-C7-C8-C9     |
| 5   | C     | 321 | BOG  | C5'-C6'-C7'-C8' |
| 2   | E     | 306 | OLC  | C13-C14-C15-C16 |
| 3   | D     | 311 | LFA  | C11-C12-C13-C14 |
| 2   | A     | 310 | OLC  | C6-C7-C8-C9     |
| 5   | E     | 321 | BOG  | C5'-C6'-C7'-C8' |
| 2   | B     | 311 | OLC  | C12-C13-C14-C15 |
| 2   | C     | 310 | OLC  | C4-C5-C6-C7     |
| 2   | D     | 306 | OLC  | C4-C5-C6-C7     |
| 2   | E     | 306 | OLC  | C11-C12-C13-C14 |
| 3   | A     | 312 | LFA  | C15-C16-C17-C18 |
| 3   | D     | 313 | LFA  | C5-C6-C7-C8     |
| 2   | B     | 301 | OLC  | O23-C22-C24-O25 |
| 2   | D     | 306 | OLC  | O23-C22-C24-O25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | B     | 310 | OLC  | O20-C21-C22-C24 |
| 2   | D     | 303 | OLC  | O20-C21-C22-C24 |
| 2   | E     | 309 | OLC  | C12-C13-C14-C15 |
| 2   | A     | 308 | OLC  | C3-C4-C5-C6     |
| 2   | B     | 304 | OLC  | C13-C14-C15-C16 |
| 3   | C     | 316 | LFA  | C9-C10-C11-C12  |
| 2   | A     | 302 | OLC  | C6-C7-C8-C9     |
| 2   | D     | 309 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 304 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 303 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 313 | OLC  | C4-C5-C6-C7     |
| 3   | A     | 318 | LFA  | C1-C2-C3-C4     |
| 3   | C     | 315 | LFA  | C17-C18-C19-C20 |
| 3   | C     | 316 | LFA  | C13-C14-C15-C16 |
| 3   | D     | 314 | LFA  | C14-C15-C16-C17 |
| 2   | B     | 313 | OLC  | C2-C1-O20-C21   |
| 3   | C     | 302 | LFA  | C13-C14-C15-C16 |
| 5   | E     | 321 | BOG  | C1'-C2'-C3'-C4' |
| 3   | D     | 311 | LFA  | C14-C15-C16-C17 |
| 3   | D     | 311 | LFA  | C10-C11-C12-C13 |
| 3   | E     | 316 | LFA  | C7-C8-C9-C10    |
| 3   | E     | 316 | LFA  | C9-C10-C11-C12  |
| 5   | A     | 320 | BOG  | O1-C1'-C2'-C3'  |
| 2   | C     | 310 | OLC  | C3-C4-C5-C6     |
| 3   | D     | 310 | LFA  | C16-C17-C18-C19 |
| 3   | D     | 311 | LFA  | C3-C4-C5-C6     |
| 2   | E     | 309 | OLC  | C14-C15-C16-C17 |
| 3   | C     | 302 | LFA  | C2-C3-C4-C5     |
| 2   | C     | 312 | OLC  | C5-C6-C7-C8     |
| 2   | C     | 301 | OLC  | C11-C12-C13-C14 |
| 3   | B     | 318 | LFA  | C1-C2-C3-C4     |
| 2   | E     | 301 | OLC  | C3-C4-C5-C6     |
| 2   | C     | 303 | OLC  | C3-C4-C5-C6     |
| 2   | D     | 301 | OLC  | C2-C3-C4-C5     |
| 2   | C     | 313 | OLC  | O19-C1-O20-C21  |
| 2   | C     | 313 | OLC  | C2-C3-C4-C5     |
| 5   | A     | 320 | BOG  | C5'-C6'-C7'-C8' |
| 2   | C     | 308 | OLC  | C2-C3-C4-C5     |
| 2   | C     | 305 | OLC  | C5-C6-C7-C8     |
| 2   | A     | 308 | OLC  | O20-C21-C22-C24 |
| 2   | C     | 309 | OLC  | O20-C21-C22-C24 |
| 2   | C     | 310 | OLC  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | B     | 311 | OLC  | C6-C7-C8-C9     |
| 2   | A     | 309 | OLC  | O20-C21-C22-O23 |
| 2   | C     | 313 | OLC  | C3-C4-C5-C6     |
| 3   | C     | 314 | LFA  | C4-C5-C6-C7     |
| 3   | C     | 319 | LFA  | C4-C5-C6-C7     |
| 2   | A     | 310 | OLC  | O23-C22-C24-O25 |
| 2   | C     | 313 | OLC  | O23-C22-C24-O25 |
| 2   | D     | 301 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 308 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 312 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 304 | OLC  | C1-C2-C3-C4     |
| 2   | E     | 306 | OLC  | C3-C4-C5-C6     |
| 2   | B     | 304 | OLC  | C10-C11-C12-C13 |
| 2   | E     | 305 | OLC  | C10-C11-C12-C13 |
| 2   | B     | 303 | OLC  | O19-C1-O20-C21  |
| 2   | D     | 308 | OLC  | O19-C1-O20-C21  |
| 5   | C     | 321 | BOG  | C3'-C4'-C5'-C6' |
| 2   | A     | 311 | OLC  | C1-C2-C3-C4     |
| 2   | D     | 303 | OLC  | C1-C2-C3-C4     |
| 2   | E     | 314 | OLC  | C14-C15-C16-C17 |
| 2   | A     | 311 | OLC  | O19-C1-O20-C21  |
| 3   | C     | 316 | LFA  | C4-C5-C6-C7     |
| 2   | B     | 308 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 304 | OLC  | O20-C21-C22-O23 |
| 2   | E     | 308 | OLC  | C21-C22-C24-O25 |
| 3   | C     | 316 | LFA  | C6-C7-C8-C9     |
| 3   | C     | 314 | LFA  | C2-C3-C4-C5     |
| 2   | B     | 313 | OLC  | O19-C1-O20-C21  |
| 2   | D     | 308 | OLC  | C2-C3-C4-C5     |
| 2   | D     | 306 | OLC  | C10-C11-C12-C13 |
| 3   | A     | 318 | LFA  | C17-C18-C19-C20 |
| 2   | E     | 304 | OLC  | C4-C5-C6-C7     |
| 2   | B     | 309 | OLC  | C5-C6-C7-C8     |
| 3   | D     | 310 | LFA  | C4-C5-C6-C7     |
| 2   | C     | 308 | OLC  | C4-C5-C6-C7     |
| 3   | D     | 310 | LFA  | C17-C18-C19-C20 |
| 2   | E     | 313 | OLC  | C4-C5-C6-C7     |
| 3   | E     | 316 | LFA  | C13-C14-C15-C16 |
| 2   | B     | 315 | OLC  | O20-C21-C22-C24 |
| 2   | B     | 310 | OLC  | C3-C4-C5-C6     |
| 3   | D     | 310 | LFA  | C7-C8-C9-C10    |
| 2   | B     | 303 | OLC  | O20-C21-C22-O23 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | B     | 311 | OLC  | C2-C3-C4-C5     |
| 2   | A     | 307 | OLC  | C6-C7-C8-C9     |
| 2   | E     | 312 | OLC  | C13-C14-C15-C16 |
| 2   | A     | 306 | OLC  | C4-C5-C6-C7     |
| 2   | B     | 309 | OLC  | C4-C5-C6-C7     |
| 2   | B     | 303 | OLC  | C2-C3-C4-C5     |
| 2   | B     | 313 | OLC  | O20-C1-C2-C3    |
| 2   | B     | 314 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 306 | OLC  | C2-C1-O20-C21   |
| 2   | E     | 312 | OLC  | C14-C15-C16-C17 |
| 3   | A     | 312 | LFA  | C17-C18-C19-C20 |
| 3   | A     | 317 | LFA  | C2-C3-C4-C5     |
| 2   | C     | 305 | OLC  | O20-C21-C22-O23 |
| 2   | C     | 309 | OLC  | O20-C21-C22-O23 |
| 3   | C     | 302 | LFA  | C17-C18-C19-C20 |
| 5   | A     | 320 | BOG  | C1'-C2'-C3'-C4' |
| 3   | A     | 312 | LFA  | C16-C17-C18-C19 |
| 2   | C     | 307 | OLC  | C12-C13-C14-C15 |
| 2   | A     | 308 | OLC  | C9-C10-C11-C12  |
| 2   | E     | 301 | OLC  | C7-C8-C9-C10    |
| 3   | A     | 315 | LFA  | C4-C5-C6-C7     |
| 2   | A     | 304 | OLC  | C5-C6-C7-C8     |
| 2   | E     | 305 | OLC  | C22-C21-O20-C1  |
| 2   | B     | 309 | OLC  | O20-C21-C22-C24 |
| 2   | D     | 306 | OLC  | C5-C6-C7-C8     |
| 2   | E     | 303 | OLC  | C2-C3-C4-C5     |
| 3   | C     | 318 | LFA  | C17-C18-C19-C20 |
| 3   | E     | 317 | LFA  | C17-C18-C19-C20 |
| 3   | B     | 302 | LFA  | C5-C6-C7-C8     |
| 2   | A     | 307 | OLC  | C5-C6-C7-C8     |
| 3   | D     | 313 | LFA  | C4-C5-C6-C7     |
| 2   | B     | 312 | OLC  | C6-C7-C8-C9     |
| 2   | E     | 306 | OLC  | O19-C1-O20-C21  |
| 2   | C     | 305 | OLC  | C9-C10-C11-C12  |
| 3   | E     | 319 | LFA  | C9-C10-C11-C12  |
| 3   | A     | 315 | LFA  | C7-C8-C9-C10    |
| 2   | A     | 302 | OLC  | C14-C15-C16-C17 |
| 2   | D     | 309 | OLC  | C5-C6-C7-C8     |
| 2   | C     | 306 | OLC  | C15-C16-C17-C18 |
| 2   | E     | 301 | OLC  | C13-C14-C15-C16 |
| 2   | A     | 309 | OLC  | C2-C3-C4-C5     |
| 2   | D     | 308 | OLC  | C3-C4-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 308 | OLC  | C12-C13-C14-C15 |
| 2   | C     | 306 | OLC  | C13-C14-C15-C16 |
| 5   | B     | 321 | BOG  | C3'-C4'-C5'-C6' |
| 2   | C     | 306 | OLC  | C1-C2-C3-C4     |
| 2   | A     | 309 | OLC  | C5-C6-C7-C8     |
| 2   | B     | 315 | OLC  | C6-C7-C8-C9     |
| 3   | C     | 314 | LFA  | C1-C2-C3-C4     |
| 3   | C     | 319 | LFA  | C15-C16-C17-C18 |
| 2   | E     | 309 | OLC  | C15-C16-C17-C18 |
| 3   | B     | 318 | LFA  | C6-C7-C8-C9     |
| 2   | D     | 305 | OLC  | C9-C10-C11-C12  |
| 2   | D     | 306 | OLC  | C7-C8-C9-C10    |
| 3   | C     | 302 | LFA  | C4-C5-C6-C7     |
| 2   | D     | 307 | OLC  | C4-C5-C6-C7     |
| 2   | C     | 304 | OLC  | C11-C12-C13-C14 |
| 3   | E     | 319 | LFA  | C7-C8-C9-C10    |
| 2   | A     | 305 | OLC  | O20-C21-C22-O23 |
| 2   | D     | 306 | OLC  | C3-C4-C5-C6     |
| 3   | C     | 302 | LFA  | C1-C2-C3-C4     |
| 2   | A     | 310 | OLC  | C3-C4-C5-C6     |
| 2   | A     | 321 | OLC  | C13-C14-C15-C16 |
| 2   | B     | 301 | OLC  | C6-C7-C8-C9     |
| 2   | A     | 304 | OLC  | C9-C10-C11-C12  |
| 2   | C     | 306 | OLC  | C7-C8-C9-C10    |
| 2   | E     | 314 | OLC  | C7-C8-C9-C10    |
| 2   | E     | 301 | OLC  | C6-C7-C8-C9     |
| 3   | A     | 314 | LFA  | C15-C16-C17-C18 |
| 3   | D     | 311 | LFA  | C16-C17-C18-C19 |
| 3   | E     | 315 | LFA  | C17-C18-C19-C20 |
| 3   | C     | 319 | LFA  | C16-C17-C18-C19 |
| 3   | C     | 316 | LFA  | C2-C3-C4-C5     |
| 2   | E     | 310 | OLC  | C2-C1-O20-C21   |
| 2   | E     | 313 | OLC  | C2-C1-O20-C21   |
| 2   | A     | 304 | OLC  | C7-C8-C9-C10    |
| 2   | B     | 309 | OLC  | C7-C8-C9-C10    |
| 2   | D     | 309 | OLC  | C7-C8-C9-C10    |
| 2   | E     | 310 | OLC  | O19-C1-O20-C21  |
| 2   | D     | 302 | OLC  | C3-C4-C5-C6     |
| 2   | B     | 301 | OLC  | C11-C12-C13-C14 |
| 3   | C     | 315 | LFA  | C15-C16-C17-C18 |
| 3   | D     | 311 | LFA  | C4-C5-C6-C7     |
| 3   | A     | 318 | LFA  | C4-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 307 | OLC  | O20-C21-C22-O23 |
| 2   | E     | 306 | OLC  | O20-C21-C22-O23 |
| 2   | E     | 313 | OLC  | C9-C10-C11-C12  |
| 2   | B     | 301 | OLC  | C5-C6-C7-C8     |
| 2   | E     | 313 | OLC  | O19-C1-O20-C21  |
| 2   | C     | 309 | OLC  | C1-C2-C3-C4     |
| 3   | E     | 316 | LFA  | C11-C12-C13-C14 |
| 2   | B     | 309 | OLC  | C2-C1-O20-C21   |
| 2   | E     | 310 | OLC  | C5-C6-C7-C8     |
| 5   | A     | 320 | BOG  | C2'-C3'-C4'-C5' |
| 2   | C     | 304 | OLC  | C21-C22-C24-O25 |
| 3   | E     | 302 | LFA  | C5-C6-C7-C8     |
| 2   | B     | 307 | OLC  | O20-C1-C2-C3    |
| 2   | C     | 304 | OLC  | O23-C22-C24-O25 |
| 2   | E     | 301 | OLC  | O23-C22-C24-O25 |
| 2   | B     | 304 | OLC  | C5-C6-C7-C8     |
| 3   | C     | 316 | LFA  | C3-C4-C5-C6     |
| 2   | B     | 309 | OLC  | O19-C1-O20-C21  |
| 3   | B     | 317 | LFA  | C1-C2-C3-C4     |
| 3   | B     | 318 | LFA  | C4-C5-C6-C7     |
| 2   | C     | 305 | OLC  | C7-C8-C9-C10    |
| 3   | B     | 317 | LFA  | C5-C6-C7-C8     |
| 3   | E     | 302 | LFA  | C4-C5-C6-C7     |
| 2   | E     | 301 | OLC  | C15-C16-C17-C18 |
| 3   | D     | 312 | LFA  | C1-C2-C3-C4     |
| 2   | E     | 305 | OLC  | C5-C6-C7-C8     |
| 2   | B     | 301 | OLC  | C7-C8-C9-C10    |
| 2   | B     | 311 | OLC  | C9-C10-C11-C12  |
| 2   | C     | 308 | OLC  | C7-C8-C9-C10    |
| 3   | E     | 319 | LFA  | C11-C10-C9-C8   |
| 3   | E     | 319 | LFA  | C11-C12-C13-C14 |
| 2   | A     | 302 | OLC  | C10-C11-C12-C13 |
| 2   | D     | 301 | OLC  | C7-C8-C9-C10    |
| 2   | B     | 311 | OLC  | C14-C15-C16-C17 |
| 2   | C     | 310 | OLC  | C11-C12-C13-C14 |
| 2   | B     | 315 | OLC  | C5-C6-C7-C8     |
| 2   | E     | 312 | OLC  | C15-C16-C17-C18 |
| 2   | A     | 301 | OLC  | O19-C1-O20-C21  |
| 3   | D     | 313 | LFA  | C10-C11-C12-C13 |
| 2   | C     | 307 | OLC  | C5-C6-C7-C8     |
| 2   | A     | 301 | OLC  | C2-C1-O20-C21   |
| 3   | D     | 311 | LFA  | C2-C3-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 321 | OLC  | C7-C8-C9-C10    |
| 2   | B     | 311 | OLC  | C15-C16-C17-C18 |
| 3   | C     | 302 | LFA  | C12-C13-C14-C15 |
| 3   | D     | 313 | LFA  | C11-C10-C9-C8   |
| 2   | A     | 303 | OLC  | C2-C3-C4-C5     |
| 2   | B     | 304 | OLC  | C7-C8-C9-C10    |
| 2   | E     | 306 | OLC  | C7-C8-C9-C10    |
| 2   | E     | 307 | OLC  | C9-C10-C11-C12  |
| 3   | C     | 316 | LFA  | C11-C10-C9-C8   |
| 2   | A     | 304 | OLC  | O20-C21-C22-C24 |
| 2   | B     | 307 | OLC  | C12-C13-C14-C15 |
| 2   | D     | 303 | OLC  | C4-C5-C6-C7     |
| 3   | B     | 319 | LFA  | C16-C17-C18-C19 |
| 2   | B     | 304 | OLC  | C9-C10-C11-C12  |
| 2   | B     | 307 | OLC  | C9-C10-C11-C12  |
| 2   | B     | 308 | OLC  | C7-C8-C9-C10    |
| 2   | D     | 303 | OLC  | C9-C10-C11-C12  |
| 2   | E     | 309 | OLC  | C9-C10-C11-C12  |
| 2   | E     | 312 | OLC  | C7-C8-C9-C10    |
| 3   | E     | 302 | LFA  | C14-C15-C16-C17 |
| 2   | E     | 308 | OLC  | O19-C1-O20-C21  |
| 2   | A     | 310 | OLC  | C2-C3-C4-C5     |
| 2   | A     | 303 | OLC  | C9-C10-C11-C12  |
| 2   | C     | 301 | OLC  | C7-C8-C9-C10    |
| 2   | D     | 308 | OLC  | C4-C5-C6-C7     |
| 2   | A     | 301 | OLC  | C3-C4-C5-C6     |
| 3   | D     | 310 | LFA  | C14-C15-C16-C17 |
| 2   | A     | 304 | OLC  | C15-C16-C17-C18 |
| 3   | E     | 302 | LFA  | C11-C12-C13-C14 |
| 2   | A     | 302 | OLC  | C9-C10-C11-C12  |
| 2   | E     | 306 | OLC  | C9-C10-C11-C12  |
| 2   | E     | 309 | OLC  | C13-C14-C15-C16 |
| 2   | C     | 306 | OLC  | C4-C5-C6-C7     |
| 3   | C     | 319 | LFA  | C17-C18-C19-C20 |
| 2   | D     | 302 | OLC  | C2-C3-C4-C5     |
| 2   | B     | 308 | OLC  | C9-C10-C11-C12  |
| 2   | D     | 306 | OLC  | C9-C10-C11-C12  |
| 2   | E     | 308 | OLC  | O20-C1-C2-C3    |
| 3   | C     | 302 | LFA  | C14-C15-C16-C17 |
| 3   | A     | 314 | LFA  | C14-C15-C16-C17 |
| 2   | E     | 308 | OLC  | C2-C1-O20-C21   |
| 2   | D     | 303 | OLC  | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | E     | 302 | LFA  | C17-C18-C19-C20 |
| 2   | B     | 306 | OLC  | C9-C10-C11-C12  |
| 2   | E     | 314 | OLC  | C9-C10-C11-C12  |
| 2   | C     | 308 | OLC  | C12-C13-C14-C15 |
| 2   | D     | 308 | OLC  | O20-C1-C2-C3    |
| 2   | A     | 304 | OLC  | C3-C4-C5-C6     |
| 3   | D     | 310 | LFA  | C13-C14-C15-C16 |
| 2   | C     | 301 | OLC  | C3-C4-C5-C6     |
| 2   | E     | 314 | OLC  | C10-C11-C12-C13 |
| 2   | C     | 311 | OLC  | C2-C3-C4-C5     |
| 2   | A     | 304 | OLC  | O20-C1-C2-C3    |
| 3   | B     | 302 | LFA  | C11-C12-C13-C14 |
| 2   | A     | 308 | OLC  | C2-C3-C4-C5     |
| 3   | D     | 310 | LFA  | C15-C16-C17-C18 |
| 2   | B     | 309 | OLC  | O20-C21-C22-O23 |
| 3   | C     | 316 | LFA  | C14-C15-C16-C17 |
| 2   | B     | 307 | OLC  | O20-C21-C22-C24 |
| 2   | D     | 307 | OLC  | O20-C1-C2-C3    |
| 2   | B     | 312 | OLC  | C3-C4-C5-C6     |
| 2   | B     | 306 | OLC  | C10-C11-C12-C13 |
| 2   | C     | 312 | OLC  | O20-C1-C2-C3    |
| 2   | A     | 321 | OLC  | C14-C15-C16-C17 |
| 2   | E     | 307 | OLC  | O20-C21-C22-O23 |
| 2   | B     | 309 | OLC  | C21-C22-C24-O25 |
| 3   | E     | 319 | LFA  | C15-C16-C17-C18 |
| 3   | E     | 323 | LFA  | C6-C7-C8-C9     |
| 3   | C     | 319 | LFA  | C3-C4-C5-C6     |
| 2   | E     | 301 | OLC  | C2-C3-C4-C5     |
| 2   | A     | 304 | OLC  | O19-C1-C2-C3    |
| 2   | D     | 307 | OLC  | O19-C1-C2-C3    |
| 2   | B     | 313 | OLC  | O19-C1-C2-C3    |
| 2   | C     | 312 | OLC  | O19-C1-C2-C3    |
| 2   | E     | 307 | OLC  | C1-C2-C3-C4     |
| 3   | B     | 302 | LFA  | C17-C18-C19-C20 |
| 2   | A     | 311 | OLC  | C5-C6-C7-C8     |
| 2   | E     | 308 | OLC  | O19-C1-C2-C3    |
| 2   | A     | 306 | OLC  | O23-C22-C24-O25 |
| 2   | B     | 312 | OLC  | C5-C6-C7-C8     |
| 2   | A     | 311 | OLC  | C6-C7-C8-C9     |
| 2   | B     | 313 | OLC  | C3-C4-C5-C6     |
| 3   | E     | 302 | LFA  | C15-C16-C17-C18 |
| 3   | A     | 315 | LFA  | C9-C10-C11-C12  |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 321 | OLC  | C15-C16-C17-C18 |
| 2   | D     | 304 | OLC  | C3-C4-C5-C6     |
| 2   | B     | 306 | OLC  | C7-C8-C9-C10    |
| 2   | D     | 303 | OLC  | O20-C1-C2-C3    |
| 2   | D     | 308 | OLC  | O19-C1-C2-C3    |
| 2   | E     | 306 | OLC  | O20-C1-C2-C3    |
| 3   | A     | 317 | LFA  | C1-C2-C3-C4     |

There are no ring outliers.

42 monomers are involved in 50 short contacts:

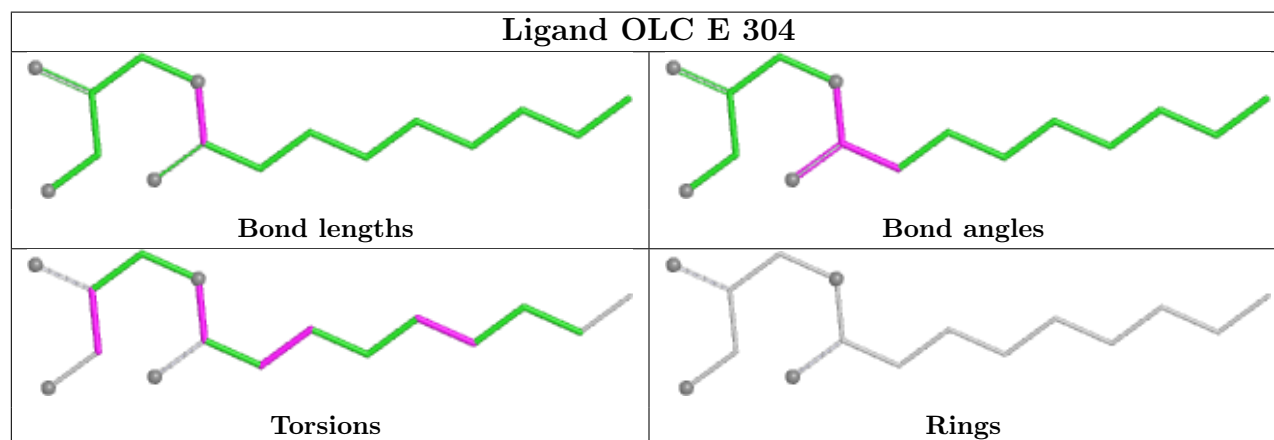
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | E     | 304 | OLC  | 2       | 0            |
| 3   | E     | 315 | LFA  | 3       | 0            |
| 2   | C     | 305 | OLC  | 1       | 0            |
| 2   | E     | 305 | OLC  | 3       | 0            |
| 2   | E     | 303 | OLC  | 3       | 0            |
| 3   | C     | 302 | LFA  | 1       | 0            |
| 5   | A     | 320 | BOG  | 3       | 0            |
| 2   | B     | 306 | OLC  | 1       | 0            |
| 2   | A     | 304 | OLC  | 1       | 0            |
| 2   | A     | 301 | OLC  | 1       | 0            |
| 3   | C     | 318 | LFA  | 3       | 0            |
| 2   | A     | 302 | OLC  | 1       | 0            |
| 2   | A     | 311 | OLC  | 2       | 0            |
| 2   | E     | 312 | OLC  | 4       | 0            |
| 2   | E     | 306 | OLC  | 1       | 0            |
| 2   | E     | 310 | OLC  | 1       | 0            |
| 2   | B     | 304 | OLC  | 1       | 0            |
| 2   | B     | 313 | OLC  | 1       | 0            |
| 2   | E     | 309 | OLC  | 1       | 0            |
| 3   | D     | 311 | LFA  | 1       | 0            |
| 2   | A     | 310 | OLC  | 1       | 0            |
| 2   | C     | 311 | OLC  | 1       | 0            |
| 3   | B     | 316 | LFA  | 1       | 0            |
| 2   | D     | 302 | OLC  | 1       | 0            |
| 3   | A     | 315 | LFA  | 1       | 0            |
| 2   | C     | 309 | OLC  | 1       | 0            |
| 5   | B     | 321 | BOG  | 4       | 0            |
| 3   | E     | 317 | LFA  | 2       | 0            |
| 2   | B     | 315 | OLC  | 1       | 0            |
| 3   | C     | 314 | LFA  | 2       | 0            |

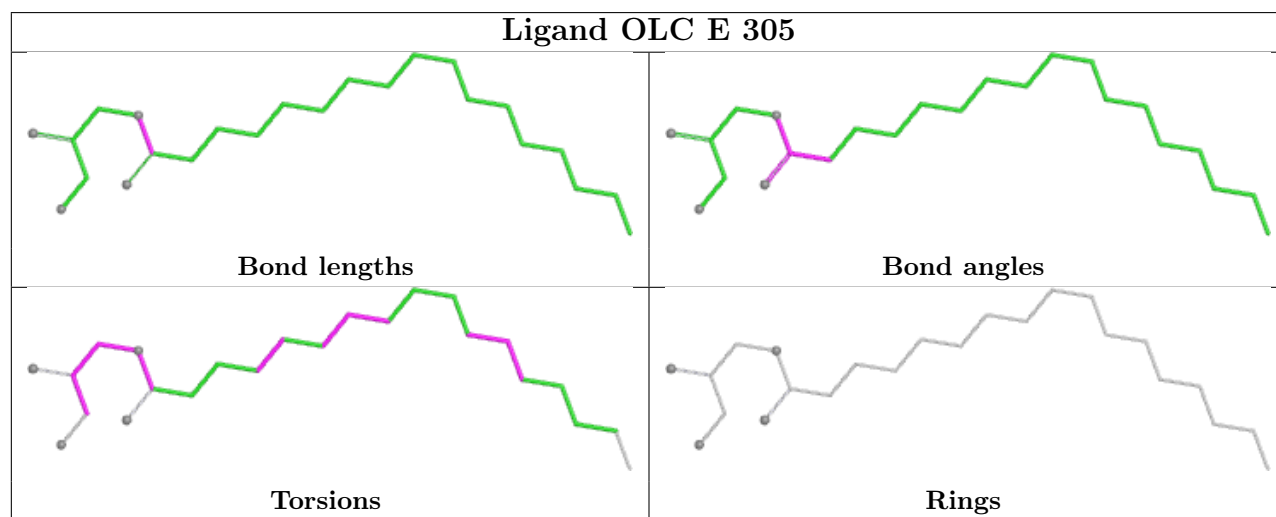
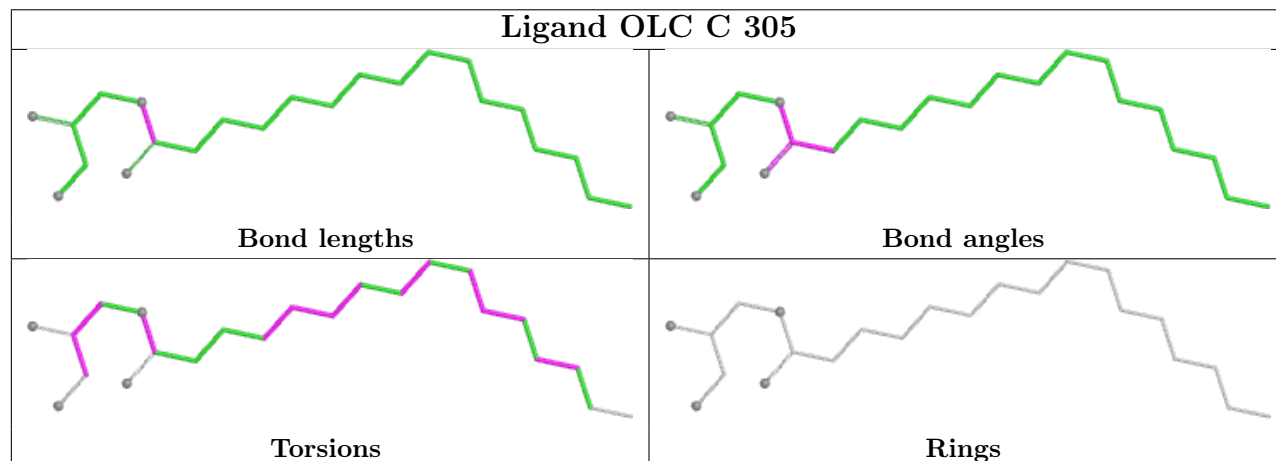
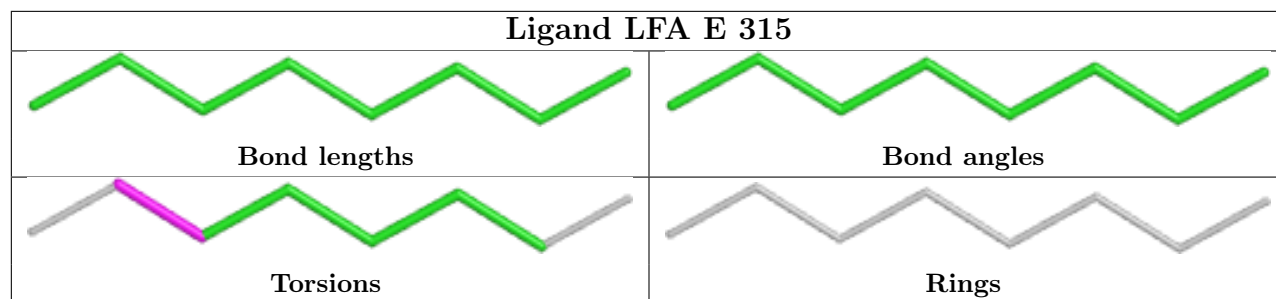
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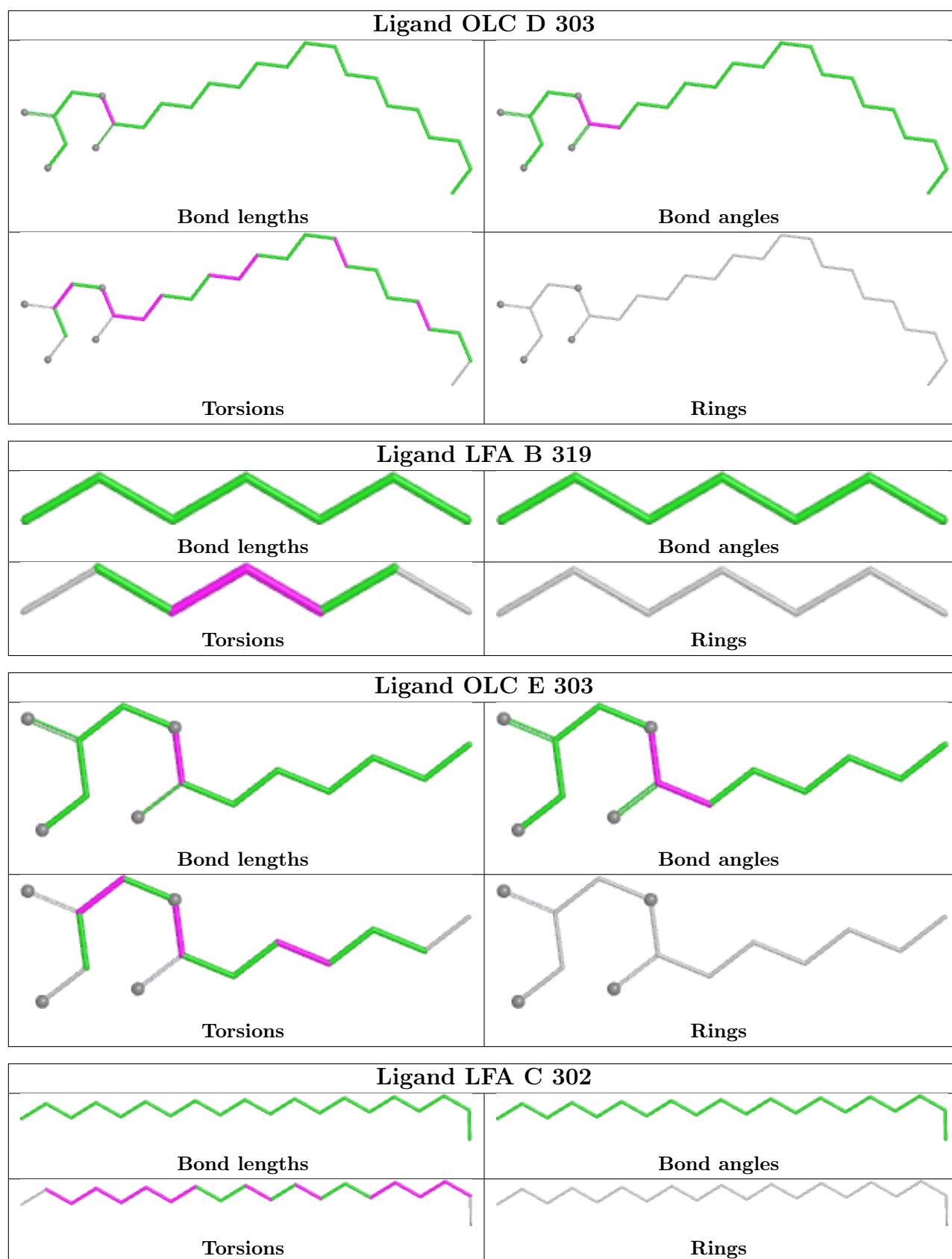
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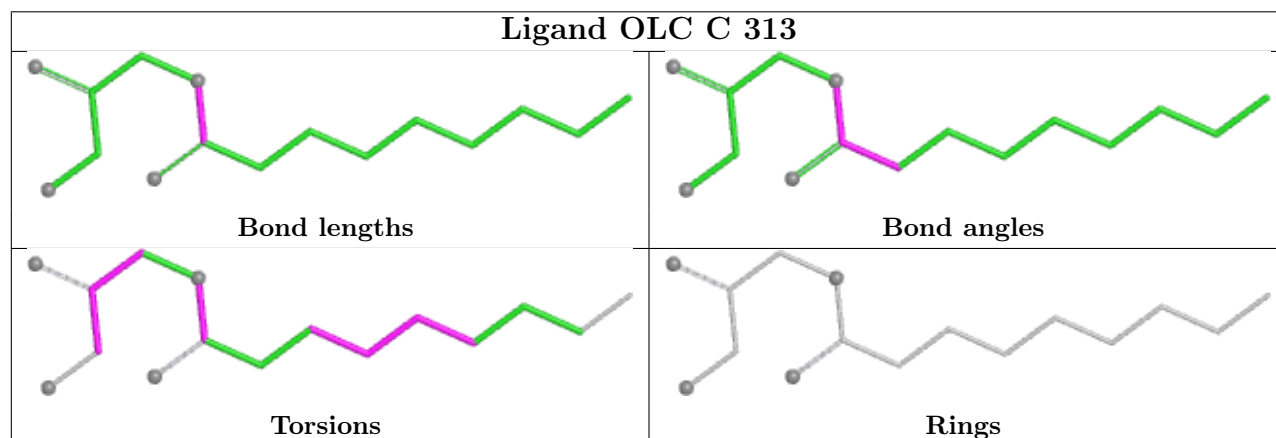
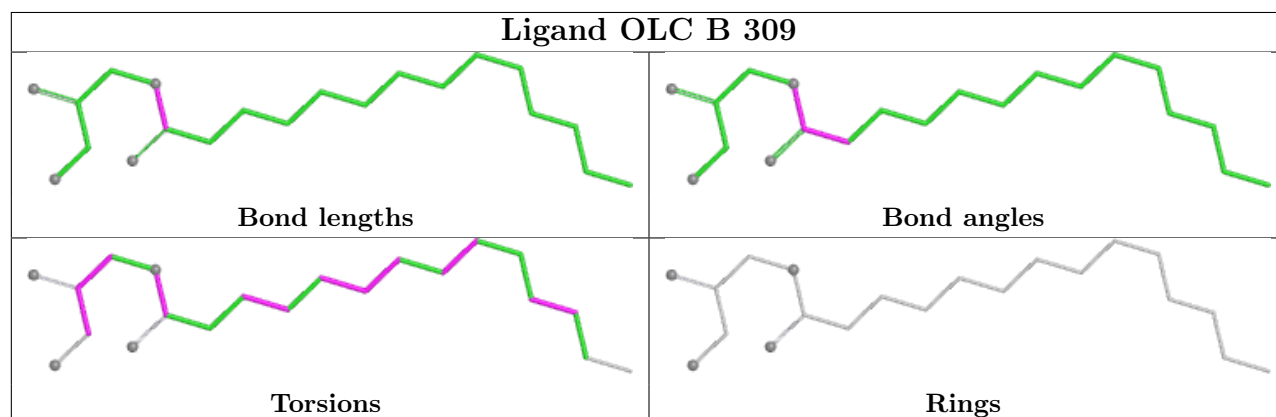
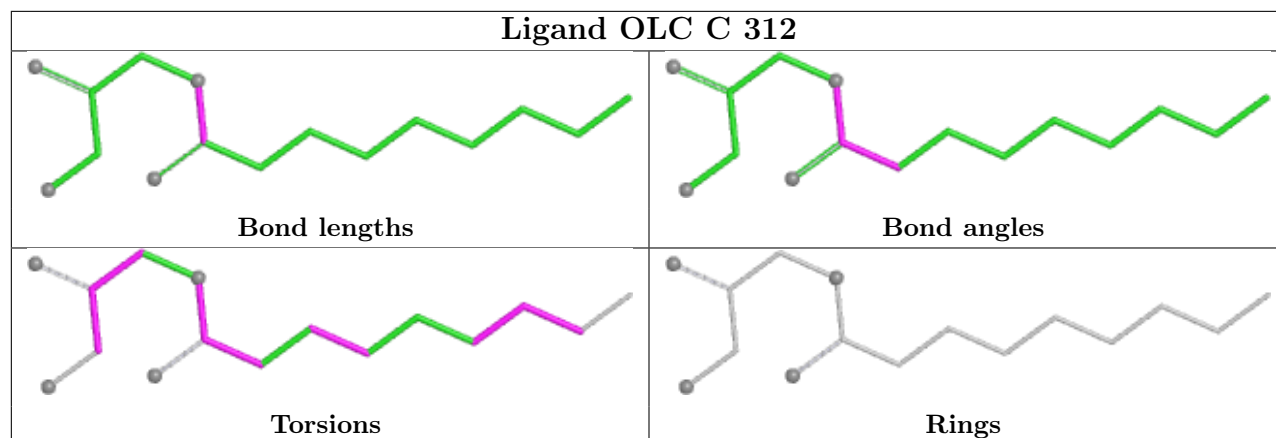
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | E     | 323 | LFA  | 1       | 0            |
| 2   | C     | 304 | OLC  | 2       | 0            |
| 5   | C     | 321 | BOG  | 1       | 0            |
| 2   | E     | 301 | OLC  | 2       | 0            |
| 2   | A     | 307 | OLC  | 1       | 0            |
| 3   | D     | 313 | LFA  | 2       | 0            |
| 2   | A     | 308 | OLC  | 1       | 0            |
| 2   | D     | 304 | OLC  | 1       | 0            |
| 5   | D     | 317 | BOG  | 1       | 0            |
| 3   | E     | 316 | LFA  | 2       | 0            |
| 2   | B     | 301 | OLC  | 4       | 0            |
| 2   | A     | 306 | OLC  | 1       | 0            |

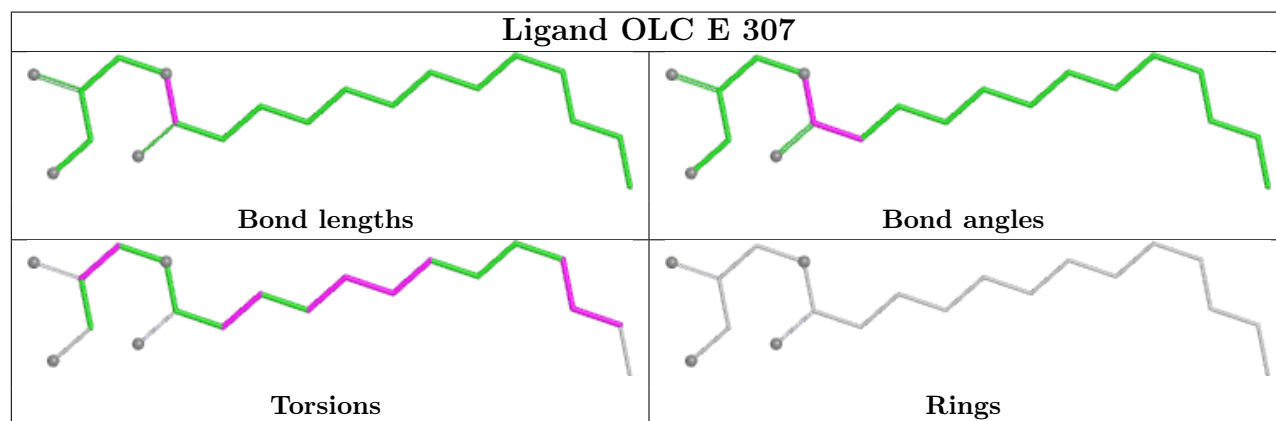
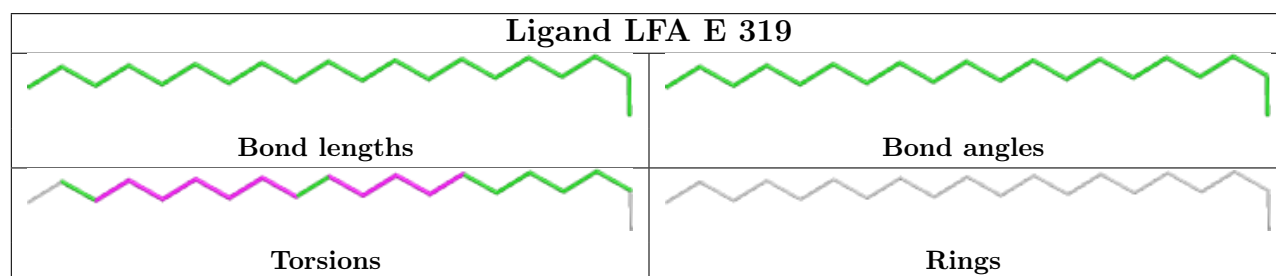
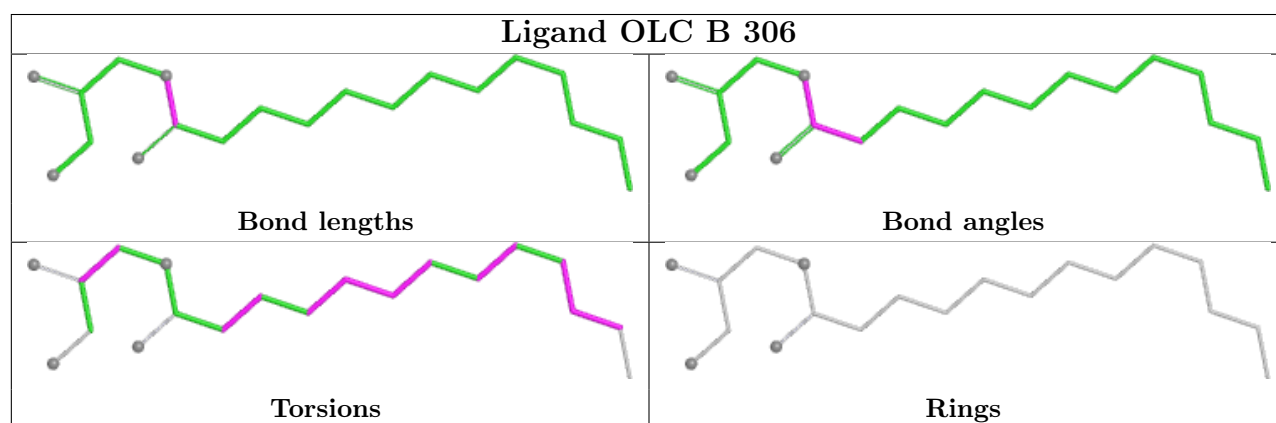
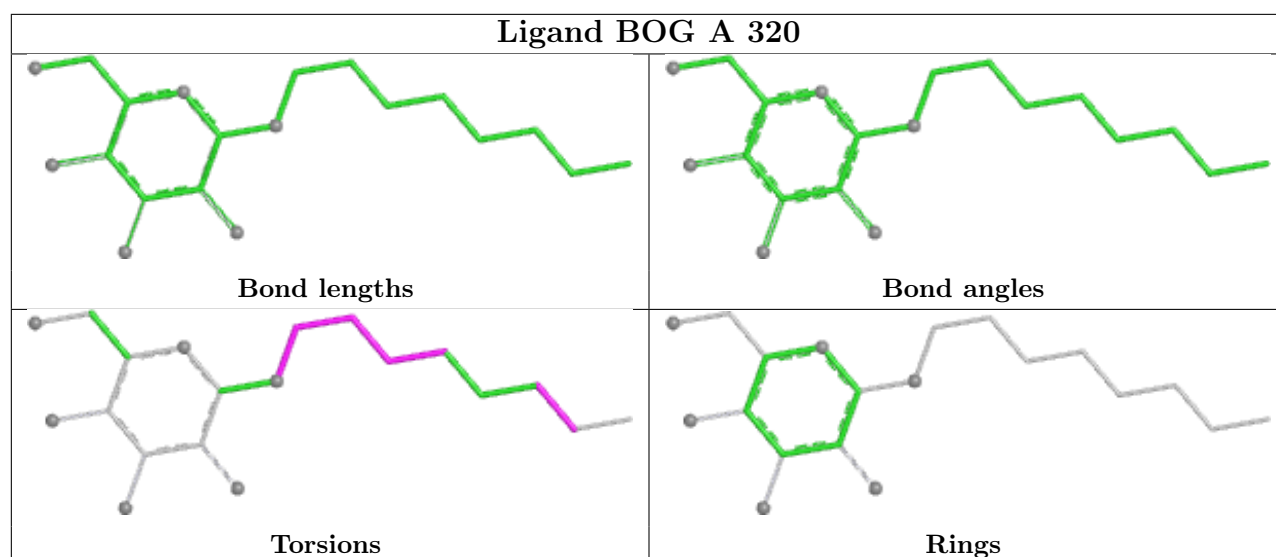
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

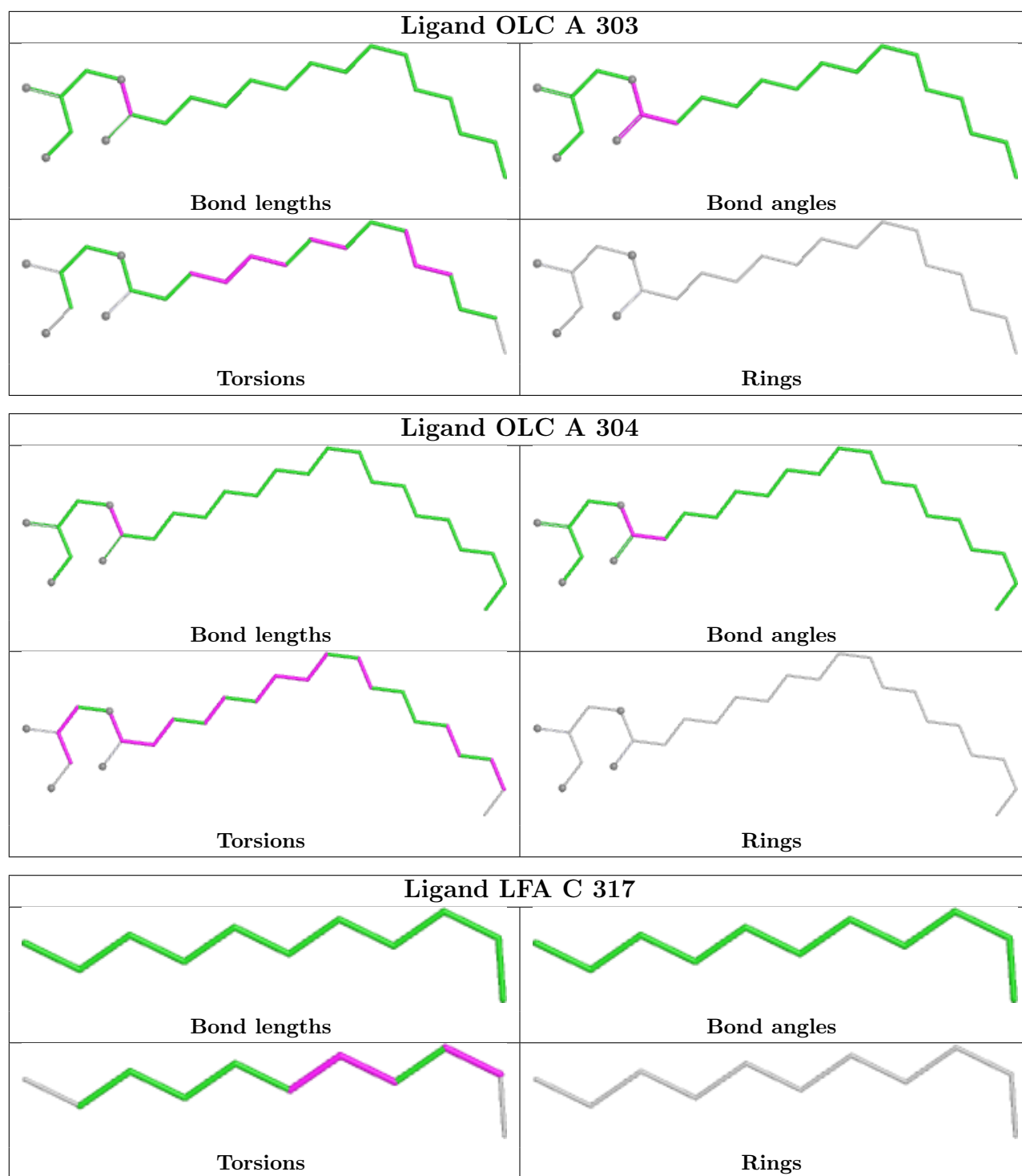




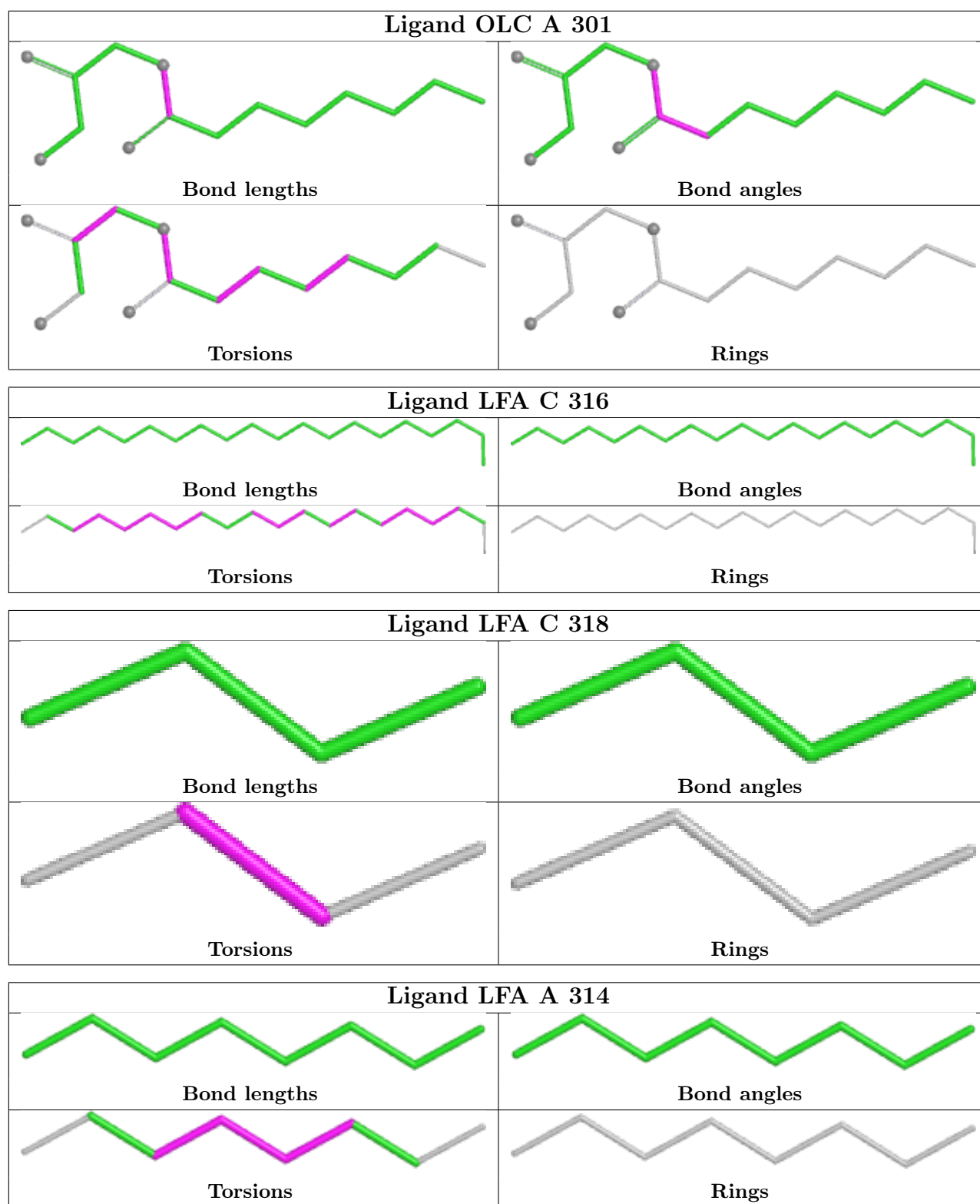


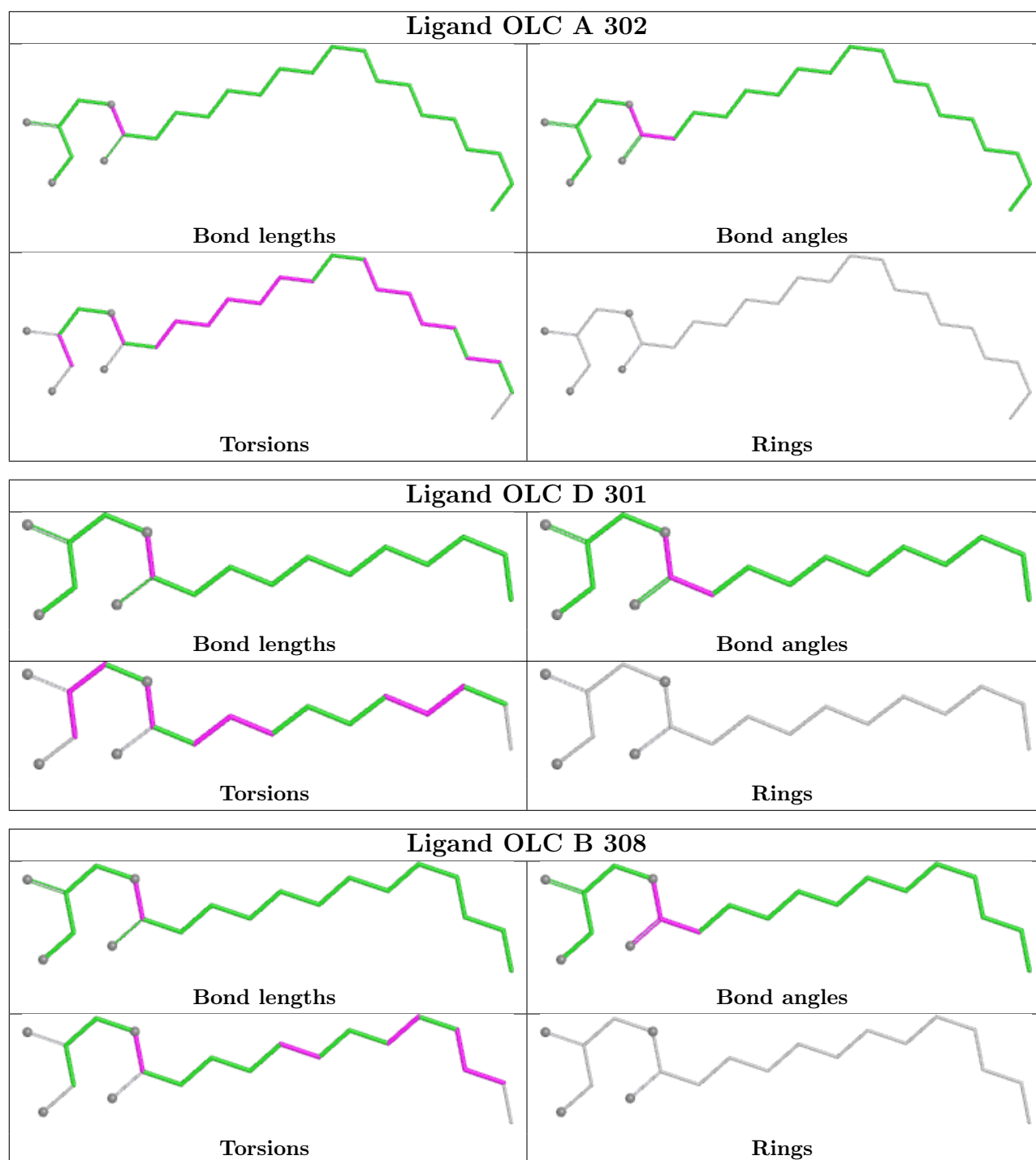


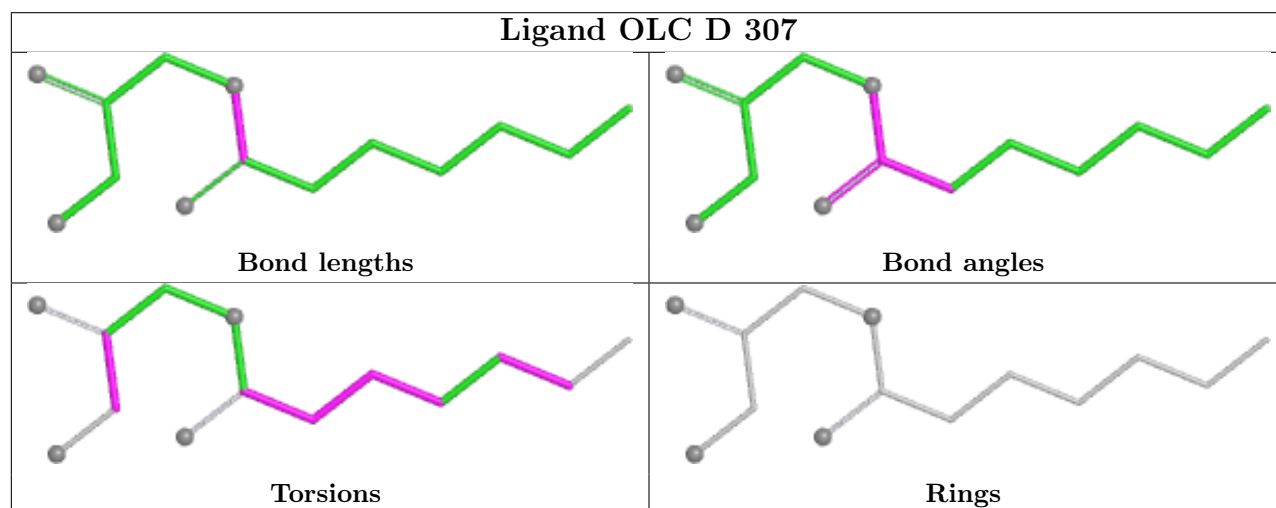
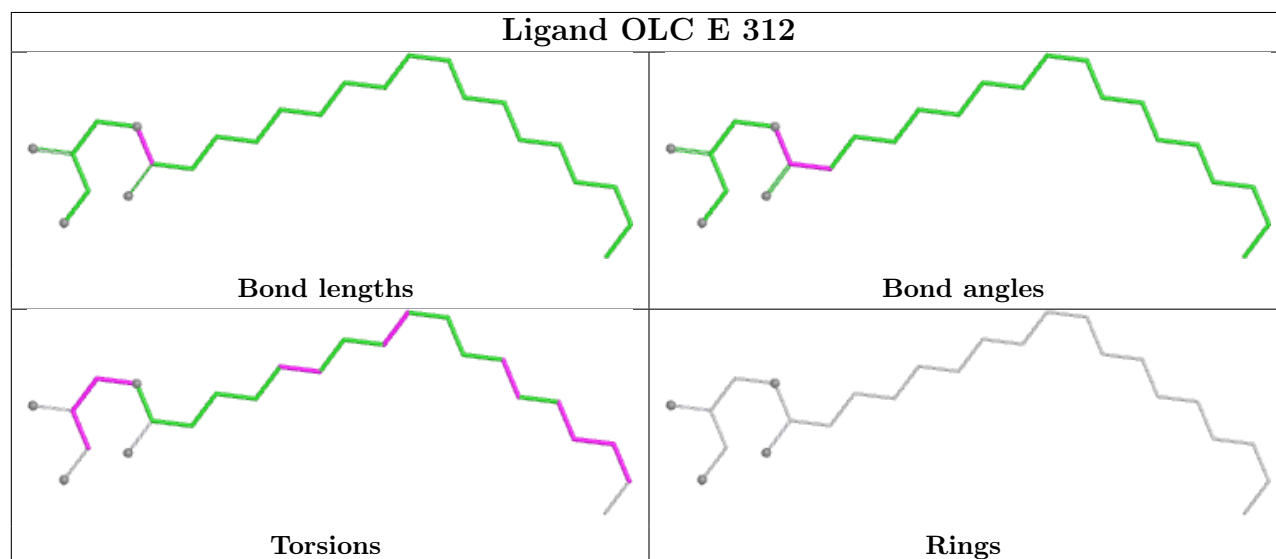
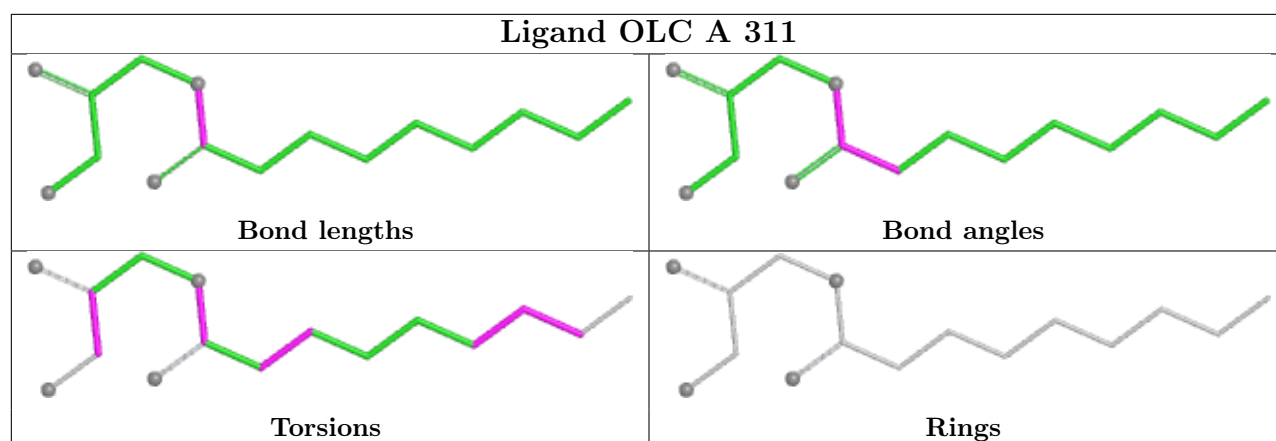


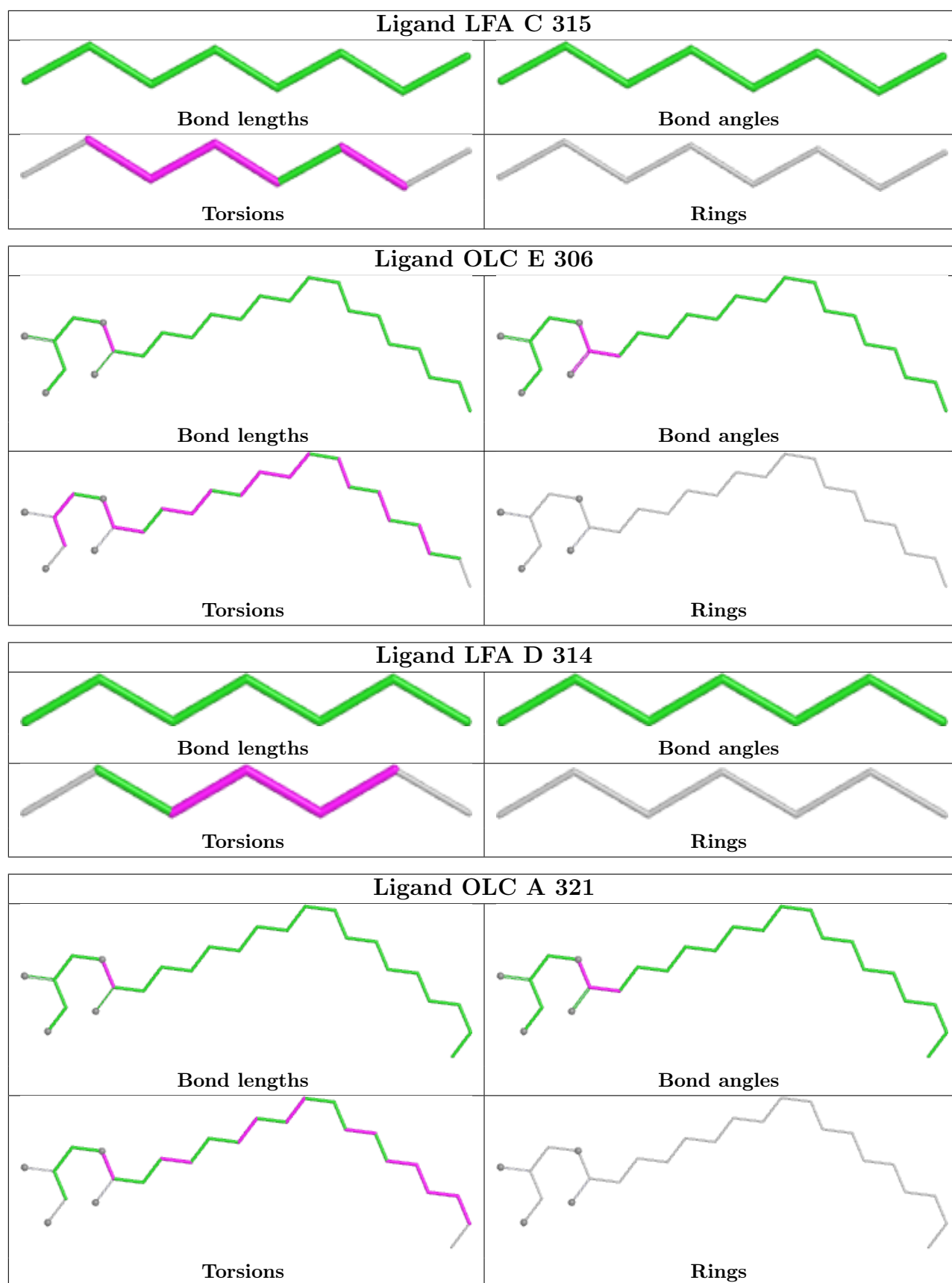


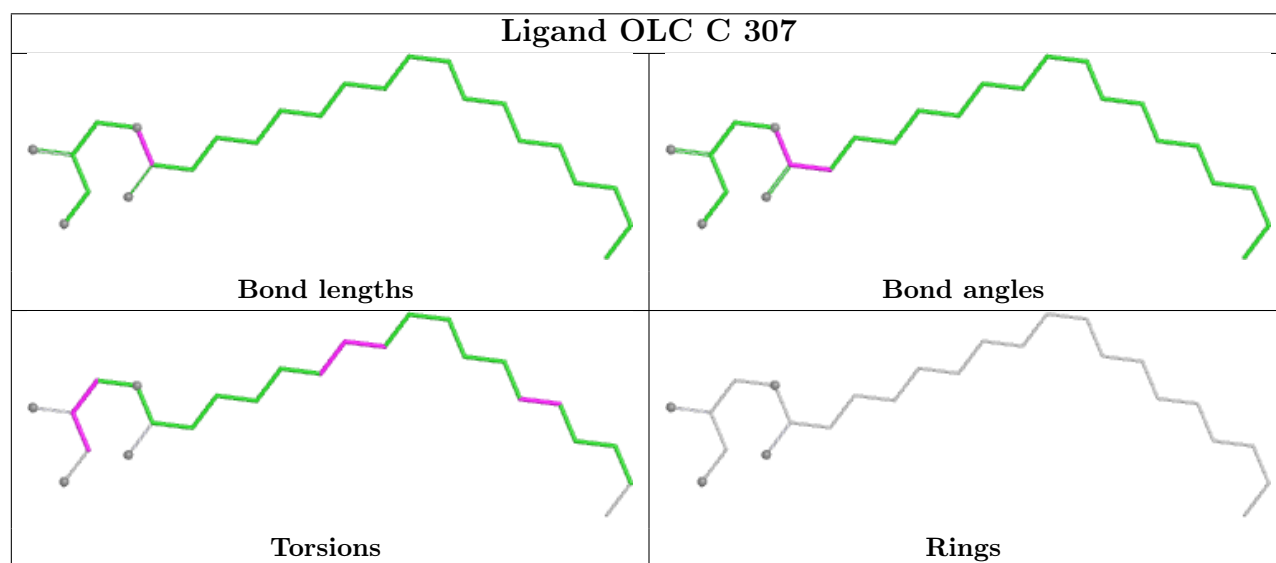
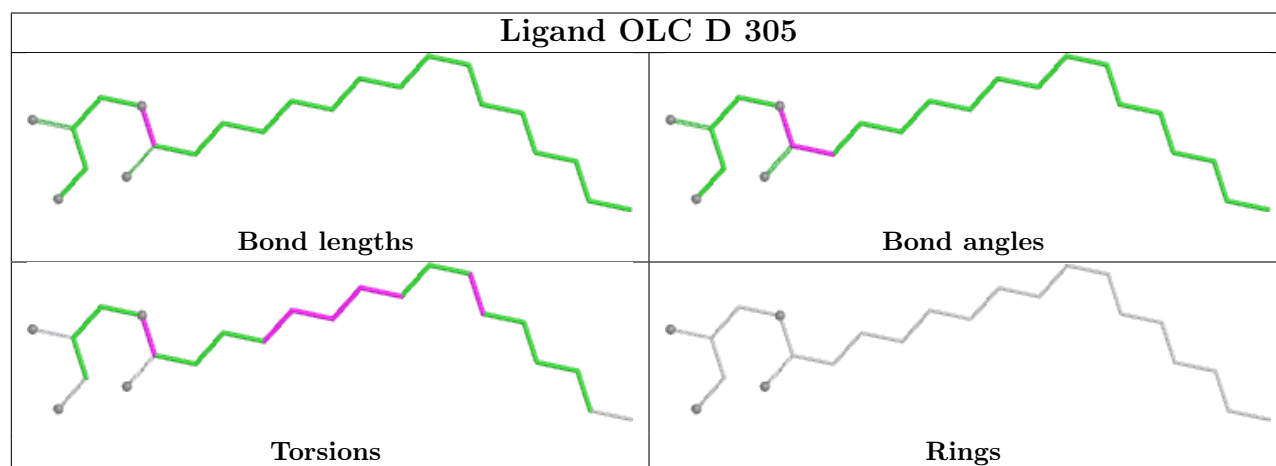
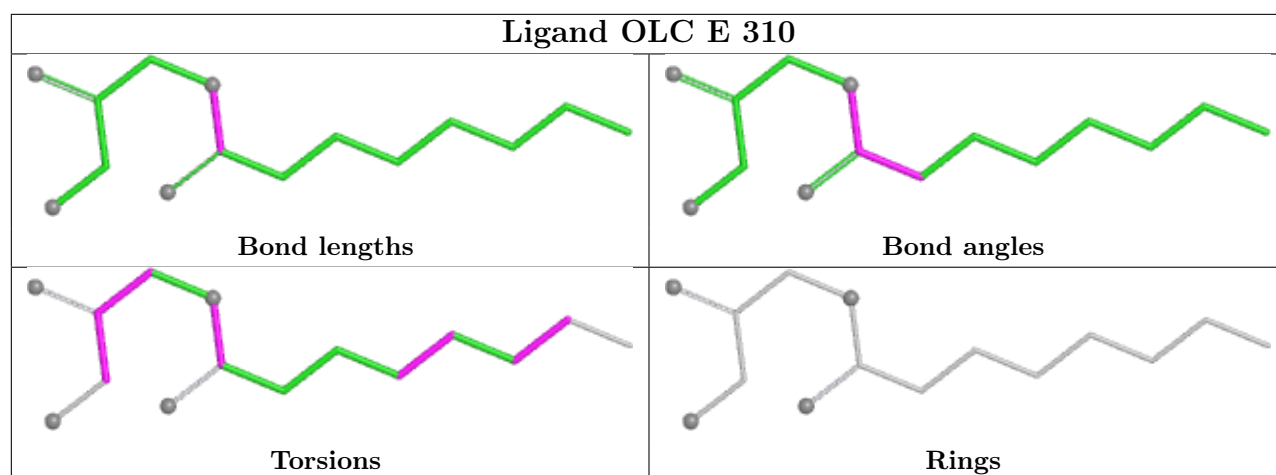


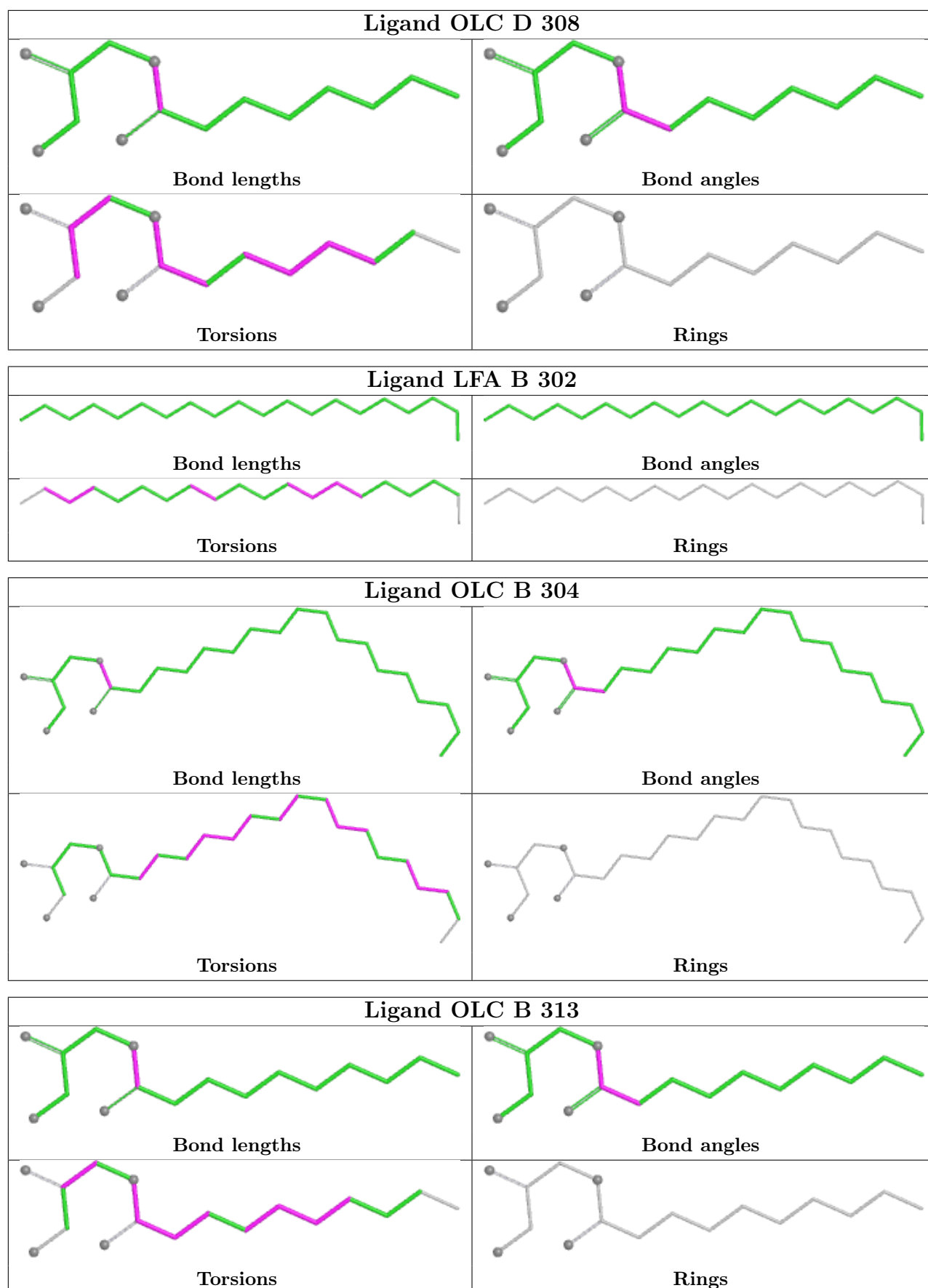


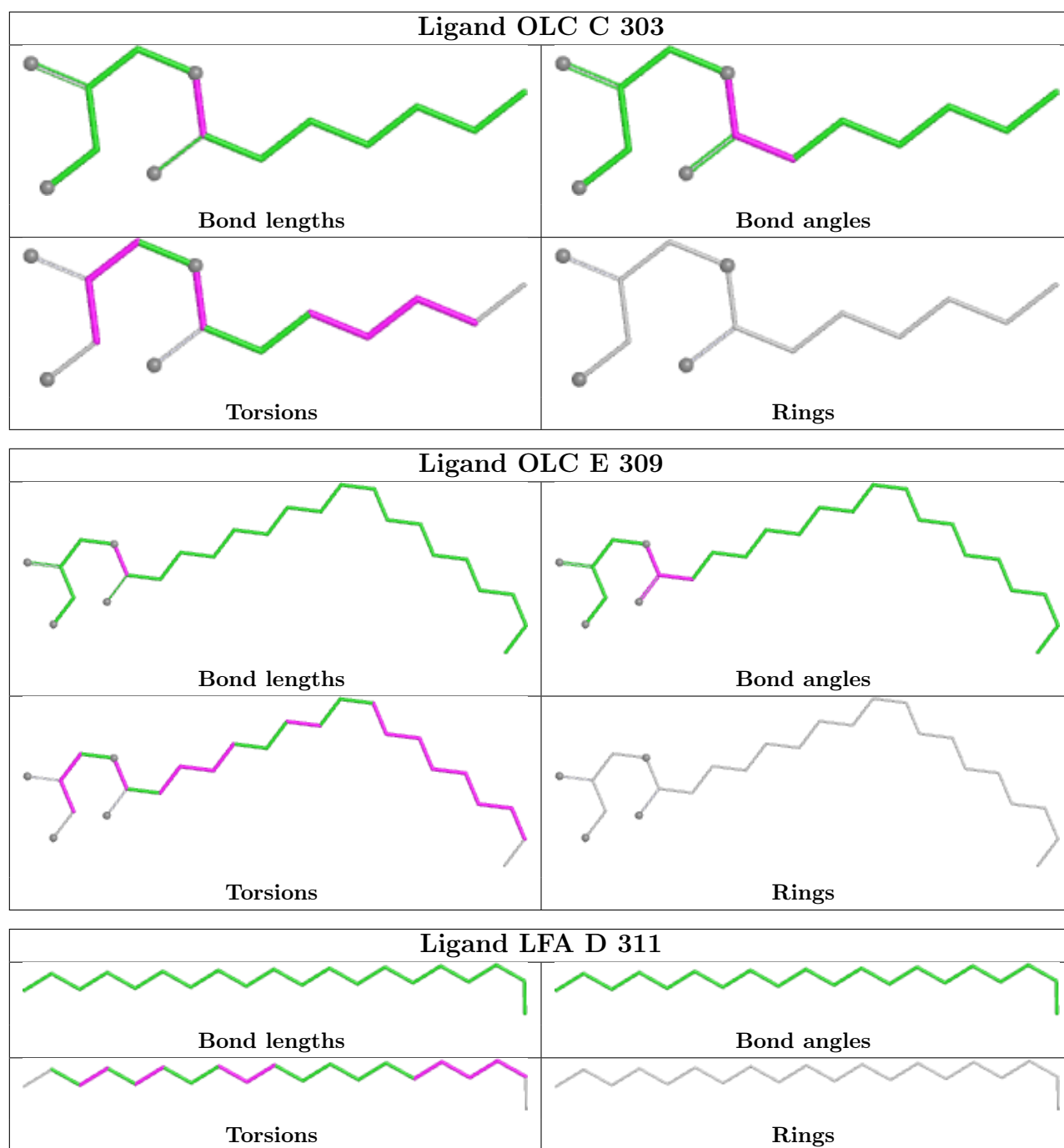


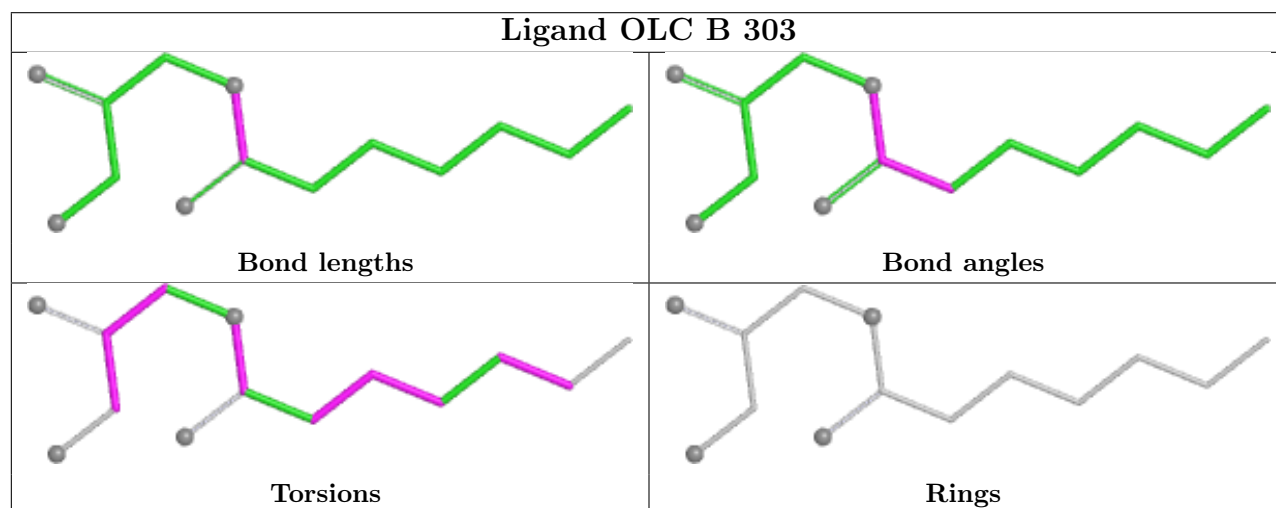
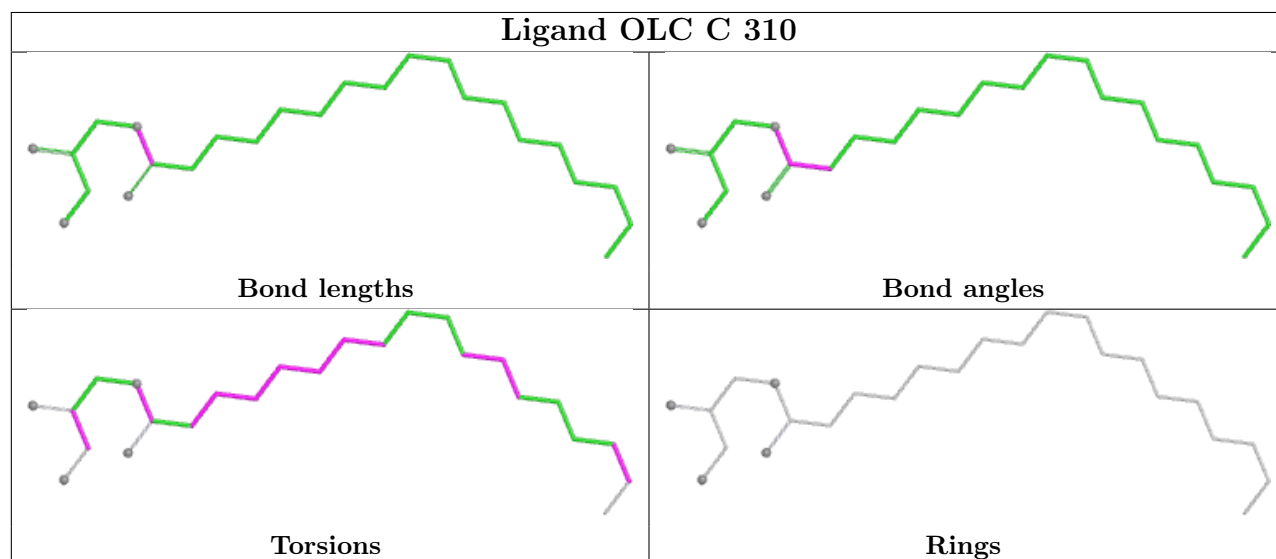
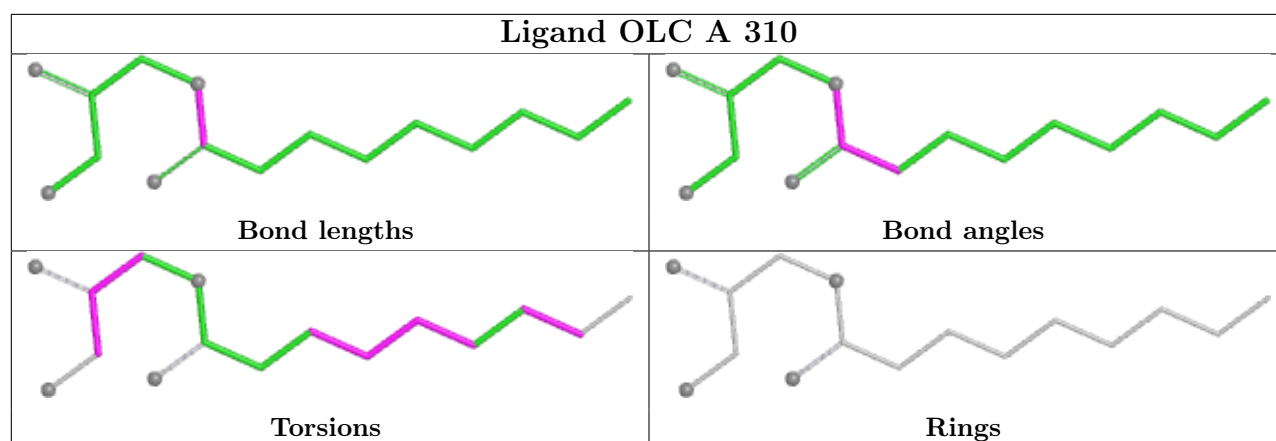




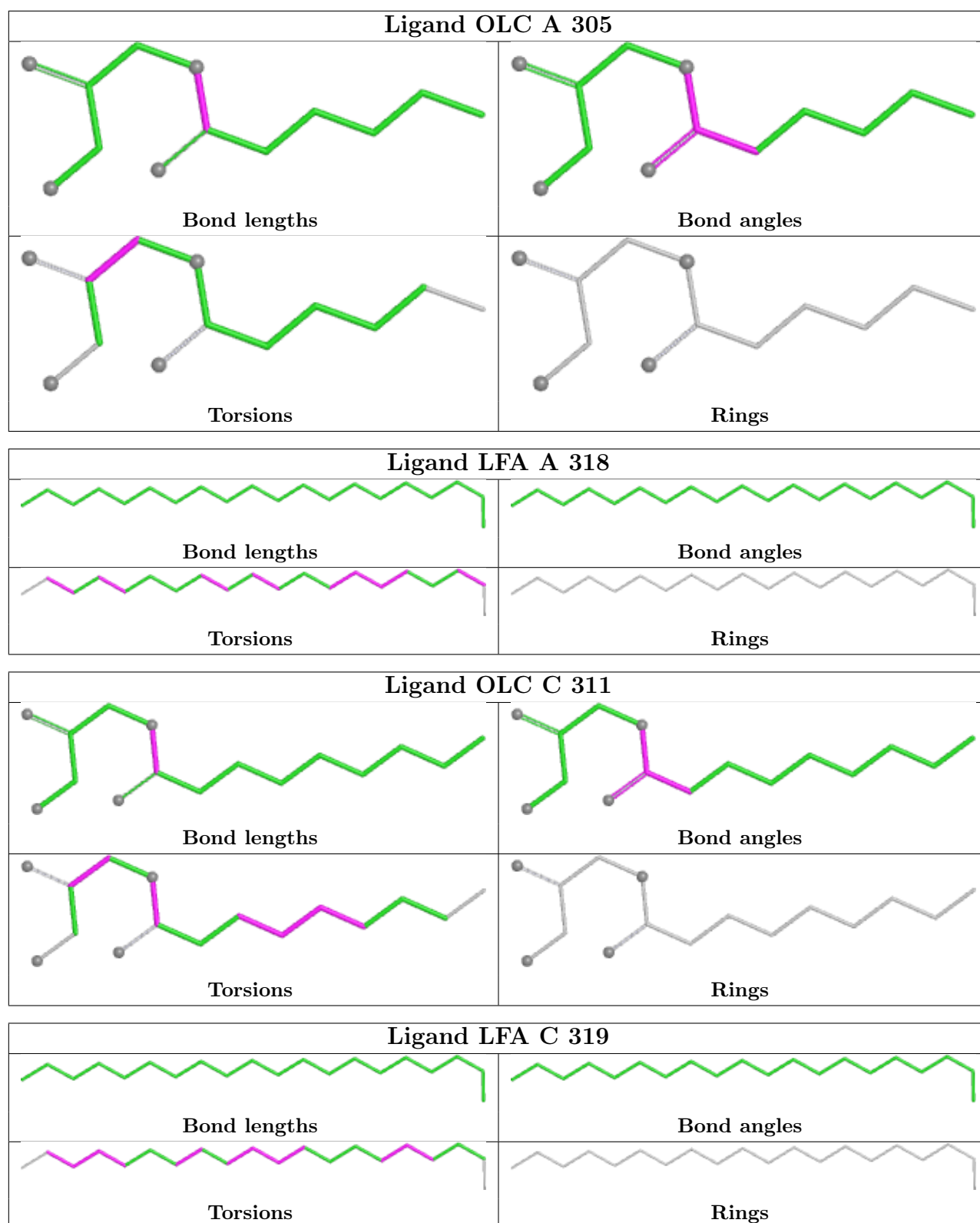


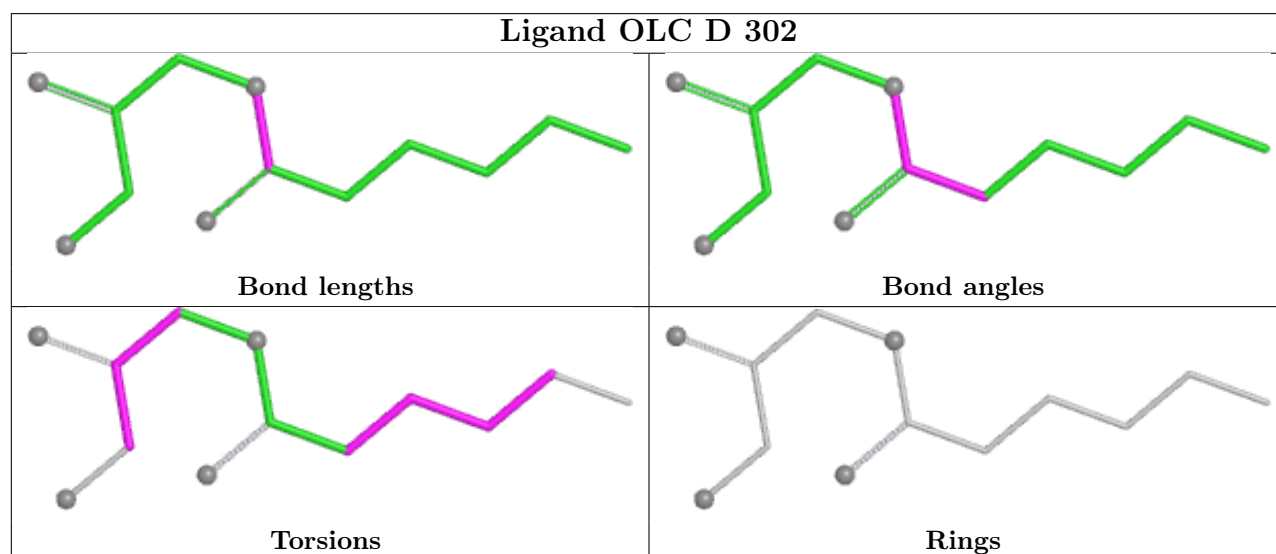
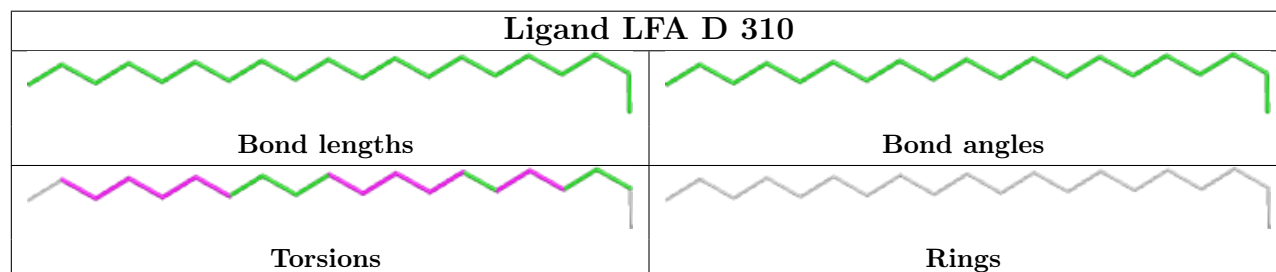
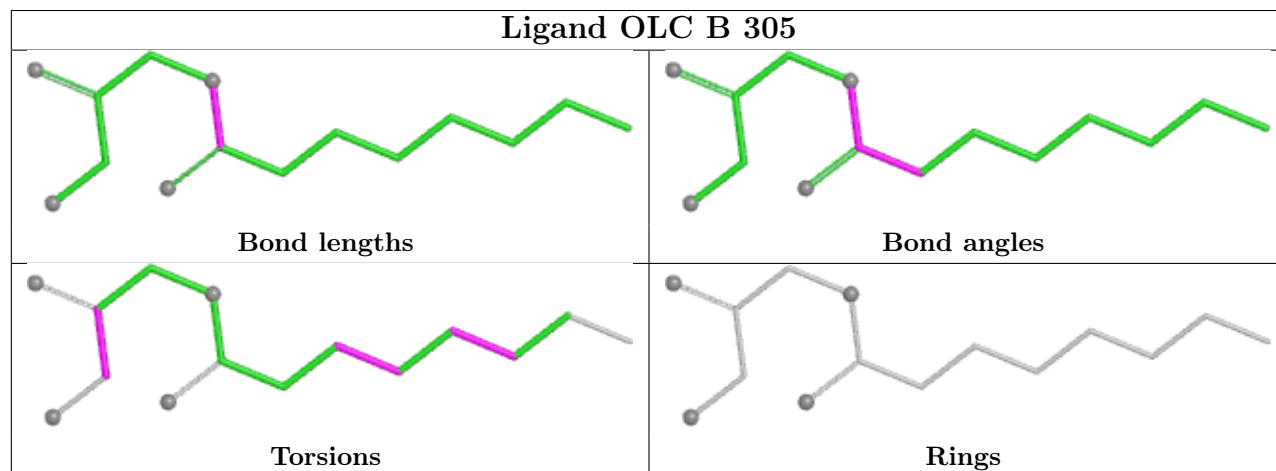
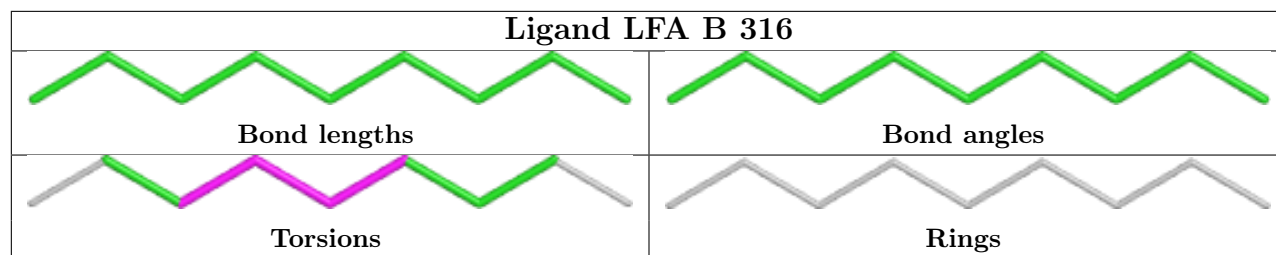


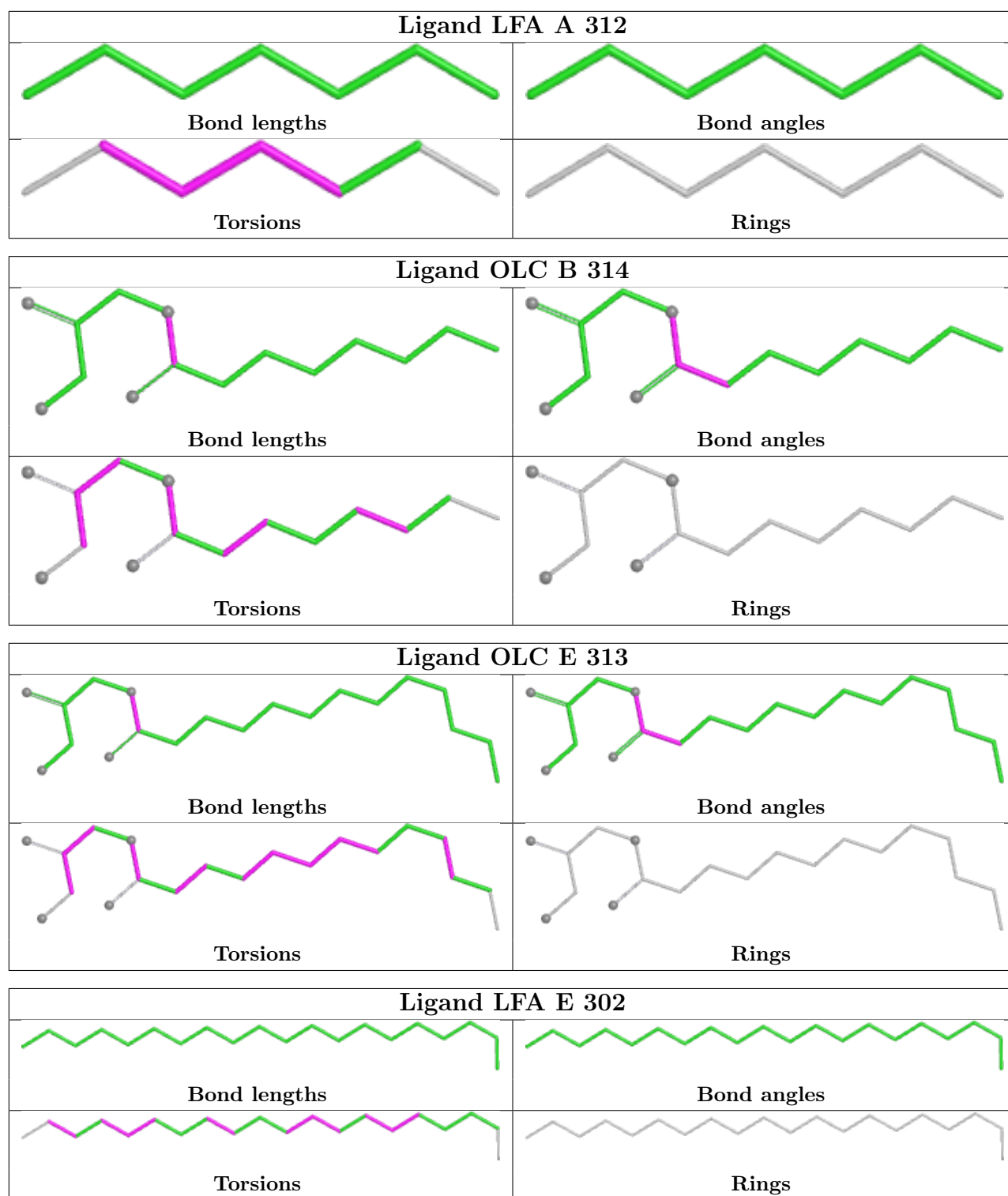


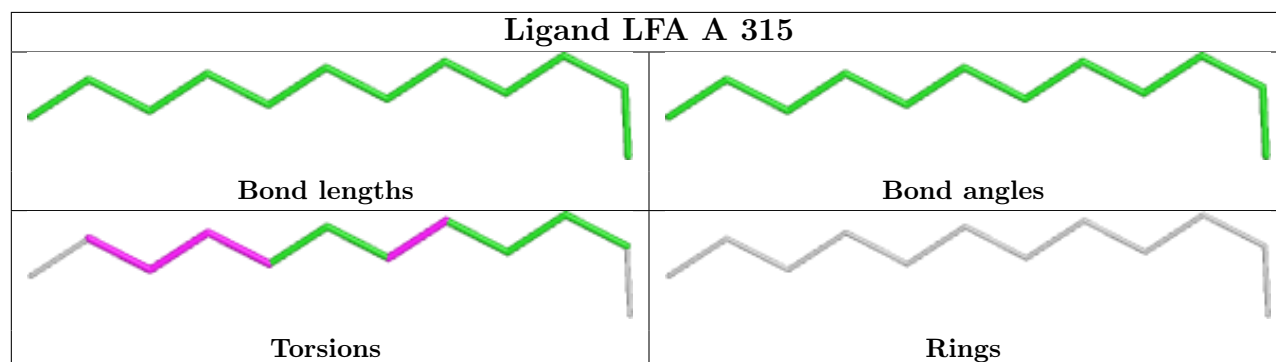
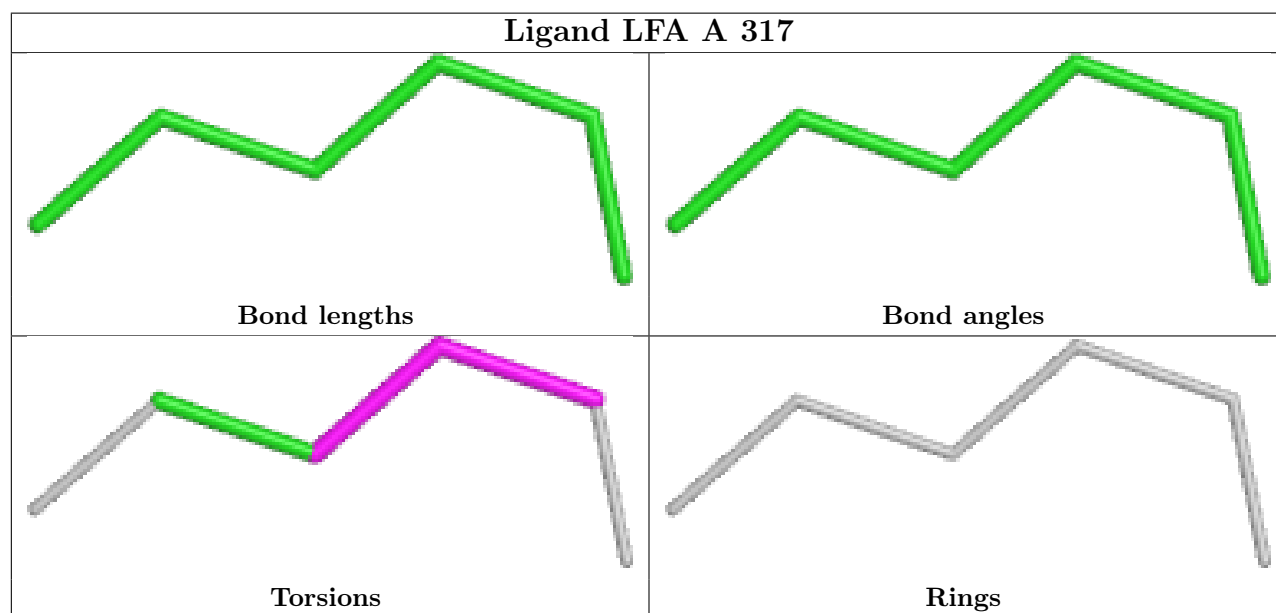
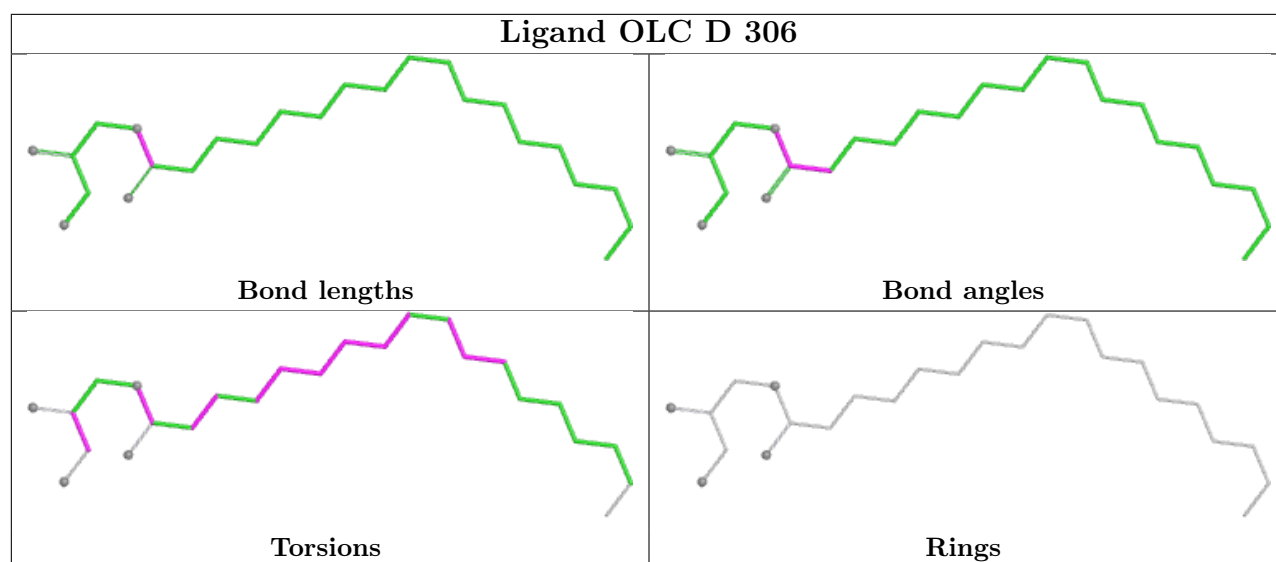


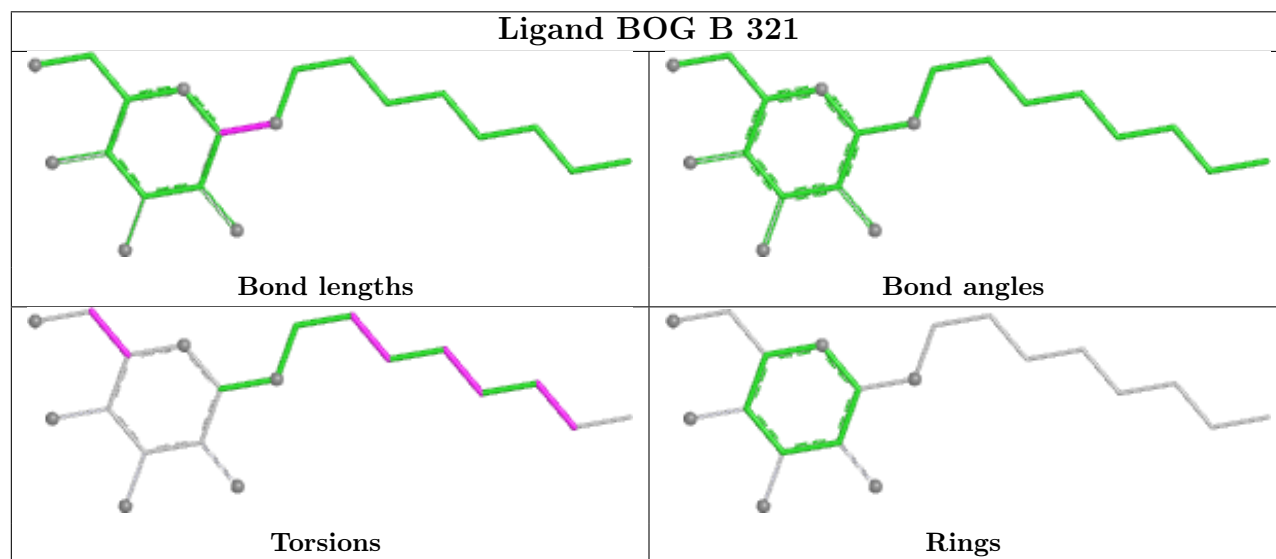
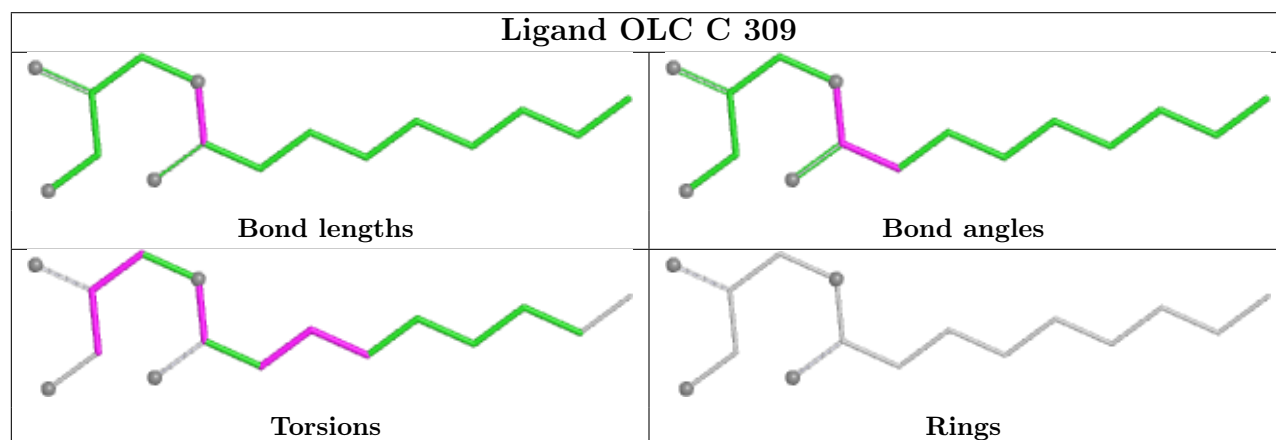
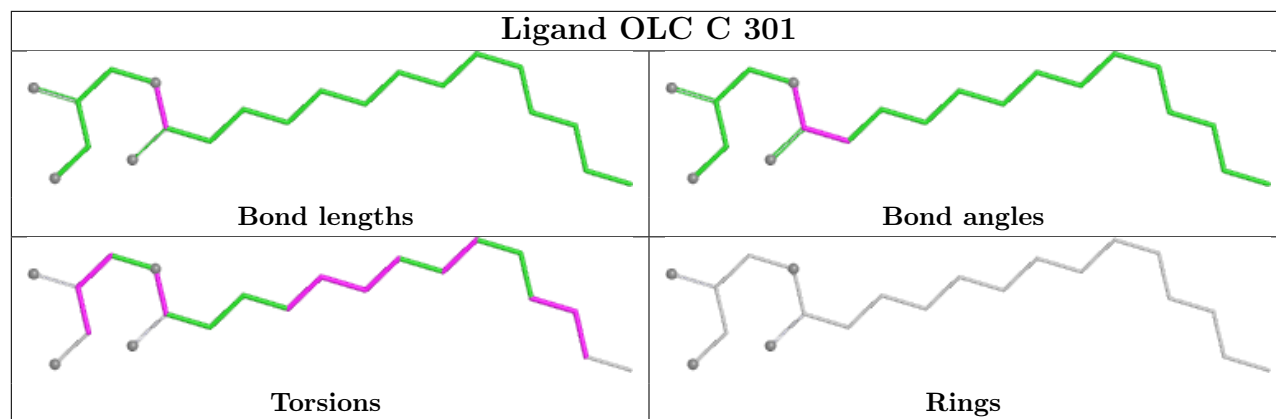


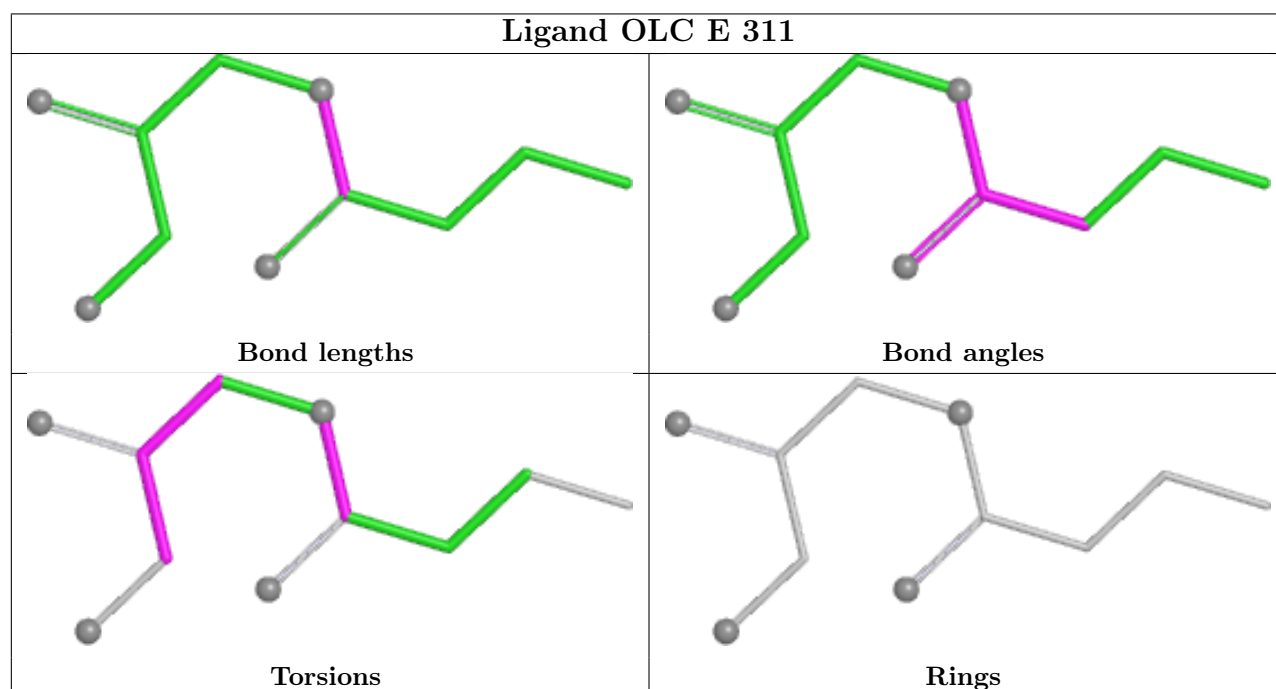
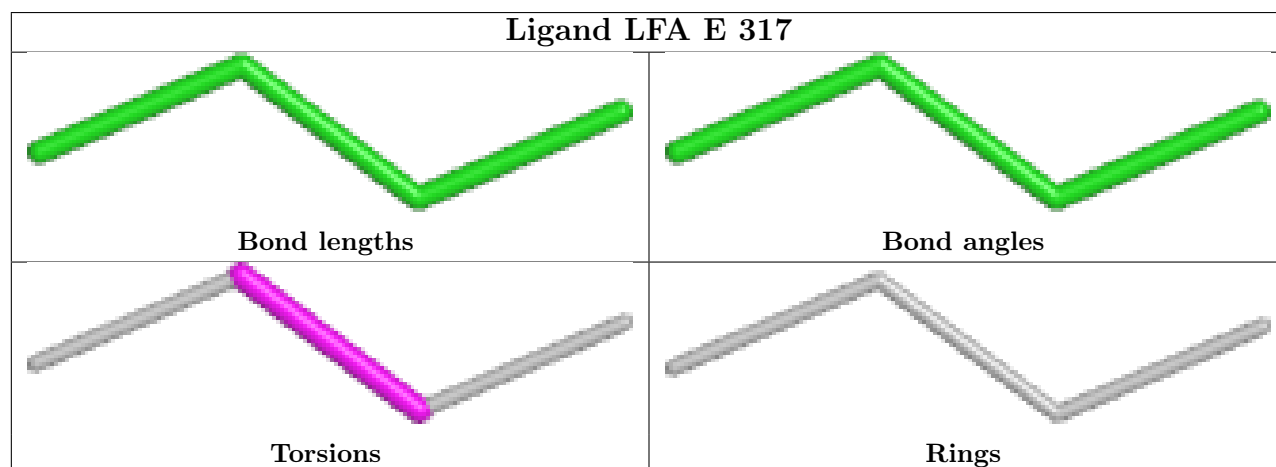
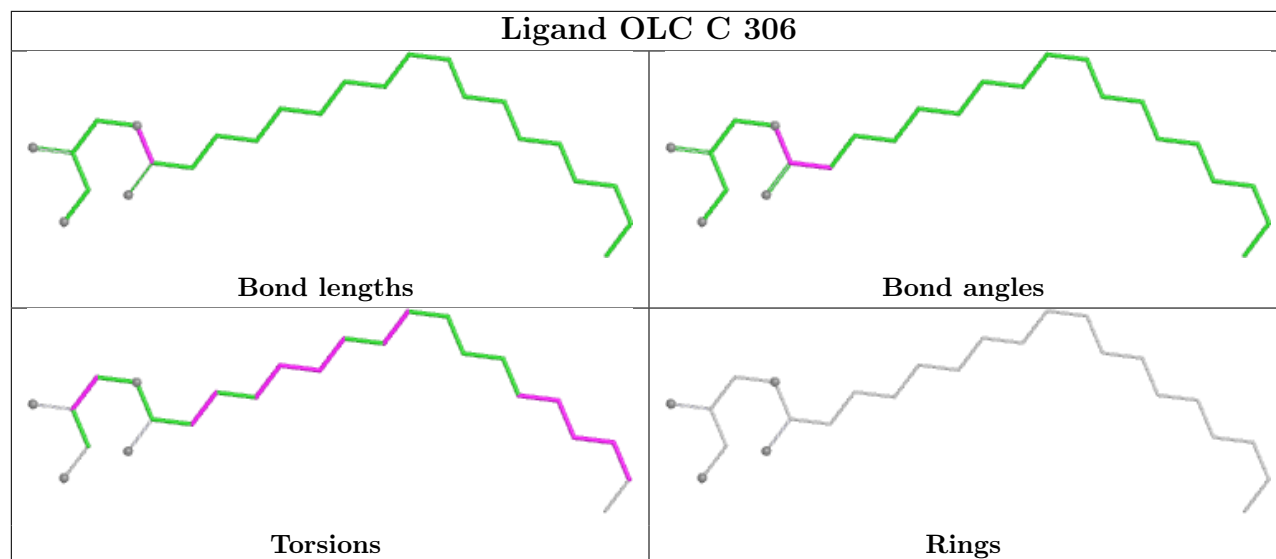


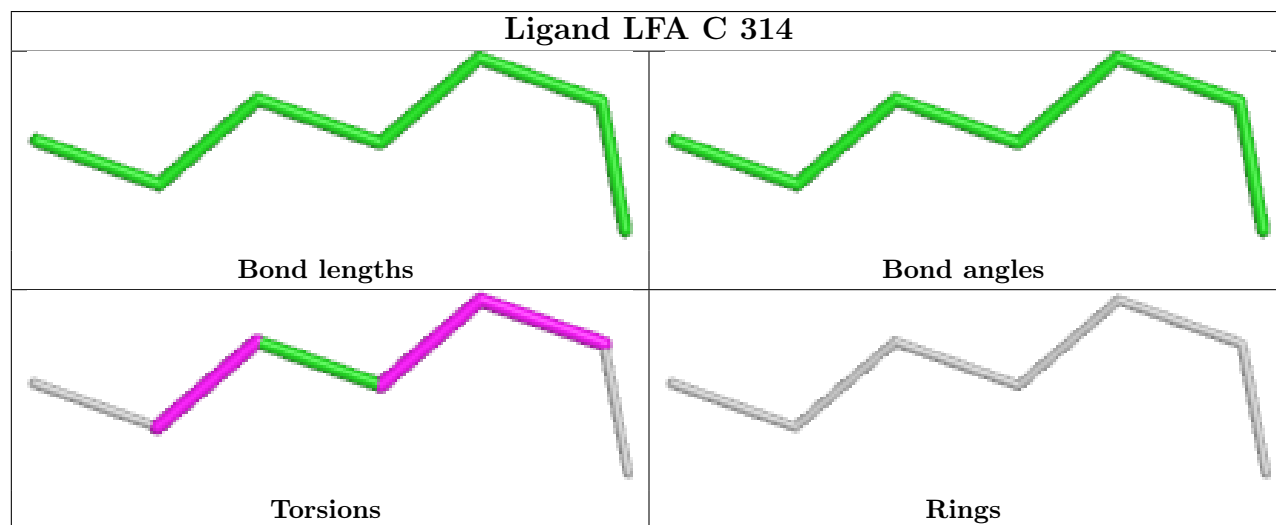
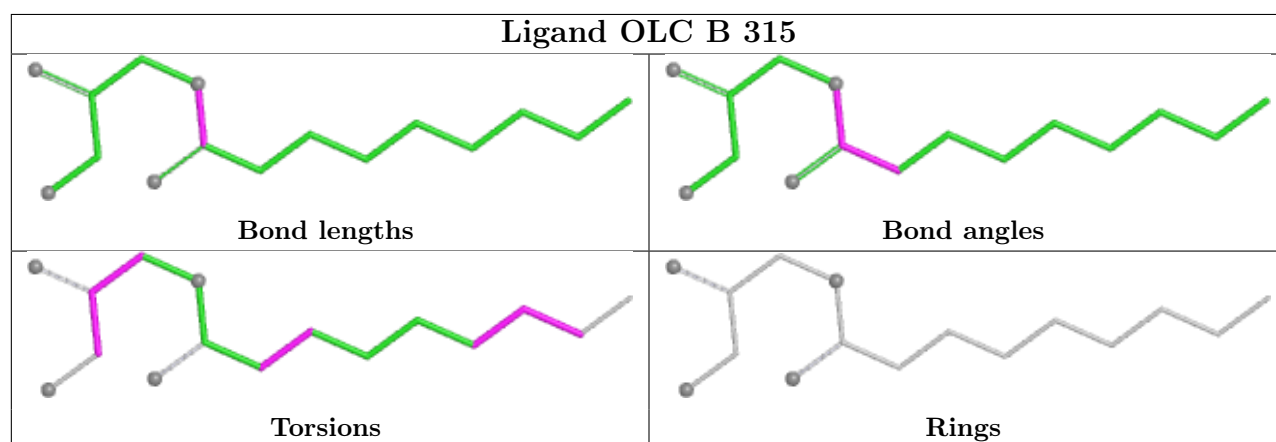
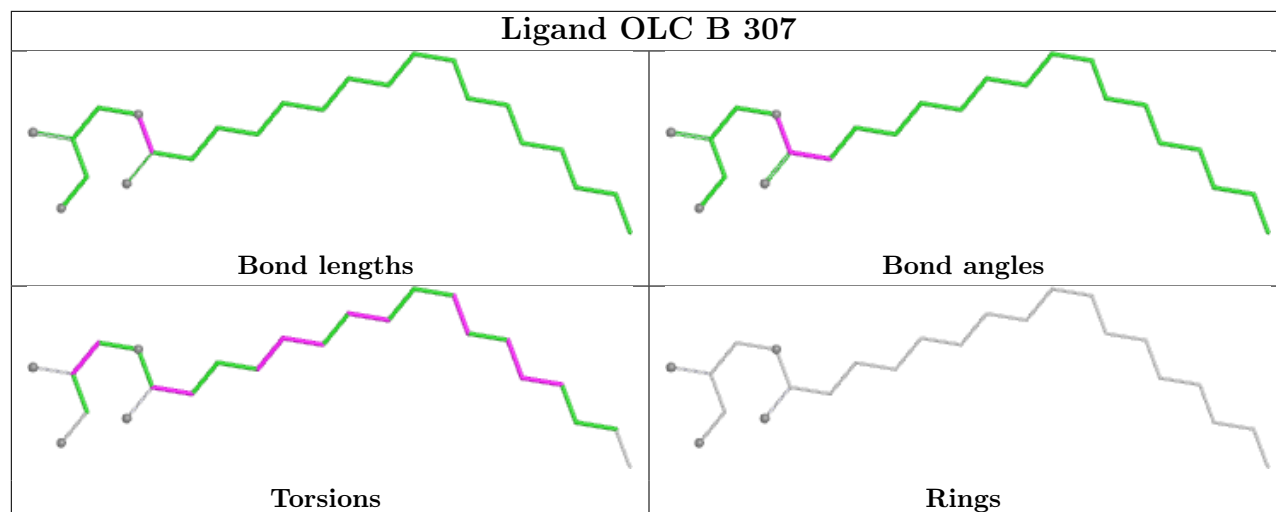


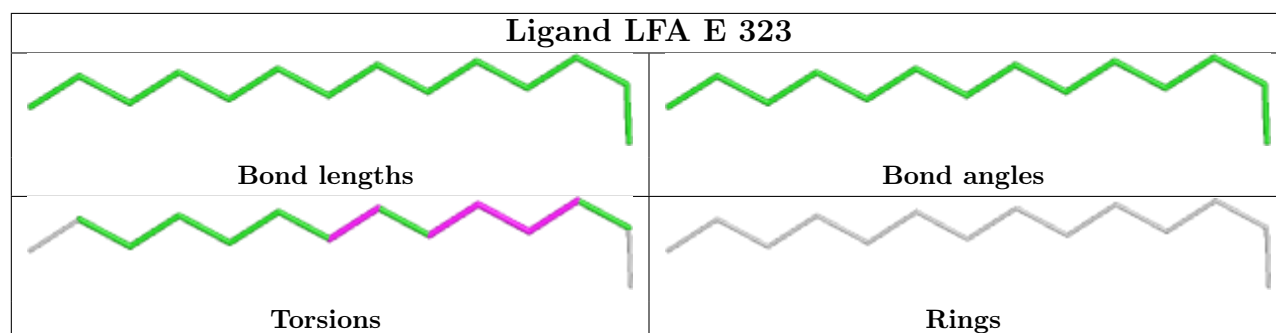
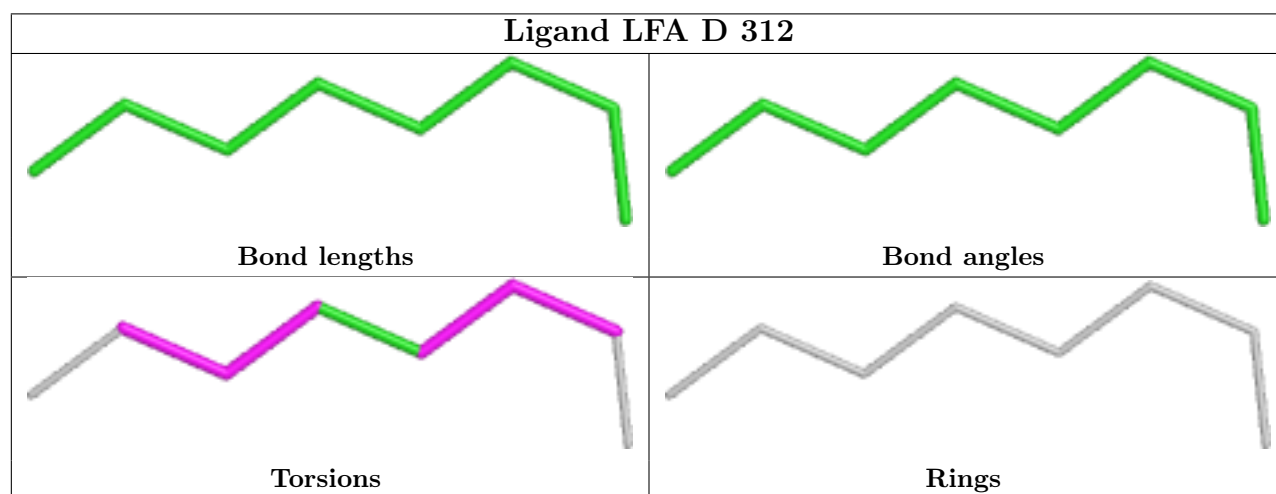
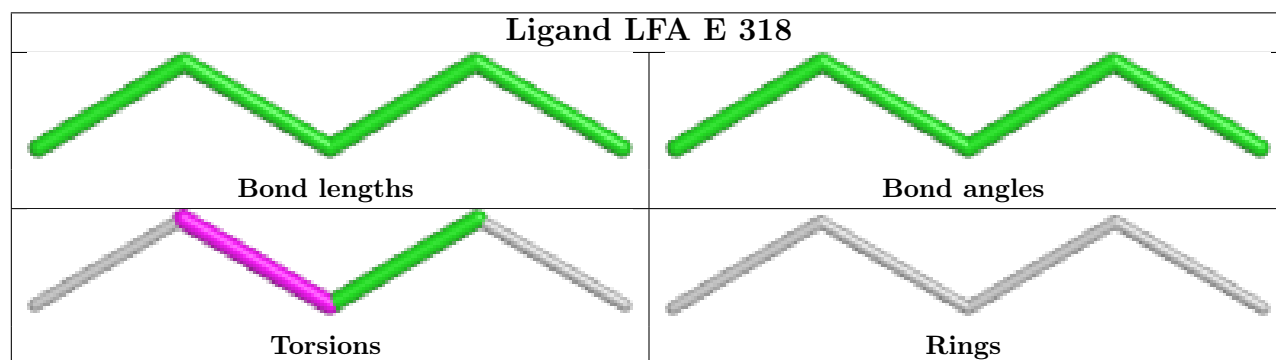
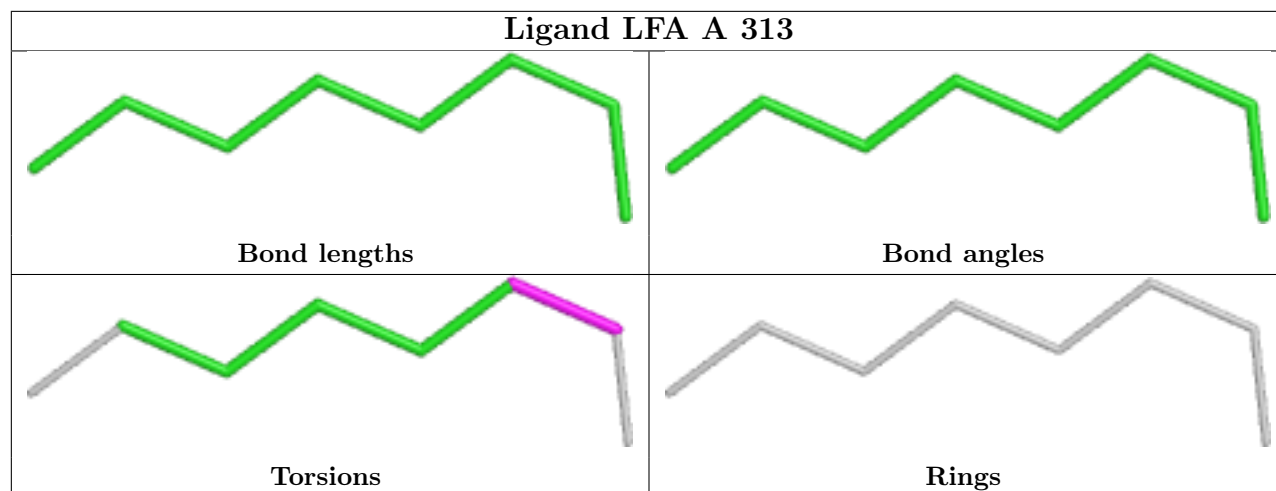




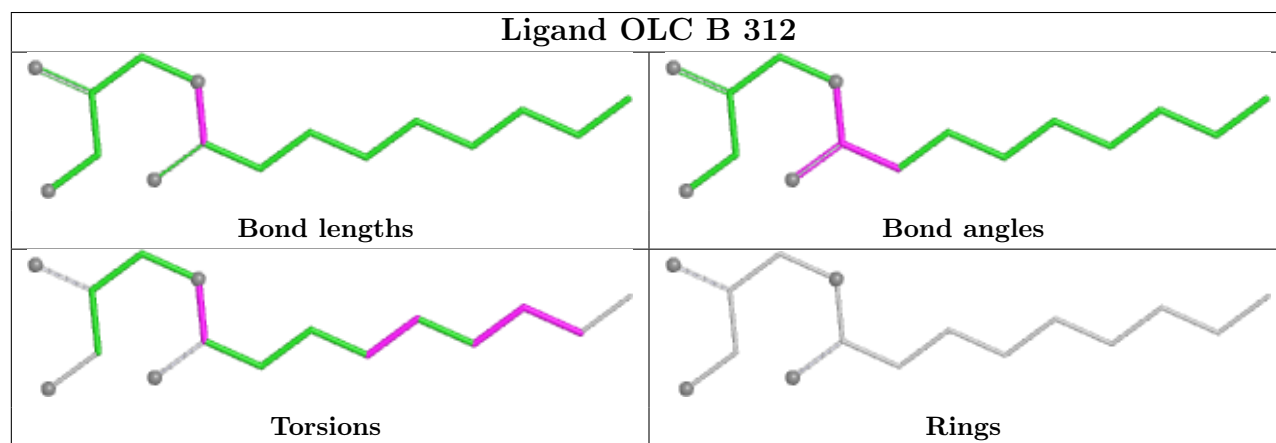
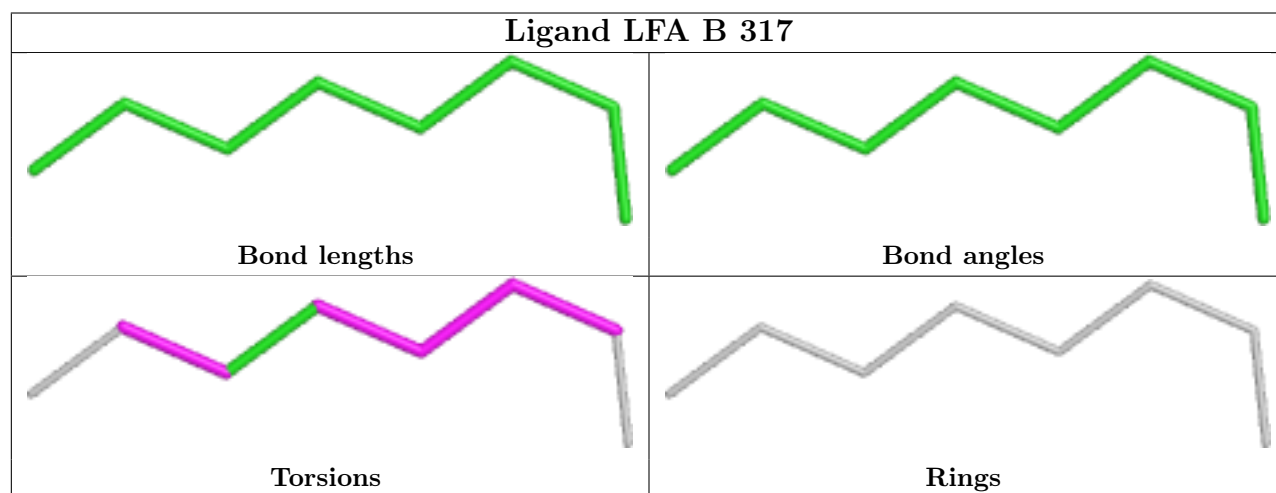
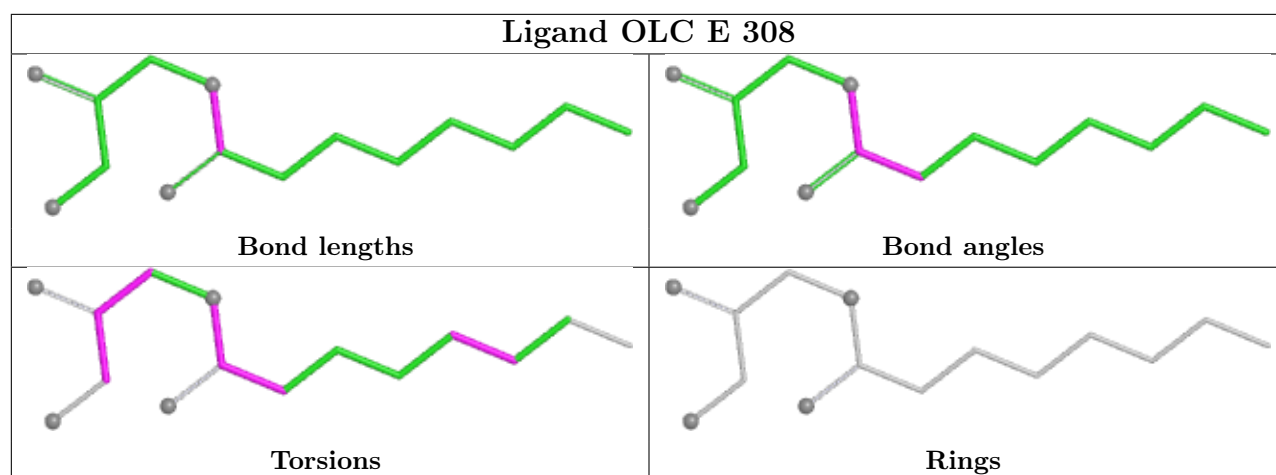


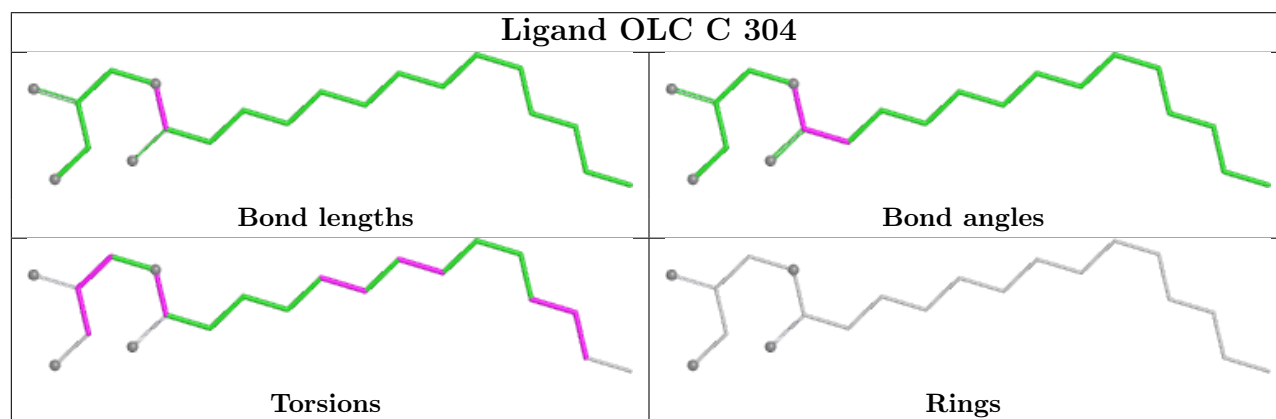
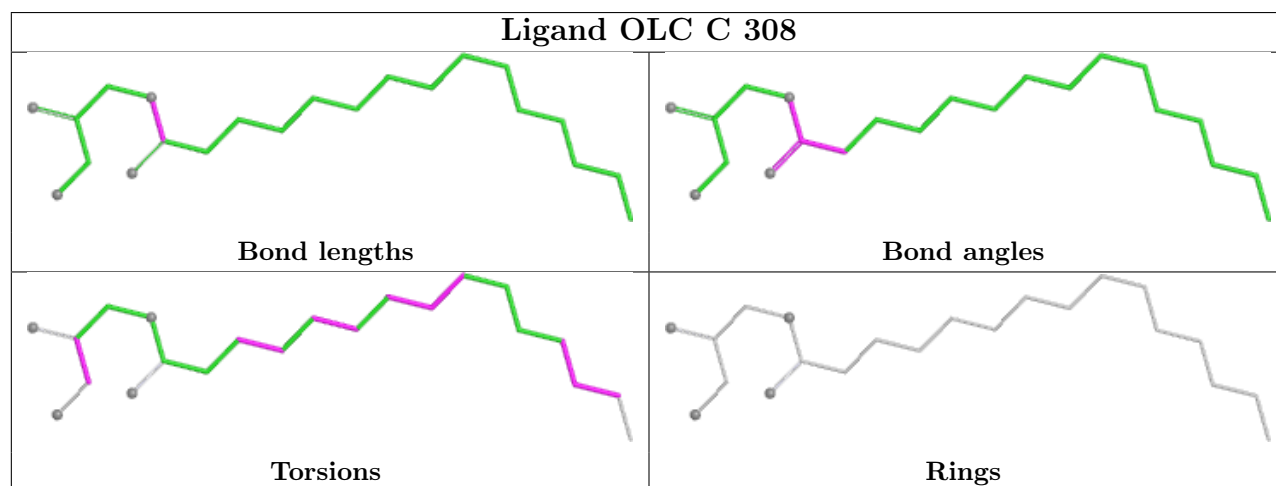
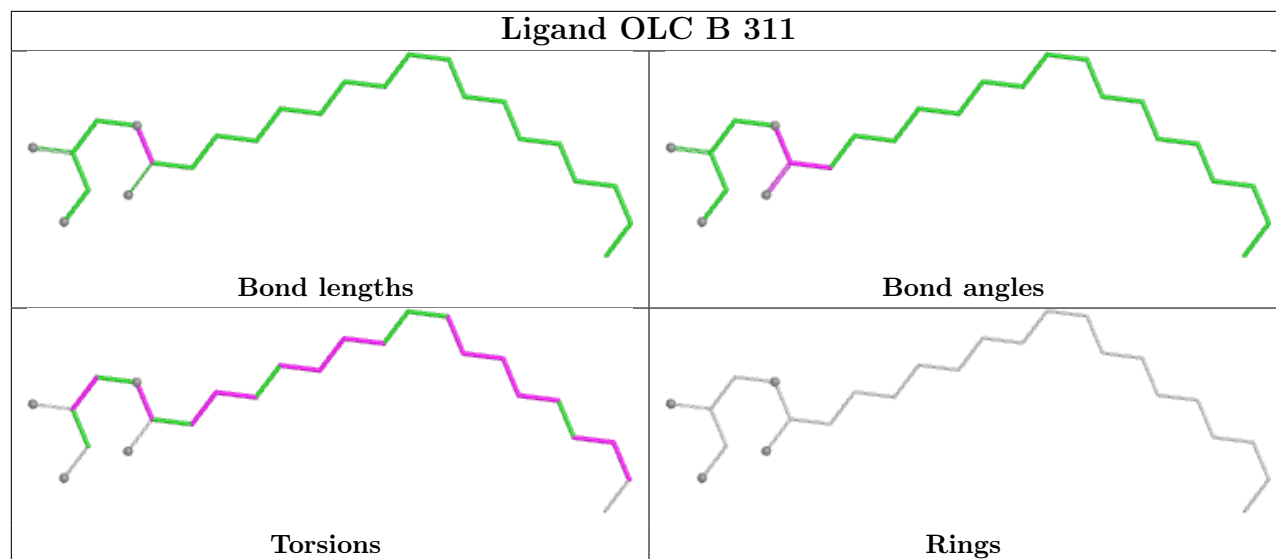


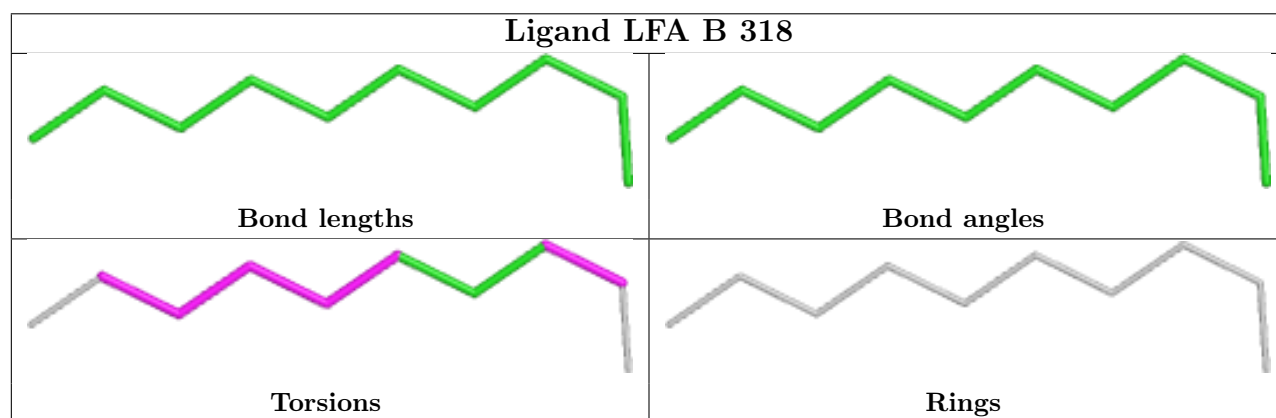
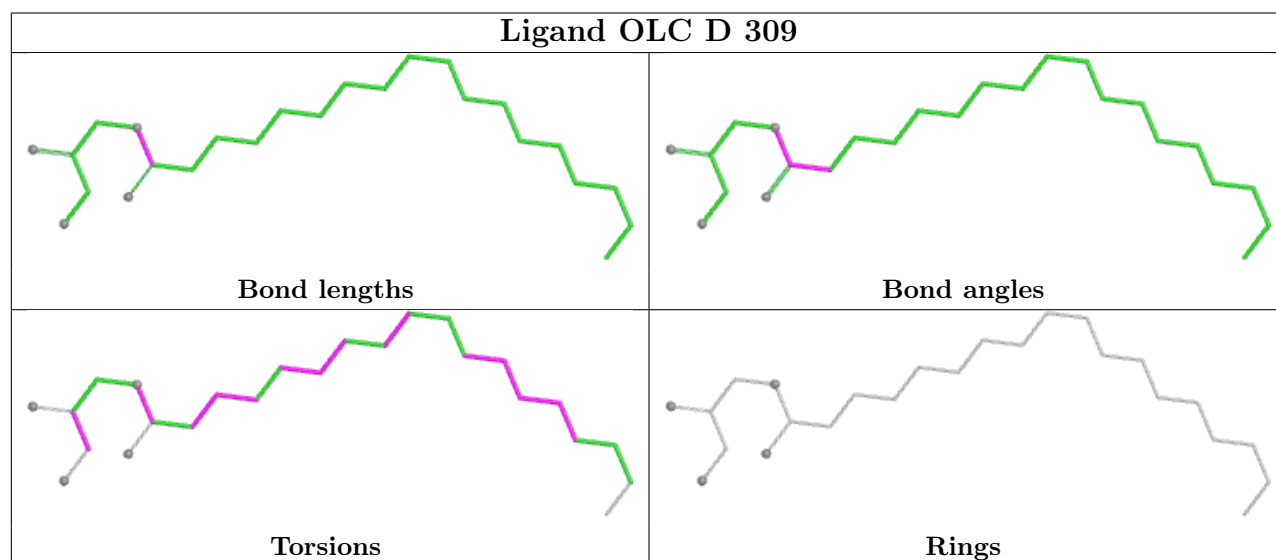
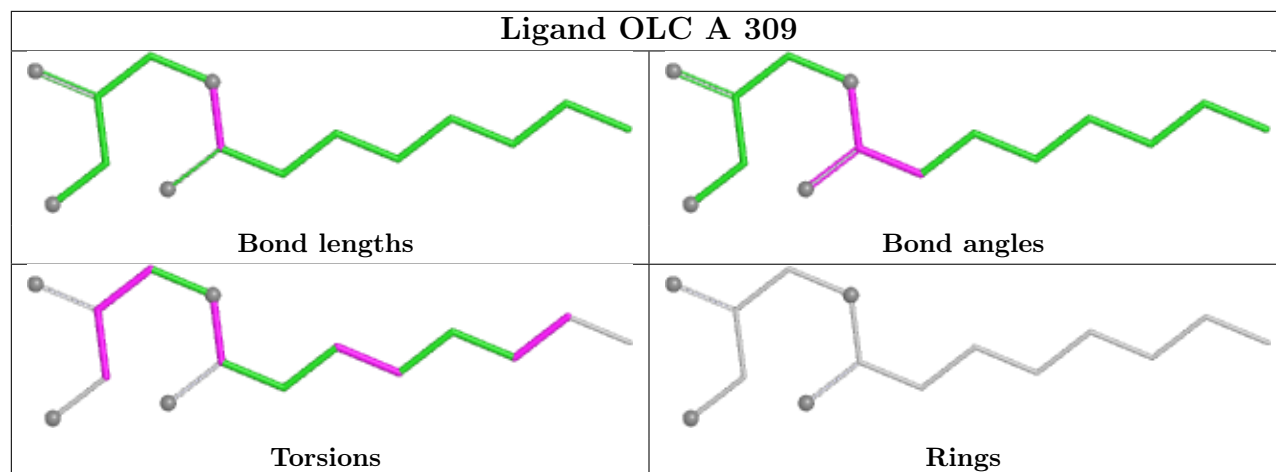


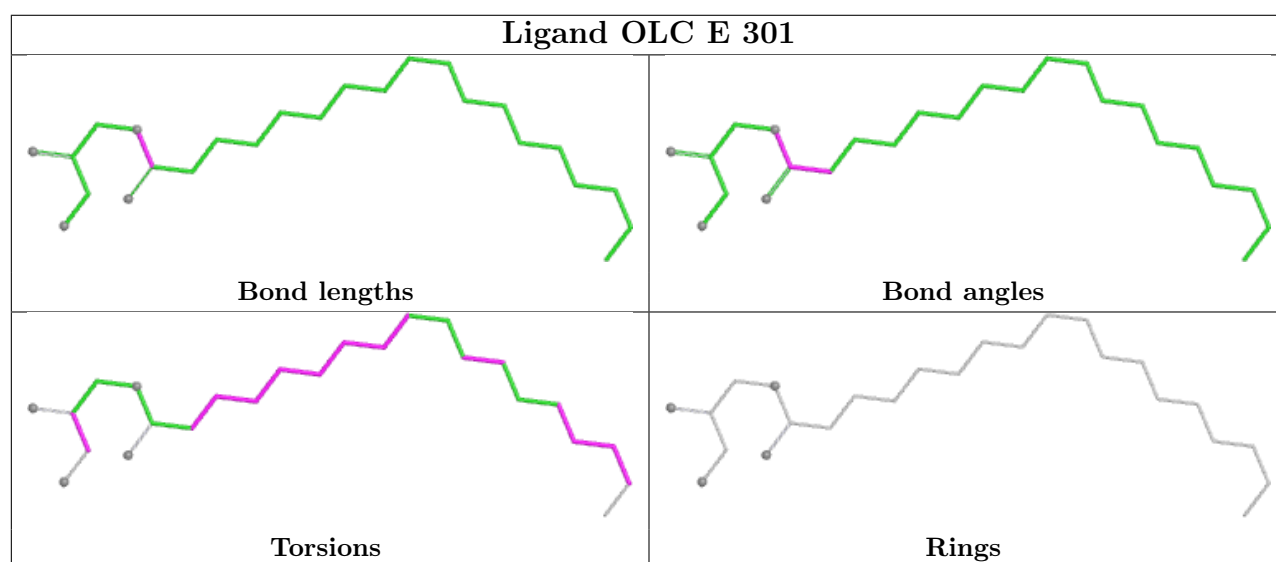
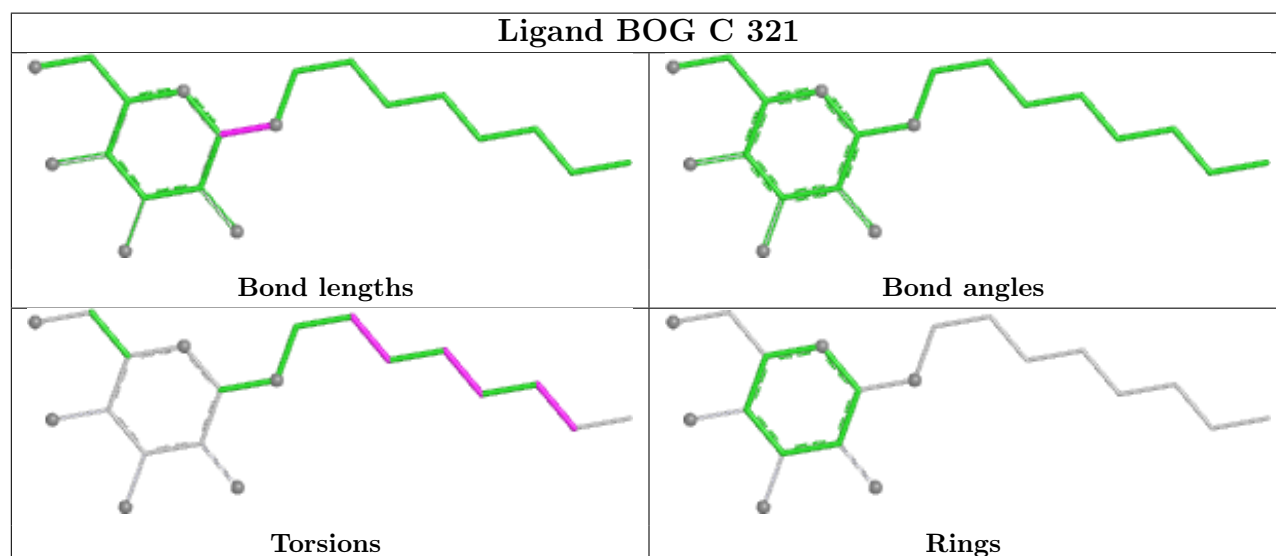
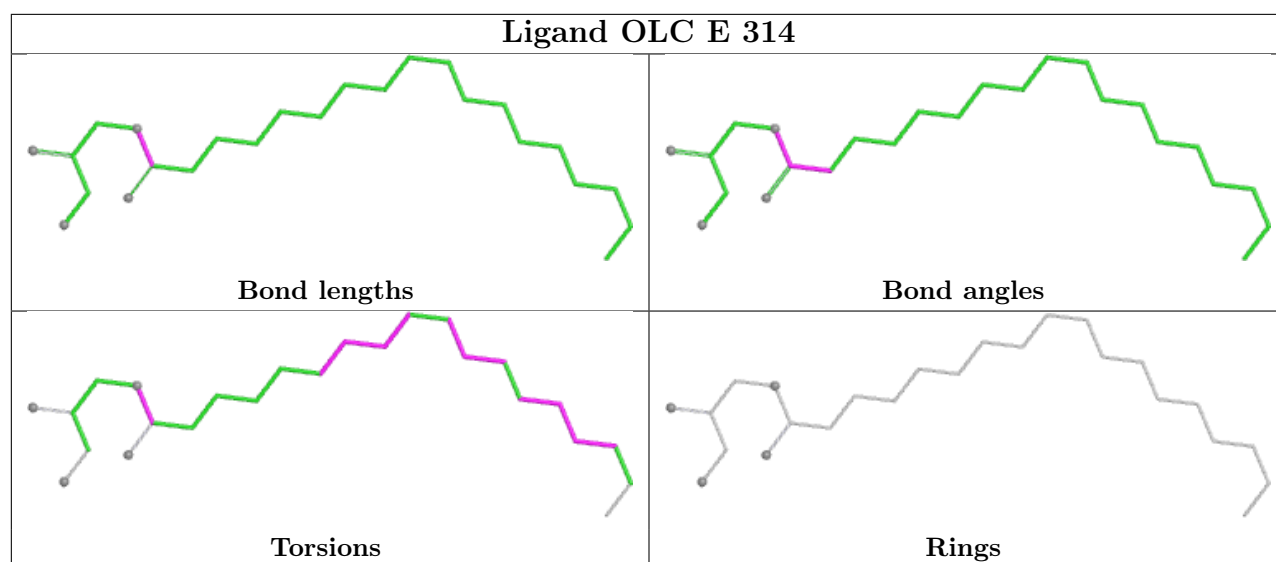


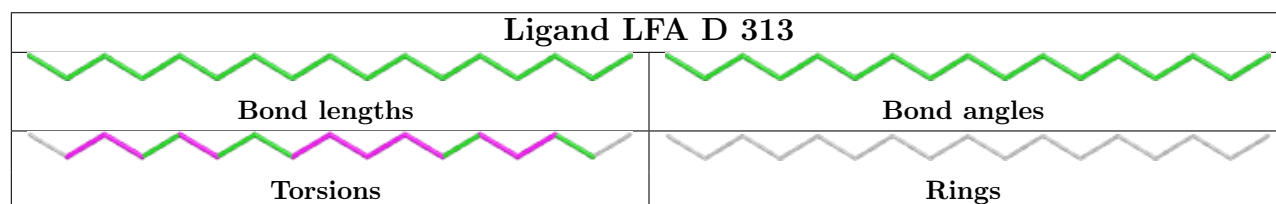
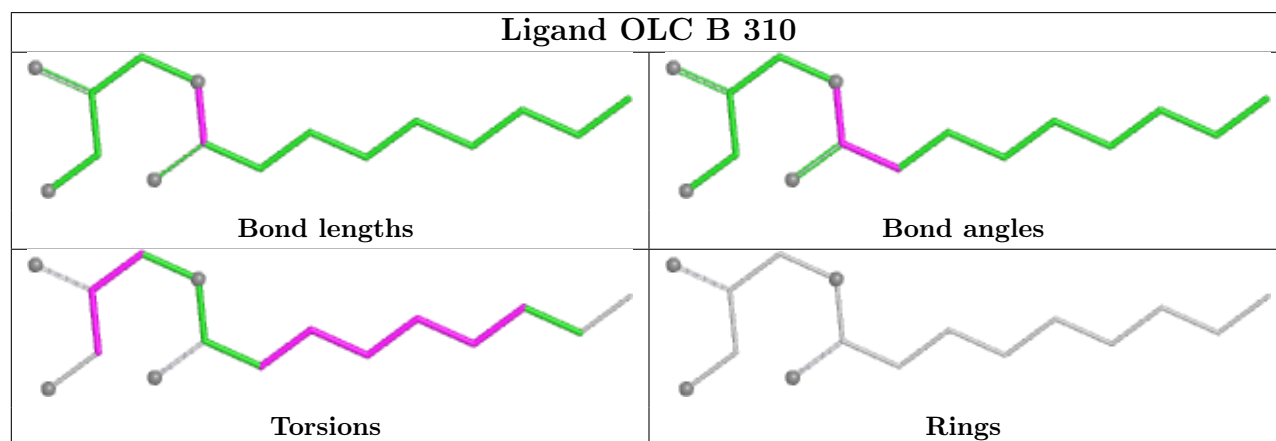
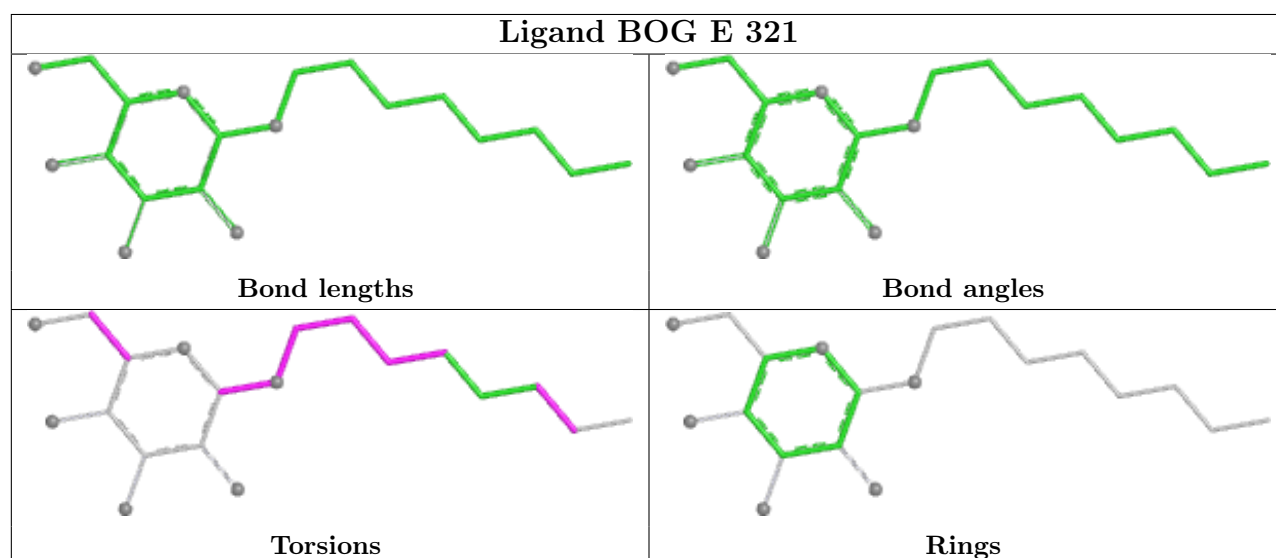
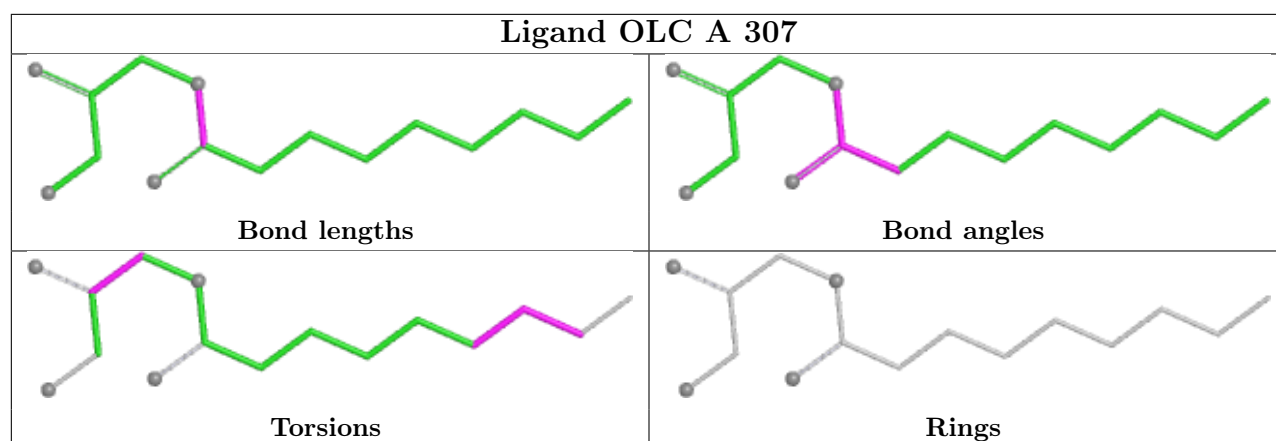


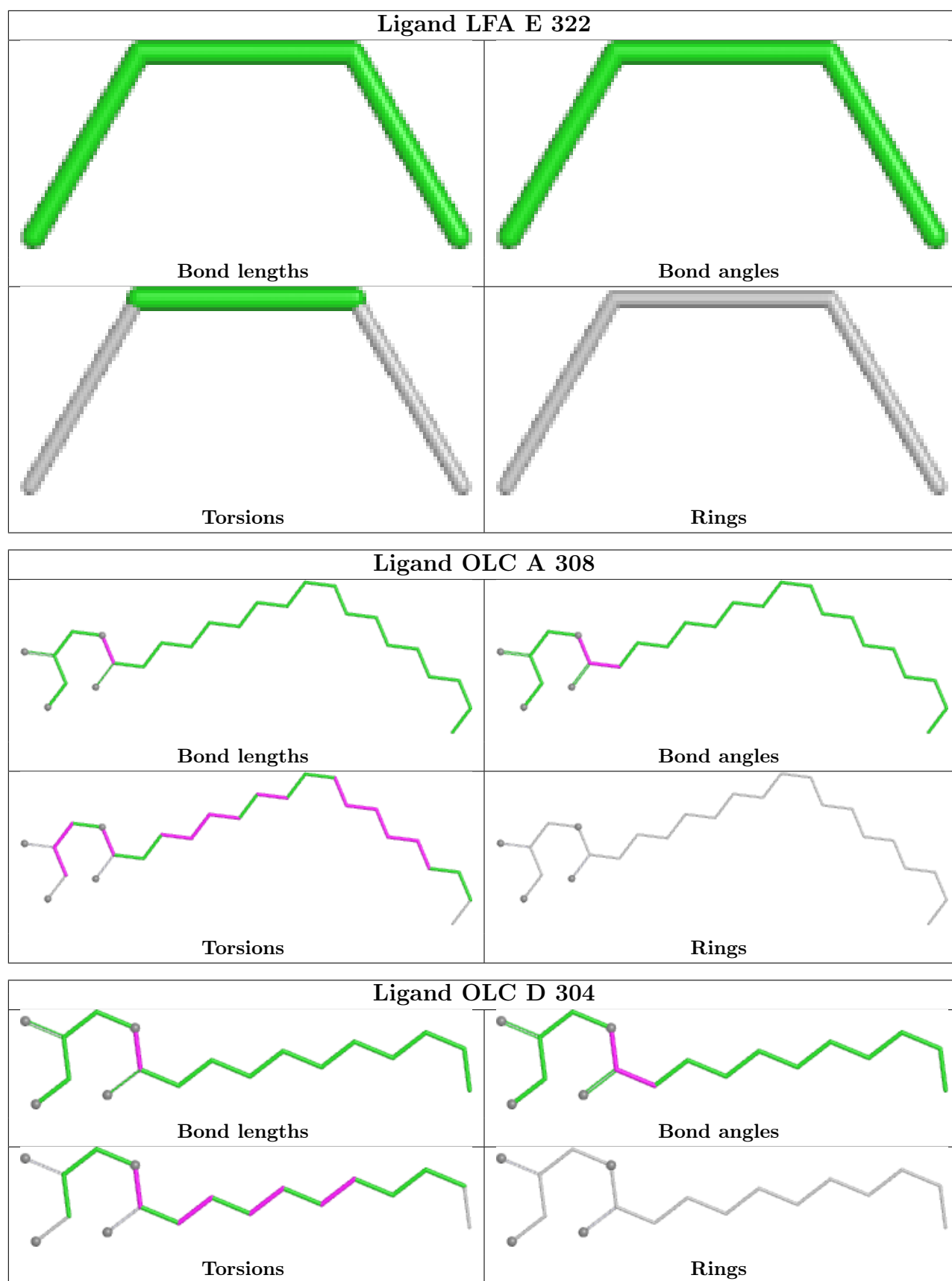


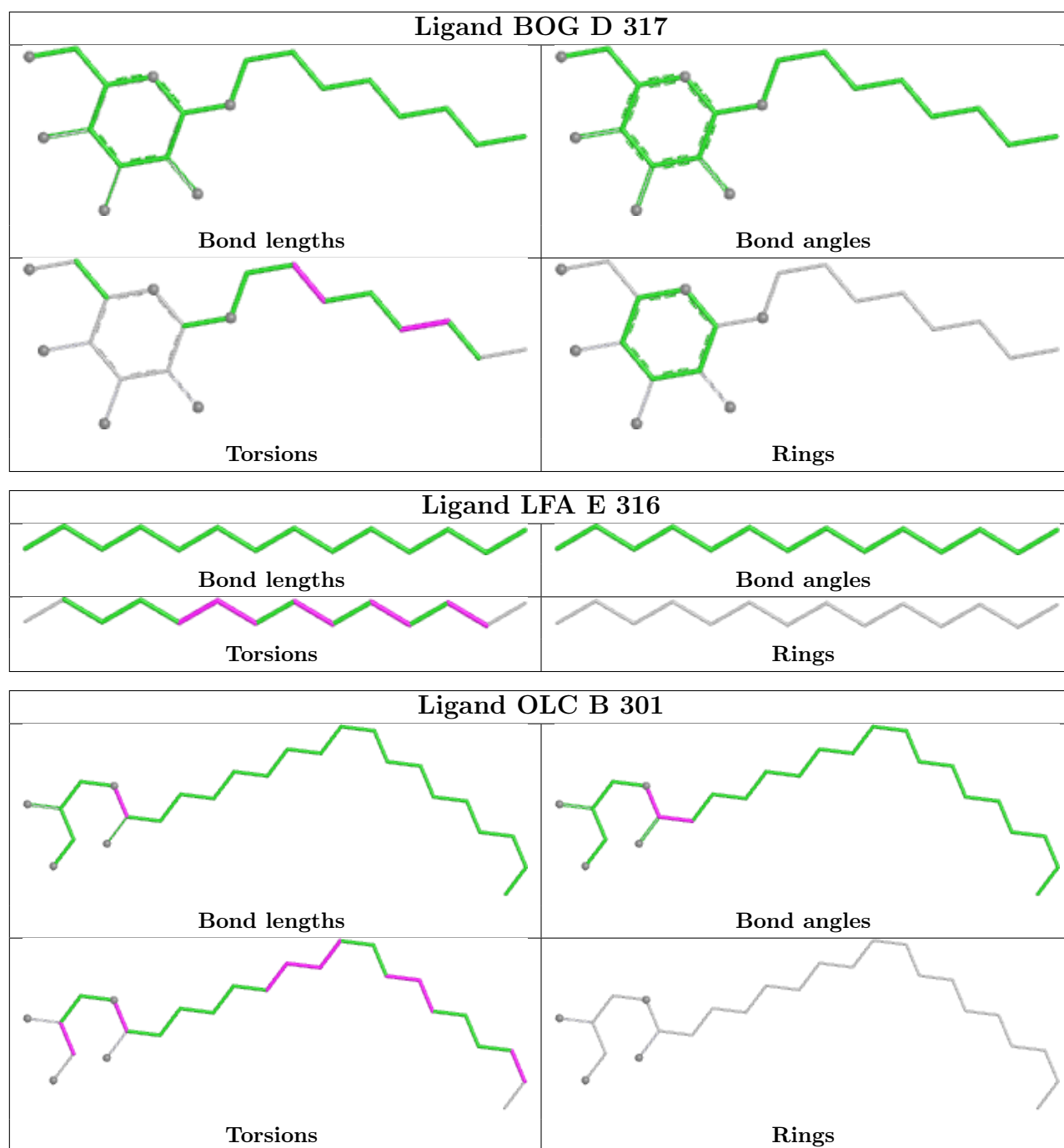


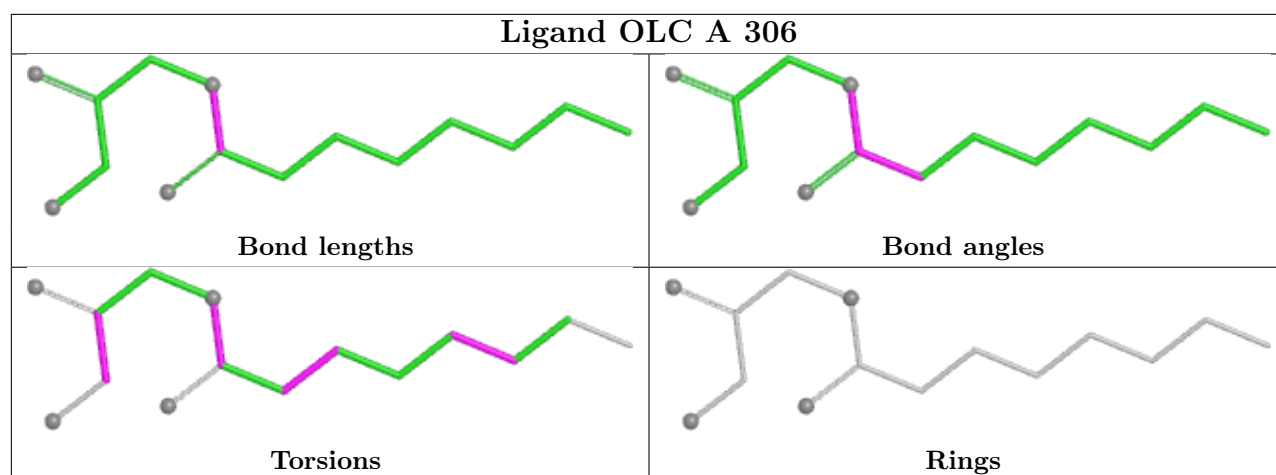












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 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     | 272/288 (94%)   | -0.33  | 3 (1%) 78 74  | 34, 45, 68, 152       | 0     |
| 1   | B     | 272/288 (94%)   | -0.25  | 2 (0%) 84 81  | 36, 45, 69, 148       | 0     |
| 1   | C     | 272/288 (94%)   | -0.20  | 3 (1%) 78 74  | 35, 45, 68, 179       | 0     |
| 1   | D     | 272/288 (94%)   | -0.18  | 5 (1%) 67 63  | 35, 47, 74, 176       | 0     |
| 1   | E     | 272/288 (94%)   | -0.19  | 4 (1%) 72 68  | 33, 45, 69, 179       | 0     |
| All | All   | 1360/1440 (94%) | -0.23  | 17 (1%) 75 71 | 33, 45, 70, 179       | 0     |

All (17) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 275 | LEU  | 7.0  |
| 1   | E     | 275 | LEU  | 5.1  |
| 1   | A     | 275 | LEU  | 4.4  |
| 1   | B     | 275 | LEU  | 4.0  |
| 1   | D     | 274 | GLU  | 3.2  |
| 1   | E     | 274 | GLU  | 3.0  |
| 1   | D     | 271 | LYS  | 2.7  |
| 1   | B     | 273 | LYS  | 2.7  |
| 1   | E     | 272 | ASN  | 2.6  |
| 1   | D     | 3   | GLN  | 2.5  |
| 1   | D     | 275 | LEU  | 2.4  |
| 1   | A     | 90  | GLU  | 2.4  |
| 1   | E     | 91  | GLU  | 2.3  |
| 1   | C     | 91  | GLU  | 2.2  |
| 1   | D     | 183 | TRP  | 2.2  |
| 1   | C     | 92  | VAL  | 2.1  |
| 1   | A     | 3   | GLN  | 2.1  |

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

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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 1   | LYR  | D     | 255 | 29/30 | 0.93 | 0.09 | 35,42,49,49                | 0     |
| 1   | LYR  | E     | 255 | 29/30 | 0.93 | 0.10 | 34,39,44,47                | 0     |
| 1   | LYR  | C     | 255 | 29/30 | 0.94 | 0.09 | 34,42,48,52                | 0     |
| 1   | LYR  | B     | 255 | 29/30 | 0.96 | 0.08 | 33,39,53,57                | 0     |
| 1   | LYR  | A     | 255 | 29/30 | 0.96 | 0.08 | 34,40,48,51                | 0     |

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | LFA  | E     | 322 | 4/20  | 0.66 | 0.49 | 73,79,81,83                | 0     |
| 2   | OLC  | C     | 309 | 16/25 | 0.70 | 0.24 | 82,110,137,140             | 0     |
| 2   | OLC  | A     | 307 | 16/25 | 0.70 | 0.23 | 90,107,122,128             | 0     |
| 2   | OLC  | E     | 311 | 11/25 | 0.71 | 0.20 | 94,110,127,133             | 0     |
| 2   | OLC  | D     | 306 | 25/25 | 0.72 | 0.22 | 80,101,115,122             | 0     |
| 3   | LFA  | D     | 315 | 6/20  | 0.73 | 0.30 | 73,87,99,104               | 0     |
| 2   | OLC  | E     | 313 | 20/25 | 0.73 | 0.23 | 65,112,127,135             | 0     |
| 2   | OLC  | B     | 314 | 15/25 | 0.74 | 0.23 | 90,107,125,126             | 0     |
| 2   | OLC  | E     | 303 | 14/25 | 0.75 | 0.21 | 104,126,146,183            | 0     |
| 2   | OLC  | A     | 306 | 15/25 | 0.76 | 0.19 | 69,96,128,137              | 0     |
| 2   | OLC  | B     | 303 | 14/25 | 0.76 | 0.21 | 101,136,164,188            | 0     |
| 3   | LFA  | E     | 317 | 4/20  | 0.76 | 0.36 | 68,71,76,85                | 0     |
| 2   | OLC  | D     | 303 | 25/25 | 0.76 | 0.24 | 75,101,114,115             | 0     |
| 2   | OLC  | C     | 306 | 25/25 | 0.77 | 0.22 | 72,95,117,128              | 0     |
| 3   | LFA  | B     | 316 | 9/20  | 0.77 | 0.30 | 75,92,99,101               | 0     |
| 2   | OLC  | B     | 307 | 24/25 | 0.77 | 0.24 | 83,112,130,134             | 0     |
| 2   | OLC  | E     | 308 | 15/25 | 0.77 | 0.19 | 84,107,142,147             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | OLC  | A     | 301 | 15/25 | 0.77 | 0.18 | 95,124,172,178              | 0     |
| 2   | OLC  | C     | 307 | 25/25 | 0.78 | 0.19 | 69,93,114,123               | 0     |
| 2   | OLC  | B     | 305 | 15/25 | 0.79 | 0.23 | 87,114,139,139              | 0     |
| 2   | OLC  | A     | 308 | 25/25 | 0.79 | 0.20 | 78,103,127,132              | 0     |
| 3   | LFA  | E     | 302 | 20/20 | 0.79 | 0.24 | 57,76,93,105                | 0     |
| 2   | OLC  | D     | 302 | 13/25 | 0.79 | 0.21 | 116,129,142,171             | 0     |
| 3   | LFA  | A     | 316 | 4/20  | 0.79 | 0.32 | 81,85,93,95                 | 0     |
| 2   | OLC  | A     | 304 | 25/25 | 0.80 | 0.20 | 70,98,119,137               | 0     |
| 3   | LFA  | C     | 317 | 11/20 | 0.80 | 0.29 | 72,88,105,107               | 0     |
| 3   | LFA  | A     | 312 | 7/20  | 0.81 | 0.29 | 86,90,92,101                | 0     |
| 3   | LFA  | C     | 314 | 7/20  | 0.81 | 0.25 | 67,79,104,106               | 0     |
| 3   | LFA  | B     | 302 | 20/20 | 0.81 | 0.23 | 59,75,86,93                 | 0     |
| 3   | LFA  | E     | 319 | 20/20 | 0.81 | 0.21 | 52,75,89,95                 | 0     |
| 3   | LFA  | D     | 310 | 20/20 | 0.81 | 0.26 | 81,94,105,115               | 0     |
| 5   | BOG  | A     | 320 | 20/20 | 0.81 | 0.17 | 76,107,122,122              | 0     |
| 2   | OLC  | E     | 306 | 24/25 | 0.82 | 0.21 | 85,103,140,162              | 0     |
| 2   | OLC  | B     | 311 | 25/25 | 0.82 | 0.19 | 82,102,121,127              | 0     |
| 3   | LFA  | C     | 319 | 20/20 | 0.82 | 0.20 | 55,68,79,80                 | 0     |
| 2   | OLC  | A     | 310 | 16/25 | 0.82 | 0.25 | 76,105,138,148              | 0     |
| 3   | LFA  | E     | 323 | 14/20 | 0.82 | 0.34 | 101,125,159,162             | 0     |
| 2   | OLC  | B     | 304 | 25/25 | 0.82 | 0.20 | 78,107,124,133              | 0     |
| 5   | BOG  | E     | 321 | 20/20 | 0.82 | 0.15 | 73,106,121,123              | 0     |
| 2   | OLC  | B     | 310 | 16/25 | 0.83 | 0.17 | 71,96,130,131               | 0     |
| 2   | OLC  | B     | 312 | 16/25 | 0.83 | 0.17 | 65,83,97,111                | 0     |
| 2   | OLC  | C     | 310 | 25/25 | 0.83 | 0.21 | 89,100,121,127              | 0     |
| 3   | LFA  | B     | 318 | 10/20 | 0.83 | 0.28 | 75,92,103,104               | 0     |
| 3   | LFA  | B     | 319 | 7/20  | 0.83 | 0.27 | 65,76,100,111               | 0     |
| 5   | BOG  | B     | 321 | 20/20 | 0.83 | 0.17 | 75,102,116,129              | 0     |
| 3   | LFA  | C     | 302 | 20/20 | 0.83 | 0.20 | 61,71,77,81                 | 0     |
| 2   | OLC  | C     | 303 | 14/25 | 0.84 | 0.19 | 93,115,149,167              | 0     |
| 2   | OLC  | C     | 308 | 22/25 | 0.84 | 0.19 | 58,98,127,148               | 0     |
| 2   | OLC  | E     | 312 | 25/25 | 0.84 | 0.24 | 80,98,116,135               | 0     |
| 5   | BOG  | C     | 321 | 20/20 | 0.84 | 0.16 | 76,93,115,115               | 0     |
| 2   | OLC  | D     | 305 | 23/25 | 0.84 | 0.20 | 60,112,160,166              | 0     |
| 2   | OLC  | E     | 314 | 25/25 | 0.85 | 0.19 | 86,115,149,161              | 0     |
| 3   | LFA  | A     | 318 | 20/20 | 0.85 | 0.23 | 80,107,126,131              | 0     |
| 3   | LFA  | E     | 318 | 5/20  | 0.85 | 0.24 | 83,83,92,101                | 0     |
| 2   | OLC  | A     | 302 | 25/25 | 0.85 | 0.24 | 74,111,124,141              | 0     |
| 3   | LFA  | A     | 315 | 12/20 | 0.85 | 0.23 | 92,99,111,112               | 0     |
| 2   | OLC  | D     | 309 | 25/25 | 0.86 | 0.25 | 79,95,116,131               | 0     |
| 2   | OLC  | B     | 309 | 21/25 | 0.86 | 0.17 | 58,87,118,143               | 0     |
| 2   | OLC  | B     | 315 | 16/25 | 0.87 | 0.24 | 75,88,123,145               | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | OLC  | D     | 304 | 18/25 | 0.87 | 0.17 | 74,96,115,118               | 0     |
| 2   | OLC  | E     | 304 | 16/25 | 0.87 | 0.16 | 67,116,151,155              | 0     |
| 2   | OLC  | B     | 308 | 20/25 | 0.87 | 0.16 | 64,86,109,114               | 0     |
| 2   | OLC  | C     | 304 | 21/25 | 0.87 | 0.25 | 74,115,144,153              | 0     |
| 3   | LFA  | A     | 313 | 8/20  | 0.87 | 0.23 | 74,83,90,91                 | 0     |
| 3   | LFA  | E     | 316 | 14/20 | 0.87 | 0.23 | 69,91,104,110               | 0     |
| 5   | BOG  | D     | 317 | 20/20 | 0.87 | 0.17 | 89,102,112,114              | 0     |
| 2   | OLC  | E     | 310 | 15/25 | 0.87 | 0.20 | 58,97,131,132               | 0     |
| 3   | LFA  | C     | 315 | 8/20  | 0.88 | 0.26 | 79,90,98,101                | 0     |
| 3   | LFA  | C     | 316 | 20/20 | 0.88 | 0.22 | 63,92,121,125               | 0     |
| 3   | LFA  | E     | 315 | 8/20  | 0.88 | 0.23 | 72,99,104,104               | 0     |
| 2   | OLC  | B     | 301 | 25/25 | 0.88 | 0.18 | 74,90,122,124               | 0     |
| 2   | OLC  | A     | 305 | 13/25 | 0.88 | 0.14 | 64,73,86,86                 | 0     |
| 2   | OLC  | D     | 308 | 15/25 | 0.88 | 0.18 | 66,90,129,139               | 0     |
| 3   | LFA  | D     | 312 | 8/20  | 0.88 | 0.24 | 74,83,108,109               | 0     |
| 2   | OLC  | C     | 313 | 16/25 | 0.89 | 0.21 | 64,85,112,122               | 0     |
| 3   | LFA  | D     | 314 | 7/20  | 0.89 | 0.19 | 71,82,99,105                | 0     |
| 2   | OLC  | D     | 301 | 18/25 | 0.89 | 0.20 | 77,96,118,128               | 0     |
| 2   | OLC  | E     | 307 | 20/25 | 0.89 | 0.17 | 75,96,108,113               | 0     |
| 2   | OLC  | A     | 311 | 16/25 | 0.89 | 0.20 | 73,91,128,145               | 0     |
| 3   | LFA  | B     | 317 | 8/20  | 0.89 | 0.26 | 75,103,106,107              | 0     |
| 2   | OLC  | C     | 311 | 16/25 | 0.89 | 0.15 | 60,86,99,103                | 0     |
| 2   | OLC  | C     | 312 | 16/25 | 0.89 | 0.17 | 65,90,118,120               | 0     |
| 2   | OLC  | E     | 301 | 25/25 | 0.90 | 0.20 | 63,92,133,149               | 0     |
| 3   | LFA  | D     | 311 | 20/20 | 0.90 | 0.23 | 70,98,113,113               | 0     |
| 3   | LFA  | A     | 314 | 8/20  | 0.90 | 0.23 | 66,91,111,123               | 0     |
| 2   | OLC  | A     | 321 | 25/25 | 0.90 | 0.20 | 65,91,126,134               | 0     |
| 3   | LFA  | C     | 318 | 4/20  | 0.90 | 0.24 | 87,93,94,97                 | 0     |
| 2   | OLC  | B     | 313 | 17/25 | 0.90 | 0.20 | 73,99,129,136               | 0     |
| 2   | OLC  | E     | 309 | 25/25 | 0.91 | 0.19 | 56,98,132,140               | 0     |
| 2   | OLC  | A     | 309 | 15/25 | 0.91 | 0.14 | 60,76,101,104               | 0     |
| 2   | OLC  | D     | 307 | 14/25 | 0.91 | 0.14 | 56,82,98,102                | 0     |
| 2   | OLC  | A     | 303 | 22/25 | 0.91 | 0.16 | 48,65,121,170               | 0     |
| 2   | OLC  | C     | 305 | 23/25 | 0.91 | 0.16 | 49,66,121,135               | 0     |
| 2   | OLC  | B     | 306 | 20/25 | 0.91 | 0.17 | 75,90,119,120               | 0     |
| 2   | OLC  | E     | 305 | 24/25 | 0.92 | 0.15 | 51,66,129,145               | 0     |
| 3   | LFA  | A     | 317 | 6/20  | 0.92 | 0.18 | 64,73,82,82                 | 0     |
| 3   | LFA  | D     | 313 | 17/20 | 0.92 | 0.15 | 49,57,84,85                 | 0     |
| 2   | OLC  | C     | 301 | 21/25 | 0.94 | 0.14 | 48,62,101,113               | 0     |
| 4   | NA   | B     | 320 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 4   | NA   | A     | 319 | 1/1   | 0.98 | 0.09 | 45,45,45,45                 | 0     |
| 4   | NA   | E     | 320 | 1/1   | 0.99 | 0.04 | 38,38,38,38                 | 0     |

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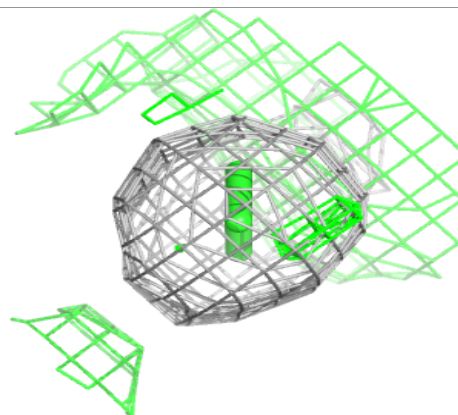
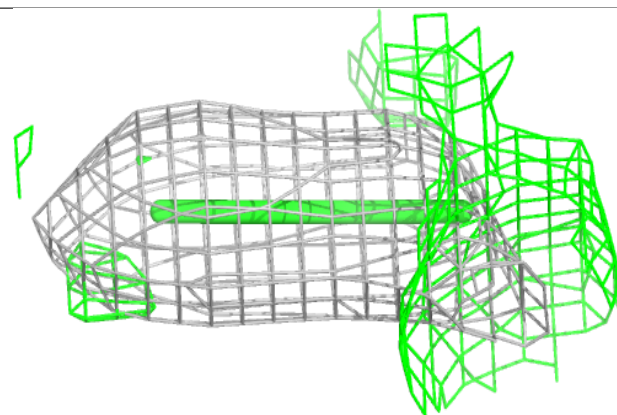
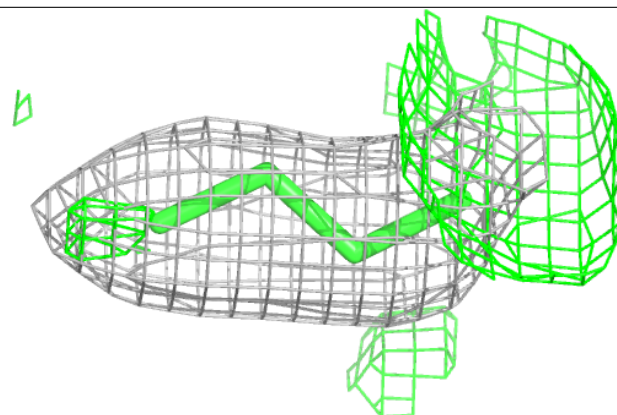
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | NA   | C     | 320 | 1/1   | 0.99 | 0.03 | 42,42,42,42                 | 0     |
| 4   | NA   | D     | 316 | 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.

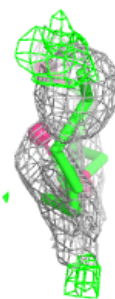
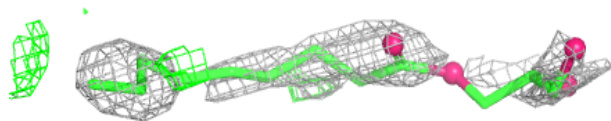
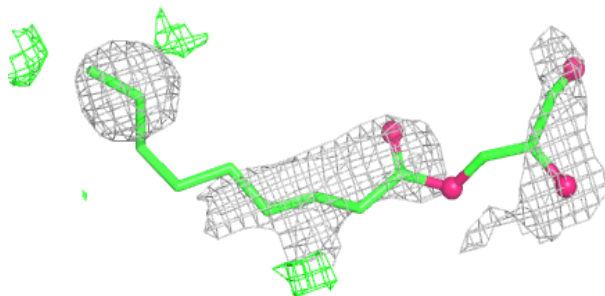
**Electron density around LFA E 322:**

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

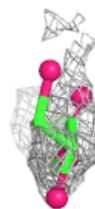
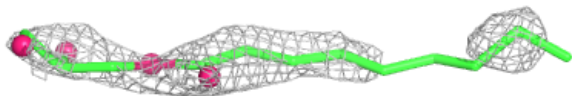
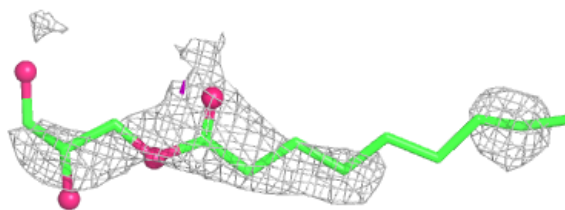


**Electron density around OLC C 309:**

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

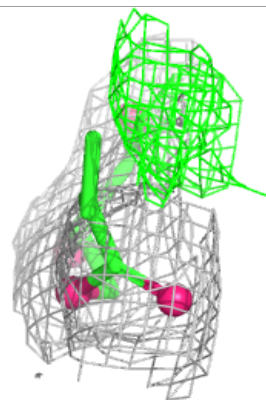
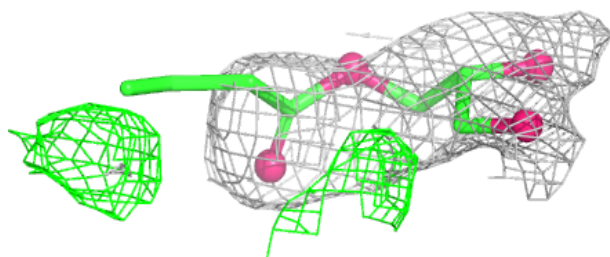
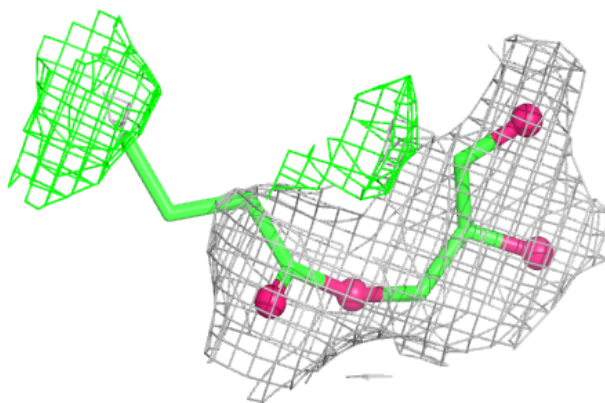
**Electron density around OLC A 307:**

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

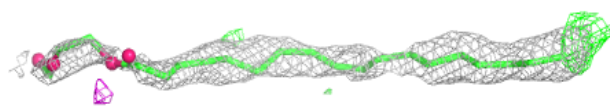
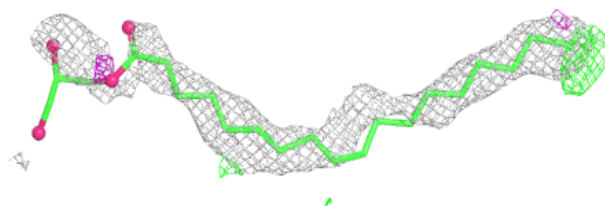


**Electron density around OLC E 311:**

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

**Electron density around OLC D 306:**

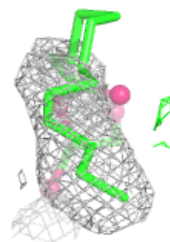
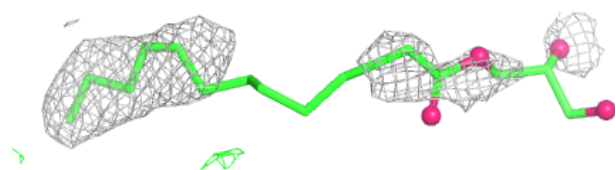
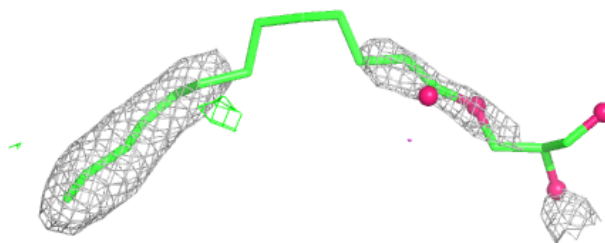
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



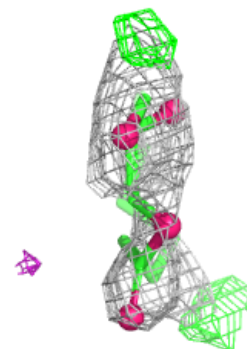
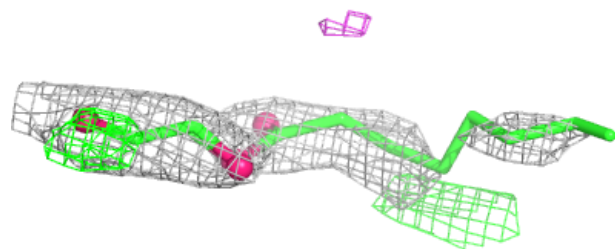
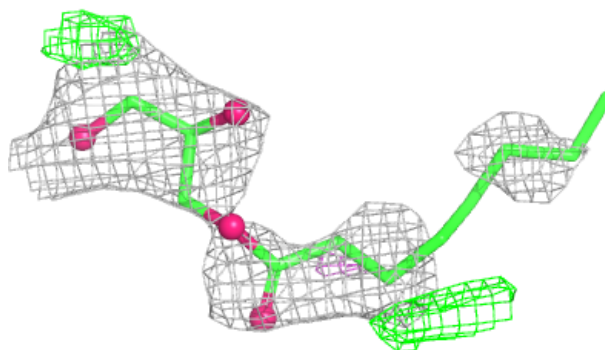


**Electron density around OLC E 313:**

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

**Electron density around OLC B 314:**

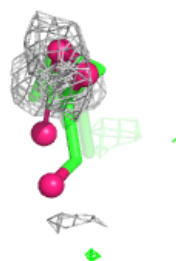
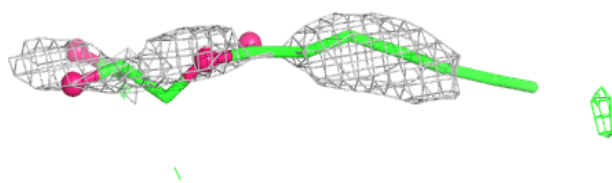
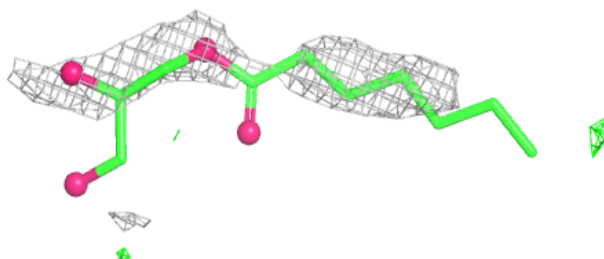
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



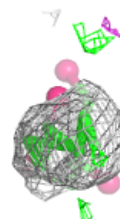
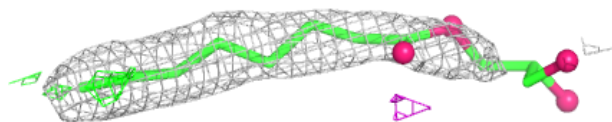
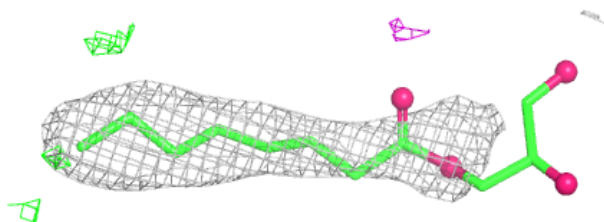


**Electron density around OLC E 303:**

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

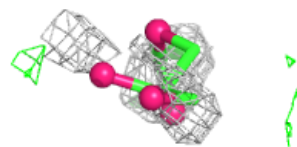
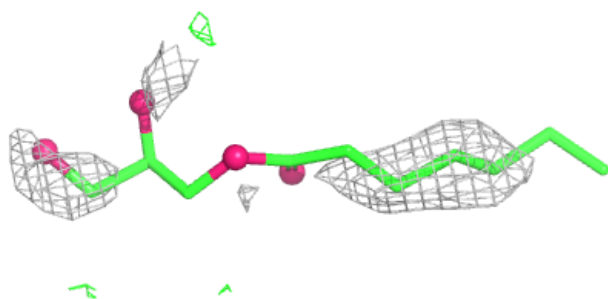
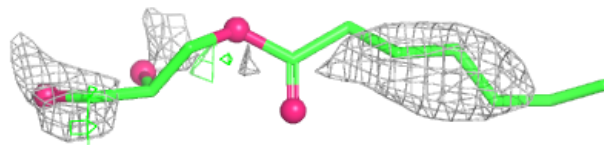
**Electron density around OLC A 306:**

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



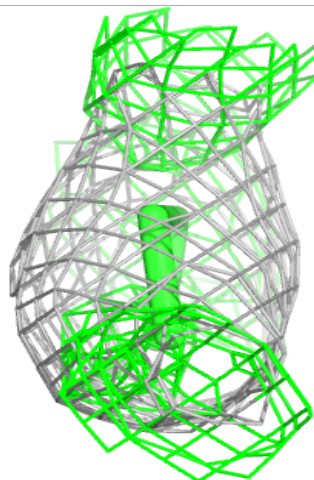
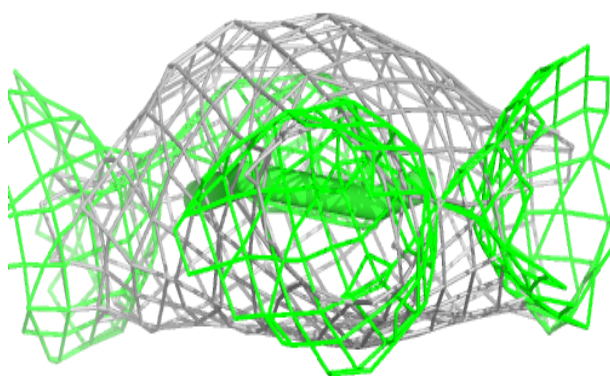
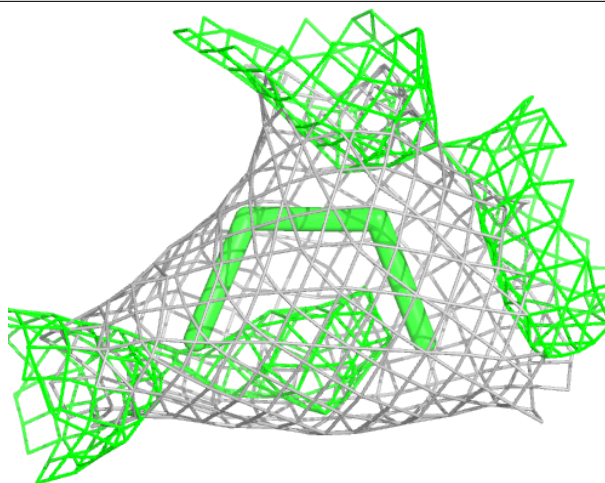
**Electron density around OLC B 303:**

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



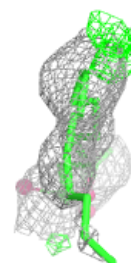
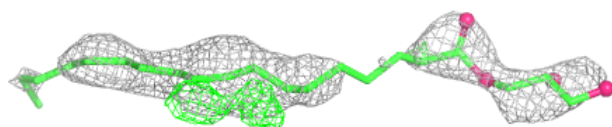
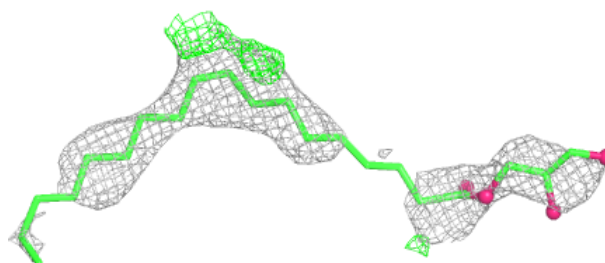
**Electron density around LFA E 317:**

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

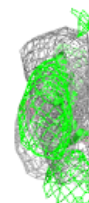
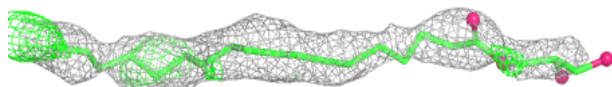
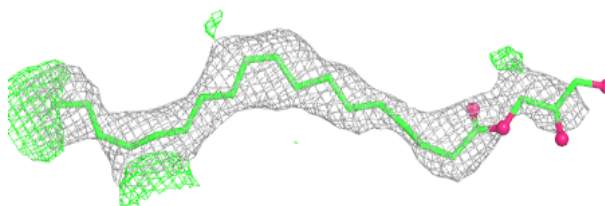


**Electron density around OLC D 303:**

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

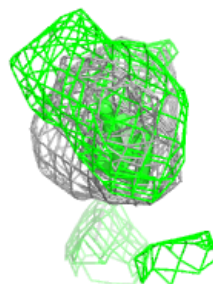
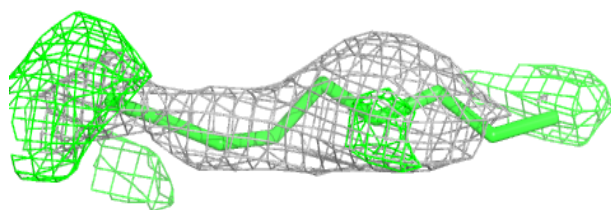
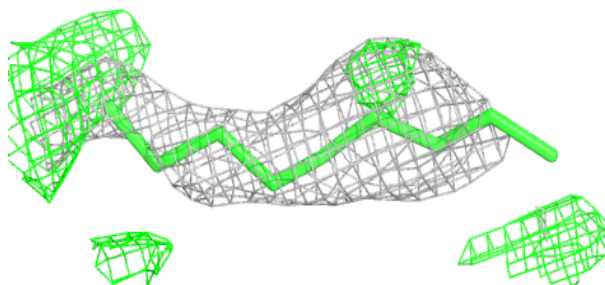
**Electron density around OLC C 306:**

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

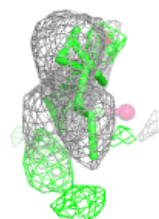
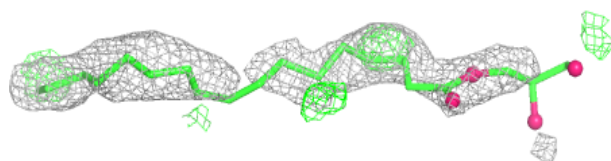
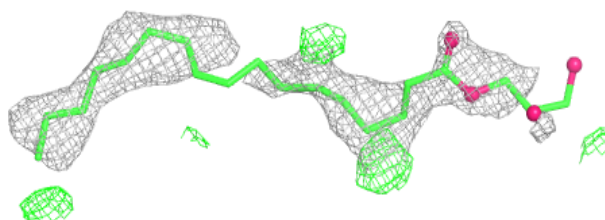


**Electron density around LFA B 316:**

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

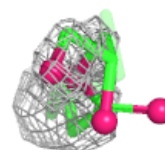
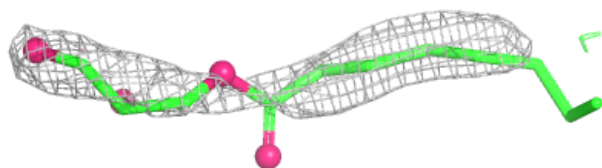
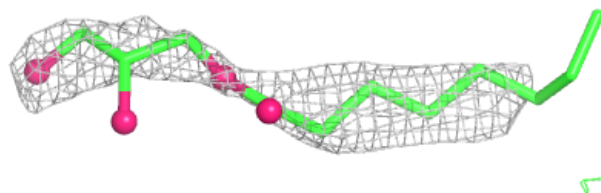
**Electron density around OLC B 307:**

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

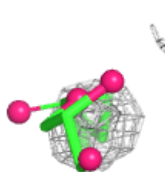
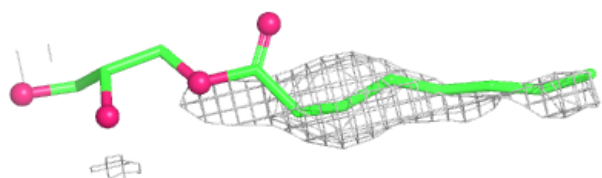
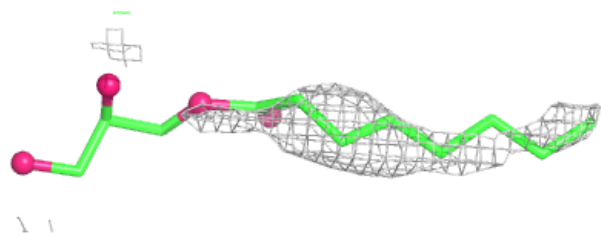


**Electron density around OLC E 308:**

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

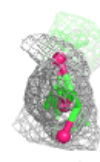
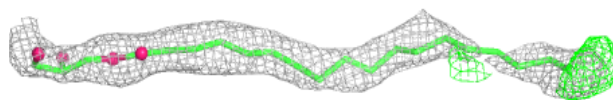
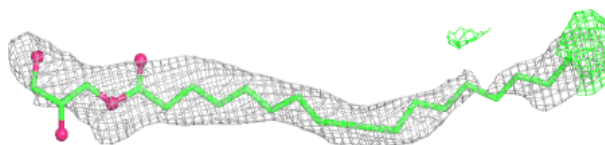
**Electron density around OLC A 301:**

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

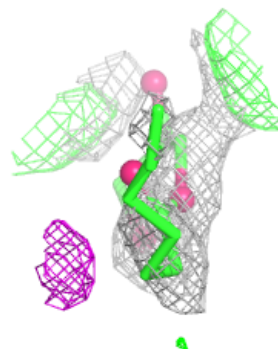
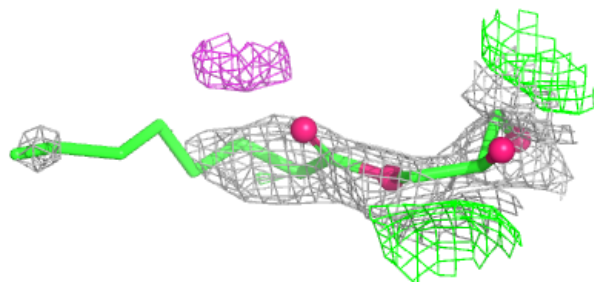
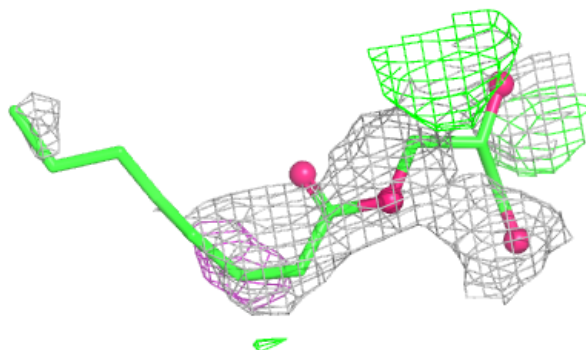


**Electron density around OLC C 307:**

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

**Electron density around OLC B 305:**

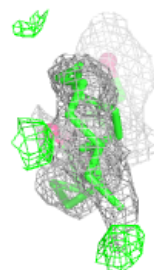
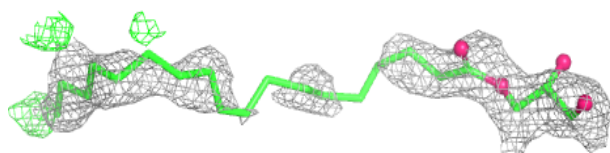
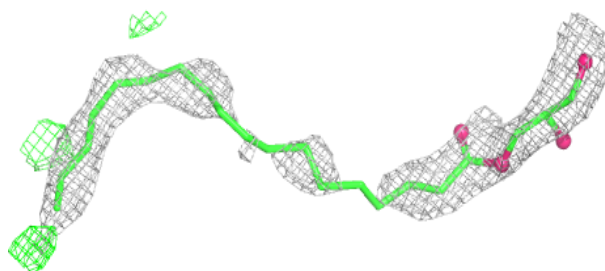
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



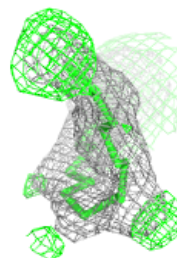
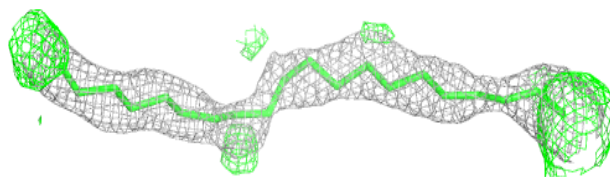
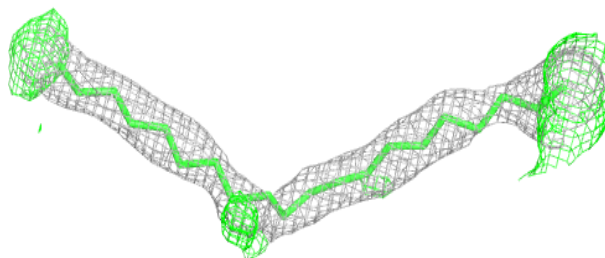


**Electron density around OLC A 308:**

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

**Electron density around LFA E 302:**

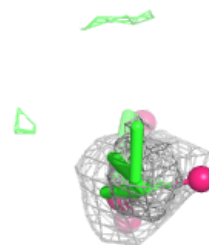
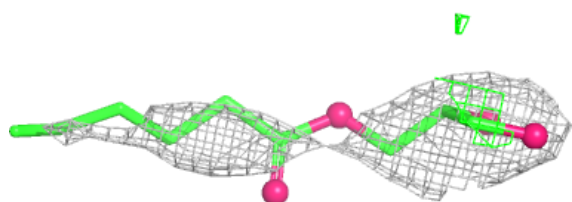
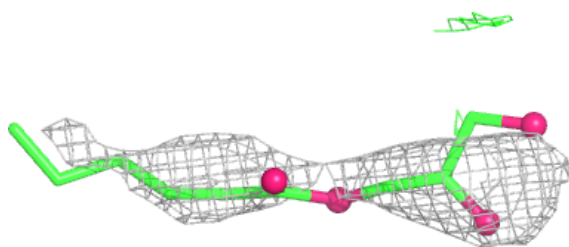
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



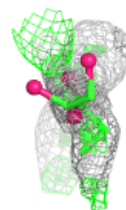
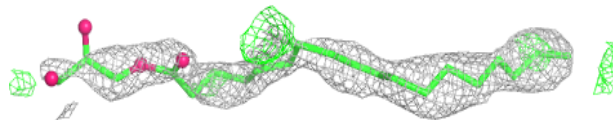
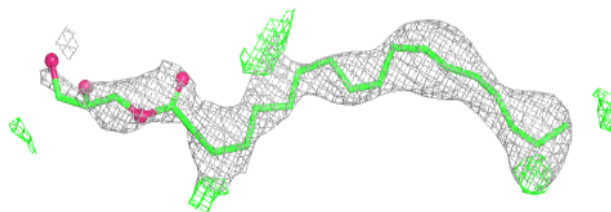


**Electron density around OLC D 302:**

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

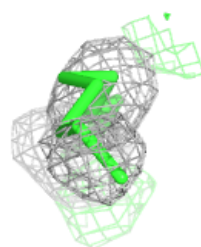
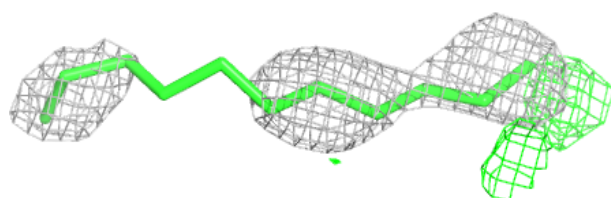
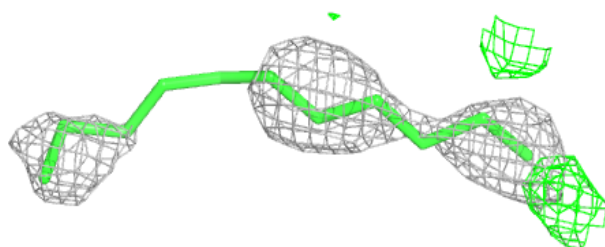
**Electron density around OLC A 304:**

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

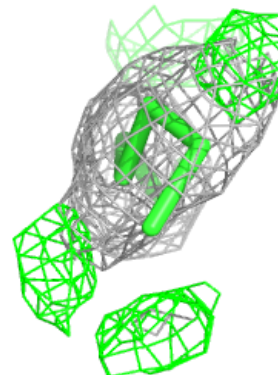
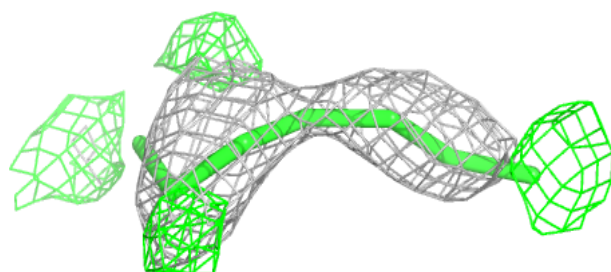
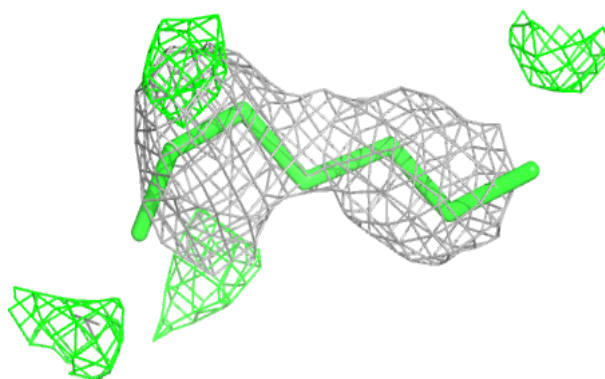


**Electron density around LFA C 317:**

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

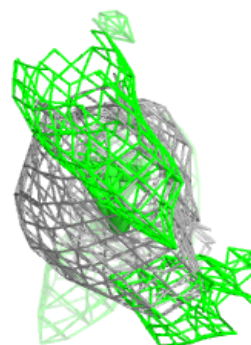
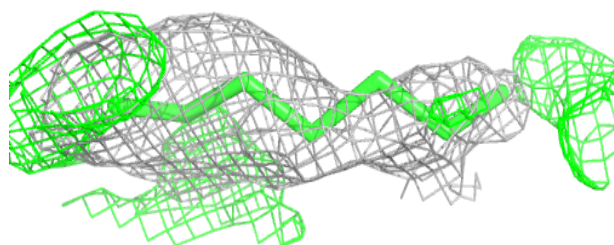
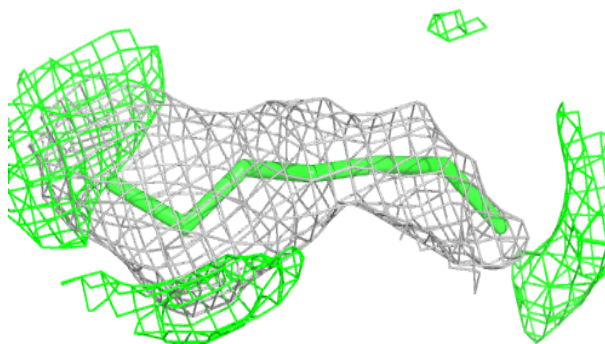
**Electron density around LFA A 312:**

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

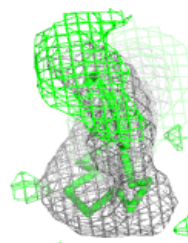
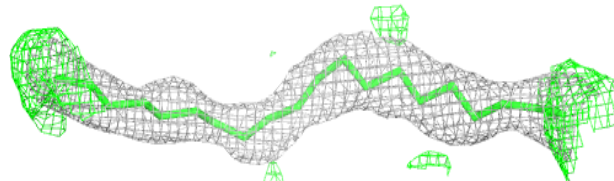
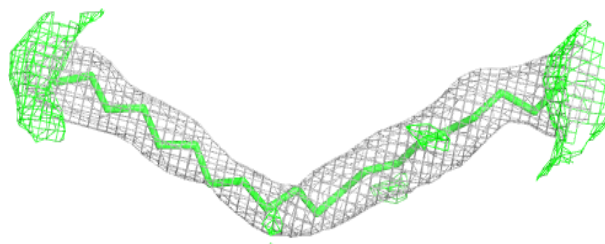


**Electron density around LFA C 314:**

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

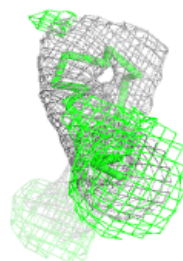
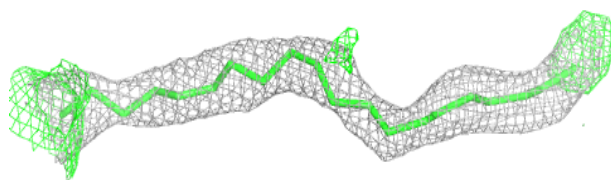
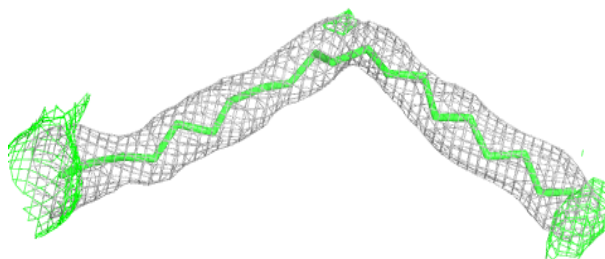
**Electron density around LFA B 302:**

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

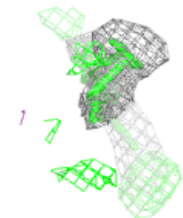
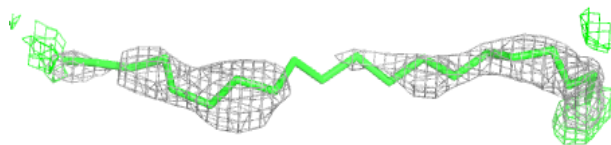
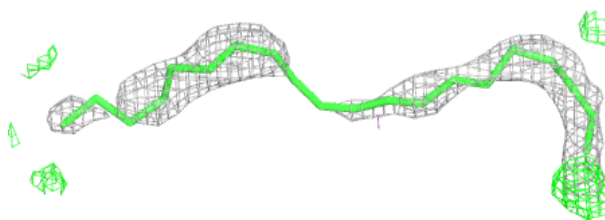


**Electron density around LFA E 319:**

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

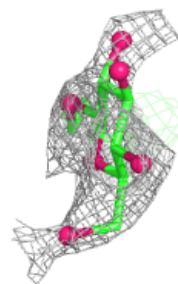
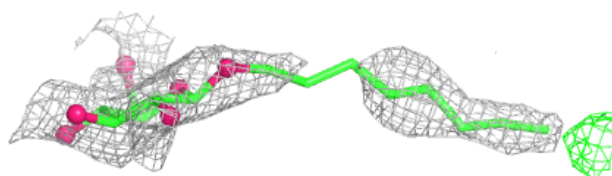
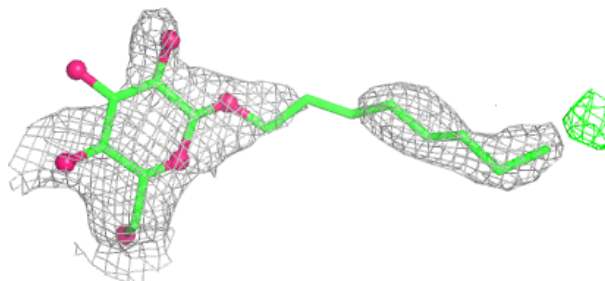
**Electron density around LFA D 310:**

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

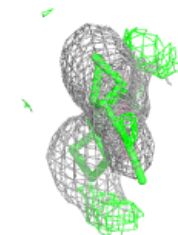
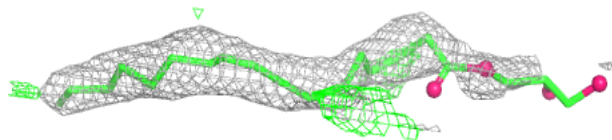
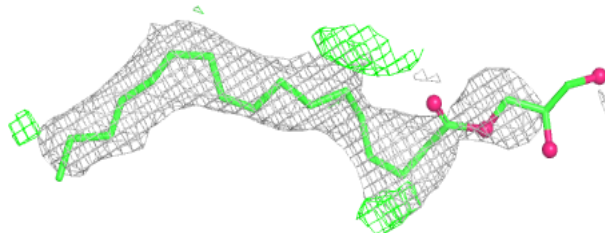


**Electron density around BOG A 320:**

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

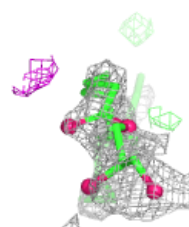
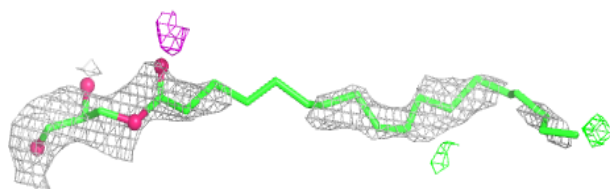
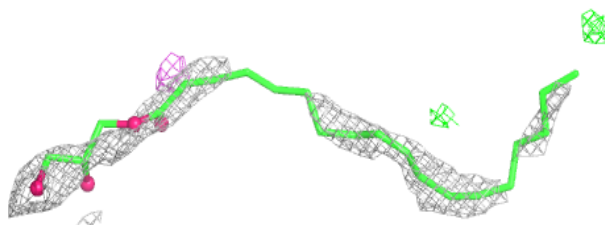
**Electron density around OLC E 306:**

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

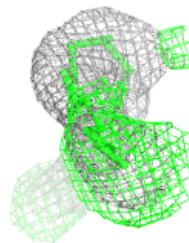
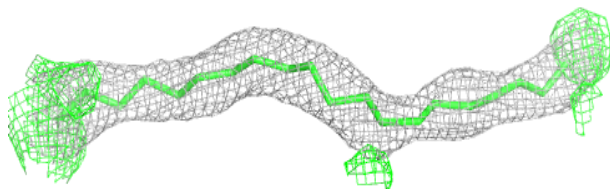
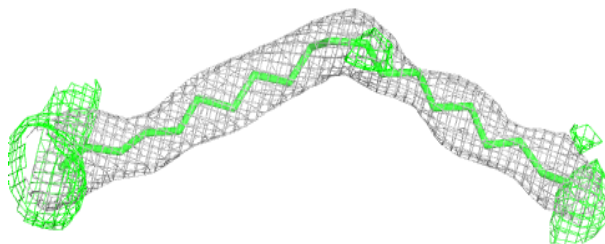


**Electron density around OLC B 311:**

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

**Electron density around LFA C 319:**

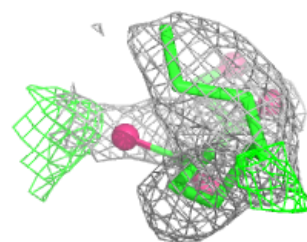
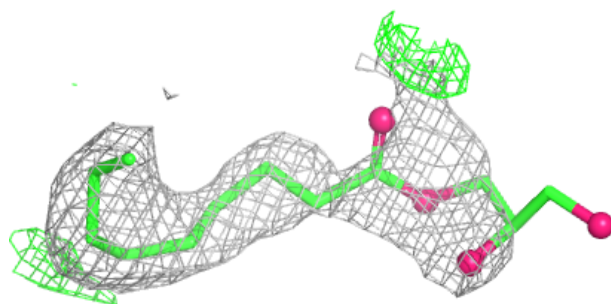
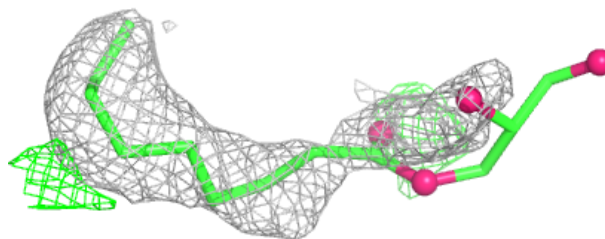
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



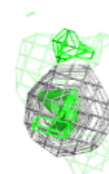
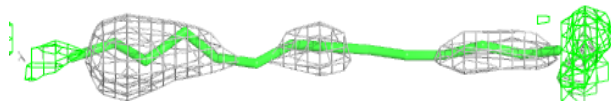
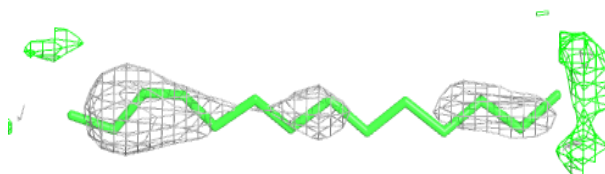


**Electron density around OLC A 310:**

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

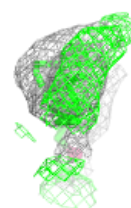
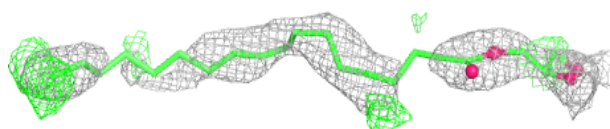
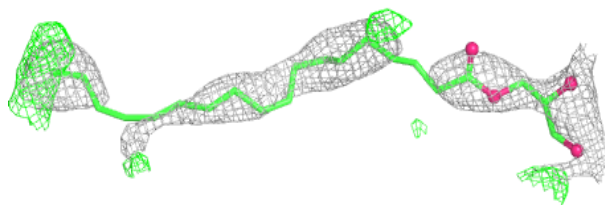
**Electron density around LFA E 323:**

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

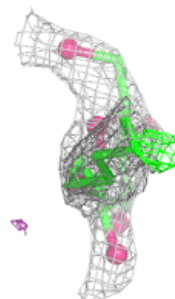
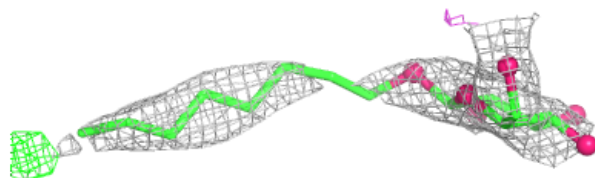
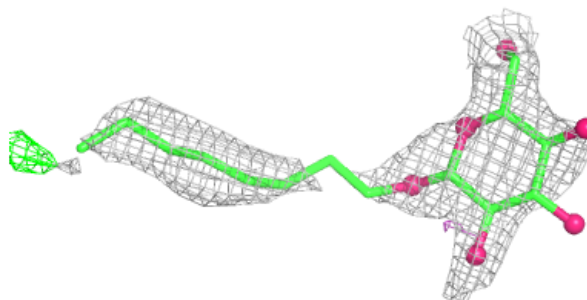


**Electron density around OLC B 304:**

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

**Electron density around BOG E 321:**

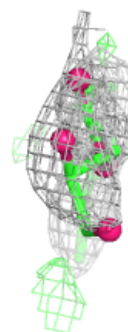
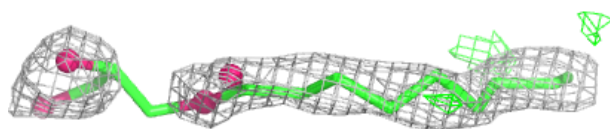
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



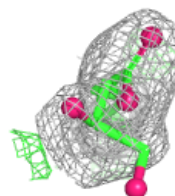
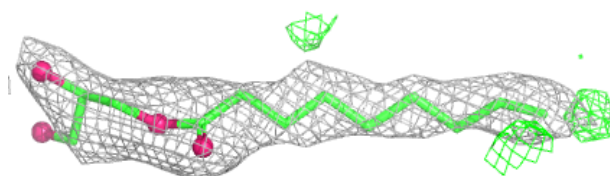
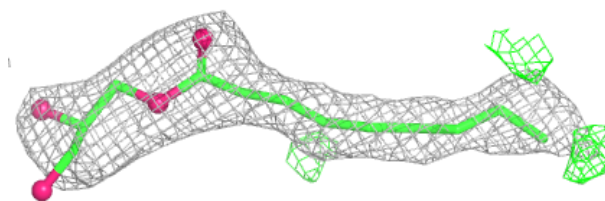


**Electron density around OLC B 310:**

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

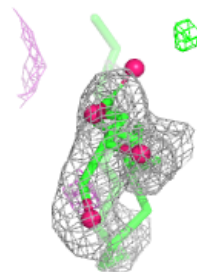
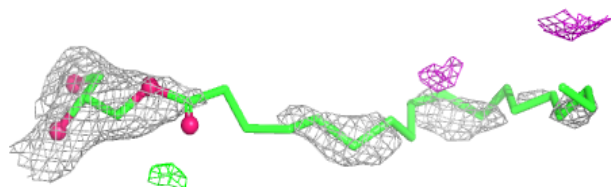
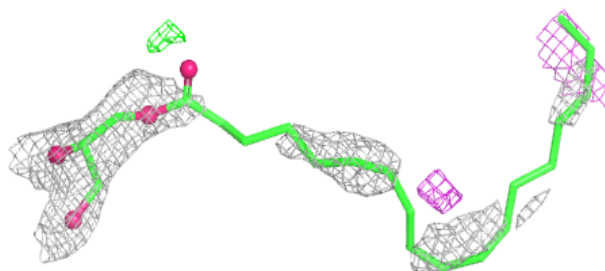
**Electron density around OLC B 312:**

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

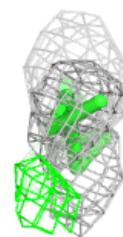
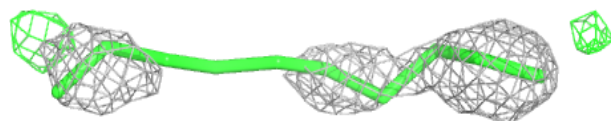
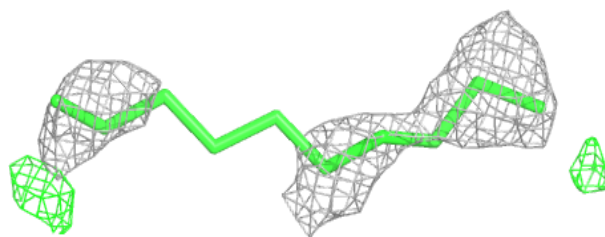


**Electron density around OLC C 310:**

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

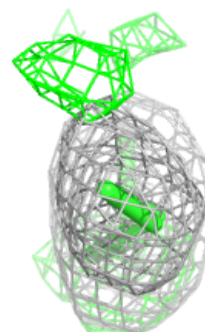
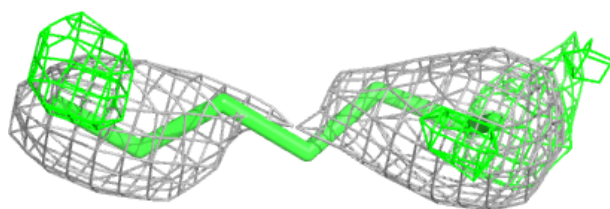
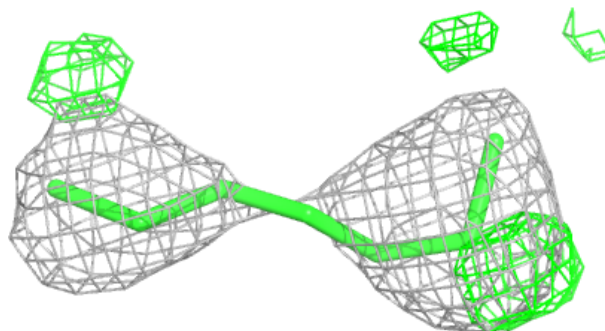
**Electron density around LFA B 318:**

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

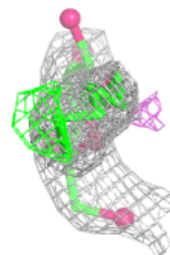
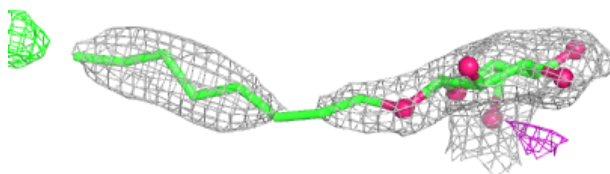
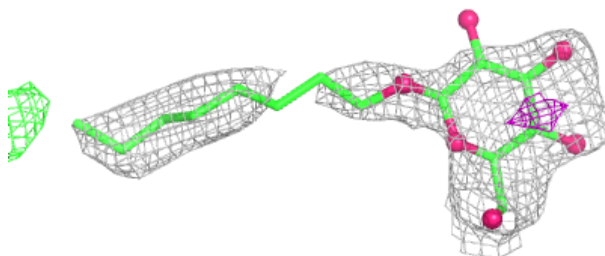


**Electron density around LFA B 319:**

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

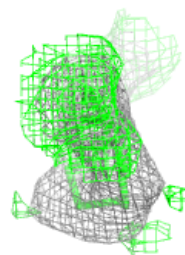
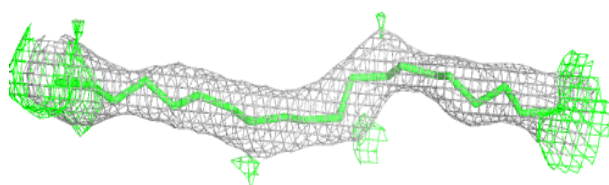
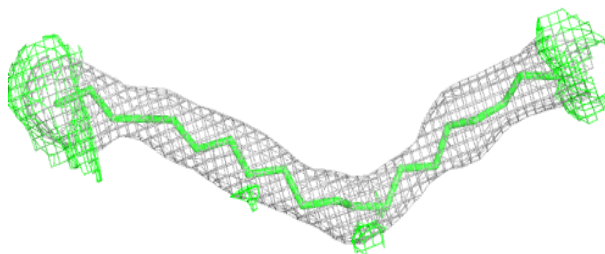
**Electron density around BOG B 321:**

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

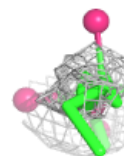
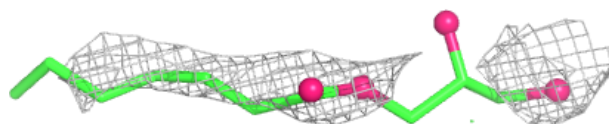
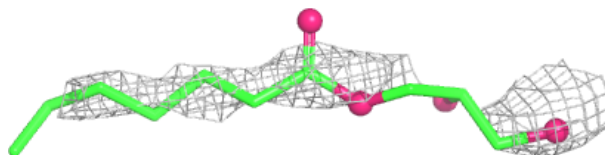


**Electron density around LFA C 302:**

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

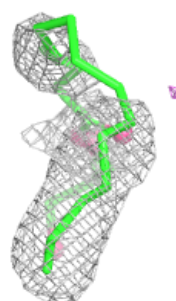
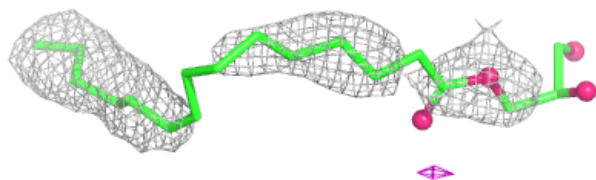
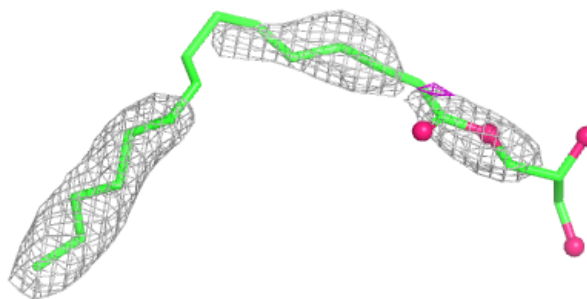
**Electron density around OLC C 303:**

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

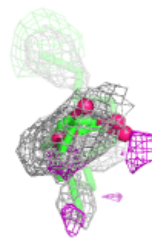
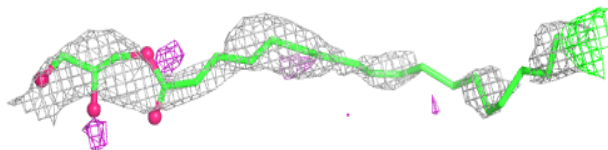
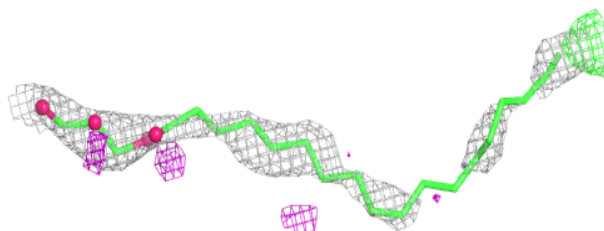


**Electron density around OLC C 308:**

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

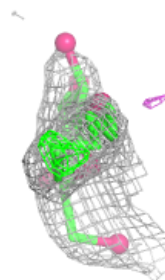
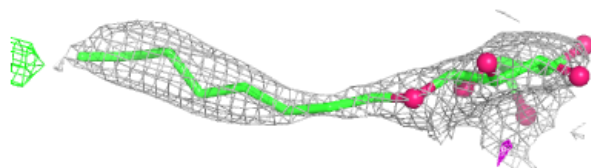
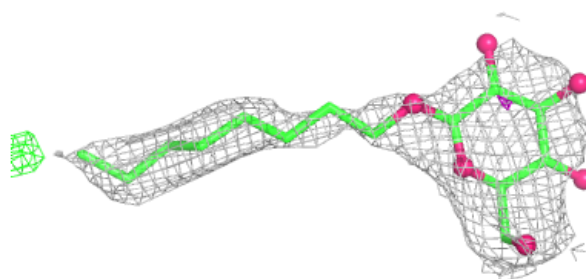
**Electron density around OLC E 312:**

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

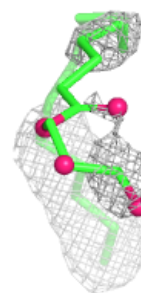
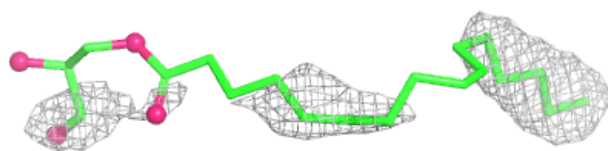
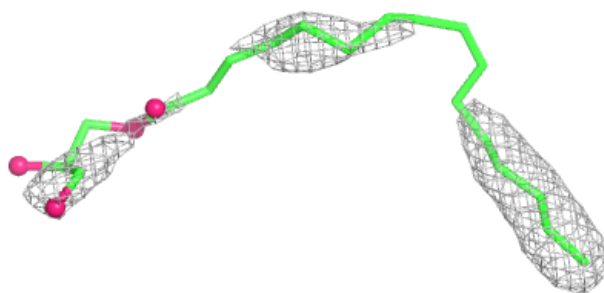


**Electron density around BOG C 321:**

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

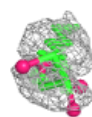
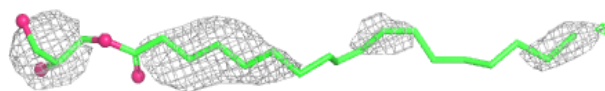
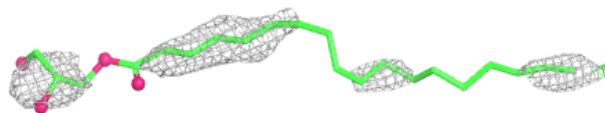
**Electron density around OLC D 305:**

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

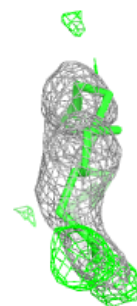
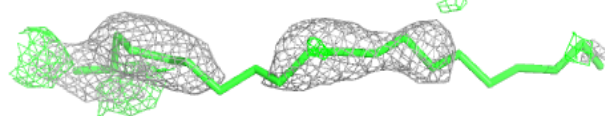
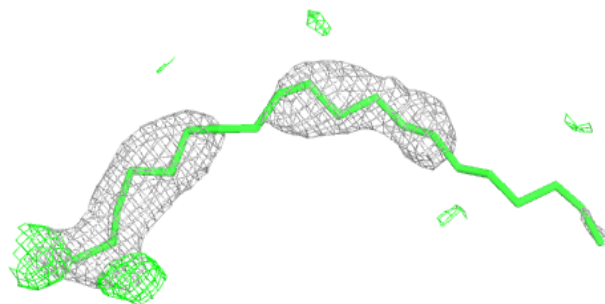


**Electron density around OLC E 314:**

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

**Electron density around LFA A 318:**

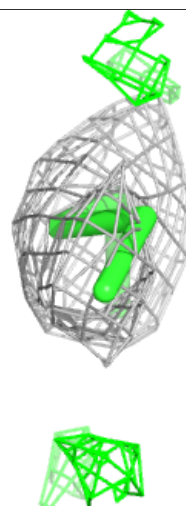
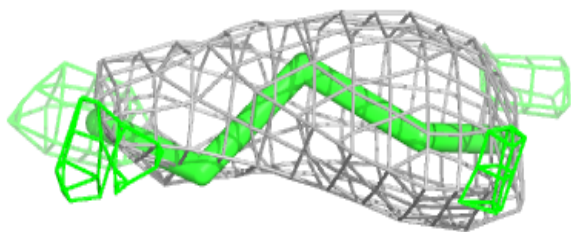
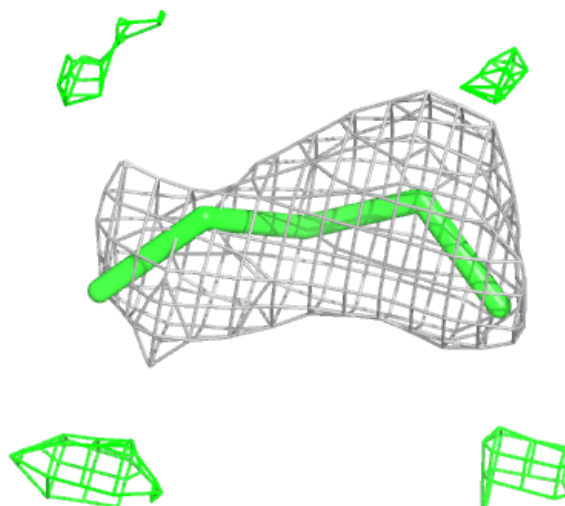
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around LFA E 318:**

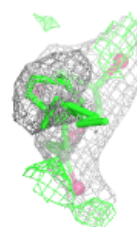
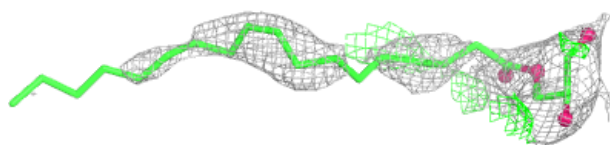
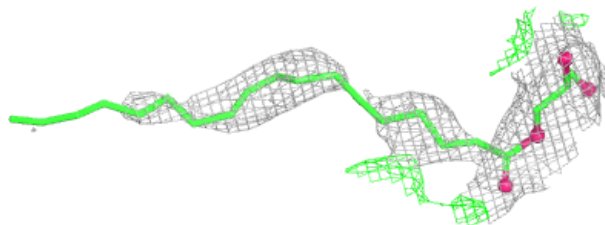
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



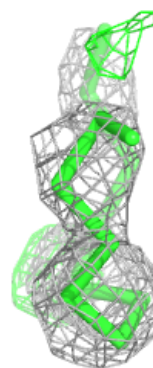
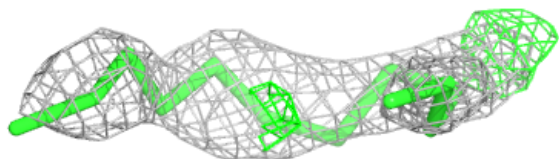
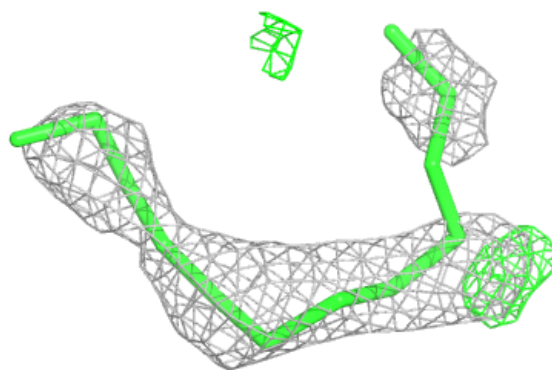


**Electron density around OLC A 302:**

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

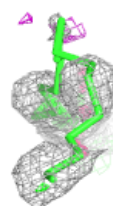
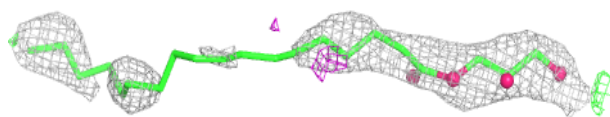
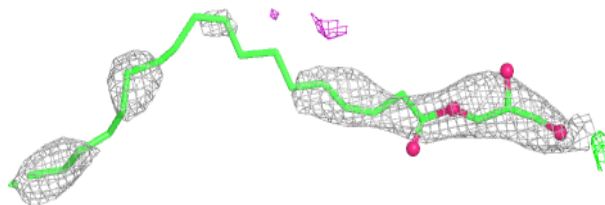
**Electron density around LFA A 315:**

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

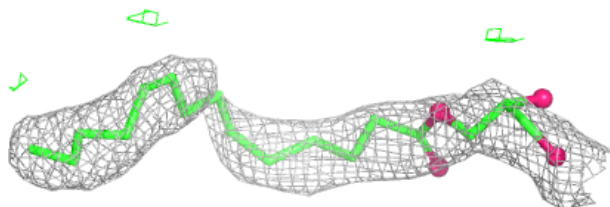
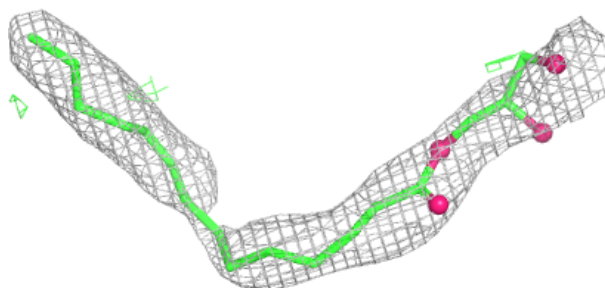


**Electron density around OLC D 309:**

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

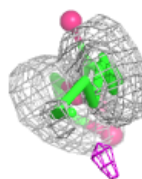
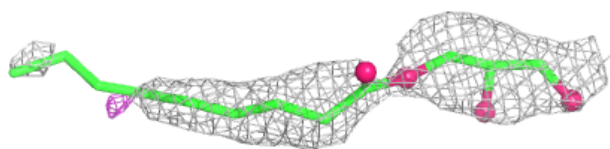
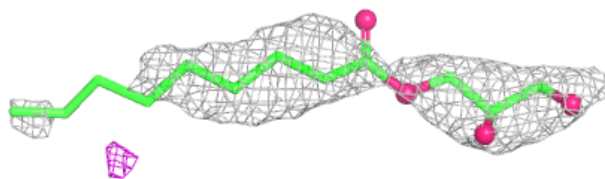
**Electron density around OLC B 309:**

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

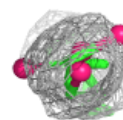
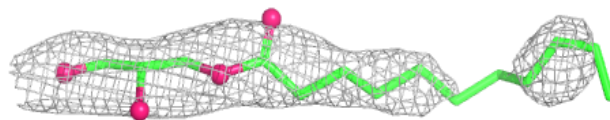
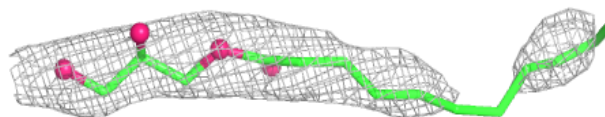


**Electron density around OLC B 315:**

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

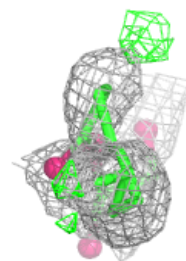
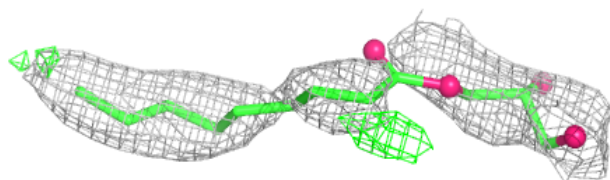
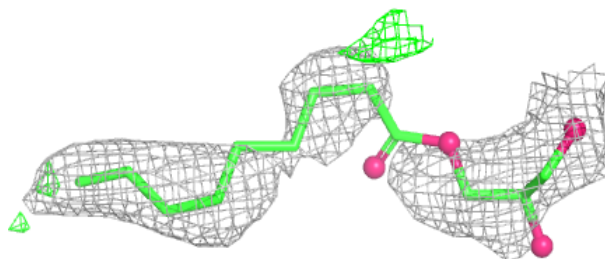
**Electron density around OLC D 304:**

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

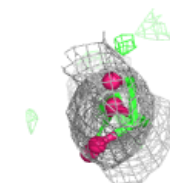
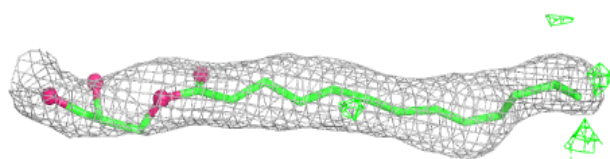
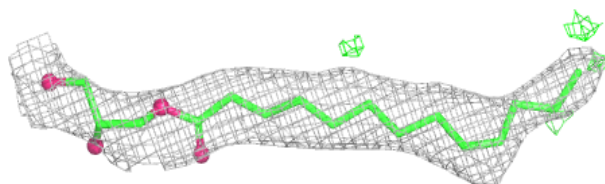


**Electron density around OLC E 304:**

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

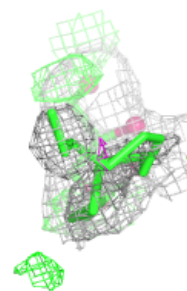
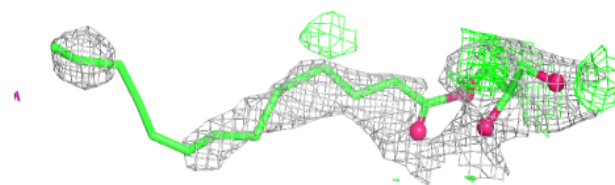
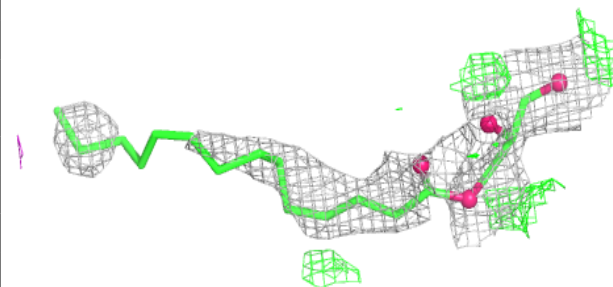
**Electron density around OLC B 308:**

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

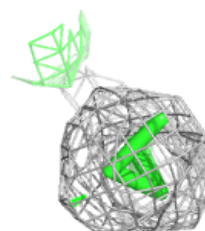
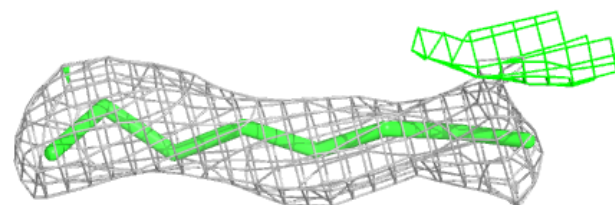
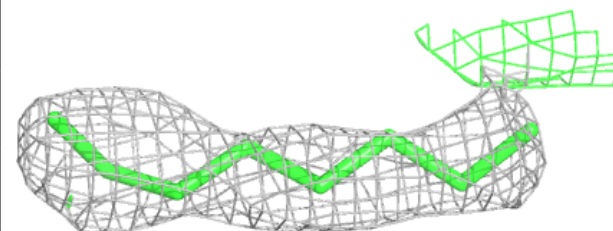


**Electron density around OLC C 304:**

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

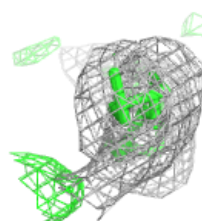
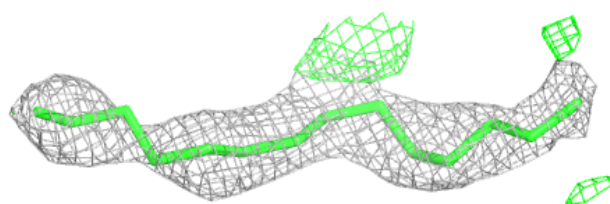
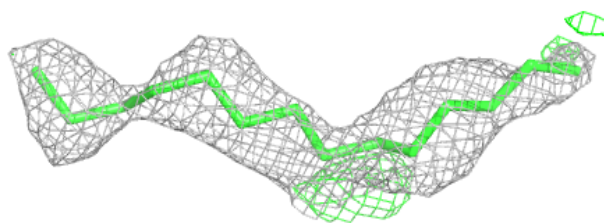
**Electron density around LFA A 313:**

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

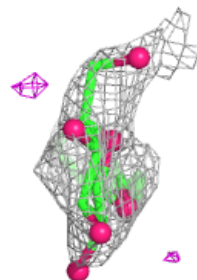
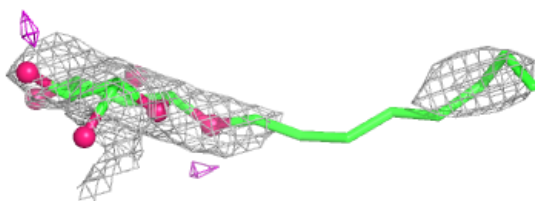
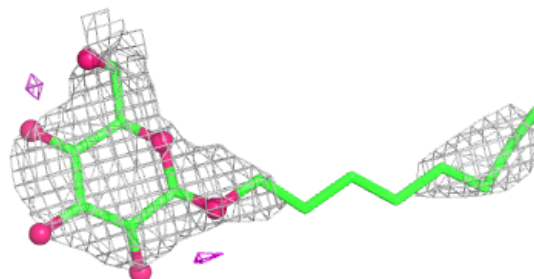


**Electron density around LFA E 316:**

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

**Electron density around BOG D 317:**

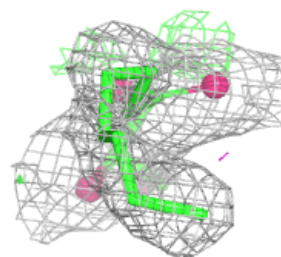
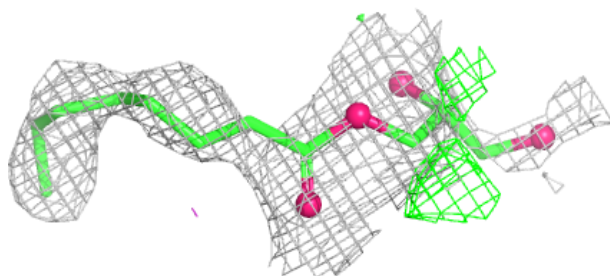
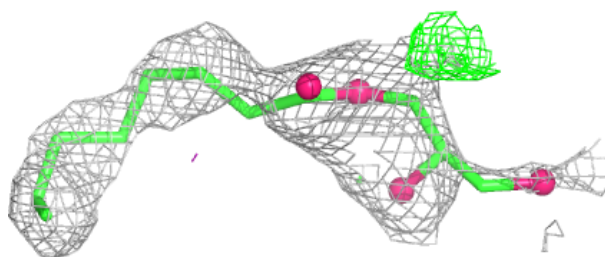
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



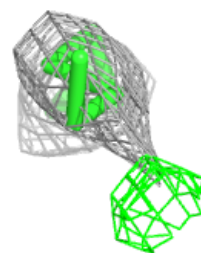
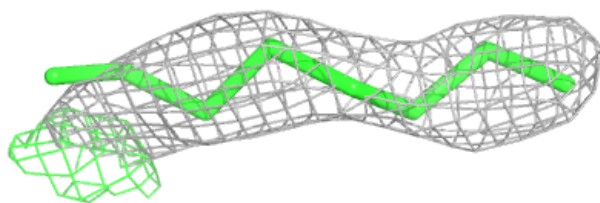
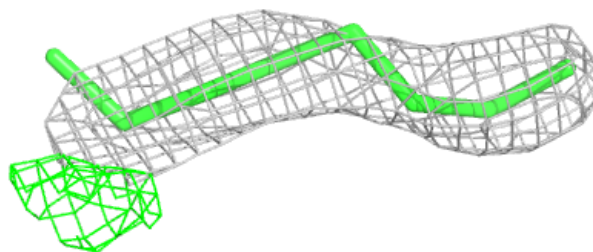


**Electron density around OLC E 310:**

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

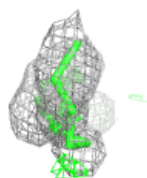
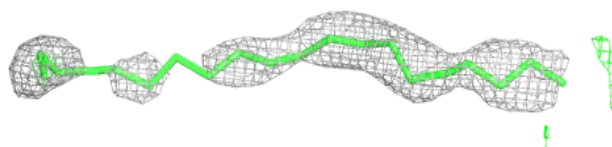
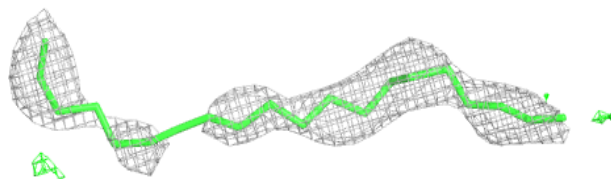
**Electron density around LFA C 315:**

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

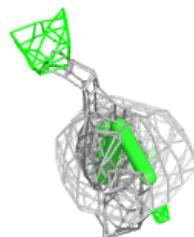
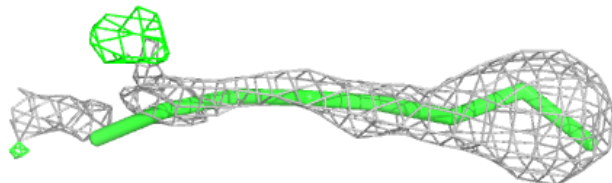
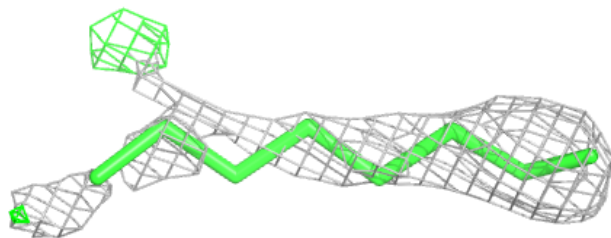


**Electron density around LFA C 316:**

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

**Electron density around LFA E 315:**

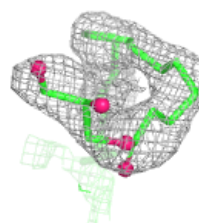
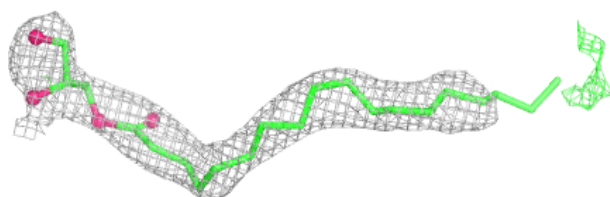
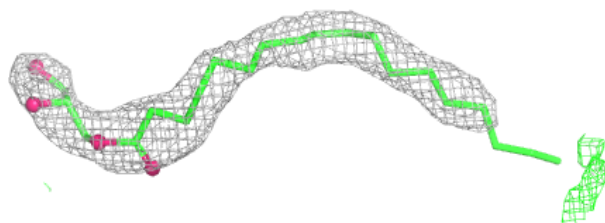
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



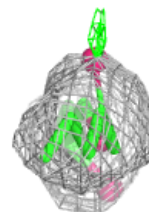
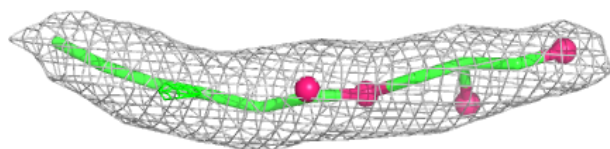
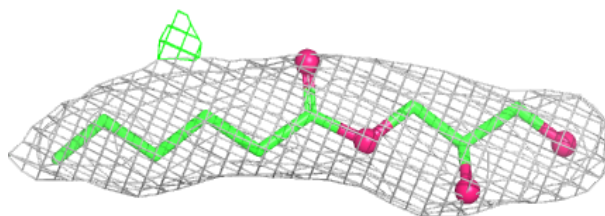


**Electron density around OLC B 301:**

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

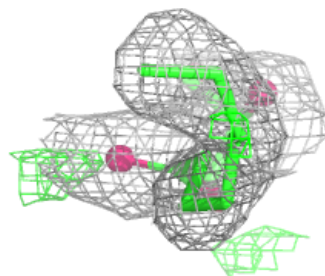
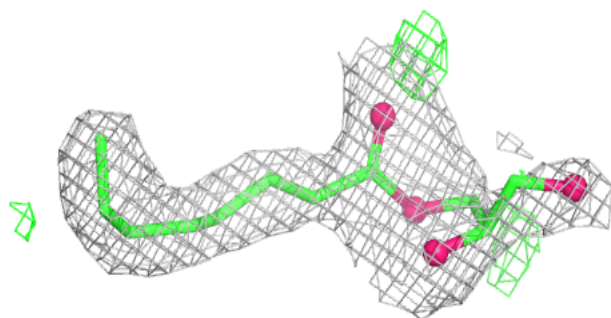
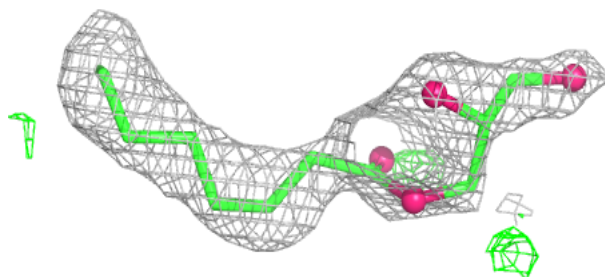
**Electron density around OLC A 305:**

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

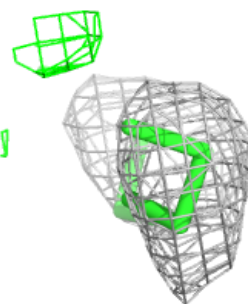
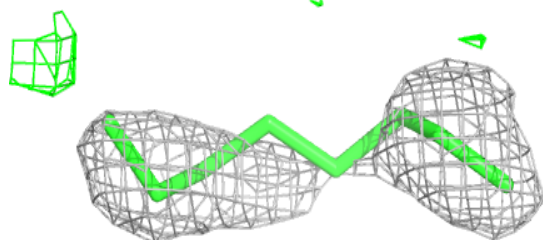
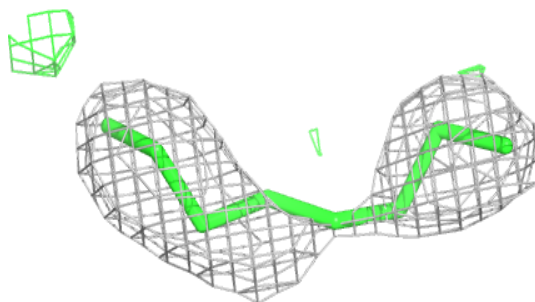


**Electron density around OLC D 308:**

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

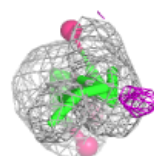
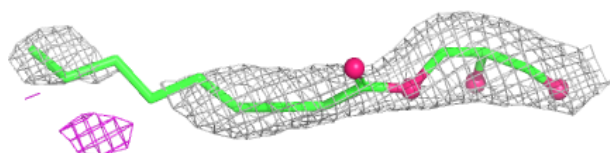
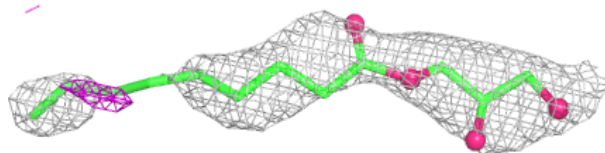
**Electron density around LFA D 312:**

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

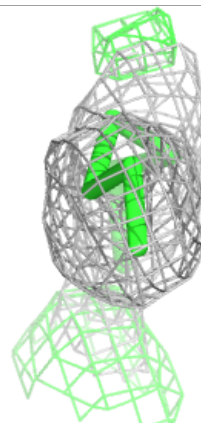
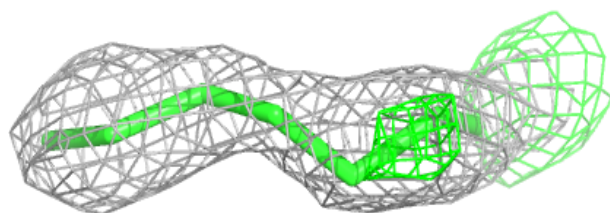
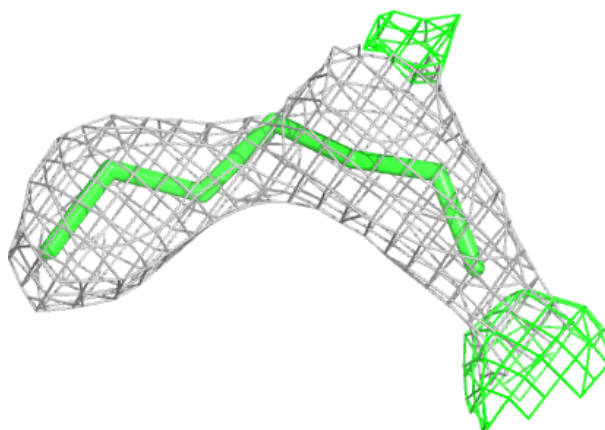


**Electron density around OLC C 313:**

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

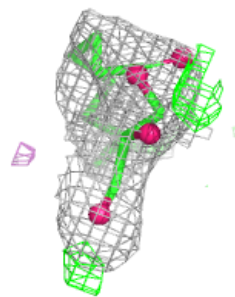
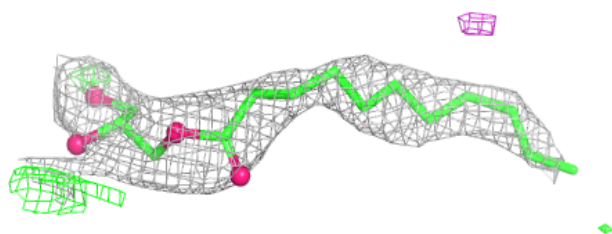
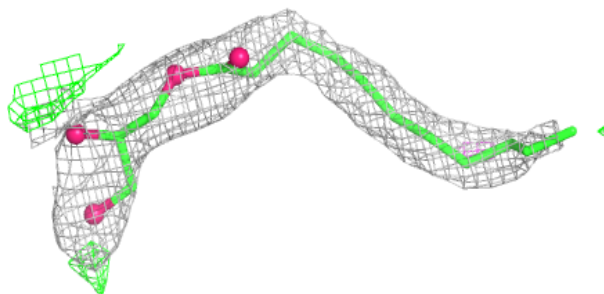
**Electron density around LFA D 314:**

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

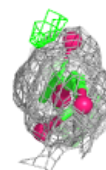
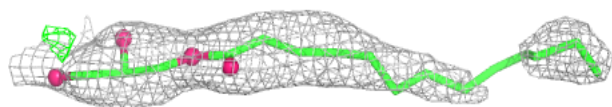
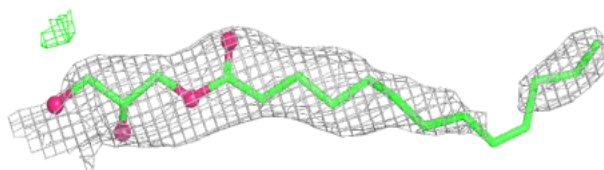


**Electron density around OLC D 301:**

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

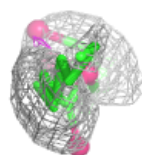
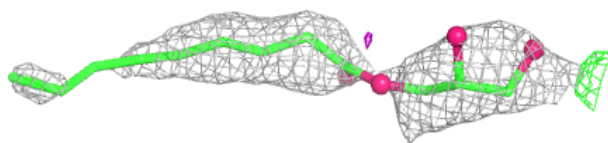
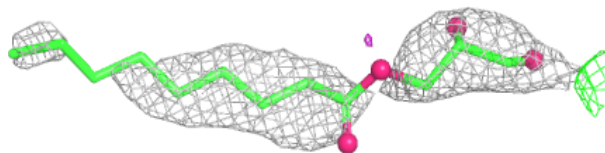
**Electron density around OLC E 307:**

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

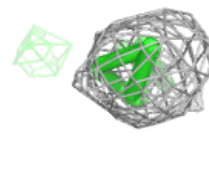
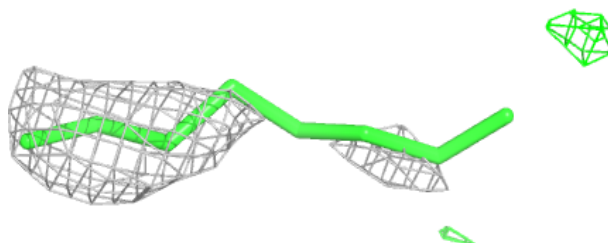
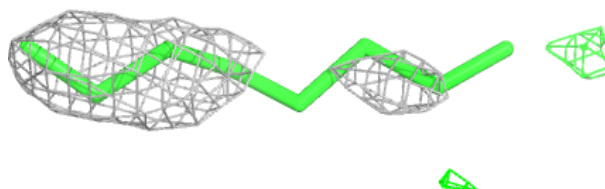


**Electron density around OLC A 311:**

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

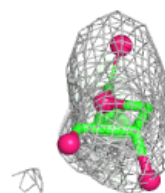
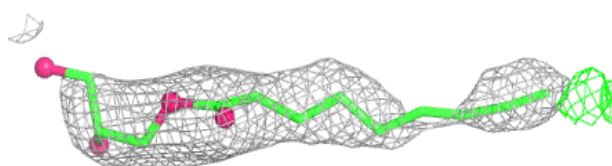
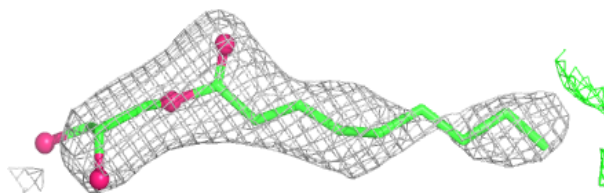
**Electron density around LFA B 317:**

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

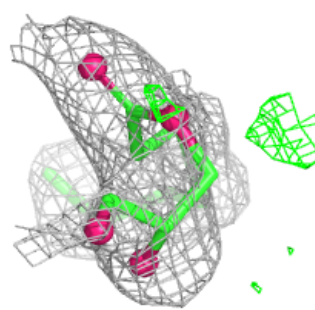
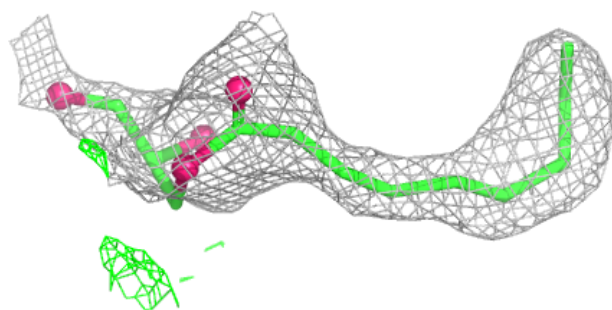
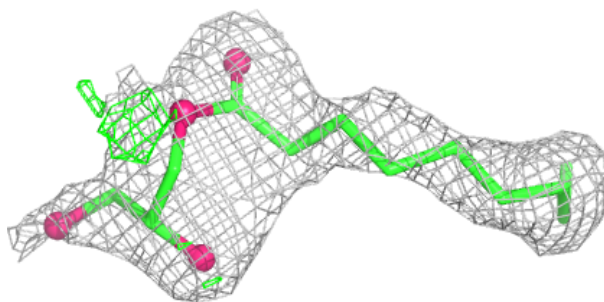


**Electron density around OLC C 311:**

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

**Electron density around OLC C 312:**

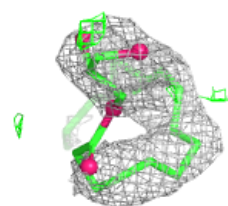
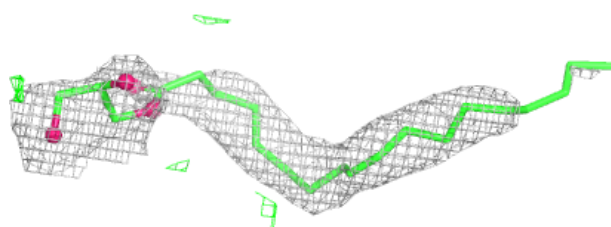
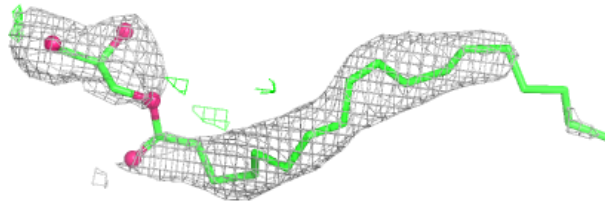
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



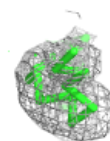
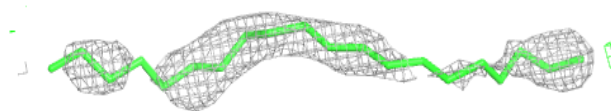
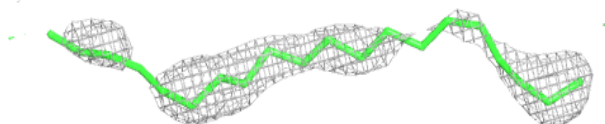


**Electron density around OLC E 301:**

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

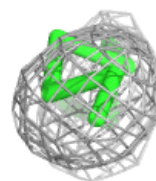
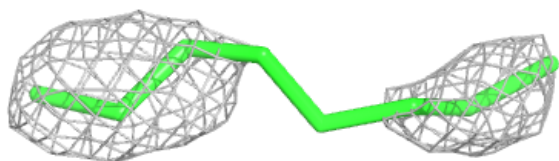
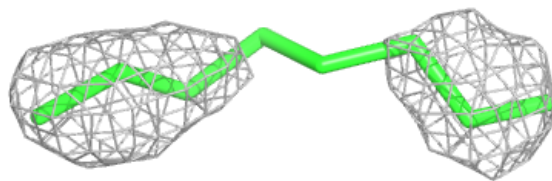
**Electron density around LFA D 311:**

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

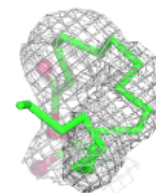
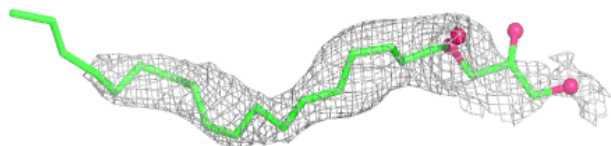
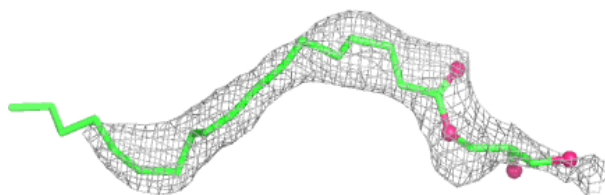


**Electron density around LFA A 314:**

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

**Electron density around OLC A 321:**

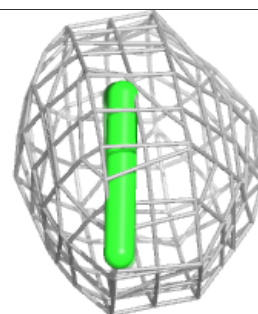
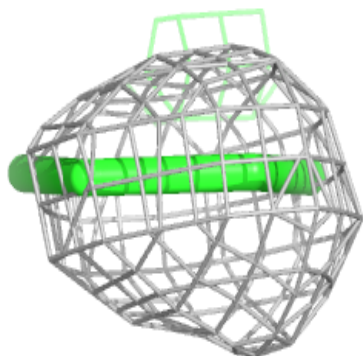
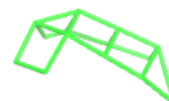
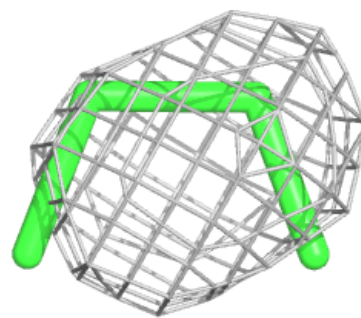
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





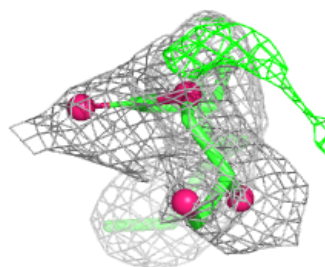
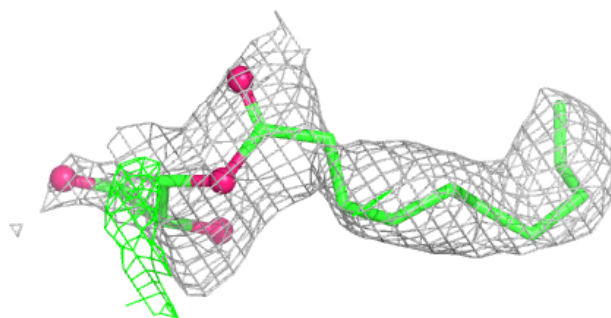
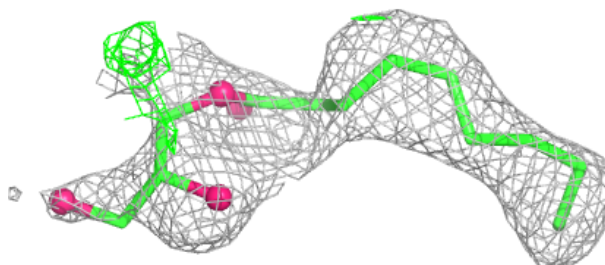
**Electron density around LFA C 318:**

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

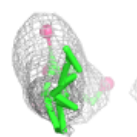
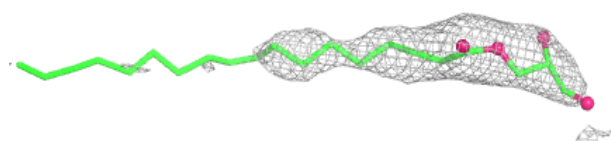
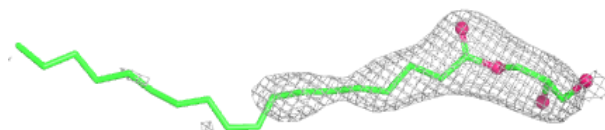


**Electron density around OLC B 313:**

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

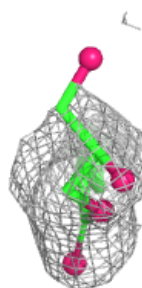
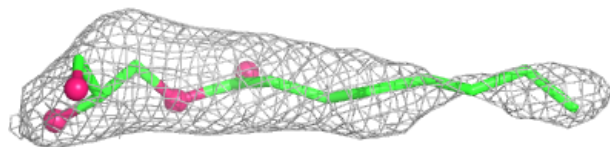
**Electron density around OLC E 309:**

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

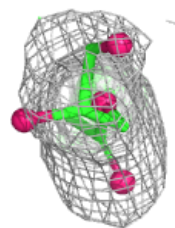
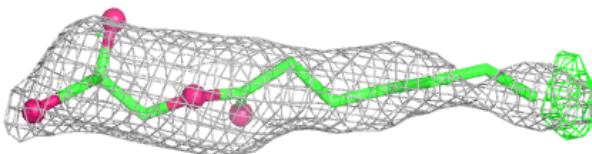
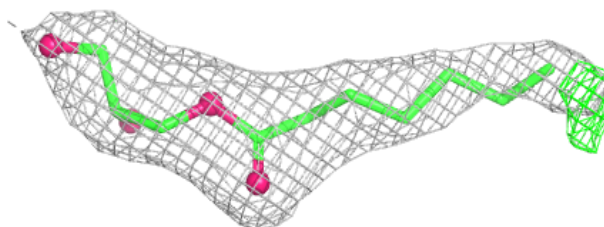


**Electron density around OLC A 309:**

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

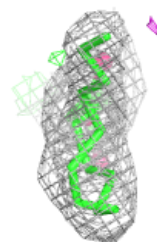
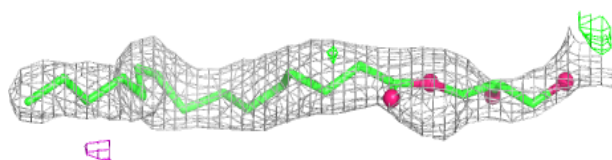
**Electron density around OLC D 307:**

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

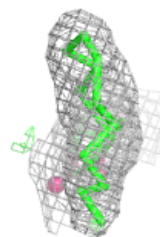
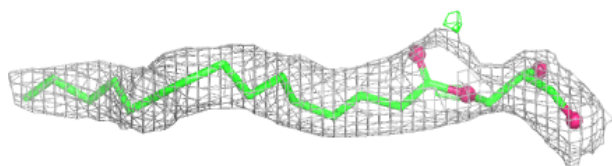
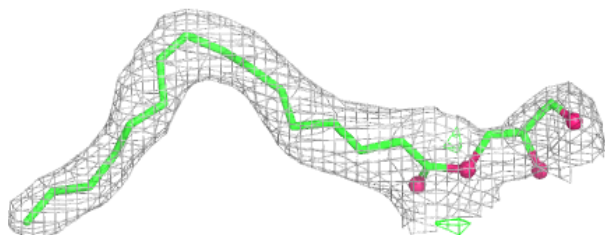


**Electron density around OLC A 303:**

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

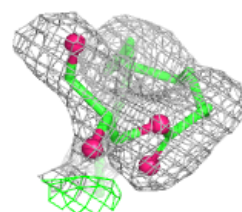
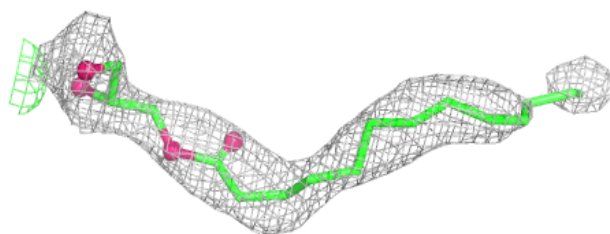
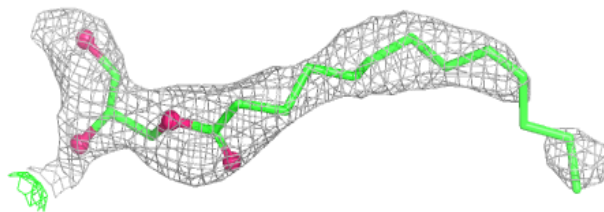
**Electron density around OLC C 305:**

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

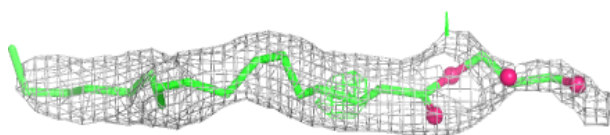
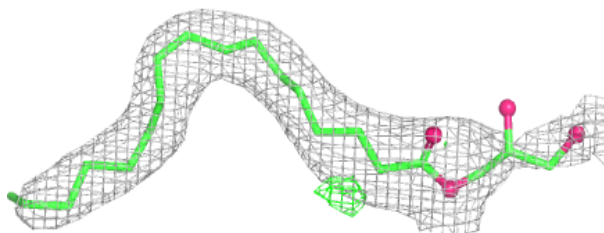


**Electron density around OLC B 306:**

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

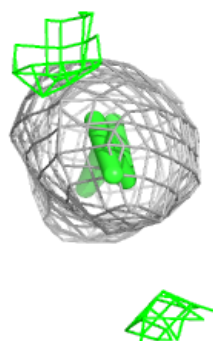
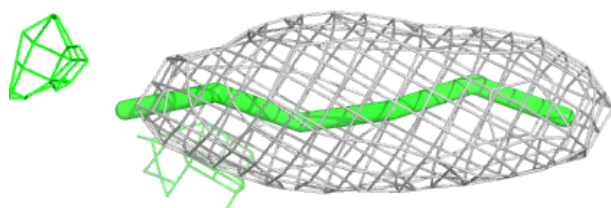
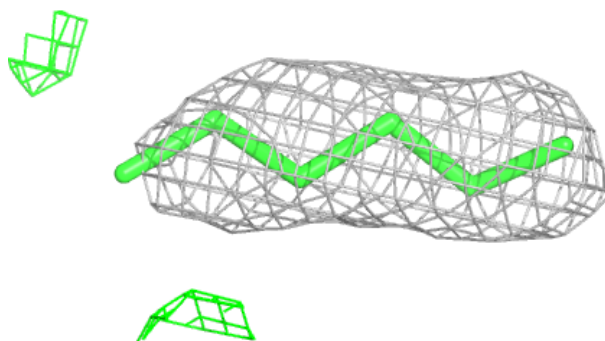
**Electron density around OLC E 305:**

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

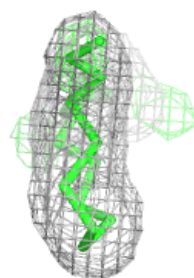
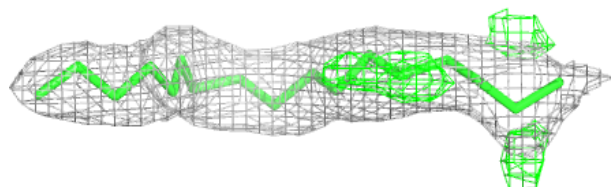
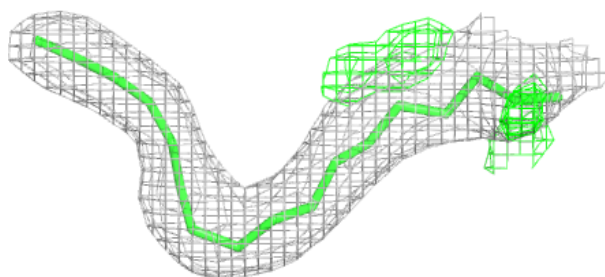


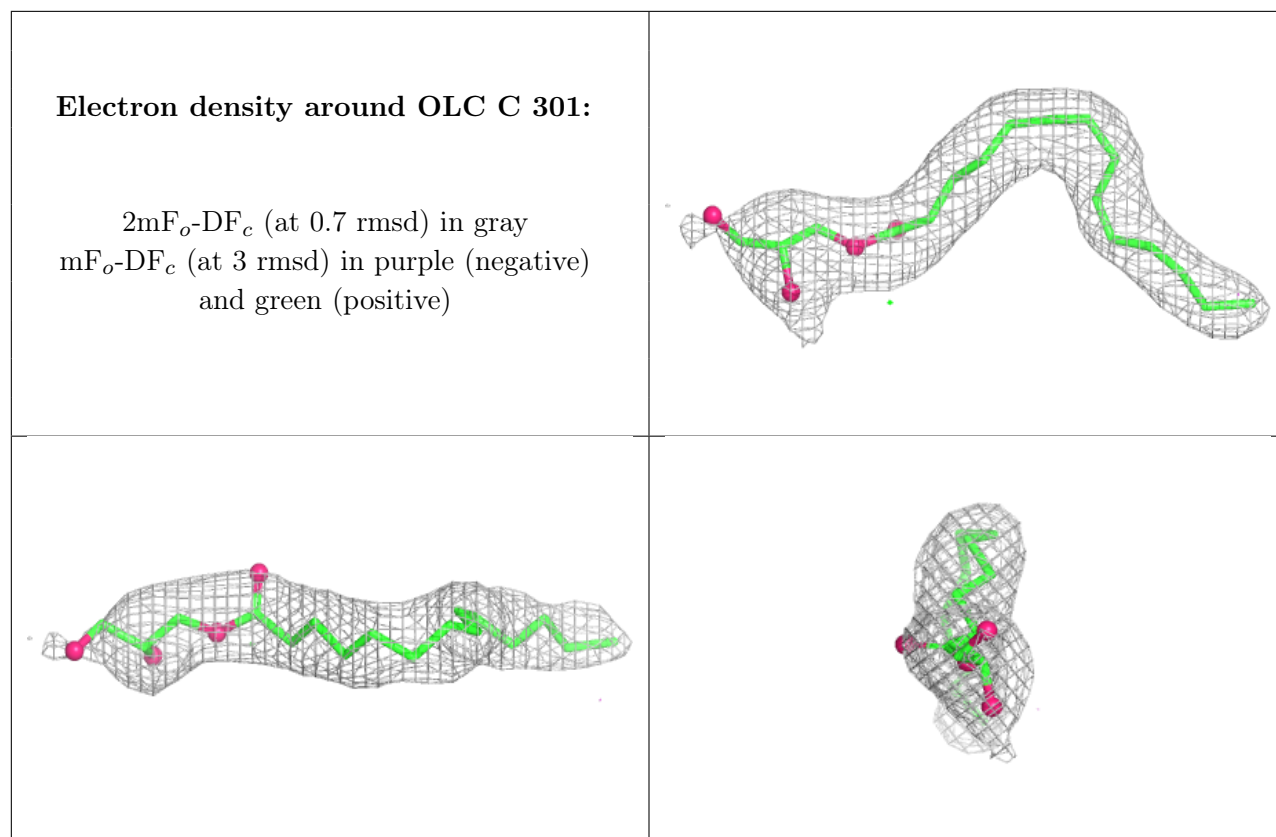
**Electron density around LFA A 317:**

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

**Electron density around LFA D 313:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.