



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:47 PM JST

PDB ID : 6JUW / pdb\_00006juw  
Title : BOVINE HEART CYTOCHROME C OXIDASE IN CATALYTIC INTER-MEDIATES AT 1.80 ANGSTROM RESOLUTION  
Authors : Shimada, A.; Muramoto, K.; Shinzawa-Itoh, K.; Yoshikawa, S.; Tsukihara, T.  
Deposited on : 2019-04-15  
Resolution : 1.80 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:

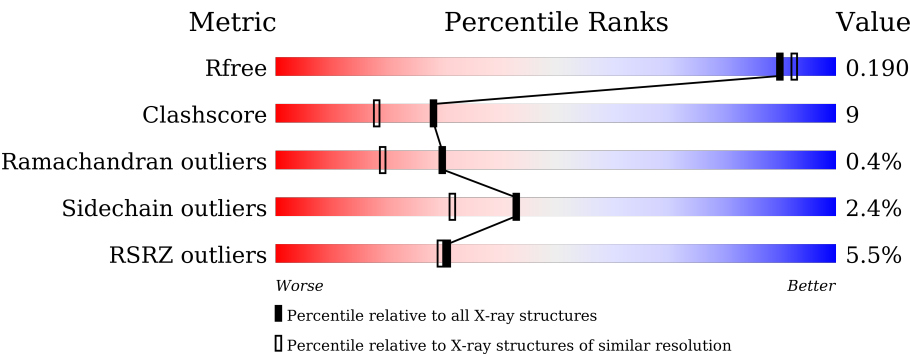
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 1.8.5 (274361), CSD as541be (2020)                               |
| 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                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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                      | 7662 (1.80-1.80)                                      |
| Clashscore            | 190562                      | 8479 (1.80-1.80)                                      |
| Ramachandran outliers | 187476                      | 8391 (1.80-1.80)                                      |
| Sidechain outliers    | 187428                      | 8390 (1.80-1.80)                                      |
| RSRZ outliers         | 180081                      | 7663 (1.80-1.80)                                      |

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     | 514    | <div><div></div><div>87%13%.</div></div>   |
| 1   | N     | 514    | <div><div>%</div><div>86%14%</div></div>   |
| 2   | B     | 227    | <div><div>5%</div><div>81%17%.</div></div> |
| 2   | O     | 227    | <div><div>5%</div><div>75%22%.</div></div> |
| 3   | C     | 259    | <div><div>%</div><div>89%11%</div></div>   |
| 3   | P     | 259    | <div><div>3%</div><div>88%12%</div></div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | D     | 144    |                  |
| 4   | Q     | 144    |                  |
| 5   | E     | 105    |                  |
| 5   | R     | 105    |                  |
| 6   | F     | 98     |                  |
| 6   | S     | 98     |                  |
| 7   | G     | 84     |                  |
| 7   | T     | 84     |                  |
| 8   | H     | 79     |                  |
| 8   | U     | 79     |                  |
| 9   | I     | 73     |                  |
| 9   | V     | 73     |                  |
| 10  | J     | 58     |                  |
| 10  | W     | 58     |                  |
| 11  | K     | 49     |                  |
| 11  | X     | 49     |                  |
| 12  | L     | 46     |                  |
| 12  | Y     | 46     |                  |
| 13  | M     | 43     |                  |
| 13  | Z     | 43     |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | EDO  | N     | 612 | -         | -        | X       | -                |
| 22  | EDO  | N     | 617 | -         | -        | X       | -                |
| 22  | EDO  | U     | 102 | -         | -        | X       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CDL  | G     | 102 | -         | -        | X       | -                |
| 25  | CDL  | T     | 102 | -         | -        | X       | -                |

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 34360 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 Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 514      | Total | C    | N   | O   | S  | 0       | 37      | 0     |
|     |       |          | 4192  | 2794 | 643 | 710 | 45 |         |         |       |
| 1   | N     | 514      | Total | C    | N   | O   | S  | 0       | 21      | 0     |
|     |       |          | 4152  | 2770 | 639 | 703 | 40 |         |         |       |

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 227      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 1839  | 1196 | 281 | 343 | 19 |         |         |       |
| 2   | O     | 227      | Total | C    | N   | O   | S  | 0       | 7       | 0     |
|     |       |          | 1857  | 1208 | 287 | 343 | 19 |         |         |       |

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 259      | Total | C    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 2122  | 1417 | 336 | 355 | 14 |         |         |       |
| 3   | P     | 259      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 2114  | 1413 | 336 | 353 | 12 |         |         |       |

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 144      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1198  | 780 | 196 | 218 | 4 |         |         |       |
| 4   | Q     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1195  | 777 | 196 | 218 | 4 |         |         |       |

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 544 | 144 | 162 | 2 |         |         |       |
| 5   | R     | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 544 | 144 | 162 | 2 |         |         |       |

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 98       | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 751   | 465 | 135 | 146 | 5 |         |         |       |
| 6   | S     | 98       | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 751   | 465 | 134 | 147 | 5 |         |         |       |

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |   |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|---|
| 7   | G     | 84       | Total<br>676 | C<br>431 | N<br>129 | O<br>114 | P<br>1 | S<br>1  | 0       | 0     | 0 |
| 7   | T     | 84       | Total<br>685 | C<br>439 | N<br>130 | O<br>114 | P<br>1 | S<br>1  | 0       | 1     | 0 |

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 417 | 121 | 119 | 5 |         |         |       |
| 8   | U     | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 417 | 121 | 119 | 5 |         |         |       |

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | I     | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 601   | 390 | 107 | 100 | 4 |         |         |       |
| 9   | V     | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 601   | 390 | 107 | 100 | 4 |         |         |       |

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | J     | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 460   | 297 | 78 | 82 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | W     | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 460   | 297 | 78 | 82 | 3 |         |         |       |

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11  | K     | 49       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 384   | 250 | 65 | 67 | 2 |         |         |       |
| 11  | X     | 49       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 385   | 250 | 65 | 68 | 2 |         |         |       |

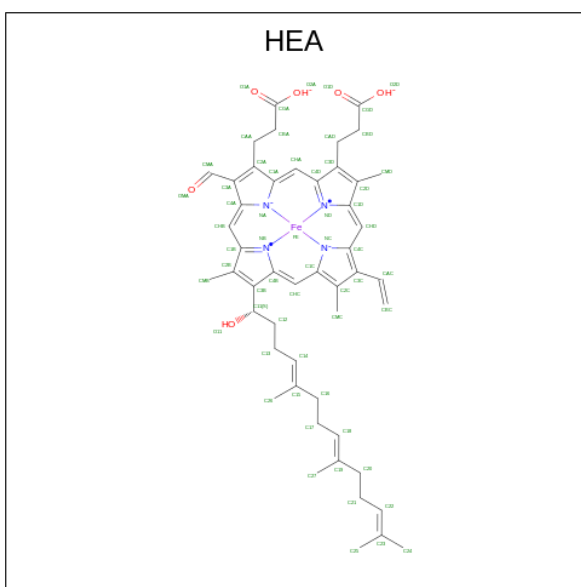
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | L     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 380   | 254 | 64 | 60 | 2 |         |         |       |
| 12  | Y     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 380   | 254 | 64 | 60 | 2 |         |         |       |

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 13  | M     | 43       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 336   | 223 | 53 | 60 |         |         |       |
| 13  | Z     | 43       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 336   | 223 | 53 | 60 |         |         |       |

- Molecule 14 is HEME-A (CCD ID: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 14  | A     | 1        | Total<br>72 | C<br>60 | Fe<br>1 | N<br>4 | O<br>7 | 0       | 1       |
| 14  | A     | 1        | Total<br>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 14  | N     | 1        | Total<br>72 | C<br>60 | Fe<br>1 | N<br>4 | O<br>7 | 0       | 1       |
| 14  | N     | 1        | Total<br>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6 | 0       | 0       |

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15  | A     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | N     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

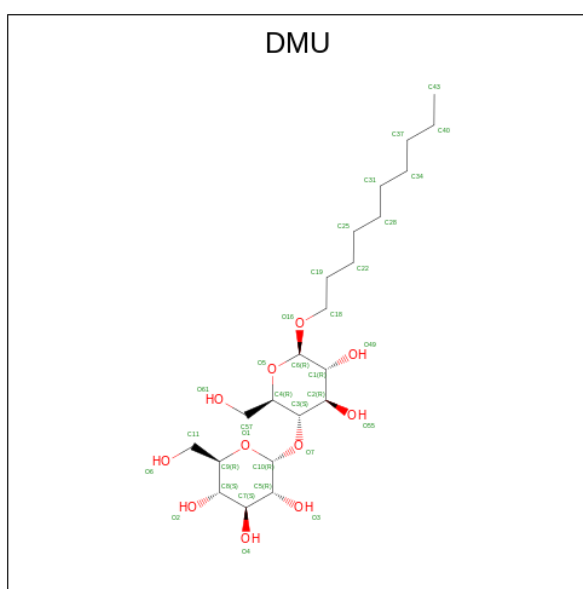
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16  | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | N     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 17  | A     | 1        | Total Na<br>1 1 | 0       | 0       |
| 17  | C     | 1        | Total Na<br>1 1 | 0       | 0       |
| 17  | N     | 1        | Total Na<br>1 1 | 0       | 0       |
| 17  | P     | 1        | Total Na<br>1 1 | 0       | 0       |

- Molecule 18 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



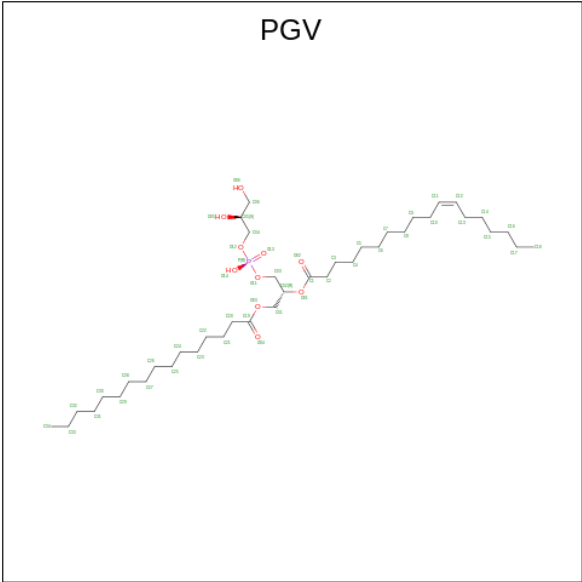
| Mol | Chain | Residues | Atoms                 | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 18  | A     | 1        | Total C O<br>13 11 2  | 0       | 0       |
| 18  | B     | 1        | Total C O<br>11 10 1  | 0       | 0       |
| 18  | C     | 1        | Total C O<br>33 22 11 | 0       | 0       |
| 18  | C     | 1        | Total C O<br>22 16 6  | 0       | 0       |
| 18  | C     | 1        | Total C O<br>11 10 1  | 0       | 0       |
| 18  | D     | 1        | Total C O<br>21 16 5  | 0       | 0       |
| 18  | J     | 1        | Total C O<br>21 16 5  | 0       | 0       |

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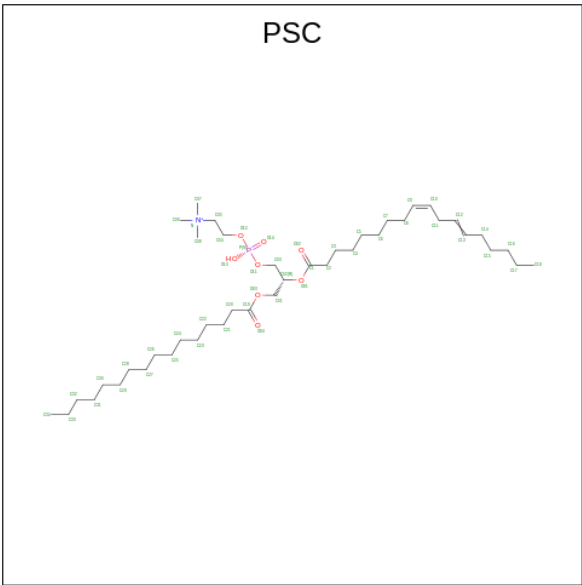
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 18  | K     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 11    | 10 | 1  |         |         |
| 18  | K     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 14    | 11 | 3  |         |         |
| 18  | K     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 22    | 16 | 6  |         |         |
| 18  | K     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 11    | 10 | 1  |         |         |
| 18  | L     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 18  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 18  | O     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 11    | 10 | 1  |         |         |
| 18  | P     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 11    | 10 | 1  |         |         |
| 18  | P     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 18  | Q     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 23    | 17 | 6  |         |         |
| 18  | W     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 21    | 16 | 5  |         |         |
| 18  | X     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 11    | 10 | 1  |         |         |
| 18  | X     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 21    | 16 | 5  |         |         |
| 18  | X     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 11    | 10 | 1  |         |         |
| 18  | X     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 11    | 10 | 1  |         |         |
| 18  | X     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 11    | 10 | 1  |         |         |
| 18  | Y     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 18  | Z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY]}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



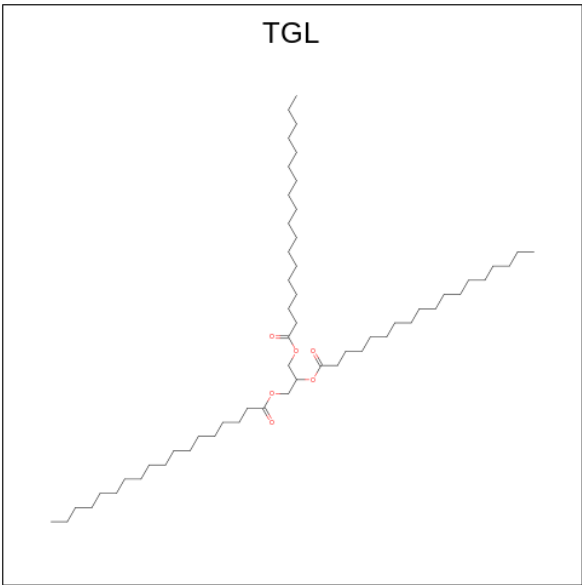
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | N     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | N     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | T     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |

- Molecule 20 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 20  | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |
| 20  | V     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |

- Molecule 21 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



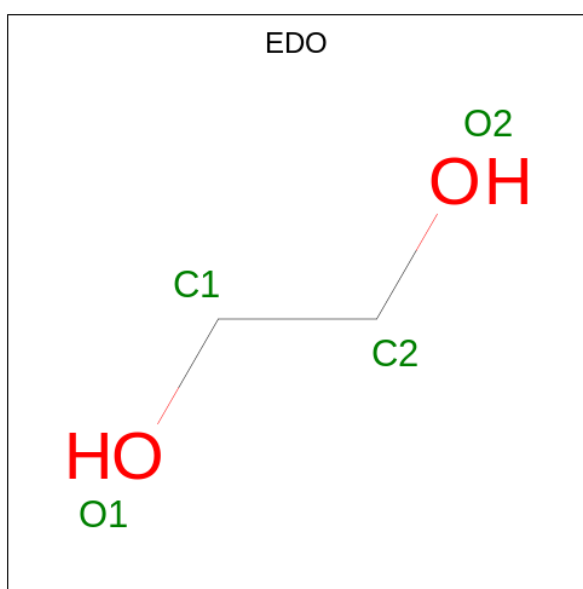
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 21  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |

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| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21  | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 21  | N     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 21  | Q     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 21  | Y     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |

- Molecule 22 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 22  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 22  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 22  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 22  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 22  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 22  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

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| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 22  | A     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | A     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | B     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | B     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | B     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | B     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | B     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | C     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | C     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | C     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | C     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | C     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | C     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | C     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | C     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | D     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | D     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | D     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | D     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | D     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | E     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | E     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 22  | E     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | F     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | F     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | F     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | F     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | F     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | F     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | F     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | F     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | G     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | H     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | J     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | L     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | L     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | M     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |

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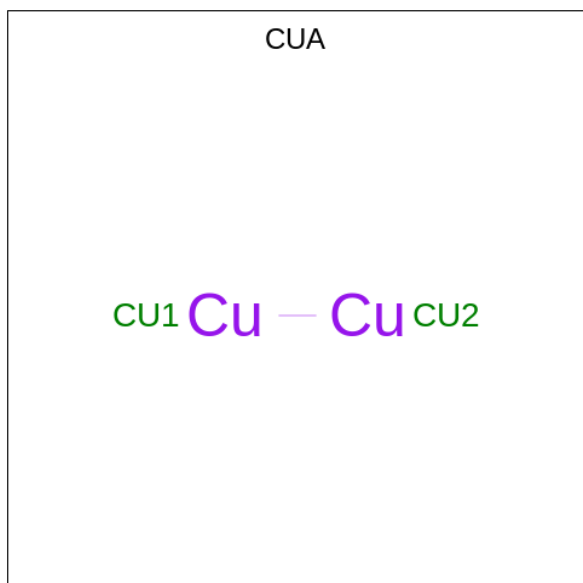
| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | N     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | O     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | O     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | P     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | P     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | P     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | P     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | P     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | P     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | P     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | Q     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | Q     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 22  | Q     | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 22  | S     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 22  | S     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 22  | S     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 22  | S     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 22  | S     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 22  | T     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 22  | T     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 22  | U     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 22  | W     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 22  | Y     | 1        | Total C O<br>4 2 2 | 0       | 0       |

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



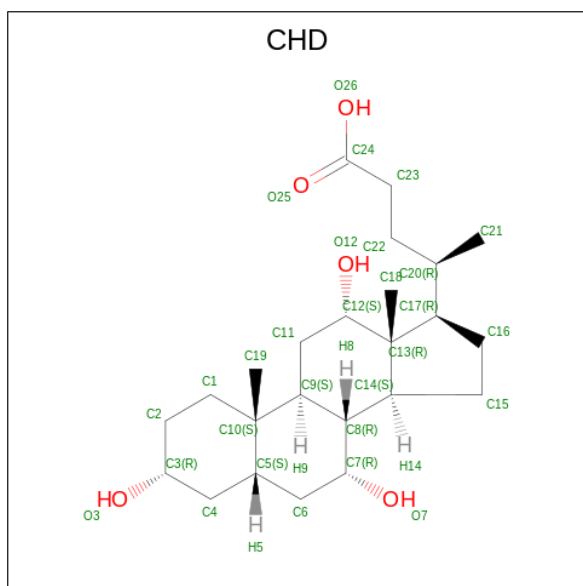
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 23  | B     | 1        | Total Cu<br>2 2 | 0       | 0       |

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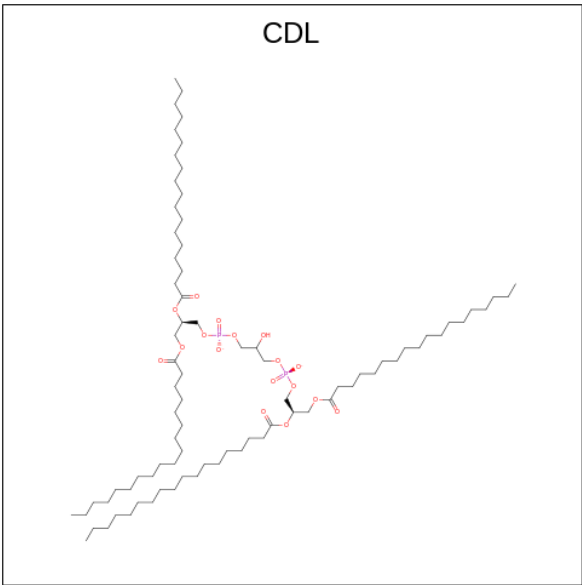
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 23  | O     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 24 is CHOLIC ACID (CCD ID: CHD) (formula:  $C_{24}H_{40}O_5$ ).



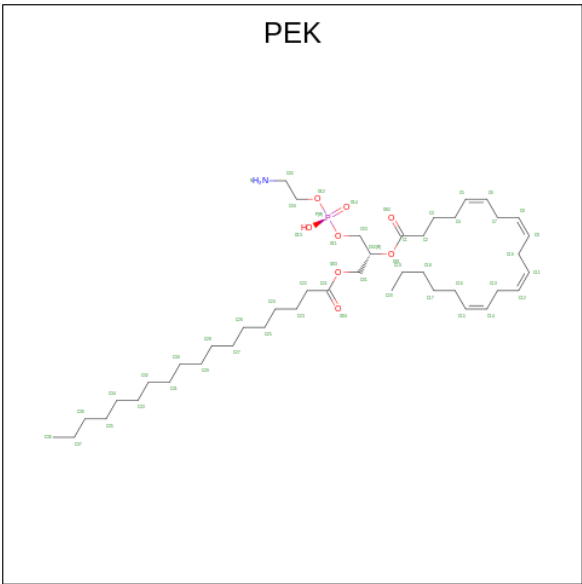
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 24  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 24  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 24  | G     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 24  | J     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 24  | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 24  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 24  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 24  | T     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 24  | Y     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 25  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 25  | G     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 25  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 25  | T     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).

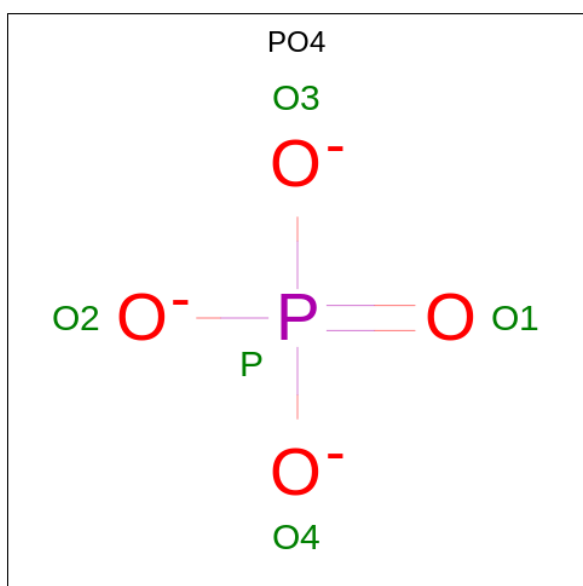


| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 26  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 26  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 26  | F     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 26  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 26  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 26  | T     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 27  | F     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 27  | S     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 28 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 28  | H     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 28  | U     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 29 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 29  | A     | 247      | Total O<br>250 250 | 0       | 4       |
| 29  | B     | 200      | Total O<br>200 200 | 0       | 0       |
| 29  | C     | 136      | Total O<br>136 136 | 0       | 0       |
| 29  | D     | 174      | Total O<br>174 174 | 0       | 0       |
| 29  | E     | 133      | Total O<br>133 133 | 0       | 0       |
| 29  | F     | 117      | Total O<br>117 117 | 0       | 0       |
| 29  | G     | 72       | Total O<br>72 72   | 0       | 0       |
| 29  | H     | 79       | Total O<br>79 79   | 0       | 0       |
| 29  | I     | 56       | Total O<br>56 56   | 0       | 0       |
| 29  | J     | 44       | Total O<br>44 44   | 0       | 0       |
| 29  | K     | 36       | Total O<br>36 36   | 0       | 0       |
| 29  | L     | 42       | Total O<br>42 42   | 0       | 0       |
| 29  | M     | 34       | Total O<br>34 34   | 0       | 0       |
| 29  | N     | 245      | Total O<br>247 247 | 0       | 3       |
| 29  | O     | 166      | Total O<br>166 166 | 0       | 0       |
| 29  | P     | 132      | Total O<br>132 132 | 0       | 0       |
| 29  | Q     | 99       | Total O<br>99 99   | 0       | 0       |
| 29  | R     | 98       | Total O<br>98 98   | 0       | 0       |
| 29  | S     | 105      | Total O<br>105 105 | 0       | 0       |
| 29  | T     | 75       | Total O<br>75 75   | 0       | 0       |
| 29  | U     | 65       | Total O<br>65 65   | 0       | 0       |

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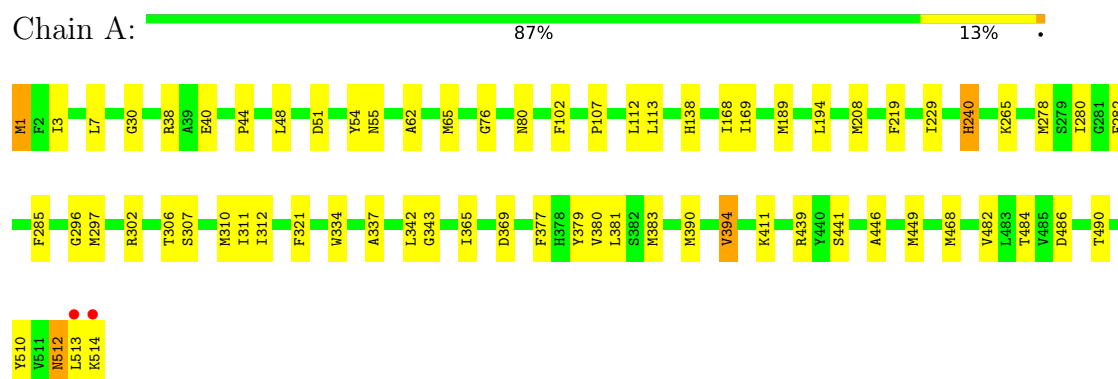
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 29  | V     | 48       | Total<br>48 | O<br>48 | 0       | 0       |
| 29  | W     | 27       | Total<br>27 | O<br>27 | 0       | 0       |
| 29  | X     | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 29  | Y     | 31       | Total<br>31 | O<br>31 | 0       | 0       |
| 29  | Z     | 20       | Total<br>20 | O<br>20 | 0       | 0       |

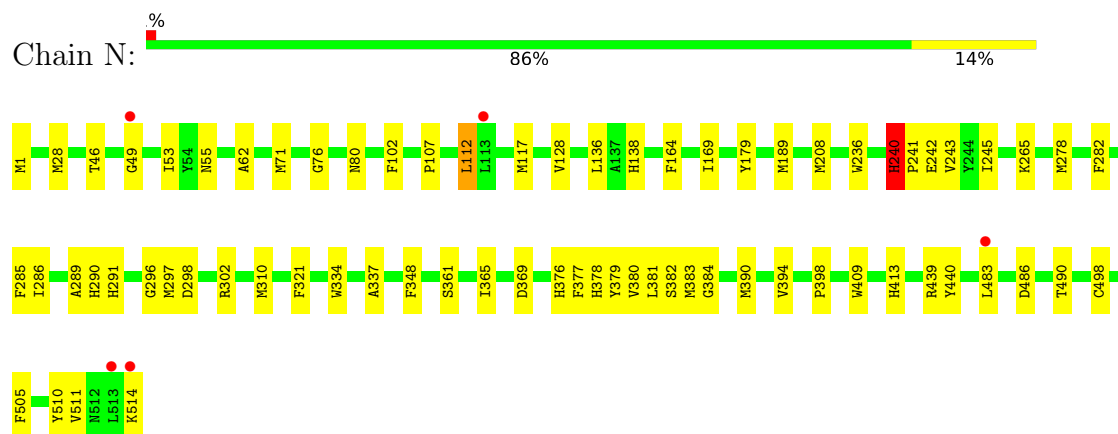
### 3 Residue-property plots

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

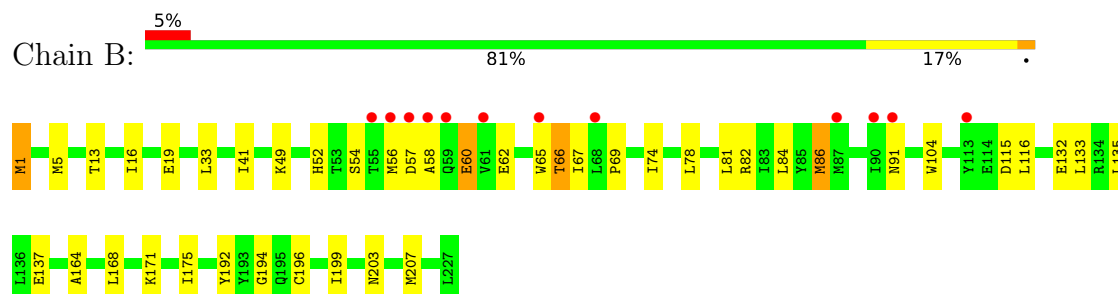
#### • Molecule 1: Cytochrome c oxidase subunit 1



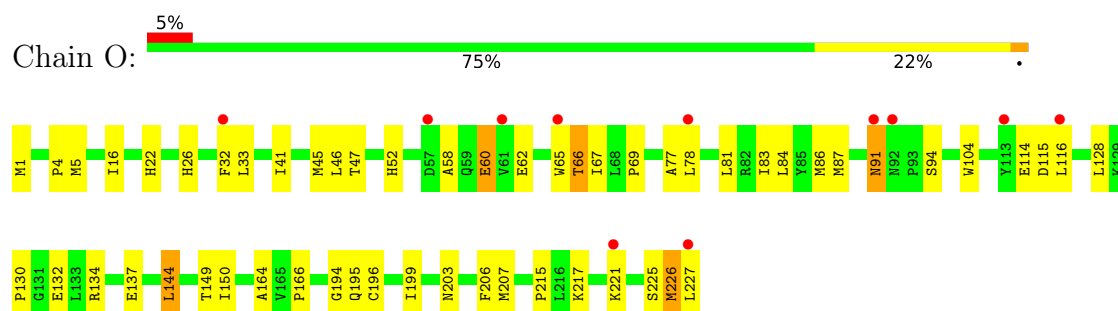
#### • Molecule 1: Cytochrome c oxidase subunit 1



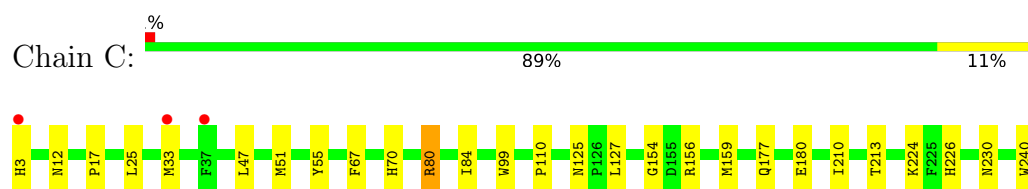
#### • Molecule 2: Cytochrome c oxidase subunit 2



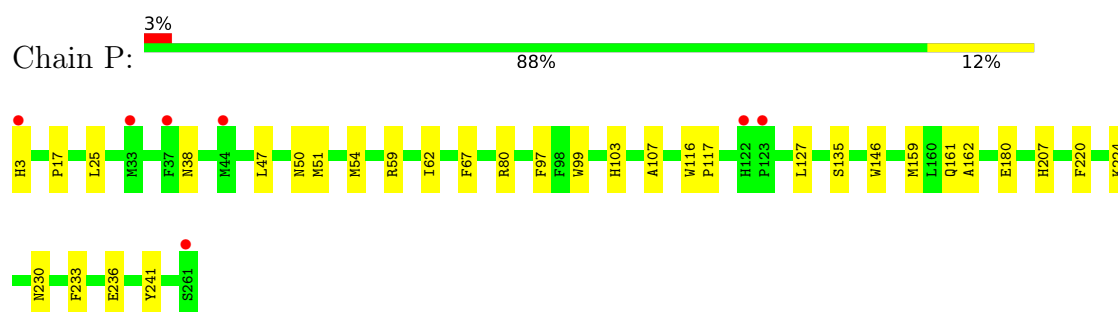
- Molecule 2: Cytochrome c oxidase subunit 2



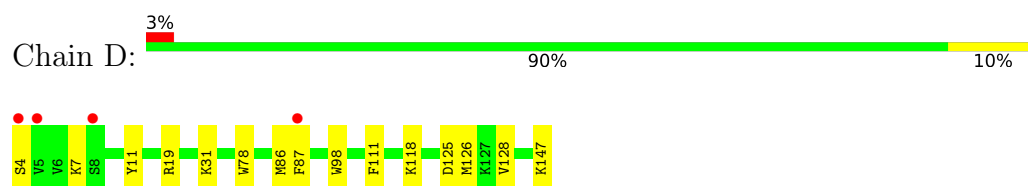
- Molecule 3: Cytochrome c oxidase subunit 3



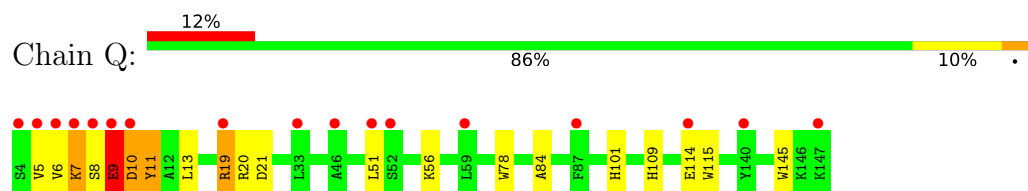
- Molecule 3: Cytochrome c oxidase subunit 3



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

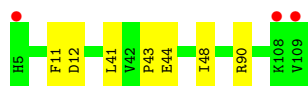


- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

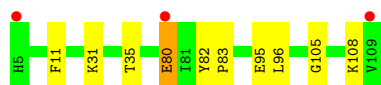
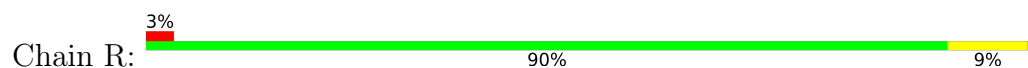


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

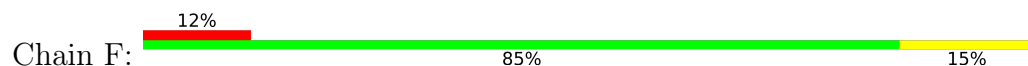




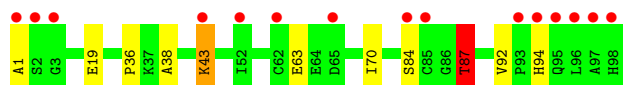
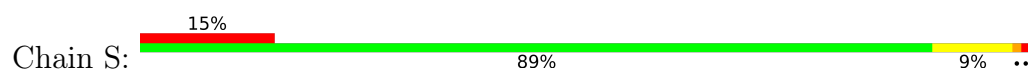
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



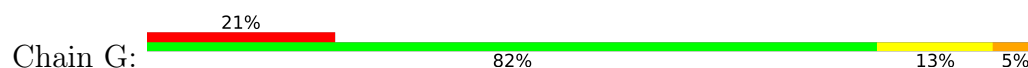
- Molecule 6: Cytochrome c oxidase subunit 5B



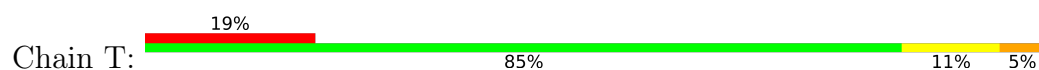
- Molecule 6: Cytochrome c oxidase subunit 5B



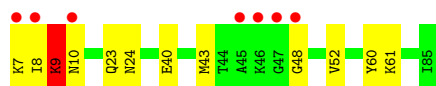
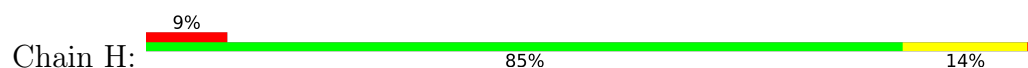
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



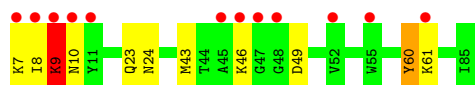
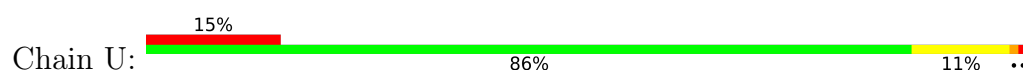
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



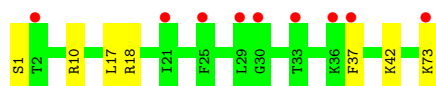
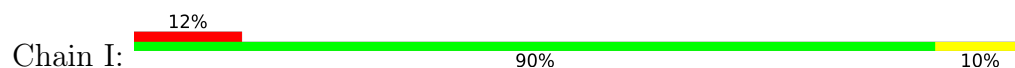
- Molecule 8: Cytochrome c oxidase subunit 6B1



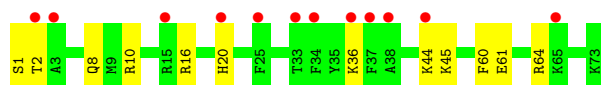
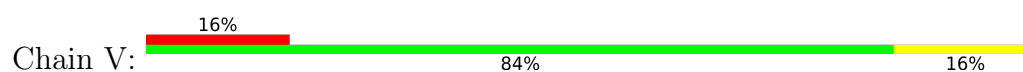
- Molecule 8: Cytochrome c oxidase subunit 6B1



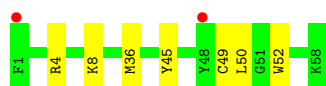
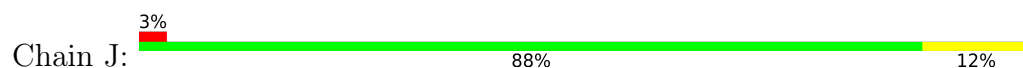
- Molecule 9: Cytochrome c oxidase subunit 6C



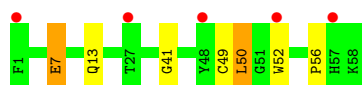
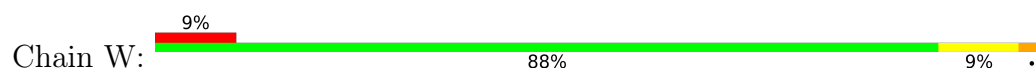
- Molecule 9: Cytochrome c oxidase subunit 6C



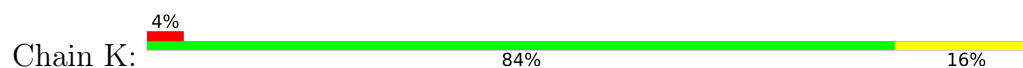
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



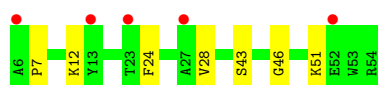
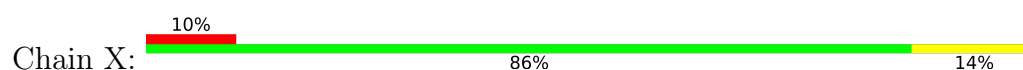
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



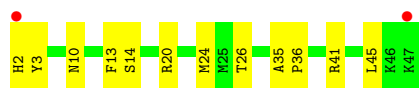
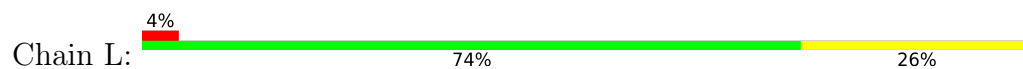
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



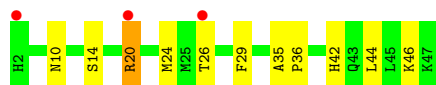
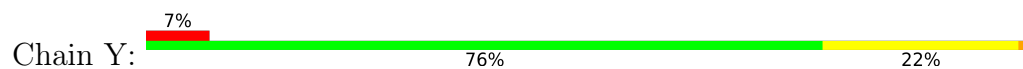
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



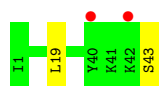
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



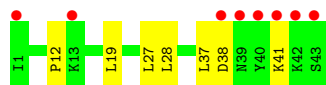
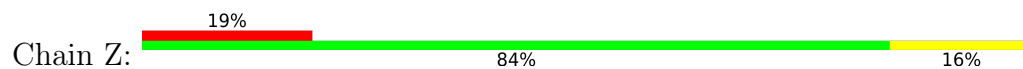
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 182.22Å 204.65Å 177.40Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 39.88 – 1.80<br>39.88 – 1.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (39.88-1.80)<br>99.8 (39.88-1.80)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.35 (at 1.80Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.13_2998: ???)                                     | Depositor        |
| R, $R_{free}$                                                           | 0.157 , 0.188<br>0.159 , 0.190                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 30366 reflections (5.01%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 29.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.685                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 79.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.005 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                        | EDS              |
| Total number of atoms                                                   | 34360                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 47.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: PO4, PSC, CHD, TPO, CU, PEK, DMU, ZN, EDO, HEA, PGV, CDL, FME, TGL, MG, NA, CUA, SAC

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     | 1.06         | 0/4445         | 1.00        | 5/6063 (0.1%)   |
| 1   | N     | 0.96         | 0/4321         | 0.92        | 3/5899 (0.1%)   |
| 2   | B     | 0.94         | 0/1896         | 0.99        | 1/2582 (0.0%)   |
| 2   | O     | 0.77         | 0/1934         | 0.92        | 2/2634 (0.1%)   |
| 3   | C     | 0.88         | 0/2236         | 0.86        | 1/3056 (0.0%)   |
| 3   | P     | 0.87         | 0/2211         | 0.83        | 0/3024          |
| 4   | D     | 0.92         | 0/1234         | 0.88        | 0/1665          |
| 4   | Q     | 0.63         | 0/1229         | 0.70        | 0/1658          |
| 5   | E     | 0.84         | 0/871          | 0.80        | 0/1182          |
| 5   | R     | 0.71         | 0/871          | 0.76        | 0/1182          |
| 6   | F     | 0.86         | 0/774          | 0.89        | 0/1050          |
| 6   | S     | 0.79         | 1/774 (0.1%)   | 0.85        | 0/1050          |
| 7   | G     | 0.79         | 0/691          | 0.85        | 0/937           |
| 7   | T     | 0.72         | 0/707          | 0.82        | 0/960           |
| 8   | H     | 0.80         | 0/682          | 0.87        | 0/921           |
| 8   | U     | 0.70         | 0/682          | 0.80        | 0/921           |
| 9   | I     | 0.70         | 0/605          | 0.77        | 0/802           |
| 9   | V     | 0.54         | 0/605          | 0.70        | 0/802           |
| 10  | J     | 0.64         | 0/471          | 0.76        | 0/636           |
| 10  | W     | 0.61         | 0/471          | 0.75        | 0/636           |
| 11  | K     | 0.78         | 0/398          | 0.81        | 0/544           |
| 11  | X     | 0.55         | 0/399          | 0.64        | 0/546           |
| 12  | L     | 0.92         | 0/393          | 0.92        | 0/526           |
| 12  | Y     | 0.74         | 0/393          | 0.75        | 0/526           |
| 13  | M     | 0.91         | 0/346          | 0.85        | 0/470           |
| 13  | Z     | 0.69         | 0/346          | 0.67        | 0/470           |
| All | All   | 0.87         | 1/29985 (0.0%) | 0.88        | 12/40742 (0.0%) |

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   | N     | 0                   | 1                   |
| 8   | H     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | S     | 87  | THR  | CB-CG2 | -5.17 | 1.35        | 1.52     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|--------|-------------|----------|
| 1   | N     | 71     | MET  | CG-SD-CE | -11.77 | 75.00       | 100.90   |
| 1   | A     | 240    | HIS  | CA-CB-CG | -6.30  | 107.50      | 113.80   |
| 1   | N     | 240    | HIS  | CA-CB-CG | -5.76  | 108.04      | 113.80   |
| 2   | B     | 192    | TYR  | CA-CB-CG | -5.62  | 103.78      | 113.90   |
| 1   | N     | 102    | PHE  | CA-CB-CG | -5.60  | 108.20      | 113.80   |
| 1   | A     | 102    | PHE  | CA-CB-CG | -5.56  | 108.24      | 113.80   |
| 3   | C     | 80     | ARG  | CG-CD-NE | -5.48  | 99.94       | 112.00   |
| 1   | A     | 512[A] | ASN  | N-CA-CB  | 5.44   | 118.68      | 110.42   |
| 1   | A     | 512[B] | ASN  | N-CA-CB  | 5.44   | 118.68      | 110.42   |
| 2   | O     | 166    | PRO  | CA-C-N   | -5.28  | 111.28      | 121.58   |
| 2   | O     | 166    | PRO  | C-N-CA   | -5.28  | 111.28      | 121.58   |
| 1   | A     | 38     | ARG  | CA-CB-CG | -5.03  | 104.04      | 114.10   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 240 | HIS  | Sidechain |
| 8   | H     | 9   | LYS  | Peptide   |
| 1   | N     | 240 | HIS  | Sidechain |

## 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     | 4192  | 0        | 4181     | 75      | 0            |
| 1   | N     | 4152  | 0        | 4129     | 73      | 0            |
| 2   | B     | 1839  | 0        | 1848     | 35      | 0            |
| 2   | O     | 1857  | 0        | 1858     | 47      | 0            |
| 3   | C     | 2122  | 0        | 2032     | 38      | 0            |
| 3   | P     | 2114  | 0        | 2028     | 28      | 0            |
| 4   | D     | 1198  | 0        | 1189     | 16      | 0            |
| 4   | Q     | 1195  | 0        | 1183     | 23      | 0            |
| 5   | E     | 852   | 0        | 845      | 5       | 0            |
| 5   | R     | 852   | 0        | 845      | 8       | 0            |
| 6   | F     | 751   | 0        | 726      | 15      | 0            |
| 6   | S     | 751   | 0        | 726      | 12      | 0            |
| 7   | G     | 676   | 0        | 644      | 17      | 0            |
| 7   | T     | 685   | 0        | 648      | 15      | 0            |
| 8   | H     | 662   | 0        | 623      | 9       | 0            |
| 8   | U     | 662   | 0        | 623      | 10      | 0            |
| 9   | I     | 601   | 0        | 613      | 7       | 0            |
| 9   | V     | 601   | 0        | 613      | 10      | 0            |
| 10  | J     | 460   | 0        | 459      | 9       | 0            |
| 10  | W     | 460   | 0        | 459      | 8       | 0            |
| 11  | K     | 384   | 0        | 366      | 11      | 0            |
| 11  | X     | 385   | 0        | 366      | 6       | 0            |
| 12  | L     | 380   | 0        | 380      | 13      | 0            |
| 12  | Y     | 380   | 0        | 380      | 12      | 0            |
| 13  | M     | 336   | 0        | 352      | 2       | 0            |
| 13  | Z     | 336   | 0        | 352      | 7       | 0            |
| 14  | A     | 132   | 0        | 93       | 5       | 0            |
| 14  | N     | 132   | 0        | 93       | 7       | 0            |
| 15  | A     | 1     | 0        | 0        | 0       | 0            |
| 15  | N     | 1     | 0        | 0        | 0       | 0            |
| 16  | A     | 1     | 0        | 0        | 0       | 0            |
| 16  | N     | 1     | 0        | 0        | 0       | 0            |
| 17  | A     | 1     | 0        | 0        | 0       | 0            |
| 17  | C     | 1     | 0        | 0        | 0       | 0            |
| 17  | N     | 1     | 0        | 0        | 0       | 0            |
| 17  | P     | 1     | 0        | 0        | 1       | 0            |
| 18  | A     | 13    | 0        | 21       | 2       | 0            |
| 18  | B     | 11    | 0        | 21       | 0       | 0            |
| 18  | C     | 66    | 0        | 94       | 2       | 0            |
| 18  | D     | 21    | 0        | 30       | 0       | 0            |
| 18  | J     | 21    | 0        | 30       | 4       | 0            |
| 18  | K     | 58    | 0        | 94       | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 18  | L     | 33    | 0        | 40       | 2       | 0            |
| 18  | M     | 33    | 0        | 42       | 1       | 0            |
| 18  | O     | 11    | 0        | 21       | 2       | 0            |
| 18  | P     | 44    | 0        | 63       | 3       | 0            |
| 18  | Q     | 23    | 0        | 31       | 2       | 0            |
| 18  | W     | 21    | 0        | 30       | 4       | 0            |
| 18  | X     | 65    | 0        | 114      | 1       | 0            |
| 18  | Y     | 33    | 0        | 42       | 3       | 0            |
| 18  | Z     | 33    | 0        | 42       | 2       | 0            |
| 19  | A     | 102   | 0        | 152      | 6       | 0            |
| 19  | C     | 51    | 0        | 76       | 6       | 0            |
| 19  | N     | 102   | 0        | 152      | 9       | 0            |
| 19  | P     | 102   | 0        | 152      | 13      | 0            |
| 19  | T     | 51    | 0        | 74       | 1       | 0            |
| 20  | A     | 52    | 0        | 79       | 17      | 0            |
| 20  | V     | 52    | 0        | 78       | 7       | 0            |
| 21  | A     | 63    | 0        | 110      | 2       | 0            |
| 21  | D     | 63    | 0        | 110      | 15      | 0            |
| 21  | L     | 63    | 0        | 110      | 16      | 0            |
| 21  | N     | 63    | 0        | 110      | 4       | 0            |
| 21  | Q     | 63    | 0        | 110      | 12      | 0            |
| 21  | Y     | 63    | 0        | 110      | 3       | 0            |
| 22  | A     | 36    | 0        | 54       | 9       | 0            |
| 22  | B     | 20    | 0        | 30       | 3       | 0            |
| 22  | C     | 28    | 0        | 42       | 3       | 0            |
| 22  | D     | 20    | 0        | 30       | 3       | 0            |
| 22  | E     | 12    | 0        | 18       | 2       | 0            |
| 22  | F     | 32    | 0        | 48       | 3       | 0            |
| 22  | G     | 4     | 0        | 6        | 0       | 0            |
| 22  | H     | 4     | 0        | 6        | 2       | 0            |
| 22  | J     | 4     | 0        | 6        | 0       | 0            |
| 22  | L     | 8     | 0        | 11       | 1       | 0            |
| 22  | M     | 4     | 0        | 6        | 0       | 0            |
| 22  | N     | 60    | 0        | 90       | 14      | 0            |
| 22  | O     | 8     | 0        | 12       | 1       | 0            |
| 22  | P     | 28    | 0        | 42       | 3       | 0            |
| 22  | Q     | 12    | 0        | 18       | 4       | 0            |
| 22  | S     | 20    | 0        | 30       | 2       | 0            |
| 22  | T     | 8     | 0        | 12       | 1       | 0            |
| 22  | U     | 4     | 0        | 6        | 4       | 0            |
| 22  | W     | 4     | 0        | 6        | 0       | 0            |
| 22  | Y     | 4     | 0        | 6        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | B     | 2     | 0        | 0        | 0       | 0            |
| 23  | O     | 2     | 0        | 0        | 0       | 0            |
| 24  | C     | 58    | 0        | 78       | 3       | 0            |
| 24  | G     | 29    | 0        | 39       | 1       | 0            |
| 24  | J     | 29    | 0        | 39       | 1       | 0            |
| 24  | L     | 29    | 0        | 39       | 0       | 0            |
| 24  | P     | 58    | 0        | 78       | 3       | 0            |
| 24  | T     | 29    | 0        | 39       | 1       | 0            |
| 24  | Y     | 29    | 0        | 39       | 1       | 0            |
| 25  | C     | 100   | 0        | 156      | 19      | 0            |
| 25  | G     | 100   | 0        | 154      | 22      | 0            |
| 25  | P     | 100   | 0        | 156      | 11      | 0            |
| 25  | T     | 100   | 0        | 154      | 29      | 0            |
| 26  | C     | 106   | 0        | 154      | 11      | 0            |
| 26  | F     | 53    | 0        | 74       | 6       | 0            |
| 26  | P     | 106   | 0        | 154      | 3       | 0            |
| 26  | T     | 53    | 0        | 77       | 9       | 0            |
| 27  | F     | 1     | 0        | 0        | 0       | 0            |
| 27  | S     | 1     | 0        | 0        | 0       | 0            |
| 28  | H     | 5     | 0        | 0        | 0       | 0            |
| 28  | U     | 5     | 0        | 0        | 0       | 0            |
| 29  | A     | 250   | 0        | 0        | 12      | 0            |
| 29  | B     | 200   | 0        | 0        | 4       | 2            |
| 29  | C     | 136   | 0        | 0        | 8       | 0            |
| 29  | D     | 174   | 0        | 0        | 3       | 2            |
| 29  | E     | 133   | 0        | 0        | 0       | 0            |
| 29  | F     | 117   | 0        | 0        | 2       | 0            |
| 29  | G     | 72    | 0        | 0        | 0       | 0            |
| 29  | H     | 79    | 0        | 0        | 3       | 0            |
| 29  | I     | 56    | 0        | 0        | 5       | 2            |
| 29  | J     | 44    | 0        | 0        | 1       | 0            |
| 29  | K     | 36    | 0        | 0        | 2       | 0            |
| 29  | L     | 42    | 0        | 0        | 2       | 0            |
| 29  | M     | 34    | 0        | 0        | 1       | 1            |
| 29  | N     | 247   | 0        | 0        | 12      | 0            |
| 29  | O     | 166   | 0        | 0        | 4       | 0            |
| 29  | P     | 132   | 0        | 0        | 4       | 0            |
| 29  | Q     | 99    | 0        | 0        | 2       | 0            |
| 29  | R     | 98    | 0        | 0        | 2       | 0            |
| 29  | S     | 105   | 0        | 0        | 4       | 0            |
| 29  | T     | 75    | 0        | 0        | 4       | 0            |
| 29  | U     | 65    | 0        | 0        | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | V     | 48    | 0        | 0        | 1       | 1            |
| 29  | W     | 27    | 0        | 0        | 1       | 0            |
| 29  | X     | 28    | 0        | 0        | 0       | 0            |
| 29  | Y     | 31    | 0        | 0        | 1       | 0            |
| 29  | Z     | 20    | 0        | 0        | 0       | 0            |
| All | All   | 34360 | 0        | 32701    | 576     | 4            |

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 9.

All (576) 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) |
|---------------------|-------------------|--------------------------|-------------------|
| 25:G:102:CDL:H512   | 25:G:102:CDL:H181 | 1.32                     | 1.09              |
| 1:A:55[B]:ASN:ND2   | 29:A:701:HOH:O    | 1.87                     | 1.05              |
| 25:G:102:CDL:H221   | 25:G:102:CDL:H551 | 1.37                     | 1.05              |
| 12:L:20:ARG:HH21    | 21:L:103:TGL:HC51 | 1.23                     | 1.04              |
| 1:A:302[B]:ARG:HH12 | 1:A:365:ILE:HD11  | 1.25                     | 1.01              |
| 8:U:24:ASN:HD21     | 22:U:102:EDO:H21  | 1.24                     | 1.00              |
| 1:N:55[B]:ASN:ND2   | 29:N:701:HOH:O    | 1.93                     | 0.98              |
| 7:T:5:LYS:NZ        | 29:T:201:HOH:O    | 1.96                     | 0.97              |
| 26:F:102:PEK:N      | 29:F:201:HOH:O    | 1.99                     | 0.93              |
| 2:O:221:LYS:O       | 29:O:401:HOH:O    | 1.88                     | 0.91              |
| 7:T:17:ARG:HH12     | 26:T:103:PEK:H041 | 1.37                     | 0.90              |
| 12:L:14:SER:H       | 21:L:103:TGL:HC31 | 1.38                     | 0.87              |
| 25:P:306:CDL:H651   | 19:P:309:PGV:H172 | 1.56                     | 0.87              |
| 4:Q:10:ASP:O        | 29:Q:301:HOH:O    | 1.93                     | 0.86              |
| 1:A:486[B]:ASP:OD2  | 4:D:19:ARG:NH1    | 2.10                     | 0.85              |
| 26:T:103:PEK:H011   | 26:T:103:PEK:H31  | 1.57                     | 0.84              |
| 26:C:308:PEK:H361   | 25:T:102:CDL:H871 | 1.57                     | 0.84              |
| 21:N:608:TGL:HA61   | 2:O:32[B]:PHE:HE1 | 1.42                     | 0.83              |
| 1:A:514:LYS:OXT     | 6:F:37:LYS:NZ     | 2.13                     | 0.82              |
| 10:J:50:LEU:HB2     | 18:J:101:DMU:H20  | 1.63                     | 0.81              |
| 1:N:510:TYR:HA      | 22:N:617:EDO:H21  | 1.63                     | 0.80              |
| 4:D:78:TRP:HB3      | 21:D:202:TGL:HB22 | 1.64                     | 0.80              |
| 11:K:20:SER:HG      | 18:K:103:DMU:H27  | 1.17                     | 0.78              |
| 1:A:446:ALA:HB2     | 22:A:615:EDO:H12  | 1.66                     | 0.78              |
| 10:W:49:CYS:HB3     | 18:W:101:DMU:H11  | 1.65                     | 0.78              |
| 3:C:67:PHE:CE2      | 25:C:307:CDL:HB22 | 2.18                     | 0.78              |
| 25:C:307:CDL:H642   | 19:C:310:PGV:H161 | 1.66                     | 0.78              |
| 2:O:22[B]:HIS:CE1   | 9:V:44:LYS:HE2    | 2.18                     | 0.78              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:L:20:ARG:NH2    | 21:L:103:TGL:HC51   | 1.99                     | 0.78              |
| 3:C:213:THR:HG23   | 25:C:307:CDL:H771   | 1.66                     | 0.77              |
| 1:A:486[B]:ASP:OD1 | 22:A:618:EDO:O1     | 2.01                     | 0.77              |
| 11:K:6:ALA:N       | 29:K:201:HOH:O      | 2.18                     | 0.76              |
| 26:F:102:PEK:H312  | 2:O:66[A]:THR:HG21  | 1.67                     | 0.76              |
| 22:N:615:EDO:H22   | 12:Y:10:ASN:HD22    | 1.52                     | 0.75              |
| 11:X:7:PRO:O       | 11:X:12:LYS:NZ      | 2.21                     | 0.74              |
| 26:F:102:PEK:H041  | 7:G:17:ARG:HH12     | 1.53                     | 0.73              |
| 1:A:302[B]:ARG:NH1 | 1:A:365:ILE:HD11    | 2.02                     | 0.73              |
| 1:A:112:LEU:HG     | 29:A:892:HOH:O      | 1.87                     | 0.72              |
| 25:G:102:CDL:H562  | 25:G:102:CDL:H762   | 1.70                     | 0.72              |
| 25:G:102:CDL:H111  | 25:G:102:CDL:H381   | 1.70                     | 0.72              |
| 21:Q:202:TGL:H352  | 9:V:16:ARG:HE       | 1.53                     | 0.72              |
| 12:Y:20:ARG:NH2    | 21:Y:103:TGL:HC32   | 2.04                     | 0.72              |
| 21:Q:202:TGL:HG12  | 21:Q:202:TGL:HC32   | 1.71                     | 0.71              |
| 1:A:302[B]:ARG:HE  | 2:B:84:LEU:HD11     | 1.56                     | 0.71              |
| 8:H:43:MET:HE1     | 8:U:43:MET:HE1      | 1.74                     | 0.70              |
| 21:L:103:TGL:HC41  | 21:L:103:TGL:OC1    | 1.89                     | 0.70              |
| 1:A:390:MET:O      | 1:A:394[A]:VAL:HG12 | 1.92                     | 0.69              |
| 1:A:468:MET:HG3    | 22:A:617:EDO:H22    | 1.74                     | 0.69              |
| 12:Y:20:ARG:HH21   | 21:Y:103:TGL:HC32   | 1.57                     | 0.69              |
| 3:P:236:GLU:HG3    | 22:P:316:EDO:H22    | 1.73                     | 0.69              |
| 25:T:102:CDL:H273  | 26:T:103:PEK:H382   | 1.74                     | 0.68              |
| 12:Y:20:ARG:NH2    | 12:Y:24:MET:HG3     | 2.08                     | 0.68              |
| 3:C:51[A]:MET:HE1  | 19:C:310:PGV:H162   | 1.76                     | 0.68              |
| 3:P:3:HIS:ND1      | 29:P:401:HOH:O      | 2.26                     | 0.68              |
| 4:D:87:PHE:CZ      | 4:D:87:PHE:CD1      | 2.79                     | 0.68              |
| 1:A:297[B]:MET:HG2 | 1:A:302[B]:ARG:HG2  | 1.75                     | 0.68              |
| 2:O:47:THR:HB      | 21:Q:202:TGL:H181   | 1.74                     | 0.68              |
| 3:C:67:PHE:HE2     | 25:C:307:CDL:HB22   | 1.58                     | 0.67              |
| 4:D:4:SER:N        | 29:D:302:HOH:O      | 2.26                     | 0.67              |
| 5:R:31:LYS:HE3     | 6:S:84:SER:O        | 1.94                     | 0.67              |
| 18:L:101:DMU:H20   | 21:L:103:TGL:H301   | 1.75                     | 0.67              |
| 1:A:482:VAL:O      | 29:A:702:HOH:O      | 2.13                     | 0.66              |
| 22:Q:204:EDO:H12   | 29:S:231:HOH:O      | 1.97                     | 0.66              |
| 12:Y:42:HIS:ND1    | 18:Y:101:DMU:O49    | 2.19                     | 0.66              |
| 21:D:202:TGL:HG12  | 21:D:202:TGL:HC42   | 1.79                     | 0.65              |
| 7:G:1:ALA:HB1      | 1:N:286:ILE:HG22    | 1.77                     | 0.65              |
| 3:P:103:HIS:HA     | 19:P:310:PGV:H012   | 1.79                     | 0.65              |
| 18:C:303:DMU:O61   | 29:C:401:HOH:O      | 2.13                     | 0.64              |
| 1:A:321:PHE:CD2    | 2:B:65:TRP:HB2      | 2.32                     | 0.64              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:A:510:TYR:OH    | 1:A:512[B]:ASN:ND2  | 2.26                     | 0.64              |
| 10:W:7:GLU:HG2    | 29:W:221:HOH:O      | 1.97                     | 0.64              |
| 7:G:37:LEU:HD23   | 25:G:102:CDL:H391   | 1.78                     | 0.64              |
| 26:F:102:PEK:H312 | 2:O:66[A]:THR:CG2   | 2.27                     | 0.64              |
| 6:S:19[B]:GLU:OE2 | 29:S:201:HOH:O      | 2.15                     | 0.64              |
| 19:N:606:PGV:H302 | 13:Z:19:LEU:HD23    | 1.79                     | 0.64              |
| 2:O:67:ILE:HD11   | 29:O:557:HOH:O      | 1.97                     | 0.63              |
| 29:N:860:HOH:O    | 6:S:87:THR:HG21     | 1.98                     | 0.63              |
| 22:B:305:EDO:H12  | 29:B:467:HOH:O      | 1.99                     | 0.63              |
| 2:O:58:ALA:O      | 2:O:62:GLU:HG3      | 1.99                     | 0.63              |
| 1:N:310:MET:HE1   | 2:O:77:ALA:HB2      | 1.81                     | 0.63              |
| 4:D:78:TRP:CB     | 21:D:202:TGL:HB22   | 2.28                     | 0.62              |
| 1:A:379:TYR:O     | 1:A:383[B]:MET:HB2  | 1.99                     | 0.62              |
| 19:N:606:PGV:H342 | 19:N:606:PGV:H162   | 1.80                     | 0.62              |
| 7:T:38:HIS:CE1    | 25:T:102:CDL:H122   | 2.34                     | 0.62              |
| 21:N:608:TGL:HA61 | 2:O:32[B]:PHE:CE1   | 2.29                     | 0.62              |
| 1:A:307:SER:CB    | 25:T:102:CDL:H182   | 2.30                     | 0.62              |
| 10:J:49:CYS:HB3   | 18:J:101:DMU:H11    | 1.80                     | 0.62              |
| 1:N:169:ILE:HG13  | 1:N:189[B]:MET:HE1  | 1.82                     | 0.62              |
| 7:G:4:ALA:HB3     | 1:N:282:PHE:HA      | 1.82                     | 0.61              |
| 2:O:225:SER:N     | 29:O:401:HOH:O      | 2.32                     | 0.61              |
| 12:Y:35:ALA:HA    | 18:Y:101:DMU:H20    | 1.82                     | 0.61              |
| 8:H:7:LYS:N       | 29:H:201:HOH:O      | 2.33                     | 0.61              |
| 25:P:306:CDL:H332 | 25:P:306:CDL:H472   | 1.81                     | 0.61              |
| 1:N:289:ALA:HB1   | 1:N:297[B]:MET:HE1  | 1.82                     | 0.61              |
| 1:A:48[B]:LEU:HB2 | 29:A:708:HOH:O      | 2.00                     | 0.61              |
| 25:C:307:CDL:H651 | 19:C:310:PGV:H182   | 1.83                     | 0.61              |
| 19:N:606:PGV:H92  | 4:Q:84:ALA:HB2      | 1.81                     | 0.61              |
| 3:C:224:LYS:CD    | 25:C:307:CDL:HB31   | 2.31                     | 0.60              |
| 22:C:313:EDO:O2   | 6:F:1:ALA:O         | 2.17                     | 0.60              |
| 13:Z:27:LEU:HD22  | 18:Z:101:DMU:H14    | 1.82                     | 0.60              |
| 1:A:334:TRP:CZ3   | 21:D:202:TGL:HA52   | 2.36                     | 0.60              |
| 20:A:609:PSC:H212 | 2:B:57:ASP:H        | 1.67                     | 0.60              |
| 20:V:101:PSC:H42  | 20:V:101:PSC:H241   | 1.83                     | 0.60              |
| 1:A:377:PHE:HA    | 1:A:380[B]:VAL:HG12 | 1.83                     | 0.60              |
| 1:N:511:VAL:H     | 22:N:617:EDO:H21    | 1.66                     | 0.60              |
| 19:N:606:PGV:H231 | 13:Z:12:PRO:HG3     | 1.82                     | 0.60              |
| 1:A:285:PHE:CD2   | 7:T:4:ALA:HB2       | 2.37                     | 0.60              |
| 1:A:297[B]:MET:CG | 1:A:302[B]:ARG:HG2  | 2.32                     | 0.59              |
| 20:A:609:PSC:C08  | 9:I:10:ARG:HH21     | 2.14                     | 0.59              |
| 4:Q:20:ARG:HG2    | 29:Q:359:HOH:O      | 2.01                     | 0.59              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:I:18:ARG:HG3     | 29:I:128:HOH:O      | 2.02                     | 0.59              |
| 2:O:60:GLU:CD      | 2:O:60:GLU:H        | 2.10                     | 0.59              |
| 17:P:301:NA:NA     | 29:P:403:HOH:O      | 1.75                     | 0.59              |
| 25:C:307:CDL:HA61  | 25:C:307:CDL:H131   | 1.84                     | 0.59              |
| 1:N:365:ILE:HD11   | 29:N:891:HOH:O      | 2.01                     | 0.59              |
| 21:N:608:TGL:H121  | 21:N:608:TGL:HA71   | 1.85                     | 0.59              |
| 6:S:43:LYS:HD2     | 6:S:43:LYS:H        | 1.68                     | 0.59              |
| 1:N:390:MET:HE2    | 1:N:413:HIS:HE1     | 1.68                     | 0.59              |
| 9:V:45:LYS:NZ      | 29:V:202:HOH:O      | 2.35                     | 0.59              |
| 22:H:102:EDO:H11   | 29:H:262:HOH:O      | 2.03                     | 0.59              |
| 4:Q:78:TRP:CA      | 21:Q:202:TGL:HB22   | 2.33                     | 0.59              |
| 1:A:3:ILE:HG23     | 1:A:7[B]:LEU:HD12   | 1.85                     | 0.58              |
| 1:A:282:PHE:HA     | 7:T:4:ALA:HB3       | 1.84                     | 0.58              |
| 19:A:607:PGV:H062  | 19:A:607:PGV:O13    | 2.03                     | 0.58              |
| 1:A:311:ILE:HD11   | 25:T:102:CDL:H421   | 1.85                     | 0.58              |
| 21:Q:202:TGL:H362  | 9:V:20:HIS:HE1      | 1.69                     | 0.58              |
| 7:G:4:ALA:HB2      | 1:N:285:PHE:CD2     | 2.38                     | 0.58              |
| 9:I:1:SAC:O        | 29:I:101:HOH:O      | 2.17                     | 0.58              |
| 1:A:381[B]:LEU:HB2 | 14:A:602:HEA:CAC    | 2.33                     | 0.58              |
| 1:A:337:ALA:HB2    | 1:A:394[B]:VAL:HG23 | 1.85                     | 0.58              |
| 25:T:102:CDL:H382  | 25:T:102:CDL:H161   | 1.85                     | 0.57              |
| 1:A:334:TRP:CD1    | 21:D:202:TGL:HC41   | 2.38                     | 0.57              |
| 3:C:156:ARG:HE     | 24:C:306:CHD:C24    | 2.17                     | 0.57              |
| 11:X:24:PHE:O      | 11:X:28:VAL:HG12    | 2.04                     | 0.57              |
| 3:C:177:GLN:HB3    | 26:C:309:PEK:H201   | 1.85                     | 0.57              |
| 1:N:514:LYS:NZ     | 29:N:707:HOH:O      | 2.38                     | 0.57              |
| 8:U:61:LYS:NZ      | 29:U:201:HOH:O      | 2.37                     | 0.57              |
| 20:A:609:PSC:O02   | 29:A:703:HOH:O      | 2.17                     | 0.56              |
| 25:T:102:CDL:C25   | 25:T:102:CDL:H751   | 2.36                     | 0.56              |
| 25:T:102:CDL:H751  | 25:T:102:CDL:H252   | 1.86                     | 0.56              |
| 4:D:78:TRP:CA      | 21:D:202:TGL:HB22   | 2.36                     | 0.56              |
| 1:N:80:ASN:HD21    | 22:N:622:EDO:H12    | 1.70                     | 0.56              |
| 22:S:105:EDO:H21   | 29:S:211:HOH:O      | 2.04                     | 0.56              |
| 3:P:54:MET:HE1     | 19:P:309:PGV:H132   | 1.88                     | 0.56              |
| 21:D:202:TGL:HC42  | 21:D:202:TGL:OG3    | 2.06                     | 0.55              |
| 2:O:144:LEU:HG     | 2:O:150:ILE:HD13    | 1.87                     | 0.55              |
| 2:O:196:CYS:HB2    | 2:O:207:MET:HG3     | 1.88                     | 0.55              |
| 1:A:112:LEU:C      | 1:A:112:LEU:HD23    | 2.32                     | 0.55              |
| 20:A:609:PSC:H251  | 2:B:56:MET:HB3      | 1.87                     | 0.55              |
| 3:C:51[B]:MET:HE1  | 25:C:307:CDL:H271   | 1.89                     | 0.55              |
| 25:G:102:CDL:HA61  | 25:G:102:CDL:H362   | 1.87                     | 0.55              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:N:297[B]:MET:CG   | 1:N:302:ARG:HG3    | 2.36                     | 0.55              |
| 2:O:132:GLU:HB3     | 2:O:137:GLU:HG3    | 1.89                     | 0.55              |
| 9:V:1:SAC:OG        | 9:V:2:THR:N        | 2.37                     | 0.55              |
| 1:N:381[B]:LEU:HB2  | 14:N:602:HEA:CAC   | 2.37                     | 0.54              |
| 6:S:19[B]:GLU:OE2   | 22:S:105:EDO:O1    | 2.26                     | 0.54              |
| 21:L:103:TGL:H362   | 21:L:103:TGL:H322  | 1.88                     | 0.54              |
| 1:N:321:PHE:HB3     | 2:O:65[A]:TRP:CE3  | 2.42                     | 0.54              |
| 7:T:38:HIS:CD2      | 25:T:102:CDL:H1    | 2.42                     | 0.54              |
| 1:N:361:SER:OG      | 2:O:84:LEU:HD13    | 2.07                     | 0.54              |
| 2:B:81:LEU:HD13     | 25:T:102:CDL:H131  | 1.89                     | 0.54              |
| 1:N:49[B]:GLY:HA3   | 13:Z:41:LYS:HE3    | 1.89                     | 0.54              |
| 1:N:505:PHE:HA      | 22:N:612:EDO:H22   | 1.90                     | 0.54              |
| 1:A:311:ILE:CD1     | 25:T:102:CDL:H421  | 2.37                     | 0.54              |
| 1:A:468:MET:CG      | 22:A:617:EDO:H22   | 2.36                     | 0.54              |
| 2:B:74:ILE:HG13     | 25:T:102:CDL:H431  | 1.90                     | 0.54              |
| 1:N:511:VAL:H       | 22:N:617:EDO:C2    | 2.21                     | 0.54              |
| 19:A:607:PGV:H321   | 19:A:607:PGV:H151  | 1.90                     | 0.54              |
| 20:A:609:PSC:C21    | 2:B:57:ASP:H       | 2.20                     | 0.54              |
| 3:C:125:ASN:HB2     | 7:G:42:ARG:HH22    | 1.73                     | 0.54              |
| 25:T:102:CDL:H581   | 25:T:102:CDL:C78   | 2.38                     | 0.54              |
| 18:Y:101:DMU:H26    | 29:Y:229:HOH:O     | 2.08                     | 0.54              |
| 20:A:609:PSC:H082   | 9:I:10:ARG:HH21    | 1.71                     | 0.53              |
| 1:A:51[B]:ASP:OD2   | 1:A:441:SER:OG     | 2.23                     | 0.53              |
| 3:P:161:GLN:NE2     | 26:T:103:PEK:H22   | 2.23                     | 0.53              |
| 21:D:202:TGL:HG32   | 29:D:336:HOH:O     | 2.08                     | 0.53              |
| 13:M:43:SER:O       | 29:M:201:HOH:O     | 2.19                     | 0.53              |
| 3:C:3:HIS:N         | 29:C:409:HOH:O     | 2.41                     | 0.53              |
| 1:N:53[B]:ILE:HG12  | 29:N:882:HOH:O     | 2.09                     | 0.53              |
| 1:N:297[B]:MET:HG2  | 1:N:302:ARG:HG3    | 1.90                     | 0.53              |
| 1:A:377:PHE:O       | 1:A:381[B]:LEU:HB3 | 2.09                     | 0.53              |
| 3:C:70:HIS:HE1      | 22:C:316:EDO:H22   | 1.74                     | 0.53              |
| 1:A:484:THR:HG22    | 29:A:921:HOH:O     | 2.09                     | 0.52              |
| 20:A:609:PSC:H22    | 20:A:609:PSC:H231  | 1.89                     | 0.52              |
| 25:G:102:CDL:H382   | 2:O:81:LEU:HD12    | 1.90                     | 0.52              |
| 2:O:83:ILE:HA       | 2:O:86:MET:HG2     | 1.91                     | 0.52              |
| 26:P:308:PEK:H101   | 26:P:308:PEK:H42   | 1.90                     | 0.52              |
| 1:A:302[B]:ARG:HH12 | 1:A:365:ILE:CD1    | 2.11                     | 0.52              |
| 1:A:514:LYS:HA      | 6:F:38:ALA:HB3     | 1.92                     | 0.52              |
| 2:B:135:LEU:HD21    | 22:B:307:EDO:H11   | 1.91                     | 0.52              |
| 4:D:86:MET:HE1      | 11:K:22:ALA:HB2    | 1.92                     | 0.52              |
| 10:J:50:LEU:HB2     | 18:J:101:DMU:C37   | 2.37                     | 0.52              |

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| Atom-1               | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 19:P:310:PGV:H71     | 19:P:310:PGV:O04    | 2.08                     | 0.52              |
| 3:C:80:ARG:NH1       | 29:C:403:HOH:O      | 2.23                     | 0.52              |
| 3:C:127:LEU:HD22     | 25:G:102:CDL:HB61   | 1.91                     | 0.52              |
| 8:H:43:MET:HE3       | 8:H:48:GLY:HA3      | 1.92                     | 0.52              |
| 21:D:202:TGL:HA21    | 21:D:202:TGL:HB31   | 1.92                     | 0.52              |
| 11:K:20:SER:HA       | 18:K:103:DMU:H5     | 1.91                     | 0.52              |
| 1:N:514:LYS:HA       | 6:S:38:ALA:HB3      | 1.92                     | 0.52              |
| 4:Q:101:HIS:ND1      | 18:Q:201:DMU:H5     | 2.25                     | 0.52              |
| 10:W:50:LEU:HG       | 18:W:101:DMU:H23    | 1.91                     | 0.52              |
| 2:B:104:TRP:CG       | 2:B:203:ASN:HB2     | 2.45                     | 0.52              |
| 4:Q:19:ARG:NH2       | 4:Q:21:ASP:OD2      | 2.42                     | 0.52              |
| 7:T:36[B]:TRP:HZ2    | 26:T:103:PEK:H201   | 1.74                     | 0.52              |
| 10:W:56:PRO:HD3      | 12:Y:46:LYS:HD2     | 1.92                     | 0.52              |
| 2:B:49:LYS:HD3       | 21:D:202:TGL:HC72   | 1.91                     | 0.51              |
| 3:C:80:ARG:HD3       | 29:C:403:HOH:O      | 2.11                     | 0.51              |
| 25:G:102:CDL:H202    | 25:G:102:CDL:H531   | 1.92                     | 0.51              |
| 3:P:224:LYS:CD       | 25:P:306:CDL:HB31   | 2.40                     | 0.51              |
| 21:L:103:TGL:HG31    | 29:L:228:HOH:O      | 2.10                     | 0.51              |
| 2:B:196:CYS:HB2      | 2:B:207:MET:HG3     | 1.92                     | 0.51              |
| 8:U:43:MET:HE3       | 8:U:49:ASP:N        | 2.26                     | 0.51              |
| 1:A:1:FME:HE2        | 1:A:1:FME:HA        | 1.93                     | 0.51              |
| 22:A:614:EDO:H12     | 2:B:58:ALA:HB3      | 1.93                     | 0.51              |
| 7:G:5:LYS:HB3        | 1:N:278[B]:MET:SD   | 2.51                     | 0.51              |
| 1:A:381[B]:LEU:HB2   | 14:A:602:HEA:HAC    | 1.93                     | 0.51              |
| 4:Q:101:HIS:HB2      | 18:Q:201:DMU:O49    | 2.10                     | 0.51              |
| 13:Z:28:LEU:HD23     | 18:Z:101:DMU:H7     | 1.93                     | 0.51              |
| 8:H:61:LYS:NZ        | 29:H:202:HOH:O      | 2.43                     | 0.51              |
| 3:P:224:LYS:HD3      | 25:P:306:CDL:HB31   | 1.92                     | 0.51              |
| 1:A:486[B]:ASP:OD1   | 4:D:19:ARG:HD2      | 2.11                     | 0.51              |
| 3:P:3:HIS:HA         | 29:P:502:HOH:O      | 2.11                     | 0.51              |
| 3:C:224:LYS:HD2      | 25:C:307:CDL:HB31   | 1.93                     | 0.50              |
| 21:A:610:TGL:H283    | 21:A:610:TGL:H101   | 1.93                     | 0.50              |
| 1:N:112:LEU:HD23     | 1:N:112:LEU:C       | 2.37                     | 0.50              |
| 1:N:337:ALA:HB2      | 1:N:394[A]:VAL:HG23 | 1.91                     | 0.50              |
| 6:F:96:LEU:C         | 6:F:98:HIS:H        | 2.20                     | 0.50              |
| 9:I:42:LYS:NZ        | 29:I:104:HOH:O      | 2.44                     | 0.50              |
| 1:N:107:PRO:HB3      | 3:P:25:LEU:HB2      | 1.92                     | 0.50              |
| 1:N:505:PHE:H        | 22:N:612:EDO:C2     | 2.24                     | 0.50              |
| 19:C:310:PGV:H161    | 19:C:310:PGV:H12    | 1.93                     | 0.50              |
| 14:N:601[B]:HEA:H122 | 29:N:854:HOH:O      | 2.10                     | 0.50              |
| 1:A:229:ILE:HD11     | 2:B:175:ILE:HD13    | 1.93                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:A:449[A]:MET:SD  | 2:B:5:MET:HG2       | 2.51                     | 0.50              |
| 3:C:226:HIS:CE1    | 25:C:307:CDL:HB32   | 2.46                     | 0.50              |
| 1:N:164:PHE:HE2    | 22:N:622:EDO:H22    | 1.77                     | 0.50              |
| 1:N:377:PHE:HA     | 1:N:380[B]:VAL:HG12 | 1.93                     | 0.50              |
| 3:P:135:SER:HB3    | 25:T:102:CDL:H562   | 1.94                     | 0.50              |
| 2:B:132:GLU:HB3    | 2:B:137:GLU:HG3     | 1.93                     | 0.50              |
| 1:N:379:TYR:O      | 1:N:383[B]:MET:HB2  | 2.11                     | 0.50              |
| 2:O:66[A]:THR:HG22 | 2:O:67:ILE:HD13     | 1.93                     | 0.50              |
| 1:N:169:ILE:HG13   | 1:N:189[A]:MET:HE1  | 1.93                     | 0.50              |
| 1:N:208:MET:HE2    | 3:P:97:PHE:CD1      | 2.46                     | 0.50              |
| 1:N:265:LYS:HB2    | 1:N:490:THR:HG21    | 1.94                     | 0.50              |
| 7:G:84:LYS:H       | 7:G:84:LYS:HE2      | 1.77                     | 0.49              |
| 3:C:224:LYS:NZ     | 25:C:307:CDL:H112   | 2.27                     | 0.49              |
| 25:T:102:CDL:H581  | 25:T:102:CDL:H772   | 1.92                     | 0.49              |
| 1:A:113:LEU:HD12   | 21:L:103:TGL:H141   | 1.94                     | 0.49              |
| 11:K:20:SER:HA     | 18:K:103:DMU:H7     | 1.93                     | 0.49              |
| 1:A:208[B]:MET:HG2 | 1:A:219:PHE:CE2     | 2.48                     | 0.49              |
| 4:Q:13:LEU:C       | 22:Q:204:EDO:H21    | 2.38                     | 0.49              |
| 3:C:84:ILE:HG21    | 26:C:308:PEK:H222   | 1.94                     | 0.49              |
| 2:O:41:ILE:O       | 2:O:45:MET:HG2      | 2.13                     | 0.49              |
| 25:G:102:CDL:C79   | 25:G:102:CDL:H571   | 2.42                     | 0.49              |
| 2:O:22[B]:HIS:HE1  | 9:V:44:LYS:HE2      | 1.75                     | 0.49              |
| 2:O:114:GLU:HG3    | 2:O:227:LEU:HD21    | 1.95                     | 0.49              |
| 3:P:80:ARG:HH21    | 22:P:316:EDO:H21    | 1.78                     | 0.49              |
| 1:A:278[B]:MET:CE  | 7:T:5:LYS:HB3       | 2.43                     | 0.49              |
| 7:G:7:ASP:OD1      | 7:G:8:HIS:N         | 2.45                     | 0.49              |
| 3:P:62:ILE:HD12    | 25:P:306:CDL:H511   | 1.94                     | 0.49              |
| 4:Q:56:LYS:NZ      | 22:Q:203:EDO:O1     | 2.46                     | 0.49              |
| 6:F:94:HIS:HB2     | 6:F:98:HIS:CD2      | 2.48                     | 0.48              |
| 3:C:240:TRP:CE2    | 26:C:308:PEK:H31    | 2.48                     | 0.48              |
| 2:O:104:TRP:CG     | 2:O:203:ASN:HB2     | 2.48                     | 0.48              |
| 20:A:609:PSC:H252  | 2:B:56:MET:SD       | 2.54                     | 0.48              |
| 6:F:92:VAL:HG23    | 6:F:92:VAL:O        | 2.14                     | 0.48              |
| 1:N:334:TRP:CZ3    | 21:Q:202:TGL:HA51   | 2.49                     | 0.48              |
| 12:Y:35:ALA:HB3    | 12:Y:36:PRO:HD3     | 1.95                     | 0.48              |
| 20:A:609:PSC:H42   | 29:I:128:HOH:O      | 2.14                     | 0.48              |
| 3:C:3:HIS:HB2      | 29:C:520:HOH:O      | 2.13                     | 0.48              |
| 3:C:180[B]:GLU:HG3 | 29:C:467:HOH:O      | 2.13                     | 0.48              |
| 20:A:609:PSC:H052  | 5:E:41:LEU:CD2      | 2.44                     | 0.48              |
| 25:G:102:CDL:H512  | 25:G:102:CDL:C18    | 2.24                     | 0.48              |
| 26:P:307:PEK:H383  | 19:P:310:PGV:H332   | 1.95                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:Q:205:EDO:H21   | 29:R:242:HOH:O    | 2.12                     | 0.48              |
| 7:T:59:PRO:O       | 22:T:105:EDO:H22  | 2.13                     | 0.48              |
| 19:A:607:PGV:H321  | 19:A:607:PGV:C15  | 2.44                     | 0.48              |
| 1:N:296:GLY:HA2    | 8:U:23:GLN:OE1    | 2.12                     | 0.48              |
| 5:R:11:PHE:CD1     | 20:V:101:PSC:H081 | 2.49                     | 0.48              |
| 20:A:609:PSC:O02   | 29:A:704:HOH:O    | 2.20                     | 0.48              |
| 22:A:611:EDO:C2    | 12:L:10:ASN:HB2   | 2.44                     | 0.48              |
| 3:C:226:HIS:HE1    | 25:C:307:CDL:HB32 | 1.79                     | 0.48              |
| 1:N:334:TRP:CE3    | 21:Q:202:TGL:HA51 | 2.49                     | 0.48              |
| 2:O:116:LEU:HD13   | 2:O:226:MET:HG2   | 1.95                     | 0.48              |
| 1:N:381[B]:LEU:HB2 | 14:N:602:HEA:HAC  | 1.96                     | 0.47              |
| 2:O:83:ILE:O       | 2:O:87[A]:MET:HG3 | 2.14                     | 0.47              |
| 25:T:102:CDL:H341  | 25:T:102:CDL:H121 | 1.96                     | 0.47              |
| 2:O:128:LEU:HD11   | 2:O:134:ARG:HA    | 1.97                     | 0.47              |
| 7:G:7:ASP:OD2      | 1:N:179:TYR:OH    | 2.28                     | 0.47              |
| 1:N:483:LEU:HD11   | 4:Q:5:VAL:O       | 2.14                     | 0.47              |
| 22:N:617:EDO:H12   | 6:S:36:PRO:HD3    | 1.96                     | 0.47              |
| 5:R:80:GLU:H       | 5:R:80:GLU:CD     | 2.21                     | 0.47              |
| 1:A:285:PHE:CE2    | 7:T:4:ALA:HB2     | 2.50                     | 0.47              |
| 6:F:94:HIS:CD2     | 6:F:98:HIS:HB2    | 2.50                     | 0.47              |
| 19:N:606:PGV:H142  | 19:N:606:PGV:H312 | 1.97                     | 0.47              |
| 1:A:107:PRO:HB3    | 3:C:25:LEU:HB2    | 1.95                     | 0.47              |
| 14:N:602:HEA:H243  | 2:O:69:PRO:HB3    | 1.94                     | 0.47              |
| 12:Y:20:ARG:HH21   | 12:Y:24:MET:HG3   | 1.78                     | 0.47              |
| 18:C:302:DMU:O6    | 29:C:402:HOH:O    | 2.20                     | 0.47              |
| 26:C:309:PEK:H101  | 26:C:309:PEK:H71  | 1.42                     | 0.47              |
| 3:P:99:TRP:CD1     | 19:P:310:PGV:H211 | 2.50                     | 0.47              |
| 18:P:303:DMU:H23   | 10:W:41:GLY:HA3   | 1.96                     | 0.47              |
| 9:V:61:GLU:OE1     | 9:V:64:ARG:NE     | 2.34                     | 0.47              |
| 24:Y:102:CHD:H112  | 24:Y:102:CHD:H12A | 1.69                     | 0.47              |
| 4:D:11:TYR:O       | 22:D:203:EDO:H21  | 2.15                     | 0.47              |
| 2:O:65[B]:TRP:HE1  | 20:V:101:PSC:H112 | 1.79                     | 0.47              |
| 4:Q:78:TRP:HA      | 21:Q:202:TGL:HB22 | 1.96                     | 0.47              |
| 20:A:609:PSC:H052  | 5:E:41:LEU:HD23   | 1.96                     | 0.47              |
| 3:C:257:TYR:O      | 3:C:261:SER:HB3   | 2.14                     | 0.47              |
| 21:L:103:TGL:H262  | 21:L:103:TGL:H231 | 1.74                     | 0.47              |
| 2:O:5:MET:HE2      | 2:O:5:MET:HB3     | 1.70                     | 0.47              |
| 25:T:102:CDL:H581  | 25:T:102:CDL:C77  | 2.44                     | 0.47              |
| 12:L:13:PHE:C      | 22:L:104:EDO:H22  | 2.40                     | 0.47              |
| 22:P:313:EDO:H12   | 10:W:13:GLN:HG2   | 1.96                     | 0.47              |
| 1:A:30:GLY:HA3     | 1:A:65[B]:MET:SD  | 2.55                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:A:169[A]:ILE:HG12 | 1:A:189[A]:MET:HE1  | 1.97                     | 0.46              |
| 25:T:102:CDL:OB3    | 25:T:102:CDL:H142   | 2.14                     | 0.46              |
| 1:A:342:LEU:HB2     | 21:D:202:TGL:HA92   | 1.97                     | 0.46              |
| 11:K:20:SER:OG      | 18:K:103:DMU:O49    | 2.02                     | 0.46              |
| 1:A:307:SER:HB3     | 25:T:102:CDL:H182   | 1.97                     | 0.46              |
| 3:C:99:TRP:CD1      | 19:T:104:PGV:H221   | 2.50                     | 0.46              |
| 24:G:101:CHD:H212   | 24:G:101:CHD:H12    | 1.97                     | 0.46              |
| 21:N:608:TGL:H121   | 21:N:608:TGL:CA7    | 2.44                     | 0.46              |
| 29:N:801:HOH:O      | 22:U:102:EDO:H11    | 2.14                     | 0.46              |
| 1:A:486[B]:ASP:CG   | 4:D:19:ARG:HD2      | 2.40                     | 0.46              |
| 20:A:609:PSC:H083   | 5:E:11:PHE:CG       | 2.51                     | 0.46              |
| 6:F:70:ILE:HG13     | 6:F:84:SER:HB3      | 1.97                     | 0.46              |
| 22:N:618:EDO:H21    | 29:N:810:HOH:O      | 2.15                     | 0.46              |
| 21:Y:103:TGL:HA91   | 21:Y:103:TGL:H222   | 1.52                     | 0.46              |
| 11:K:7:PRO:HD2      | 29:K:210:HOH:O      | 2.16                     | 0.46              |
| 20:A:609:PSC:H22    | 20:A:609:PSC:C23    | 2.45                     | 0.46              |
| 21:L:103:TGL:H362   | 21:L:103:TGL:C32    | 2.45                     | 0.46              |
| 4:Q:19:ARG:HG2      | 4:Q:21:ASP:OD1      | 2.15                     | 0.46              |
| 21:L:103:TGL:HA92   | 21:L:103:TGL:H221   | 1.30                     | 0.46              |
| 1:A:513:LEU:O       | 1:A:514:LYS:HB2     | 2.16                     | 0.46              |
| 22:F:109:EDO:H22    | 29:F:279:HOH:O      | 2.16                     | 0.46              |
| 8:H:24:ASN:HD21     | 22:H:102:EDO:C2     | 2.29                     | 0.46              |
| 12:L:45:LEU:HD23    | 12:L:45:LEU:HA      | 1.82                     | 0.46              |
| 1:N:298[B]:ASP:OD1  | 29:N:702:HOH:O      | 2.21                     | 0.46              |
| 2:O:130:PRO:HA      | 4:Q:115:TRP:CH2     | 2.51                     | 0.46              |
| 1:A:302[B]:ARG:HH21 | 2:B:84:LEU:CD1      | 2.29                     | 0.46              |
| 2:O:130:PRO:HA      | 4:Q:115:TRP:CZ3     | 2.51                     | 0.46              |
| 12:L:20:ARG:HH22    | 21:L:103:TGL:HC72   | 1.80                     | 0.45              |
| 21:Q:202:TGL:H362   | 9:V:20:HIS:CE1      | 2.51                     | 0.45              |
| 26:C:308:PEK:C36    | 25:T:102:CDL:H871   | 2.38                     | 0.45              |
| 12:L:41:ARG:HH22    | 18:L:101:DMU:H30    | 1.81                     | 0.45              |
| 1:N:348:PHE:CE1     | 1:N:380[B]:VAL:HG22 | 2.51                     | 0.45              |
| 21:A:610:TGL:H282   | 21:A:610:TGL:H251   | 1.62                     | 0.45              |
| 18:P:303:DMU:H19    | 18:P:303:DMU:H25    | 1.69                     | 0.45              |
| 25:P:306:CDL:H612   | 19:P:309:PGV:H131   | 1.99                     | 0.45              |
| 4:Q:9:GLU:O         | 4:Q:11:TYR:N        | 2.49                     | 0.45              |
| 1:N:112:LEU:HG      | 29:N:919:HOH:O      | 2.16                     | 0.45              |
| 3:P:50:ASN:ND2      | 3:P:54:MET:HE2      | 2.30                     | 0.45              |
| 1:A:468:MET:HG3     | 22:A:617:EDO:C2     | 2.44                     | 0.45              |
| 18:A:606:DMU:H6     | 11:K:30:VAL:HG21    | 1.98                     | 0.45              |
| 5:E:12:ASP:OD2      | 5:E:44:GLU:HG3      | 2.16                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:G:1:ALA:N        | 19:P:310:PGV:H262   | 2.32                     | 0.45              |
| 2:B:82:ARG:NH1     | 2:B:86:MET:HE1      | 2.31                     | 0.45              |
| 3:C:51[B]:MET:HE1  | 25:C:307:CDL:C27    | 2.47                     | 0.45              |
| 26:F:102:PEK:H372  | 25:G:102:CDL:H262   | 1.57                     | 0.45              |
| 1:N:505:PHE:H      | 22:N:612:EDO:H22    | 1.81                     | 0.45              |
| 29:O:482:HOH:O     | 21:Q:202:TGL:H331   | 2.16                     | 0.45              |
| 8:U:60:TYR:CD1     | 8:U:60:TYR:C        | 2.95                     | 0.45              |
| 10:W:52:TRP:CZ2    | 18:W:101:DMU:H4     | 2.51                     | 0.45              |
| 26:C:309:PEK:H71   | 26:C:309:PEK:H42    | 1.74                     | 0.45              |
| 8:H:9:LYS:HA       | 8:H:9:LYS:HD3       | 1.53                     | 0.45              |
| 7:G:4:ALA:HB2      | 1:N:285:PHE:CE2     | 2.51                     | 0.45              |
| 1:N:486:ASP:OD2    | 4:Q:19:ARG:HD2      | 2.16                     | 0.45              |
| 8:U:43:MET:HE3     | 8:U:49:ASP:H        | 1.80                     | 0.45              |
| 4:Q:78:TRP:HB3     | 21:Q:202:TGL:HB22   | 1.99                     | 0.45              |
| 5:R:95:GLU:HG2     | 5:R:96:LEU:HD23     | 1.99                     | 0.45              |
| 22:A:615:EDO:H22   | 2:B:133:LEU:HD22    | 1.98                     | 0.45              |
| 12:L:35:ALA:HB3    | 12:L:36:PRO:HD3     | 1.98                     | 0.45              |
| 24:P:304:CHD:C24   | 19:P:310:PGV:H011   | 2.47                     | 0.45              |
| 24:T:101:CHD:H12   | 24:T:101:CHD:H212   | 1.99                     | 0.45              |
| 3:P:127:LEU:HD22   | 25:T:102:CDL:HB61   | 1.99                     | 0.44              |
| 4:Q:114:GLU:HG3    | 11:X:51:LYS:HE2     | 1.98                     | 0.44              |
| 13:Z:37:LEU:HD23   | 13:Z:37:LEU:HA      | 1.83                     | 0.44              |
| 1:A:512[B]:ASN:ND2 | 6:F:36:PRO:HB2      | 2.32                     | 0.44              |
| 29:A:703:HOH:O     | 2:B:52:HIS:HD2      | 2.00                     | 0.44              |
| 2:B:164:ALA:O      | 2:B:194:GLY:HA3     | 2.16                     | 0.44              |
| 25:G:102:CDL:H801  | 25:G:102:CDL:H832   | 1.64                     | 0.44              |
| 1:N:377:PHE:HA     | 1:N:380[A]:VAL:HG22 | 1.98                     | 0.44              |
| 10:W:52:TRP:CE2    | 18:W:101:DMU:H4     | 2.53                     | 0.44              |
| 1:A:168:ILE:CG2    | 1:A:189[A]:MET:HE2  | 2.48                     | 0.44              |
| 2:B:54:SER:CB      | 22:E:203:EDO:H11    | 2.47                     | 0.44              |
| 1:N:377:PHE:O      | 1:N:381[B]:LEU:HB3  | 2.16                     | 0.44              |
| 2:O:52:HIS:HD2     | 29:R:247:HOH:O      | 2.00                     | 0.44              |
| 3:P:116:TRP:HA     | 3:P:117:PRO:C       | 2.42                     | 0.44              |
| 22:U:102:EDO:H22   | 29:U:227:HOH:O      | 2.15                     | 0.44              |
| 7:G:84:LYS:H       | 7:G:84:LYS:CE       | 2.30                     | 0.44              |
| 26:T:103:PEK:H5    | 26:T:103:PEK:H221   | 1.98                     | 0.44              |
| 22:A:616:EDO:H12   | 6:F:70:ILE:HD12     | 1.99                     | 0.44              |
| 6:F:28:GLN:O       | 22:F:108:EDO:O1     | 2.31                     | 0.44              |
| 10:J:4:ARG:HD3     | 29:J:222:HOH:O      | 2.16                     | 0.44              |
| 2:O:91:ASN:HB2     | 2:O:149:THR:HG21    | 1.98                     | 0.44              |
| 2:O:215:PRO:HD3    | 9:V:60:PHE:CD1      | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:V:101:PSC:C12   | 20:V:101:PSC:H343  | 2.47                     | 0.44              |
| 1:A:76:GLY:O       | 1:A:80:ASN:HB2     | 2.18                     | 0.44              |
| 25:C:307:CDL:H251  | 25:C:307:CDL:H222  | 1.53                     | 0.44              |
| 1:N:409:TRP:CZ2    | 19:N:606:PGV:H61   | 2.53                     | 0.44              |
| 2:O:26:HIS:HE1     | 18:O:302:DMU:H9    | 1.82                     | 0.44              |
| 2:B:67:ILE:HD11    | 29:T:268:HOH:O     | 2.17                     | 0.44              |
| 12:L:24:MET:HG3    | 29:L:225:HOH:O     | 2.17                     | 0.44              |
| 25:T:102:CDL:H321  | 29:T:257:HOH:O     | 2.18                     | 0.44              |
| 3:C:180[B]:GLU:HG2 | 29:C:422:HOH:O     | 2.18                     | 0.44              |
| 3:C:224:LYS:HD3    | 25:C:307:CDL:HB31  | 1.99                     | 0.44              |
| 25:G:102:CDL:H392  | 25:G:102:CDL:H122  | 1.99                     | 0.44              |
| 25:G:102:CDL:H422  | 25:G:102:CDL:H451  | 1.66                     | 0.44              |
| 1:A:265:LYS:HB2    | 1:A:490:THR:HG21   | 1.99                     | 0.44              |
| 1:A:306:THR:O      | 1:A:310[B]:MET:HG2 | 2.18                     | 0.44              |
| 21:L:103:TGL:HC22  | 21:L:103:TGL:HC52  | 1.68                     | 0.44              |
| 1:N:28:MET:HE3     | 12:Y:29:PHE:CD1    | 2.52                     | 0.44              |
| 3:C:210:ILE:HD13   | 19:C:310:PGV:H302  | 2.00                     | 0.43              |
| 1:N:240:HIS:O      | 1:N:241:PRO:C      | 2.60                     | 0.43              |
| 3:P:99:TRP:CE2     | 19:P:310:PGV:H231  | 2.53                     | 0.43              |
| 3:P:107:ALA:HB2    | 19:P:310:PGV:H031  | 1.99                     | 0.43              |
| 1:A:439:ARG:HD3    | 2:B:199:ILE:HB     | 1.99                     | 0.43              |
| 1:A:510:TYR:CZ     | 1:A:512[B]:ASN:ND2 | 2.87                     | 0.43              |
| 4:D:125:ASP:OD1    | 22:D:205:EDO:O2    | 2.36                     | 0.43              |
| 1:N:378:HIS:O      | 1:N:382[B]:SER:HB2 | 2.17                     | 0.43              |
| 3:P:47:LEU:O       | 3:P:51:MET:HG2     | 2.17                     | 0.43              |
| 18:X:102:DMU:H16   | 18:X:102:DMU:H11   | 1.78                     | 0.43              |
| 1:A:296:GLY:HA2    | 8:H:23:GLN:OE1     | 2.18                     | 0.43              |
| 9:I:18:ARG:HD3     | 29:I:148:HOH:O     | 2.18                     | 0.43              |
| 1:N:46:THR:HG22    | 1:N:49[B]:GLY:H    | 1.82                     | 0.43              |
| 19:N:607:PGV:H343  | 26:P:308:PEK:H381  | 2.00                     | 0.43              |
| 5:R:105:GLY:O      | 5:R:108:LYS:HG2    | 2.18                     | 0.43              |
| 14:A:602:HEA:H243  | 2:B:69:PRO:HB3     | 2.00                     | 0.43              |
| 24:C:306:CHD:H12A  | 24:C:306:CHD:H112  | 1.70                     | 0.43              |
| 1:A:343:GLY:HA2    | 21:D:202:TGL:H201  | 2.01                     | 0.43              |
| 18:A:606:DMU:H11   | 11:K:26:VAL:HG13   | 2.01                     | 0.43              |
| 29:A:868:HOH:O     | 21:D:202:TGL:HC32  | 2.18                     | 0.43              |
| 3:C:12:ASN:HD21    | 22:C:311:EDO:H12   | 1.83                     | 0.43              |
| 8:H:9:LYS:O        | 8:H:10:ASN:HB2     | 2.19                     | 0.43              |
| 2:O:4:PRO:HB2      | 11:X:43:SER:HA     | 2.01                     | 0.43              |
| 25:P:306:CDL:H121  | 29:P:519:HOH:O     | 2.18                     | 0.43              |
| 8:U:9:LYS:O        | 8:U:10:ASN:HB2     | 2.18                     | 0.43              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 1:N:243:VAL:HB       | 14:N:602:HEA:CAC   | 2.49                     | 0.43              |
| 22:N:623:EDO:H11     | 29:N:876:HOH:O     | 2.18                     | 0.43              |
| 3:P:146:TRP:CD2      | 3:P:162:ALA:HB2    | 2.54                     | 0.43              |
| 6:S:92:VAL:O         | 6:S:92:VAL:HG23    | 2.18                     | 0.43              |
| 25:T:102:CDL:H572    | 25:T:102:CDL:H752  | 2.01                     | 0.43              |
| 25:T:102:CDL:H801    | 25:T:102:CDL:H832  | 1.36                     | 0.43              |
| 22:B:305:EDO:H11     | 29:B:406:HOH:O     | 2.17                     | 0.43              |
| 8:H:52:VAL:O         | 8:U:46:LYS:HD3     | 2.18                     | 0.43              |
| 1:N:334:TRP:CH2      | 2:O:46:LEU:HD13    | 2.54                     | 0.43              |
| 2:O:26:HIS:CE1       | 18:O:302:DMU:H9    | 2.54                     | 0.43              |
| 2:O:206:PHE:CE1      | 22:O:304:EDO:H21   | 2.53                     | 0.43              |
| 1:A:40:GLU:HG2       | 1:A:54[B]:TYR:CD1  | 2.54                     | 0.43              |
| 7:G:1:ALA:H2         | 19:P:310:PGV:H262  | 1.84                     | 0.43              |
| 25:G:102:CDL:H511    | 25:G:102:CDL:H542  | 1.73                     | 0.43              |
| 3:C:33:MET:HE1       | 10:J:45:TYR:OH     | 2.19                     | 0.43              |
| 12:L:20:ARG:HH21     | 21:L:103:TGL:CC5   | 2.11                     | 0.43              |
| 9:V:10:ARG:HH21      | 20:V:101:PSC:H081  | 1.84                     | 0.43              |
| 25:P:306:CDL:H852    | 25:P:306:CDL:H822  | 1.87                     | 0.42              |
| 7:T:42:ARG:NH2       | 29:T:208:HOH:O     | 2.52                     | 0.42              |
| 3:C:51[A]:MET:SD     | 25:C:307:CDL:H622  | 2.59                     | 0.42              |
| 25:C:307:CDL:HB21    | 10:J:8:LYS:CE      | 2.49                     | 0.42              |
| 4:D:118:LYS:NZ       | 22:D:206:EDO:O2    | 2.49                     | 0.42              |
| 5:R:11:PHE:CG        | 20:V:101:PSC:H081  | 2.54                     | 0.42              |
| 10:J:52:TRP:CE2      | 18:J:101:DMU:H4    | 2.54                     | 0.42              |
| 3:P:220:PHE:HB2      | 25:P:306:CDL:H712  | 2.01                     | 0.42              |
| 14:A:601[B]:HEA:H122 | 29:A:819:HOH:O     | 2.18                     | 0.42              |
| 12:L:2:HIS:CG        | 12:L:3:TYR:H       | 2.37                     | 0.42              |
| 3:C:47:LEU:O         | 3:C:51[B]:MET:HG3  | 2.18                     | 0.42              |
| 3:C:125:ASN:HB2      | 7:G:42:ARG:NH2     | 2.33                     | 0.42              |
| 1:N:289:ALA:HB1      | 1:N:297[A]:MET:HE1 | 2.00                     | 0.42              |
| 2:B:1:FME:HE2        | 2:B:1:FME:HB3      | 1.58                     | 0.42              |
| 2:B:16:ILE:HD13      | 2:B:16:ILE:HA      | 1.85                     | 0.42              |
| 19:A:607:PGV:H311    | 13:M:19:LEU:HD23   | 2.00                     | 0.42              |
| 2:B:54:SER:HB2       | 22:E:203:EDO:H11   | 2.02                     | 0.42              |
| 1:N:236:TRP:CH2      | 14:N:602:HEA:HBD1  | 2.54                     | 0.42              |
| 5:R:82:TYR:HB3       | 5:R:83:PRO:HD3     | 2.01                     | 0.42              |
| 25:T:102:CDL:H622    | 25:T:102:CDL:H651  | 1.73                     | 0.42              |
| 20:A:609:PSC:H342    | 2:B:41:ILE:HD13    | 2.01                     | 0.42              |
| 4:Q:78:TRP:CB        | 21:Q:202:TGL:HB22  | 2.50                     | 0.42              |
| 4:D:126:MET:HG3      | 4:D:128:VAL:HG23   | 2.00                     | 0.42              |
| 2:O:16:ILE:HD12      | 2:O:16:ILE:HG23    | 1.83                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:B:69:PRO:HG2      | 29:B:429:HOH:O      | 2.19                     | 0.42              |
| 5:E:43:PRO:HB2      | 5:E:48:ILE:HD11     | 2.02                     | 0.42              |
| 11:K:23:THR:HB      | 18:K:103:DMU:H6     | 2.02                     | 0.42              |
| 1:N:376:HIS:CE1     | 1:N:380[B]:VAL:HG11 | 2.55                     | 0.42              |
| 2:O:114:GLU:HG3     | 2:O:227:LEU:CD2     | 2.50                     | 0.42              |
| 4:Q:109:HIS:HE1     | 4:Q:115:TRP:CZ3     | 2.37                     | 0.42              |
| 25:G:102:CDL:H761   | 1:N:282:PHE:HZ      | 1.85                     | 0.41              |
| 1:N:242:GLU:HA      | 1:N:245:ILE:HD12    | 2.01                     | 0.41              |
| 19:N:607:PGV:H262   | 19:P:309:PGV:H292   | 2.01                     | 0.41              |
| 3:P:38:ASN:O        | 18:P:303:DMU:H35    | 2.20                     | 0.41              |
| 3:P:161:GLN:HE22    | 26:T:103:PEK:H22    | 1.85                     | 0.41              |
| 4:Q:114:GLU:CD      | 11:X:51:LYS:HE2     | 2.45                     | 0.41              |
| 1:A:280:ILE:HG23    | 1:A:312[B]:ILE:HD11 | 2.01                     | 0.41              |
| 3:C:47:LEU:O        | 3:C:51[A]:MET:HG2   | 2.20                     | 0.41              |
| 26:C:309:PEK:H161   | 26:C:309:PEK:H132   | 1.79                     | 0.41              |
| 1:N:290:HIS:CD2     | 1:N:291:HIS:CD2     | 3.08                     | 0.41              |
| 26:C:308:PEK:H321   | 7:T:5:LYS:HB2       | 2.02                     | 0.41              |
| 26:F:102:PEK:H222   | 7:G:21:PHE:CD1      | 2.55                     | 0.41              |
| 2:O:41:ILE:HD13     | 20:V:101:PSC:H342   | 2.03                     | 0.41              |
| 3:P:207:HIS:HD2     | 3:P:241:TYR:OH      | 2.03                     | 0.41              |
| 6:S:94:HIS:HB2      | 29:S:214:HOH:O      | 2.19                     | 0.41              |
| 7:T:38:HIS:ND1      | 7:T:38:HIS:N        | 2.67                     | 0.41              |
| 4:D:31:LYS:NZ       | 29:D:303:HOH:O      | 2.37                     | 0.41              |
| 25:G:102:CDL:H221   | 25:G:102:CDL:C55    | 2.27                     | 0.41              |
| 22:N:613:EDO:H12    | 6:S:70:ILE:HD12     | 2.02                     | 0.41              |
| 1:A:334:TRP:CE3     | 21:D:202:TGL:HA32   | 2.56                     | 0.41              |
| 1:A:411:LYS:NZ      | 29:A:713:HOH:O      | 2.54                     | 0.41              |
| 1:A:513:LEU:HD23    | 1:A:513:LEU:HA      | 1.50                     | 0.41              |
| 21:L:103:TGL:H291   | 21:L:103:TGL:H122   | 1.81                     | 0.41              |
| 1:N:390:MET:HE2     | 1:N:413:HIS:CE1     | 2.52                     | 0.41              |
| 24:P:305:CHD:H183   | 24:P:305:CHD:H212   | 2.03                     | 0.41              |
| 1:A:512[B]:ASN:HD22 | 6:F:36:PRO:HB2      | 1.85                     | 0.41              |
| 2:B:19:GLU:OE1      | 2:B:82:ARG:NH2      | 2.54                     | 0.41              |
| 25:C:307:CDL:HB21   | 10:J:8:LYS:HE3      | 2.02                     | 0.41              |
| 7:G:84:LYS:H        | 7:G:84:LYS:CD       | 2.32                     | 0.41              |
| 1:N:240:HIS:CD2     | 1:N:240:HIS:C       | 2.99                     | 0.41              |
| 19:N:606:PGV:H251   | 13:Z:12:PRO:HB3     | 2.03                     | 0.41              |
| 2:O:164:ALA:O       | 2:O:194:GLY:HA3     | 2.20                     | 0.41              |
| 19:A:607:PGV:H011   | 19:A:607:PGV:C3     | 2.51                     | 0.41              |
| 3:P:59:ARG:HA       | 25:P:306:CDL:H512   | 2.02                     | 0.41              |
| 1:A:54[B]:TYR:HB2   | 29:A:708:HOH:O      | 2.21                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:N:76:GLY:O       | 1:N:80:ASN:HB2    | 2.20                     | 0.41              |
| 2:O:116:LEU:CD1    | 2:O:226:MET:HG2   | 2.51                     | 0.41              |
| 4:Q:145:TRP:CG     | 11:X:46:GLY:H     | 2.39                     | 0.41              |
| 5:R:31:LYS:HE2     | 5:R:35:THR:OG1    | 2.20                     | 0.41              |
| 6:S:70:ILE:HG13    | 6:S:84:SER:HB2    | 2.03                     | 0.41              |
| 7:T:36[B]:TRP:CZ2  | 26:T:103:PEK:H201 | 2.55                     | 0.41              |
| 25:G:102:CDL:H311  | 25:G:102:CDL:H341 | 1.87                     | 0.41              |
| 12:L:14:SER:N      | 21:L:103:TGL:HC31 | 2.20                     | 0.41              |
| 3:P:80:ARG:HG2     | 3:P:233:PHE:CE1   | 2.56                     | 0.41              |
| 8:U:24:ASN:ND2     | 22:U:102:EDO:H21  | 2.10                     | 0.41              |
| 1:A:194:LEU:HD11   | 7:T:4:ALA:HB1     | 2.02                     | 0.40              |
| 19:A:608:PGV:H322  | 26:C:309:PEK:H382 | 2.02                     | 0.40              |
| 20:A:609:PSC:H042  | 20:A:609:PSC:H072 | 1.62                     | 0.40              |
| 2:B:13:THR:HB      | 2:B:168:LEU:HD23  | 2.03                     | 0.40              |
| 2:B:58:ALA:O       | 2:B:62:GLU:HG3    | 2.21                     | 0.40              |
| 2:B:60:GLU:CD      | 2:B:60:GLU:H      | 2.29                     | 0.40              |
| 24:C:306:CHD:H111  | 24:C:306:CHD:H193 | 1.76                     | 0.40              |
| 4:D:98:TRP:CE2     | 18:M:101:DMU:H10  | 2.56                     | 0.40              |
| 10:J:36:MET:HG2    | 24:J:102:CHD:H221 | 2.04                     | 0.40              |
| 25:T:102:CDL:H581  | 25:T:102:CDL:H781 | 2.03                     | 0.40              |
| 2:B:66[A]:THR:CG2  | 26:T:103:PEK:H312 | 2.52                     | 0.40              |
| 3:C:51[A]:MET:HE1  | 19:C:310:PGV:C16  | 2.49                     | 0.40              |
| 11:K:54:ARG:HE     | 11:K:54:ARG:HB3   | 1.63                     | 0.40              |
| 1:N:53[B]:ILE:HD12 | 12:Y:44:LEU:CD2   | 2.51                     | 0.40              |
| 1:N:439:ARG:HD3    | 2:O:199:ILE:HB    | 2.03                     | 0.40              |
| 1:N:440:TYR:OH     | 2:O:195:GLN:HB3   | 2.22                     | 0.40              |
| 4:Q:7:LYS:HB3      | 4:Q:8:SER:H       | 1.63                     | 0.40              |
| 25:T:102:CDL:H151  | 25:T:102:CDL:H181 | 1.23                     | 0.40              |
| 12:Y:14:SER:O      | 12:Y:20:ARG:NH1   | 2.53                     | 0.40              |
| 20:A:609:PSC:H61   | 9:I:17:LEU:HD23   | 2.04                     | 0.40              |
| 1:N:136:LEU:HB2    | 29:N:909:HOH:O    | 2.21                     | 0.40              |
| 25:T:102:CDL:H751  | 25:T:102:CDL:H251 | 2.03                     | 0.40              |
| 3:C:55:TYR:OH      | 25:C:307:CDL:HA62 | 2.20                     | 0.40              |
| 3:C:154:GLY:HA2    | 6:F:6:VAL:HB      | 2.04                     | 0.40              |
| 6:F:96:LEU:HG      | 6:F:96:LEU:O      | 2.21                     | 0.40              |
| 3:P:67:PHE:HE2     | 25:P:306:CDL:H1   | 1.86                     | 0.40              |
| 24:P:305:CHD:H111  | 24:P:305:CHD:H182 | 1.86                     | 0.40              |
| 1:A:44:PRO:HG3     | 4:D:111:PHE:CZ    | 2.56                     | 0.40              |
| 29:B:552:HOH:O     | 21:D:202:TGL:HC81 | 2.22                     | 0.40              |
| 26:C:309:PEK:H182  | 26:C:309:PEK:H15  | 1.91                     | 0.40              |
| 6:F:65:ASP:OD2     | 6:S:1:ALA:N       | 2.53                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:G:102:CDL:OB3   | 25:G:102:CDL:H131  | 2.21                     | 0.40              |
| 1:N:117[A]:MET:HE3 | 1:N:117[A]:MET:HB3 | 2.00                     | 0.40              |
| 1:N:398:PRO:O      | 1:N:498:CYS:HB3    | 2.22                     | 0.40              |
| 1:N:505:PHE:CA     | 22:N:612:EDO:H22   | 2.50                     | 0.40              |
| 25:T:102:CDL:H432  | 25:T:102:CDL:H401  | 1.86                     | 0.40              |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 29:B:454:HOH:O | 29:D:303:HOH:O[2_584] | 2.03                     | 0.17              |
| 29:I:129:HOH:O | 29:V:201:HOH:O[3_647] | 2.03                     | 0.17              |
| 29:I:132:HOH:O | 29:M:226:HOH:O[2_584] | 2.09                     | 0.11              |
| 29:B:500:HOH:O | 29:D:437:HOH:O[2_584] | 2.15                     | 0.05              |

## 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     | 550/514 (107%) | 537 (98%)  | 13 (2%) | 0        | 100         | 100 |
| 1   | N     | 534/514 (104%) | 517 (97%)  | 15 (3%) | 2 (0%)   | 30          | 19  |
| 2   | B     | 229/227 (101%) | 220 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 2   | O     | 232/227 (102%) | 226 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 3   | C     | 262/259 (101%) | 256 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 3   | P     | 259/259 (100%) | 253 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 4   | D     | 143/144 (99%)  | 139 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 4   | Q     | 142/144 (99%)  | 135 (95%)  | 4 (3%)  | 3 (2%)   | 5           | 1   |
| 5   | E     | 103/105 (98%)  | 103 (100%) | 0       | 0        | 100         | 100 |
| 5   | R     | 103/105 (98%)  | 102 (99%)  | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|------------------|------------|---------|----------|-------------|-----|
| 6   | F     | 97/98 (99%)      | 95 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 6   | S     | 97/98 (99%)      | 93 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 7   | G     | 81/84 (96%)      | 71 (88%)   | 7 (9%)  | 3 (4%)   | 2           | 0   |
| 7   | T     | 82/84 (98%)      | 72 (88%)   | 6 (7%)  | 4 (5%)   | 1           | 0   |
| 8   | H     | 77/79 (98%)      | 74 (96%)   | 2 (3%)  | 1 (1%)   | 9           | 3   |
| 8   | U     | 77/79 (98%)      | 73 (95%)   | 2 (3%)  | 2 (3%)   | 4           | 0   |
| 9   | I     | 71/73 (97%)      | 69 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 9   | V     | 71/73 (97%)      | 70 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 10  | J     | 56/58 (97%)      | 56 (100%)  | 0       | 0        | 100         | 100 |
| 10  | W     | 56/58 (97%)      | 56 (100%)  | 0       | 0        | 100         | 100 |
| 11  | K     | 47/49 (96%)      | 47 (100%)  | 0       | 0        | 100         | 100 |
| 11  | X     | 47/49 (96%)      | 46 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 12  | L     | 44/46 (96%)      | 41 (93%)   | 3 (7%)  | 0        | 100         | 100 |
| 12  | Y     | 44/46 (96%)      | 42 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 13  | M     | 41/43 (95%)      | 40 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 13  | Z     | 41/43 (95%)      | 41 (100%)  | 0       | 0        | 100         | 100 |
| All | All   | 3586/3558 (101%) | 3474 (97%) | 97 (3%) | 15 (0%)  | 30          | 19  |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 7   | G     | 4      | ALA  |
| 7   | G     | 6      | GLY  |
| 4   | Q     | 9      | GLU  |
| 4   | Q     | 10     | ASP  |
| 4   | Q     | 11     | TYR  |
| 7   | T     | 6      | GLY  |
| 7   | G     | 5      | LYS  |
| 7   | T     | 2      | SER  |
| 7   | T     | 3      | ALA  |
| 7   | T     | 4      | ALA  |
| 8   | U     | 9      | LYS  |
| 1   | N     | 384[A] | GLY  |
| 1   | N     | 384[B] | GLY  |
| 8   | H     | 8      | ILE  |
| 8   | U     | 8      | ILE  |

### 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     | 461/426 (108%) | 457 (99%) | 4 (1%)   | 70          | 67  |
| 1   | N     | 445/426 (104%) | 441 (99%) | 4 (1%)   | 70          | 67  |
| 2   | B     | 214/210 (102%) | 204 (95%) | 10 (5%)  | 23          | 11  |
| 2   | O     | 217/210 (103%) | 206 (95%) | 11 (5%)  | 21          | 9   |
| 3   | C     | 229/224 (102%) | 225 (98%) | 4 (2%)   | 53          | 45  |
| 3   | P     | 226/224 (101%) | 222 (98%) | 4 (2%)   | 51          | 43  |
| 4   | D     | 129/128 (101%) | 127 (98%) | 2 (2%)   | 55          | 47  |
| 4   | Q     | 128/128 (100%) | 123 (96%) | 5 (4%)   | 28          | 16  |
| 5   | E     | 92/92 (100%)   | 91 (99%)  | 1 (1%)   | 65          | 60  |
| 5   | R     | 92/92 (100%)   | 91 (99%)  | 1 (1%)   | 65          | 60  |
| 6   | F     | 82/81 (101%)   | 79 (96%)  | 3 (4%)   | 30          | 18  |
| 6   | S     | 82/81 (101%)   | 79 (96%)  | 3 (4%)   | 30          | 18  |
| 7   | G     | 67/67 (100%)   | 62 (92%)  | 5 (8%)   | 12          | 4   |
| 7   | T     | 68/67 (102%)   | 63 (93%)  | 5 (7%)   | 13          | 4   |
| 8   | H     | 71/71 (100%)   | 68 (96%)  | 3 (4%)   | 26          | 14  |
| 8   | U     | 71/71 (100%)   | 68 (96%)  | 3 (4%)   | 26          | 14  |
| 9   | I     | 57/57 (100%)   | 55 (96%)  | 2 (4%)   | 32          | 19  |
| 9   | V     | 57/57 (100%)   | 55 (96%)  | 2 (4%)   | 32          | 19  |
| 10  | J     | 49/49 (100%)   | 49 (100%) | 0        | 100         | 100 |
| 10  | W     | 49/49 (100%)   | 47 (96%)  | 2 (4%)   | 27          | 15  |
| 11  | K     | 39/39 (100%)   | 39 (100%) | 0        | 100         | 100 |
| 11  | X     | 39/39 (100%)   | 39 (100%) | 0        | 100         | 100 |
| 12  | L     | 39/39 (100%)   | 38 (97%)  | 1 (3%)   | 40          | 28  |
| 12  | Y     | 39/39 (100%)   | 37 (95%)  | 2 (5%)   | 21          | 9   |
| 13  | M     | 37/37 (100%)   | 37 (100%) | 0        | 100         | 100 |
| 13  | Z     | 37/37 (100%)   | 36 (97%)  | 1 (3%)   | 39          | 27  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |
|-----|-------|------------------|------------|----------|-------------|
| All | All   | 3116/3040 (102%) | 3038 (98%) | 78 (2%)  | 43 30       |

All (78) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 138    | HIS  |
| 1   | A     | 369    | ASP  |
| 1   | A     | 394[A] | VAL  |
| 1   | A     | 394[B] | VAL  |
| 2   | B     | 33     | LEU  |
| 2   | B     | 60     | GLU  |
| 2   | B     | 66[A]  | THR  |
| 2   | B     | 66[B]  | THR  |
| 2   | B     | 78     | LEU  |
| 2   | B     | 86     | MET  |
| 2   | B     | 91     | ASN  |
| 2   | B     | 115    | ASP  |
| 2   | B     | 116    | LEU  |
| 2   | B     | 171    | LYS  |
| 3   | C     | 17     | PRO  |
| 3   | C     | 110    | PRO  |
| 3   | C     | 159    | MET  |
| 3   | C     | 230    | ASN  |
| 4   | D     | 7      | LYS  |
| 4   | D     | 147    | LYS  |
| 5   | E     | 90     | ARG  |
| 6   | F     | 63     | GLU  |
| 6   | F     | 80[A]  | GLN  |
| 6   | F     | 80[B]  | GLN  |
| 7   | G     | 2      | SER  |
| 7   | G     | 33     | LEU  |
| 7   | G     | 36     | TRP  |
| 7   | G     | 37     | LEU  |
| 7   | G     | 84     | LYS  |
| 8   | H     | 9      | LYS  |
| 8   | H     | 40     | GLU  |
| 8   | H     | 60     | TYR  |
| 9   | I     | 37     | PHE  |
| 9   | I     | 73     | LYS  |
| 12  | L     | 26     | THR  |
| 1   | N     | 112    | LEU  |
| 1   | N     | 128    | VAL  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | N     | 138   | HIS  |
| 1   | N     | 369   | ASP  |
| 2   | O     | 33    | LEU  |
| 2   | O     | 60    | GLU  |
| 2   | O     | 66[A] | THR  |
| 2   | O     | 66[B] | THR  |
| 2   | O     | 78    | LEU  |
| 2   | O     | 91    | ASN  |
| 2   | O     | 94    | SER  |
| 2   | O     | 115   | ASP  |
| 2   | O     | 144   | LEU  |
| 2   | O     | 217   | LYS  |
| 2   | O     | 226   | MET  |
| 3   | P     | 17    | PRO  |
| 3   | P     | 159   | MET  |
| 3   | P     | 180   | GLU  |
| 3   | P     | 230   | ASN  |
| 4   | Q     | 6     | VAL  |
| 4   | Q     | 7     | LYS  |
| 4   | Q     | 9     | GLU  |
| 4   | Q     | 19    | ARG  |
| 4   | Q     | 51    | LEU  |
| 5   | R     | 80    | GLU  |
| 6   | S     | 43    | LYS  |
| 6   | S     | 63    | GLU  |
| 6   | S     | 87    | THR  |
| 7   | T     | 2     | SER  |
| 7   | T     | 5     | LYS  |
| 7   | T     | 33    | LEU  |
| 7   | T     | 37    | LEU  |
| 7   | T     | 38    | HIS  |
| 8   | U     | 7     | LYS  |
| 8   | U     | 9     | LYS  |
| 8   | U     | 60    | TYR  |
| 9   | V     | 8     | GLN  |
| 9   | V     | 36    | LYS  |
| 10  | W     | 7     | GLU  |
| 10  | W     | 50    | LEU  |
| 12  | Y     | 20    | ARG  |
| 12  | Y     | 26    | THR  |
| 13  | Z     | 38    | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | GLN  |
| 1   | A     | 422 | ASN  |
| 2   | B     | 203 | ASN  |
| 3   | C     | 3   | HIS  |
| 3   | C     | 4   | GLN  |
| 3   | C     | 149 | HIS  |
| 4   | D     | 109 | HIS  |
| 4   | D     | 119 | GLN  |
| 6   | F     | 98  | HIS  |
| 7   | G     | 71  | HIS  |
| 8   | H     | 25  | GLN  |
| 8   | H     | 28  | ASN  |
| 8   | H     | 32  | ASN  |
| 1   | N     | 422 | ASN  |
| 3   | P     | 38  | ASN  |
| 3   | P     | 50  | ASN  |
| 4   | Q     | 101 | HIS  |
| 4   | Q     | 109 | HIS  |
| 7   | T     | 41  | HIS  |
| 8   | U     | 25  | GLN  |
| 8   | U     | 28  | ASN  |
| 8   | U     | 32  | ASN  |
| 9   | V     | 20  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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 |
| 9   | SAC  | I     | 1   | 9    | 7,8,9        | 0.64 | 0        | 8,9,11      | 0.96 | 0        |
| 2   | FME  | O     | 1   | 2    | 8,9,10       | 0.66 | 0        | 7,9,11      | 1.70 | 2 (28%)  |
| 7   | TPO  | T     | 11  | 7    | 8,10,11      | 1.34 | 1 (12%)  | 10,14,16    | 1.23 | 1 (10%)  |
| 7   | TPO  | G     | 11  | 7    | 8,10,11      | 1.33 | 1 (12%)  | 10,14,16    | 1.35 | 1 (10%)  |
| 1   | FME  | N     | 1   | 1    | 8,9,10       | 0.51 | 0        | 7,9,11      | 1.62 | 1 (14%)  |
| 9   | SAC  | V     | 1   | 9    | 7,8,9        | 0.58 | 0        | 8,9,11      | 0.61 | 0        |
| 1   | FME  | A     | 1   | 1    | 8,9,10       | 0.65 | 0        | 7,9,11      | 1.62 | 1 (14%)  |
| 2   | FME  | B     | 1   | 2    | 8,9,10       | 0.96 | 0        | 7,9,11      | 2.08 | 3 (42%)  |

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 |
|-----|------|-------|-----|------|---------|-----------|-------|
| 9   | SAC  | I     | 1   | 9    | -       | 3/7/8/10  | -     |
| 2   | FME  | O     | 1   | 2    | -       | 0/7/9/11  | -     |
| 7   | TPO  | T     | 11  | 7    | -       | 6/9/11/13 | -     |
| 7   | TPO  | G     | 11  | 7    | -       | 5/9/11/13 | -     |
| 1   | FME  | N     | 1   | 1    | -       | 4/7/9/11  | -     |
| 9   | SAC  | V     | 1   | 9    | -       | 4/7/8/10  | -     |
| 1   | FME  | A     | 1   | 1    | -       | 4/7/9/11  | -     |
| 2   | FME  | B     | 1   | 2    | -       | 1/7/9/11  | -     |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 7   | G     | 11  | TPO  | P-O1P | 2.94 | 1.60        | 1.50     |
| 7   | T     | 11  | TPO  | P-O1P | 2.73 | 1.59        | 1.50     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 1   | FME  | CG-CB-CA  | -3.56 | 103.07      | 112.95   |
| 2   | O     | 1   | FME  | CG-CB-CA  | -3.51 | 103.19      | 112.95   |
| 1   | N     | 1   | FME  | CE-SD-CG  | 3.25  | 111.55      | 100.40   |
| 7   | G     | 11  | TPO  | CG2-CB-CA | 3.09  | 119.27      | 113.16   |
| 1   | A     | 1   | FME  | CE-SD-CG  | 2.87  | 110.25      | 100.40   |
| 7   | T     | 11  | TPO  | CG2-CB-CA | 2.47  | 118.04      | 113.16   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 1   | FME  | O-C-CA   | -2.41 | 118.46      | 124.78   |
| 2   | O     | 1   | FME  | O-C-CA   | -2.30 | 118.76      | 124.78   |
| 2   | B     | 1   | FME  | CB-CG-SD | -2.04 | 102.53      | 113.48   |

There are no chirality outliers.

All (27) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | A     | 1   | FME  | N-CA-CB-CG   |
| 7   | G     | 11  | TPO  | N-CA-CB-CG2  |
| 7   | G     | 11  | TPO  | N-CA-CB-OG1  |
| 7   | G     | 11  | TPO  | C-CA-CB-CG2  |
| 7   | G     | 11  | TPO  | O-C-CA-CB    |
| 9   | I     | 1   | SAC  | O-C-CA-CB    |
| 1   | N     | 1   | FME  | O1-CN-N-CA   |
| 1   | N     | 1   | FME  | N-CA-CB-CG   |
| 1   | N     | 1   | FME  | C-CA-CB-CG   |
| 7   | T     | 11  | TPO  | N-CA-CB-CG2  |
| 7   | T     | 11  | TPO  | N-CA-CB-OG1  |
| 7   | T     | 11  | TPO  | C-CA-CB-CG2  |
| 7   | T     | 11  | TPO  | O-C-CA-CB    |
| 9   | V     | 1   | SAC  | C2A-C1A-N-CA |
| 9   | V     | 1   | SAC  | OAC-C1A-N-CA |
| 9   | V     | 1   | SAC  | C-CA-N-C1A   |
| 9   | V     | 1   | SAC  | O-C-CA-CB    |
| 1   | N     | 1   | FME  | CB-CG-SD-CE  |
| 9   | I     | 1   | SAC  | N-CA-CB-OG   |
| 1   | A     | 1   | FME  | O1-CN-N-CA   |
| 2   | B     | 1   | FME  | CB-CG-SD-CE  |
| 7   | T     | 11  | TPO  | CB-OG1-P-O2P |
| 1   | A     | 1   | FME  | C-CA-CB-CG   |
| 9   | I     | 1   | SAC  | C-CA-CB-OG   |
| 7   | G     | 11  | TPO  | CB-OG1-P-O3P |
| 7   | T     | 11  | TPO  | CB-OG1-P-O3P |
| 1   | A     | 1   | FME  | CB-CA-N-CN   |

There are no ring outliers.

4 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | I     | 1   | SAC  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | V     | 1   | SAC  | 1       | 0            |
| 1   | A     | 1   | FME  | 1       | 0            |
| 2   | B     | 1   | FME  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 160 ligands modelled in this entry, 10 are monoatomic - leaving 150 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 | $\# Z  > 2$ |
| 22  | EDO  | N     | 623 | -    | 3,3,3        | 0.61 | 0           | 2,2,2       | 0.55 | 0           |
| 22  | EDO  | N     | 615 | -    | 3,3,3        | 0.68 | 0           | 2,2,2       | 0.39 | 0           |
| 22  | EDO  | F     | 110 | -    | 3,3,3        | 0.70 | 0           | 2,2,2       | 0.18 | 0           |
| 26  | PEK  | C     | 309 | -    | 52,52,52     | 0.88 | 2 (3%)      | 55,57,57    | 1.23 | 6 (10%)     |
| 18  | DMU  | P     | 302 | -    | 10,10,34     | 0.44 | 0           | 9,9,45      | 0.38 | 0           |
| 22  | EDO  | D     | 207 | -    | 3,3,3        | 0.58 | 0           | 2,2,2       | 0.31 | 0           |
| 18  | DMU  | X     | 102 | -    | 21,21,34     | 0.57 | 0           | 24,25,45    | 1.40 | 2 (8%)      |
| 22  | EDO  | P     | 314 | -    | 3,3,3        | 0.92 | 0           | 2,2,2       | 0.07 | 0           |
| 22  | EDO  | J     | 103 | -    | 3,3,3        | 0.63 | 0           | 2,2,2       | 0.24 | 0           |
| 14  | HEA  | A     | 602 | 29,1 | 66,67,67     | 1.86 | 20 (30%)    | 78,103,103  | 2.47 | 30 (38%)    |
| 22  | EDO  | A     | 611 | -    | 3,3,3        | 0.69 | 0           | 2,2,2       | 0.50 | 0           |
| 21  | TGL  | N     | 608 | -    | 62,62,62     | 1.15 | 3 (4%)      | 65,65,65    | 1.32 | 6 (9%)      |
| 22  | EDO  | S     | 102 | -    | 3,3,3        | 0.74 | 0           | 2,2,2       | 0.65 | 0           |
| 25  | CDL  | C     | 307 | -    | 99,99,99     | 1.40 | 14 (14%)    | 105,111,111 | 1.66 | 17 (16%)    |
| 18  | DMU  | Y     | 101 | -    | 34,34,34     | 0.73 | 0           | 45,45,45    | 1.13 | 3 (6%)      |
| 19  | PGV  | P     | 309 | -    | 50,50,50     | 0.82 | 4 (8%)      | 53,56,56    | 1.08 | 4 (7%)      |
| 22  | EDO  | P     | 311 | -    | 3,3,3        | 0.60 | 0           | 2,2,2       | 0.28 | 0           |
| 18  | DMU  | M     | 101 | -    | 34,34,34     | 0.46 | 0           | 45,45,45    | 1.12 | 4 (8%)      |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | EDO  | S     | 104    | -    | 3,3,3        | 0.76 | 0        | 2,2,2       | 0.34 | 0        |
| 22  | EDO  | S     | 105    | -    | 3,3,3        | 0.36 | 0        | 2,2,2       | 0.28 | 0        |
| 26  | PEK  | F     | 102    | 6,25 | 52,52,52     | 1.06 | 2 (3%)   | 55,57,57    | 1.50 | 5 (9%)   |
| 14  | HEA  | A     | 601[B] | -    | 66,67,67     | 1.94 | 20 (30%) | 78,103,103  | 2.47 | 36 (46%) |
| 18  | DMU  | P     | 303    | -    | 34,34,34     | 0.64 | 0        | 45,45,45    | 2.08 | 15 (33%) |
| 22  | EDO  | F     | 103    | -    | 3,3,3        | 0.72 | 0        | 2,2,2       | 0.55 | 0        |
| 22  | EDO  | P     | 315    | -    | 3,3,3        | 1.08 | 0        | 2,2,2       | 0.66 | 0        |
| 18  | DMU  | O     | 302    | -    | 10,10,34     | 0.40 | 0        | 9,9,45      | 0.40 | 0        |
| 22  | EDO  | N     | 618    | -    | 3,3,3        | 0.83 | 0        | 2,2,2       | 0.36 | 0        |
| 22  | EDO  | L     | 104    | -    | 3,3,3        | 0.68 | 0        | 2,2,2       | 0.54 | 0        |
| 22  | EDO  | A     | 616    | -    | 3,3,3        | 0.61 | 0        | 2,2,2       | 0.27 | 0        |
| 19  | PGV  | A     | 608    | -    | 50,50,50     | 0.89 | 4 (8%)   | 53,56,56    | 1.28 | 2 (3%)   |
| 22  | EDO  | S     | 103    | -    | 3,3,3        | 0.65 | 0        | 2,2,2       | 0.57 | 0        |
| 22  | EDO  | C     | 313    | -    | 3,3,3        | 0.38 | 0        | 2,2,2       | 0.68 | 0        |
| 19  | PGV  | A     | 607    | -    | 50,50,50     | 1.10 | 3 (6%)   | 53,56,56    | 1.31 | 7 (13%)  |
| 14  | HEA  | N     | 601[B] | -    | 66,67,67     | 1.69 | 20 (30%) | 78,103,103  | 2.06 | 28 (35%) |
| 14  | HEA  | N     | 602    | 29,1 | 66,67,67     | 1.76 | 17 (25%) | 78,103,103  | 2.26 | 36 (46%) |
| 22  | EDO  | A     | 614    | -    | 3,3,3        | 0.41 | 0        | 2,2,2       | 0.24 | 0        |
| 22  | EDO  | M     | 102    | -    | 3,3,3        | 0.40 | 0        | 2,2,2       | 0.19 | 0        |
| 22  | EDO  | F     | 108    | -    | 3,3,3        | 0.47 | 0        | 2,2,2       | 0.24 | 0        |
| 22  | EDO  | Q     | 205    | -    | 3,3,3        | 0.75 | 0        | 2,2,2       | 0.28 | 0        |
| 18  | DMU  | X     | 105    | -    | 10,10,34     | 0.38 | 0        | 9,9,45      | 0.32 | 0        |
| 18  | DMU  | X     | 101    | -    | 10,10,34     | 0.44 | 0        | 9,9,45      | 0.45 | 0        |
| 24  | CHD  | G     | 101    | -    | 32,32,32     | 0.88 | 0        | 51,51,51    | 1.39 | 8 (15%)  |
| 22  | EDO  | N     | 620    | -    | 3,3,3        | 0.64 | 0        | 2,2,2       | 0.19 | 0        |
| 20  | PSC  | V     | 101    | 9    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.56 | 11 (19%) |
| 26  | PEK  | P     | 308    | -    | 52,52,52     | 0.77 | 2 (3%)   | 55,57,57    | 1.30 | 5 (9%)   |
| 18  | DMU  | W     | 101    | -    | 21,21,34     | 0.92 | 1 (4%)   | 24,25,45    | 1.54 | 5 (20%)  |
| 22  | EDO  | E     | 203    | -    | 3,3,3        | 0.42 | 0        | 2,2,2       | 0.55 | 0        |
| 22  | EDO  | N     | 613    | -    | 3,3,3        | 0.61 | 0        | 2,2,2       | 0.25 | 0        |
| 25  | CDL  | P     | 306    | -    | 99,99,99     | 1.33 | 12 (12%) | 105,111,111 | 1.58 | 18 (17%) |
| 22  | EDO  | C     | 317    | -    | 3,3,3        | 0.72 | 0        | 2,2,2       | 0.24 | 0        |
| 22  | EDO  | N     | 616    | -    | 3,3,3        | 0.68 | 0        | 2,2,2       | 0.26 | 0        |
| 22  | EDO  | H     | 102    | -    | 3,3,3        | 0.27 | 0        | 2,2,2       | 0.79 | 0        |
| 22  | EDO  | U     | 102    | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.13 | 0        |
| 24  | CHD  | C     | 305    | -    | 32,32,32     | 1.08 | 1 (3%)   | 51,51,51    | 1.43 | 6 (11%)  |
| 21  | TGL  | D     | 202    | -    | 62,62,62     | 1.33 | 5 (8%)   | 65,65,65    | 1.16 | 6 (9%)   |
| 24  | CHD  | P     | 304    | -    | 32,32,32     | 0.89 | 0        | 51,51,51    | 1.57 | 7 (13%)  |
| 18  | DMU  | B     | 302    | -    | 10,10,34     | 0.42 | 0        | 9,9,45      | 0.44 | 0        |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | PGV  | P     | 310    | -    | 50,50,50     | 1.04 | 2 (4%)   | 53,56,56    | 1.30 | 5 (9%)   |
| 18  | DMU  | C     | 303    | -    | 22,22,34     | 0.80 | 1 (4%)   | 27,27,45    | 1.56 | 3 (11%)  |
| 22  | EDO  | F     | 104    | -    | 3,3,3        | 0.39 | 0        | 2,2,2       | 0.29 | 0        |
| 22  | EDO  | P     | 312    | -    | 3,3,3        | 0.39 | 0        | 2,2,2       | 0.78 | 0        |
| 26  | PEK  | C     | 308    | -    | 52,52,52     | 1.17 | 2 (3%)   | 55,57,57    | 1.40 | 6 (10%)  |
| 14  | HEA  | A     | 601[A] | -    | 66,67,67     | 1.95 | 20 (30%) | 78,103,103  | 2.46 | 33 (42%) |
| 20  | PSC  | A     | 609    | 1    | 51,51,51     | 1.13 | 3 (5%)   | 57,59,59    | 1.53 | 6 (10%)  |
| 22  | EDO  | B     | 306    | -    | 3,3,3        | 0.76 | 0        | 2,2,2       | 0.39 | 0        |
| 22  | EDO  | N     | 617    | -    | 3,3,3        | 0.29 | 0        | 2,2,2       | 0.75 | 0        |
| 22  | EDO  | E     | 201    | -    | 3,3,3        | 0.49 | 0        | 2,2,2       | 0.26 | 0        |
| 22  | EDO  | A     | 618    | -    | 3,3,3        | 0.66 | 0        | 2,2,2       | 0.24 | 0        |
| 19  | PGV  | C     | 310    | -    | 50,50,50     | 0.76 | 1 (2%)   | 53,56,56    | 1.16 | 5 (9%)   |
| 19  | PGV  | N     | 606    | -    | 50,50,50     | 1.02 | 2 (4%)   | 53,56,56    | 1.28 | 6 (11%)  |
| 14  | HEA  | N     | 601[A] | -    | 66,67,67     | 1.70 | 19 (28%) | 78,103,103  | 1.92 | 23 (29%) |
| 18  | DMU  | D     | 201    | -    | 21,21,34     | 0.89 | 1 (4%)   | 24,25,45    | 1.55 | 5 (20%)  |
| 22  | EDO  | D     | 205    | -    | 3,3,3        | 0.55 | 0        | 2,2,2       | 0.37 | 0        |
| 18  | DMU  | C     | 302    | -    | 34,34,34     | 0.51 | 0        | 45,45,45    | 2.14 | 15 (33%) |
| 18  | DMU  | A     | 606    | -    | 11,11,34     | 0.36 | 0        | 9,9,45      | 0.71 | 0        |
| 24  | CHD  | P     | 305    | -    | 32,32,32     | 0.72 | 0        | 51,51,51    | 1.73 | 9 (17%)  |
| 21  | TGL  | L     | 103    | -    | 62,62,62     | 1.32 | 4 (6%)   | 65,65,65    | 2.12 | 16 (24%) |
| 22  | EDO  | P     | 313    | -    | 3,3,3        | 0.95 | 0        | 2,2,2       | 0.34 | 0        |
| 22  | EDO  | A     | 613    | -    | 3,3,3        | 0.92 | 0        | 2,2,2       | 0.62 | 0        |
| 18  | DMU  | C     | 304    | -    | 10,10,34     | 0.40 | 0        | 9,9,45      | 0.29 | 0        |
| 22  | EDO  | Q     | 203    | -    | 3,3,3        | 0.48 | 0        | 2,2,2       | 0.27 | 0        |
| 22  | EDO  | O     | 304    | -    | 3,3,3        | 0.60 | 0        | 2,2,2       | 0.24 | 0        |
| 26  | PEK  | P     | 307    | -    | 52,52,52     | 1.09 | 2 (3%)   | 55,57,57    | 1.38 | 7 (12%)  |
| 22  | EDO  | B     | 304    | -    | 3,3,3        | 0.41 | 0        | 2,2,2       | 0.49 | 0        |
| 22  | EDO  | A     | 615    | -    | 3,3,3        | 0.34 | 0        | 2,2,2       | 0.92 | 0        |
| 22  | EDO  | C     | 314    | -    | 3,3,3        | 0.75 | 0        | 2,2,2       | 1.02 | 0        |
| 22  | EDO  | N     | 611    | -    | 3,3,3        | 1.12 | 0        | 2,2,2       | 0.36 | 0        |
| 19  | PGV  | N     | 607    | -    | 50,50,50     | 1.01 | 2 (4%)   | 53,56,56    | 1.37 | 7 (13%)  |
| 22  | EDO  | N     | 622    | -    | 3,3,3        | 1.10 | 0        | 2,2,2       | 1.30 | 0        |
| 18  | DMU  | L     | 101    | 22   | 34,34,34     | 0.68 | 0        | 45,45,45    | 1.64 | 9 (20%)  |
| 22  | EDO  | A     | 619    | -    | 3,3,3        | 0.43 | 0        | 2,2,2       | 0.65 | 0        |
| 26  | PEK  | T     | 103    | -    | 52,52,52     | 1.09 | 2 (3%)   | 55,57,57    | 1.48 | 6 (10%)  |
| 22  | EDO  | F     | 105    | -    | 3,3,3        | 0.65 | 0        | 2,2,2       | 0.64 | 0        |
| 18  | DMU  | K     | 102    | -    | 12,12,34     | 0.49 | 0        | 10,11,45    | 0.47 | 0        |
| 22  | EDO  | T     | 105    | -    | 3,3,3        | 0.57 | 0        | 2,2,2       | 0.31 | 0        |
| 22  | EDO  | C     | 311    | -    | 3,3,3        | 0.90 | 0        | 2,2,2       | 0.45 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | CHD  | C     | 306 | -    | 32,32,32     | 0.85 | 1 (3%)   | 51,51,51    | 2.03 | 16 (31%) |
| 22  | EDO  | N     | 612 | -    | 3,3,3        | 0.45 | 0        | 2,2,2       | 0.19 | 0        |
| 22  | EDO  | N     | 610 | -    | 3,3,3        | 0.61 | 0        | 2,2,2       | 0.39 | 0        |
| 18  | DMU  | J     | 101 | -    | 21,21,34     | 0.93 | 1 (4%)   | 24,25,45    | 1.36 | 4 (16%)  |
| 22  | EDO  | B     | 303 | -    | 3,3,3        | 0.67 | 0        | 2,2,2       | 0.65 | 0        |
| 25  | CDL  | T     | 102 | 7    | 99,99,99     | 1.36 | 12 (12%) | 105,111,111 | 1.42 | 14 (13%) |
| 22  | EDO  | A     | 612 | -    | 3,3,3        | 0.72 | 0        | 2,2,2       | 1.12 | 0        |
| 22  | EDO  | D     | 203 | -    | 3,3,3        | 0.75 | 0        | 2,2,2       | 0.28 | 0        |
| 22  | EDO  | D     | 204 | -    | 3,3,3        | 0.41 | 0        | 2,2,2       | 0.50 | 0        |
| 24  | CHD  | J     | 102 | -    | 32,32,32     | 0.82 | 0        | 51,51,51    | 1.65 | 13 (25%) |
| 22  | EDO  | G     | 103 | -    | 3,3,3        | 0.88 | 0        | 2,2,2       | 0.54 | 0        |
| 22  | EDO  | C     | 315 | -    | 3,3,3        | 0.50 | 0        | 2,2,2       | 0.57 | 0        |
| 22  | EDO  | N     | 614 | -    | 3,3,3        | 0.54 | 0        | 2,2,2       | 0.22 | 0        |
| 18  | DMU  | K     | 103 | -    | 22,22,34     | 1.01 | 1 (4%)   | 27,27,45    | 1.33 | 4 (14%)  |
| 22  | EDO  | S     | 106 | -    | 3,3,3        | 0.73 | 0        | 2,2,2       | 0.32 | 0        |
| 22  | EDO  | C     | 312 | -    | 3,3,3        | 0.93 | 0        | 2,2,2       | 0.13 | 0        |
| 22  | EDO  | Y     | 104 | -    | 3,3,3        | 0.56 | 0        | 2,2,2       | 0.12 | 0        |
| 22  | EDO  | P     | 316 | -    | 3,3,3        | 0.64 | 0        | 2,2,2       | 0.45 | 0        |
| 23  | CUA  | O     | 301 | 2    | 0,1,1        | -    | -        | -           | -    | -        |
| 22  | EDO  | F     | 109 | -    | 3,3,3        | 0.59 | 0        | 2,2,2       | 0.30 | 0        |
| 22  | EDO  | O     | 303 | -    | 3,3,3        | 0.71 | 0        | 2,2,2       | 0.62 | 0        |
| 22  | EDO  | P     | 317 | -    | 3,3,3        | 0.69 | 0        | 2,2,2       | 0.60 | 0        |
| 22  | EDO  | Q     | 204 | -    | 3,3,3        | 0.40 | 0        | 2,2,2       | 0.54 | 0        |
| 22  | EDO  | T     | 106 | -    | 3,3,3        | 0.86 | 0        | 2,2,2       | 1.06 | 0        |
| 21  | TGL  | A     | 610 | -    | 62,62,62     | 1.18 | 3 (4%)   | 65,65,65    | 1.34 | 6 (9%)   |
| 22  | EDO  | B     | 305 | -    | 3,3,3        | 0.37 | 0        | 2,2,2       | 0.24 | 0        |
| 28  | PO4  | H     | 101 | -    | 4,4,4        | 0.99 | 0        | 6,6,6       | 0.39 | 0        |
| 22  | EDO  | B     | 307 | -    | 3,3,3        | 0.77 | 0        | 2,2,2       | 0.69 | 0        |
| 18  | DMU  | Z     | 101 | -    | 34,34,34     | 0.63 | 1 (2%)   | 45,45,45    | 1.06 | 3 (6%)   |
| 18  | DMU  | X     | 103 | -    | 10,10,34     | 0.38 | 0        | 9,9,45      | 0.27 | 0        |
| 19  | PGV  | T     | 104 | 7    | 50,50,50     | 1.07 | 2 (4%)   | 53,56,56    | 1.50 | 7 (13%)  |
| 18  | DMU  | K     | 104 | -    | 10,10,34     | 0.31 | 0        | 9,9,45      | 0.50 | 0        |
| 22  | EDO  | D     | 206 | -    | 3,3,3        | 0.46 | 0        | 2,2,2       | 0.60 | 0        |
| 22  | EDO  | F     | 107 | -    | 3,3,3        | 0.73 | 0        | 2,2,2       | 0.31 | 0        |
| 22  | EDO  | C     | 316 | -    | 3,3,3        | 0.89 | 0        | 2,2,2       | 0.53 | 0        |
| 22  | EDO  | F     | 106 | -    | 3,3,3        | 0.96 | 0        | 2,2,2       | 0.29 | 0        |
| 21  | TGL  | Q     | 202 | -    | 62,62,62     | 1.12 | 3 (4%)   | 65,65,65    | 0.95 | 5 (7%)   |
| 22  | EDO  | N     | 619 | -    | 3,3,3        | 0.54 | 0        | 2,2,2       | 0.41 | 0        |
| 22  | EDO  | W     | 102 | -    | 3,3,3        | 0.47 | 0        | 2,2,2       | 0.41 | 0        |
| 18  | DMU  | K     | 101 | -    | 10,10,34     | 0.27 | 0        | 9,9,45      | 0.78 | 0        |
| 22  | EDO  | N     | 609 | -    | 3,3,3        | 0.58 | 0        | 2,2,2       | 0.87 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | CHD  | T     | 101 | -    | 32,32,32     | 1.10 | 2 (6%)   | 51,51,51    | 1.54 | 9 (17%)  |
| 22  | EDO  | L     | 105 | 18   | 3,3,3        | 0.49 | 0        | 2,2,2       | 0.27 | 0        |
| 23  | CUA  | B     | 301 | 2    | 0,1,1        | -    | -        | -           | -    | -        |
| 24  | CHD  | Y     | 102 | -    | 32,32,32     | 0.64 | 0        | 51,51,51    | 2.18 | 15 (29%) |
| 21  | TGL  | Y     | 103 | -    | 62,62,62     | 1.33 | 3 (4%)   | 65,65,65    | 1.57 | 9 (13%)  |
| 22  | EDO  | N     | 621 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.81 | 0        |
| 25  | CDL  | G     | 102 | 26   | 99,99,99     | 1.41 | 12 (12%) | 105,111,111 | 1.25 | 9 (8%)   |
| 22  | EDO  | A     | 617 | -    | 3,3,3        | 0.39 | 0        | 2,2,2       | 0.65 | 0        |
| 24  | CHD  | L     | 102 | -    | 32,32,32     | 0.62 | 0        | 51,51,51    | 2.45 | 20 (39%) |
| 18  | DMU  | X     | 104 | -    | 10,10,34     | 0.31 | 0        | 9,9,45      | 0.44 | 0        |
| 28  | PO4  | U     | 101 | -    | 4,4,4        | 0.91 | 0        | 6,6,6       | 0.58 | 0        |
| 22  | EDO  | E     | 202 | -    | 3,3,3        | 0.45 | 0        | 2,2,2       | 0.40 | 0        |
| 18  | DMU  | Q     | 201 | -    | 22,22,34     | 0.86 | 1 (4%)   | 27,27,45    | 1.74 | 7 (25%)  |

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   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 22  | EDO  | N     | 623 | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | N     | 615 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | F     | 110 | -    | -       | 1/1/1/1        | -       |
| 26  | PEK  | C     | 309 | -    | -       | 16/56/56/56    | -       |
| 18  | DMU  | P     | 302 | -    | -       | 0/8/8/59       | -       |
| 22  | EDO  | D     | 207 | -    | -       | 0/1/1/1        | -       |
| 18  | DMU  | X     | 102 | -    | -       | 8/13/29/59     | 0/1/1/2 |
| 22  | EDO  | P     | 314 | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | J     | 103 | -    | -       | 1/1/1/1        | -       |
| 14  | HEA  | A     | 602 | 29,1 | -       | 5/36/76/76     | -       |
| 22  | EDO  | A     | 611 | -    | -       | 1/1/1/1        | -       |
| 21  | TGL  | N     | 608 | -    | -       | 33/65/65/65    | -       |
| 22  | EDO  | S     | 102 | -    | -       | 0/1/1/1        | -       |
| 25  | CDL  | C     | 307 | -    | -       | 43/110/110/110 | -       |
| 18  | DMU  | Y     | 101 | -    | -       | 5/19/59/59     | 0/2/2/2 |
| 19  | PGV  | P     | 309 | -    | -       | 10/55/55/55    | -       |
| 22  | EDO  | P     | 311 | -    | -       | 0/1/1/1        | -       |
| 18  | DMU  | M     | 101 | -    | -       | 7/19/59/59     | 0/2/2/2 |
| 22  | EDO  | S     | 104 | -    | -       | 0/1/1/1        | -       |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|--------|------|---------|----------------|---------|
| 22  | EDO  | S     | 105    | -    | -       | 0/1/1/1        | -       |
| 26  | PEK  | F     | 102    | 6,25 | -       | 24/56/56/56    | -       |
| 14  | HEA  | A     | 601[B] | -    | -       | 4/36/76/76     | -       |
| 18  | DMU  | P     | 303    | -    | -       | 6/19/59/59     | 0/2/2/2 |
| 22  | EDO  | F     | 103    | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | P     | 315    | -    | -       | 1/1/1/1        | -       |
| 18  | DMU  | O     | 302    | -    | -       | 0/8/8/59       | -       |
| 22  | EDO  | N     | 618    | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | L     | 104    | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | A     | 616    | -    | -       | 0/1/1/1        | -       |
| 19  | PGV  | A     | 608    | -    | -       | 4/55/55/55     | -       |
| 22  | EDO  | S     | 103    | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | C     | 313    | -    | -       | 0/1/1/1        | -       |
| 19  | PGV  | A     | 607    | -    | -       | 18/55/55/55    | -       |
| 14  | HEA  | N     | 601[B] | -    | -       | 4/36/76/76     | -       |
| 14  | HEA  | N     | 602    | 29,1 | -       | 6/36/76/76     | -       |
| 22  | EDO  | A     | 614    | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | M     | 102    | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | F     | 108    | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | Q     | 205    | -    | -       | 1/1/1/1        | -       |
| 18  | DMU  | X     | 105    | -    | -       | 4/8/8/59       | -       |
| 18  | DMU  | X     | 101    | -    | -       | 1/8/8/59       | -       |
| 24  | CHD  | G     | 101    | -    | -       | 2/9/74/74      | 0/4/4/4 |
| 22  | EDO  | N     | 620    | -    | -       | 0/1/1/1        | -       |
| 20  | PSC  | V     | 101    | 9    | -       | 20/55/55/55    | -       |
| 26  | PEK  | P     | 308    | -    | -       | 11/56/56/56    | -       |
| 18  | DMU  | W     | 101    | -    | -       | 4/13/29/59     | 0/1/1/2 |
| 22  | EDO  | E     | 203    | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | N     | 613    | -    | -       | 0/1/1/1        | -       |
| 25  | CDL  | P     | 306    | -    | -       | 42/110/110/110 | -       |
| 22  | EDO  | C     | 317    | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | N     | 616    | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | H     | 102    | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | U     | 102    | -    | -       | 1/1/1/1        | -       |
| 24  | CHD  | C     | 305    | -    | -       | 1/9/74/74      | 0/4/4/4 |
| 21  | TGL  | D     | 202    | -    | -       | 21/65/65/65    | -       |
| 24  | CHD  | P     | 304    | -    | -       | 2/9/74/74      | 0/4/4/4 |
| 18  | DMU  | B     | 302    | -    | -       | 3/8/8/59       | -       |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|--------|------|---------|-------------|---------|
| 19  | PGV  | P     | 310    | -    | -       | 16/55/55/55 | -       |
| 18  | DMU  | C     | 303    | -    | -       | 7/13/33/59  | 0/1/1/2 |
| 22  | EDO  | F     | 104    | -    | -       | 0/1/1/1     | -       |
| 22  | EDO  | P     | 312    | -    | -       | 1/1/1/1     | -       |
| 26  | PEK  | C     | 308    | -    | -       | 17/56/56/56 | -       |
| 14  | HEA  | A     | 601[A] | -    | -       | 7/36/76/76  | -       |
| 20  | PSC  | A     | 609    | 1    | -       | 15/55/55/55 | -       |
| 22  | EDO  | B     | 306    | -    | -       | 1/1/1/1     | -       |
| 22  | EDO  | N     | 617    | -    | -       | 1/1/1/1     | -       |
| 22  | EDO  | E     | 201    | -    | -       | 0/1/1/1     | -       |
| 22  | EDO  | A     | 618    | -    | -       | 1/1/1/1     | -       |
| 19  | PGV  | C     | 310    | -    | -       | 8/55/55/55  | -       |
| 19  | PGV  | N     | 606    | -    | -       | 15/55/55/55 | -       |
| 14  | HEA  | N     | 601[A] | -    | -       | 11/36/76/76 | -       |
| 18  | DMU  | D     | 201    | -    | -       | 4/13/29/59  | 0/1/1/2 |
| 22  | EDO  | D     | 205    | -    | -       | 0/1/1/1     | -       |
| 18  | DMU  | C     | 302    | -    | -       | 10/19/59/59 | 0/2/2/2 |
| 18  | DMU  | A     | 606    | -    | -       | 2/8/8/59    | -       |
| 24  | CHD  | P     | 305    | -    | -       | 5/9/74/74   | 0/4/4/4 |
| 21  | TGL  | L     | 103    | -    | -       | 32/65/65/65 | -       |
| 22  | EDO  | P     | 313    | -    | -       | 1/1/1/1     | -       |
| 22  | EDO  | A     | 613    | -    | -       | 0/1/1/1     | -       |
| 18  | DMU  | C     | 304    | -    | -       | 5/8/8/59    | -       |
| 22  | EDO  | Q     | 203    | -    | -       | 1/1/1/1     | -       |
| 22  | EDO  | O     | 304    | -    | -       | 0/1/1/1     | -       |
| 26  | PEK  | P     | 307    | -    | -       | 22/56/56/56 | -       |
| 22  | EDO  | B     | 304    | -    | -       | 1/1/1/1     | -       |
| 22  | EDO  | A     | 615    | -    | -       | 1/1/1/1     | -       |
| 22  | EDO  | C     | 314    | -    | -       | 0/1/1/1     | -       |
| 22  | EDO  | N     | 611    | -    | -       | 0/1/1/1     | -       |
| 19  | PGV  | N     | 607    | -    | -       | 7/55/55/55  | -       |
| 22  | EDO  | N     | 622    | -    | -       | 1/1/1/1     | -       |
| 18  | DMU  | L     | 101    | 22   | -       | 8/19/59/59  | 0/2/2/2 |
| 22  | EDO  | A     | 619    | -    | -       | 1/1/1/1     | -       |
| 26  | PEK  | T     | 103    | -    | -       | 24/56/56/56 | -       |
| 22  | EDO  | F     | 105    | -    | -       | 0/1/1/1     | -       |
| 18  | DMU  | K     | 102    | -    | -       | 4/9/10/59   | -       |
| 22  | EDO  | T     | 105    | -    | -       | 1/1/1/1     | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 22  | EDO  | C     | 311 | -    | -       | 1/1/1/1        | -       |
| 24  | CHD  | C     | 306 | -    | -       | 9/9/74/74      | 0/4/4/4 |
| 22  | EDO  | N     | 612 | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | N     | 610 | -    | -       | 0/1/1/1        | -       |
| 18  | DMU  | J     | 101 | -    | -       | 4/13/29/59     | 0/1/1/2 |
| 22  | EDO  | B     | 303 | -    | -       | 0/1/1/1        | -       |
| 25  | CDL  | T     | 102 | 7    | -       | 43/110/110/110 | -       |
| 22  | EDO  | A     | 612 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | D     | 203 | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | D     | 204 | -    | -       | 0/1/1/1        | -       |
| 24  | CHD  | J     | 102 | -    | -       | 5/9/74/74      | 0/4/4/4 |
| 22  | EDO  | G     | 103 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | C     | 315 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | N     | 614 | -    | -       | 0/1/1/1        | -       |
| 18  | DMU  | K     | 103 | -    | -       | 6/13/33/59     | 0/1/1/2 |
| 22  | EDO  | S     | 106 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | C     | 312 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | Y     | 104 | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | P     | 316 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | F     | 109 | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | O     | 303 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | P     | 317 | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | Q     | 204 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | T     | 106 | -    | -       | 0/1/1/1        | -       |
| 21  | TGL  | A     | 610 | -    | -       | 36/65/65/65    | -       |
| 22  | EDO  | B     | 305 | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | B     | 307 | -    | -       | 1/1/1/1        | -       |
| 18  | DMU  | Z     | 101 | -    | -       | 5/19/59/59     | 0/2/2/2 |
| 18  | DMU  | X     | 103 | -    | -       | 4/8/8/59       | -       |
| 19  | PGV  | T     | 104 | 7    | -       | 19/55/55/55    | -       |
| 18  | DMU  | K     | 104 | -    | -       | 4/8/8/59       | -       |
| 22  | EDO  | D     | 206 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | F     | 107 | -    | -       | 0/1/1/1        | -       |
| 22  | EDO  | C     | 316 | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | F     | 106 | -    | -       | 0/1/1/1        | -       |
| 21  | TGL  | Q     | 202 | -    | -       | 28/65/65/65    | -       |
| 22  | EDO  | N     | 619 | -    | -       | 1/1/1/1        | -       |
| 22  | EDO  | W     | 102 | -    | -       | 1/1/1/1        | -       |
| 18  | DMU  | K     | 101 | -    | -       | 3/8/8/59       | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 22  | EDO  | N     | 609 | -    | -       | 0/1/1/1        | -       |
| 24  | CHD  | T     | 101 | -    | -       | 2/9/74/74      | 0/4/4/4 |
| 22  | EDO  | L     | 105 | 18   | -       | 0/1/1/1        | -       |
| 24  | CHD  | Y     | 102 | -    | -       | 1/9/74/74      | 0/4/4/4 |
| 21  | TGL  | Y     | 103 | -    | -       | 32/65/65/65    | -       |
| 22  | EDO  | N     | 621 | -    | -       | 0/1/1/1        | -       |
| 25  | CDL  | G     | 102 | 26   | -       | 40/110/110/110 | -       |
| 22  | EDO  | A     | 617 | -    | -       | 0/1/1/1        | -       |
| 24  | CHD  | L     | 102 | -    | -       | 5/9/74/74      | 0/4/4/4 |
| 18  | DMU  | X     | 104 | -    | -       | 3/8/8/59       | -       |
| 22  | EDO  | E     | 202 | -    | -       | 1/1/1/1        | -       |
| 18  | DMU  | Q     | 201 | -    | -       | 5/13/33/59     | 0/1/1/2 |

All (237) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 21  | L     | 103 | TGL  | OG2-CB1 | 6.24 | 1.51        | 1.34     |
| 21  | Y     | 103 | TGL  | OG2-CB1 | 6.12 | 1.51        | 1.34     |
| 21  | Y     | 103 | TGL  | OG3-CC1 | 5.88 | 1.50        | 1.33     |
| 14  | A     | 602 | HEA  | CHD-C1D | 5.79 | 1.50        | 1.38     |
| 25  | G     | 102 | CDL  | OA6-CA5 | 5.48 | 1.49        | 1.34     |
| 21  | N     | 608 | TGL  | OG2-CB1 | 5.38 | 1.49        | 1.34     |
| 26  | C     | 308 | PEK  | O03-C21 | 5.35 | 1.49        | 1.33     |
| 21  | A     | 610 | TGL  | OG2-CB1 | 5.23 | 1.49        | 1.34     |
| 21  | A     | 610 | TGL  | OG1-CA1 | 5.09 | 1.48        | 1.33     |
| 21  | D     | 202 | TGL  | OG2-CB1 | 5.07 | 1.48        | 1.34     |
| 21  | L     | 103 | TGL  | OG3-CC1 | 5.04 | 1.48        | 1.33     |
| 19  | N     | 606 | PGV  | O03-C19 | 5.03 | 1.48        | 1.33     |
| 26  | C     | 308 | PEK  | O01-C1  | 4.98 | 1.48        | 1.34     |
| 21  | D     | 202 | TGL  | OG3-CC1 | 4.94 | 1.47        | 1.33     |
| 19  | A     | 607 | PGV  | O03-C19 | 4.93 | 1.47        | 1.33     |
| 21  | Y     | 103 | TGL  | OG1-CA1 | 4.92 | 1.47        | 1.33     |
| 25  | G     | 102 | CDL  | OA8-CA7 | 4.92 | 1.47        | 1.33     |
| 26  | P     | 307 | PEK  | O01-C1  | 4.87 | 1.48        | 1.34     |
| 25  | G     | 102 | CDL  | OB8-CB7 | 4.86 | 1.47        | 1.33     |
| 25  | T     | 102 | CDL  | OA6-CA5 | 4.85 | 1.48        | 1.34     |
| 26  | T     | 103 | PEK  | O03-C21 | 4.84 | 1.47        | 1.33     |
| 26  | F     | 102 | PEK  | O03-C21 | 4.82 | 1.47        | 1.33     |
| 19  | T     | 104 | PGV  | O01-C1  | 4.79 | 1.47        | 1.34     |
| 26  | P     | 307 | PEK  | O03-C21 | 4.79 | 1.47        | 1.33     |
| 19  | P     | 310 | PGV  | O03-C19 | 4.77 | 1.47        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 20  | A     | 609    | PSC  | O01-C1  | 4.77  | 1.47        | 1.34     |
| 21  | Q     | 202    | TGL  | OG2-CB1 | 4.76  | 1.47        | 1.34     |
| 25  | T     | 102    | CDL  | OB8-CB7 | 4.75  | 1.47        | 1.33     |
| 26  | F     | 102    | PEK  | O01-C1  | 4.75  | 1.47        | 1.34     |
| 25  | P     | 306    | CDL  | OA8-CA7 | 4.75  | 1.47        | 1.33     |
| 25  | C     | 307    | CDL  | OB8-CB7 | 4.69  | 1.47        | 1.33     |
| 21  | L     | 103    | TGL  | OG1-CA1 | 4.69  | 1.47        | 1.33     |
| 20  | V     | 101    | PSC  | O01-C1  | 4.64  | 1.47        | 1.34     |
| 26  | T     | 103    | PEK  | O01-C1  | 4.62  | 1.47        | 1.34     |
| 19  | T     | 104    | PGV  | O03-C19 | 4.57  | 1.46        | 1.33     |
| 21  | A     | 610    | TGL  | OG3-CC1 | 4.57  | 1.46        | 1.33     |
| 21  | N     | 608    | TGL  | OG1-CA1 | 4.57  | 1.46        | 1.33     |
| 25  | P     | 306    | CDL  | OA6-CA5 | 4.47  | 1.46        | 1.34     |
| 21  | D     | 202    | TGL  | OG1-CA1 | 4.47  | 1.46        | 1.33     |
| 14  | N     | 602    | HEA  | CHB-C4A | 4.43  | 1.47        | 1.38     |
| 14  | A     | 601[A] | HEA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 14  | A     | 601[B] | HEA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 21  | N     | 608    | TGL  | OG3-CC1 | 4.39  | 1.46        | 1.33     |
| 21  | Q     | 202    | TGL  | OG1-CA1 | 4.38  | 1.46        | 1.33     |
| 19  | P     | 310    | PGV  | O01-C1  | 4.37  | 1.46        | 1.34     |
| 19  | A     | 607    | PGV  | O01-C1  | 4.36  | 1.46        | 1.34     |
| 20  | V     | 101    | PSC  | O03-C19 | 4.32  | 1.46        | 1.33     |
| 25  | C     | 307    | CDL  | OA8-CA7 | 4.28  | 1.45        | 1.33     |
| 25  | T     | 102    | CDL  | OB6-CB5 | 4.23  | 1.46        | 1.34     |
| 25  | G     | 102    | CDL  | OB6-CB5 | 4.19  | 1.46        | 1.34     |
| 14  | A     | 601[A] | HEA  | CBD-CGD | 4.16  | 1.60        | 1.50     |
| 14  | A     | 601[B] | HEA  | CBD-CGD | 4.16  | 1.60        | 1.50     |
| 19  | N     | 606    | PGV  | O01-C1  | 4.16  | 1.46        | 1.34     |
| 25  | C     | 307    | CDL  | OA6-CA5 | 4.09  | 1.45        | 1.34     |
| 14  | N     | 601[A] | HEA  | CHA-C1A | 4.02  | 1.46        | 1.38     |
| 14  | N     | 601[B] | HEA  | CHA-C1A | 4.02  | 1.46        | 1.38     |
| 14  | N     | 601[A] | HEA  | CHC-C4B | 4.00  | 1.46        | 1.38     |
| 14  | N     | 601[B] | HEA  | CHC-C4B | 4.00  | 1.46        | 1.38     |
| 26  | C     | 309    | PEK  | O03-C21 | 3.97  | 1.44        | 1.33     |
| 14  | N     | 602    | HEA  | CHA-C1A | 3.94  | 1.46        | 1.38     |
| 14  | A     | 602    | HEA  | C1A-C2A | -3.94 | 1.38        | 1.45     |
| 20  | V     | 101    | PSC  | C13-C12 | 3.91  | 1.54        | 1.31     |
| 25  | T     | 102    | CDL  | OA8-CA7 | 3.91  | 1.44        | 1.33     |
| 14  | A     | 601[A] | HEA  | C1D-ND  | -3.91 | 1.33        | 1.40     |
| 14  | A     | 601[B] | HEA  | C1D-ND  | -3.91 | 1.33        | 1.40     |
| 25  | P     | 306    | CDL  | OB8-CB7 | 3.90  | 1.44        | 1.33     |
| 21  | Q     | 202    | TGL  | OG3-CC1 | 3.89  | 1.44        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 14  | A     | 601[A] | HEA  | C4C-NC  | -3.87 | 1.32        | 1.39     |
| 14  | A     | 601[B] | HEA  | C4C-NC  | -3.87 | 1.32        | 1.39     |
| 14  | A     | 601[A] | HEA  | CBA-CGA | 3.81  | 1.59        | 1.50     |
| 14  | A     | 601[B] | HEA  | CBA-CGA | 3.81  | 1.59        | 1.50     |
| 21  | D     | 202    | TGL  | OB1-CB1 | 3.75  | 1.33        | 1.22     |
| 20  | A     | 609    | PSC  | C13-C12 | 3.73  | 1.53        | 1.31     |
| 25  | C     | 307    | CDL  | C59-C58 | -3.70 | 1.30        | 1.51     |
| 14  | N     | 602    | HEA  | C4C-NC  | -3.69 | 1.32        | 1.39     |
| 14  | N     | 601[A] | HEA  | C4B-NB  | -3.67 | 1.34        | 1.40     |
| 14  | N     | 601[B] | HEA  | C4B-NB  | -3.67 | 1.34        | 1.40     |
| 20  | A     | 609    | PSC  | O03-C19 | 3.67  | 1.44        | 1.33     |
| 14  | A     | 601[A] | HEA  | CMC-C2C | 3.64  | 1.58        | 1.50     |
| 14  | A     | 601[B] | HEA  | CMC-C2C | 3.64  | 1.58        | 1.50     |
| 18  | K     | 103    | DMU  | O16-C6  | 3.61  | 1.46        | 1.40     |
| 25  | C     | 307    | CDL  | OB6-CB5 | 3.61  | 1.44        | 1.34     |
| 14  | N     | 602    | HEA  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 25  | P     | 306    | CDL  | OB6-CB5 | 3.49  | 1.44        | 1.34     |
| 18  | W     | 101    | DMU  | O16-C6  | 3.49  | 1.46        | 1.40     |
| 14  | A     | 601[A] | HEA  | C1A-C2A | -3.49 | 1.39        | 1.45     |
| 14  | A     | 601[B] | HEA  | C1A-C2A | -3.49 | 1.39        | 1.45     |
| 25  | C     | 307    | CDL  | C79-C78 | -3.48 | 1.32        | 1.51     |
| 25  | T     | 102    | CDL  | C59-C58 | -3.45 | 1.32        | 1.51     |
| 25  | T     | 102    | CDL  | C19-C18 | -3.45 | 1.32        | 1.51     |
| 18  | J     | 101    | DMU  | O16-C6  | 3.44  | 1.46        | 1.40     |
| 19  | N     | 607    | PGV  | O01-C1  | 3.40  | 1.43        | 1.34     |
| 14  | A     | 602    | HEA  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 26  | P     | 308    | PEK  | O03-C21 | 3.35  | 1.43        | 1.33     |
| 14  | A     | 602    | HEA  | C4A-NA  | -3.35 | 1.33        | 1.39     |
| 25  | T     | 102    | CDL  | C82-C81 | -3.35 | 1.32        | 1.51     |
| 14  | N     | 601[A] | HEA  | C3A-C4A | -3.34 | 1.40        | 1.46     |
| 14  | N     | 601[B] | HEA  | C3A-C4A | -3.34 | 1.40        | 1.46     |
| 25  | G     | 102    | CDL  | C59-C58 | -3.32 | 1.32        | 1.51     |
| 25  | P     | 306    | CDL  | C79-C78 | -3.30 | 1.33        | 1.51     |
| 19  | N     | 607    | PGV  | O03-C19 | 3.29  | 1.43        | 1.33     |
| 14  | A     | 601[A] | HEA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 14  | A     | 601[B] | HEA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 25  | C     | 307    | CDL  | C39-C38 | -3.26 | 1.33        | 1.51     |
| 25  | T     | 102    | CDL  | C22-C21 | -3.23 | 1.33        | 1.51     |
| 25  | C     | 307    | CDL  | C82-C81 | -3.22 | 1.33        | 1.51     |
| 25  | P     | 306    | CDL  | C22-C21 | -3.21 | 1.33        | 1.51     |
| 25  | T     | 102    | CDL  | C79-C78 | -3.21 | 1.33        | 1.51     |
| 25  | P     | 306    | CDL  | C19-C18 | -3.21 | 1.33        | 1.51     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 25  | G     | 102    | CDL  | C62-C61 | -3.21 | 1.33        | 1.51     |
| 25  | T     | 102    | CDL  | C62-C61 | -3.20 | 1.33        | 1.51     |
| 25  | G     | 102    | CDL  | C82-C81 | -3.20 | 1.33        | 1.51     |
| 25  | T     | 102    | CDL  | C42-C41 | -3.20 | 1.33        | 1.51     |
| 14  | A     | 601[A] | HEA  | CHC-C4B | 3.20  | 1.45        | 1.38     |
| 14  | A     | 601[B] | HEA  | CHC-C4B | 3.20  | 1.45        | 1.38     |
| 25  | C     | 307    | CDL  | C42-C41 | -3.19 | 1.33        | 1.51     |
| 14  | A     | 602    | HEA  | C1C-NC  | -3.19 | 1.33        | 1.39     |
| 25  | G     | 102    | CDL  | C79-C78 | -3.19 | 1.33        | 1.51     |
| 25  | C     | 307    | CDL  | C22-C21 | -3.15 | 1.33        | 1.51     |
| 25  | C     | 307    | CDL  | C62-C61 | -3.15 | 1.33        | 1.51     |
| 25  | C     | 307    | CDL  | C19-C18 | -3.15 | 1.33        | 1.51     |
| 14  | A     | 602    | HEA  | CHB-C4A | 3.13  | 1.44        | 1.38     |
| 14  | N     | 601[A] | HEA  | CHB-C4A | 3.11  | 1.44        | 1.38     |
| 14  | N     | 601[B] | HEA  | CHB-C4A | 3.11  | 1.44        | 1.38     |
| 14  | N     | 602    | HEA  | FE-NA   | 3.10  | 2.05        | 1.95     |
| 25  | T     | 102    | CDL  | C39-C38 | -3.09 | 1.34        | 1.51     |
| 14  | A     | 602    | HEA  | C4D-C3D | -3.08 | 1.39        | 1.45     |
| 25  | P     | 306    | CDL  | C59-C58 | -3.04 | 1.34        | 1.51     |
| 25  | P     | 306    | CDL  | C82-C81 | -3.04 | 1.34        | 1.51     |
| 25  | P     | 306    | CDL  | C39-C38 | -3.03 | 1.34        | 1.51     |
| 18  | D     | 201    | DMU  | O16-C6  | 3.02  | 1.45        | 1.40     |
| 25  | G     | 102    | CDL  | C42-C41 | -3.02 | 1.34        | 1.51     |
| 25  | P     | 306    | CDL  | C62-C61 | -3.01 | 1.34        | 1.51     |
| 14  | A     | 602    | HEA  | FE-NC   | 3.00  | 2.05        | 1.95     |
| 25  | G     | 102    | CDL  | C39-C38 | -2.99 | 1.34        | 1.51     |
| 14  | A     | 602    | HEA  | CHA-C4D | 2.99  | 1.46        | 1.39     |
| 25  | C     | 307    | CDL  | O1-C1   | 2.96  | 1.52        | 1.43     |
| 14  | N     | 601[A] | HEA  | FE-NA   | 2.95  | 2.05        | 1.95     |
| 14  | N     | 601[B] | HEA  | FE-NA   | 2.95  | 2.05        | 1.95     |
| 25  | P     | 306    | CDL  | C42-C41 | -2.95 | 1.35        | 1.51     |
| 24  | C     | 305    | CHD  | O12-C12 | 2.91  | 1.48        | 1.43     |
| 14  | N     | 602    | HEA  | CHA-C4D | 2.90  | 1.45        | 1.39     |
| 14  | A     | 601[A] | HEA  | C4A-NA  | -2.90 | 1.34        | 1.39     |
| 14  | A     | 601[B] | HEA  | C4A-NA  | -2.90 | 1.34        | 1.39     |
| 18  | C     | 303    | DMU  | O16-C6  | 2.89  | 1.45        | 1.40     |
| 19  | P     | 309    | PGV  | O01-C1  | 2.87  | 1.42        | 1.34     |
| 19  | P     | 309    | PGV  | O01-C02 | -2.85 | 1.39        | 1.46     |
| 25  | G     | 102    | CDL  | C19-C18 | -2.85 | 1.35        | 1.51     |
| 26  | C     | 309    | PEK  | O01-C1  | 2.83  | 1.42        | 1.34     |
| 14  | A     | 601[A] | HEA  | C1B-NB  | -2.81 | 1.33        | 1.38     |
| 14  | A     | 601[B] | HEA  | C1B-NB  | -2.81 | 1.33        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 19  | A     | 608    | PGV  | O01-C1  | 2.80  | 1.42        | 1.34     |
| 25  | G     | 102    | CDL  | C22-C21 | -2.75 | 1.36        | 1.51     |
| 14  | A     | 602    | HEA  | CHC-C4B | 2.74  | 1.44        | 1.38     |
| 18  | Q     | 201    | DMU  | O16-C6  | 2.72  | 1.44        | 1.40     |
| 24  | T     | 101    | CHD  | O7-C7   | 2.68  | 1.49        | 1.43     |
| 14  | N     | 601[A] | HEA  | CHA-C4D | 2.65  | 1.45        | 1.39     |
| 14  | N     | 601[B] | HEA  | CHA-C4D | 2.65  | 1.45        | 1.39     |
| 14  | N     | 602    | HEA  | C3A-C4A | -2.64 | 1.41        | 1.46     |
| 14  | N     | 602    | HEA  | C4B-NB  | -2.63 | 1.35        | 1.40     |
| 14  | A     | 602    | HEA  | C18-C19 | 2.62  | 1.39        | 1.33     |
| 14  | A     | 601[A] | HEA  | FE-NB   | 2.60  | 2.02        | 1.94     |
| 14  | A     | 601[B] | HEA  | FE-NB   | 2.60  | 2.02        | 1.94     |
| 14  | N     | 601[A] | HEA  | CBA-CGA | 2.60  | 1.56        | 1.50     |
| 14  | N     | 601[B] | HEA  | CBA-CGA | 2.60  | 1.56        | 1.50     |
| 18  | Z     | 101    | DMU  | O16-C6  | 2.58  | 1.44        | 1.40     |
| 14  | A     | 601[A] | HEA  | CHA-C4D | 2.57  | 1.45        | 1.39     |
| 14  | A     | 601[B] | HEA  | CHA-C4D | 2.57  | 1.45        | 1.39     |
| 21  | D     | 202    | TGL  | CB2-CB1 | 2.54  | 1.58        | 1.50     |
| 14  | A     | 601[A] | HEA  | CAD-C3D | 2.54  | 1.57        | 1.51     |
| 14  | A     | 601[B] | HEA  | CAD-C3D | 2.54  | 1.57        | 1.51     |
| 19  | A     | 608    | PGV  | O03-C19 | 2.53  | 1.40        | 1.33     |
| 24  | C     | 306    | CHD  | C10-C9  | -2.51 | 1.51        | 1.56     |
| 14  | A     | 602    | HEA  | CBA-CGA | 2.48  | 1.56        | 1.50     |
| 26  | P     | 308    | PEK  | C05-C04 | 2.46  | 1.60        | 1.50     |
| 14  | A     | 602    | HEA  | CMC-C2C | 2.45  | 1.56        | 1.50     |
| 14  | N     | 601[A] | HEA  | CHD-C1D | 2.45  | 1.43        | 1.38     |
| 14  | N     | 601[B] | HEA  | CHD-C1D | 2.45  | 1.43        | 1.38     |
| 14  | A     | 601[A] | HEA  | CAA-C2A | 2.44  | 1.57        | 1.51     |
| 14  | A     | 601[B] | HEA  | CAA-C2A | 2.44  | 1.57        | 1.51     |
| 21  | L     | 103    | TGL  | CC2-CC1 | 2.33  | 1.57        | 1.50     |
| 14  | N     | 601[A] | HEA  | O1A-CGA | 2.32  | 1.29        | 1.22     |
| 14  | N     | 601[B] | HEA  | O1A-CGA | 2.32  | 1.29        | 1.22     |
| 14  | N     | 601[A] | HEA  | CHD-C4C | 2.31  | 1.44        | 1.39     |
| 14  | N     | 601[B] | HEA  | CHD-C4C | 2.31  | 1.44        | 1.39     |
| 14  | N     | 602    | HEA  | C1A-C2A | -2.30 | 1.41        | 1.45     |
| 14  | A     | 602    | HEA  | C3C-C4C | 2.30  | 1.48        | 1.42     |
| 14  | N     | 601[A] | HEA  | C1A-C2A | -2.29 | 1.41        | 1.45     |
| 14  | N     | 601[B] | HEA  | C1A-C2A | -2.29 | 1.41        | 1.45     |
| 14  | A     | 601[A] | HEA  | O1A-CGA | 2.29  | 1.29        | 1.22     |
| 14  | A     | 601[B] | HEA  | O1A-CGA | 2.29  | 1.29        | 1.22     |
| 24  | T     | 101    | CHD  | C13-C17 | -2.29 | 1.51        | 1.55     |
| 14  | A     | 602    | HEA  | C14-C15 | 2.29  | 1.38        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 14  | N     | 601[A] | HEA  | CMC-C2C | 2.28  | 1.55        | 1.50     |
| 14  | N     | 601[B] | HEA  | CMC-C2C | 2.28  | 1.55        | 1.50     |
| 14  | N     | 602    | HEA  | C18-C19 | 2.27  | 1.38        | 1.33     |
| 14  | N     | 602    | HEA  | CMC-C2C | 2.26  | 1.55        | 1.50     |
| 19  | A     | 608    | PGV  | C20-C19 | 2.24  | 1.57        | 1.50     |
| 14  | N     | 602    | HEA  | FE-NB   | 2.23  | 2.01        | 1.94     |
| 19  | A     | 607    | PGV  | O02-C1  | 2.22  | 1.29        | 1.22     |
| 14  | N     | 601[A] | HEA  | C4C-NC  | -2.22 | 1.35        | 1.39     |
| 14  | N     | 601[B] | HEA  | C4C-NC  | -2.22 | 1.35        | 1.39     |
| 14  | A     | 601[A] | HEA  | C12-C13 | 2.21  | 1.60        | 1.53     |
| 14  | A     | 601[A] | HEA  | C3D-C2D | 2.20  | 1.41        | 1.36     |
| 14  | A     | 601[B] | HEA  | C3D-C2D | 2.20  | 1.41        | 1.36     |
| 14  | A     | 602    | HEA  | C3B-C2B | 2.18  | 1.39        | 1.34     |
| 25  | C     | 307    | CDL  | PB2-OB3 | 2.17  | 1.58        | 1.50     |
| 14  | N     | 601[A] | HEA  | CAD-C3D | 2.17  | 1.56        | 1.51     |
| 14  | N     | 601[B] | HEA  | CAD-C3D | 2.17  | 1.56        | 1.51     |
| 14  | N     | 602    | HEA  | C1A-NA  | -2.17 | 1.35        | 1.39     |
| 14  | N     | 602    | HEA  | C4B-C3B | -2.17 | 1.40        | 1.44     |
| 19  | P     | 309    | PGV  | P-O14   | -2.17 | 1.45        | 1.55     |
| 14  | A     | 601[A] | HEA  | C3A-C4A | -2.16 | 1.42        | 1.46     |
| 14  | A     | 601[B] | HEA  | C3A-C4A | -2.16 | 1.42        | 1.46     |
| 14  | A     | 601[A] | HEA  | C1C-NC  | -2.16 | 1.35        | 1.39     |
| 14  | A     | 601[B] | HEA  | C1C-NC  | -2.16 | 1.35        | 1.39     |
| 14  | N     | 602    | HEA  | C14-C15 | 2.15  | 1.38        | 1.33     |
| 14  | A     | 602    | HEA  | FE-ND   | 2.13  | 2.01        | 1.94     |
| 14  | A     | 602    | HEA  | C4C-NC  | -2.12 | 1.35        | 1.39     |
| 14  | A     | 601[B] | HEA  | C12-C11 | -2.12 | 1.49        | 1.52     |
| 19  | P     | 309    | PGV  | O03-C19 | 2.11  | 1.39        | 1.33     |
| 19  | C     | 310    | PGV  | O01-C1  | 2.11  | 1.40        | 1.34     |
| 14  | N     | 602    | HEA  | CBD-CGD | 2.10  | 1.55        | 1.50     |
| 19  | A     | 608    | PGV  | O03-C01 | 2.09  | 1.49        | 1.45     |
| 20  | V     | 101    | PSC  | C08-N   | -2.08 | 1.43        | 1.50     |
| 14  | A     | 602    | HEA  | O2D-CGD | -2.08 | 1.23        | 1.30     |
| 14  | N     | 601[A] | HEA  | C1A-NA  | -2.08 | 1.35        | 1.39     |
| 14  | N     | 601[B] | HEA  | C1A-NA  | -2.08 | 1.35        | 1.39     |
| 14  | N     | 601[A] | HEA  | CHC-C1C | 2.07  | 1.44        | 1.39     |
| 14  | N     | 601[B] | HEA  | CHC-C1C | 2.07  | 1.44        | 1.39     |
| 14  | N     | 601[A] | HEA  | C4D-ND  | -2.07 | 1.34        | 1.38     |
| 14  | N     | 601[B] | HEA  | C4D-ND  | -2.07 | 1.34        | 1.38     |
| 14  | N     | 601[B] | HEA  | O11-C11 | 2.07  | 1.47        | 1.42     |
| 14  | N     | 602    | HEA  | CHD-C4C | 2.06  | 1.44        | 1.39     |
| 14  | N     | 601[A] | HEA  | O2D-CGD | -2.04 | 1.23        | 1.30     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 14  | N     | 601[B] | HEA  | O2D-CGD | -2.04 | 1.23        | 1.30     |
| 14  | A     | 602    | HEA  | FE-NB   | 2.01  | 2.01        | 1.94     |

All (569) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | L     | 102    | CHD  | C10-C9-C8   | 7.39  | 119.75      | 111.82   |
| 21  | L     | 103    | TGL  | OG2-CB1-CB2 | 7.35  | 127.34      | 111.50   |
| 20  | A     | 609    | PSC  | C03-C02-C01 | -7.04 | 95.14       | 111.79   |
| 21  | Y     | 103    | TGL  | OG2-CB1-CB2 | 6.56  | 125.64      | 111.50   |
| 14  | A     | 602    | HEA  | C3C-C2C-C1C | -6.49 | 99.32       | 107.16   |
| 14  | A     | 602    | HEA  | C2C-C1C-NC  | 6.38  | 119.80      | 110.08   |
| 14  | N     | 601[B] | HEA  | C13-C12-C11 | -6.35 | 104.81      | 114.35   |
| 21  | A     | 610    | TGL  | OG2-CB1-CB2 | 6.30  | 125.08      | 111.50   |
| 18  | C     | 302    | DMU  | C10-O1-C9   | 6.26  | 125.97      | 113.69   |
| 25  | P     | 306    | CDL  | CB4-OB6-CB5 | -6.25 | 102.41      | 117.79   |
| 24  | Y     | 102    | CHD  | C6-C5-C4    | -6.14 | 104.12      | 111.19   |
| 14  | A     | 601[A] | HEA  | C2B-C1B-NB  | 5.94  | 117.00      | 109.88   |
| 14  | A     | 601[B] | HEA  | C2B-C1B-NB  | 5.94  | 117.00      | 109.88   |
| 14  | A     | 602    | HEA  | C26-C15-C16 | 5.94  | 125.26      | 115.27   |
| 21  | L     | 103    | TGL  | OG3-CC1-OC1 | -5.85 | 108.83      | 123.59   |
| 21  | N     | 608    | TGL  | OG2-CB1-CB2 | 5.56  | 123.47      | 111.50   |
| 19  | T     | 104    | PGV  | O03-C19-C20 | 5.54  | 129.29      | 111.91   |
| 21  | L     | 103    | TGL  | CG2-OG2-CB1 | 5.49  | 131.30      | 117.79   |
| 14  | N     | 601[A] | HEA  | C13-C12-C11 | -5.34 | 106.33      | 114.35   |
| 14  | N     | 602    | HEA  | CHA-C1A-NA  | 5.32  | 130.20      | 124.44   |
| 18  | X     | 102    | DMU  | C6-O5-C4    | 5.29  | 119.00      | 113.13   |
| 18  | C     | 303    | DMU  | O16-C6-C1   | 5.22  | 116.46      | 108.30   |
| 25  | P     | 306    | CDL  | C52-C51-CB5 | -5.19 | 94.74       | 113.62   |
| 26  | T     | 103    | PEK  | O01-C1-C2   | 5.18  | 122.66      | 111.50   |
| 26  | F     | 102    | PEK  | O03-C21-C22 | 5.16  | 128.09      | 111.91   |
| 14  | A     | 601[A] | HEA  | CHD-C4C-NC  | 5.16  | 133.33      | 123.85   |
| 14  | A     | 601[B] | HEA  | CHD-C4C-NC  | 5.16  | 133.33      | 123.85   |
| 14  | A     | 601[A] | HEA  | C13-C12-C11 | -5.08 | 106.72      | 114.35   |
| 14  | A     | 601[A] | HEA  | C26-C15-C16 | 5.05  | 123.77      | 115.27   |
| 24  | L     | 102    | CHD  | C6-C5-C4    | -5.04 | 105.39      | 111.19   |
| 14  | N     | 602    | HEA  | C13-C12-C11 | -5.04 | 106.78      | 114.35   |
| 24  | Y     | 102    | CHD  | C1-C10-C5   | 5.03  | 115.21      | 107.77   |
| 26  | T     | 103    | PEK  | O03-C21-C22 | 5.03  | 127.68      | 111.91   |
| 20  | V     | 101    | PSC  | O01-C1-C2   | 4.99  | 122.25      | 111.50   |
| 26  | C     | 308    | PEK  | O01-C1-C2   | 4.97  | 122.22      | 111.50   |
| 24  | Y     | 102    | CHD  | C14-C8-C7   | 4.97  | 118.40      | 111.81   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 18  | L     | 101    | DMU  | C10-O1-C9   | 4.94  | 123.38      | 113.69   |
| 25  | C     | 307    | CDL  | O1-C1-CB2   | 4.94  | 126.87      | 109.56   |
| 14  | A     | 601[B] | HEA  | C13-C12-C11 | -4.94 | 106.93      | 114.35   |
| 24  | L     | 102    | CHD  | C11-C12-C13 | 4.85  | 116.23      | 111.24   |
| 24  | L     | 102    | CHD  | C13-C17-C20 | 4.83  | 125.26      | 119.50   |
| 25  | C     | 307    | CDL  | CB4-OB6-CB5 | -4.82 | 105.92      | 117.79   |
| 14  | A     | 602    | HEA  | C27-C19-C20 | 4.81  | 123.36      | 115.27   |
| 19  | P     | 310    | PGV  | O03-C19-C20 | 4.80  | 126.97      | 111.91   |
| 21  | D     | 202    | TGL  | OG3-CC1-CC2 | 4.79  | 126.95      | 111.91   |
| 14  | A     | 601[A] | HEA  | CAA-CBA-CGA | -4.79 | 103.29      | 113.60   |
| 14  | A     | 601[B] | HEA  | CAA-CBA-CGA | -4.79 | 103.29      | 113.60   |
| 18  | P     | 303    | DMU  | O1-C10-C5   | 4.79  | 120.48      | 110.35   |
| 25  | G     | 102    | CDL  | OA6-CA5-C11 | 4.77  | 121.77      | 111.50   |
| 24  | C     | 305    | CHD  | C18-C13-C12 | 4.76  | 113.91      | 109.07   |
| 25  | C     | 307    | CDL  | CB2-C1-CA2  | -4.72 | 98.91       | 112.79   |
| 24  | Y     | 102    | CHD  | C19-C10-C1  | -4.71 | 100.67      | 108.26   |
| 24  | L     | 102    | CHD  | C11-C9-C10  | -4.69 | 108.89      | 113.73   |
| 25  | C     | 307    | CDL  | OB8-CB7-C71 | 4.68  | 126.60      | 111.91   |
| 14  | A     | 602    | HEA  | CHB-C4A-NA  | 4.64  | 129.46      | 124.44   |
| 19  | T     | 104    | PGV  | C01-O03-C19 | 4.63  | 134.28      | 117.12   |
| 18  | L     | 101    | DMU  | O7-C3-C2    | 4.62  | 119.57      | 107.28   |
| 19  | P     | 310    | PGV  | O01-C1-C2   | 4.59  | 121.40      | 111.50   |
| 24  | C     | 306    | CHD  | C14-C8-C9   | -4.59 | 103.41      | 109.71   |
| 18  | P     | 303    | DMU  | C10-O1-C9   | 4.57  | 122.67      | 113.69   |
| 21  | L     | 103    | TGL  | OG3-CC1-CC2 | 4.56  | 126.23      | 111.91   |
| 18  | C     | 302    | DMU  | C8-C7-C5    | 4.52  | 118.71      | 110.82   |
| 21  | L     | 103    | TGL  | CG3-CG2-CG1 | -4.50 | 101.13      | 111.79   |
| 14  | A     | 601[A] | HEA  | C2D-C1D-ND  | 4.50  | 115.18      | 109.84   |
| 14  | A     | 601[B] | HEA  | C2D-C1D-ND  | 4.50  | 115.18      | 109.84   |
| 14  | A     | 601[A] | HEA  | CHB-C4A-NA  | 4.47  | 129.28      | 124.44   |
| 14  | A     | 601[B] | HEA  | CHB-C4A-NA  | 4.47  | 129.28      | 124.44   |
| 24  | C     | 306    | CHD  | C23-C22-C20 | -4.44 | 106.41      | 114.52   |
| 14  | A     | 601[B] | HEA  | C17-C18-C19 | -4.44 | 116.97      | 127.66   |
| 26  | C     | 308    | PEK  | O03-C01-C02 | 4.42  | 121.29      | 108.43   |
| 24  | P     | 304    | CHD  | C22-C20-C17 | -4.41 | 101.17      | 110.28   |
| 18  | Q     | 201    | DMU  | O5-C4-C3    | 4.38  | 117.64      | 109.69   |
| 24  | J     | 102    | CHD  | C13-C17-C20 | 4.38  | 124.72      | 119.50   |
| 20  | A     | 609    | PSC  | O01-C1-C2   | 4.37  | 120.92      | 111.50   |
| 25  | P     | 306    | CDL  | OB8-CB7-C71 | 4.36  | 125.58      | 111.91   |
| 26  | P     | 307    | PEK  | O03-C21-C22 | 4.33  | 125.50      | 111.91   |
| 26  | C     | 308    | PEK  | O03-C21-C22 | 4.33  | 125.49      | 111.91   |
| 25  | T     | 102    | CDL  | OB6-CB5-C51 | 4.29  | 120.75      | 111.50   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | C     | 306    | CHD  | C11-C9-C10  | -4.29 | 109.31      | 113.73   |
| 14  | A     | 601[A] | HEA  | C4C-CHD-C1D | -4.28 | 116.18      | 126.34   |
| 14  | A     | 601[B] | HEA  | C4C-CHD-C1D | -4.28 | 116.18      | 126.34   |
| 24  | P     | 305    | CHD  | C15-C14-C13 | 4.24  | 107.71      | 103.55   |
| 14  | A     | 602    | HEA  | C4A-CHB-C1B | -4.23 | 116.92      | 126.06   |
| 26  | F     | 102    | PEK  | C01-O03-C21 | 4.23  | 132.77      | 117.12   |
| 14  | N     | 601[A] | HEA  | O2A-CGA-CBA | 4.22  | 127.59      | 114.03   |
| 14  | N     | 601[B] | HEA  | O2A-CGA-CBA | 4.22  | 127.59      | 114.03   |
| 25  | C     | 307    | CDL  | OB2-PB2-OB3 | 4.21  | 125.53      | 109.07   |
| 24  | P     | 305    | CHD  | C1-C2-C3    | 4.20  | 115.86      | 110.47   |
| 24  | P     | 304    | CHD  | C16-C17-C13 | 4.18  | 107.66      | 103.55   |
| 21  | Y     | 103    | TGL  | CG2-OG2-CB1 | 4.15  | 128.02      | 117.79   |
| 26  | F     | 102    | PEK  | O01-C1-C2   | 4.14  | 120.43      | 111.50   |
| 14  | N     | 601[A] | HEA  | C3D-C4D-ND  | 4.13  | 114.36      | 110.36   |
| 14  | N     | 601[B] | HEA  | C3D-C4D-ND  | 4.13  | 114.36      | 110.36   |
| 14  | A     | 601[A] | HEA  | C3D-C4D-ND  | 4.12  | 114.35      | 110.36   |
| 14  | A     | 601[B] | HEA  | C3D-C4D-ND  | 4.12  | 114.35      | 110.36   |
| 19  | N     | 606    | PGV  | C03-C02-C01 | -4.12 | 102.04      | 111.79   |
| 25  | P     | 306    | CDL  | OB6-CB5-C51 | 4.11  | 120.37      | 111.50   |
| 14  | A     | 602    | HEA  | CAD-CBD-CGD | -4.09 | 104.80      | 113.60   |
| 19  | A     | 607    | PGV  | C4-C3-C2    | -4.08 | 98.51       | 113.19   |
| 19  | A     | 608    | PGV  | O03-C19-O04 | -4.06 | 113.33      | 123.59   |
| 21  | N     | 608    | TGL  | CG3-CG2-CG1 | -4.05 | 102.21      | 111.79   |
| 24  | C     | 305    | CHD  | C22-C20-C17 | -4.03 | 101.96      | 110.28   |
| 24  | P     | 305    | CHD  | C18-C13-C12 | -4.03 | 104.96      | 109.07   |
| 19  | A     | 608    | PGV  | O03-C19-C20 | 4.02  | 124.54      | 111.91   |
| 25  | T     | 102    | CDL  | OA8-CA7-C31 | 4.01  | 124.48      | 111.91   |
| 18  | P     | 303    | DMU  | O1-C9-C11   | 3.94  | 116.22      | 106.44   |
| 26  | F     | 102    | PEK  | O03-C21-O04 | -3.89 | 113.78      | 123.59   |
| 24  | P     | 304    | CHD  | C15-C14-C13 | 3.89  | 107.36      | 103.55   |
| 25  | P     | 306    | CDL  | OB8-CB7-OB9 | -3.89 | 113.78      | 123.59   |
| 18  | C     | 302    | DMU  | O1-C10-C5   | 3.89  | 118.57      | 110.35   |
| 14  | A     | 602    | HEA  | C16-C15-C14 | -3.88 | 113.26      | 121.12   |
| 14  | N     | 602    | HEA  | C16-C15-C14 | -3.87 | 113.29      | 121.12   |
| 14  | N     | 602    | HEA  | CAA-CBA-CGA | -3.87 | 105.28      | 113.60   |
| 14  | N     | 601[A] | HEA  | C1D-ND-C4D  | -3.85 | 101.09      | 105.07   |
| 14  | N     | 601[B] | HEA  | C1D-ND-C4D  | -3.85 | 101.09      | 105.07   |
| 24  | C     | 306    | CHD  | C18-C13-C12 | -3.85 | 105.14      | 109.07   |
| 14  | A     | 601[A] | HEA  | O2A-CGA-CBA | 3.85  | 126.39      | 114.03   |
| 14  | A     | 601[B] | HEA  | O2A-CGA-CBA | 3.85  | 126.39      | 114.03   |
| 14  | A     | 601[A] | HEA  | C16-C15-C14 | -3.81 | 113.41      | 121.12   |
| 25  | T     | 102    | CDL  | OA6-CA5-C11 | 3.80  | 119.68      | 111.50   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 14  | N     | 601[A] | HEA  | C1B-C2B-C3B | -3.78 | 102.28      | 106.80   |
| 14  | N     | 601[B] | HEA  | C1B-C2B-C3B | -3.78 | 102.28      | 106.80   |
| 24  | L     | 102    | CHD  | C14-C13-C12 | 3.78  | 110.92      | 107.40   |
| 14  | A     | 602    | HEA  | C20-C19-C18 | -3.77 | 113.48      | 121.12   |
| 14  | N     | 602    | HEA  | C3C-C2C-C1C | -3.77 | 102.61      | 107.16   |
| 24  | C     | 306    | CHD  | C19-C10-C9  | -3.77 | 105.99      | 111.18   |
| 24  | L     | 102    | CHD  | C15-C14-C8  | 3.77  | 123.60      | 118.33   |
| 14  | N     | 602    | HEA  | C2D-C1D-ND  | 3.75  | 114.29      | 109.84   |
| 26  | P     | 308    | PEK  | O03-C21-C22 | 3.72  | 123.58      | 111.91   |
| 25  | C     | 307    | CDL  | OB6-CB5-C51 | 3.72  | 119.51      | 111.50   |
| 24  | C     | 306    | CHD  | C14-C13-C12 | 3.71  | 110.86      | 107.40   |
| 24  | L     | 102    | CHD  | C21-C20-C17 | 3.71  | 118.59      | 112.92   |
| 14  | A     | 601[A] | HEA  | CAD-CBD-CGD | -3.70 | 105.63      | 113.60   |
| 14  | A     | 601[B] | HEA  | CAD-CBD-CGD | -3.70 | 105.63      | 113.60   |
| 24  | G     | 101    | CHD  | C13-C17-C20 | -3.70 | 115.07      | 119.50   |
| 18  | C     | 302    | DMU  | O5-C6-O16   | -3.70 | 101.21      | 109.97   |
| 24  | L     | 102    | CHD  | C5-C6-C7    | 3.69  | 118.54      | 114.46   |
| 19  | T     | 104    | PGV  | O03-C19-O04 | -3.69 | 114.27      | 123.59   |
| 18  | D     | 201    | DMU  | O5-C4-C57   | 3.68  | 112.73      | 106.83   |
| 14  | A     | 602    | HEA  | C4C-CHD-C1D | -3.67 | 117.63      | 126.34   |
| 25  | C     | 307    | CDL  | OB8-CB7-OB9 | -3.67 | 114.34      | 123.59   |
| 19  | N     | 606    | PGV  | O03-C19-C20 | 3.66  | 123.40      | 111.91   |
| 25  | G     | 102    | CDL  | CB6-OB8-CB7 | 3.65  | 130.66      | 117.12   |
| 26  | P     | 307    | PEK  | O03-C21-O04 | -3.65 | 114.38      | 123.59   |
| 24  | T     | 101    | CHD  | C13-C14-C8  | -3.64 | 110.08      | 114.74   |
| 21  | Y     | 103    | TGL  | OG3-CG3-CG2 | 3.64  | 119.04      | 108.43   |
| 14  | A     | 602    | HEA  | C2A-C1A-NA  | 3.62  | 113.85      | 110.32   |
| 24  | Y     | 102    | CHD  | C21-C20-C17 | 3.62  | 118.46      | 112.92   |
| 14  | A     | 601[A] | HEA  | CHB-C4A-C3A | -3.61 | 119.08      | 125.26   |
| 14  | A     | 601[B] | HEA  | CHB-C4A-C3A | -3.61 | 119.08      | 125.26   |
| 18  | P     | 303    | DMU  | O1-C9-C8    | 3.60  | 116.22      | 109.69   |
| 14  | A     | 602    | HEA  | CHD-C4C-NC  | 3.58  | 130.44      | 123.85   |
| 18  | L     | 101    | DMU  | O1-C10-C5   | 3.58  | 117.94      | 110.35   |
| 19  | N     | 607    | PGV  | O03-C19-C20 | 3.58  | 123.15      | 111.91   |
| 14  | A     | 602    | HEA  | CHA-C1A-C2A | -3.58 | 119.13      | 124.94   |
| 14  | N     | 602    | HEA  | CAA-C2A-C1A | 3.58  | 131.65      | 124.89   |
| 21  | L     | 103    | TGL  | CC5-CC4-CC3 | -3.57 | 96.31       | 114.42   |
| 14  | A     | 602    | HEA  | C3A-C2A-C1A | -3.53 | 103.71      | 107.08   |
| 19  | N     | 606    | PGV  | O01-C1-C2   | 3.52  | 119.09      | 111.50   |
| 24  | C     | 306    | CHD  | C15-C14-C13 | 3.52  | 107.01      | 103.55   |
| 19  | N     | 607    | PGV  | O01-C1-O02  | -3.51 | 115.22      | 123.70   |
| 14  | N     | 602    | HEA  | CHA-C1A-C2A | -3.51 | 119.25      | 124.94   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 14  | N     | 602    | HEA  | C27-C19-C20 | 3.49  | 121.15      | 115.27   |
| 19  | T     | 104    | PGV  | O01-C1-C2   | 3.49  | 119.02      | 111.50   |
| 14  | N     | 602    | HEA  | C4A-C3A-C2A | 3.46  | 109.60      | 106.75   |
| 14  | A     | 601[B] | HEA  | C20-C19-C18 | 3.45  | 128.11      | 121.12   |
| 24  | Y     | 102    | CHD  | C13-C17-C20 | 3.44  | 123.61      | 119.50   |
| 14  | N     | 601[A] | HEA  | CHC-C4B-NB  | 3.43  | 128.61      | 124.37   |
| 14  | N     | 601[B] | HEA  | CHC-C4B-NB  | 3.43  | 128.61      | 124.37   |
| 20  | V     | 101    | PSC  | C21-C20-C19 | -3.43 | 101.13      | 113.62   |
| 21  | A     | 610    | TGL  | OG1-CA1-CA2 | 3.43  | 122.68      | 111.91   |
| 14  | N     | 601[A] | HEA  | C1C-CHC-C4B | -3.43 | 118.20      | 126.34   |
| 14  | N     | 601[B] | HEA  | C1C-CHC-C4B | -3.43 | 118.20      | 126.34   |
| 18  | Q     | 201    | DMU  | C3-C2-C1    | -3.41 | 104.86      | 110.82   |
| 24  | P     | 305    | CHD  | C19-C10-C9  | -3.40 | 106.50      | 111.18   |
| 24  | Y     | 102    | CHD  | C10-C9-C8   | 3.40  | 115.47      | 111.82   |
| 26  | T     | 103    | PEK  | O03-C21-O04 | -3.40 | 115.02      | 123.59   |
| 14  | A     | 601[B] | HEA  | C27-C19-C18 | -3.39 | 114.99      | 123.68   |
| 25  | G     | 102    | CDL  | OB6-CB5-C51 | 3.38  | 118.80      | 111.50   |
| 24  | P     | 305    | CHD  | C11-C12-C13 | -3.37 | 107.78      | 111.24   |
| 26  | P     | 308    | PEK  | O03-C21-O04 | -3.34 | 115.15      | 123.59   |
| 20  | A     | 609    | PSC  | C04-C05-N   | -3.33 | 104.64      | 115.78   |
| 21  | Y     | 103    | TGL  | OG3-CC1-CC2 | 3.33  | 122.37      | 111.91   |
| 24  | T     | 101    | CHD  | C6-C5-C4    | -3.33 | 107.35      | 111.19   |
| 14  | N     | 602    | HEA  | C4A-NA-C1A  | 3.33  | 108.61      | 105.35   |
| 14  | N     | 602    | HEA  | C2C-C1C-NC  | 3.33  | 115.15      | 110.08   |
| 24  | T     | 101    | CHD  | C11-C9-C10  | -3.33 | 110.30      | 113.73   |
| 26  | P     | 307    | PEK  | C03-C02-C01 | -3.30 | 103.98      | 111.79   |
| 24  | P     | 305    | CHD  | C16-C17-C13 | 3.30  | 106.79      | 103.55   |
| 18  | P     | 303    | DMU  | C10-O7-C3   | -3.29 | 109.83      | 117.96   |
| 19  | N     | 607    | PGV  | O03-C19-O04 | -3.28 | 115.30      | 123.59   |
| 18  | C     | 302    | DMU  | O5-C4-C3    | 3.28  | 116.67      | 109.75   |
| 24  | C     | 306    | CHD  | C6-C5-C4    | -3.28 | 107.41      | 111.19   |
| 18  | K     | 103    | DMU  | C3-C2-C1    | -3.28 | 105.09      | 110.82   |
| 18  | P     | 303    | DMU  | C7-C8-C9    | 3.26  | 116.06      | 110.24   |
| 14  | A     | 601[A] | HEA  | CMB-C2B-C1B | 3.25  | 129.99      | 125.04   |
| 14  | A     | 601[B] | HEA  | CMB-C2B-C1B | 3.25  | 129.99      | 125.04   |
| 24  | L     | 102    | CHD  | C14-C8-C7   | 3.25  | 116.12      | 111.81   |
| 14  | A     | 601[A] | HEA  | C20-C21-C22 | -3.24 | 101.22      | 111.88   |
| 14  | A     | 601[B] | HEA  | C20-C21-C22 | -3.24 | 101.22      | 111.88   |
| 18  | C     | 302    | DMU  | C10-O7-C3   | -3.23 | 109.97      | 117.96   |
| 24  | L     | 102    | CHD  | C1-C10-C9   | -3.22 | 106.28      | 111.35   |
| 18  | Y     | 101    | DMU  | O1-C9-C11   | 3.22  | 114.44      | 106.44   |
| 21  | L     | 103    | TGL  | C20-CA9-CA8 | -3.22 | 98.10       | 114.42   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 18  | C     | 302    | DMU  | O5-C6-C1    | 3.20  | 117.12      | 110.35   |
| 24  | T     | 101    | CHD  | C19-C10-C1  | -3.20 | 103.11      | 108.26   |
| 18  | C     | 302    | DMU  | C7-C8-C9    | 3.19  | 115.93      | 110.24   |
| 14  | A     | 602    | HEA  | C3C-C4C-NC  | -3.19 | 108.29      | 110.25   |
| 18  | P     | 303    | DMU  | O6-C11-C9   | 3.17  | 122.17      | 111.29   |
| 18  | P     | 303    | DMU  | C8-C7-C5    | 3.17  | 116.35      | 110.82   |
| 14  | N     | 601[A] | HEA  | C2D-C1D-ND  | 3.16  | 113.59      | 109.84   |
| 14  | N     | 601[B] | HEA  | C2D-C1D-ND  | 3.16  | 113.59      | 109.84   |
| 24  | Y     | 102    | CHD  | C2-C1-C10   | 3.16  | 118.21      | 112.78   |
| 18  | L     | 101    | DMU  | C10-O7-C3   | 3.16  | 125.79      | 117.96   |
| 21  | N     | 608    | TGL  | OG3-CC1-CC2 | 3.16  | 121.82      | 111.91   |
| 26  | P     | 307    | PEK  | O01-C1-C2   | 3.15  | 118.29      | 111.50   |
| 24  | P     | 305    | CHD  | C14-C8-C9   | -3.13 | 105.42      | 109.71   |
| 21  | D     | 202    | TGL  | OG3-CC1-OC1 | -3.13 | 115.70      | 123.59   |
| 14  | A     | 601[A] | HEA  | C4B-NB-C1B  | -3.12 | 101.85      | 105.07   |
| 14  | A     | 601[B] | HEA  | C4B-NB-C1B  | -3.12 | 101.85      | 105.07   |
| 25  | P     | 306    | CDL  | OA8-CA7-C31 | 3.12  | 121.69      | 111.91   |
| 18  | P     | 303    | DMU  | O16-C6-C1   | 3.12  | 113.17      | 108.30   |
| 24  | Y     | 102    | CHD  | C11-C12-C13 | 3.11  | 114.44      | 111.24   |
| 18  | D     | 201    | DMU  | O16-C6-C1   | 3.09  | 113.13      | 108.30   |
| 14  | A     | 601[A] | HEA  | C20-C19-C18 | -3.09 | 114.87      | 121.12   |
| 14  | A     | 601[A] | HEA  | C1D-ND-C4D  | -3.08 | 101.89      | 105.07   |
| 14  | A     | 601[B] | HEA  | C1D-ND-C4D  | -3.08 | 101.89      | 105.07   |
| 14  | A     | 602    | HEA  | CAA-C2A-C1A | 3.08  | 130.69      | 124.89   |
| 25  | C     | 307    | CDL  | OA8-CA7-C31 | 3.08  | 121.56      | 111.91   |
| 14  | N     | 601[A] | HEA  | CAA-CBA-CGA | -3.07 | 106.99      | 113.60   |
| 14  | N     | 601[B] | HEA  | CAA-CBA-CGA | -3.07 | 106.99      | 113.60   |
| 24  | T     | 101    | CHD  | C5-C4-C3    | -3.07 | 108.25      | 112.76   |
| 25  | T     | 102    | CDL  | OA8-CA7-OA9 | -3.07 | 115.86      | 123.59   |
| 14  | A     | 601[A] | HEA  | CHD-C1D-C2D | -3.06 | 118.22      | 126.73   |
| 14  | A     | 601[B] | HEA  | CHD-C1D-C2D | -3.06 | 118.22      | 126.73   |
| 21  | L     | 103    | TGL  | CC4-CC3-CC2 | -3.06 | 102.19      | 113.19   |
| 18  | Q     | 201    | DMU  | O16-C6-C1   | 3.05  | 113.06      | 108.30   |
| 21  | D     | 202    | TGL  | CG3-CG2-CG1 | -3.04 | 104.59      | 111.79   |
| 18  | P     | 303    | DMU  | C6-O5-C4    | -3.04 | 107.72      | 113.69   |
| 19  | A     | 607    | PGV  | O01-C1-C2   | 3.04  | 118.06      | 111.50   |
| 14  | A     | 601[A] | HEA  | CHA-C4D-C3D | -3.04 | 120.37      | 124.84   |
| 14  | A     | 601[B] | HEA  | CHA-C4D-C3D | -3.04 | 120.37      | 124.84   |
| 14  | N     | 602    | HEA  | C26-C15-C16 | 3.04  | 120.38      | 115.27   |
| 14  | A     | 602    | HEA  | CMB-C2B-C3B | -3.03 | 124.57      | 130.34   |
| 14  | A     | 601[A] | HEA  | CBD-CAD-C3D | -3.02 | 104.24      | 112.63   |
| 14  | A     | 601[B] | HEA  | CBD-CAD-C3D | -3.02 | 104.24      | 112.63   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 14  | N     | 601[A] | HEA  | CHA-C4D-C3D | -3.01 | 120.42      | 124.84   |
| 14  | N     | 601[B] | HEA  | CHA-C4D-C3D | -3.01 | 120.42      | 124.84   |
| 24  | G     | 101    | CHD  | C11-C12-C13 | 3.00  | 114.33      | 111.24   |
| 18  | P     | 303    | DMU  | C10-C5-C7   | 3.00  | 116.24      | 110.00   |
| 19  | A     | 607    | PGV  | O03-C19-C20 | 2.99  | 121.30      | 111.91   |
| 18  | Y     | 101    | DMU  | O7-C10-C5   | 2.99  | 115.85      | 108.10   |
| 19  | N     | 606    | PGV  | C4-C3-C2    | -2.99 | 102.44      | 113.19   |
| 26  | P     | 308    | PEK  | C11-C10-C9  | -2.98 | 97.35       | 112.02   |
| 19  | C     | 310    | PGV  | O03-C19-O04 | -2.98 | 116.07      | 123.59   |
| 14  | N     | 602    | HEA  | C1D-ND-C4D  | -2.97 | 102.00      | 105.07   |
| 26  | P     | 307    | PEK  | O03-C01-C02 | 2.97  | 117.08      | 108.43   |
| 14  | A     | 602    | HEA  | CAA-CBA-CGA | -2.97 | 107.21      | 113.60   |
| 24  | J     | 102    | CHD  | C5-C6-C7    | 2.97  | 117.74      | 114.46   |
| 25  | C     | 307    | CDL  | C61-C60-C59 | -2.97 | 99.36       | 114.42   |
| 24  | G     | 101    | CHD  | C15-C14-C13 | 2.97  | 106.46      | 103.55   |
| 24  | J     | 102    | CHD  | C6-C5-C4    | -2.96 | 107.78      | 111.19   |
| 14  | N     | 602    | HEA  | C3C-C4C-NC  | 2.95  | 112.06      | 110.25   |
| 24  | C     | 306    | CHD  | C13-C17-C20 | -2.95 | 115.98      | 119.50   |
| 14  | N     | 602    | HEA  | C1A-CHA-C4D | -2.95 | 119.70      | 126.06   |
| 14  | N     | 601[A] | HEA  | O1A-CGA-CBA | -2.94 | 113.64      | 123.08   |
| 14  | N     | 601[B] | HEA  | O1A-CGA-CBA | -2.94 | 113.64      | 123.08   |
| 18  | C     | 302    | DMU  | O4-C7-C5    | -2.94 | 103.56      | 110.35   |
| 24  | C     | 306    | CHD  | C1-C10-C5   | 2.94  | 112.11      | 107.77   |
| 24  | T     | 101    | CHD  | C15-C14-C13 | 2.92  | 106.42      | 103.55   |
| 21  | L     | 103    | TGL  | OB1-CB1-CB2 | -2.92 | 112.33      | 123.73   |
| 24  | J     | 102    | CHD  | C22-C20-C17 | 2.92  | 116.32      | 110.28   |
| 18  | W     | 101    | DMU  | O16-C18-C19 | 2.91  | 119.78      | 109.56   |
| 19  | P     | 310    | PGV  | O03-C19-O04 | -2.91 | 116.25      | 123.59   |
| 24  | Y     | 102    | CHD  | C4-C5-C10   | 2.91  | 115.75      | 112.66   |
| 14  | N     | 602    | HEA  | O1D-CGD-CBD | -2.91 | 113.75      | 123.08   |
| 18  | K     | 103    | DMU  | C18-O16-C6  | 2.90  | 118.66      | 113.84   |
| 21  | L     | 103    | TGL  | C26-C25-C24 | -2.90 | 99.69       | 114.42   |
| 26  | T     | 103    | PEK  | C01-O03-C21 | 2.90  | 127.84      | 117.12   |
| 14  | A     | 601[B] | HEA  | C16-C17-C18 | 2.89  | 121.39      | 111.88   |
| 14  | N     | 601[B] | HEA  | C17-C18-C19 | -2.89 | 120.69      | 127.66   |
| 21  | N     | 608    | TGL  | OG1-CA1-CA2 | 2.89  | 120.98      | 111.91   |
| 24  | T     | 101    | CHD  | C6-C7-C8    | -2.89 | 108.40      | 111.48   |
| 25  | P     | 306    | CDL  | OB2-PB2-OB3 | 2.89  | 120.34      | 109.07   |
| 26  | C     | 309    | PEK  | O03-C21-C22 | 2.88  | 120.95      | 111.91   |
| 19  | N     | 607    | PGV  | O01-C1-C2   | 2.88  | 117.71      | 111.50   |
| 20  | V     | 101    | PSC  | O01-C02-C03 | 2.87  | 118.81      | 108.40   |
| 14  | A     | 601[A] | HEA  | C4C-NC-C1C  | 2.87  | 108.16      | 105.35   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 14  | A     | 601[B] | HEA  | C4C-NC-C1C  | 2.87  | 108.16      | 105.35   |
| 18  | Q     | 201    | DMU  | O55-C2-C3   | 2.87  | 116.99      | 110.35   |
| 14  | N     | 602    | HEA  | C4A-CHB-C1B | -2.87 | 119.88      | 126.06   |
| 26  | C     | 308    | PEK  | O01-C1-O02  | -2.86 | 116.79      | 123.70   |
| 21  | A     | 610    | TGL  | CG3-OG3-CC1 | 2.86  | 127.71      | 117.12   |
| 14  | N     | 602    | HEA  | C3A-C2A-C1A | -2.86 | 104.35      | 107.08   |
| 24  | P     | 304    | CHD  | C1-C2-C3    | -2.85 | 106.81      | 110.47   |
| 25  | P     | 306    | CDL  | OA6-CA5-C11 | 2.84  | 117.62      | 111.50   |
| 20  | V     | 101    | PSC  | C07-N-C06   | 2.83  | 116.24      | 108.97   |
| 18  | C     | 302    | DMU  | C6-O5-C4    | 2.82  | 119.22      | 113.69   |
| 21  | D     | 202    | TGL  | CB3-CB2-CB1 | 2.82  | 123.87      | 113.62   |
| 18  | Q     | 201    | DMU  | C6-O5-C4    | 2.82  | 119.21      | 113.69   |
| 18  | W     | 101    | DMU  | O16-C6-C1   | 2.81  | 112.69      | 108.30   |
| 14  | A     | 602    | HEA  | C21-C20-C19 | 2.81  | 122.22      | 112.98   |
| 24  | J     | 102    | CHD  | C11-C9-C10  | -2.81 | 110.83      | 113.73   |
| 19  | P     | 310    | PGV  | C01-O03-C19 | 2.80  | 127.50      | 117.12   |
| 21  | Q     | 202    | TGL  | OG2-CB1-CB2 | 2.80  | 117.53      | 111.50   |
| 14  | N     | 601[A] | HEA  | C1A-CHA-C4D | -2.80 | 120.02      | 126.06   |
| 14  | N     | 601[B] | HEA  | C1A-CHA-C4D | -2.80 | 120.02      | 126.06   |
| 14  | N     | 602    | HEA  | CAD-CBD-CGD | -2.78 | 107.61      | 113.60   |
| 24  | L     | 102    | CHD  | C21-C20-C22 | -2.78 | 106.00      | 110.36   |
| 20  | V     | 101    | PSC  | C08-N-C07   | -2.77 | 101.84      | 108.97   |
| 14  | A     | 602    | HEA  | CMC-C2C-C1C | 2.77  | 129.59      | 125.37   |
| 14  | N     | 601[A] | HEA  | OMA-CMA-C3A | -2.76 | 119.44      | 125.69   |
| 14  | N     | 601[B] | HEA  | OMA-CMA-C3A | -2.76 | 119.44      | 125.69   |
| 21  | Y     | 103    | TGL  | OB1-CB1-CB2 | -2.76 | 112.96      | 123.73   |
| 21  | L     | 103    | TGL  | OG1-CA1-CA2 | 2.76  | 120.56      | 111.91   |
| 21  | L     | 103    | TGL  | CC3-CC2-CC1 | 2.75  | 123.63      | 113.62   |
| 20  | V     | 101    | PSC  | C01-O03-C19 | 2.75  | 127.31      | 117.12   |
| 18  | J     | 101    | DMU  | C6-O5-C4    | 2.75  | 116.17      | 113.13   |
| 18  | Z     | 101    | DMU  | O16-C6-C1   | 2.75  | 112.59      | 108.30   |
| 21  | L     | 103    | TGL  | CB9-CB8-CB7 | -2.73 | 100.56      | 114.42   |
| 24  | C     | 306    | CHD  | C4-C5-C10   | 2.73  | 115.56      | 112.66   |
| 21  | L     | 103    | TGL  | OG3-CG3-CG2 | 2.73  | 116.37      | 108.43   |
| 14  | N     | 602    | HEA  | OMA-CMA-C3A | -2.71 | 119.56      | 125.69   |
| 14  | N     | 601[A] | HEA  | C3C-C4C-NC  | 2.70  | 111.91      | 110.25   |
| 14  | N     | 601[B] | HEA  | C3C-C4C-NC  | 2.70  | 111.91      | 110.25   |
| 21  | N     | 608    | TGL  | OG3-CC1-OC1 | -2.70 | 116.78      | 123.59   |
| 26  | P     | 308    | PEK  | C2-C3-C4    | -2.70 | 108.42      | 113.23   |
| 25  | T     | 102    | CDL  | OA6-CA4-CA3 | 2.69  | 118.15      | 108.40   |
| 24  | Y     | 102    | CHD  | C15-C14-C8  | 2.68  | 122.08      | 118.33   |
| 19  | P     | 309    | PGV  | O01-C1-O02  | -2.68 | 117.23      | 123.70   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25  | C     | 307    | CDL  | C53-C52-C51 | -2.67 | 103.58      | 113.19   |
| 19  | A     | 607    | PGV  | C3-C2-C1    | 2.67  | 123.34      | 113.62   |
| 14  | A     | 601[A] | HEA  | C1B-C2B-C3B | -2.67 | 103.61      | 106.80   |
| 14  | A     | 601[B] | HEA  | C1B-C2B-C3B | -2.67 | 103.61      | 106.80   |
| 24  | L     | 102    | CHD  | C1-C10-C5   | 2.67  | 111.71      | 107.77   |
| 14  | A     | 601[A] | HEA  | O1A-CGA-CBA | -2.66 | 114.52      | 123.08   |
| 14  | A     | 601[B] | HEA  | O1A-CGA-CBA | -2.66 | 114.52      | 123.08   |
| 21  | Q     | 202    | TGL  | OG3-CC1-OC1 | -2.66 | 116.87      | 123.59   |
| 26  | C     | 309    | PEK  | O11-P-O14   | -2.66 | 98.69       | 109.07   |
| 18  | C     | 302    | DMU  | O49-C1-C2   | -2.65 | 104.22      | 110.35   |
| 20  | V     | 101    | PSC  | C02-O01-C1  | 2.65  | 124.31      | 117.79   |
| 25  | T     | 102    | CDL  | CA6-OA8-CA7 | 2.65  | 126.92      | 117.12   |
| 14  | N     | 602    | HEA  | C4C-NC-C1C  | -2.65 | 102.76      | 105.35   |
| 20  | V     | 101    | PSC  | C3-C2-C1    | -2.64 | 104.01      | 113.62   |
| 19  | A     | 607    | PGV  | C04-C05-C06 | -2.64 | 102.28      | 111.67   |
| 18  | W     | 101    | DMU  | C6-O5-C4    | 2.64  | 116.05      | 113.13   |
| 14  | N     | 602    | HEA  | C20-C19-C18 | -2.63 | 115.78      | 121.12   |
| 14  | A     | 602    | HEA  | C25-C23-C24 | 2.63  | 120.41      | 114.60   |
| 18  | J     | 101    | DMU  | O5-C4-C57   | 2.61  | 111.02      | 106.83   |
| 26  | C     | 309    | PEK  | C11-C10-C9  | -2.61 | 99.17       | 112.02   |
| 24  | Y     | 102    | CHD  | O7-C7-C8    | 2.61  | 115.25      | 109.43   |
| 21  | L     | 103    | TGL  | C25-C24-C23 | -2.60 | 101.21      | 114.42   |
| 25  | P     | 306    | CDL  | C82-C81-C80 | 2.60  | 127.63      | 114.42   |
| 21  | Q     | 202    | TGL  | OG3-CC1-CC2 | 2.60  | 120.06      | 111.91   |
| 25  | C     | 307    | CDL  | CA6-CA4-CA3 | -2.60 | 105.64      | 111.79   |
| 24  | C     | 305    | CHD  | C22-C23-C24 | -2.60 | 105.62      | 112.51   |
| 14  | N     | 602    | HEA  | CHB-C4A-NA  | 2.58  | 127.23      | 124.44   |
| 19  | A     | 607    | PGV  | O02-C1-C2   | -2.58 | 113.65      | 123.73   |
| 26  | P     | 307    | PEK  | C3-C4-C5    | -2.58 | 97.66       | 112.43   |
| 14  | N     | 601[A] | HEA  | C2B-C1B-NB  | 2.57  | 112.96      | 109.88   |
| 14  | N     | 601[B] | HEA  | C2B-C1B-NB  | 2.57  | 112.96      | 109.88   |
| 19  | T     | 104    | PGV  | C21-C20-C19 | -2.57 | 104.28      | 113.62   |
| 25  | T     | 102    | CDL  | OA8-CA6-CA4 | -2.57 | 100.96      | 108.43   |
| 14  | A     | 602    | HEA  | C4A-C3A-C2A | 2.56  | 108.86      | 106.75   |
| 24  | G     | 101    | CHD  | C19-C10-C5  | -2.56 | 106.02      | 110.36   |
| 14  | N     | 602    | HEA  | O2A-CGA-CBA | 2.56  | 122.25      | 114.03   |
| 24  | J     | 102    | CHD  | C18-C13-C17 | 2.56  | 115.21      | 111.21   |
| 21  | Y     | 103    | TGL  | OG1-CA1-CA2 | 2.55  | 119.91      | 111.91   |
| 14  | A     | 602    | HEA  | CHC-C1C-C2C | -2.55 | 120.04      | 127.24   |
| 19  | P     | 309    | PGV  | C27-C26-C25 | -2.55 | 101.49      | 114.42   |
| 14  | N     | 601[A] | HEA  | C3C-C2C-C1C | -2.55 | 104.08      | 107.16   |
| 14  | N     | 601[B] | HEA  | C3C-C2C-C1C | -2.55 | 104.08      | 107.16   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 14  | A     | 601[A] | HEA  | CHB-C1B-NB  | -2.55 | 121.65      | 124.42   |
| 14  | A     | 601[B] | HEA  | CHB-C1B-NB  | -2.55 | 121.65      | 124.42   |
| 14  | N     | 601[A] | HEA  | CAD-CBD-CGD | -2.55 | 108.12      | 113.60   |
| 14  | N     | 601[B] | HEA  | CAD-CBD-CGD | -2.55 | 108.12      | 113.60   |
| 14  | N     | 602    | HEA  | CHC-C1C-C2C | -2.53 | 120.08      | 127.24   |
| 21  | A     | 610    | TGL  | OB1-CB1-CB2 | -2.53 | 113.87      | 123.73   |
| 14  | N     | 602    | HEA  | C13-C14-C15 | -2.53 | 121.58      | 127.66   |
| 18  | C     | 302    | DMU  | O55-C2-C1   | -2.53 | 104.51      | 110.35   |
| 14  | N     | 601[A] | HEA  | O2D-CGD-CBD | 2.53  | 122.14      | 114.03   |
| 14  | N     | 601[B] | HEA  | O2D-CGD-CBD | 2.53  | 122.14      | 114.03   |
| 25  | G     | 102    | CDL  | OA8-CA7-C31 | 2.52  | 119.82      | 111.91   |
| 14  | N     | 602    | HEA  | C3D-C4D-ND  | 2.52  | 112.80      | 110.36   |
| 18  | D     | 201    | DMU  | O5-C6-O16   | 2.52  | 115.94      | 109.97   |
| 18  | Z     | 101    | DMU  | O2-C8-C7    | -2.51 | 104.54      | 110.35   |
| 14  | A     | 601[A] | HEA  | C4D-C3D-C2D | -2.51 | 103.24      | 106.90   |
| 14  | A     | 601[B] | HEA  | C4D-C3D-C2D | -2.51 | 103.24      | 106.90   |
| 19  | C     | 310    | PGV  | C22-C21-C20 | -2.51 | 104.17      | 113.19   |
| 25  | G     | 102    | CDL  | OA8-CA6-CA4 | 2.50  | 115.72      | 108.43   |
| 18  | K     | 103    | DMU  | C6-O5-C4    | 2.50  | 118.60      | 113.69   |
| 18  | D     | 201    | DMU  | C3-C4-C57   | -2.50 | 108.21      | 112.60   |
| 14  | N     | 602    | HEA  | CHB-C1B-C2B | -2.50 | 121.07      | 124.98   |
| 18  | C     | 302    | DMU  | O1-C9-C8    | 2.49  | 114.22      | 109.69   |
| 14  | N     | 601[B] | HEA  | C16-C17-C18 | 2.49  | 120.05      | 111.88   |
| 24  | P     | 304    | CHD  | C19-C10-C1  | -2.49 | 104.26      | 108.26   |
| 18  | J     | 101    | DMU  | O16-C18-C19 | 2.48  | 118.26      | 109.56   |
| 14  | N     | 601[B] | HEA  | C13-C14-C15 | -2.48 | 121.69      | 127.66   |
| 19  | C     | 310    | PGV  | C26-C25-C24 | -2.47 | 101.87      | 114.42   |
| 24  | C     | 305    | CHD  | C23-C22-C20 | -2.47 | 110.00      | 114.52   |
| 24  | L     | 102    | CHD  | C9-C10-C5   | 2.47  | 112.05      | 108.58   |
| 14  | A     | 601[A] | HEA  | CMD-C2D-C1D | 2.46  | 128.79      | 125.04   |
| 14  | A     | 601[B] | HEA  | CMD-C2D-C1D | 2.46  | 128.79      | 125.04   |
| 18  | J     | 101    | DMU  | O16-C6-C1   | 2.45  | 112.14      | 108.30   |
| 14  | N     | 601[A] | HEA  | C16-C17-C18 | -2.45 | 103.82      | 111.88   |
| 21  | Y     | 103    | TGL  | CG3-CG2-CG1 | -2.45 | 105.99      | 111.79   |
| 19  | P     | 309    | PGV  | O03-C01-C02 | -2.45 | 101.30      | 108.43   |
| 19  | N     | 606    | PGV  | O14-P-O13   | 2.45  | 124.34      | 112.24   |
| 25  | P     | 306    | CDL  | C59-C58-C57 | 2.45  | 126.84      | 114.42   |
| 24  | Y     | 102    | CHD  | C5-C6-C7    | 2.44  | 117.16      | 114.46   |
| 14  | A     | 602    | HEA  | C2D-C1D-ND  | 2.44  | 112.73      | 109.84   |
| 18  | X     | 102    | DMU  | O5-C4-C3    | 2.44  | 113.93      | 110.04   |
| 26  | T     | 103    | PEK  | C2-C3-C4    | 2.44  | 117.58      | 113.23   |
| 25  | P     | 306    | CDL  | C83-C82-C81 | 2.44  | 126.80      | 114.42   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 21  | A     | 610    | TGL  | OG2-CG2-CG3 | 2.43  | 117.19      | 108.40   |
| 19  | N     | 607    | PGV  | C9-C10-C11  | -2.43 | 98.53       | 112.43   |
| 18  | Q     | 201    | DMU  | O49-C1-C6   | 2.43  | 115.94      | 110.05   |
| 14  | A     | 601[A] | HEA  | CHD-C4C-C3C | -2.42 | 116.94      | 127.71   |
| 14  | A     | 601[B] | HEA  | CHD-C4C-C3C | -2.42 | 116.94      | 127.71   |
| 25  | T     | 102    | CDL  | C19-C18-C17 | 2.42  | 126.70      | 114.42   |
| 25  | P     | 306    | CDL  | OA8-CA6-CA4 | 2.42  | 115.47      | 108.43   |
| 25  | G     | 102    | CDL  | OA6-CA4-CA3 | 2.42  | 117.15      | 108.40   |
| 14  | N     | 602    | HEA  | C1D-C2D-C3D | -2.41 | 104.42      | 106.96   |
| 20  | V     | 101    | PSC  | C04-C05-N   | 2.41  | 123.83      | 115.78   |
| 14  | N     | 601[A] | HEA  | C1D-C2D-C3D | -2.41 | 104.42      | 106.96   |
| 14  | N     | 601[B] | HEA  | C1D-C2D-C3D | -2.41 | 104.42      | 106.96   |
| 19  | C     | 310    | PGV  | O03-C19-C20 | 2.40  | 119.44      | 111.91   |
| 24  | J     | 102    | CHD  | C9-C8-C7    | -2.40 | 109.01      | 111.88   |
| 24  | L     | 102    | CHD  | C23-C22-C20 | -2.39 | 110.14      | 114.52   |
| 25  | P     | 306    | CDL  | CB2-C1-CA2  | -2.39 | 105.75      | 112.79   |
| 24  | T     | 101    | CHD  | C5-C6-C7    | 2.39  | 117.10      | 114.46   |
| 26  | C     | 309    | PEK  | O01-C1-O02  | -2.39 | 117.93      | 123.70   |
| 24  | L     | 102    | CHD  | O25-C24-C23 | -2.39 | 115.41      | 123.08   |
| 24  | C     | 306    | CHD  | C1-C10-C9   | -2.39 | 107.60      | 111.35   |
| 21  | N     | 608    | TGL  | OG2-CG2-CG3 | 2.37  | 116.99      | 108.40   |
| 14  | A     | 602    | HEA  | CHA-C1A-NA  | 2.37  | 127.00      | 124.44   |
| 14  | N     | 601[B] | HEA  | C26-C15-C14 | -2.37 | 117.60      | 123.68   |
| 24  | T     | 101    | CHD  | C16-C17-C13 | 2.36  | 105.86      | 103.55   |
| 25  | T     | 102    | CDL  | C61-C60-C59 | -2.35 | 102.47      | 114.42   |
| 14  | A     | 602    | HEA  | C13-C14-C15 | -2.35 | 122.01      | 127.66   |
| 19  | A     | 607    | PGV  | C22-C21-C20 | -2.35 | 104.75      | 113.19   |
| 24  | L     | 102    | CHD  | C6-C7-C8    | 2.34  | 113.98      | 111.48   |
| 24  | C     | 306    | CHD  | C22-C23-C24 | -2.34 | 106.31      | 112.51   |
| 24  | P     | 304    | CHD  | C6-C5-C4    | -2.33 | 108.51      | 111.19   |
| 25  | T     | 102    | CDL  | OB8-CB7-C71 | 2.33  | 119.21      | 111.91   |
| 14  | A     | 601[A] | HEA  | CHB-C1B-C2B | -2.32 | 121.35      | 124.98   |
| 14  | A     | 601[B] | HEA  | CHB-C1B-C2B | -2.32 | 121.35      | 124.98   |
| 14  | A     | 602    | HEA  | C4C-NC-C1C  | -2.32 | 103.07      | 105.35   |
| 26  | T     | 103    | PEK  | O01-C1-O02  | -2.32 | 118.10      | 123.70   |
| 18  | L     | 101    | DMU  | O1-C9-C11   | 2.32  | 112.20      | 106.44   |
| 26  | C     | 308    | PEK  | O03-C21-O04 | -2.32 | 117.74      | 123.59   |
| 18  | C     | 302    | DMU  | C10-C5-C7   | 2.31  | 114.81      | 110.00   |
| 25  | T     | 102    | CDL  | C60-C59-C58 | 2.31  | 126.16      | 114.42   |
| 19  | P     | 309    | PGV  | C03-C02-C01 | -2.31 | 106.33      | 111.79   |
| 19  | N     | 607    | PGV  | O12-P-O13   | 2.31  | 118.09      | 109.07   |
| 14  | N     | 601[B] | HEA  | C26-C15-C16 | 2.29  | 119.13      | 115.27   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24  | J     | 102    | CHD  | C1-C10-C5   | 2.29  | 111.16      | 107.77   |
| 25  | C     | 307    | CDL  | PB2-OB2-CB2 | 2.29  | 135.09      | 121.68   |
| 21  | Y     | 103    | TGL  | C26-C25-C24 | -2.28 | 102.83      | 114.42   |
| 25  | P     | 306    | CDL  | OA8-CA7-OA9 | -2.28 | 117.83      | 123.59   |
| 18  | P     | 303    | DMU  | C6-C1-C2    | 2.28  | 114.74      | 110.00   |
| 24  | P     | 304    | CHD  | C11-C12-C13 | -2.28 | 108.91      | 111.24   |
| 25  | C     | 307    | CDL  | OA6-CA5-C11 | 2.27  | 116.40      | 111.50   |
| 18  | K     | 103    | DMU  | O7-C3-C4    | 2.27  | 114.93      | 109.30   |
| 26  | C     | 308    | PEK  | C03-C02-C01 | 2.27  | 117.15      | 111.79   |
| 14  | N     | 602    | HEA  | CHA-C4D-C3D | -2.26 | 121.52      | 124.84   |
| 24  | L     | 102    | CHD  | C6-C5-C10   | 2.26  | 115.06      | 112.66   |
| 25  | G     | 102    | CDL  | C19-C18-C17 | 2.26  | 125.89      | 114.42   |
| 24  | G     | 101    | CHD  | C11-C9-C10  | -2.26 | 111.40      | 113.73   |
| 20  | V     | 101    | PSC  | C08-N-C05   | -2.26 | 100.69      | 109.92   |
| 24  | J     | 102    | CHD  | C6-C5-C10   | 2.25  | 115.05      | 112.66   |
| 18  | L     | 101    | DMU  | O5-C4-C3    | 2.25  | 114.50      | 109.75   |
| 19  | T     | 104    | PGV  | C22-C21-C20 | 2.25  | 121.28      | 113.19   |
| 24  | G     | 101    | CHD  | O3-C3-C4    | -2.24 | 105.39      | 109.85   |
| 25  | C     | 307    | CDL  | C62-C61-C60 | 2.24  | 125.80      | 114.42   |
| 18  | P     | 303    | DMU  | O5-C6-O16   | -2.24 | 104.67      | 109.97   |
| 25  | G     | 102    | CDL  | CA6-CA4-CA3 | -2.24 | 106.50      | 111.79   |
| 24  | J     | 102    | CHD  | C17-C13-C14 | -2.24 | 97.84       | 100.09   |
| 21  | Q     | 202    | TGL  | CG2-OG2-CB1 | -2.24 | 112.29      | 117.79   |
| 18  | M     | 101    | DMU  | O1-C9-C8    | 2.23  | 113.75      | 109.69   |
| 21  | Q     | 202    | TGL  | OG1-CA1-CA2 | 2.22  | 118.86      | 111.91   |
| 24  | L     | 102    | CHD  | O26-C24-C23 | 2.22  | 121.15      | 114.03   |
| 14  | A     | 601[A] | HEA  | C4A-CHB-C1B | -2.21 | 121.28      | 126.06   |
| 14  | A     | 601[B] | HEA  | C4A-CHB-C1B | -2.21 | 121.28      | 126.06   |
| 24  | J     | 102    | CHD  | C19-C10-C9  | -2.21 | 108.14      | 111.18   |
| 25  | P     | 306    | CDL  | OA4-PA1-OA3 | 2.20  | 123.13      | 112.24   |
| 26  | C     | 309    | PEK  | C03-C02-C01 | -2.20 | 106.58      | 111.79   |
| 14  | N     | 602    | HEA  | C2B-C1B-NB  | 2.20  | 112.51      | 109.88   |
| 21  | D     | 202    | TGL  | OG1-CA1-OA1 | -2.20 | 118.05      | 123.59   |
| 18  | M     | 101    | DMU  | C22-C19-C18 | -2.19 | 103.79      | 113.49   |
| 18  | M     | 101    | DMU  | C31-C28-C25 | -2.19 | 103.31      | 114.42   |
| 24  | P     | 305    | CHD  | C6-C5-C4    | -2.19 | 108.67      | 111.19   |
| 24  | J     | 102    | CHD  | C9-C10-C5   | 2.19  | 111.65      | 108.58   |
| 24  | C     | 306    | CHD  | O7-C7-C8    | 2.18  | 114.31      | 109.43   |
| 18  | L     | 101    | DMU  | O55-C2-C1   | -2.18 | 105.30      | 110.35   |
| 14  | N     | 602    | HEA  | CMC-C2C-C3C | 2.18  | 131.87      | 126.59   |
| 18  | Q     | 201    | DMU  | C6-C1-C2    | -2.18 | 105.46      | 110.00   |
| 25  | C     | 307    | CDL  | OA8-CA7-OA9 | -2.18 | 118.09      | 123.59   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 18  | Z     | 101    | DMU  | O7-C10-C5   | 2.18  | 113.74      | 108.10   |
| 19  | N     | 606    | PGV  | O03-C19-O04 | -2.17 | 118.11      | 123.59   |
| 25  | T     | 102    | CDL  | C62-C61-C60 | 2.17  | 125.44      | 114.42   |
| 14  | A     | 602    | HEA  | CHB-C4A-C3A | -2.16 | 121.56      | 125.26   |
| 24  | C     | 305    | CHD  | C6-C5-C10   | -2.16 | 110.36      | 112.66   |
| 18  | W     | 101    | DMU  | O5-C6-C1    | -2.16 | 105.78      | 110.35   |
| 18  | Y     | 101    | DMU  | O6-C11-C9   | 2.16  | 118.69      | 111.29   |
| 26  | F     | 102    | PEK  | O11-P-O14   | -2.16 | 100.64      | 109.07   |
| 20  | A     | 609    | PSC  | C29-C28-C27 | -2.16 | 103.48      | 114.42   |
| 21  | A     | 610    | TGL  | CB3-CB2-CB1 | -2.15 | 105.80      | 113.62   |
| 20  | A     | 609    | PSC  | C27-C26-C25 | -2.14 | 103.57      | 114.42   |
| 24  | C     | 305    | CHD  | C5-C6-C7    | 2.13  | 116.81      | 114.46   |
| 26  | P     | 308    | PEK  | O01-C1-C2   | 2.12  | 116.08      | 111.50   |
| 25  | P     | 306    | CDL  | O1-C1-CA2   | -2.12 | 102.11      | 109.56   |
| 19  | T     | 104    | PGV  | C02-O01-C1  | 2.12  | 123.01      | 117.79   |
| 14  | N     | 601[A] | HEA  | CAD-C3D-C2D | 2.12  | 131.82      | 127.88   |
| 14  | N     | 601[B] | HEA  | CAD-C3D-C2D | 2.12  | 131.82      | 127.88   |
| 25  | T     | 102    | CDL  | OB6-CB5-OB7 | -2.11 | 118.59      | 123.70   |
| 14  | N     | 601[B] | HEA  | O11-C11-C12 | 2.11  | 115.32      | 109.42   |
| 19  | P     | 310    | PGV  | O01-C1-O02  | -2.11 | 118.60      | 123.70   |
| 18  | P     | 303    | DMU  | C37-C34-C31 | -2.11 | 103.72      | 114.42   |
| 19  | C     | 310    | PGV  | O01-C1-C2   | 2.11  | 116.05      | 111.50   |
| 14  | N     | 602    | HEA  | C12-C13-C14 | -2.11 | 106.67      | 112.23   |
| 21  | Y     | 103    | TGL  | CG1-OG1-CA1 | 2.11  | 124.92      | 117.12   |
| 14  | A     | 601[A] | HEA  | C1A-CHA-C4D | -2.10 | 121.52      | 126.06   |
| 14  | A     | 601[B] | HEA  | C1A-CHA-C4D | -2.10 | 121.52      | 126.06   |
| 24  | Y     | 102    | CHD  | C14-C13-C12 | 2.10  | 109.36      | 107.40   |
| 14  | A     | 601[A] | HEA  | CMB-C2B-C3B | -2.10 | 126.34      | 130.34   |
| 14  | A     | 601[B] | HEA  | CMB-C2B-C3B | -2.10 | 126.34      | 130.34   |
| 18  | D     | 201    | DMU  | O49-C1-C6   | 2.10  | 115.15      | 110.05   |
| 26  | P     | 307    | PEK  | C8-C7-C6    | -2.09 | 101.72      | 112.02   |
| 18  | C     | 303    | DMU  | C3-C2-C1    | 2.09  | 114.48      | 110.82   |
| 19  | N     | 607    | PGV  | O11-P-O13   | -2.09 | 100.89      | 109.07   |
| 14  | N     | 602    | HEA  | C3B-C4B-NB  | 2.09  | 112.31      | 109.84   |
| 24  | G     | 101    | CHD  | C6-C5-C4    | -2.08 | 108.79      | 111.19   |
| 25  | G     | 102    | CDL  | C39-C38-C37 | 2.08  | 125.00      | 114.42   |
| 24  | C     | 306    | CHD  | C16-C15-C14 | -2.08 | 101.01      | 105.13   |
| 25  | P     | 306    | CDL  | O1-C1-CB2   | 2.08  | 116.84      | 109.56   |
| 14  | A     | 601[A] | HEA  | O1D-CGD-CBD | -2.08 | 116.41      | 123.08   |
| 14  | A     | 601[B] | HEA  | O1D-CGD-CBD | -2.08 | 116.41      | 123.08   |
| 26  | C     | 309    | PEK  | C3-C2-C1    | -2.07 | 106.08      | 113.62   |
| 20  | V     | 101    | PSC  | O03-C01-C02 | -2.07 | 102.40      | 108.43   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25  | C     | 307    | CDL  | OA6-CA4-CA3 | 2.06  | 115.87      | 108.40   |
| 18  | L     | 101    | DMU  | O7-C3-C4    | -2.06 | 103.80      | 109.45   |
| 18  | M     | 101    | DMU  | O7-C10-C5   | 2.06  | 113.43      | 108.10   |
| 24  | J     | 102    | CHD  | C6-C7-C8    | 2.05  | 113.67      | 111.48   |
| 14  | A     | 602    | HEA  | C1C-CHC-C4B | 2.05  | 131.21      | 126.34   |
| 18  | W     | 101    | DMU  | O5-C4-C57   | 2.05  | 110.12      | 106.83   |
| 24  | P     | 305    | CHD  | C22-C20-C17 | -2.05 | 106.06      | 110.28   |
| 24  | G     | 101    | CHD  | C4-C5-C10   | -2.04 | 110.49      | 112.66   |
| 21  | L     | 103    | TGL  | C21-C20-CA9 | -2.04 | 104.08      | 114.42   |
| 25  | C     | 307    | CDL  | OA4-PA1-OA3 | 2.04  | 122.30      | 112.24   |
| 18  | C     | 303    | DMU  | O55-C2-C3   | -2.04 | 105.64      | 110.35   |
| 18  | P     | 303    | DMU  | O4-C7-C5    | -2.04 | 105.64      | 110.35   |
| 18  | C     | 302    | DMU  | O5-C4-C57   | 2.03  | 111.49      | 106.44   |
| 18  | L     | 101    | DMU  | O55-C2-C3   | 2.03  | 115.33      | 109.94   |
| 14  | N     | 601[A] | HEA  | CBD-CAD-C3D | -2.03 | 107.00      | 112.63   |
| 14  | N     | 601[B] | HEA  | CBD-CAD-C3D | -2.03 | 107.00      | 112.63   |
| 25  | T     | 102    | CDL  | OB8-CB6-CB4 | 2.02  | 114.32      | 108.43   |
| 14  | A     | 601[B] | HEA  | C26-C15-C16 | 2.02  | 118.67      | 115.27   |
| 14  | N     | 601[A] | HEA  | C4C-NC-C1C  | -2.02 | 103.37      | 105.35   |
| 14  | N     | 601[B] | HEA  | C4C-NC-C1C  | -2.02 | 103.37      | 105.35   |
| 24  | L     | 102    | CHD  | C22-C23-C24 | -2.02 | 107.14      | 112.51   |
| 14  | A     | 601[B] | HEA  | O11-C11-C12 | 2.02  | 115.05      | 109.42   |
| 14  | A     | 602    | HEA  | CHC-C1C-NC  | -2.02 | 120.14      | 123.85   |
| 24  | C     | 306    | CHD  | C9-C10-C5   | 2.01  | 111.40      | 108.58   |
| 24  | Y     | 102    | CHD  | C21-C20-C22 | -2.01 | 107.22      | 110.36   |
| 25  | P     | 306    | CDL  | C39-C38-C37 | 2.01  | 124.61      | 114.42   |
| 20  | A     | 609    | PSC  | O01-C1-O02  | -2.00 | 118.86      | 123.70   |
| 14  | N     | 602    | HEA  | O2A-CGA-O1A | -2.00 | 118.31      | 123.30   |
| 21  | D     | 202    | TGL  | OG1-CA1-CA2 | 2.00  | 118.18      | 111.91   |

There are no chirality outliers.

All (811) torsion outliers are listed below:

| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 14  | N     | 601[A] | HEA  | C18-C19-C20-C21 |
| 14  | N     | 601[A] | HEA  | C27-C19-C20-C21 |
| 18  | C     | 302    | DMU  | C1-C6-O16-C18   |
| 18  | C     | 302    | DMU  | O5-C6-O16-C18   |
| 18  | W     | 101    | DMU  | O5-C6-O16-C18   |
| 18  | X     | 102    | DMU  | C3-C4-C57-O61   |
| 18  | X     | 102    | DMU  | O5-C4-C57-O61   |
| 19  | A     | 607    | PGV  | C2-C1-O01-C02   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 607 | PGV  | O04-C19-O03-C01 |
| 19  | A     | 607 | PGV  | C20-C19-O03-C01 |
| 19  | N     | 606 | PGV  | O02-C1-O01-C02  |
| 19  | N     | 606 | PGV  | C2-C1-O01-C02   |
| 19  | N     | 606 | PGV  | O04-C19-O03-C01 |
| 19  | N     | 606 | PGV  | C20-C19-O03-C01 |
| 19  | P     | 309 | PGV  | C10-C11-C12-C13 |
| 19  | P     | 310 | PGV  | O04-C19-O03-C01 |
| 19  | P     | 310 | PGV  | C20-C19-O03-C01 |
| 19  | T     | 104 | PGV  | C03-O11-P-O13   |
| 19  | T     | 104 | PGV  | C03-O11-P-O14   |
| 19  | T     | 104 | PGV  | O04-C19-O03-C01 |
| 19  | T     | 104 | PGV  | C20-C19-O03-C01 |
| 20  | A     | 609 | PSC  | O12-C04-C05-N   |
| 20  | A     | 609 | PSC  | O02-C1-O01-C02  |
| 20  | A     | 609 | PSC  | C2-C1-O01-C02   |
| 20  | V     | 101 | PSC  | C2-C1-O01-C02   |
| 21  | L     | 103 | TGL  | OB1-CB1-OG2-CG2 |
| 21  | Y     | 103 | TGL  | CB2-CB1-OG2-CG2 |
| 22  | N     | 619 | EDO  | O1-C1-C2-O2     |
| 25  | C     | 307 | CDL  | OA9-CA7-OA8-CA6 |
| 25  | C     | 307 | CDL  | C31-CA7-OA8-CA6 |
| 25  | C     | 307 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | C     | 307 | CDL  | CB3-OB5-PB2-OB3 |
| 25  | C     | 307 | CDL  | C51-CB5-OB6-CB4 |
| 25  | G     | 102 | CDL  | OA9-CA7-OA8-CA6 |
| 25  | G     | 102 | CDL  | C31-CA7-OA8-CA6 |
| 25  | G     | 102 | CDL  | CB2-OB2-PB2-OB3 |
| 25  | P     | 306 | CDL  | CA2-OA2-PA1-OA3 |
| 25  | P     | 306 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | P     | 306 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | P     | 306 | CDL  | OA9-CA7-OA8-CA6 |
| 25  | P     | 306 | CDL  | C31-CA7-OA8-CA6 |
| 25  | P     | 306 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | P     | 306 | CDL  | CB3-OB5-PB2-OB4 |
| 25  | T     | 102 | CDL  | CA3-OA5-PA1-OA4 |
| 26  | C     | 308 | PEK  | C03-O11-P-O12   |
| 26  | C     | 308 | PEK  | C03-O11-P-O13   |
| 26  | C     | 308 | PEK  | C03-O11-P-O14   |
| 26  | C     | 308 | PEK  | O04-C21-O03-C01 |
| 26  | C     | 308 | PEK  | C22-C21-O03-C01 |
| 26  | C     | 308 | PEK  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | C     | 308 | PEK  | C9-C10-C11-C12  |
| 26  | F     | 102 | PEK  | C04-O12-P-O13   |
| 26  | P     | 307 | PEK  | O04-C21-O03-C01 |
| 26  | P     | 307 | PEK  | C22-C21-O03-C01 |
| 26  | P     | 307 | PEK  | C11-C12-C13-C14 |
| 26  | T     | 103 | PEK  | O04-C21-O03-C01 |
| 26  | T     | 103 | PEK  | C22-C21-O03-C01 |
| 26  | T     | 103 | PEK  | C5-C6-C7-C8     |
| 25  | T     | 102 | CDL  | OA9-CA7-OA8-CA6 |
| 26  | F     | 102 | PEK  | O04-C21-O03-C01 |
| 18  | L     | 101 | DMU  | O1-C10-O7-C3    |
| 26  | F     | 102 | PEK  | C22-C21-O03-C01 |
| 20  | A     | 609 | PSC  | O04-C19-O03-C01 |
| 21  | Y     | 103 | TGL  | OA1-CA1-OG1-CG1 |
| 24  | L     | 102 | CHD  | C13-C17-C20-C21 |
| 19  | A     | 607 | PGV  | O02-C1-O01-C02  |
| 20  | V     | 101 | PSC  | O02-C1-O01-C02  |
| 21  | Y     | 103 | TGL  | OB1-CB1-OG2-CG2 |
| 25  | C     | 307 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | C     | 307 | CDL  | OB7-CB5-OB6-CB4 |
| 26  | T     | 103 | PEK  | O02-C1-O01-C02  |
| 21  | L     | 103 | TGL  | CA2-CA1-OG1-CG1 |
| 25  | T     | 102 | CDL  | C31-CA7-OA8-CA6 |
| 21  | L     | 103 | TGL  | CB2-CB1-OG2-CG2 |
| 26  | T     | 103 | PEK  | C2-C1-O01-C02   |
| 24  | C     | 306 | CHD  | C20-C22-C23-C24 |
| 20  | A     | 609 | PSC  | C20-C19-O03-C01 |
| 21  | Y     | 103 | TGL  | CA2-CA1-OG1-CG1 |
| 19  | P     | 310 | PGV  | C10-C11-C12-C13 |
| 20  | V     | 101 | PSC  | C11-C10-C9-C8   |
| 26  | C     | 308 | PEK  | C4-C5-C6-C7     |
| 26  | C     | 308 | PEK  | C7-C8-C9-C10    |
| 26  | P     | 307 | PEK  | C4-C5-C6-C7     |
| 26  | T     | 103 | PEK  | C13-C14-C15-C16 |
| 21  | L     | 103 | TGL  | OA1-CA1-OG1-CG1 |
| 18  | C     | 302 | DMU  | O6-C11-C9-O1    |
| 19  | A     | 607 | PGV  | O12-C04-C05-O05 |
| 18  | K     | 103 | DMU  | C3-C4-C57-O61   |
| 25  | C     | 307 | CDL  | C11-CA5-OA6-CA4 |
| 21  | L     | 103 | TGL  | CC1-CC2-CC3-CC4 |
| 18  | K     | 103 | DMU  | O5-C4-C57-O61   |
| 25  | P     | 306 | CDL  | C80-C81-C82-C83 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 24  | L     | 102    | CHD  | C16-C17-C20-C22 |
| 18  | C     | 302    | DMU  | O5-C4-C57-O61   |
| 18  | C     | 303    | DMU  | O5-C4-C57-O61   |
| 18  | Y     | 101    | DMU  | O5-C4-C57-O61   |
| 25  | T     | 102    | CDL  | C15-C16-C17-C18 |
| 24  | P     | 305    | CHD  | C21-C20-C22-C23 |
| 24  | C     | 306    | CHD  | C17-C20-C22-C23 |
| 24  | P     | 305    | CHD  | C17-C20-C22-C23 |
| 19  | N     | 606    | PGV  | C19-C20-C21-C22 |
| 21  | N     | 608    | TGL  | CC2-CC1-OG3-CG3 |
| 18  | C     | 302    | DMU  | C3-C4-C57-O61   |
| 18  | C     | 303    | DMU  | C3-C4-C57-O61   |
| 18  | Y     | 101    | DMU  | C3-C4-C57-O61   |
| 24  | C     | 306    | CHD  | C21-C20-C22-C23 |
| 21  | A     | 610    | TGL  | C22-C23-C24-C25 |
| 21  | N     | 608    | TGL  | CA1-CA2-CA3-CA4 |
| 25  | G     | 102    | CDL  | CA5-C11-C12-C13 |
| 21  | N     | 608    | TGL  | OC1-CC1-OG3-CG3 |
| 21  | N     | 608    | TGL  | CC1-CC2-CC3-CC4 |
| 26  | F     | 102    | PEK  | C10-C11-C12-C13 |
| 18  | L     | 101    | DMU  | C4-C3-O7-C10    |
| 25  | G     | 102    | CDL  | C80-C81-C82-C83 |
| 21  | D     | 202    | TGL  | OB1-CB1-OG2-CG2 |
| 21  | A     | 610    | TGL  | CA9-C20-C21-C22 |
| 22  | W     | 102    | EDO  | O1-C1-C2-O2     |
| 18  | C     | 302    | DMU  | O16-C18-C19-C22 |
| 24  | J     | 102    | CHD  | C13-C17-C20-C21 |
| 24  | J     | 102    | CHD  | C13-C17-C20-C22 |
| 14  | A     | 601[A] | HEA  | C15-C16-C17-C18 |
| 14  | N     | 601[A] | HEA  | C15-C16-C17-C18 |
| 18  | M     | 101    | DMU  | O16-C18-C19-C22 |
| 25  | T     | 102    | CDL  | C80-C81-C82-C83 |
| 21  | L     | 103    | TGL  | C21-C22-C23-C24 |
| 21  | N     | 608    | TGL  | CC6-CC7-CC8-CC9 |
| 24  | J     | 102    | CHD  | C16-C17-C20-C21 |
| 18  | L     | 101    | DMU  | C2-C3-O7-C10    |
| 18  | K     | 102    | DMU  | O16-C18-C19-C22 |
| 19  | A     | 607    | PGV  | C10-C11-C12-C13 |
| 19  | A     | 608    | PGV  | C10-C11-C12-C13 |
| 21  | D     | 202    | TGL  | CB2-CB1-OG2-CG2 |
| 25  | P     | 306    | CDL  | C11-CA5-OA6-CA4 |
| 25  | P     | 306    | CDL  | C51-CB5-OB6-CB4 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | T     | 104 | PGV  | C03-O11-P-O12   |
| 25  | C     | 307 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | C     | 307 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | C     | 307 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | G     | 102 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | P     | 306 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | P     | 306 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | T     | 102 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | T     | 102 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | T     | 102 | CDL  | CB3-OB5-PB2-OB2 |
| 26  | F     | 102 | PEK  | C04-O12-P-O11   |
| 21  | L     | 103 | TGL  | CB1-CB2-CB3-CB4 |
| 18  | J     | 101 | DMU  | O16-C18-C19-C22 |
| 18  | X     | 102 | DMU  | O16-C18-C19-C22 |
| 25  | C     | 307 | CDL  | C63-C64-C65-C66 |
| 25  | P     | 306 | CDL  | OA7-CA5-OA6-CA4 |
| 20  | V     | 101 | PSC  | C04-C05-N-C06   |
| 20  | V     | 101 | PSC  | C04-C05-N-C08   |
| 21  | Q     | 202 | TGL  | CC2-CC1-OG3-CG3 |
| 21  | Y     | 103 | TGL  | CA9-C20-C21-C22 |
| 21  | Q     | 202 | TGL  | CC1-CC2-CC3-CC4 |
| 21  | A     | 610 | TGL  | C16-C17-C18-C19 |
| 26  | P     | 307 | PEK  | C2-C1-O01-C02   |
| 18  | X     | 105 | DMU  | C31-C34-C37-C40 |
| 20  | V     | 101 | PSC  | C21-C22-C23-C24 |
| 21  | D     | 202 | TGL  | C21-C20-CA9-CA8 |
| 21  | N     | 608 | TGL  | C21-C20-CA9-CA8 |
| 25  | T     | 102 | CDL  | C57-C58-C59-C60 |
| 25  | T     | 102 | CDL  | C77-C78-C79-C80 |
| 26  | C     | 309 | PEK  | C31-C32-C33-C34 |
| 18  | X     | 103 | DMU  | C19-C22-C25-C28 |
| 25  | C     | 307 | CDL  | C40-C41-C42-C43 |
| 25  | G     | 102 | CDL  | C54-C55-C56-C57 |
| 21  | A     | 610 | TGL  | OB1-CB1-OG2-CG2 |
| 25  | P     | 306 | CDL  | OB7-CB5-OB6-CB4 |
| 26  | P     | 307 | PEK  | O02-C1-O01-C02  |
| 19  | N     | 607 | PGV  | C26-C27-C28-C29 |
| 26  | P     | 308 | PEK  | C4-C5-C6-C7     |
| 18  | Z     | 101 | DMU  | C22-C25-C28-C31 |
| 21  | N     | 608 | TGL  | CB1-CB2-CB3-CB4 |
| 21  | Q     | 202 | TGL  | CB1-CB2-CB3-CB4 |
| 18  | P     | 303 | DMU  | C1-C6-O16-C18   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | W     | 101 | DMU  | C1-C6-O16-C18   |
| 21  | A     | 610 | TGL  | CC2-CC1-OG3-CG3 |
| 18  | X     | 105 | DMU  | C25-C28-C31-C34 |
| 21  | Y     | 103 | TGL  | CA4-CA5-CA6-CA7 |
| 19  | N     | 606 | PGV  | C20-C21-C22-C23 |
| 19  | P     | 309 | PGV  | C7-C8-C9-C10    |
| 21  | N     | 608 | TGL  | CB4-CB5-CB6-CB7 |
| 25  | C     | 307 | CDL  | C17-C18-C19-C20 |
| 25  | G     | 102 | CDL  | C57-C58-C59-C60 |
| 18  | Q     | 201 | DMU  | C28-C31-C34-C37 |
| 21  | Q     | 202 | TGL  | C15-C16-C17-C18 |
| 21  | D     | 202 | TGL  | C16-C17-C18-C19 |
| 21  | L     | 103 | TGL  | CB5-CB6-CB7-CB8 |
| 21  | N     | 608 | TGL  | CA7-CA8-CA9-C20 |
| 21  | A     | 610 | TGL  | CB2-CB1-OG2-CG2 |
| 21  | L     | 103 | TGL  | C10-C11-C12-C13 |
| 25  | C     | 307 | CDL  | C80-C81-C82-C83 |
| 18  | L     | 101 | DMU  | C31-C34-C37-C40 |
| 19  | C     | 310 | PGV  | C7-C8-C9-C10    |
| 19  | N     | 606 | PGV  | C3-C4-C5-C6     |
| 21  | D     | 202 | TGL  | C20-C21-C22-C23 |
| 21  | Y     | 103 | TGL  | CA6-CA7-CA8-CA9 |
| 21  | Y     | 103 | TGL  | CB5-CB6-CB7-CB8 |
| 21  | Y     | 103 | TGL  | CC3-CC4-CC5-CC6 |
| 21  | Y     | 103 | TGL  | C21-C22-C23-C24 |
| 25  | G     | 102 | CDL  | C40-C41-C42-C43 |
| 25  | P     | 306 | CDL  | C60-C61-C62-C63 |
| 26  | C     | 308 | PEK  | C30-C31-C32-C33 |
| 26  | F     | 102 | PEK  | C29-C30-C31-C32 |
| 18  | P     | 303 | DMU  | O5-C6-O16-C18   |
| 19  | C     | 310 | PGV  | C27-C28-C29-C30 |
| 21  | N     | 608 | TGL  | CC5-CC6-CC7-CC8 |
| 26  | C     | 309 | PEK  | O12-C04-C05-N   |
| 21  | Y     | 103 | TGL  | CA2-CA3-CA4-CA5 |
| 21  | A     | 610 | TGL  | CC4-CC5-CC6-CC7 |
| 21  | D     | 202 | TGL  | C19-C33-C34-C35 |
| 21  | N     | 608 | TGL  | CA6-CA7-CA8-CA9 |
| 25  | C     | 307 | CDL  | C51-C52-C53-C54 |
| 18  | Q     | 201 | DMU  | C22-C25-C28-C31 |
| 20  | A     | 609 | PSC  | C24-C25-C26-C27 |
| 21  | N     | 608 | TGL  | CA4-CA5-CA6-CA7 |
| 21  | Q     | 202 | TGL  | C11-C10-CB9-CB8 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | P     | 303 | DMU  | C19-C18-O16-C6  |
| 18  | C     | 303 | DMU  | C22-C25-C28-C31 |
| 18  | M     | 101 | DMU  | C25-C28-C31-C34 |
| 21  | L     | 103 | TGL  | CA3-CA4-CA5-CA6 |
| 21  | Q     | 202 | TGL  | C19-C33-C34-C35 |
| 25  | G     | 102 | CDL  | C55-C56-C57-C58 |
| 19  | P     | 310 | PGV  | C1-C2-C3-C4     |
| 21  | L     | 103 | TGL  | C18-C19-C33-C34 |
| 26  | F     | 102 | PEK  | C26-C27-C28-C29 |
| 18  | K     | 102 | DMU  | C25-C28-C31-C34 |
| 18  | X     | 103 | DMU  | C25-C28-C31-C34 |
| 19  | T     | 104 | PGV  | C3-C4-C5-C6     |
| 21  | D     | 202 | TGL  | CB5-CB6-CB7-CB8 |
| 25  | C     | 307 | CDL  | C59-C60-C61-C62 |
| 25  | G     | 102 | CDL  | C77-C78-C79-C80 |
| 18  | C     | 302 | DMU  | O6-C11-C9-C8    |
| 18  | C     | 302 | DMU  | O1-C10-O7-C3    |
| 21  | Q     | 202 | TGL  | CA6-CA7-CA8-CA9 |
| 25  | P     | 306 | CDL  | C36-C37-C38-C39 |
| 25  | C     | 307 | CDL  | O1-C1-CA2-OA2   |
| 19  | P     | 310 | PGV  | C20-C21-C22-C23 |
| 21  | A     | 610 | TGL  | CC9-C15-C16-C17 |
| 21  | D     | 202 | TGL  | CC7-CC8-CC9-C15 |
| 21  | N     | 608 | TGL  | CB6-CB7-CB8-CB9 |
| 21  | Y     | 103 | TGL  | C22-C23-C24-C25 |
| 21  | A     | 610 | TGL  | C10-C11-C12-C13 |
| 21  | Q     | 202 | TGL  | C13-C14-C29-C30 |
| 21  | D     | 202 | TGL  | C11-C10-CB9-CB8 |
| 21  | Y     | 103 | TGL  | CB9-C10-C11-C12 |
| 21  | Q     | 202 | TGL  | OC1-CC1-OG3-CG3 |
| 18  | C     | 303 | DMU  | C19-C22-C25-C28 |
| 19  | P     | 309 | PGV  | C30-C31-C32-C33 |
| 21  | N     | 608 | TGL  | C20-C21-C22-C23 |
| 26  | C     | 309 | PEK  | C32-C33-C34-C35 |
| 20  | V     | 101 | PSC  | C04-C05-N-C07   |
| 22  | A     | 611 | EDO  | O1-C1-C2-O2     |
| 22  | A     | 615 | EDO  | O1-C1-C2-O2     |
| 22  | C     | 311 | EDO  | O1-C1-C2-O2     |
| 22  | P     | 312 | EDO  | O1-C1-C2-O2     |
| 22  | P     | 315 | EDO  | O1-C1-C2-O2     |
| 22  | Q     | 205 | EDO  | O1-C1-C2-O2     |
| 22  | T     | 105 | EDO  | O1-C1-C2-O2     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | D     | 201 | DMU  | O16-C18-C19-C22 |
| 21  | A     | 610 | TGL  | C16-C15-CC9-CC8 |
| 21  | L     | 103 | TGL  | CA2-CA3-CA4-CA5 |
| 25  | C     | 307 | CDL  | C31-C32-C33-C34 |
| 25  | G     | 102 | CDL  | C56-C57-C58-C59 |
| 18  | K     | 104 | DMU  | C18-C19-C22-C25 |
| 24  | L     | 102 | CHD  | C16-C17-C20-C21 |
| 18  | J     | 101 | DMU  | C31-C34-C37-C40 |
| 21  | A     | 610 | TGL  | CA5-CA6-CA7-CA8 |
| 25  | C     | 307 | CDL  | C20-C21-C22-C23 |
| 24  | L     | 102 | CHD  | C13-C17-C20-C22 |
| 21  | N     | 608 | TGL  | OB1-CB1-OG2-CG2 |
| 21  | Q     | 202 | TGL  | OB1-CB1-OG2-CG2 |
| 21  | D     | 202 | TGL  | CC9-C15-C16-C17 |
| 21  | L     | 103 | TGL  | C11-C12-C13-C14 |
| 19  | T     | 104 | PGV  | C24-C25-C26-C27 |
| 21  | N     | 608 | TGL  | C11-C10-CB9-CB8 |
| 21  | Q     | 202 | TGL  | CC2-CC3-CC4-CC5 |
| 25  | T     | 102 | CDL  | C20-C21-C22-C23 |
| 18  | Y     | 101 | DMU  | C28-C31-C34-C37 |
| 25  | P     | 306 | CDL  | C58-C59-C60-C61 |
| 26  | C     | 309 | PEK  | C26-C27-C28-C29 |
| 20  | V     | 101 | PSC  | C20-C19-O03-C01 |
| 18  | X     | 102 | DMU  | C18-C19-C22-C25 |
| 18  | K     | 103 | DMU  | C19-C22-C25-C28 |
| 21  | A     | 610 | TGL  | C24-C25-C26-C27 |
| 21  | D     | 202 | TGL  | C16-C15-CC9-CC8 |
| 25  | G     | 102 | CDL  | C37-C38-C39-C40 |
| 25  | G     | 102 | CDL  | C60-C61-C62-C63 |
| 25  | T     | 102 | CDL  | C14-C15-C16-C17 |
| 21  | N     | 608 | TGL  | CB2-CB1-OG2-CG2 |
| 21  | Q     | 202 | TGL  | CB2-CB1-OG2-CG2 |
| 25  | G     | 102 | CDL  | C51-CB5-OB6-CB4 |
| 25  | T     | 102 | CDL  | C11-CA5-OA6-CA4 |
| 19  | P     | 310 | PGV  | O01-C02-C03-O11 |
| 21  | A     | 610 | TGL  | CB4-CB5-CB6-CB7 |
| 20  | A     | 609 | PSC  | C3-C4-C5-C6     |
| 25  | G     | 102 | CDL  | OB7-CB5-OB6-CB4 |
| 18  | X     | 102 | DMU  | C28-C31-C34-C37 |
| 21  | N     | 608 | TGL  | C16-C15-CC9-CC8 |
| 21  | Y     | 103 | TGL  | C19-C33-C34-C35 |
| 18  | L     | 101 | DMU  | O5-C4-C57-O61   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | P     | 310 | PGV  | C28-C29-C30-C31 |
| 21  | Q     | 202 | TGL  | C22-C23-C24-C25 |
| 25  | T     | 102 | CDL  | OA7-CA5-OA6-CA4 |
| 18  | X     | 104 | DMU  | C22-C25-C28-C31 |
| 18  | M     | 101 | DMU  | C19-C22-C25-C28 |
| 21  | N     | 608 | TGL  | CA2-CA1-OG1-CG1 |
| 25  | C     | 307 | CDL  | OA5-CA3-CA4-CA6 |
| 25  | G     | 102 | CDL  | OB5-CB3-CB4-CB6 |
| 26  | T     | 103 | PEK  | C01-C02-C03-O11 |
| 26  | C     | 308 | PEK  | C21-C22-C23-C24 |
| 26  | P     | 308 | PEK  | C26-C27-C28-C29 |
| 18  | Y     | 101 | DMU  | C25-C28-C31-C34 |
| 21  | N     | 608 | TGL  | CC9-C15-C16-C17 |
| 26  | F     | 102 | PEK  | C27-C28-C29-C30 |
| 18  | X     | 102 | DMU  | C34-C37-C40-C43 |
| 25  | T     | 102 | CDL  | CB3-CB4-CB6-OB8 |
| 26  | P     | 308 | PEK  | C10-C11-C12-C13 |
| 20  | V     | 101 | PSC  | O04-C19-O03-C01 |
| 21  | A     | 610 | TGL  | OC1-CC1-OG3-CG3 |
| 25  | G     | 102 | CDL  | C24-C25-C26-C27 |
| 20  | A     | 609 | PSC  | C2-C3-C4-C5     |
| 25  | T     | 102 | CDL  | C79-C80-C81-C82 |
| 18  | L     | 101 | DMU  | C25-C28-C31-C34 |
| 18  | X     | 101 | DMU  | C18-C19-C22-C25 |
| 19  | A     | 607 | PGV  | C2-C3-C4-C5     |
| 25  | P     | 306 | CDL  | C77-C78-C79-C80 |
| 18  | K     | 102 | DMU  | C18-C19-C22-C25 |
| 20  | V     | 101 | PSC  | C03-C02-O01-C1  |
| 18  | A     | 606 | DMU  | C22-C25-C28-C31 |
| 21  | Y     | 103 | TGL  | C13-C14-C29-C30 |
| 25  | C     | 307 | CDL  | C58-C59-C60-C61 |
| 25  | C     | 307 | CDL  | C83-C84-C85-C86 |
| 18  | Q     | 201 | DMU  | O5-C4-C57-O61   |
| 18  | Z     | 101 | DMU  | C25-C28-C31-C34 |
| 21  | Q     | 202 | TGL  | C21-C20-CA9-CA8 |
| 21  | Q     | 202 | TGL  | CC9-C15-C16-C17 |
| 19  | N     | 607 | PGV  | C29-C30-C31-C32 |
| 25  | C     | 307 | CDL  | OA5-CA3-CA4-OA6 |
| 25  | T     | 102 | CDL  | OA5-CA3-CA4-OA6 |
| 26  | C     | 309 | PEK  | C13-C14-C15-C16 |
| 26  | P     | 308 | PEK  | C7-C8-C9-C10    |
| 26  | P     | 308 | PEK  | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | T     | 103 | PEK  | C4-C5-C6-C7     |
| 18  | K     | 104 | DMU  | C22-C25-C28-C31 |
| 20  | V     | 101 | PSC  | C23-C24-C25-C26 |
| 18  | K     | 101 | DMU  | C18-C19-C22-C25 |
| 22  | C     | 316 | EDO  | O1-C1-C2-O2     |
| 22  | F     | 110 | EDO  | O1-C1-C2-O2     |
| 21  | L     | 103 | TGL  | C11-C10-CB9-CB8 |
| 18  | P     | 303 | DMU  | O6-C11-C9-C8    |
| 21  | Y     | 103 | TGL  | CB1-CB2-CB3-CB4 |
| 18  | K     | 103 | DMU  | C1-C6-O16-C18   |
| 20  | V     | 101 | PSC  | O03-C01-C02-O01 |
| 21  | Y     | 103 | TGL  | OG2-CG2-CG3-OG3 |
| 25  | T     | 102 | CDL  | OB6-CB4-CB6-OB8 |
| 21  | Y     | 103 | TGL  | CB4-CB5-CB6-CB7 |
| 25  | C     | 307 | CDL  | C37-C38-C39-C40 |
| 21  | N     | 608 | TGL  | OA1-CA1-OG1-CG1 |
| 19  | N     | 606 | PGV  | C4-C5-C6-C7     |
| 26  | C     | 309 | PEK  | C30-C31-C32-C33 |
| 24  | C     | 306 | CHD  | C16-C17-C20-C21 |
| 19  | A     | 607 | PGV  | O12-C04-C05-C06 |
| 25  | T     | 102 | CDL  | C39-C40-C41-C42 |
| 21  | L     | 103 | TGL  | CC2-CC1-OG3-CG3 |
| 18  | M     | 101 | DMU  | C34-C37-C40-C43 |
| 19  | T     | 104 | PGV  | C31-C32-C33-C34 |
| 21  | A     | 610 | TGL  | C12-C13-C14-C29 |
| 26  | F     | 102 | PEK  | C13-C14-C15-C16 |
| 19  | P     | 310 | PGV  | C01-C02-C03-O11 |
| 25  | P     | 306 | CDL  | OA5-CA3-CA4-CA6 |
| 18  | X     | 104 | DMU  | O16-C18-C19-C22 |
| 21  | A     | 610 | TGL  | C15-C16-C17-C18 |
| 26  | C     | 308 | PEK  | C27-C28-C29-C30 |
| 19  | A     | 607 | PGV  | C20-C21-C22-C23 |
| 25  | T     | 102 | CDL  | CA7-C31-C32-C33 |
| 25  | G     | 102 | CDL  | C71-CB7-OB8-CB6 |
| 21  | A     | 610 | TGL  | C14-C29-C30-C31 |
| 18  | M     | 101 | DMU  | C22-C25-C28-C31 |
| 21  | D     | 202 | TGL  | CC5-CC6-CC7-CC8 |
| 20  | V     | 101 | PSC  | C3-C4-C5-C6     |
| 19  | N     | 606 | PGV  | O03-C01-C02-C03 |
| 21  | L     | 103 | TGL  | OG1-CG1-CG2-CG3 |
| 25  | C     | 307 | CDL  | CB3-CB4-CB6-OB8 |
| 25  | G     | 102 | CDL  | CB3-CB4-CB6-OB8 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 25  | P     | 306    | CDL  | CB3-CB4-CB6-OB8 |
| 26  | F     | 102    | PEK  | O03-C01-C02-C03 |
| 18  | B     | 302    | DMU  | C31-C34-C37-C40 |
| 19  | N     | 606    | PGV  | C10-C11-C12-C13 |
| 19  | N     | 607    | PGV  | C10-C11-C12-C13 |
| 26  | C     | 309    | PEK  | C4-C5-C6-C7     |
| 26  | F     | 102    | PEK  | C4-C5-C6-C7     |
| 21  | Q     | 202    | TGL  | C17-C18-C19-C33 |
| 18  | X     | 103    | DMU  | C22-C25-C28-C31 |
| 25  | C     | 307    | CDL  | C55-C56-C57-C58 |
| 25  | C     | 307    | CDL  | C82-C83-C84-C85 |
| 25  | P     | 306    | CDL  | C17-C18-C19-C20 |
| 25  | C     | 307    | CDL  | C78-C79-C80-C81 |
| 25  | P     | 306    | CDL  | C59-C60-C61-C62 |
| 14  | A     | 601[A] | HEA  | C2A-C3A-CMA-OMA |
| 14  | A     | 601[B] | HEA  | C2A-C3A-CMA-OMA |
| 14  | A     | 602    | HEA  | C2A-C3A-CMA-OMA |
| 14  | N     | 601[A] | HEA  | C2A-C3A-CMA-OMA |
| 14  | N     | 601[B] | HEA  | C2A-C3A-CMA-OMA |
| 20  | A     | 609    | PSC  | C03-O11-P-O12   |
| 20  | A     | 609    | PSC  | C9-C10-C11-C12  |
| 20  | A     | 609    | PSC  | C10-C11-C12-C13 |
| 20  | V     | 101    | PSC  | C10-C11-C12-C13 |
| 26  | C     | 308    | PEK  | C5-C6-C7-C8     |
| 26  | C     | 308    | PEK  | C11-C10-C9-C8   |
| 26  | C     | 308    | PEK  | C11-C12-C13-C14 |
| 26  | C     | 308    | PEK  | C12-C13-C14-C15 |
| 26  | C     | 309    | PEK  | C5-C6-C7-C8     |
| 26  | C     | 309    | PEK  | C9-C10-C11-C12  |
| 26  | C     | 309    | PEK  | C11-C12-C13-C14 |
| 26  | F     | 102    | PEK  | C5-C6-C7-C8     |
| 26  | F     | 102    | PEK  | C6-C7-C8-C9     |
| 26  | F     | 102    | PEK  | C11-C10-C9-C8   |
| 26  | F     | 102    | PEK  | C9-C10-C11-C12  |
| 26  | F     | 102    | PEK  | C11-C12-C13-C14 |
| 26  | F     | 102    | PEK  | C12-C13-C14-C15 |
| 26  | P     | 307    | PEK  | C5-C6-C7-C8     |
| 26  | P     | 307    | PEK  | C6-C7-C8-C9     |
| 26  | P     | 307    | PEK  | C11-C10-C9-C8   |
| 26  | P     | 307    | PEK  | C12-C13-C14-C15 |
| 26  | P     | 308    | PEK  | C11-C12-C13-C14 |
| 26  | P     | 308    | PEK  | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | T     | 103 | PEK  | C6-C7-C8-C9     |
| 26  | T     | 103 | PEK  | C11-C10-C9-C8   |
| 26  | T     | 103 | PEK  | C9-C10-C11-C12  |
| 26  | T     | 103 | PEK  | C11-C12-C13-C14 |
| 26  | T     | 103 | PEK  | C12-C13-C14-C15 |
| 21  | A     | 610 | TGL  | CB1-CB2-CB3-CB4 |
| 25  | G     | 102 | CDL  | OB9-CB7-OB8-CB6 |
| 18  | C     | 304 | DMU  | C34-C37-C40-C43 |
| 21  | D     | 202 | TGL  | CB4-CB5-CB6-CB7 |
| 21  | Y     | 103 | TGL  | C11-C10-CB9-CB8 |
| 25  | G     | 102 | CDL  | C33-C34-C35-C36 |
| 25  | G     | 102 | CDL  | OB5-CB3-CB4-OB6 |
| 25  | P     | 306 | CDL  | OA5-CA3-CA4-OA6 |
| 18  | X     | 105 | DMU  | C22-C25-C28-C31 |
| 21  | L     | 103 | TGL  | C15-C16-C17-C18 |
| 24  | C     | 306 | CHD  | C13-C17-C20-C21 |
| 19  | N     | 606 | PGV  | O03-C01-C02-O01 |
| 25  | G     | 102 | CDL  | OB6-CB4-CB6-OB8 |
| 21  | N     | 608 | TGL  | C13-C14-C29-C30 |
| 18  | W     | 101 | DMU  | C18-C19-C22-C25 |
| 25  | G     | 102 | CDL  | C81-C82-C83-C84 |
| 25  | T     | 102 | CDL  | C56-C57-C58-C59 |
| 19  | T     | 104 | PGV  | O02-C1-O01-C02  |
| 18  | B     | 302 | DMU  | C19-C22-C25-C28 |
| 18  | C     | 304 | DMU  | C31-C34-C37-C40 |
| 19  | C     | 310 | PGV  | C24-C25-C26-C27 |
| 25  | T     | 102 | CDL  | C82-C83-C84-C85 |
| 18  | C     | 304 | DMU  | C18-C19-C22-C25 |
| 20  | V     | 101 | PSC  | C24-C25-C26-C27 |
| 19  | P     | 309 | PGV  | C02-C03-O11-P   |
| 21  | L     | 103 | TGL  | C14-C29-C30-C31 |
| 24  | P     | 305 | CHD  | C20-C22-C23-C24 |
| 25  | T     | 102 | CDL  | C71-C72-C73-C74 |
| 22  | N     | 623 | EDO  | O1-C1-C2-O2     |
| 22  | P     | 313 | EDO  | O1-C1-C2-O2     |
| 18  | X     | 102 | DMU  | C22-C25-C28-C31 |
| 21  | L     | 103 | TGL  | C12-C13-C14-C29 |
| 25  | G     | 102 | CDL  | C14-C15-C16-C17 |
| 25  | T     | 102 | CDL  | OB7-CB5-OB6-CB4 |
| 19  | T     | 104 | PGV  | C2-C1-O01-C02   |
| 25  | T     | 102 | CDL  | C51-CB5-OB6-CB4 |
| 25  | T     | 102 | CDL  | C40-C41-C42-C43 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | Z     | 101 | DMU  | O6-C11-C9-C8    |
| 24  | C     | 306 | CHD  | C16-C17-C20-C22 |
| 25  | T     | 102 | CDL  | C33-C34-C35-C36 |
| 25  | C     | 307 | CDL  | CA7-C31-C32-C33 |
| 20  | A     | 609 | PSC  | C15-C16-C17-C18 |
| 21  | N     | 608 | TGL  | CB7-CB8-CB9-C10 |
| 26  | P     | 307 | PEK  | C29-C30-C31-C32 |
| 21  | Q     | 202 | TGL  | CC5-CC6-CC7-CC8 |
| 21  | Y     | 103 | TGL  | C20-C21-C22-C23 |
| 18  | Q     | 201 | DMU  | C25-C28-C31-C34 |
| 21  | Y     | 103 | TGL  | C12-C13-C14-C29 |
| 24  | C     | 306 | CHD  | C13-C17-C20-C22 |
| 21  | L     | 103 | TGL  | C17-C18-C19-C33 |
| 21  | D     | 202 | TGL  | CA1-CA2-CA3-CA4 |
| 21  | Q     | 202 | TGL  | CA9-C20-C21-C22 |
| 25  | T     | 102 | CDL  | C71-CB7-OB8-CB6 |
| 21  | A     | 610 | TGL  | C29-C30-C31-C32 |
| 18  | Z     | 101 | DMU  | C28-C31-C34-C37 |
| 26  | P     | 308 | PEK  | C22-C23-C24-C25 |
| 19  | C     | 310 | PGV  | C13-C14-C15-C16 |
| 19  | T     | 104 | PGV  | C1-C2-C3-C4     |
| 21  | A     | 610 | TGL  | CG1-CG2-CG3-OG3 |
| 21  | Y     | 103 | TGL  | CG1-CG2-CG3-OG3 |
| 25  | G     | 102 | CDL  | CA3-CA4-CA6-OA8 |
| 25  | T     | 102 | CDL  | CA3-CA4-CA6-OA8 |
| 21  | L     | 103 | TGL  | OG1-CA1-CA2-CA3 |
| 21  | Q     | 202 | TGL  | CB9-C10-C11-C12 |
| 25  | T     | 102 | CDL  | O1-C1-CA2-OA2   |
| 25  | P     | 306 | CDL  | C72-C73-C74-C75 |
| 21  | A     | 610 | TGL  | OG2-CG2-CG3-OG3 |
| 21  | L     | 103 | TGL  | OG1-CG1-CG2-OG2 |
| 25  | C     | 307 | CDL  | OB6-CB4-CB6-OB8 |
| 25  | P     | 306 | CDL  | OB6-CB4-CB6-OB8 |
| 18  | C     | 304 | DMU  | C19-C22-C25-C28 |
| 21  | L     | 103 | TGL  | OC1-CC1-OG3-CG3 |
| 21  | N     | 608 | TGL  | CC7-CC8-CC9-C15 |
| 25  | T     | 102 | CDL  | OB9-CB7-OB8-CB6 |
| 19  | N     | 607 | PGV  | C14-C15-C16-C17 |
| 21  | Y     | 103 | TGL  | CB7-CB8-CB9-C10 |
| 19  | P     | 309 | PGV  | C24-C25-C26-C27 |
| 21  | Y     | 103 | TGL  | C33-C34-C35-C36 |
| 18  | D     | 201 | DMU  | C3-C4-C57-O61   |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 19  | C     | 310    | PGV  | C1-C2-C3-C4     |
| 18  | C     | 302    | DMU  | C34-C37-C40-C43 |
| 26  | T     | 103    | PEK  | C04-O12-P-O11   |
| 21  | Y     | 103    | TGL  | C25-C26-C27-C28 |
| 19  | C     | 310    | PGV  | C02-C03-O11-P   |
| 19  | P     | 310    | PGV  | C02-C03-O11-P   |
| 19  | T     | 104    | PGV  | C02-C03-O11-P   |
| 25  | C     | 307    | CDL  | CA3-OA5-PA1-OA3 |
| 25  | C     | 307    | CDL  | CB3-OB5-PB2-OB4 |
| 25  | G     | 102    | CDL  | CA3-OA5-PA1-OA3 |
| 25  | P     | 306    | CDL  | CA3-OA5-PA1-OA3 |
| 25  | P     | 306    | CDL  | CB2-OB2-PB2-OB3 |
| 25  | T     | 102    | CDL  | CB2-OB2-PB2-OB3 |
| 25  | T     | 102    | CDL  | CB3-OB5-PB2-OB3 |
| 26  | F     | 102    | PEK  | C04-O12-P-O14   |
| 25  | T     | 102    | CDL  | OA5-CA3-CA4-CA6 |
| 22  | A     | 619    | EDO  | O1-C1-C2-O2     |
| 22  | E     | 202    | EDO  | O1-C1-C2-O2     |
| 22  | N     | 618    | EDO  | O1-C1-C2-O2     |
| 22  | P     | 317    | EDO  | O1-C1-C2-O2     |
| 19  | P     | 310    | PGV  | C25-C26-C27-C28 |
| 26  | C     | 309    | PEK  | C7-C8-C9-C10    |
| 18  | C     | 303    | DMU  | O16-C18-C19-C22 |
| 25  | G     | 102    | CDL  | CA7-C31-C32-C33 |
| 19  | A     | 607    | PGV  | C14-C15-C16-C17 |
| 19  | P     | 309    | PGV  | C12-C13-C14-C15 |
| 19  | T     | 104    | PGV  | C29-C30-C31-C32 |
| 25  | C     | 307    | CDL  | CB7-C71-C72-C73 |
| 18  | M     | 101    | DMU  | O6-C11-C9-C8    |
| 26  | T     | 103    | PEK  | O01-C02-C03-O11 |
| 18  | K     | 101    | DMU  | C25-C28-C31-C34 |
| 20  | V     | 101    | PSC  | C20-C21-C22-C23 |
| 21  | L     | 103    | TGL  | C24-C25-C26-C27 |
| 21  | N     | 608    | TGL  | CB3-CB4-CB5-CB6 |
| 14  | N     | 601[A] | HEA  | C4A-C3A-CMA-OMA |
| 14  | N     | 601[B] | HEA  | C4A-C3A-CMA-OMA |
| 14  | N     | 602    | HEA  | C4A-C3A-CMA-OMA |
| 26  | T     | 103    | PEK  | C28-C29-C30-C31 |
| 26  | F     | 102    | PEK  | O03-C01-C02-O01 |
| 18  | K     | 104    | DMU  | C25-C28-C31-C34 |
| 21  | L     | 103    | TGL  | C25-C26-C27-C28 |
| 26  | F     | 102    | PEK  | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | P     | 306 | CDL  | C37-C38-C39-C40 |
| 25  | P     | 306 | CDL  | C55-C56-C57-C58 |
| 18  | Z     | 101 | DMU  | C34-C37-C40-C43 |
| 18  | J     | 101 | DMU  | C25-C28-C31-C34 |
| 21  | Q     | 202 | TGL  | OG3-CC1-CC2-CC3 |
| 25  | T     | 102 | CDL  | C32-C31-CA7-OA8 |
| 25  | C     | 307 | CDL  | C61-C62-C63-C64 |
| 21  | L     | 103 | TGL  | C16-C15-CC9-CC8 |
| 19  | A     | 607 | PGV  | C11-C10-C9-C8   |
| 21  | Y     | 103 | TGL  | CB6-CB7-CB8-CB9 |
| 18  | K     | 104 | DMU  | C31-C34-C37-C40 |
| 21  | A     | 610 | TGL  | CB9-C10-C11-C12 |
| 21  | Q     | 202 | TGL  | C12-C13-C14-C29 |
| 21  | A     | 610 | TGL  | CB6-CB7-CB8-CB9 |
| 21  | Y     | 103 | TGL  | CC2-CC3-CC4-CC5 |
| 18  | Q     | 201 | DMU  | C31-C34-C37-C40 |
| 25  | P     | 306 | CDL  | C42-C43-C44-C45 |
| 25  | T     | 102 | CDL  | CA3-CA4-OA6-CA5 |
| 26  | F     | 102 | PEK  | C16-C17-C18-C19 |
| 18  | D     | 201 | DMU  | C18-C19-C22-C25 |
| 18  | C     | 303 | DMU  | C28-C31-C34-C37 |
| 21  | A     | 610 | TGL  | C17-C18-C19-C33 |
| 25  | C     | 307 | CDL  | CA4-CA3-OA5-PA1 |
| 26  | P     | 307 | PEK  | C10-C11-C12-C13 |
| 21  | Y     | 103 | TGL  | C24-C25-C26-C27 |
| 22  | N     | 612 | EDO  | O1-C1-C2-O2     |
| 22  | P     | 314 | EDO  | O1-C1-C2-O2     |
| 22  | S     | 103 | EDO  | O1-C1-C2-O2     |
| 18  | X     | 104 | DMU  | C31-C34-C37-C40 |
| 18  | K     | 103 | DMU  | O5-C6-O16-C18   |
| 19  | N     | 606 | PGV  | C11-C12-C13-C14 |
| 24  | L     | 102 | CHD  | C20-C22-C23-C24 |
| 21  | A     | 610 | TGL  | OG1-CG1-CG2-OG2 |
| 19  | P     | 310 | PGV  | C03-O11-P-O12   |
| 25  | G     | 102 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | G     | 102 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | G     | 102 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | T     | 102 | CDL  | CA2-OA2-PA1-OA5 |
| 19  | P     | 309 | PGV  | C1-C2-C3-C4     |
| 21  | A     | 610 | TGL  | CC7-CC8-CC9-C15 |
| 21  | L     | 103 | TGL  | C21-C20-CA9-CA8 |
| 18  | J     | 101 | DMU  | C18-C19-C22-C25 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 21  | A     | 610    | TGL  | C11-C12-C13-C14 |
| 18  | P     | 303    | DMU  | C34-C37-C40-C43 |
| 19  | P     | 309    | PGV  | C20-C21-C22-C23 |
| 21  | D     | 202    | TGL  | CA3-CA4-CA5-CA6 |
| 26  | C     | 309    | PEK  | C25-C26-C27-C28 |
| 21  | A     | 610    | TGL  | CA4-CA5-CA6-CA7 |
| 19  | A     | 607    | PGV  | C05-C04-O12-P   |
| 25  | C     | 307    | CDL  | C1-CA2-OA2-PA1  |
| 19  | A     | 608    | PGV  | C11-C12-C13-C14 |
| 20  | V     | 101    | PSC  | C7-C8-C9-C10    |
| 19  | P     | 309    | PGV  | C28-C29-C30-C31 |
| 25  | P     | 306    | CDL  | CB7-C71-C72-C73 |
| 21  | A     | 610    | TGL  | CA2-CA1-OG1-CG1 |
| 25  | P     | 306    | CDL  | C41-C42-C43-C44 |
| 14  | N     | 602    | HEA  | CAA-CBA-CGA-O1A |
| 24  | T     | 101    | CHD  | C22-C23-C24-O26 |
| 19  | T     | 104    | PGV  | C19-C20-C21-C22 |
| 21  | Q     | 202    | TGL  | CC6-CC7-CC8-CC9 |
| 14  | N     | 601[A] | HEA  | C19-C20-C21-C22 |
| 21  | Q     | 202    | TGL  | CA4-CA5-CA6-CA7 |
| 26  | P     | 308    | PEK  | O12-C04-C05-N   |
| 24  | Y     | 102    | CHD  | C13-C17-C20-C21 |
| 21  | N     | 608    | TGL  | CC2-CC3-CC4-CC5 |
| 25  | G     | 102    | CDL  | C72-C73-C74-C75 |
| 24  | C     | 306    | CHD  | C22-C23-C24-O26 |
| 24  | J     | 102    | CHD  | C22-C23-C24-O26 |
| 21  | Y     | 103    | TGL  | CB3-CB4-CB5-CB6 |
| 21  | Y     | 103    | TGL  | C17-C18-C19-C33 |
| 25  | P     | 306    | CDL  | C73-C74-C75-C76 |
| 14  | A     | 601[A] | HEA  | CAD-CBD-CGD-O1D |
| 14  | A     | 601[B] | HEA  | CAD-CBD-CGD-O1D |
| 22  | D     | 203    | EDO  | O1-C1-C2-O2     |
| 24  | J     | 102    | CHD  | C22-C23-C24-O25 |
| 18  | X     | 105    | DMU  | C19-C22-C25-C28 |
| 25  | P     | 306    | CDL  | C20-C21-C22-C23 |
| 24  | T     | 101    | CHD  | C22-C23-C24-O25 |
| 26  | P     | 307    | PEK  | C7-C8-C9-C10    |
| 21  | N     | 608    | TGL  | CA2-CA3-CA4-CA5 |
| 19  | T     | 104    | PGV  | C14-C15-C16-C17 |
| 24  | G     | 101    | CHD  | C22-C23-C24-O26 |
| 21  | Q     | 202    | TGL  | C11-C12-C13-C14 |
| 14  | A     | 602    | HEA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 26  | P     | 307    | PEK  | C03-C02-O01-C1  |
| 14  | A     | 602    | HEA  | CAA-CBA-CGA-O1A |
| 14  | N     | 602    | HEA  | C2A-C3A-CMA-OMA |
| 20  | V     | 101    | PSC  | C9-C10-C11-C12  |
| 26  | C     | 309    | PEK  | C12-C13-C14-C15 |
| 26  | P     | 307    | PEK  | C9-C10-C11-C12  |
| 26  | P     | 308    | PEK  | C6-C7-C8-C9     |
| 24  | G     | 101    | CHD  | C22-C23-C24-O25 |
| 18  | C     | 303    | DMU  | C18-C19-C22-C25 |
| 14  | N     | 602    | HEA  | CAD-CBD-CGD-O1D |
| 19  | A     | 607    | PGV  | C4-C5-C6-C7     |
| 18  | L     | 101    | DMU  | C5-C10-O7-C3    |
| 14  | A     | 602    | HEA  | CAD-CBD-CGD-O2D |
| 19  | A     | 607    | PGV  | C19-C20-C21-C22 |
| 14  | N     | 602    | HEA  | CAA-CBA-CGA-O2A |
| 18  | M     | 101    | DMU  | C28-C31-C34-C37 |
| 18  | X     | 102    | DMU  | C31-C34-C37-C40 |
| 21  | Q     | 202    | TGL  | CB3-CB4-CB5-CB6 |
| 25  | P     | 306    | CDL  | OA6-CA4-CA6-OA8 |
| 19  | P     | 310    | PGV  | C5-C6-C7-C8     |
| 21  | D     | 202    | TGL  | OC1-CC1-OG3-CG3 |
| 18  | X     | 103    | DMU  | O16-C18-C19-C22 |
| 18  | A     | 606    | DMU  | C28-C31-C34-C37 |
| 18  | K     | 103    | DMU  | O16-C18-C19-C22 |
| 21  | L     | 103    | TGL  | CC3-CC4-CC5-CC6 |
| 14  | A     | 601[A] | HEA  | C19-C20-C21-C22 |
| 14  | N     | 602    | HEA  | CAD-CBD-CGD-O2D |
| 19  | N     | 606    | PGV  | C31-C32-C33-C34 |
| 25  | P     | 306    | CDL  | C51-C52-C53-C54 |
| 18  | P     | 303    | DMU  | C31-C34-C37-C40 |
| 26  | P     | 307    | PEK  | C27-C28-C29-C30 |
| 21  | L     | 103    | TGL  | CA9-C20-C21-C22 |
| 26  | T     | 103    | PEK  | C34-C35-C36-C37 |
| 19  | A     | 608    | PGV  | O03-C19-C20-C21 |
| 25  | P     | 306    | CDL  | C38-C39-C40-C41 |
| 14  | A     | 602    | HEA  | CAA-CBA-CGA-O2A |
| 22  | J     | 103    | EDO  | O1-C1-C2-O2     |
| 22  | Q     | 203    | EDO  | O1-C1-C2-O2     |
| 26  | T     | 103    | PEK  | C33-C34-C35-C36 |
| 25  | G     | 102    | CDL  | C11-C12-C13-C14 |
| 25  | P     | 306    | CDL  | C34-C35-C36-C37 |
| 21  | L     | 103    | TGL  | C33-C34-C35-C36 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 19  | P     | 310    | PGV  | C11-C12-C13-C14 |
| 26  | C     | 308    | PEK  | C3-C4-C5-C6     |
| 26  | T     | 103    | PEK  | C14-C15-C16-C17 |
| 18  | C     | 302    | DMU  | C5-C10-O7-C3    |
| 24  | P     | 304    | CHD  | C22-C23-C24-O25 |
| 19  | A     | 607    | PGV  | O01-C1-C2-C3    |
| 14  | N     | 601[A] | HEA  | CAD-CBD-CGD-O1D |
| 14  | N     | 601[B] | HEA  | CAD-CBD-CGD-O1D |
| 21  | D     | 202    | TGL  | CC2-CC1-OG3-CG3 |
| 25  | C     | 307    | CDL  | C72-C73-C74-C75 |
| 25  | P     | 306    | CDL  | C24-C25-C26-C27 |
| 25  | G     | 102    | CDL  | OA6-CA4-CA6-OA8 |
| 18  | B     | 302    | DMU  | C22-C25-C28-C31 |
| 20  | V     | 101    | PSC  | C5-C6-C7-C8     |
| 24  | C     | 306    | CHD  | C22-C23-C24-O25 |
| 24  | P     | 305    | CHD  | C22-C23-C24-O26 |
| 21  | N     | 608    | TGL  | CA9-C20-C21-C22 |
| 19  | A     | 607    | PGV  | C23-C24-C25-C26 |
| 26  | C     | 309    | PEK  | C14-C15-C16-C17 |
| 26  | F     | 102    | PEK  | C3-C4-C5-C6     |
| 26  | P     | 307    | PEK  | C3-C4-C5-C6     |
| 25  | G     | 102    | CDL  | C59-C60-C61-C62 |
| 26  | P     | 307    | PEK  | O03-C21-C22-C23 |
| 26  | C     | 309    | PEK  | C23-C24-C25-C26 |
| 26  | T     | 103    | PEK  | C35-C36-C37-C38 |
| 19  | C     | 310    | PGV  | C9-C10-C11-C12  |
| 19  | N     | 606    | PGV  | C9-C10-C11-C12  |
| 19  | N     | 607    | PGV  | C11-C12-C13-C14 |
| 19  | T     | 104    | PGV  | C9-C10-C11-C12  |
| 20  | A     | 609    | PSC  | C7-C8-C9-C10    |
| 20  | V     | 101    | PSC  | C12-C13-C14-C15 |
| 26  | P     | 308    | PEK  | C14-C15-C16-C17 |
| 25  | P     | 306    | CDL  | C82-C83-C84-C85 |
| 24  | P     | 304    | CHD  | C22-C23-C24-O26 |
| 25  | T     | 102    | CDL  | C32-C31-CA7-OA9 |
| 21  | A     | 610    | TGL  | OA1-CA1-OG1-CG1 |
| 25  | C     | 307    | CDL  | C21-C22-C23-C24 |
| 19  | P     | 310    | PGV  | C15-C16-C17-C18 |
| 21  | A     | 610    | TGL  | OG1-CA1-CA2-CA3 |
| 18  | Y     | 101    | DMU  | C19-C22-C25-C28 |
| 26  | P     | 307    | PEK  | C24-C25-C26-C27 |
| 19  | T     | 104    | PGV  | C11-C12-C13-C14 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 26  | T     | 103    | PEK  | C3-C4-C5-C6     |
| 14  | A     | 601[A] | HEA  | C12-C11-C3B-C2B |
| 14  | N     | 601[A] | HEA  | C12-C11-C3B-C2B |
| 18  | C     | 304    | DMU  | C25-C28-C31-C34 |
| 21  | A     | 610    | TGL  | CA3-CA4-CA5-CA6 |
| 21  | A     | 610    | TGL  | CC5-CC6-CC7-CC8 |
| 19  | N     | 607    | PGV  | O03-C19-C20-C21 |
| 25  | P     | 306    | CDL  | C72-C71-CB7-OB8 |
| 24  | P     | 305    | CHD  | C22-C23-C24-O25 |
| 21  | Q     | 202    | TGL  | CA2-CA3-CA4-CA5 |
| 22  | A     | 618    | EDO  | O1-C1-C2-O2     |
| 22  | B     | 304    | EDO  | O1-C1-C2-O2     |
| 22  | B     | 305    | EDO  | O1-C1-C2-O2     |
| 22  | B     | 306    | EDO  | O1-C1-C2-O2     |
| 22  | B     | 307    | EDO  | O1-C1-C2-O2     |
| 22  | F     | 109    | EDO  | O1-C1-C2-O2     |
| 22  | N     | 617    | EDO  | O1-C1-C2-O2     |
| 22  | N     | 622    | EDO  | O1-C1-C2-O2     |
| 22  | U     | 102    | EDO  | O1-C1-C2-O2     |
| 22  | Y     | 104    | EDO  | O1-C1-C2-O2     |
| 24  | C     | 305    | CHD  | C22-C23-C24-O25 |
| 21  | Q     | 202    | TGL  | OG1-CA1-CA2-CA3 |
| 21  | D     | 202    | TGL  | CC1-CC2-CC3-CC4 |
| 14  | N     | 601[A] | HEA  | CAD-CBD-CGD-O2D |
| 14  | N     | 601[B] | HEA  | CAD-CBD-CGD-O2D |
| 21  | N     | 608    | TGL  | OG3-CC1-CC2-CC3 |
| 21  | N     | 608    | TGL  | OG2-CG2-CG3-OG3 |
| 18  | W     | 101    | DMU  | C22-C25-C28-C31 |
| 18  | K     | 101    | DMU  | C34-C37-C40-C43 |
| 21  | Y     | 103    | TGL  | C29-C30-C31-C32 |
| 18  | D     | 201    | DMU  | C19-C22-C25-C28 |
| 19  | A     | 607    | PGV  | C31-C32-C33-C34 |
| 19  | P     | 310    | PGV  | C24-C25-C26-C27 |
| 19  | C     | 310    | PGV  | C11-C12-C13-C14 |
| 26  | F     | 102    | PEK  | C14-C15-C16-C17 |
| 21  | D     | 202    | TGL  | OG1-CA1-CA2-CA3 |
| 14  | A     | 601[A] | HEA  | CAD-CBD-CGD-O2D |
| 14  | A     | 601[B] | HEA  | CAD-CBD-CGD-O2D |
| 25  | C     | 307    | CDL  | C22-C23-C24-C25 |
| 21  | A     | 610    | TGL  | OA1-CA1-CA2-CA3 |
| 19  | A     | 608    | PGV  | C26-C27-C28-C29 |
| 21  | L     | 103    | TGL  | OA1-CA1-CA2-CA3 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 26  | P     | 307    | PEK  | O04-C21-C22-C23 |
| 25  | T     | 102    | CDL  | C24-C25-C26-C27 |
| 14  | N     | 601[A] | HEA  | C12-C13-C14-C15 |
| 25  | G     | 102    | CDL  | C32-C31-CA7-OA8 |
| 25  | P     | 306    | CDL  | C72-C71-CB7-OB9 |
| 20  | A     | 609    | PSC  | C23-C24-C25-C26 |
| 21  | A     | 610    | TGL  | CA1-CA2-CA3-CA4 |
| 26  | C     | 309    | PEK  | C17-C18-C19-C20 |
| 21  | N     | 608    | TGL  | CC3-CC4-CC5-CC6 |
| 19  | T     | 104    | PGV  | C21-C22-C23-C24 |
| 21  | A     | 610    | TGL  | CA6-CA7-CA8-CA9 |
| 21  | Y     | 103    | TGL  | C16-C17-C18-C19 |
| 26  | F     | 102    | PEK  | C30-C31-C32-C33 |
| 19  | N     | 606    | PGV  | C04-O12-P-O13   |
| 25  | C     | 307    | CDL  | CA2-OA2-PA1-OA3 |
| 25  | G     | 102    | CDL  | CB3-OB5-PB2-OB3 |
| 25  | T     | 102    | CDL  | CA2-OA2-PA1-OA3 |
| 26  | T     | 103    | PEK  | C04-O12-P-O13   |
| 26  | T     | 103    | PEK  | C04-O12-P-O14   |
| 26  | T     | 103    | PEK  | C30-C31-C32-C33 |
| 21  | D     | 202    | TGL  | OA1-CA1-CA2-CA3 |
| 21  | N     | 608    | TGL  | OC1-CC1-CC2-CC3 |
| 26  | P     | 307    | PEK  | O12-C04-C05-N   |
| 19  | T     | 104    | PGV  | C5-C6-C7-C8     |
| 22  | C     | 317    | EDO  | O1-C1-C2-O2     |
| 19  | A     | 607    | PGV  | O03-C19-C20-C21 |
| 26  | P     | 307    | PEK  | C01-C02-O01-C1  |
| 20  | A     | 609    | PSC  | C12-C13-C14-C15 |
| 19  | N     | 607    | PGV  | C30-C31-C32-C33 |
| 19  | P     | 310    | PGV  | C26-C27-C28-C29 |
| 25  | T     | 102    | CDL  | C31-C32-C33-C34 |
| 25  | G     | 102    | CDL  | C32-C31-CA7-OA9 |
| 18  | L     | 101    | DMU  | C34-C37-C40-C43 |
| 25  | C     | 307    | CDL  | C42-C43-C44-C45 |
| 14  | N     | 601[A] | HEA  | O11-C11-C3B-C2B |
| 21  | D     | 202    | TGL  | OG2-CB1-CB2-CB3 |
| 19  | P     | 309    | PGV  | C9-C10-C11-C12  |
| 25  | G     | 102    | CDL  | C17-C18-C19-C20 |
| 21  | L     | 103    | TGL  | CB2-CB3-CB4-CB5 |
| 21  | N     | 608    | TGL  | OG1-CA1-CA2-CA3 |
| 25  | T     | 102    | CDL  | C37-C38-C39-C40 |
| 25  | T     | 102    | CDL  | C43-C44-C45-C46 |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 21  | Q     | 202    | TGL  | OG2-CB1-CB2-CB3 |
| 25  | C     | 307    | CDL  | C32-C31-CA7-OA8 |
| 18  | K     | 102    | DMU  | C28-C31-C34-C37 |
| 14  | A     | 601[A] | HEA  | CAA-CBA-CGA-O2A |
| 14  | A     | 601[B] | HEA  | CAA-CBA-CGA-O2A |

There are no ring outliers.

89 monomers are involved in 317 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 22  | N     | 623    | EDO  | 1       | 0            |
| 22  | N     | 615    | EDO  | 1       | 0            |
| 22  | F     | 110    | EDO  | 1       | 0            |
| 26  | C     | 309    | PEK  | 6       | 0            |
| 18  | X     | 102    | DMU  | 1       | 0            |
| 14  | A     | 602    | HEA  | 3       | 0            |
| 22  | A     | 611    | EDO  | 1       | 0            |
| 21  | N     | 608    | TGL  | 4       | 0            |
| 25  | C     | 307    | CDL  | 19      | 0            |
| 18  | Y     | 101    | DMU  | 3       | 0            |
| 19  | P     | 309    | PGV  | 4       | 0            |
| 18  | M     | 101    | DMU  | 1       | 0            |
| 22  | S     | 105    | EDO  | 2       | 0            |
| 26  | F     | 102    | PEK  | 6       | 0            |
| 14  | A     | 601[B] | HEA  | 1       | 0            |
| 18  | P     | 303    | DMU  | 3       | 0            |
| 18  | O     | 302    | DMU  | 2       | 0            |
| 22  | N     | 618    | EDO  | 1       | 0            |
| 22  | L     | 104    | EDO  | 1       | 0            |
| 22  | A     | 616    | EDO  | 1       | 0            |
| 19  | A     | 608    | PGV  | 1       | 0            |
| 22  | C     | 313    | EDO  | 1       | 0            |
| 19  | A     | 607    | PGV  | 5       | 0            |
| 14  | N     | 601[B] | HEA  | 1       | 0            |
| 14  | N     | 602    | HEA  | 5       | 0            |
| 22  | A     | 614    | EDO  | 1       | 0            |
| 22  | F     | 108    | EDO  | 1       | 0            |
| 22  | Q     | 205    | EDO  | 1       | 0            |
| 24  | G     | 101    | CHD  | 1       | 0            |
| 20  | V     | 101    | PSC  | 7       | 0            |
| 26  | P     | 308    | PEK  | 2       | 0            |
| 18  | W     | 101    | DMU  | 4       | 0            |

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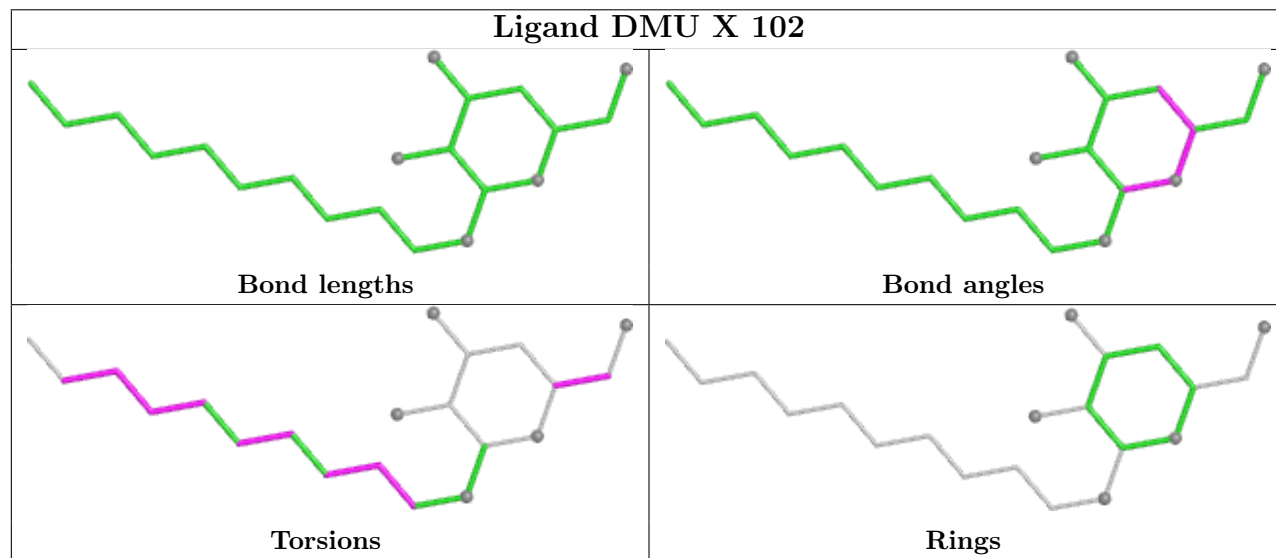
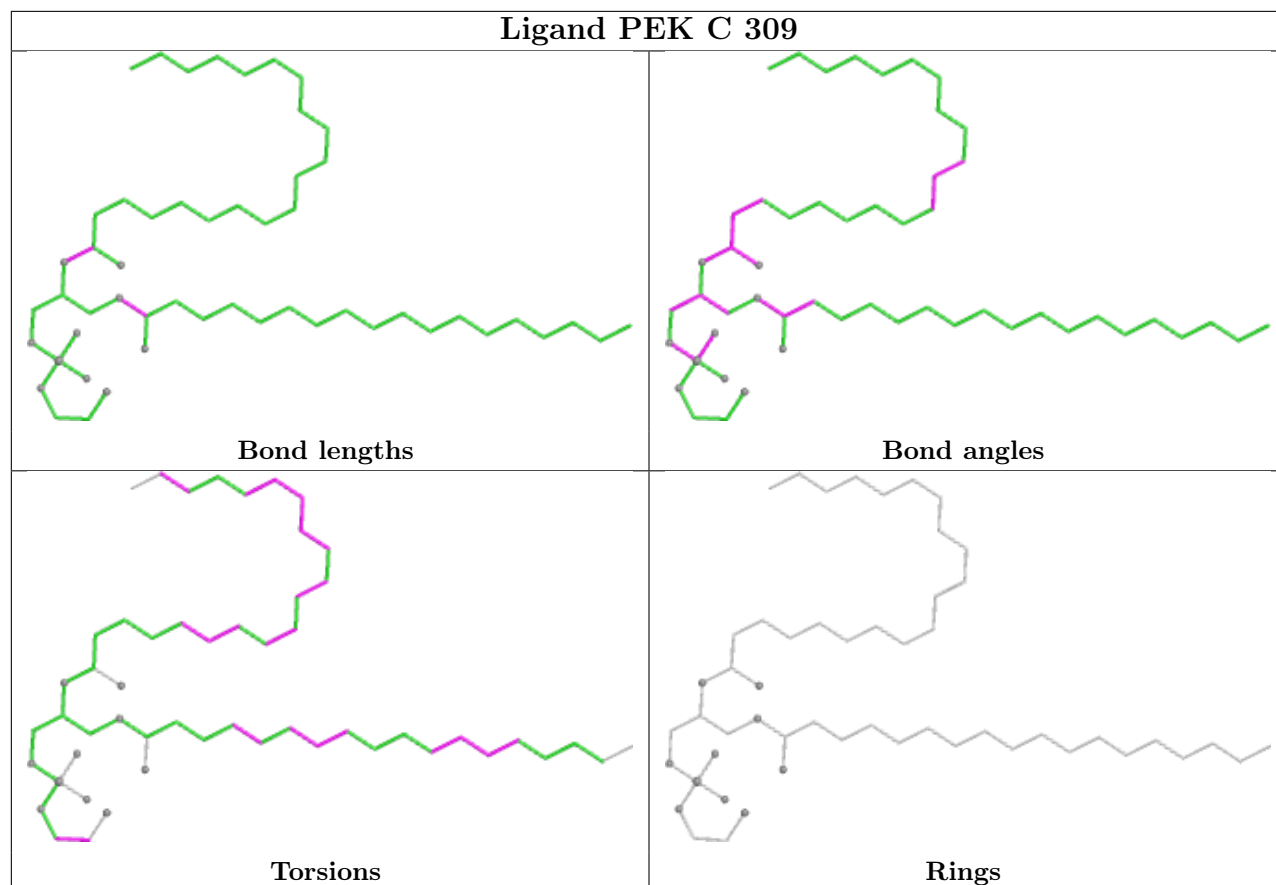
| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 22  | E     | 203    | EDO  | 2       | 0            |
| 22  | N     | 613    | EDO  | 1       | 0            |
| 25  | P     | 306    | CDL  | 11      | 0            |
| 22  | H     | 102    | EDO  | 2       | 0            |
| 22  | U     | 102    | EDO  | 4       | 0            |
| 21  | D     | 202    | TGL  | 15      | 0            |
| 24  | P     | 304    | CHD  | 1       | 0            |
| 19  | P     | 310    | PGV  | 9       | 0            |
| 18  | C     | 303    | DMU  | 1       | 0            |
| 26  | C     | 308    | PEK  | 5       | 0            |
| 14  | A     | 601[A] | HEA  | 1       | 0            |
| 20  | A     | 609    | PSC  | 17      | 0            |
| 22  | N     | 617    | EDO  | 4       | 0            |
| 22  | A     | 618    | EDO  | 1       | 0            |
| 19  | C     | 310    | PGV  | 6       | 0            |
| 19  | N     | 606    | PGV  | 7       | 0            |
| 14  | N     | 601[A] | HEA  | 1       | 0            |
| 22  | D     | 205    | EDO  | 1       | 0            |
| 18  | C     | 302    | DMU  | 1       | 0            |
| 18  | A     | 606    | DMU  | 2       | 0            |
| 24  | P     | 305    | CHD  | 2       | 0            |
| 21  | L     | 103    | TGL  | 16      | 0            |
| 22  | P     | 313    | EDO  | 1       | 0            |
| 22  | Q     | 203    | EDO  | 1       | 0            |
| 22  | O     | 304    | EDO  | 1       | 0            |
| 26  | P     | 307    | PEK  | 1       | 0            |
| 22  | A     | 615    | EDO  | 2       | 0            |
| 19  | N     | 607    | PGV  | 2       | 0            |
| 22  | N     | 622    | EDO  | 2       | 0            |
| 18  | L     | 101    | DMU  | 2       | 0            |
| 26  | T     | 103    | PEK  | 9       | 0            |
| 22  | T     | 105    | EDO  | 1       | 0            |
| 22  | C     | 311    | EDO  | 1       | 0            |
| 24  | C     | 306    | CHD  | 3       | 0            |
| 22  | N     | 612    | EDO  | 4       | 0            |
| 18  | J     | 101    | DMU  | 4       | 0            |
| 25  | T     | 102    | CDL  | 29      | 0            |
| 22  | D     | 203    | EDO  | 1       | 0            |
| 24  | J     | 102    | CHD  | 1       | 0            |
| 18  | K     | 103    | DMU  | 5       | 0            |
| 22  | P     | 316    | EDO  | 2       | 0            |
| 22  | F     | 109    | EDO  | 1       | 0            |

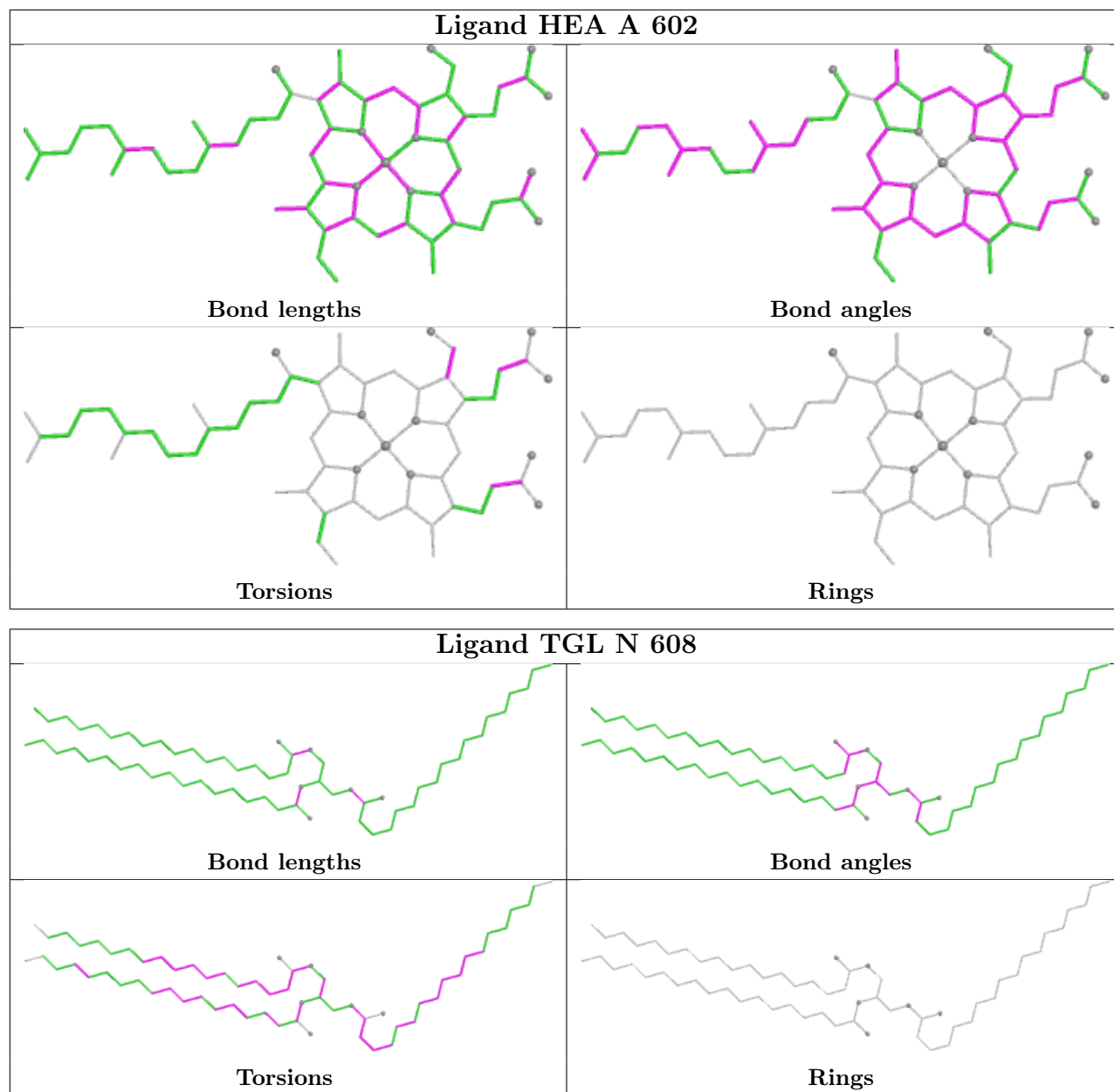
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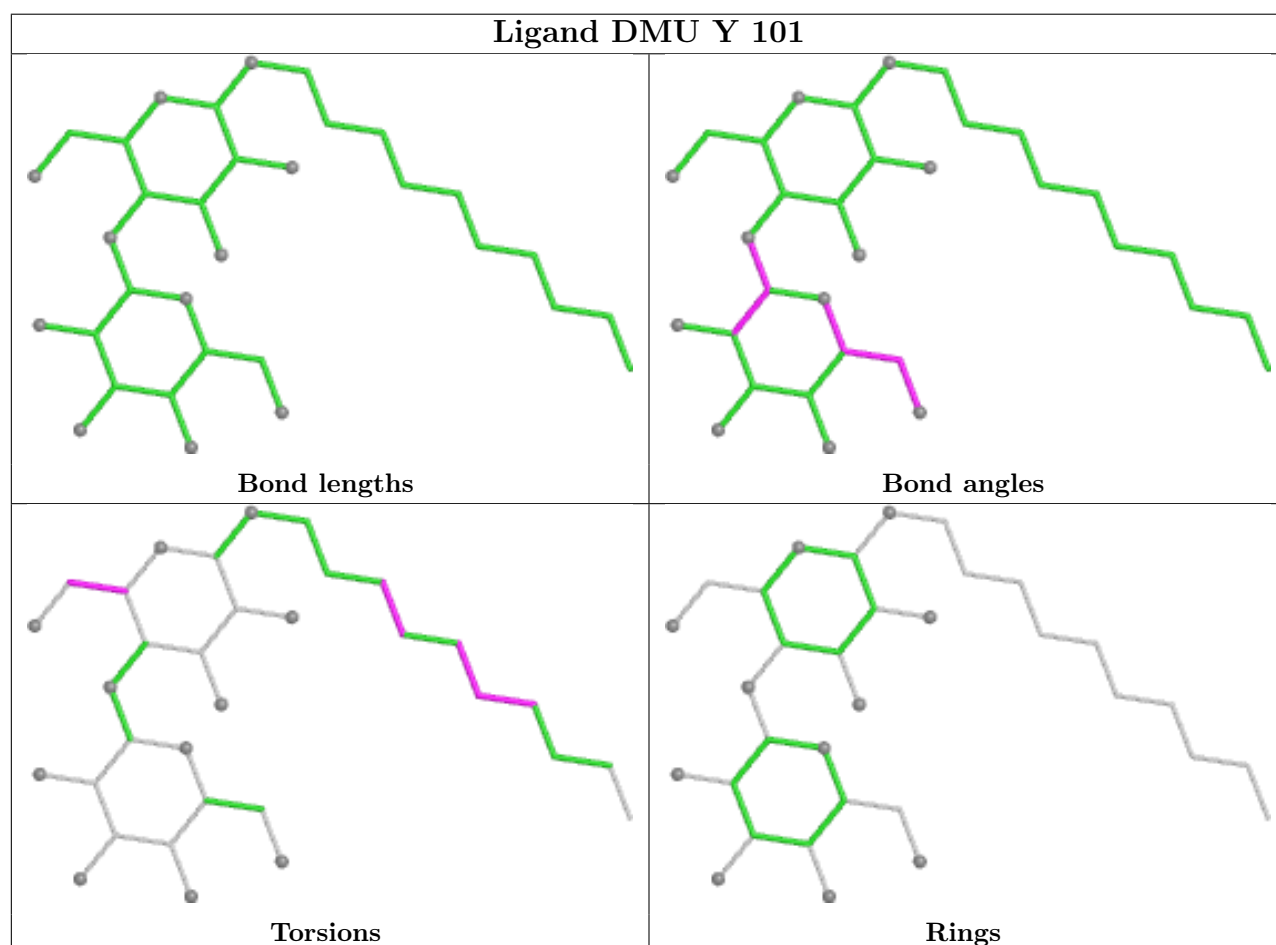
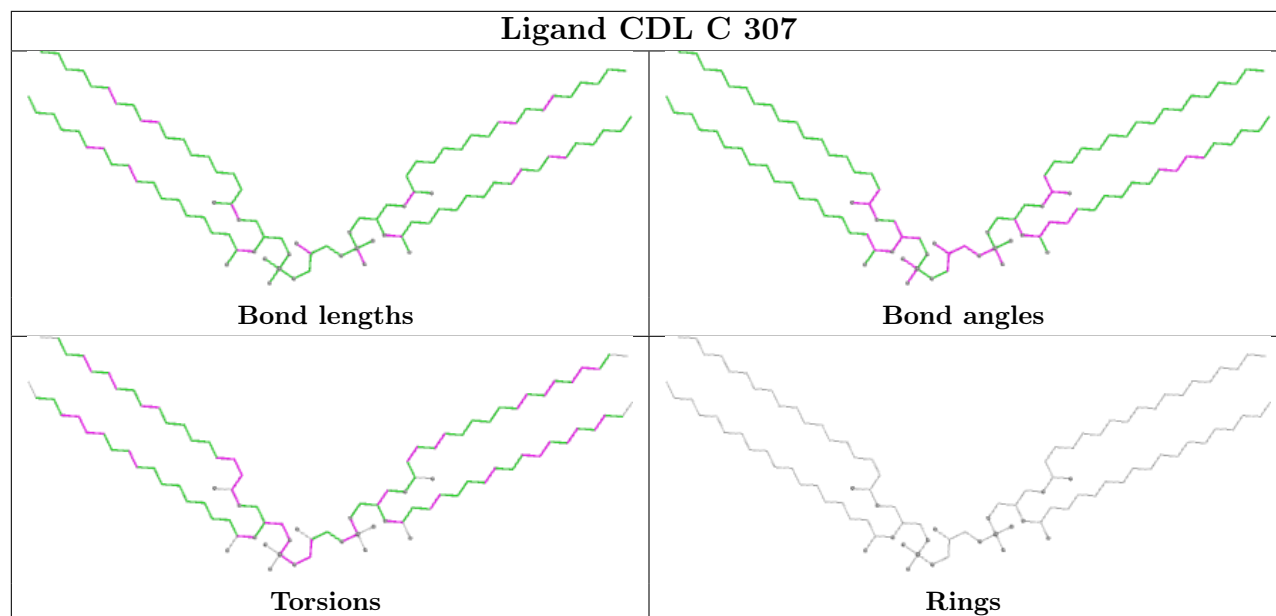
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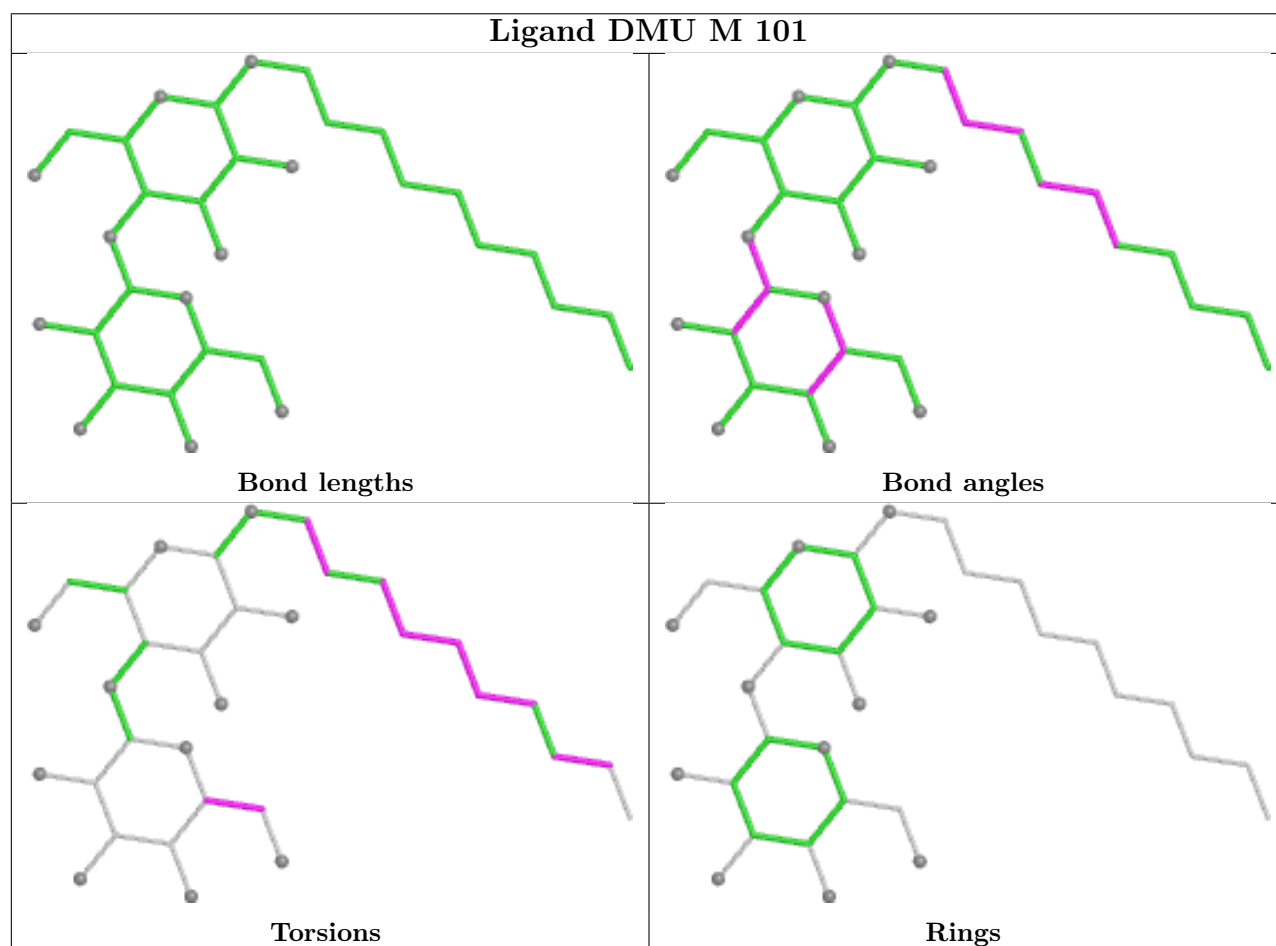
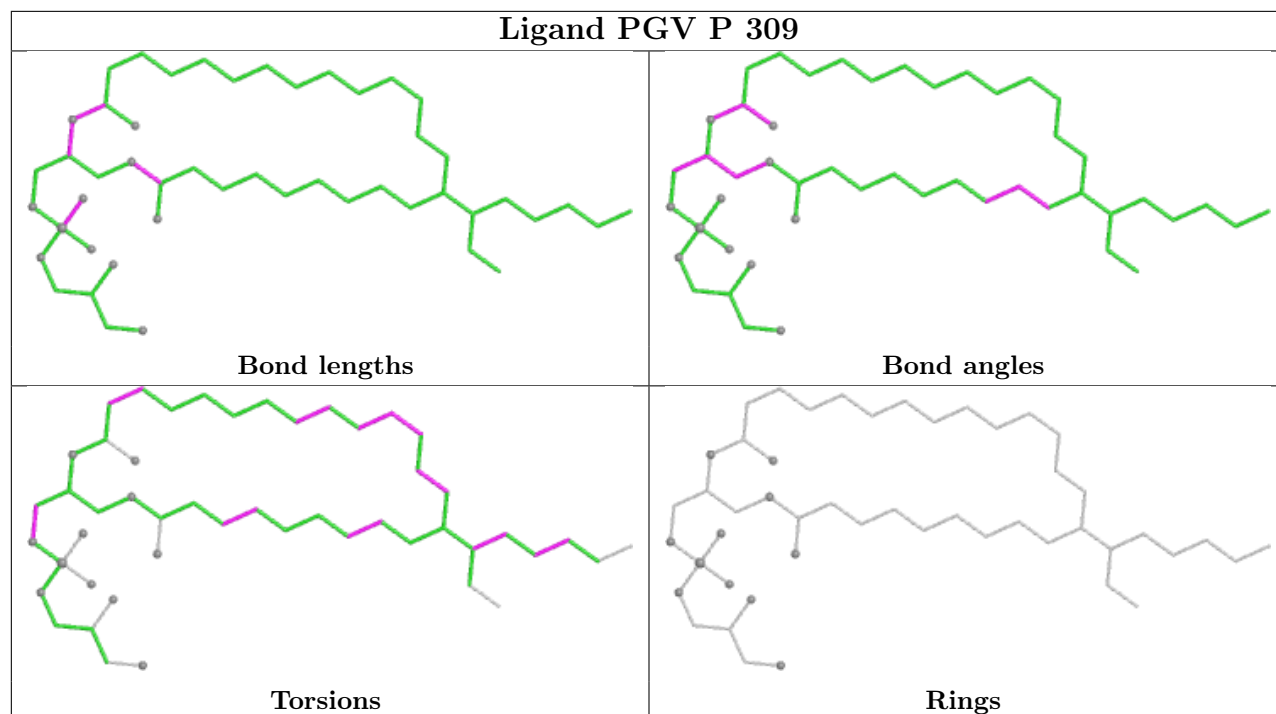
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | Q     | 204 | EDO  | 2       | 0            |
| 21  | A     | 610 | TGL  | 2       | 0            |
| 22  | B     | 305 | EDO  | 2       | 0            |
| 22  | B     | 307 | EDO  | 1       | 0            |
| 18  | Z     | 101 | DMU  | 2       | 0            |
| 19  | T     | 104 | PGV  | 1       | 0            |
| 22  | D     | 206 | EDO  | 1       | 0            |
| 22  | C     | 316 | EDO  | 1       | 0            |
| 21  | Q     | 202 | TGL  | 12      | 0            |
| 24  | T     | 101 | CHD  | 1       | 0            |
| 24  | Y     | 102 | CHD  | 1       | 0            |
| 21  | Y     | 103 | TGL  | 3       | 0            |
| 25  | G     | 102 | CDL  | 22      | 0            |
| 22  | A     | 617 | EDO  | 3       | 0            |
| 18  | Q     | 201 | DMU  | 2       | 0            |

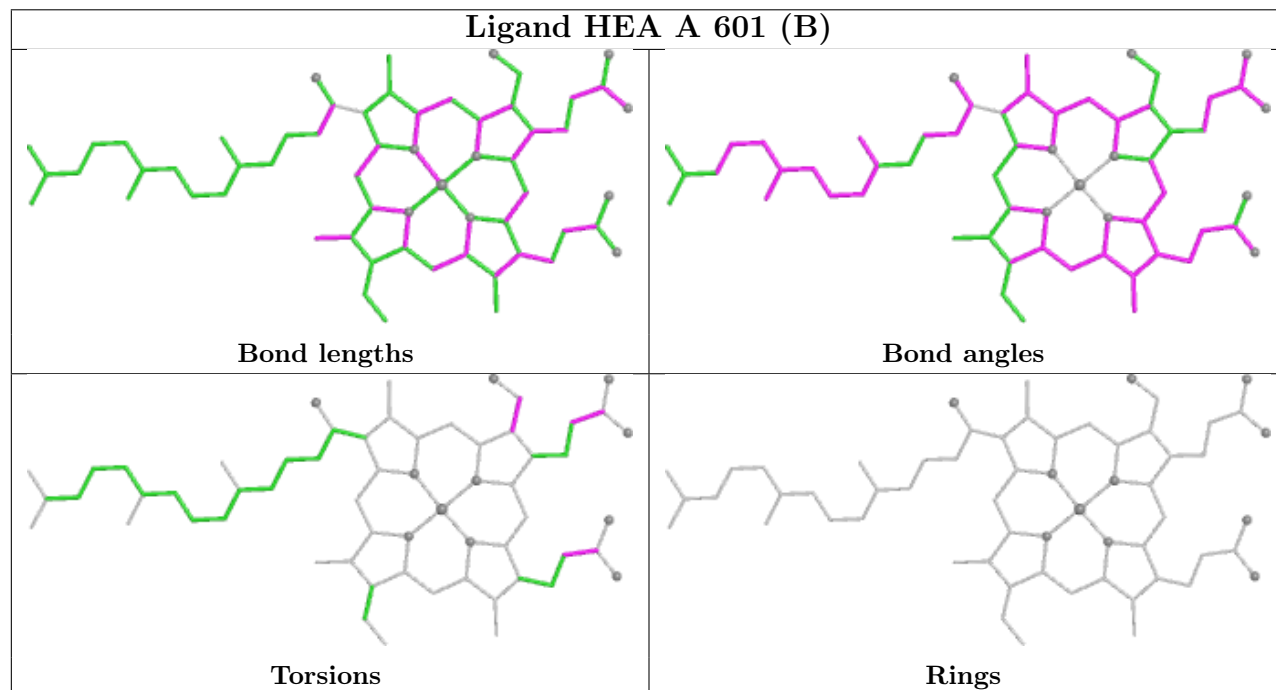
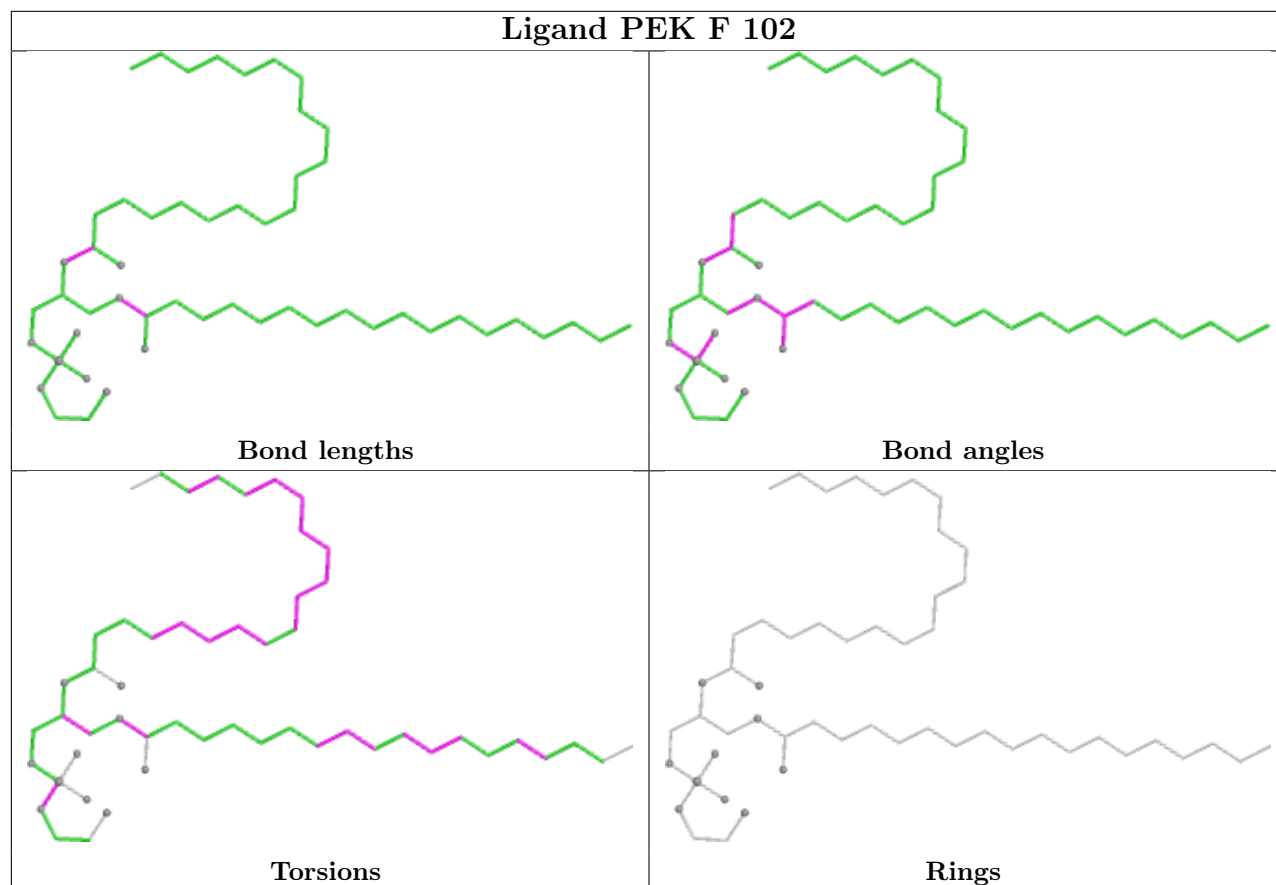
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

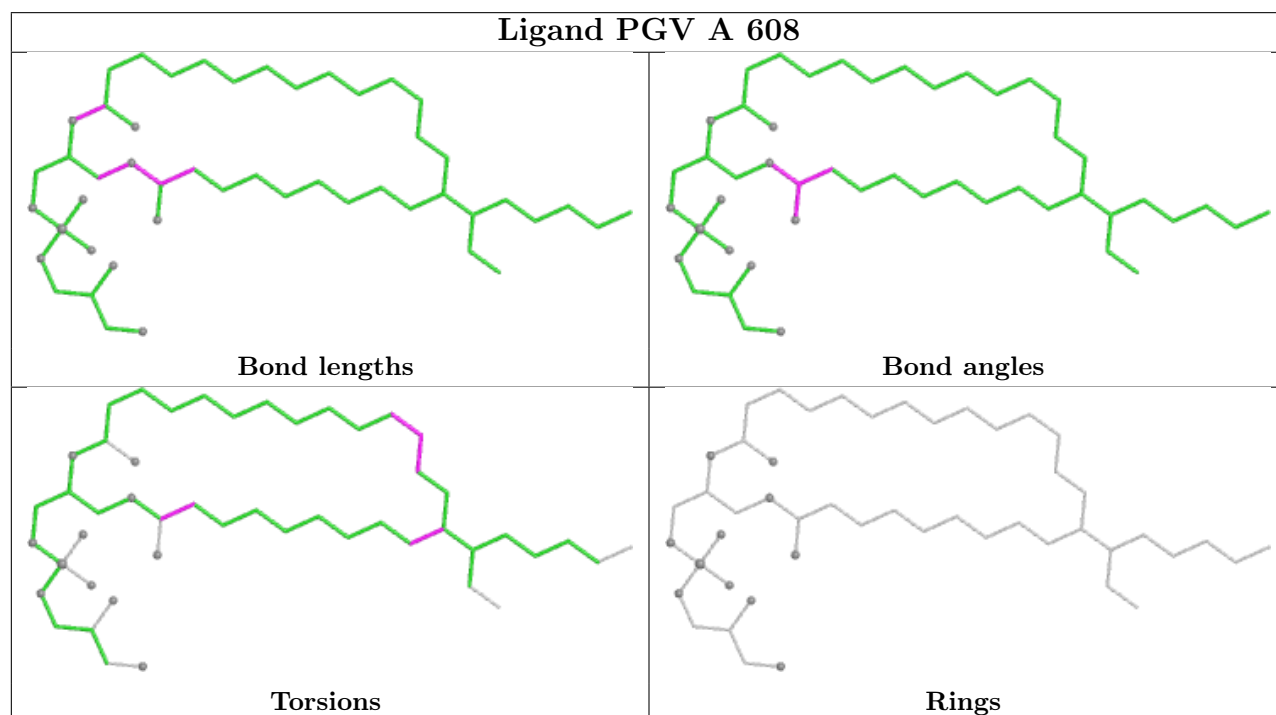
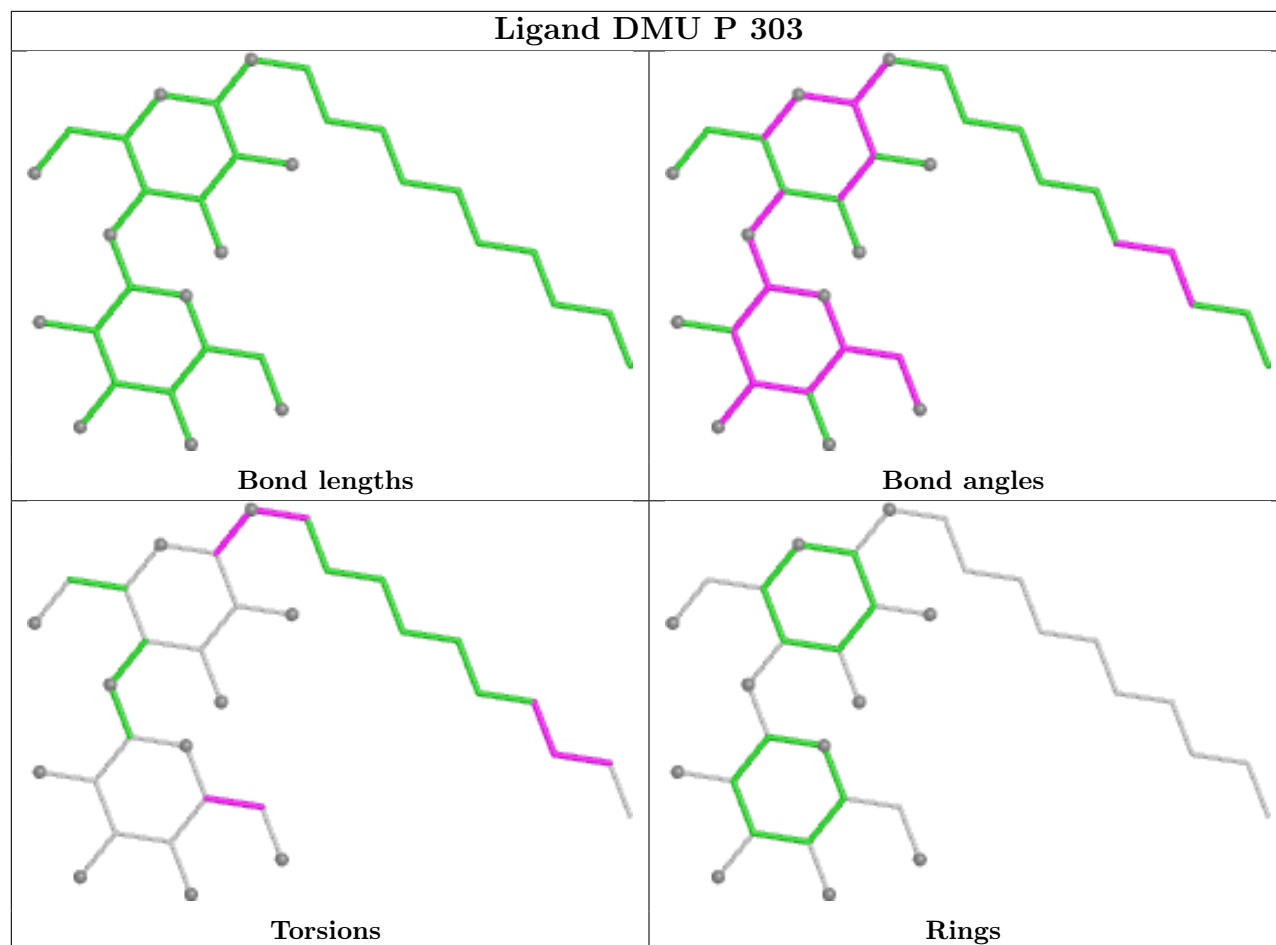


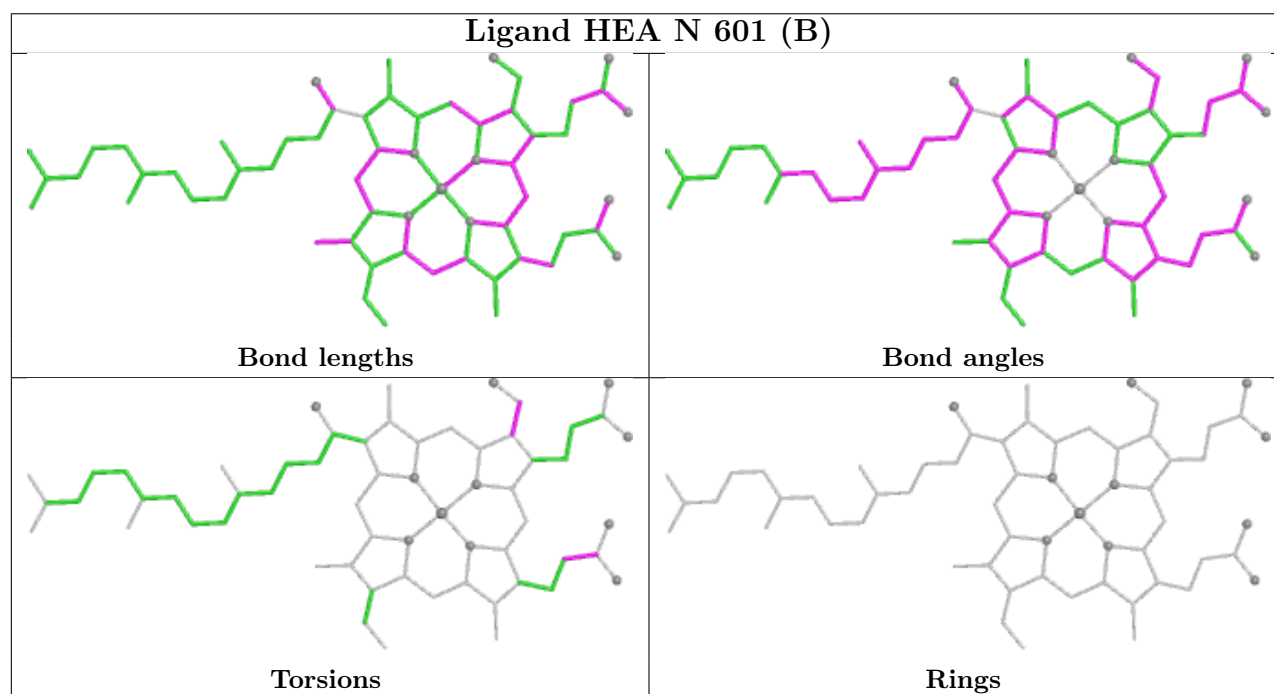
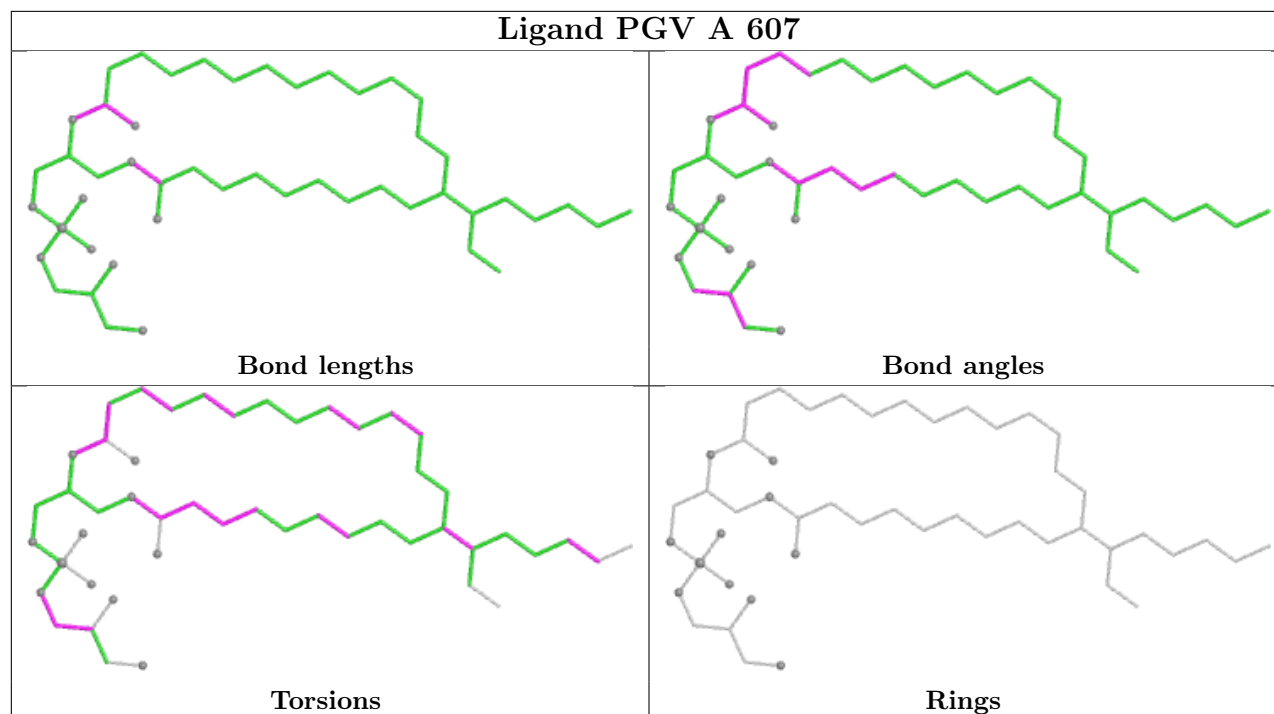


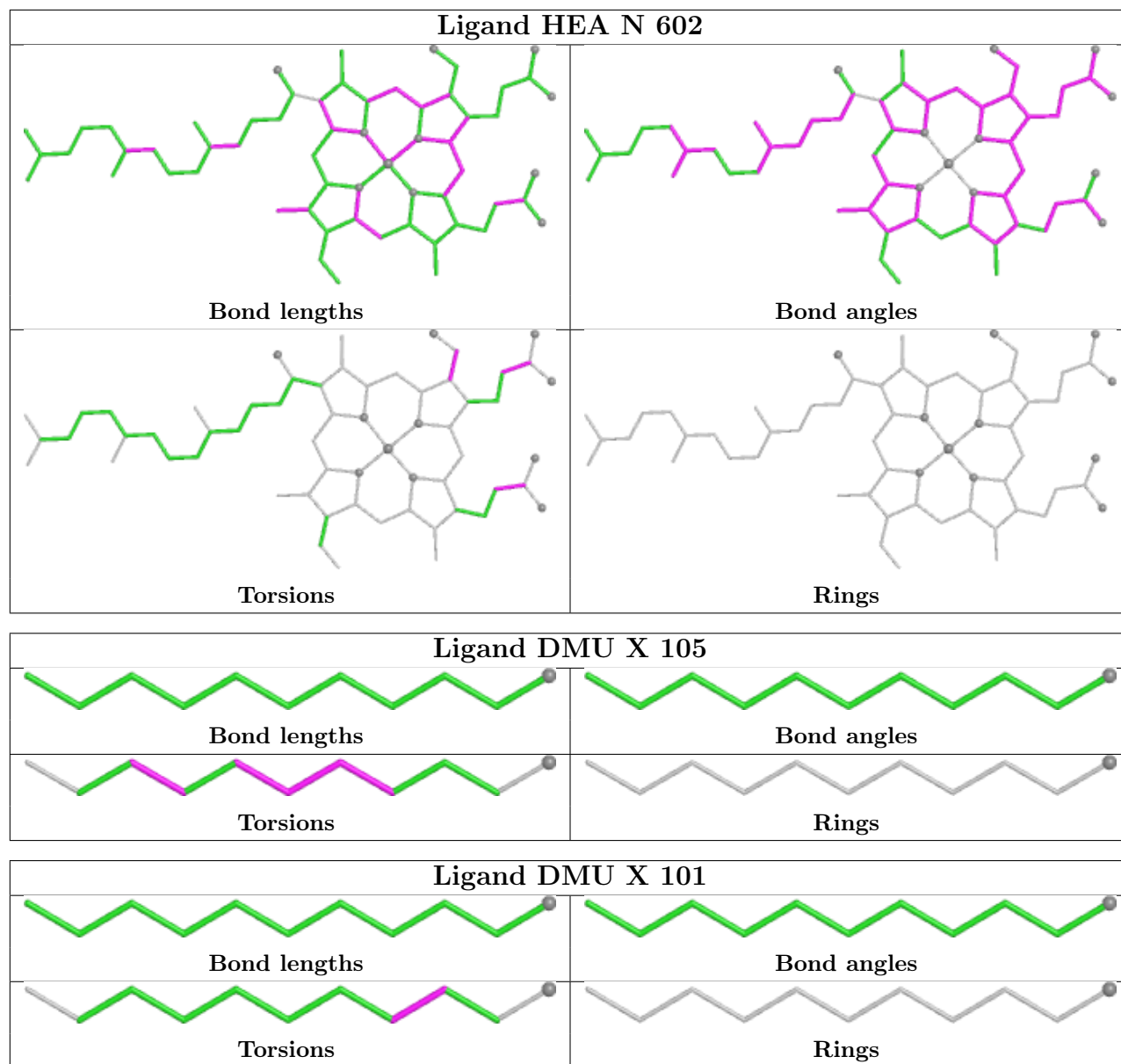


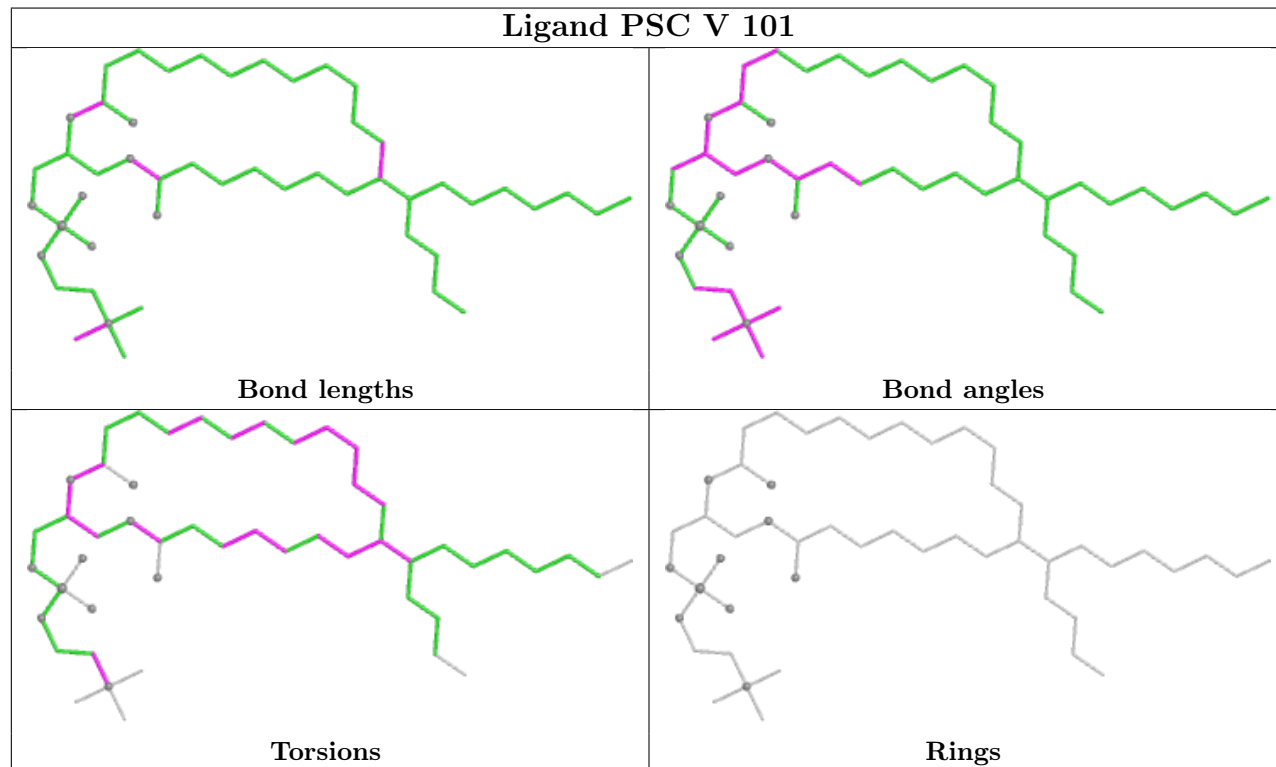
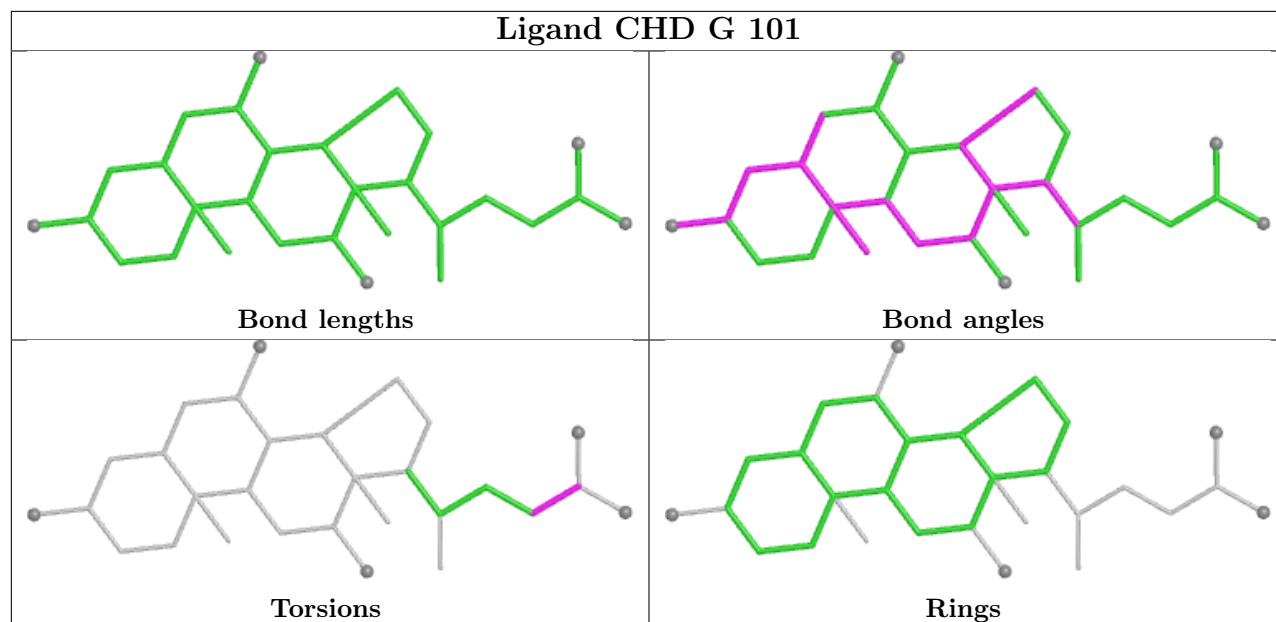




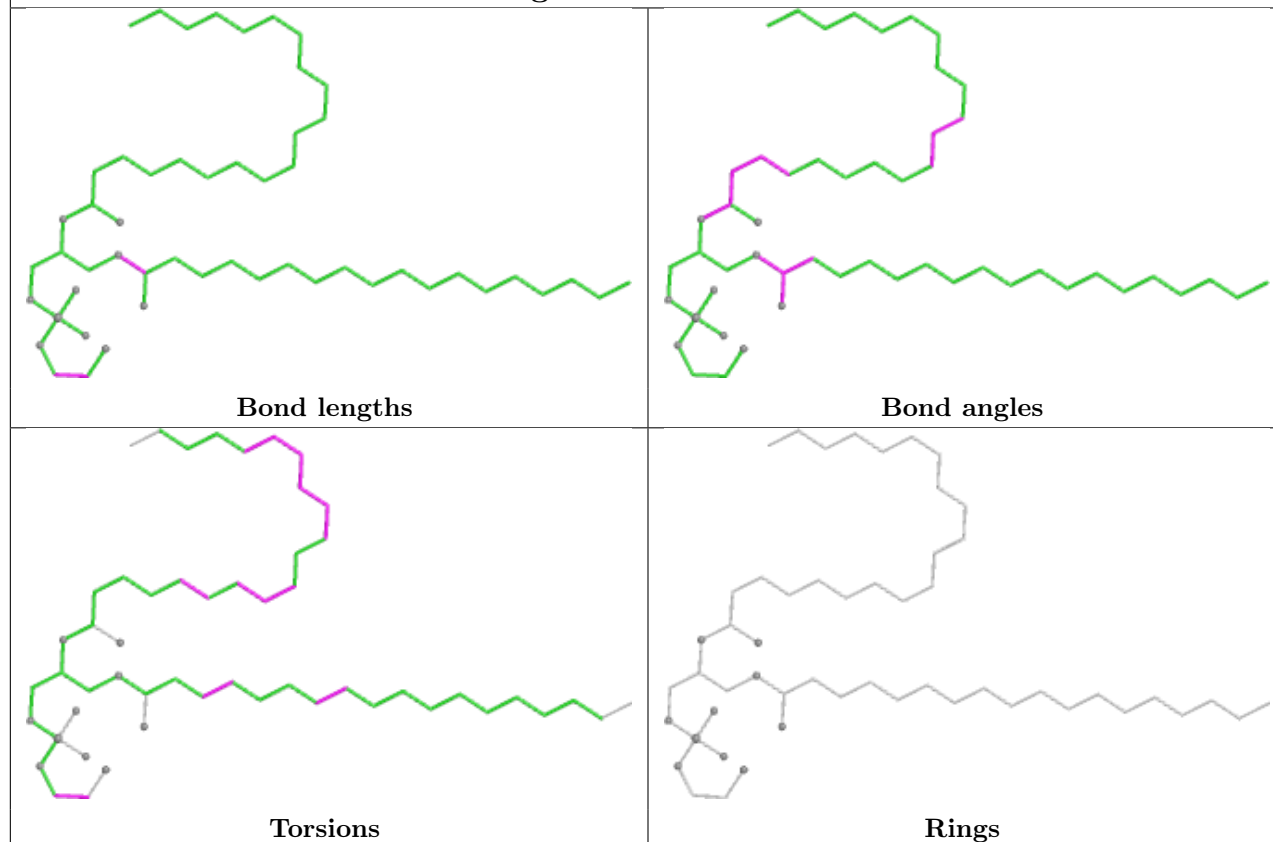




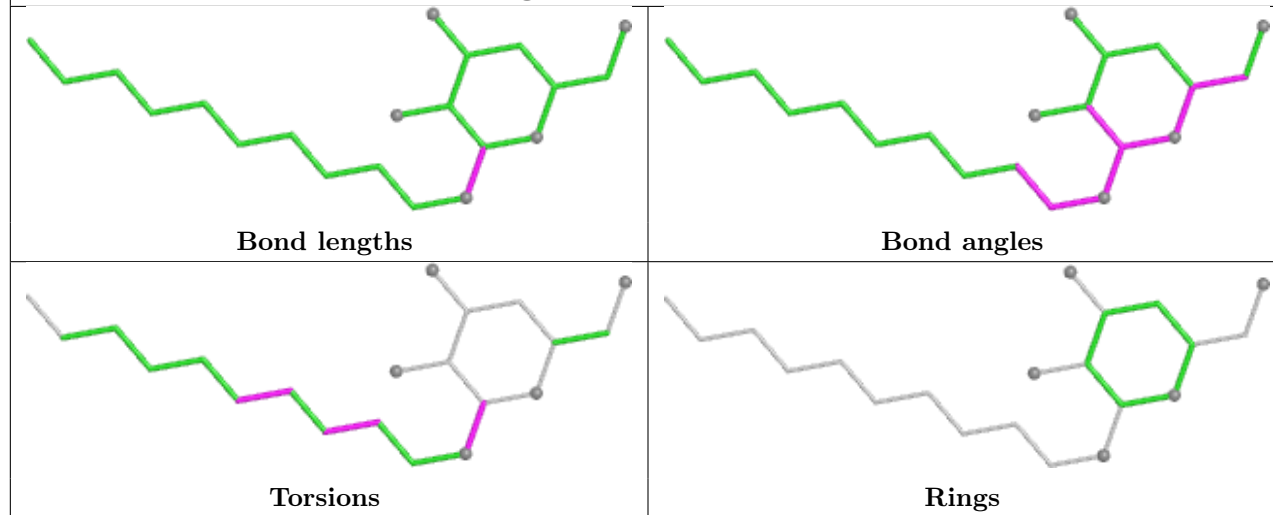


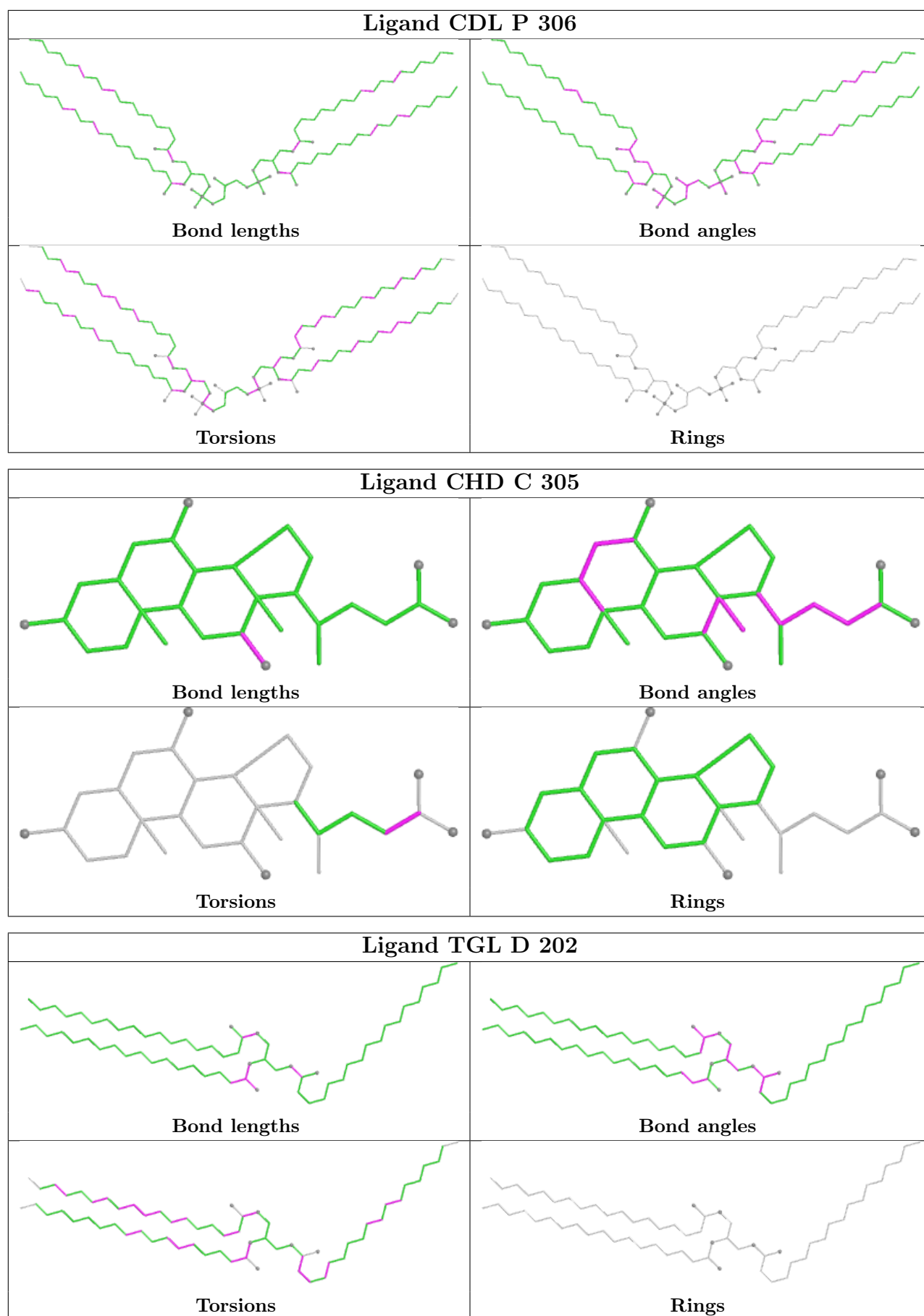


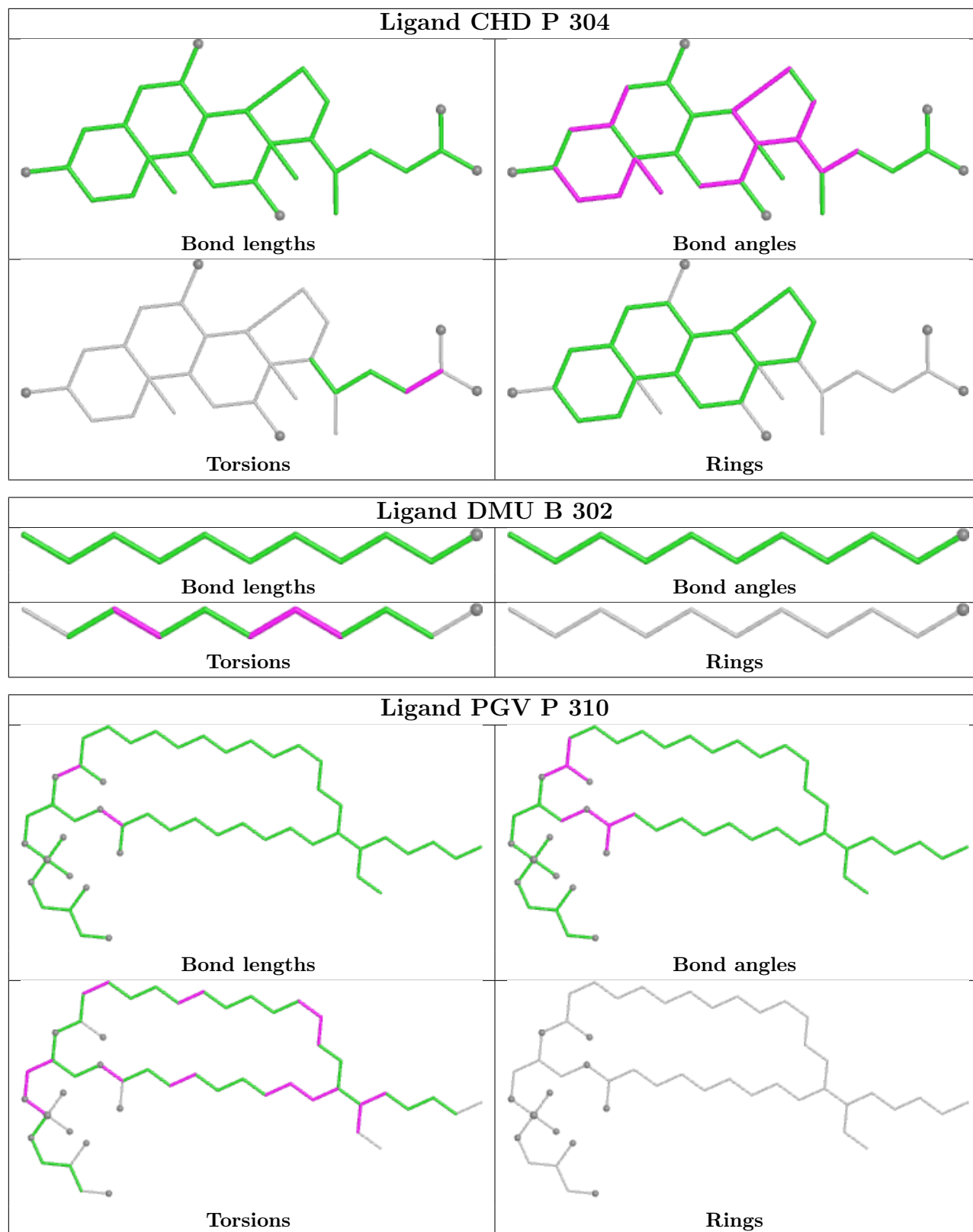
## Ligand PEK P 308

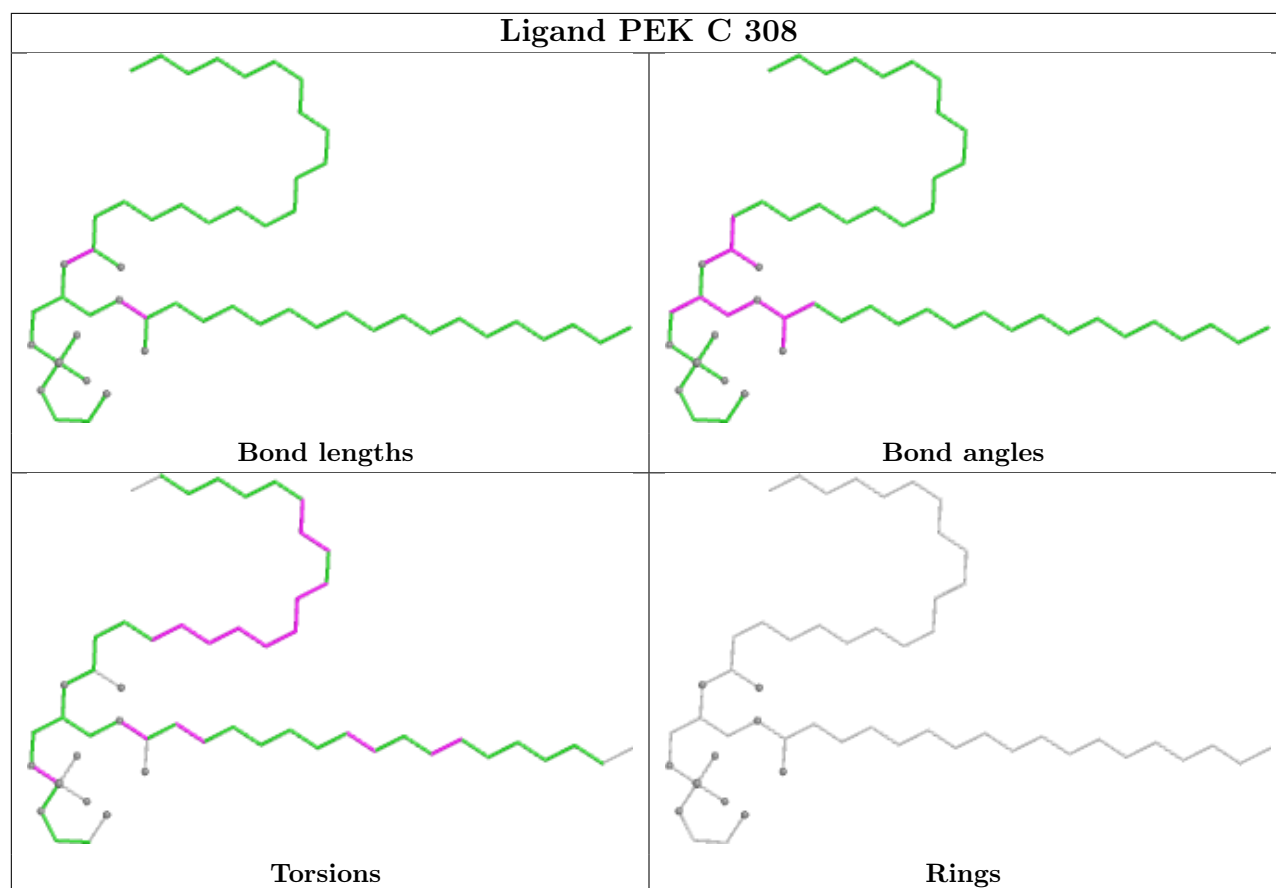
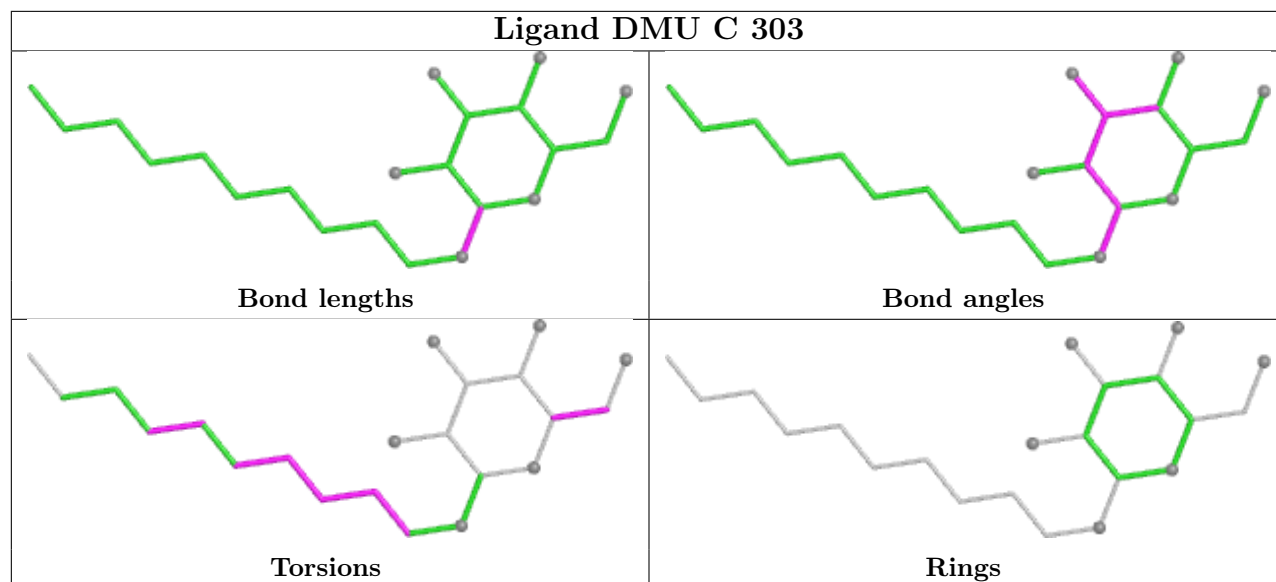


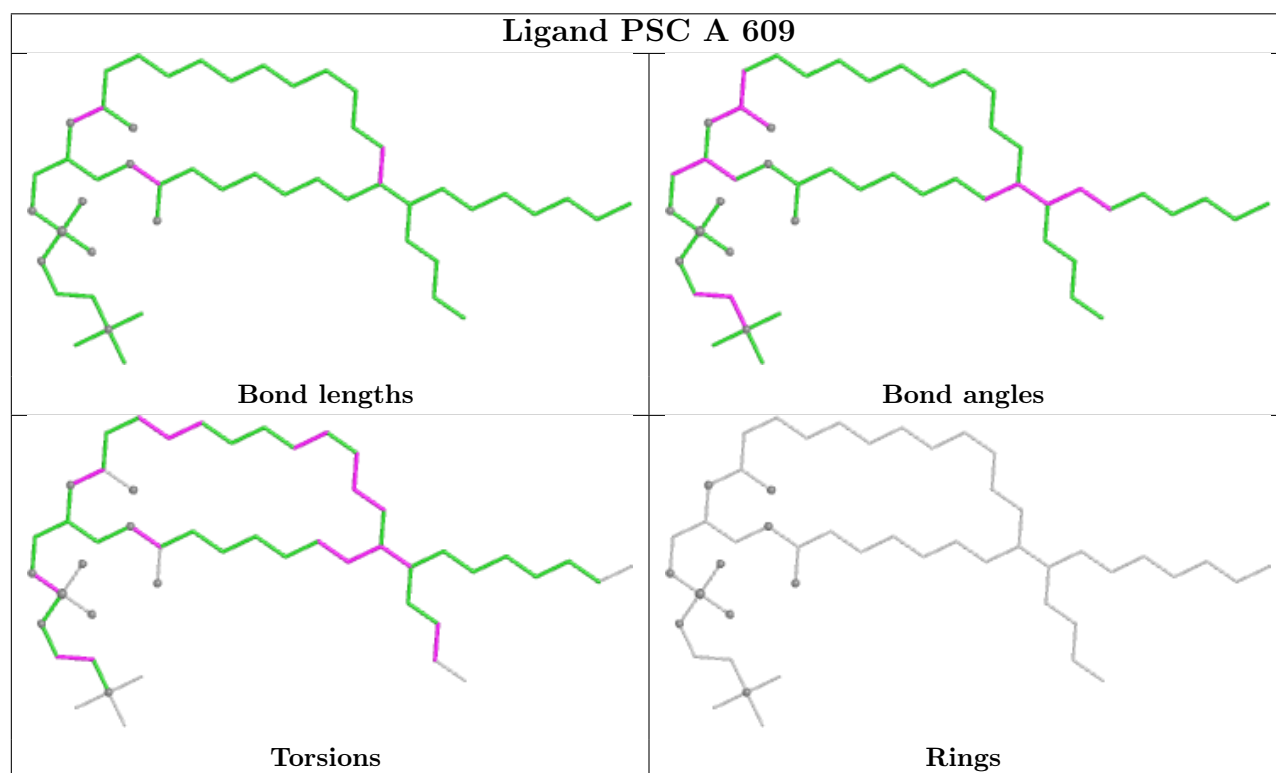
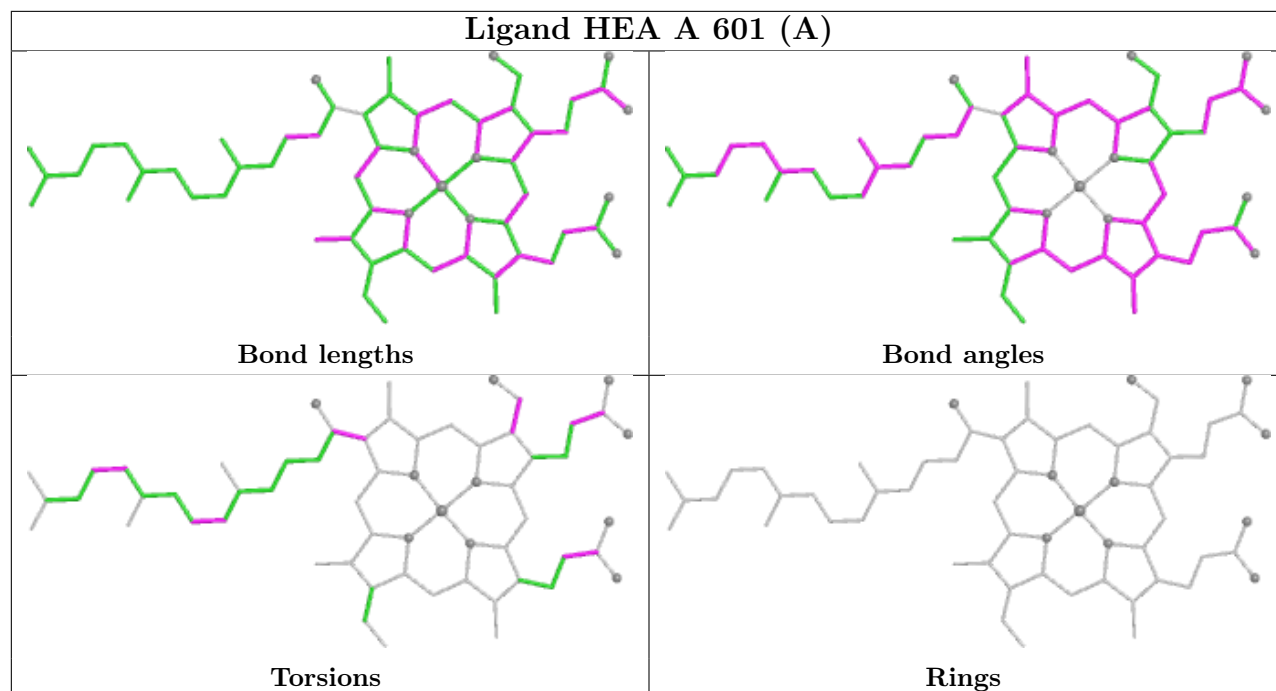
## Ligand DMU W 101

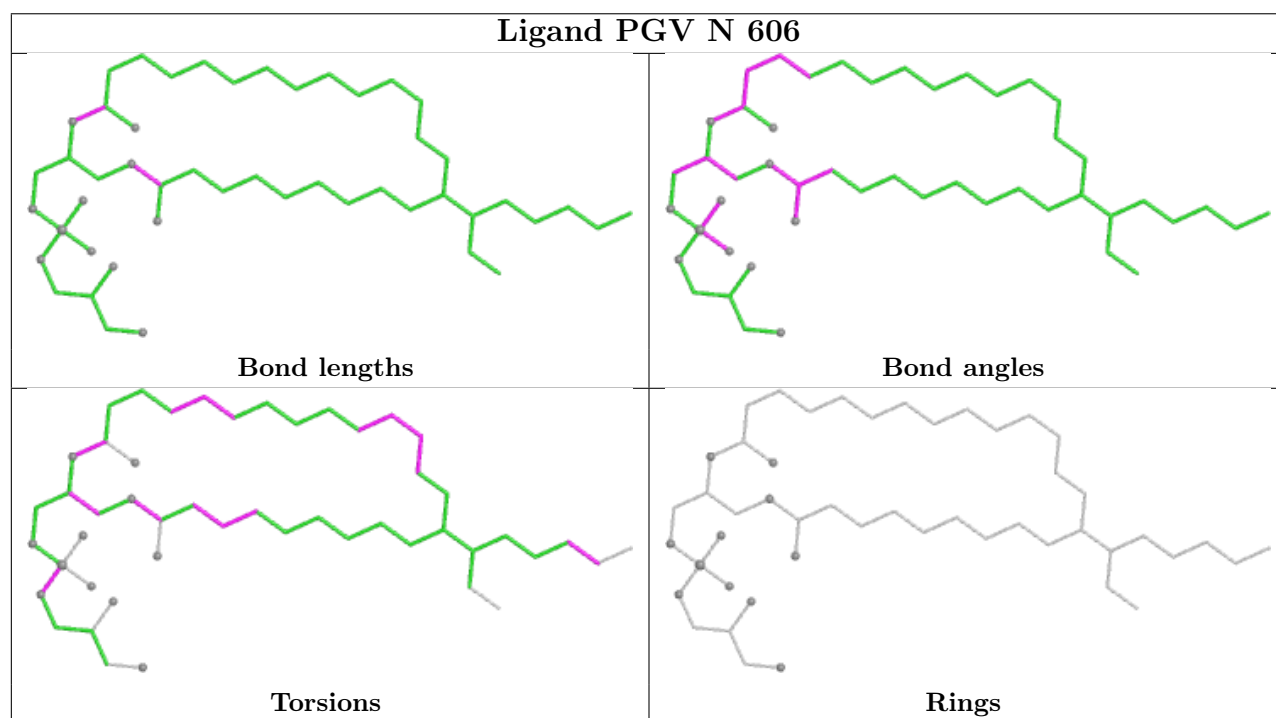
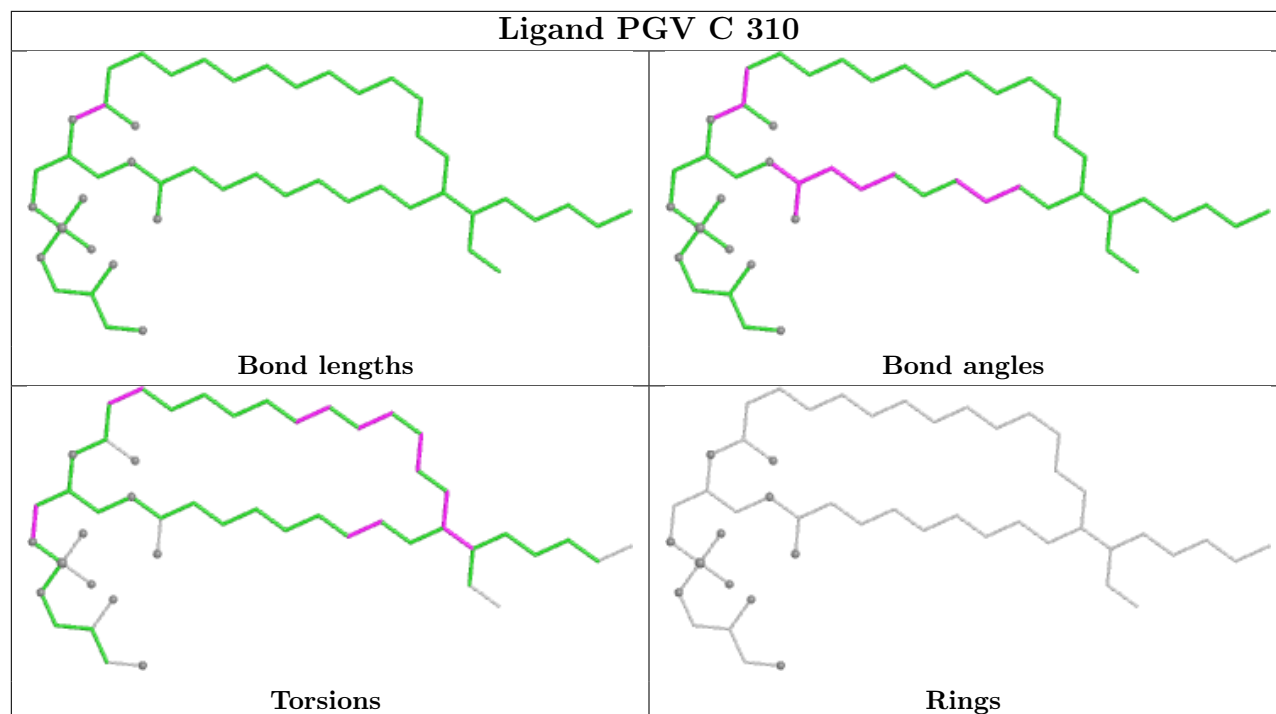


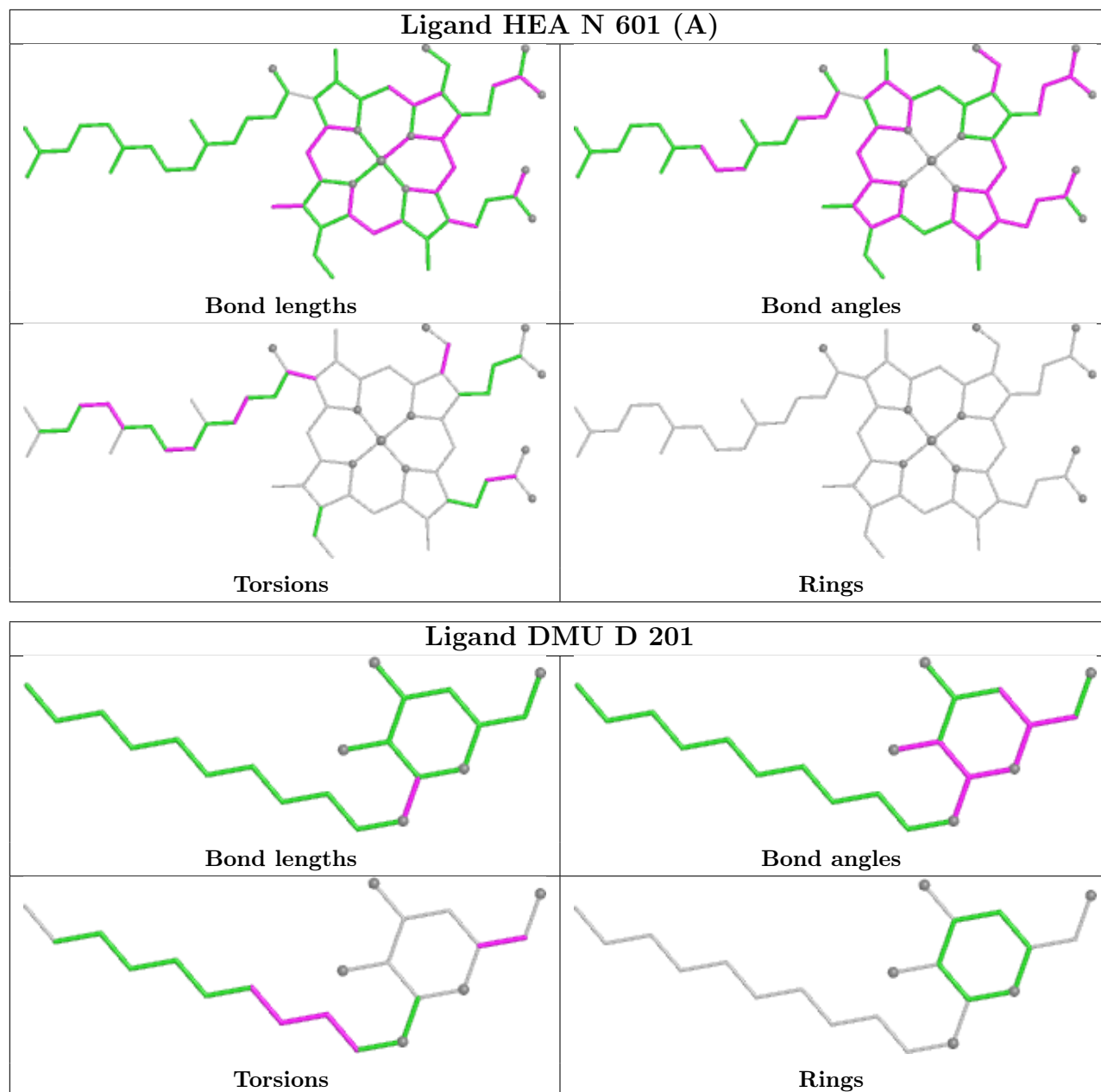


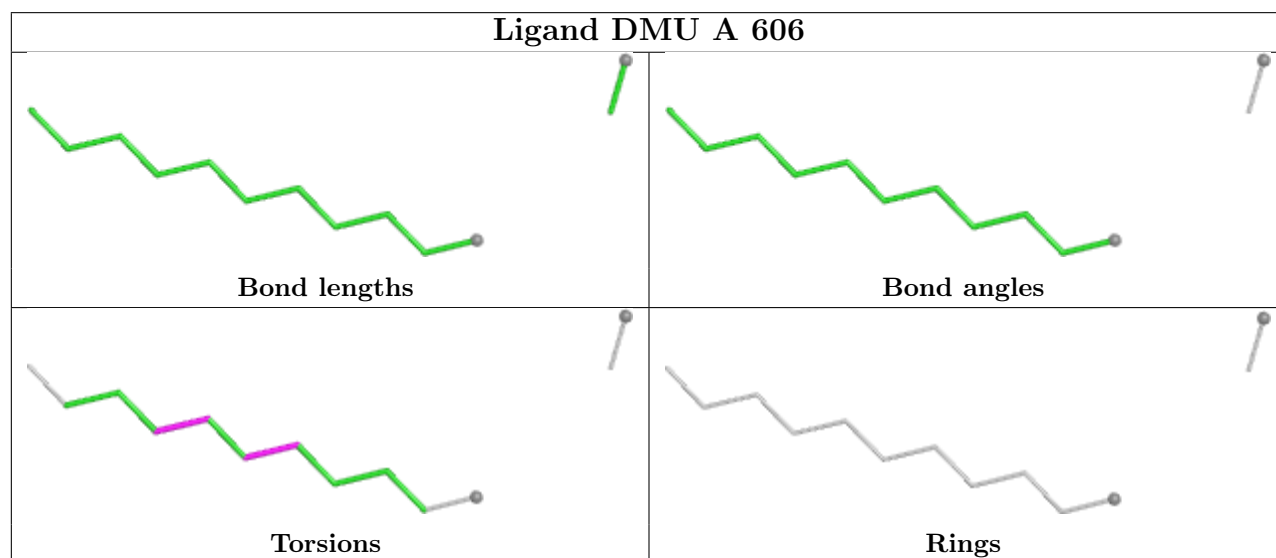
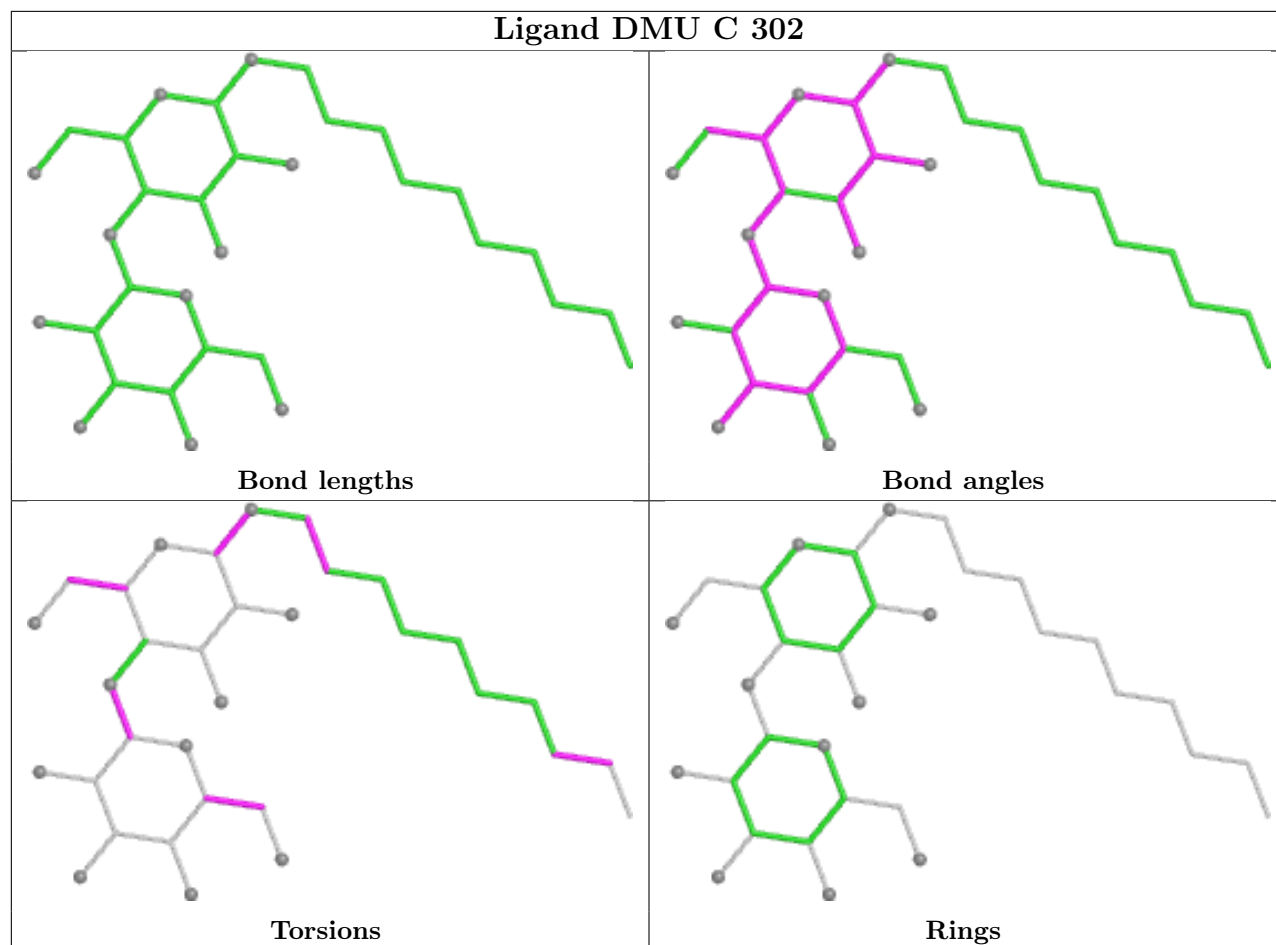


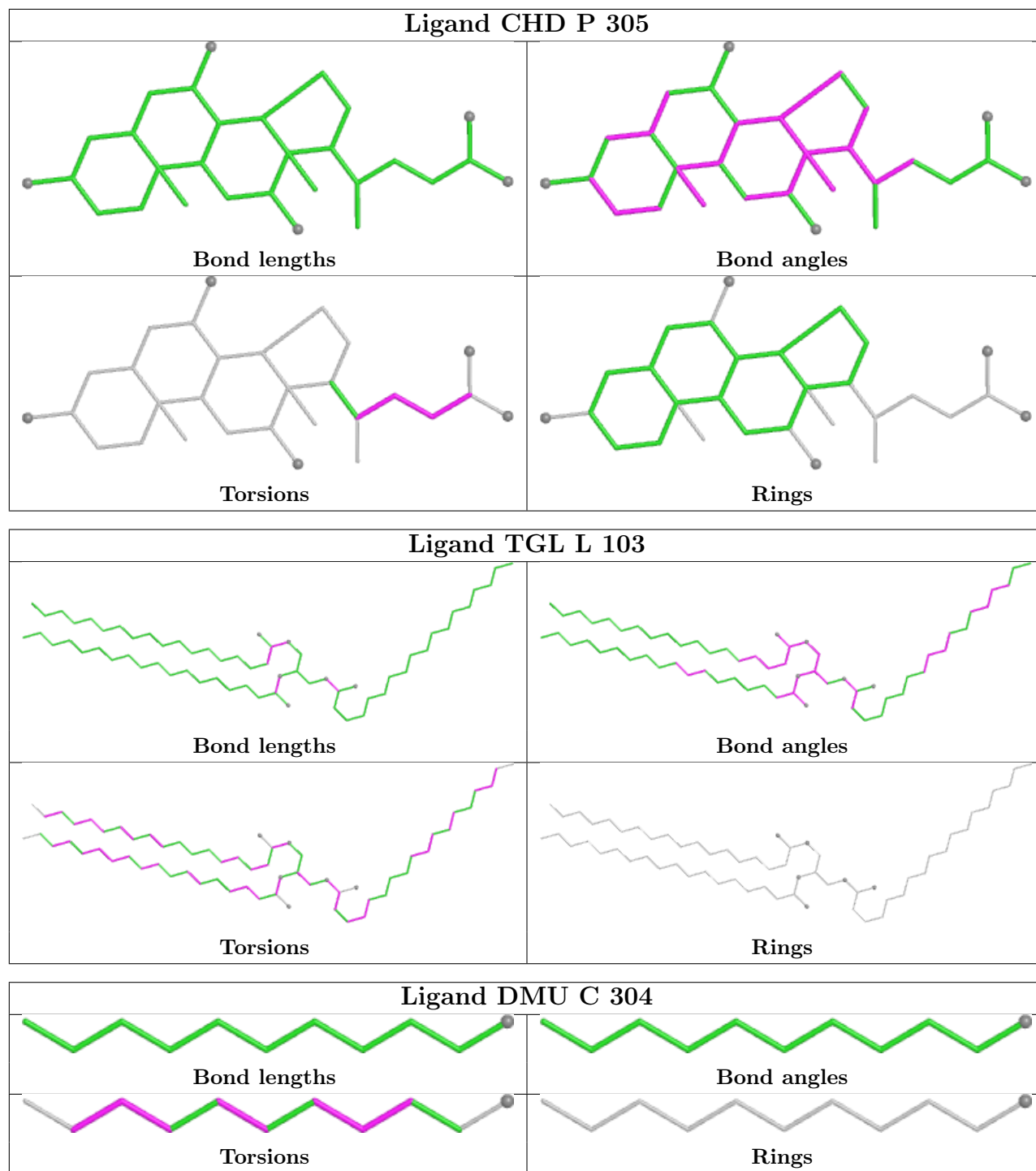




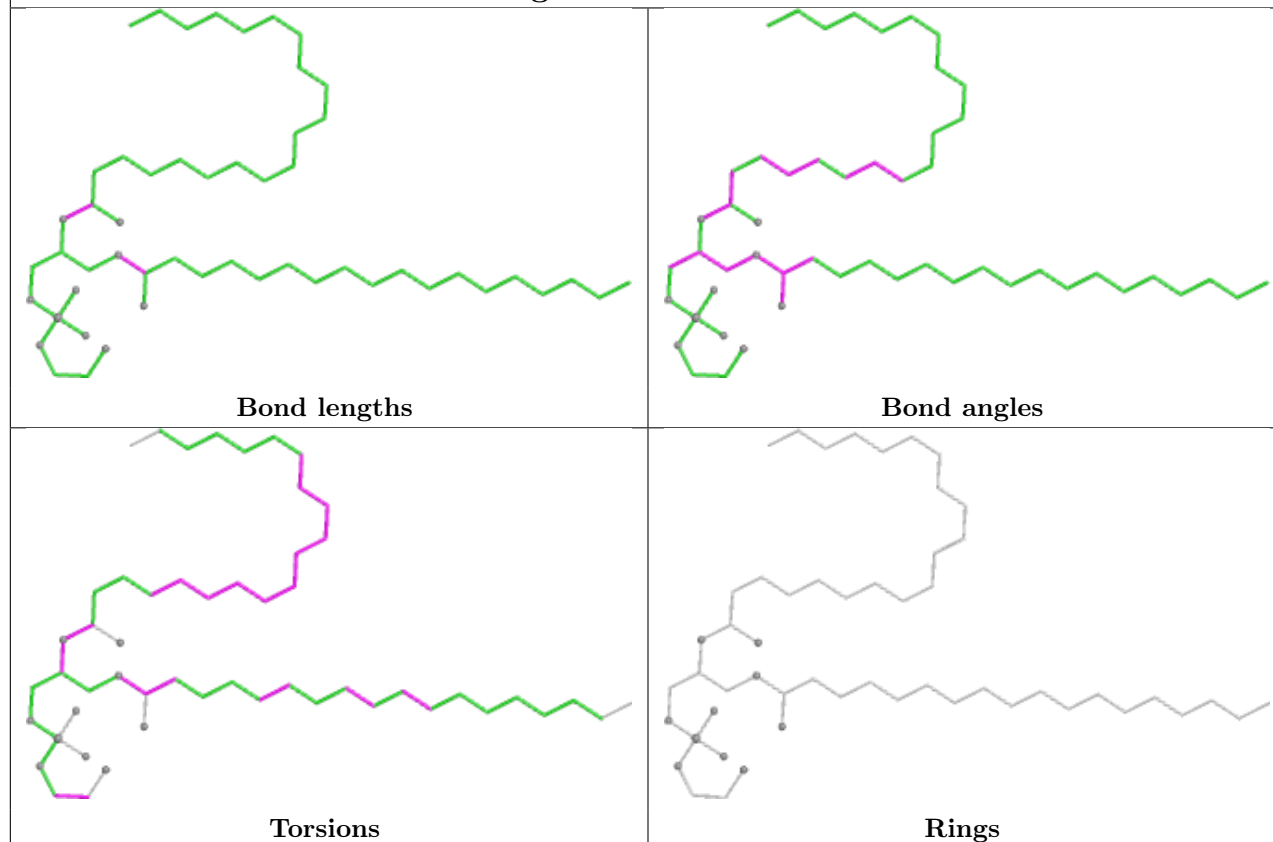




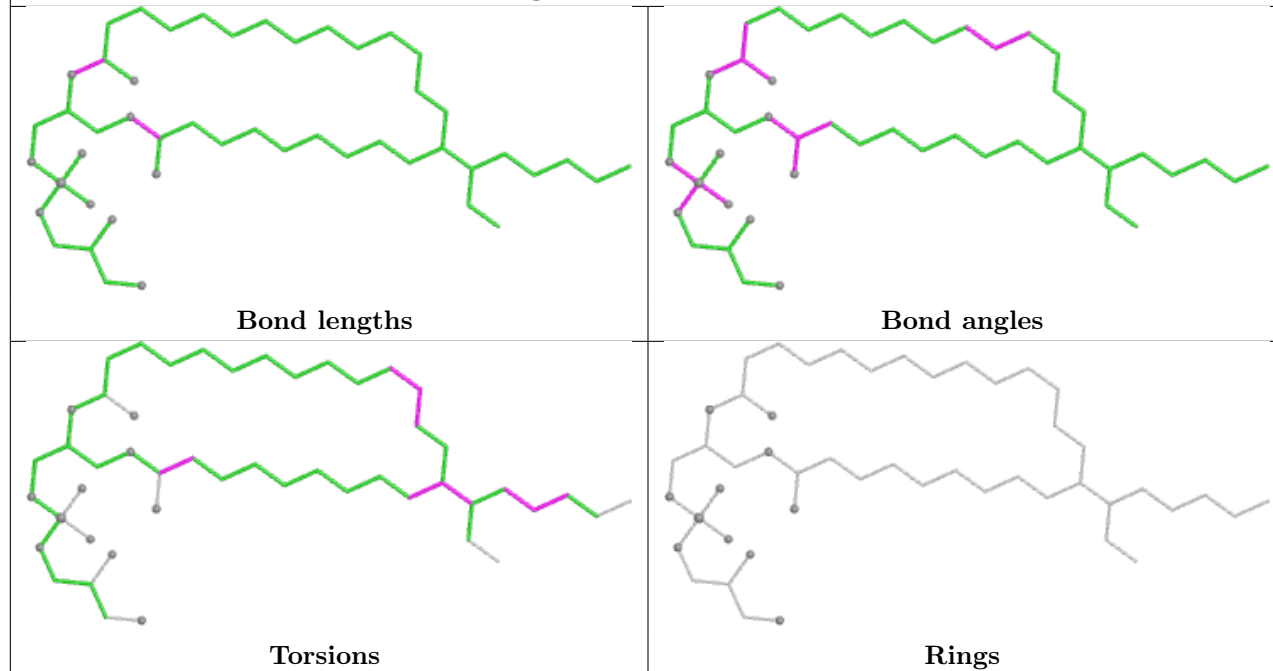


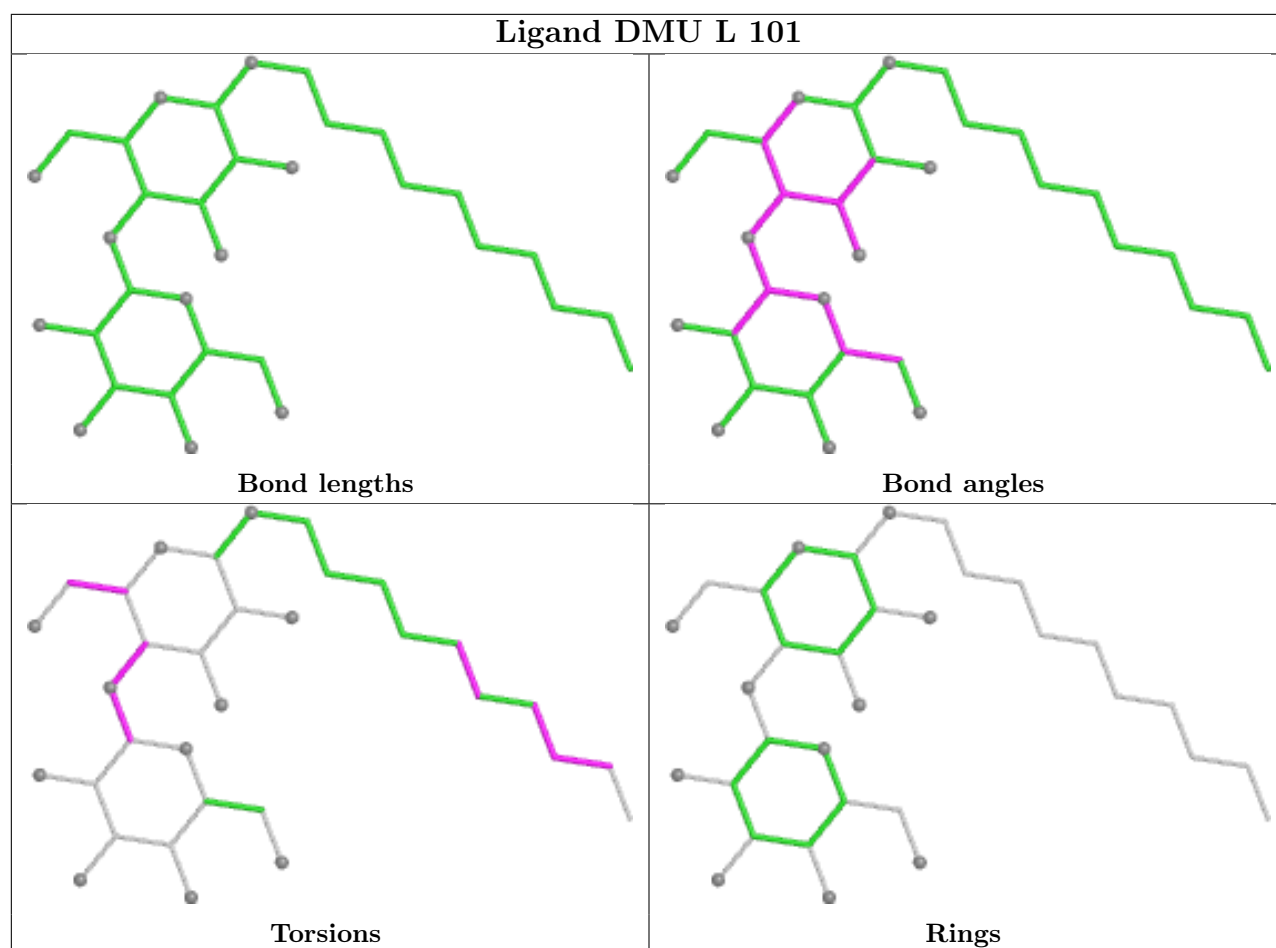


## Ligand PEK P 307

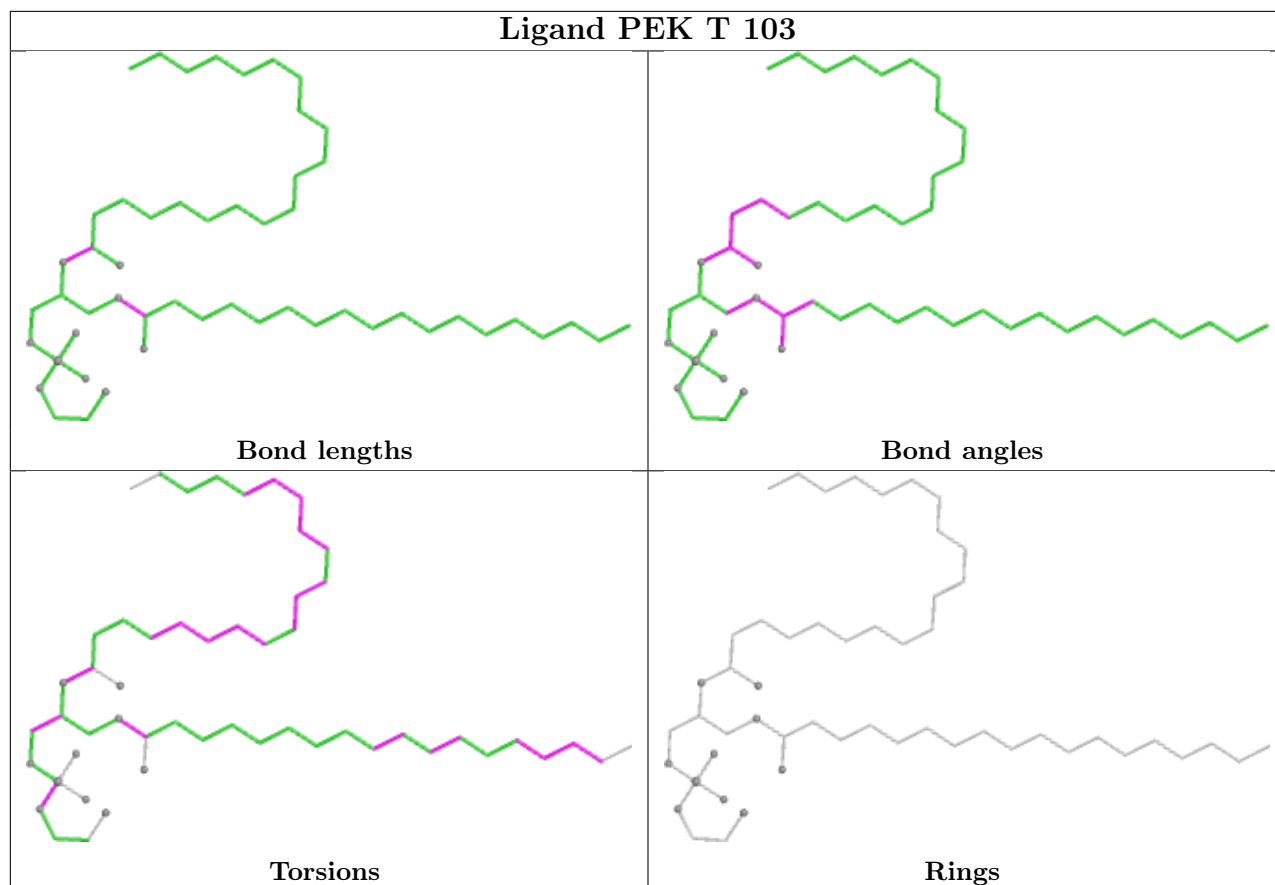


## Ligand PGV N 607

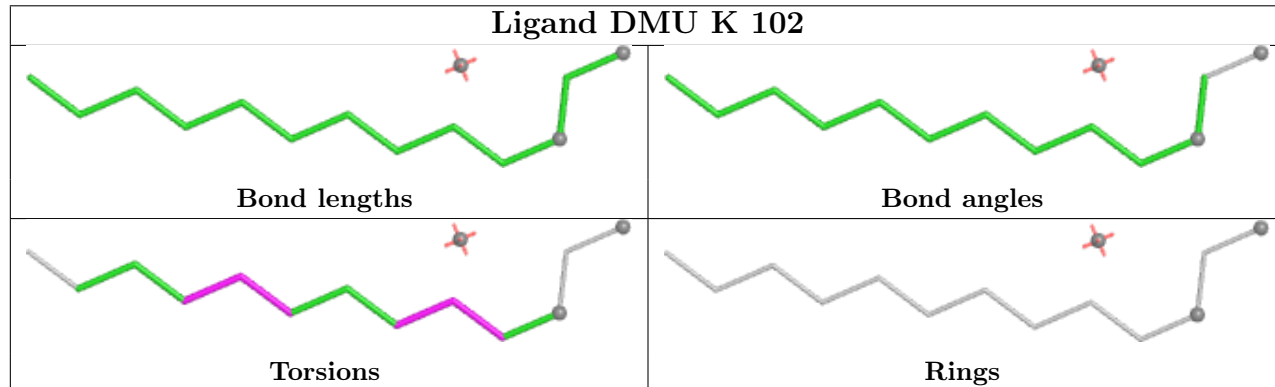


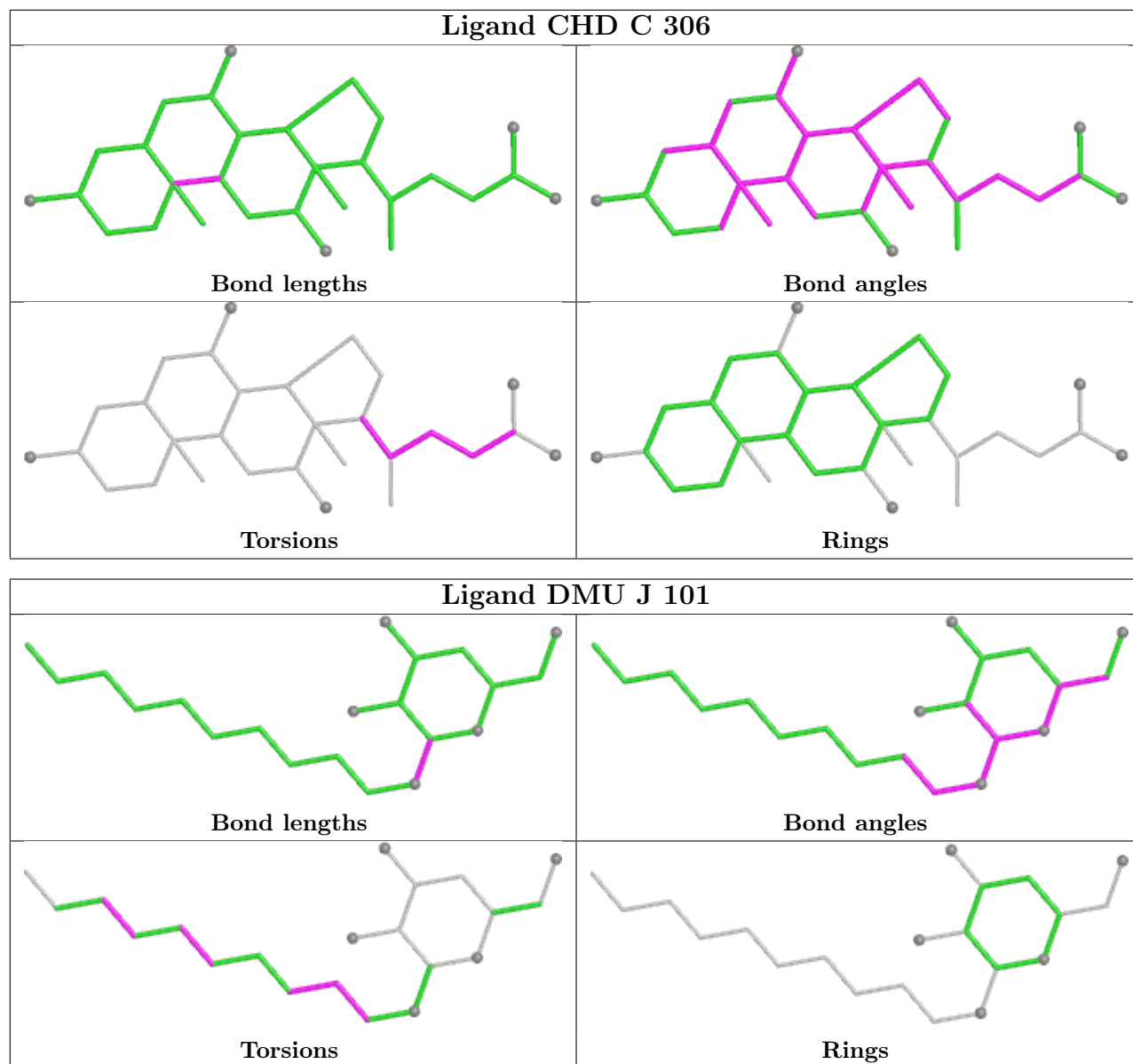


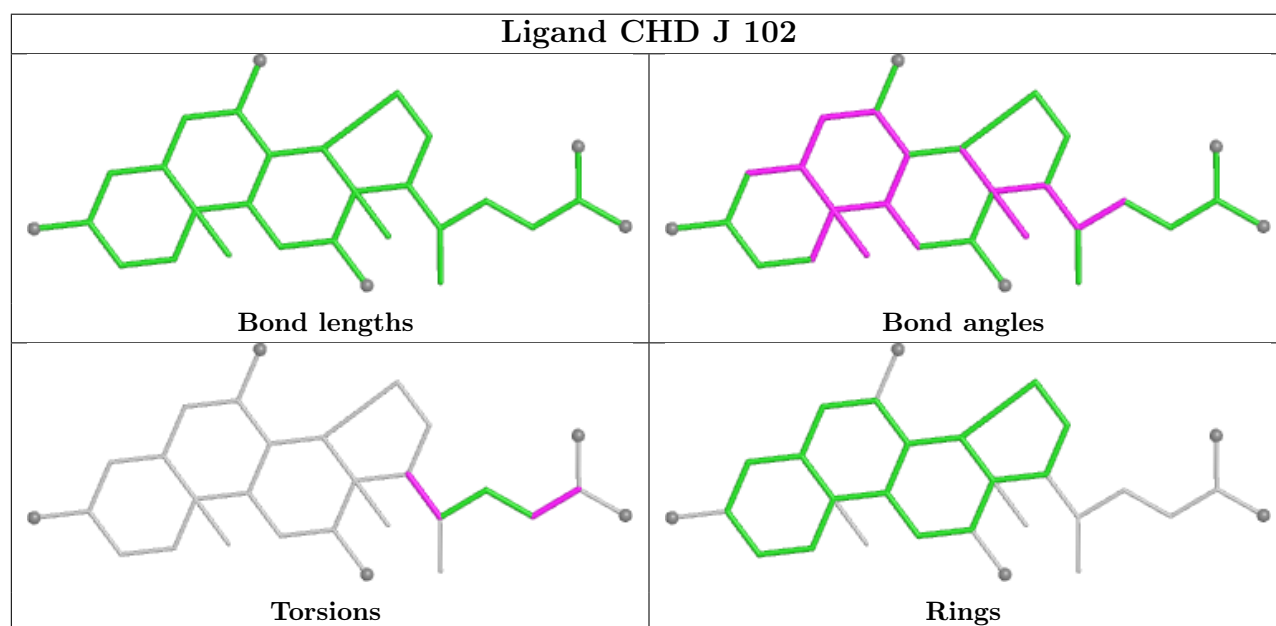
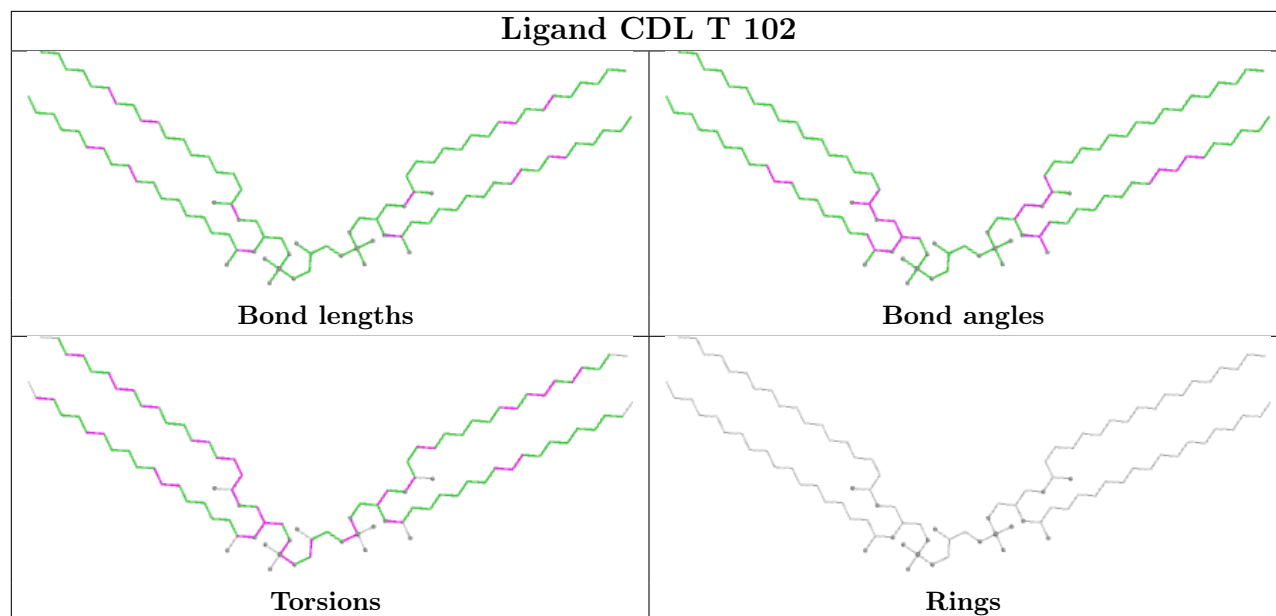
## Ligand PEK T 103

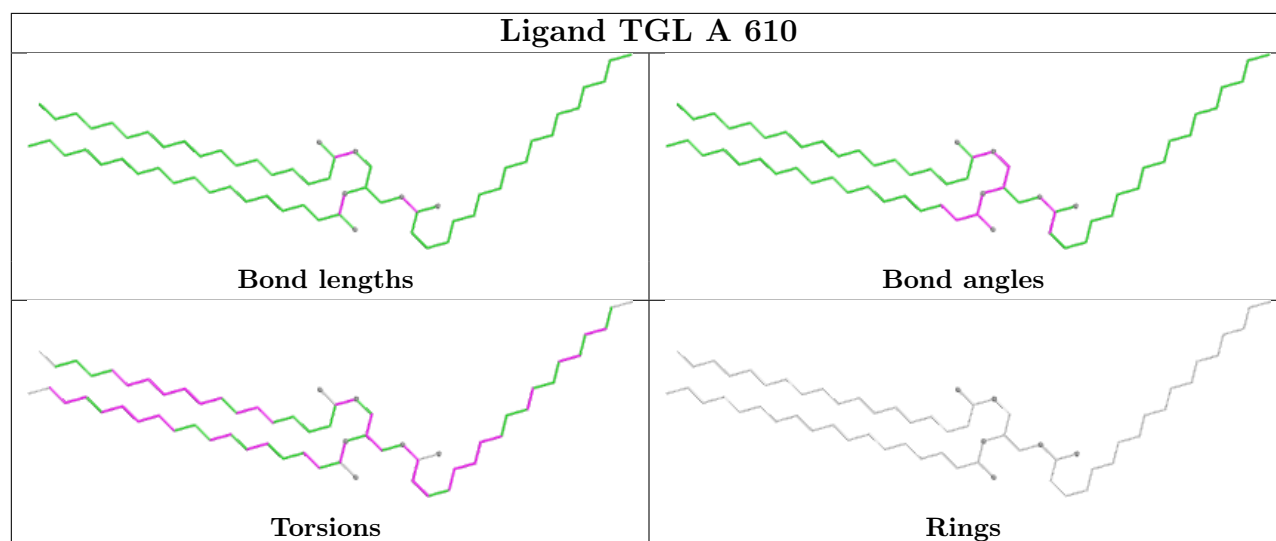
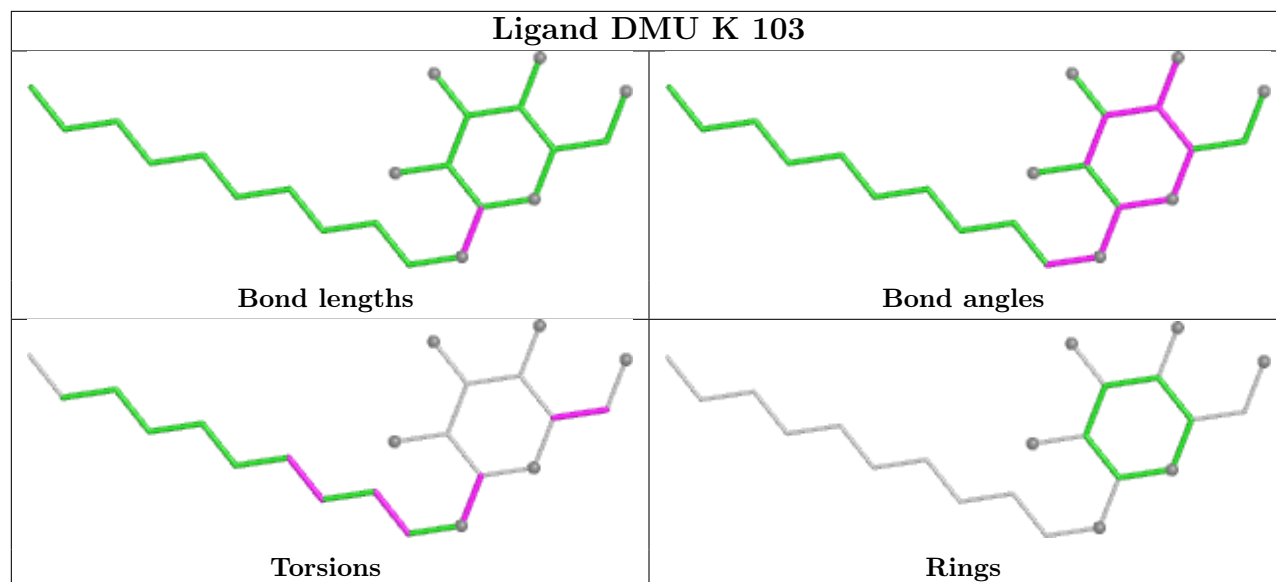


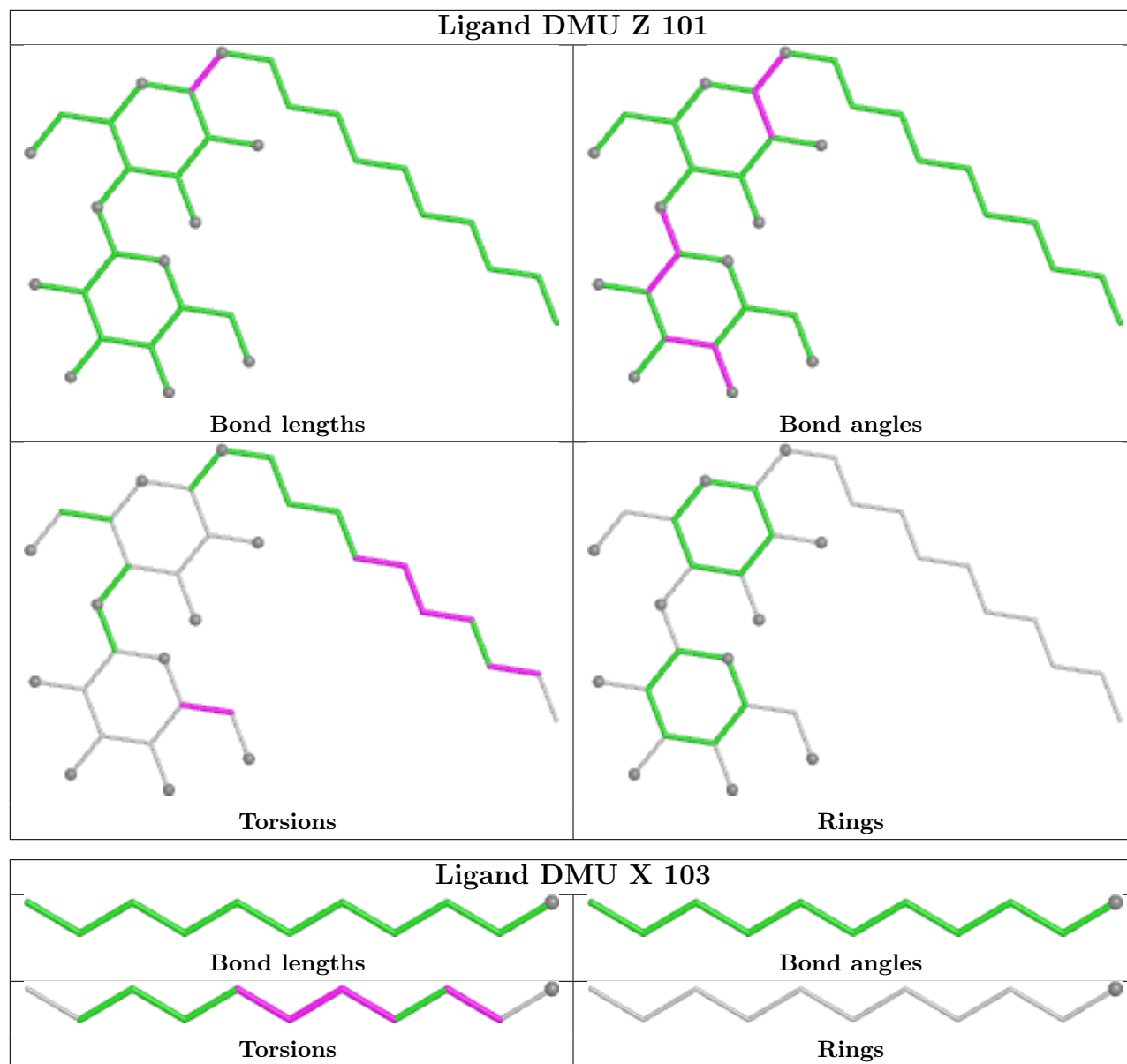
## Ligand DMU K 102

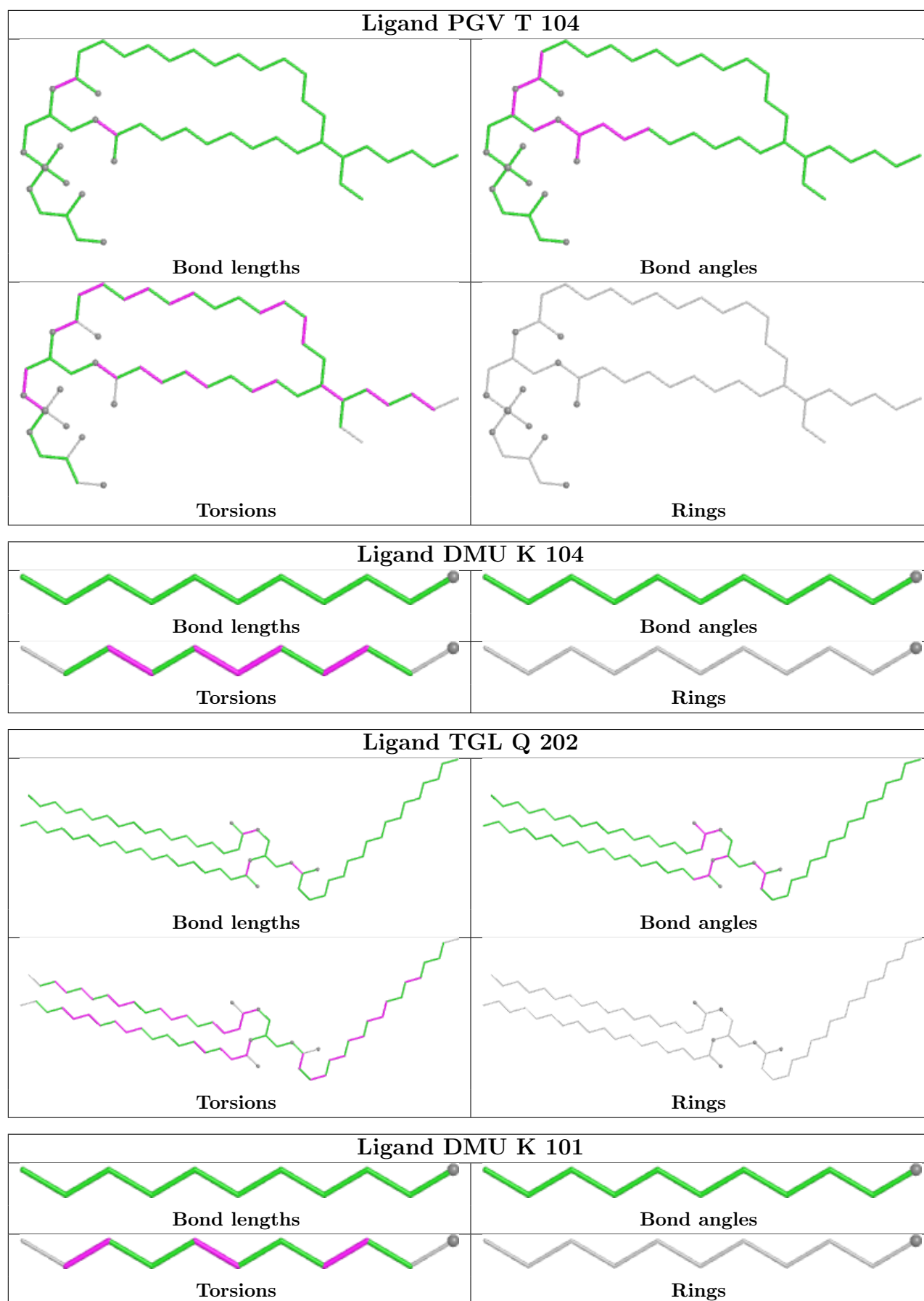


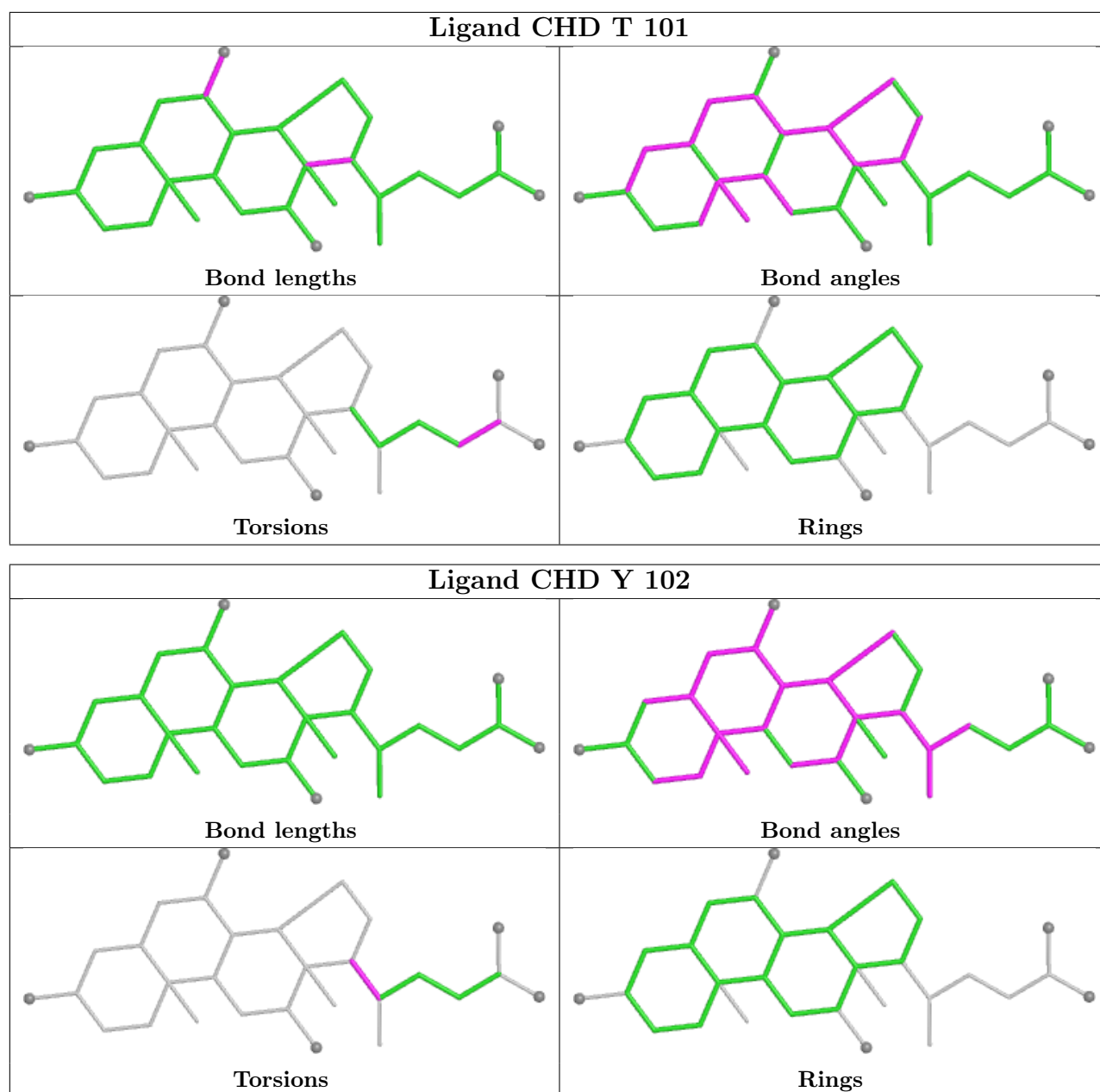


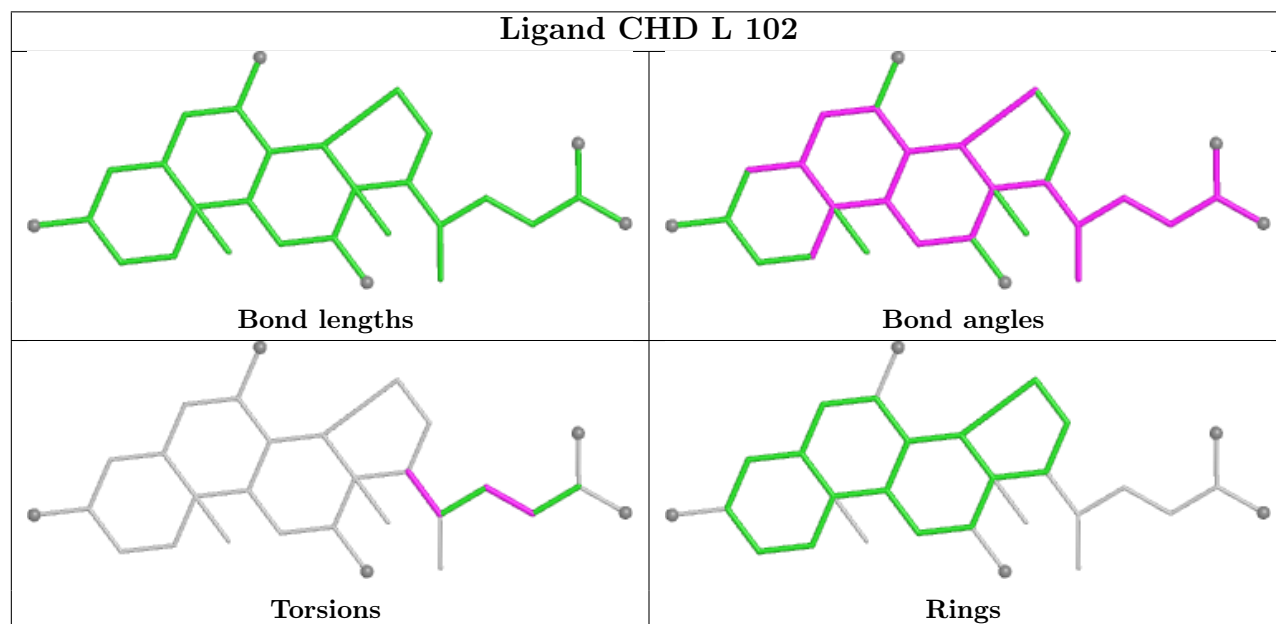
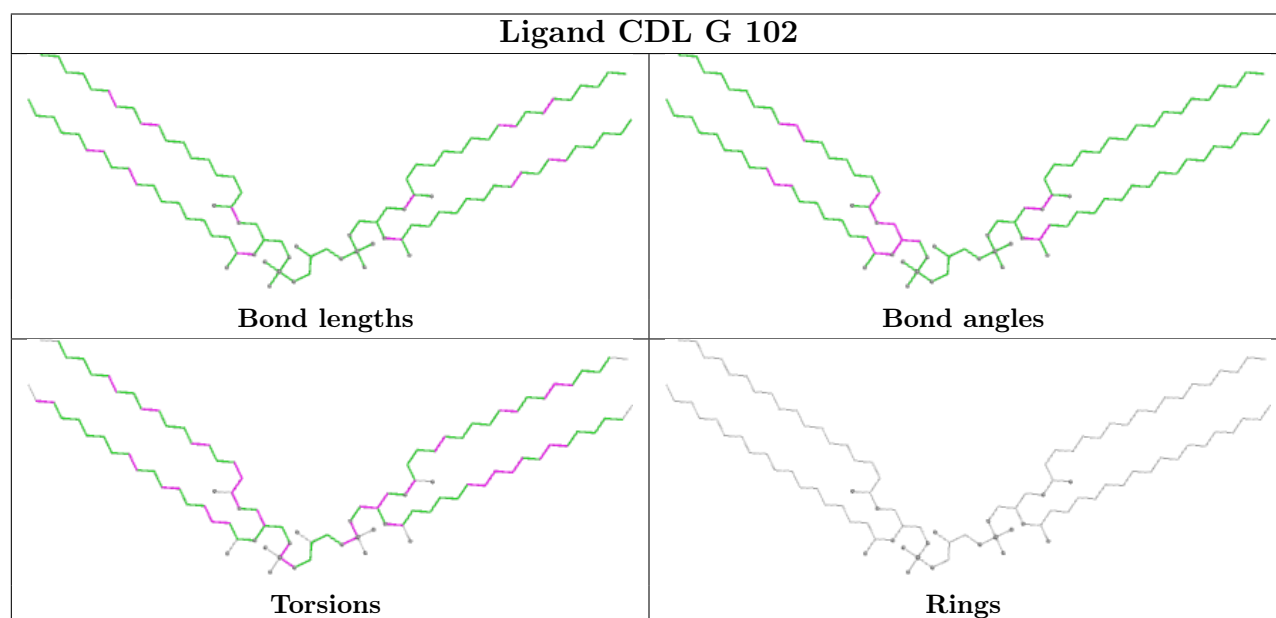
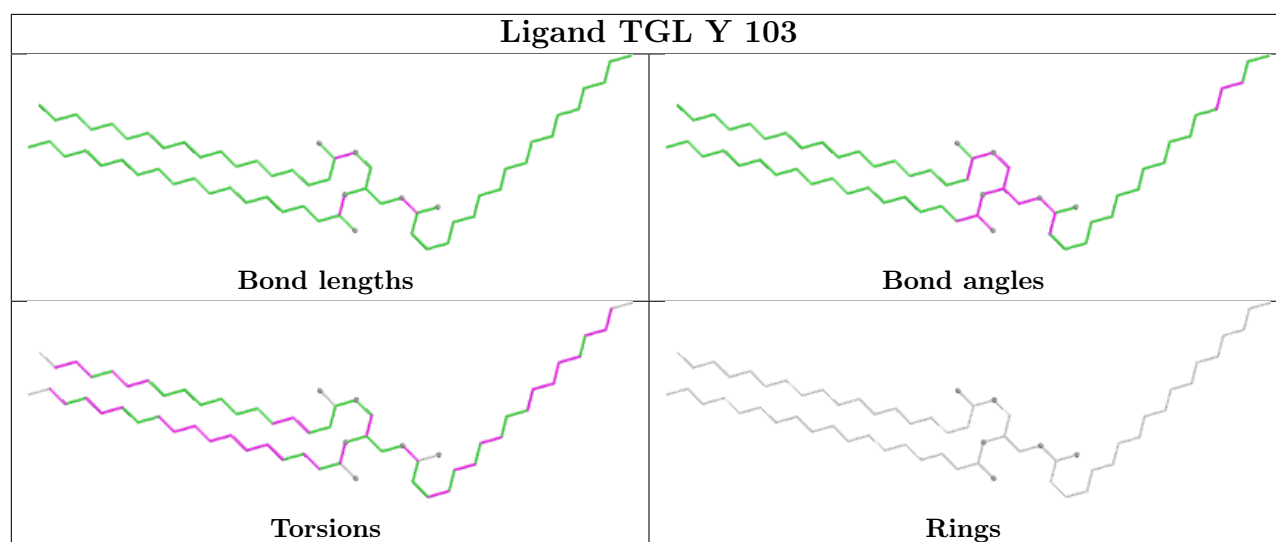


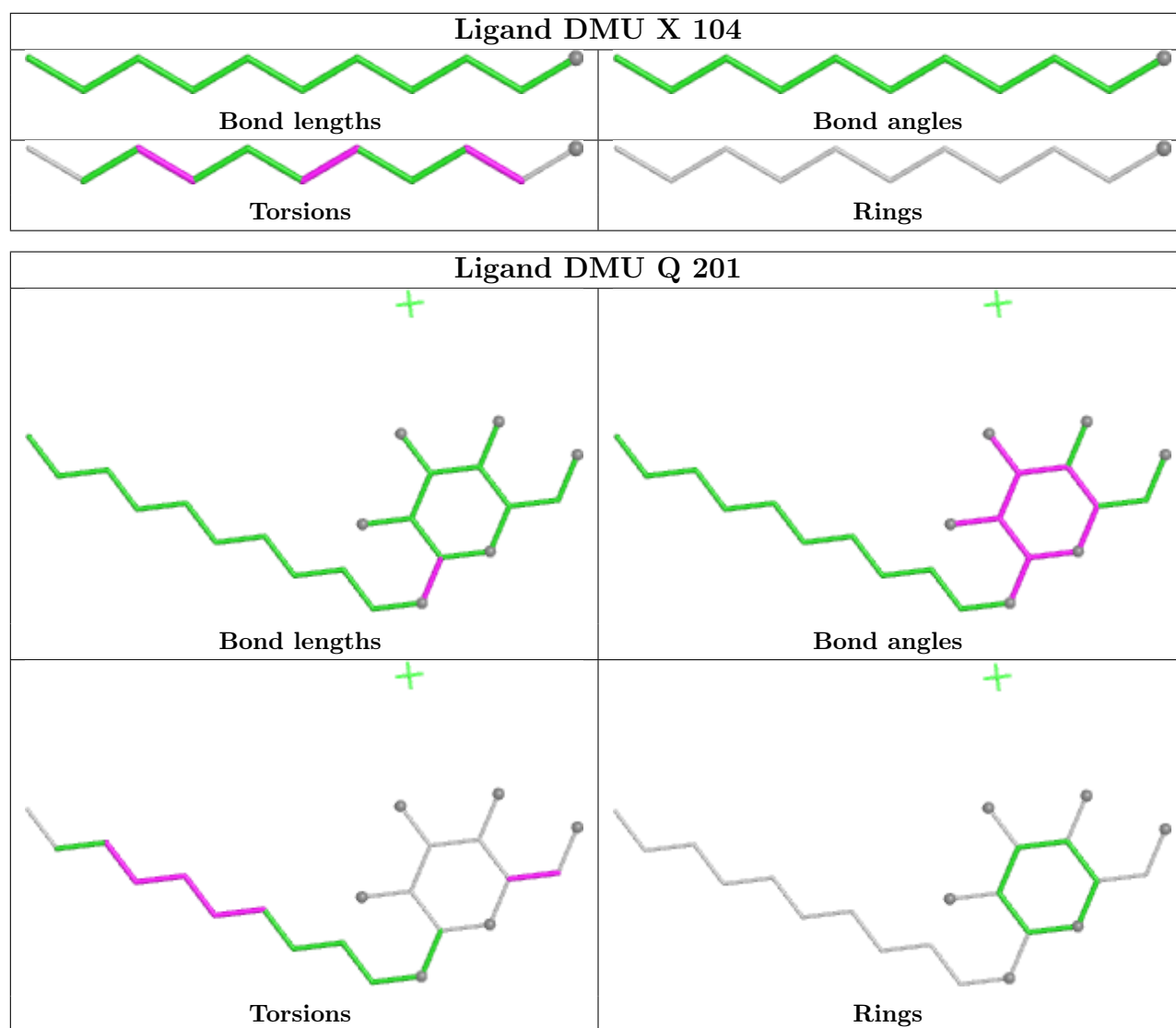












## 5.7 Other polymers [i](#)

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     | 513/514 (99%)  | -0.37  | 2 (0%) 88 89  | 12, 28, 36, 103       | 37 (7%) |
| 1   | N     | 513/514 (99%)  | -0.33  | 5 (0%) 79 80  | 13, 31, 42, 111       | 21 (4%) |
| 2   | B     | 226/227 (99%)  | 0.21   | 12 (5%) 32 31 | 26, 37, 73, 143       | 4 (1%)  |
| 2   | O     | 226/227 (99%)  | 0.29   | 11 (4%) 35 33 | 29, 42, 81, 124       | 7 (3%)  |
| 3   | C     | 259/259 (100%) | -0.12  | 3 (1%) 76 77  | 25, 32, 50, 99        | 5 (1%)  |
| 3   | P     | 259/259 (100%) | -0.05  | 7 (2%) 56 56  | 26, 33, 55, 94        | 2 (0%)  |
| 4   | D     | 144/144 (100%) | 0.09   | 4 (2%) 55 55  | 23, 39, 64, 120       | 1 (0%)  |
| 4   | Q     | 144/144 (100%) | 0.82   | 17 (11%) 9 7  | 36, 52, 106, 286      | 0       |
| 5   | E     | 105/105 (100%) | 0.02   | 3 (2%) 53 53  | 29, 37, 72, 132       | 0       |
| 5   | R     | 105/105 (100%) | 0.29   | 3 (2%) 53 53  | 33, 47, 83, 161       | 0       |
| 6   | F     | 98/98 (100%)   | 0.64   | 12 (12%) 8 7  | 28, 41, 147, 232      | 1 (1%)  |
| 6   | S     | 98/98 (100%)   | 0.68   | 15 (15%) 5 4  | 29, 42, 130, 198      | 1 (1%)  |
| 7   | G     | 83/84 (98%)    | 1.38   | 18 (21%) 2 2  | 29, 41, 129, 212      | 0       |
| 7   | T     | 83/84 (98%)    | 0.99   | 16 (19%) 3 2  | 28, 45, 138, 226      | 1 (1%)  |
| 8   | H     | 79/79 (100%)   | 0.65   | 7 (8%) 15 13  | 33, 45, 118, 155      | 0       |
| 8   | U     | 79/79 (100%)   | 0.76   | 12 (15%) 5 4  | 36, 48, 144, 220      | 0       |
| 9   | I     | 72/73 (98%)    | 0.88   | 9 (12%) 8 6   | 34, 54, 87, 116       | 0       |
| 9   | V     | 72/73 (98%)    | 1.12   | 12 (16%) 4 3  | 34, 61, 104, 191      | 0       |
| 10  | J     | 58/58 (100%)   | 0.41   | 2 (3%) 48 48  | 31, 43, 94, 131       | 0       |
| 10  | W     | 58/58 (100%)   | 0.60   | 5 (8%) 16 14  | 33, 47, 94, 161       | 0       |
| 11  | K     | 49/49 (100%)   | 0.35   | 2 (4%) 41 41  | 35, 43, 67, 78        | 0       |
| 11  | X     | 49/49 (100%)   | 0.67   | 5 (10%) 12 10 | 43, 54, 93, 113       | 0       |
| 12  | L     | 46/46 (100%)   | 0.20   | 2 (4%) 40 39  | 29, 33, 62, 118       | 0       |
| 12  | Y     | 46/46 (100%)   | 0.28   | 3 (6%) 25 23  | 34, 42, 87, 126       | 0       |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|----------------|-----------------------|---------|
| 13  | M     | 43/43 (100%)    | 0.14   | 2 (4%) 36 35   | 29, 34, 83, 143       | 0       |
| 13  | Z     | 43/43 (100%)    | 0.64   | 8 (18%) 3 2    | 40, 46, 123, 185      | 0       |
| All | All   | 3550/3558 (99%) | 0.17   | 197 (5%) 30 29 | 12, 37, 85, 286       | 80 (2%) |

All (197) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 4   | Q     | 6     | VAL  | 10.7 |
| 6   | S     | 1     | ALA  | 10.4 |
| 7   | G     | 3     | ALA  | 10.0 |
| 6   | F     | 1     | ALA  | 9.9  |
| 7   | G     | 1     | ALA  | 9.3  |
| 7   | T     | 3     | ALA  | 8.4  |
| 7   | G     | 6     | GLY  | 8.2  |
| 7   | G     | 8     | HIS  | 7.5  |
| 4   | Q     | 5     | VAL  | 7.3  |
| 7   | G     | 9     | GLY  | 6.7  |
| 7   | T     | 36[A] | TRP  | 6.6  |
| 7   | G     | 7     | ASP  | 6.5  |
| 7   | G     | 36    | TRP  | 6.4  |
| 7   | T     | 4     | ALA  | 6.0  |
| 6   | S     | 97    | ALA  | 5.7  |
| 4   | Q     | 8     | SER  | 5.7  |
| 8   | U     | 45    | ALA  | 5.6  |
| 9   | V     | 37    | PHE  | 5.6  |
| 7   | G     | 5     | LYS  | 5.4  |
| 6   | S     | 96    | LEU  | 5.4  |
| 7   | G     | 2     | SER  | 5.4  |
| 2   | O     | 113   | TYR  | 5.3  |
| 7   | G     | 10    | GLY  | 5.2  |
| 7   | G     | 4     | ALA  | 5.2  |
| 6   | S     | 94    | HIS  | 5.2  |
| 8   | U     | 8     | ILE  | 5.1  |
| 7   | T     | 8     | HIS  | 5.0  |
| 7   | T     | 2     | SER  | 5.0  |
| 6   | F     | 96    | LEU  | 5.0  |
| 9   | V     | 3     | ALA  | 4.9  |
| 7   | T     | 7     | ASP  | 4.8  |
| 7   | T     | 9     | GLY  | 4.8  |
| 6   | F     | 84    | SER  | 4.7  |
| 6   | F     | 97    | ALA  | 4.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | D     | 4   | SER  | 4.6  |
| 9   | I     | 29  | LEU  | 4.6  |
| 8   | H     | 47  | GLY  | 4.6  |
| 4   | Q     | 4   | SER  | 4.5  |
| 2   | O     | 227 | LEU  | 4.5  |
| 6   | S     | 93  | PRO  | 4.5  |
| 6   | S     | 84  | SER  | 4.5  |
| 7   | T     | 6   | GLY  | 4.3  |
| 8   | H     | 8   | ILE  | 4.3  |
| 9   | V     | 65  | LYS  | 4.2  |
| 13  | Z     | 40  | TYR  | 4.1  |
| 9   | I     | 25  | PHE  | 4.1  |
| 10  | J     | 1   | PHE  | 4.1  |
| 9   | V     | 2   | THR  | 4.0  |
| 6   | F     | 2   | SER  | 4.0  |
| 7   | T     | 5   | LYS  | 3.9  |
| 8   | H     | 48  | GLY  | 3.8  |
| 2   | B     | 65  | TRP  | 3.8  |
| 6   | F     | 98  | HIS  | 3.7  |
| 2   | B     | 61  | VAL  | 3.7  |
| 6   | S     | 2   | SER  | 3.7  |
| 6   | F     | 95  | GLN  | 3.7  |
| 6   | F     | 3   | GLY  | 3.6  |
| 7   | T     | 10  | GLY  | 3.6  |
| 8   | H     | 45  | ALA  | 3.5  |
| 4   | Q     | 7   | LYS  | 3.5  |
| 2   | B     | 113 | TYR  | 3.5  |
| 12  | L     | 2   | HIS  | 3.5  |
| 6   | S     | 95  | GLN  | 3.4  |
| 7   | G     | 37  | LEU  | 3.4  |
| 13  | Z     | 39  | ASN  | 3.4  |
| 8   | H     | 46  | LYS  | 3.3  |
| 8   | U     | 7   | LYS  | 3.3  |
| 11  | X     | 52  | GLU  | 3.3  |
| 6   | S     | 62  | CYS  | 3.3  |
| 2   | O     | 221 | LYS  | 3.3  |
| 8   | U     | 46  | LYS  | 3.3  |
| 12  | L     | 47  | LYS  | 3.3  |
| 5   | R     | 109 | VAL  | 3.2  |
| 9   | I     | 2   | THR  | 3.2  |
| 11  | X     | 6   | ALA  | 3.2  |
| 2   | B     | 87  | MET  | 3.2  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 2   | B     | 58    | ALA  | 3.2  |
| 2   | O     | 32[A] | PHE  | 3.2  |
| 3   | C     | 3     | HIS  | 3.2  |
| 10  | W     | 57    | HIS  | 3.2  |
| 4   | Q     | 147   | LYS  | 3.1  |
| 3   | P     | 33    | MET  | 3.1  |
| 6   | F     | 62    | CYS  | 3.1  |
| 2   | O     | 65[A] | TRP  | 3.1  |
| 8   | U     | 47    | GLY  | 3.1  |
| 1   | N     | 514   | LYS  | 3.0  |
| 13  | M     | 40    | TYR  | 3.0  |
| 12  | Y     | 20    | ARG  | 3.0  |
| 6   | S     | 43    | LYS  | 3.0  |
| 2   | O     | 116   | LEU  | 3.0  |
| 10  | W     | 52    | TRP  | 3.0  |
| 7   | G     | 40    | GLY  | 3.0  |
| 4   | Q     | 46    | ALA  | 3.0  |
| 4   | Q     | 10    | ASP  | 2.9  |
| 9   | I     | 37    | PHE  | 2.9  |
| 8   | U     | 55    | TRP  | 2.9  |
| 4   | Q     | 51    | LEU  | 2.9  |
| 5   | E     | 109   | VAL  | 2.9  |
| 9   | I     | 21    | ILE  | 2.9  |
| 7   | G     | 12    | GLY  | 2.9  |
| 8   | U     | 48    | GLY  | 2.9  |
| 2   | B     | 91    | ASN  | 2.8  |
| 6   | S     | 98    | HIS  | 2.8  |
| 10  | W     | 1     | PHE  | 2.8  |
| 9   | V     | 15    | ARG  | 2.8  |
| 3   | P     | 44    | MET  | 2.8  |
| 7   | G     | 39    | SER  | 2.8  |
| 2   | O     | 91    | ASN  | 2.8  |
| 1   | A     | 514   | LYS  | 2.8  |
| 1   | N     | 49[A] | GLY  | 2.8  |
| 8   | U     | 9     | LYS  | 2.8  |
| 13  | M     | 42    | LYS  | 2.8  |
| 2   | B     | 55    | THR  | 2.8  |
| 6   | S     | 52    | ILE  | 2.8  |
| 13  | Z     | 38    | ASP  | 2.7  |
| 6   | S     | 3     | GLY  | 2.7  |
| 3   | P     | 37    | PHE  | 2.7  |
| 2   | O     | 92    | ASN  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | P     | 3   | HIS  | 2.7  |
| 12  | Y     | 2   | HIS  | 2.7  |
| 10  | W     | 48  | TYR  | 2.7  |
| 5   | R     | 80  | GLU  | 2.7  |
| 9   | V     | 44  | LYS  | 2.7  |
| 11  | K     | 47  | ARG  | 2.6  |
| 13  | Z     | 42  | LYS  | 2.6  |
| 8   | H     | 10  | ASN  | 2.6  |
| 9   | I     | 36  | LYS  | 2.6  |
| 6   | F     | 85  | CYS  | 2.6  |
| 7   | G     | 41  | HIS  | 2.6  |
| 7   | T     | 46  | ALA  | 2.6  |
| 9   | V     | 34  | PHE  | 2.5  |
| 2   | O     | 57  | ASP  | 2.5  |
| 9   | V     | 33  | THR  | 2.5  |
| 6   | S     | 85  | CYS  | 2.5  |
| 2   | B     | 57  | ASP  | 2.5  |
| 13  | Z     | 41  | LYS  | 2.5  |
| 7   | T     | 12  | GLY  | 2.5  |
| 3   | P     | 261 | SER  | 2.5  |
| 5   | R     | 5   | HIS  | 2.5  |
| 4   | D     | 5   | VAL  | 2.5  |
| 10  | W     | 27  | THR  | 2.5  |
| 4   | D     | 8   | SER  | 2.5  |
| 3   | C     | 33  | MET  | 2.5  |
| 2   | B     | 68  | LEU  | 2.4  |
| 1   | N     | 113 | LEU  | 2.4  |
| 6   | S     | 65  | ASP  | 2.4  |
| 9   | I     | 73  | LYS  | 2.4  |
| 9   | V     | 20  | HIS  | 2.3  |
| 7   | T     | 39  | SER  | 2.3  |
| 4   | Q     | 9   | GLU  | 2.3  |
| 2   | B     | 56  | MET  | 2.3  |
| 8   | U     | 61  | LYS  | 2.3  |
| 11  | K     | 54  | ARG  | 2.3  |
| 4   | Q     | 59  | LEU  | 2.3  |
| 11  | X     | 23  | THR  | 2.3  |
| 8   | U     | 11  | TYR  | 2.2  |
| 10  | J     | 48  | TYR  | 2.2  |
| 11  | X     | 13  | TYR  | 2.2  |
| 2   | B     | 90  | ILE  | 2.2  |
| 13  | Z     | 13  | LYS  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 513 | LEU  | 2.2  |
| 1   | N     | 483 | LEU  | 2.2  |
| 7   | T     | 1   | ALA  | 2.2  |
| 11  | X     | 27  | ALA  | 2.2  |
| 3   | P     | 122 | HIS  | 2.2  |
| 7   | G     | 42  | ARG  | 2.2  |
| 8   | U     | 10  | ASN  | 2.2  |
| 8   | U     | 52  | VAL  | 2.2  |
| 9   | I     | 33  | THR  | 2.2  |
| 13  | Z     | 43  | SER  | 2.2  |
| 1   | N     | 513 | LEU  | 2.2  |
| 2   | O     | 78  | LEU  | 2.2  |
| 7   | T     | 38  | HIS  | 2.1  |
| 3   | C     | 37  | PHE  | 2.1  |
| 7   | G     | 35  | SER  | 2.1  |
| 3   | P     | 123 | PRO  | 2.1  |
| 6   | F     | 43  | LYS  | 2.1  |
| 8   | H     | 7   | LYS  | 2.1  |
| 7   | T     | 41  | HIS  | 2.1  |
| 9   | V     | 38  | ALA  | 2.1  |
| 2   | B     | 59  | GLN  | 2.1  |
| 9   | V     | 25  | PHE  | 2.1  |
| 4   | Q     | 140 | TYR  | 2.1  |
| 5   | E     | 5   | HIS  | 2.1  |
| 6   | F     | 65  | ASP  | 2.1  |
| 4   | D     | 87  | PHE  | 2.0  |
| 4   | Q     | 87  | PHE  | 2.0  |
| 4   | Q     | 114 | GLU  | 2.0  |
| 4   | Q     | 52  | SER  | 2.0  |
| 9   | I     | 30  | GLY  | 2.0  |
| 4   | Q     | 33  | LEU  | 2.0  |
| 5   | E     | 108 | LYS  | 2.0  |
| 9   | V     | 36  | LYS  | 2.0  |
| 13  | Z     | 1   | ILE  | 2.0  |
| 12  | Y     | 26  | THR  | 2.0  |
| 2   | O     | 61  | VAL  | 2.0  |
| 4   | Q     | 19  | ARG  | 2.0  |

## 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 9   | SAC  | V     | 1   | 9/10  | 0.44 | 0.18 | 210,249,270,285            | 0     |
| 7   | TPO  | T     | 11  | 11/12 | 0.67 | 0.25 | 124,161,188,220            | 0     |
| 9   | SAC  | I     | 1   | 9/10  | 0.67 | 0.21 | 131,136,147,157            | 0     |
| 7   | TPO  | G     | 11  | 11/12 | 0.73 | 0.26 | 137,171,213,223            | 0     |
| 1   | FME  | N     | 1   | 10/11 | 0.92 | 0.13 | 38,54,95,119               | 0     |
| 1   | FME  | A     | 1   | 10/11 | 0.93 | 0.14 | 39,52,94,106               | 0     |
| 2   | FME  | B     | 1   | 10/11 | 0.97 | 0.09 | 32,35,43,114               | 0     |
| 2   | FME  | O     | 1   | 10/11 | 0.97 | 0.09 | 35,40,46,125               | 0     |

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 18  | DMU  | K     | 104 | 11/33 | 0.68 | 0.17 | 73,94,107,107              | 0     |
| 18  | DMU  | K     | 103 | 22/33 | 0.69 | 0.21 | 66,110,139,152             | 0     |
| 22  | EDO  | E     | 203 | 4/4   | 0.69 | 0.17 | 67,79,81,82                | 0     |
| 18  | DMU  | Q     | 201 | 23/33 | 0.70 | 0.24 | 52,92,138,154              | 0     |
| 24  | CHD  | Y     | 102 | 29/29 | 0.71 | 0.22 | 68,98,143,174              | 0     |
| 18  | DMU  | X     | 103 | 11/33 | 0.72 | 0.19 | 67,83,110,113              | 0     |
| 18  | DMU  | X     | 105 | 11/33 | 0.72 | 0.20 | 80,95,123,124              | 0     |
| 26  | PEK  | C     | 308 | 53/53 | 0.72 | 0.22 | 48,101,182,205             | 0     |
| 18  | DMU  | C     | 302 | 33/33 | 0.75 | 0.16 | 53,103,152,162             | 0     |
| 18  | DMU  | C     | 303 | 22/33 | 0.75 | 0.19 | 53,89,148,160              | 0     |
| 18  | DMU  | P     | 303 | 33/33 | 0.75 | 0.15 | 49,107,135,152             | 0     |
| 22  | EDO  | C     | 317 | 4/4   | 0.77 | 0.25 | 45,73,80,84                | 0     |
| 24  | CHD  | J     | 102 | 29/29 | 0.78 | 0.17 | 61,109,143,153             | 0     |
| 22  | EDO  | D     | 203 | 4/4   | 0.78 | 0.27 | 45,66,83,84                | 0     |
| 19  | PGV  | T     | 104 | 51/51 | 0.78 | 0.22 | 50,97,182,229              | 0     |
| 19  | PGV  | P     | 310 | 51/51 | 0.79 | 0.20 | 51,97,153,200              | 0     |
| 21  | TGL  | A     | 610 | 63/63 | 0.79 | 0.20 | 36,73,112,133              | 0     |
| 26  | PEK  | T     | 103 | 53/53 | 0.79 | 0.22 | 49,78,169,233              | 0     |

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| Mol | Type | Chain | Res | Atoms   | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|---------|------|------|-----------------------------|-------|
| 18  | DMU  | C     | 304 | 11/33   | 0.80 | 0.16 | 56,65,86,100                | 0     |
| 18  | DMU  | L     | 101 | 33/33   | 0.80 | 0.15 | 49,102,136,160              | 0     |
| 25  | CDL  | T     | 102 | 100/100 | 0.80 | 0.22 | 42,103,168,206              | 0     |
| 18  | DMU  | Y     | 101 | 33/33   | 0.80 | 0.14 | 52,105,145,149              | 0     |
| 22  | EDO  | N     | 618 | 4/4     | 0.80 | 0.22 | 41,54,66,72                 | 0     |
| 21  | TGL  | N     | 608 | 63/63   | 0.81 | 0.20 | 48,70,116,129               | 0     |
| 20  | PSC  | V     | 101 | 52/52   | 0.81 | 0.24 | 43,92,191,241               | 0     |
| 20  | PSC  | A     | 609 | 52/52   | 0.81 | 0.21 | 42,101,181,243              | 0     |
| 26  | PEK  | P     | 307 | 53/53   | 0.81 | 0.21 | 50,74,159,190               | 0     |
| 24  | CHD  | L     | 102 | 29/29   | 0.81 | 0.21 | 51,91,123,145               | 0     |
| 19  | PGV  | N     | 606 | 51/51   | 0.82 | 0.21 | 41,94,148,194               | 0     |
| 22  | EDO  | C     | 311 | 4/4     | 0.82 | 0.23 | 35,61,78,103                | 0     |
| 24  | CHD  | P     | 305 | 29/29   | 0.82 | 0.14 | 59,75,113,132               | 0     |
| 18  | DMU  | D     | 201 | 21/33   | 0.82 | 0.21 | 51,85,132,140               | 0     |
| 18  | DMU  | X     | 102 | 21/33   | 0.83 | 0.15 | 68,102,136,151              | 0     |
| 18  | DMU  | K     | 102 | 14/33   | 0.83 | 0.19 | 60,80,119,123               | 0     |
| 22  | EDO  | C     | 314 | 4/4     | 0.83 | 0.21 | 41,45,49,59                 | 0     |
| 22  | EDO  | F     | 110 | 4/4     | 0.83 | 0.20 | 66,70,80,81                 | 0     |
| 25  | CDL  | G     | 102 | 100/100 | 0.83 | 0.20 | 51,99,177,197               | 0     |
| 25  | CDL  | P     | 306 | 100/100 | 0.83 | 0.23 | 40,100,173,211              | 0     |
| 22  | EDO  | C     | 316 | 4/4     | 0.83 | 0.29 | 52,60,77,128                | 0     |
| 22  | EDO  | P     | 317 | 4/4     | 0.83 | 0.16 | 61,66,67,80                 | 0     |
| 22  | EDO  | S     | 103 | 4/4     | 0.83 | 0.18 | 61,71,80,83                 | 0     |
| 22  | EDO  | S     | 105 | 4/4     | 0.83 | 0.19 | 73,85,94,103                | 0     |
| 18  | DMU  | A     | 606 | 13/33   | 0.84 | 0.17 | 43,67,113,117               | 0     |
| 22  | EDO  | C     | 315 | 4/4     | 0.84 | 0.23 | 51,65,79,108                | 0     |
| 21  | TGL  | D     | 202 | 63/63   | 0.84 | 0.21 | 34,68,120,140               | 0     |
| 22  | EDO  | Q     | 203 | 4/4     | 0.84 | 0.19 | 78,86,87,105                | 0     |
| 19  | PGV  | A     | 607 | 51/51   | 0.85 | 0.22 | 31,70,159,167               | 0     |
| 26  | PEK  | F     | 102 | 53/53   | 0.85 | 0.20 | 46,79,162,232               | 0     |
| 24  | CHD  | C     | 306 | 29/29   | 0.85 | 0.15 | 51,80,118,135               | 0     |
| 21  | TGL  | Q     | 202 | 63/63   | 0.85 | 0.20 | 37,73,125,139               | 0     |
| 21  | TGL  | Y     | 103 | 63/63   | 0.86 | 0.20 | 39,73,128,179               | 0     |
| 22  | EDO  | L     | 104 | 4/4     | 0.86 | 0.21 | 41,94,96,97                 | 0     |
| 21  | TGL  | L     | 103 | 63/63   | 0.86 | 0.20 | 29,63,125,169               | 0     |
| 22  | EDO  | P     | 315 | 4/4     | 0.86 | 0.20 | 41,52,78,113                | 0     |
| 18  | DMU  | X     | 101 | 11/33   | 0.86 | 0.16 | 48,75,115,125               | 0     |
| 18  | DMU  | X     | 104 | 11/33   | 0.86 | 0.20 | 56,71,105,109               | 0     |
| 22  | EDO  | Q     | 205 | 4/4     | 0.86 | 0.24 | 67,78,84,107                | 0     |
| 22  | EDO  | A     | 613 | 4/4     | 0.87 | 0.21 | 39,40,46,80                 | 0     |
| 22  | EDO  | F     | 107 | 4/4     | 0.87 | 0.18 | 54,60,63,83                 | 0     |
| 22  | EDO  | F     | 109 | 4/4     | 0.87 | 0.22 | 53,57,67,98                 | 0     |

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| Mol | Type | Chain | Res | Atoms   | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|---------|------|------|-----------------------------|-------|
| 22  | EDO  | B     | 304 | 4/4     | 0.87 | 0.21 | 59,73,85,88                 | 0     |
| 18  | DMU  | J     | 101 | 21/33   | 0.87 | 0.18 | 32,68,123,131               | 0     |
| 18  | DMU  | W     | 101 | 21/33   | 0.87 | 0.17 | 42,75,111,128               | 0     |
| 25  | CDL  | C     | 307 | 100/100 | 0.88 | 0.17 | 39,85,148,175               | 0     |
| 22  | EDO  | T     | 105 | 4/4     | 0.88 | 0.21 | 58,81,89,108                | 0     |
| 22  | EDO  | D     | 206 | 4/4     | 0.88 | 0.19 | 46,59,99,113                | 0     |
| 22  | EDO  | P     | 314 | 4/4     | 0.88 | 0.19 | 46,48,65,82                 | 0     |
| 22  | EDO  | P     | 313 | 4/4     | 0.89 | 0.19 | 50,57,70,84                 | 0     |
| 22  | EDO  | W     | 102 | 4/4     | 0.89 | 0.18 | 53,80,80,128                | 0     |
| 18  | DMU  | O     | 302 | 11/33   | 0.89 | 0.15 | 57,67,89,89                 | 0     |
| 22  | EDO  | D     | 205 | 4/4     | 0.89 | 0.16 | 53,58,60,87                 | 0     |
| 18  | DMU  | P     | 302 | 11/33   | 0.89 | 0.14 | 52,60,93,94                 | 0     |
| 28  | PO4  | H     | 101 | 5/5     | 0.89 | 0.09 | 63,70,118,149               | 0     |
| 22  | EDO  | N     | 623 | 4/4     | 0.90 | 0.24 | 67,76,79,96                 | 0     |
| 18  | DMU  | K     | 101 | 11/33   | 0.90 | 0.14 | 47,70,93,99                 | 0     |
| 18  | DMU  | Z     | 101 | 33/33   | 0.90 | 0.13 | 44,58,89,96                 | 0     |
| 24  | CHD  | C     | 305 | 29/29   | 0.90 | 0.11 | 35,42,60,67                 | 0     |
| 22  | EDO  | M     | 102 | 4/4     | 0.90 | 0.16 | 71,76,76,93                 | 0     |
| 22  | EDO  | N     | 611 | 4/4     | 0.90 | 0.19 | 37,37,43,56                 | 0     |
| 22  | EDO  | D     | 207 | 4/4     | 0.90 | 0.17 | 42,70,72,108                | 0     |
| 22  | EDO  | N     | 620 | 4/4     | 0.90 | 0.17 | 45,56,92,96                 | 0     |
| 22  | EDO  | N     | 622 | 4/4     | 0.90 | 0.20 | 29,50,67,70                 | 0     |
| 22  | EDO  | F     | 106 | 4/4     | 0.91 | 0.12 | 43,43,53,54                 | 0     |
| 22  | EDO  | A     | 617 | 4/4     | 0.91 | 0.25 | 49,69,96,141                | 0     |
| 22  | EDO  | N     | 613 | 4/4     | 0.91 | 0.16 | 52,55,73,74                 | 0     |
| 22  | EDO  | D     | 204 | 4/4     | 0.91 | 0.14 | 54,55,56,95                 | 0     |
| 22  | EDO  | A     | 619 | 4/4     | 0.91 | 0.14 | 59,67,69,89                 | 0     |
| 22  | EDO  | Y     | 104 | 4/4     | 0.91 | 0.16 | 56,71,73,83                 | 0     |
| 22  | EDO  | F     | 104 | 4/4     | 0.91 | 0.20 | 60,66,79,83                 | 0     |
| 28  | PO4  | U     | 101 | 5/5     | 0.91 | 0.09 | 59,65,141,151               | 0     |
| 22  | EDO  | N     | 616 | 4/4     | 0.92 | 0.14 | 49,54,55,66                 | 0     |
| 22  | EDO  | B     | 305 | 4/4     | 0.92 | 0.16 | 44,56,58,76                 | 0     |
| 22  | EDO  | J     | 103 | 4/4     | 0.92 | 0.15 | 44,70,75,83                 | 0     |
| 22  | EDO  | A     | 618 | 4/4     | 0.92 | 0.17 | 38,57,68,73                 | 0     |
| 22  | EDO  | A     | 611 | 4/4     | 0.93 | 0.16 | 37,41,41,94                 | 0     |
| 22  | EDO  | Q     | 204 | 4/4     | 0.93 | 0.14 | 35,64,73,77                 | 0     |
| 22  | EDO  | N     | 619 | 4/4     | 0.93 | 0.15 | 49,65,71,83                 | 0     |
| 22  | EDO  | L     | 105 | 4/4     | 0.93 | 0.11 | 56,59,64,85                 | 0     |
| 22  | EDO  | B     | 306 | 4/4     | 0.93 | 0.16 | 35,46,51,94                 | 0     |
| 18  | DMU  | B     | 302 | 11/33   | 0.93 | 0.13 | 61,78,97,105                | 0     |
| 22  | EDO  | T     | 106 | 4/4     | 0.93 | 0.13 | 38,40,45,52                 | 0     |
| 22  | EDO  | U     | 102 | 4/4     | 0.93 | 0.15 | 42,53,67,72                 | 0     |

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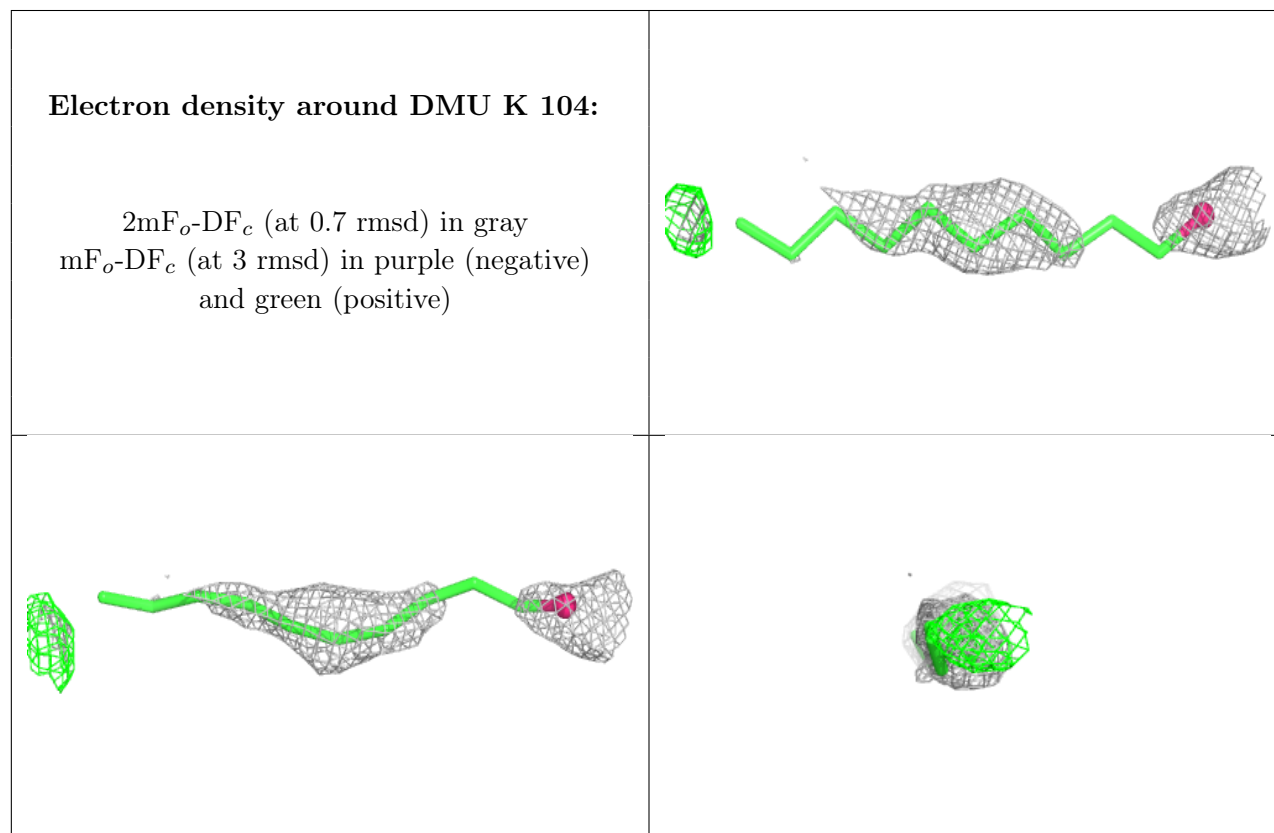
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 22  | EDO  | N     | 612 | 4/4   | 0.93 | 0.15 | 40,55,59,61                 | 0     |
| 22  | EDO  | C     | 312 | 4/4   | 0.93 | 0.13 | 38,46,49,49                 | 0     |
| 22  | EDO  | N     | 615 | 4/4   | 0.93 | 0.17 | 40,56,59,88                 | 0     |
| 22  | EDO  | P     | 316 | 4/4   | 0.93 | 0.19 | 32,52,92,94                 | 0     |
| 18  | DMU  | M     | 101 | 33/33 | 0.93 | 0.10 | 36,46,68,80                 | 0     |
| 22  | EDO  | A     | 614 | 4/4   | 0.94 | 0.14 | 36,57,62,82                 | 0     |
| 22  | EDO  | N     | 621 | 4/4   | 0.94 | 0.15 | 37,47,53,79                 | 0     |
| 22  | EDO  | H     | 102 | 4/4   | 0.94 | 0.12 | 41,41,57,84                 | 0     |
| 22  | EDO  | N     | 610 | 4/4   | 0.94 | 0.15 | 33,57,77,86                 | 0     |
| 22  | EDO  | O     | 303 | 4/4   | 0.94 | 0.09 | 33,35,37,38                 | 0     |
| 22  | EDO  | O     | 304 | 4/4   | 0.94 | 0.17 | 56,64,81,84                 | 0     |
| 22  | EDO  | N     | 617 | 4/4   | 0.94 | 0.14 | 48,48,58,79                 | 0     |
| 24  | CHD  | P     | 304 | 29/29 | 0.94 | 0.09 | 34,44,64,70                 | 0     |
| 22  | EDO  | F     | 108 | 4/4   | 0.94 | 0.12 | 74,76,86,88                 | 0     |
| 22  | EDO  | A     | 616 | 4/4   | 0.94 | 0.16 | 48,53,72,112                | 0     |
| 22  | EDO  | A     | 615 | 4/4   | 0.95 | 0.18 | 30,61,69,139                | 0     |
| 26  | PEK  | C     | 309 | 53/53 | 0.95 | 0.12 | 31,48,111,119               | 0     |
| 22  | EDO  | B     | 307 | 4/4   | 0.95 | 0.15 | 36,57,74,101                | 0     |
| 22  | EDO  | C     | 313 | 4/4   | 0.95 | 0.12 | 34,41,56,57                 | 0     |
| 26  | PEK  | P     | 308 | 53/53 | 0.95 | 0.12 | 31,50,93,125                | 0     |
| 22  | EDO  | E     | 201 | 4/4   | 0.95 | 0.09 | 44,47,50,56                 | 0     |
| 22  | EDO  | E     | 202 | 4/4   | 0.95 | 0.10 | 37,40,47,53                 | 0     |
| 22  | EDO  | S     | 102 | 4/4   | 0.95 | 0.13 | 33,33,35,39                 | 0     |
| 22  | EDO  | B     | 303 | 4/4   | 0.96 | 0.08 | 30,31,32,40                 | 0     |
| 22  | EDO  | G     | 103 | 4/4   | 0.96 | 0.08 | 31,37,40,44                 | 0     |
| 22  | EDO  | F     | 105 | 4/4   | 0.96 | 0.11 | 36,39,40,42                 | 0     |
| 22  | EDO  | A     | 612 | 4/4   | 0.96 | 0.08 | 24,28,31,31                 | 0     |
| 22  | EDO  | N     | 614 | 4/4   | 0.96 | 0.11 | 38,45,67,71                 | 0     |
| 19  | PGV  | N     | 607 | 51/51 | 0.96 | 0.10 | 26,38,64,78                 | 0     |
| 19  | PGV  | C     | 310 | 51/51 | 0.96 | 0.11 | 26,33,93,120                | 0     |
| 22  | EDO  | P     | 312 | 4/4   | 0.96 | 0.12 | 37,43,47,68                 | 0     |
| 19  | PGV  | A     | 608 | 51/51 | 0.96 | 0.11 | 26,33,69,92                 | 0     |
| 22  | EDO  | S     | 106 | 4/4   | 0.96 | 0.11 | 38,45,59,63                 | 0     |
| 27  | ZN   | F     | 101 | 1/1   | 0.96 | 0.32 | 55,55,55,55                 | 0     |
| 27  | ZN   | S     | 101 | 1/1   | 0.96 | 0.31 | 55,55,55,55                 | 0     |
| 24  | CHD  | T     | 101 | 29/29 | 0.96 | 0.07 | 28,33,41,65                 | 0     |
| 22  | EDO  | N     | 609 | 4/4   | 0.96 | 0.08 | 29,32,35,37                 | 0     |
| 19  | PGV  | P     | 309 | 51/51 | 0.97 | 0.10 | 26,37,83,126                | 0     |
| 22  | EDO  | F     | 103 | 4/4   | 0.97 | 0.09 | 31,35,37,40                 | 0     |
| 22  | EDO  | S     | 104 | 4/4   | 0.97 | 0.07 | 32,35,38,42                 | 0     |
| 22  | EDO  | P     | 311 | 4/4   | 0.97 | 0.09 | 40,46,48,56                 | 0     |
| 24  | CHD  | G     | 101 | 29/29 | 0.97 | 0.06 | 27,32,38,49                 | 0     |

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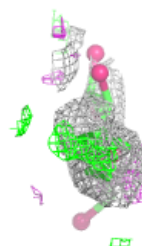
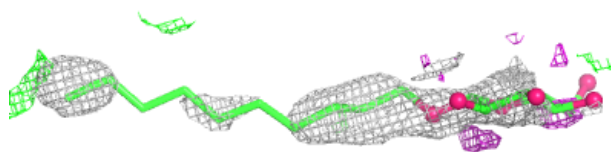
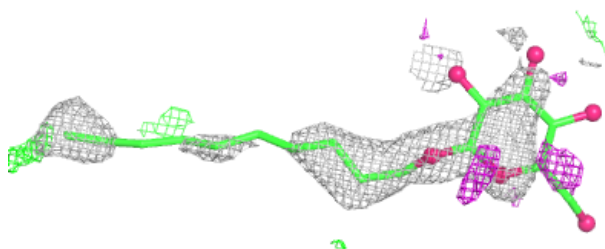
| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 14  | HEA  | A     | 602    | 60/60 | 0.98 | 0.07 | 22,27,38,47                 | 0     |
| 14  | HEA  | N     | 602    | 60/60 | 0.98 | 0.07 | 24,28,33,47                 | 0     |
| 16  | MG   | A     | 604    | 1/1   | 0.98 | 0.06 | 29,29,29,29                 | 0     |
| 17  | NA   | P     | 301    | 1/1   | 0.98 | 0.15 | 22,22,22,22                 | 0     |
| 14  | HEA  | N     | 601[B] | 60/60 | 0.99 | 0.06 | 24,30,48,56                 | 12    |
| 14  | HEA  | A     | 601[B] | 60/60 | 0.99 | 0.06 | 20,24,41,51                 | 12    |
| 15  | CU   | N     | 603    | 1/1   | 0.99 | 0.02 | 30,30,30,30                 | 0     |
| 14  | HEA  | A     | 601[A] | 60/60 | 0.99 | 0.06 | 20,24,41,51                 | 12    |
| 16  | MG   | N     | 604    | 1/1   | 0.99 | 0.05 | 31,31,31,31                 | 0     |
| 17  | NA   | A     | 605    | 1/1   | 0.99 | 0.05 | 29,29,29,29                 | 0     |
| 17  | NA   | C     | 301    | 1/1   | 0.99 | 0.13 | 22,22,22,22                 | 0     |
| 17  | NA   | N     | 605    | 1/1   | 0.99 | 0.06 | 34,34,34,34                 | 0     |
| 14  | HEA  | N     | 601[A] | 60/60 | 0.99 | 0.06 | 23,30,48,53                 | 12    |
| 23  | CUA  | O     | 301    | 2/2   | 1.00 | 0.01 | 32,32,32,33                 | 0     |
| 15  | CU   | A     | 603    | 1/1   | 1.00 | 0.03 | 29,29,29,29                 | 0     |
| 23  | CUA  | B     | 301    | 2/2   | 1.00 | 0.02 | 28,28,28,29                 | 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.

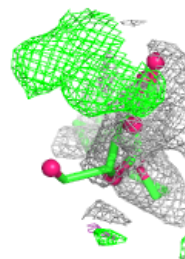
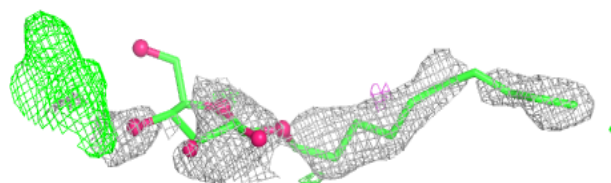
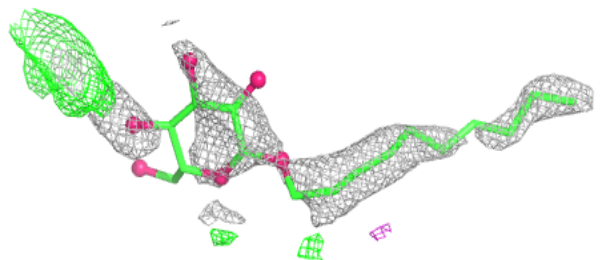


**Electron density around DMU K 103:**

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

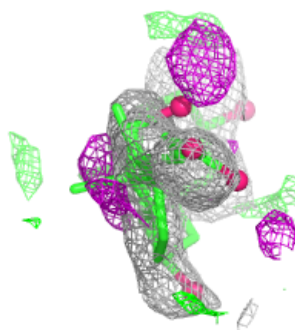
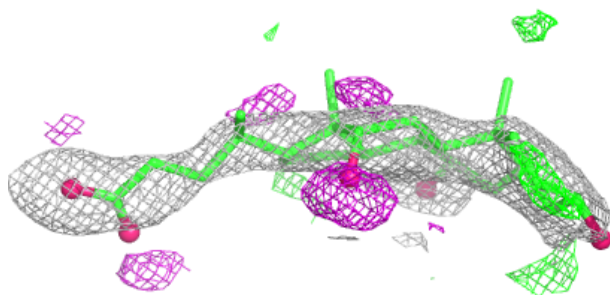
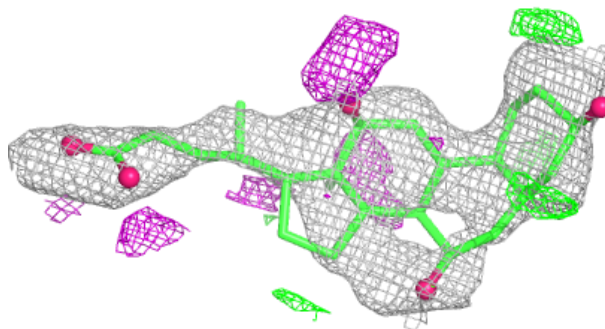
**Electron density around DMU Q 201:**

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

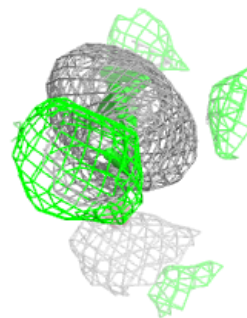
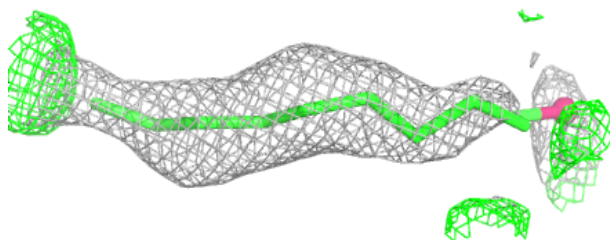
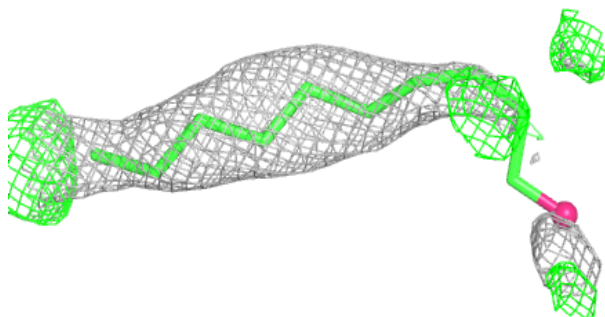


**Electron density around CHD Y 102:**

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

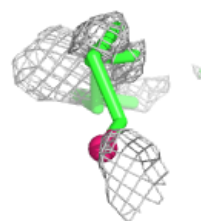
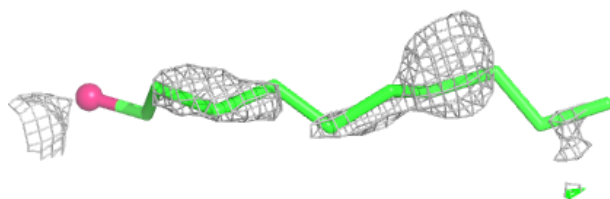
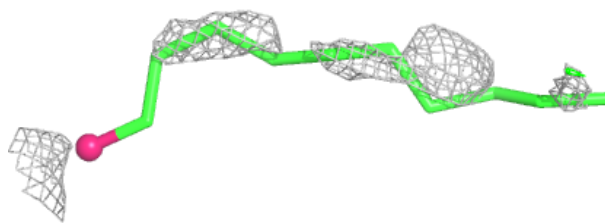
**Electron density around DMU X 103:**

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



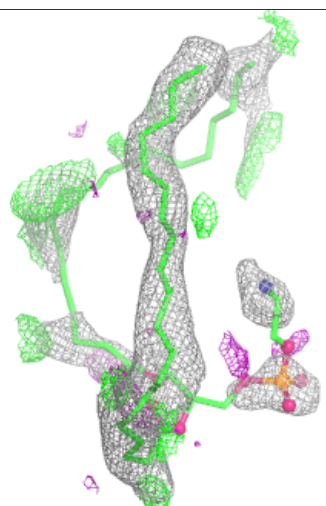
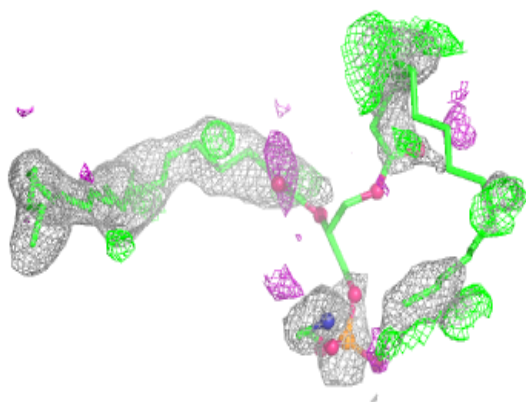
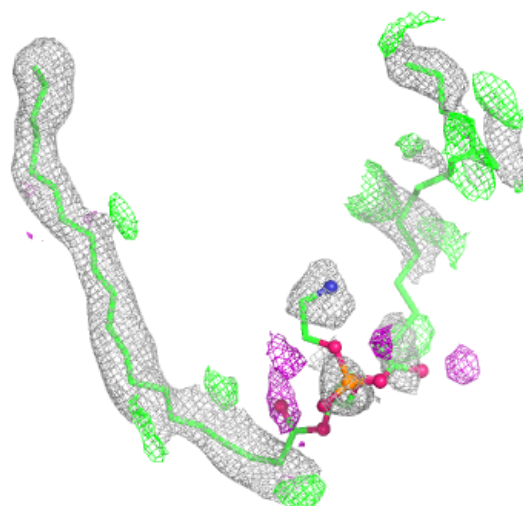
**Electron density around DMU X 105:**

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



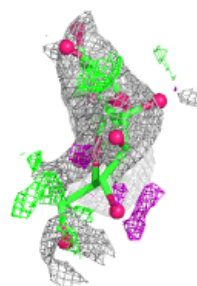
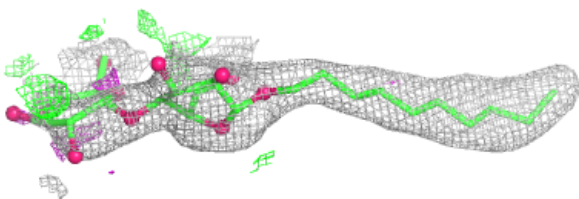
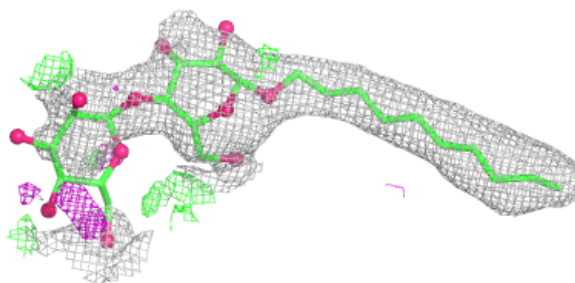
**Electron density around PEK C 308:**

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

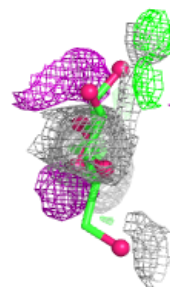
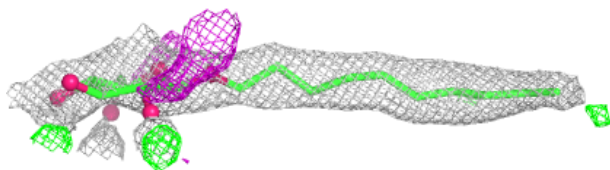
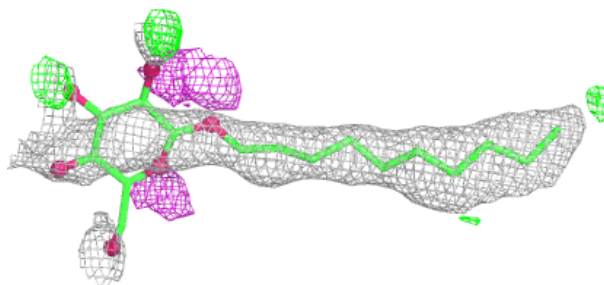


**Electron density around DMU C 302:**

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

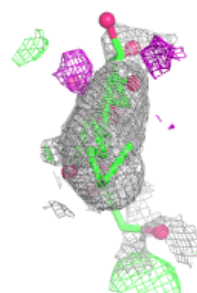
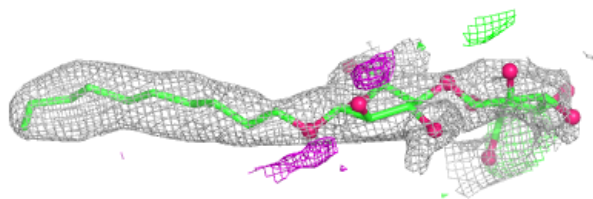
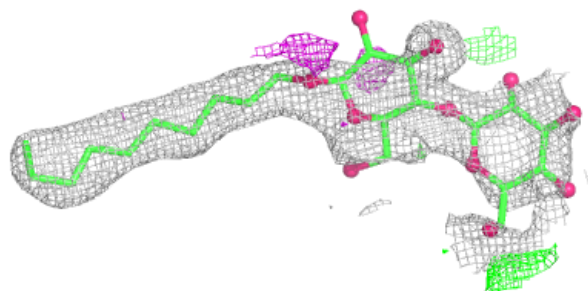
**Electron density around DMU C 303:**

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

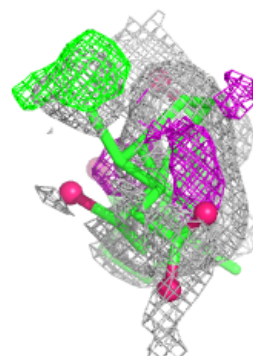
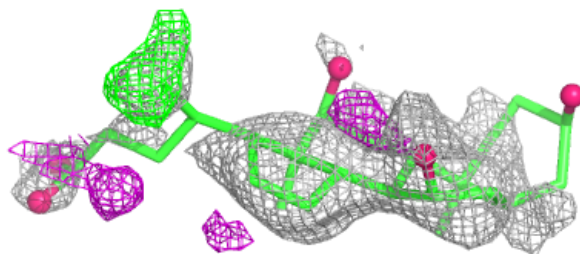
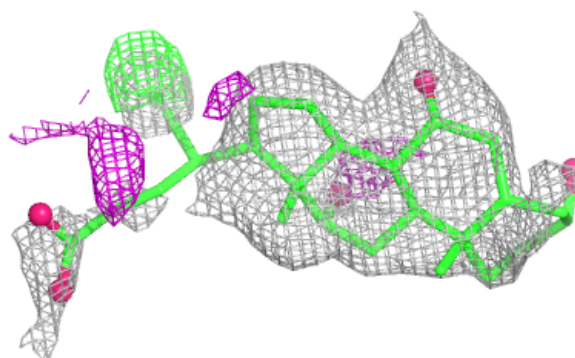


**Electron density around DMU P 303:**

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

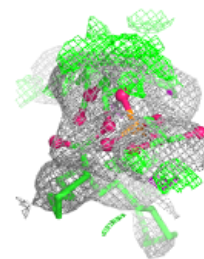
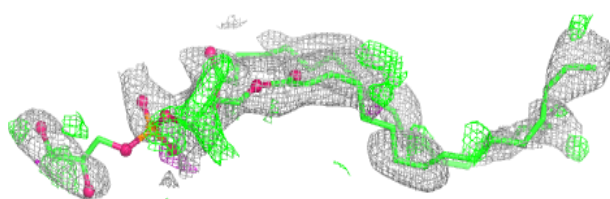
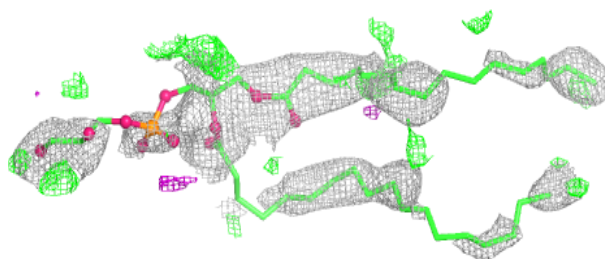
**Electron density around CHD J 102:**

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

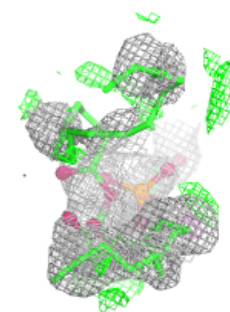
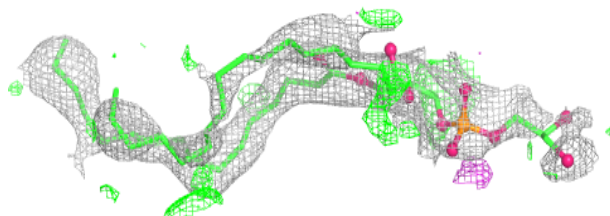
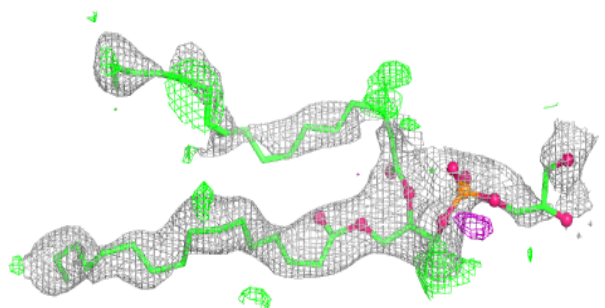


**Electron density around PGV T 104:**

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

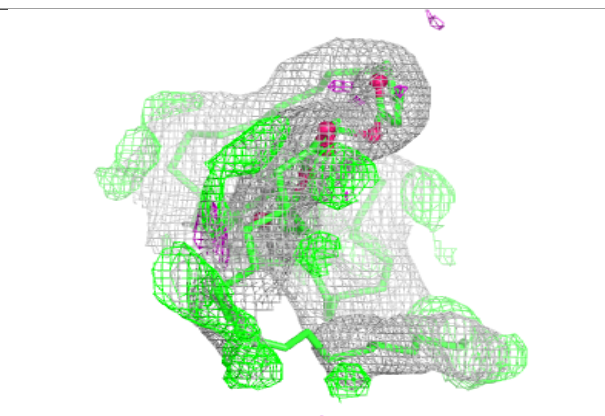
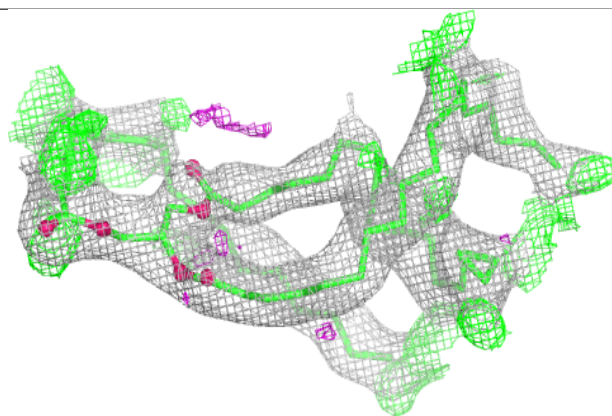
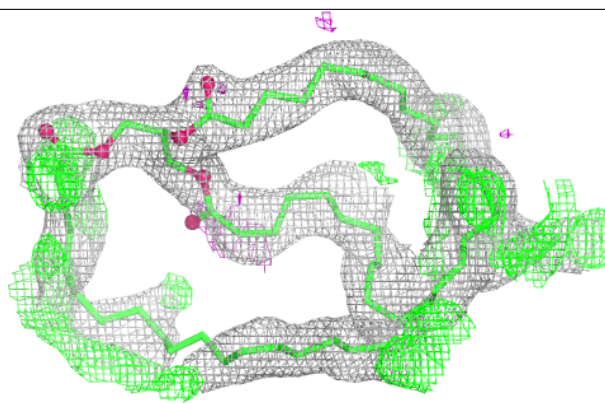
**Electron density around PGV P 310:**

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

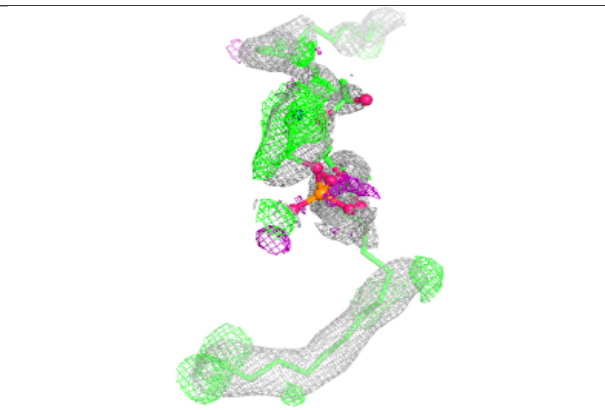
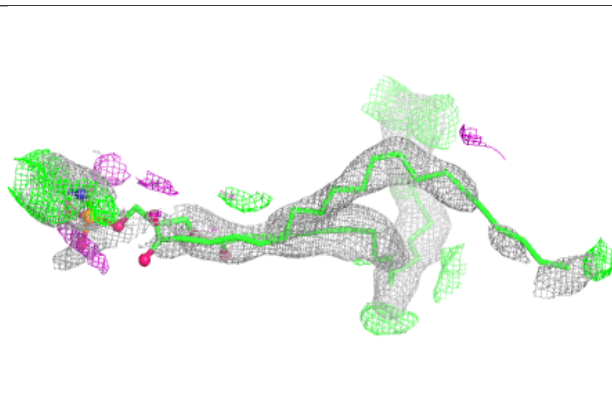
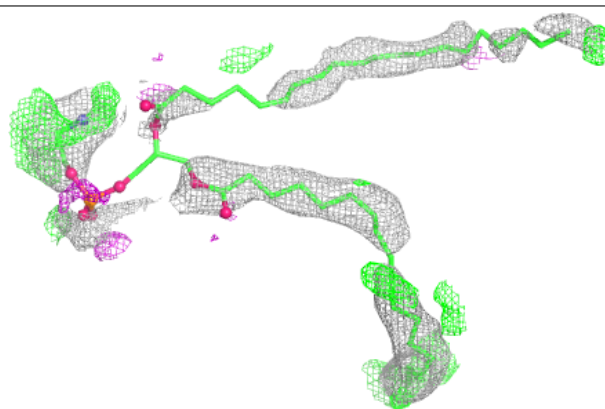


**Electron density around TGL A 610:**

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

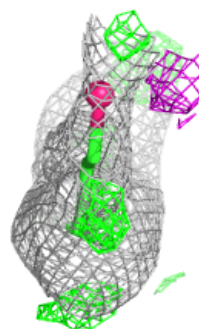
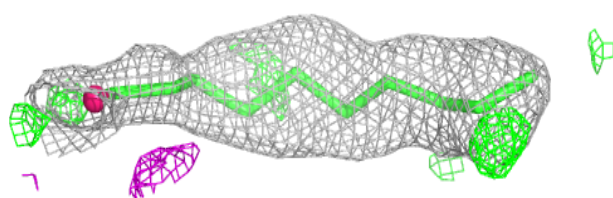
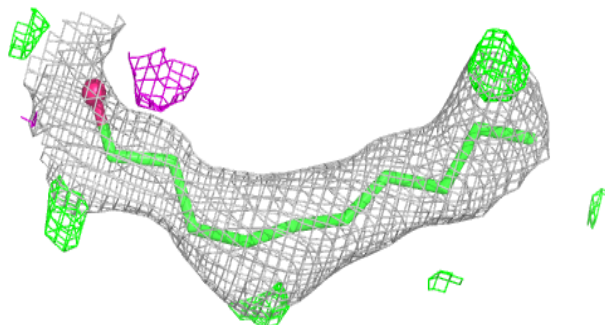
**Electron density around PEK T 103:**

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

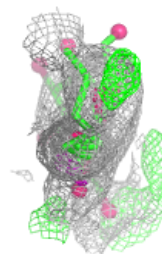
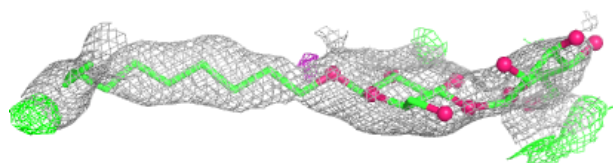
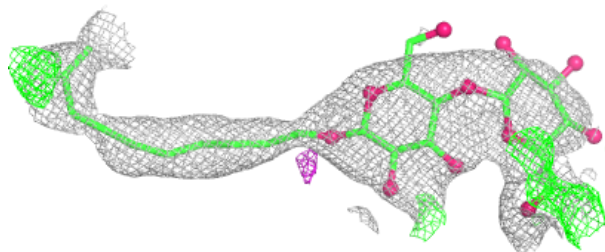


**Electron density around DMU C 304:**

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

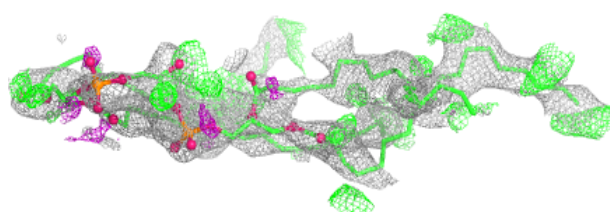
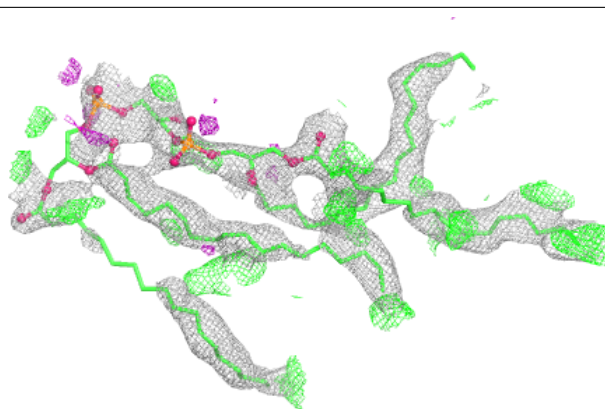
**Electron density around DMU L 101:**

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

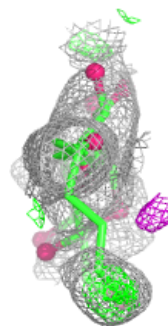
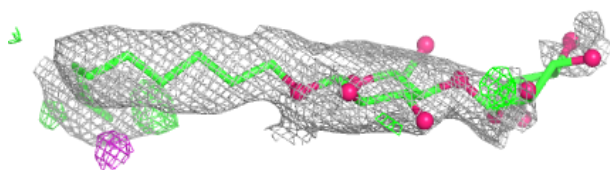
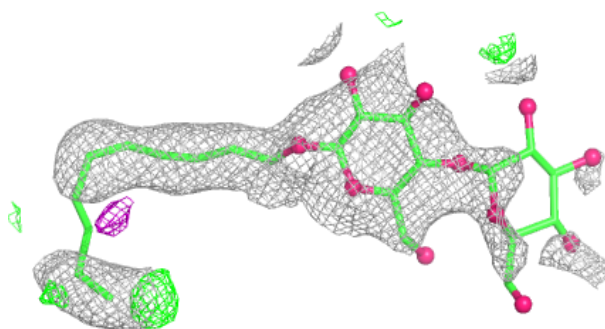


**Electron density around CDL T 102:**

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

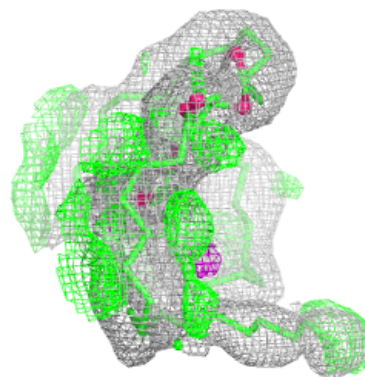
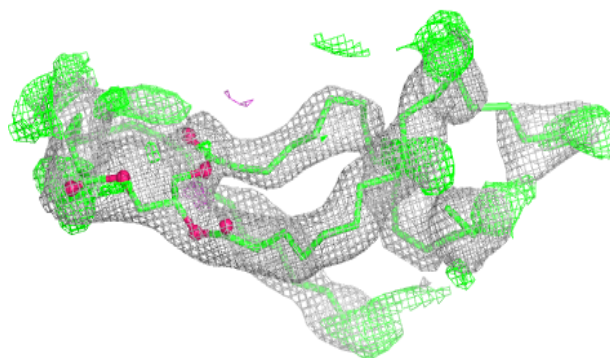
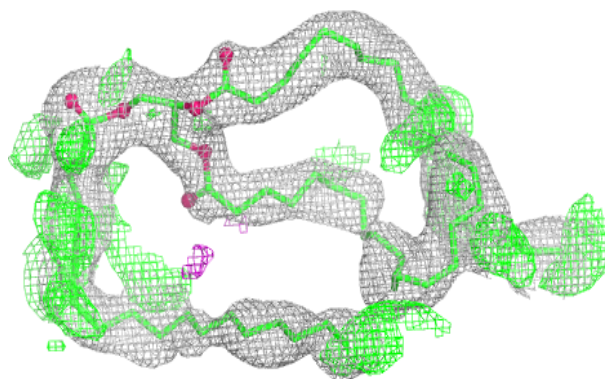
**Electron density around DMU Y 101:**

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

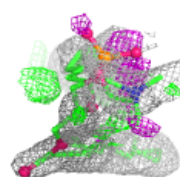
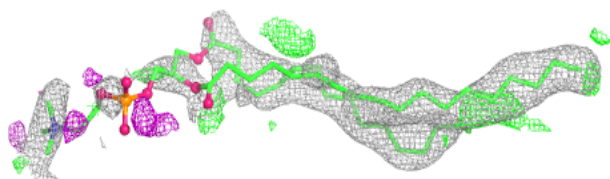
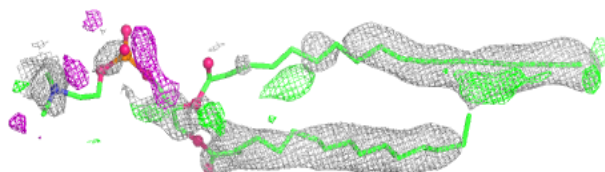


**Electron density around TGL N 608:**

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

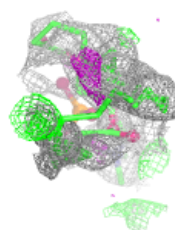
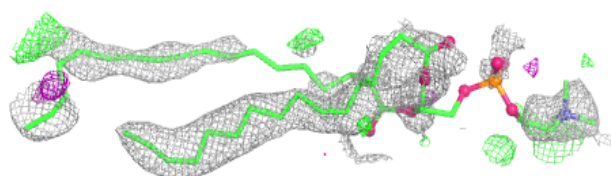
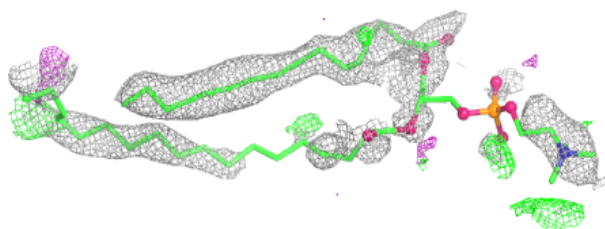
**Electron density around PSC V 101:**

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

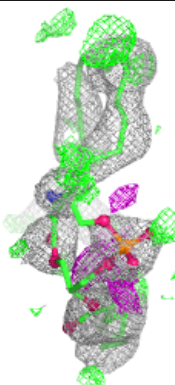
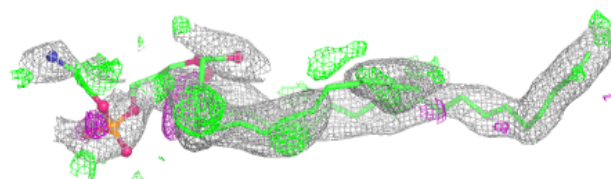
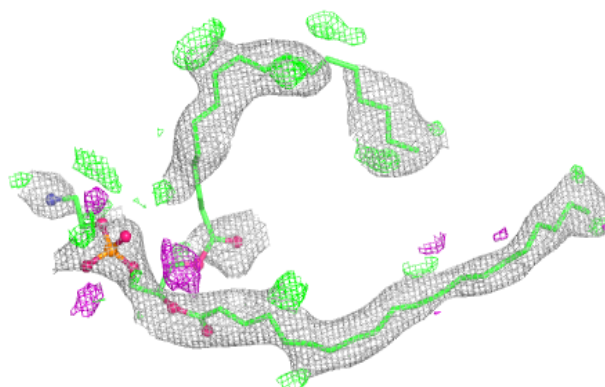


**Electron density around PSC A 609:**

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

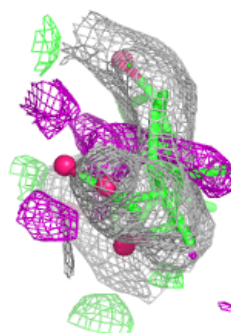
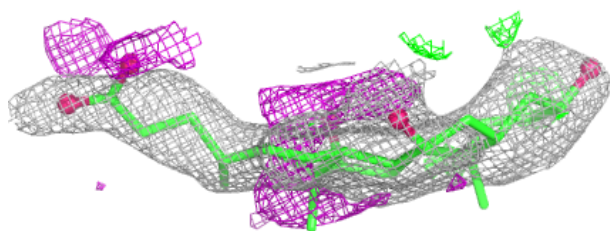
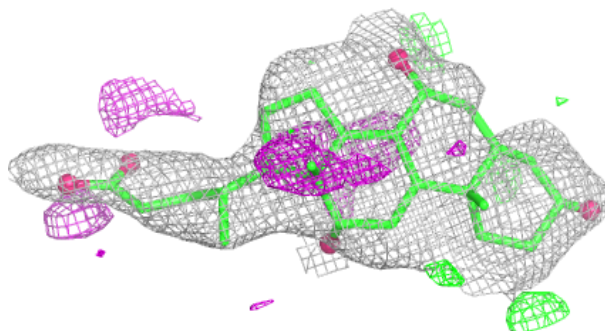
**Electron density around PEK P 307:**

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

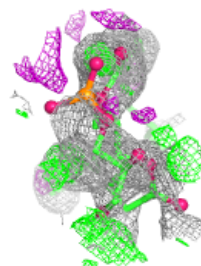
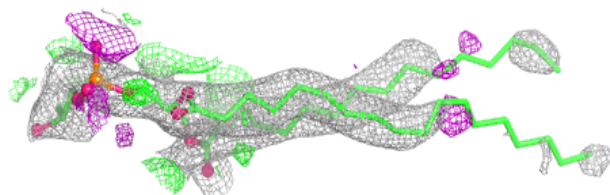
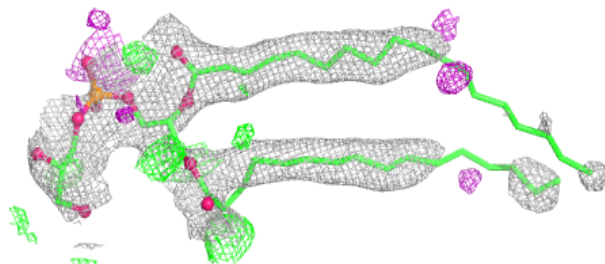


**Electron density around CHD L 102:**

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

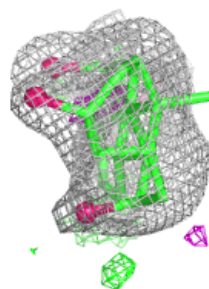
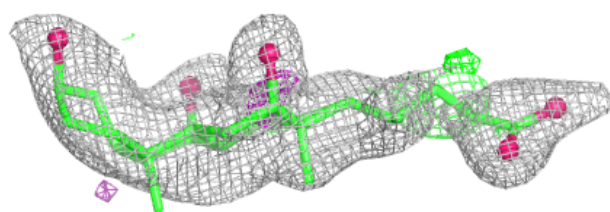
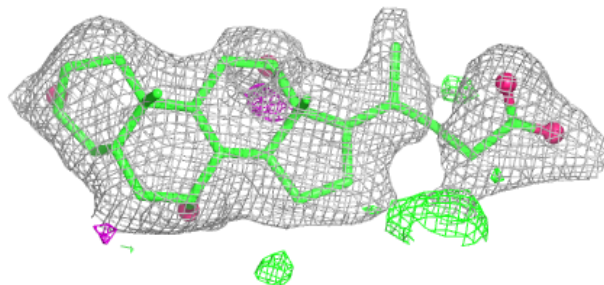
**Electron density around PGV N 606:**

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

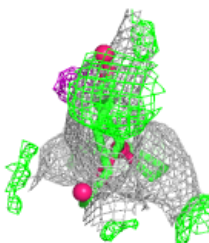
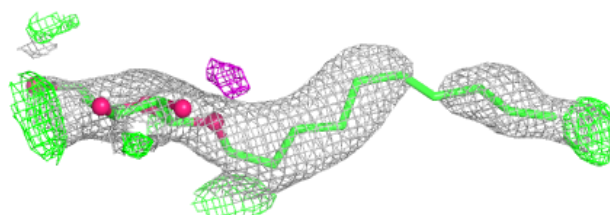
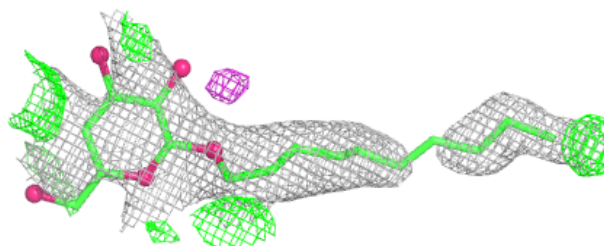


**Electron density around CHD P 305:**

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

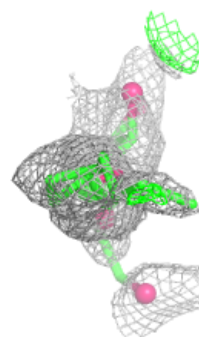
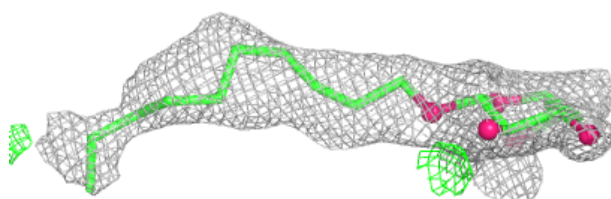
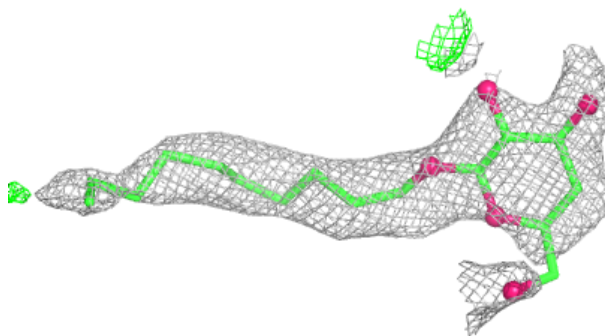
**Electron density around DMU D 201:**

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

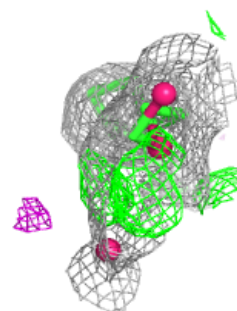
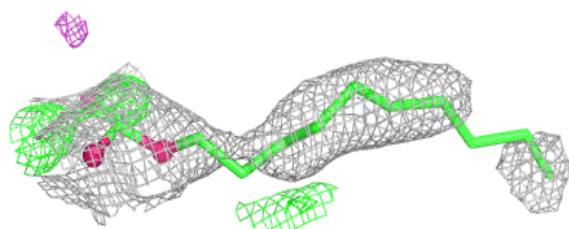
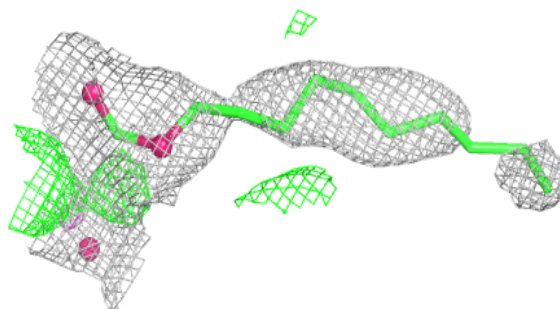


**Electron density around DMU X 102:**

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

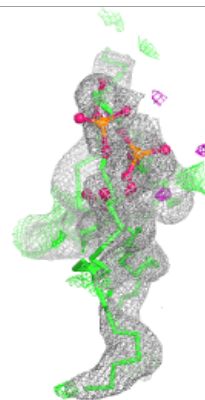
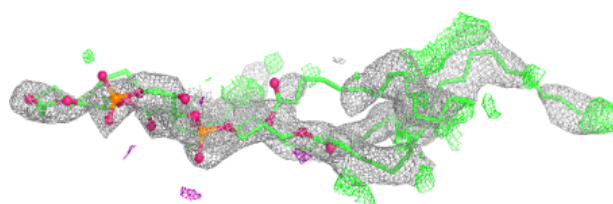
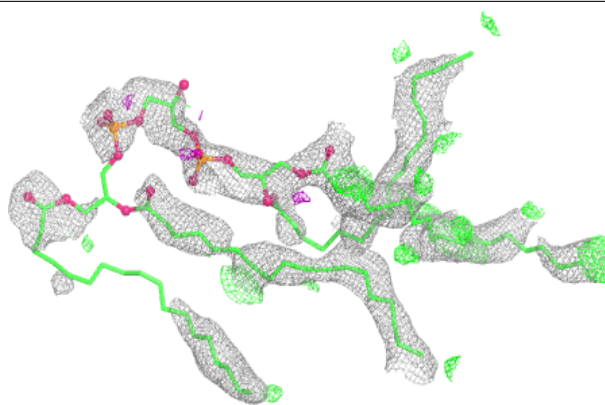
**Electron density around DMU K 102:**

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



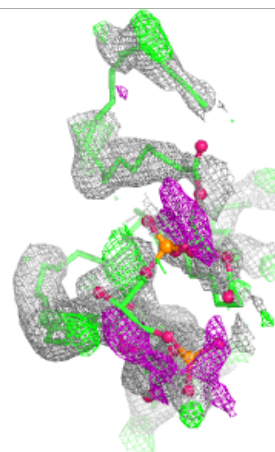
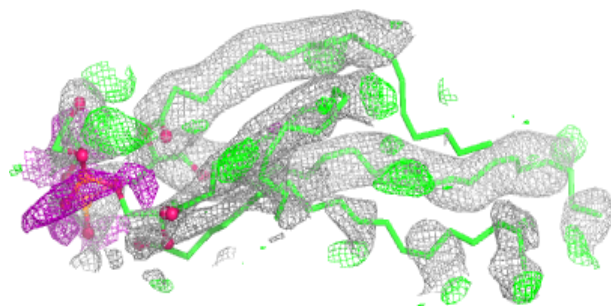
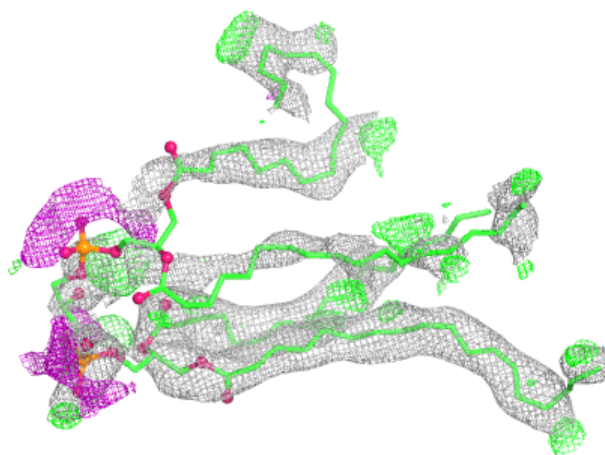
**Electron density around CDL G 102:**

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



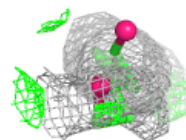
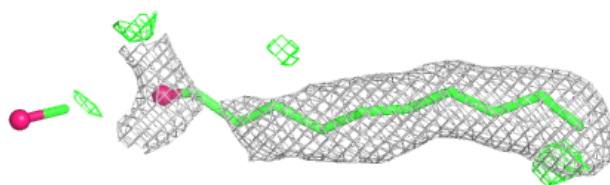
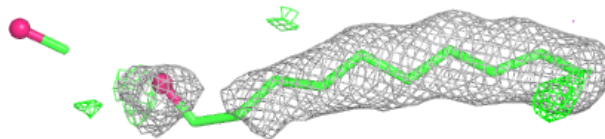
**Electron density around CDL P 306:**

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

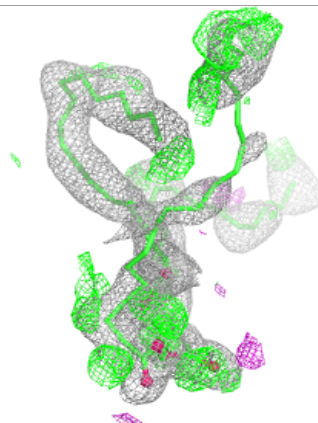
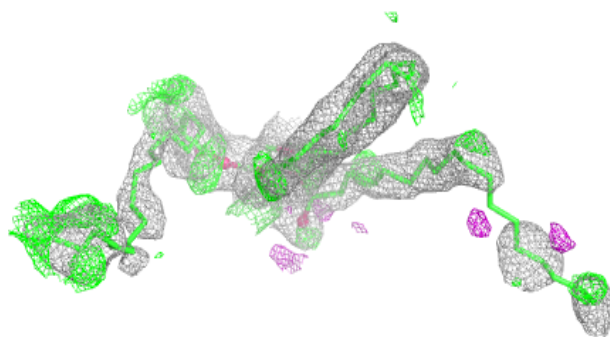
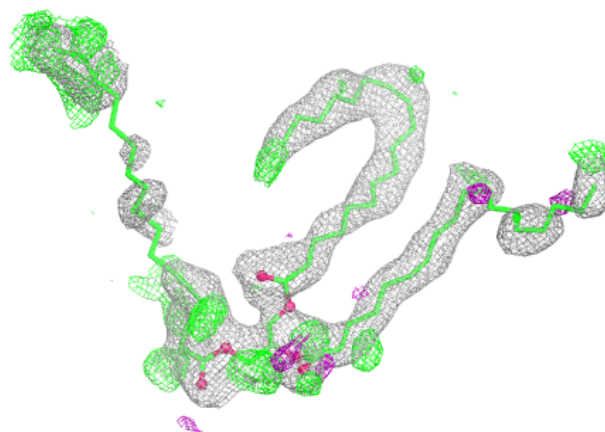


**Electron density around DMU A 606:**

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

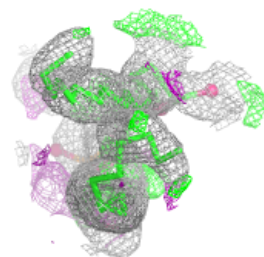
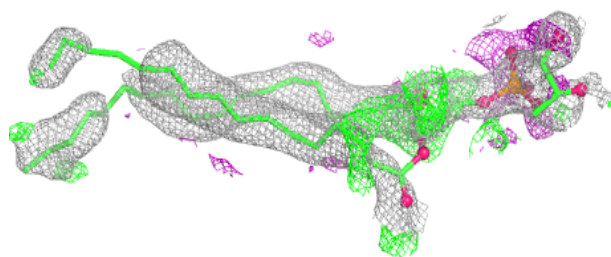
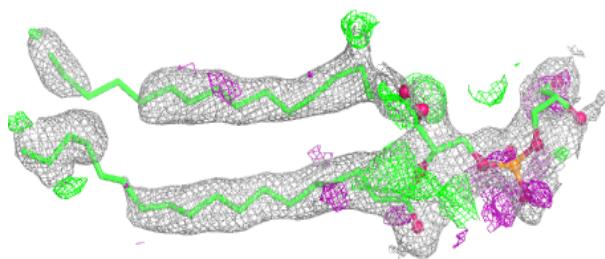
**Electron density around TGL D 202:**

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

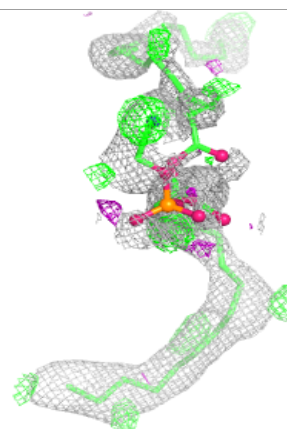
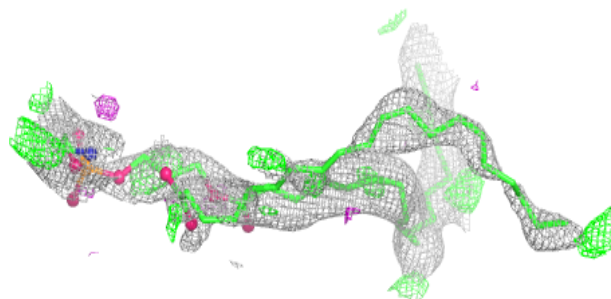
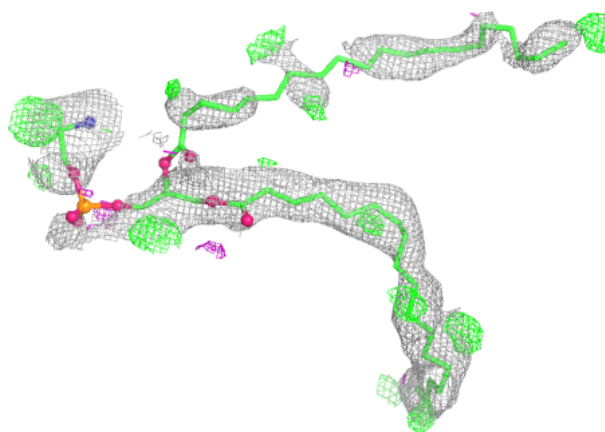


**Electron density around PGV A 607:**

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

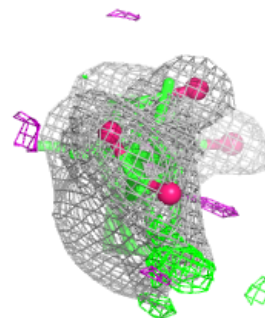
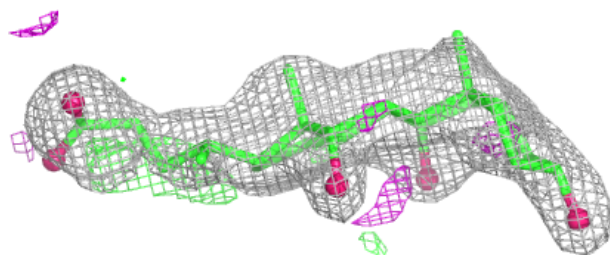
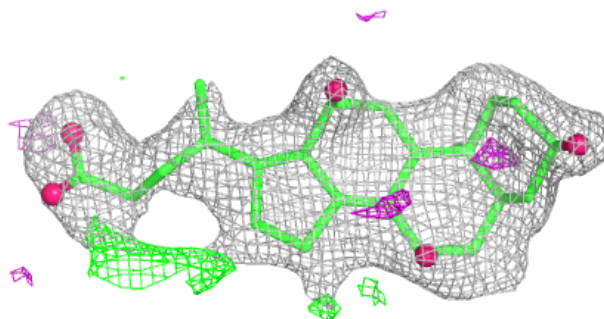
**Electron density around PEK F 102:**

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

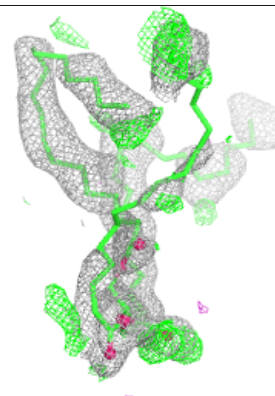
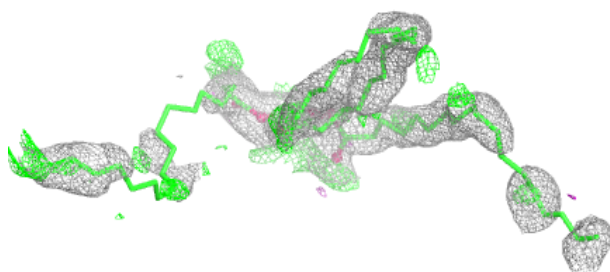
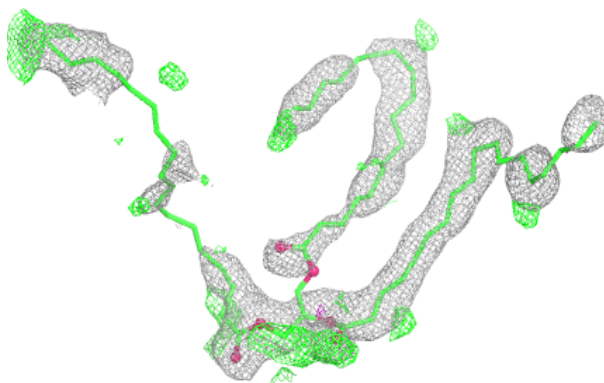


**Electron density around CHD C 306:**

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

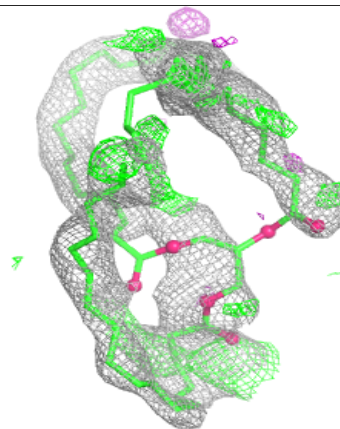
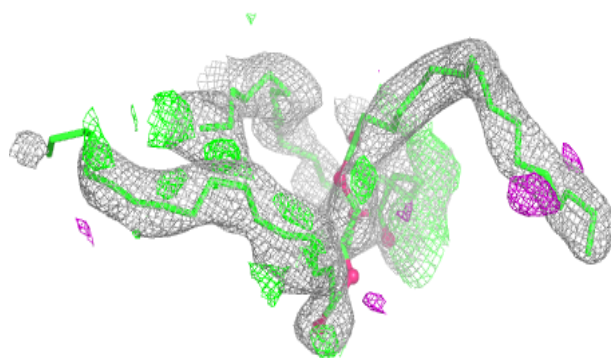
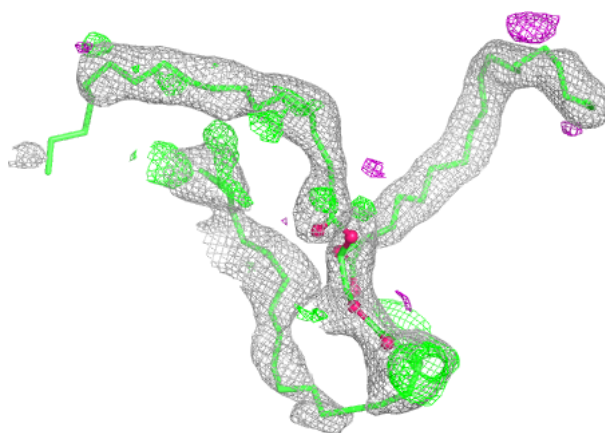
**Electron density around TGL Q 202:**

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



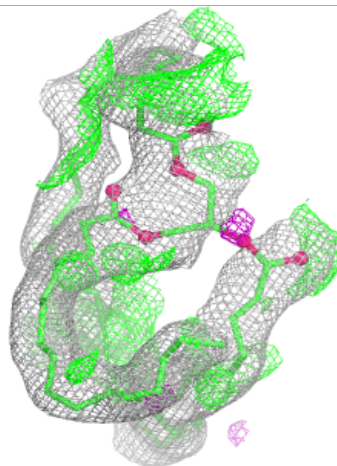
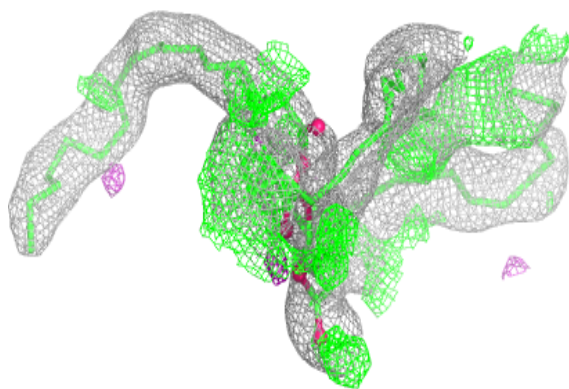
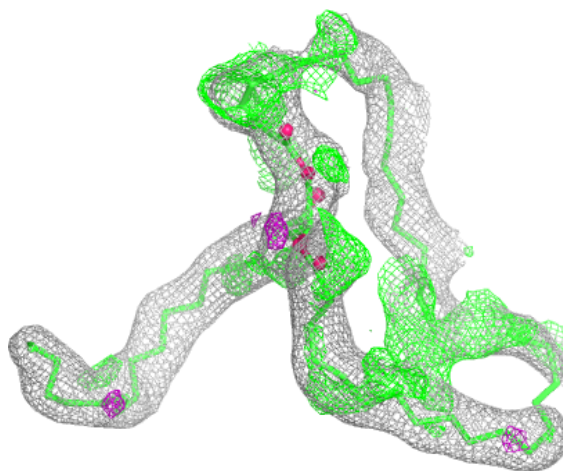
**Electron density around TGL Y 103:**

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



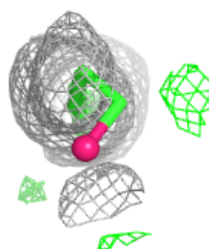
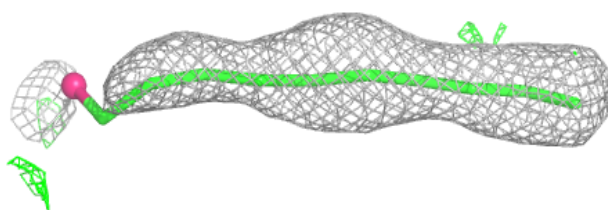
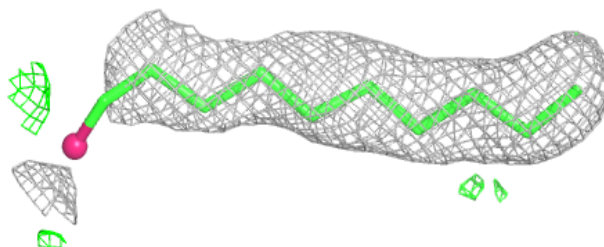
**Electron density around TGL L 103:**

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

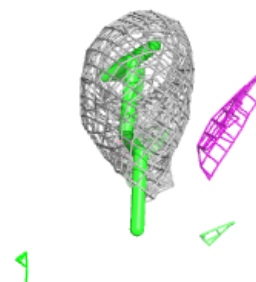
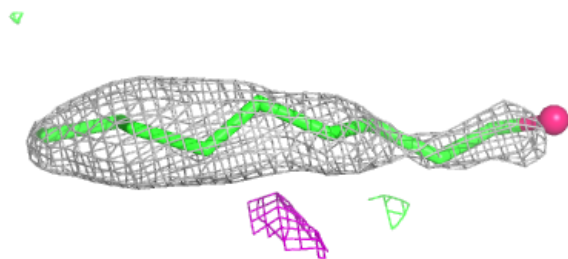
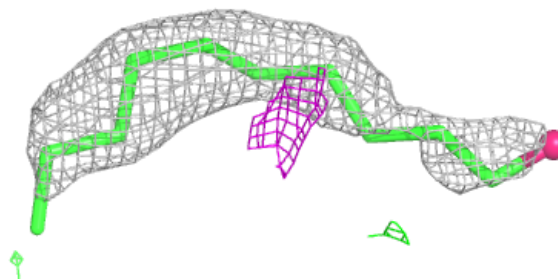


**Electron density around DMU X 101:**

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

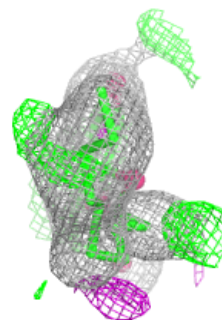
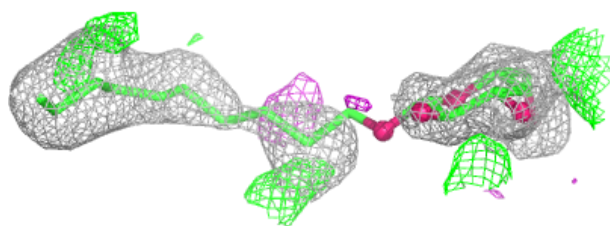
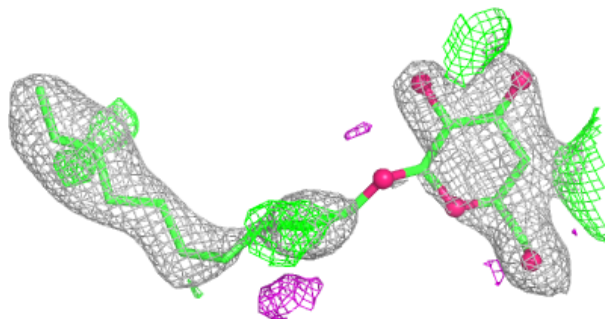
**Electron density around DMU X 104:**

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

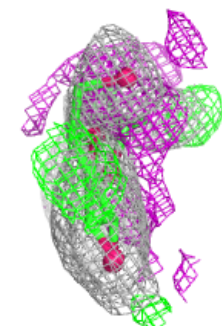
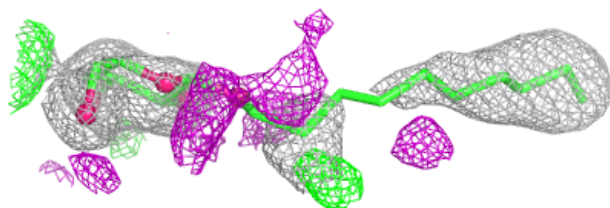
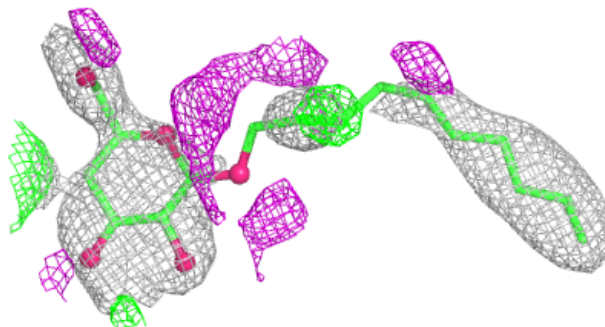


**Electron density around DMU J 101:**

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

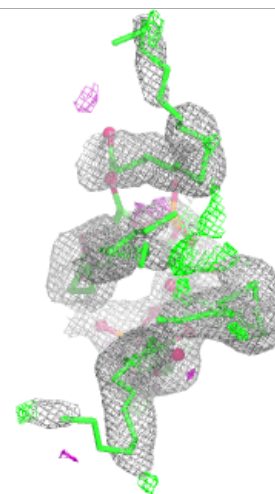
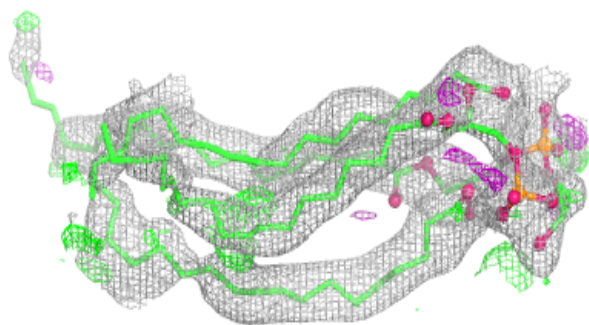
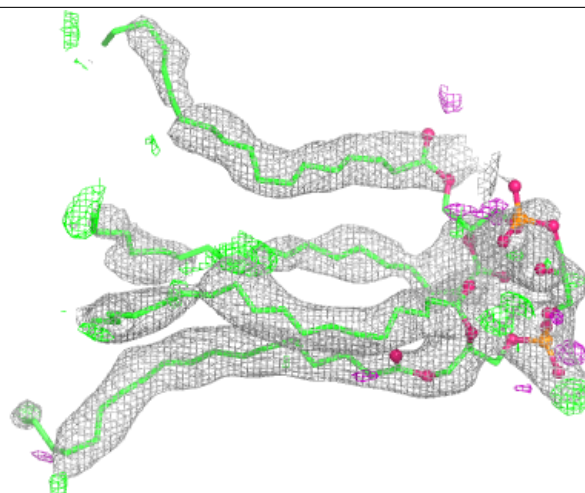
**Electron density around DMU W 101:**

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



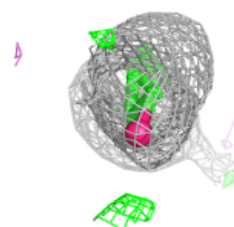
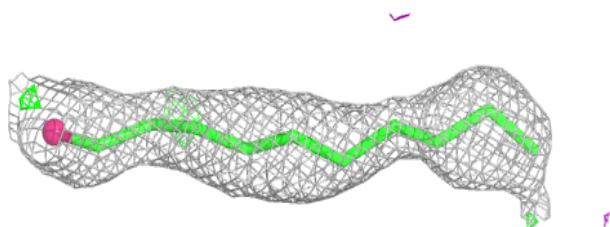
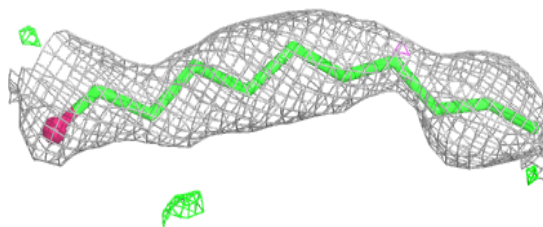
**Electron density around CDL C 307:**

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

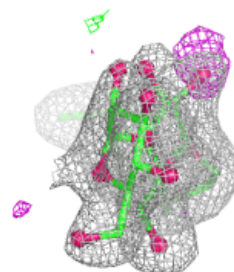
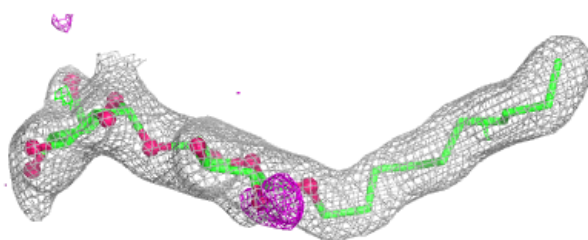
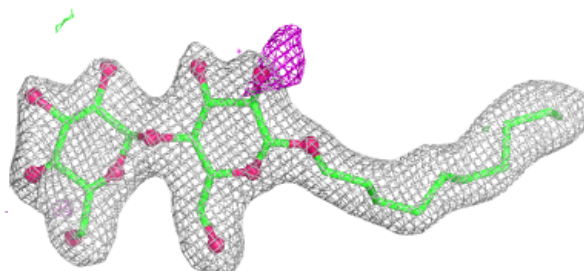


**Electron density around DMU K 101:**

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

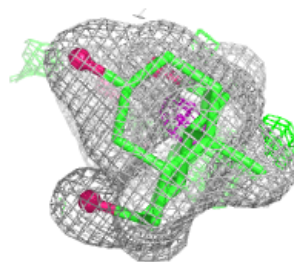
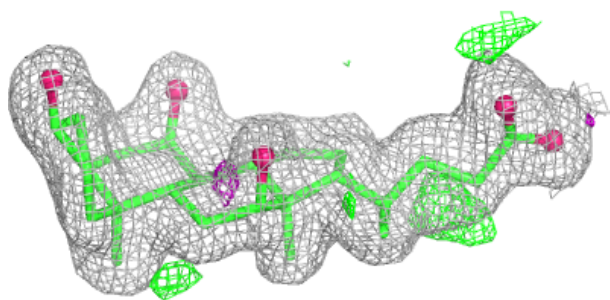
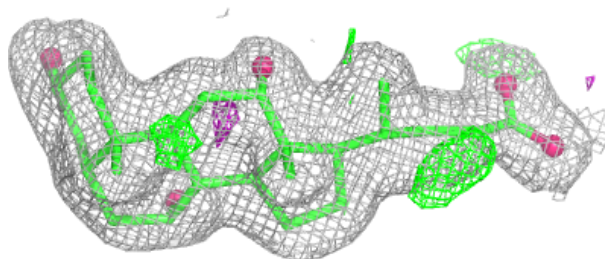
**Electron density around DMU Z 101:**

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

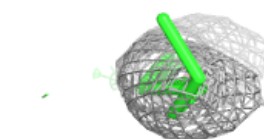
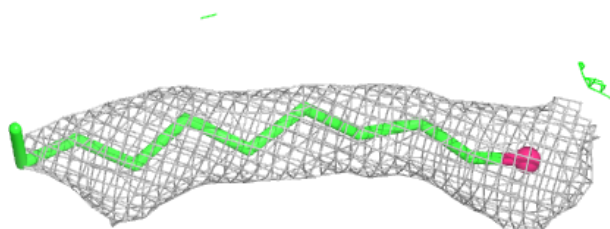
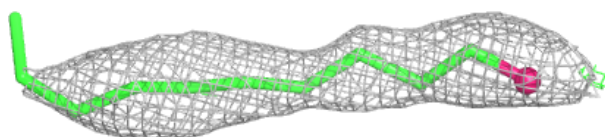


**Electron density around CHD C 305:**

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

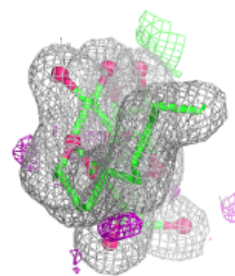
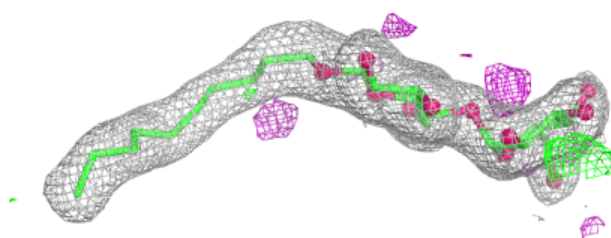
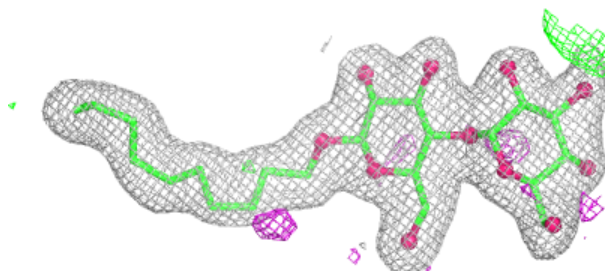
**Electron density around DMU B 302:**

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

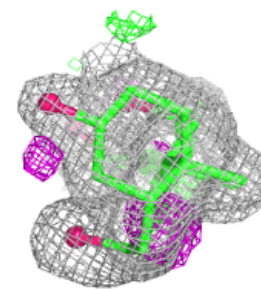
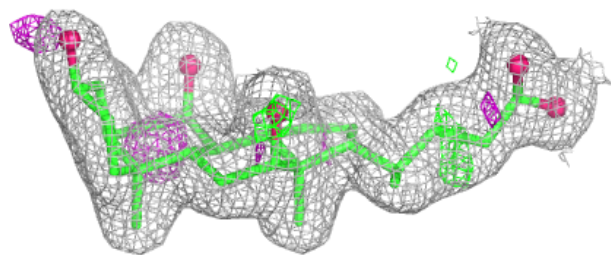
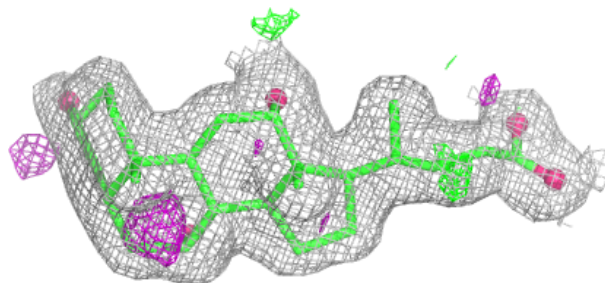


**Electron density around DMU M 101:**

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

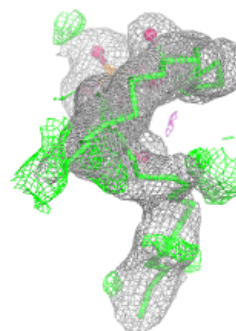
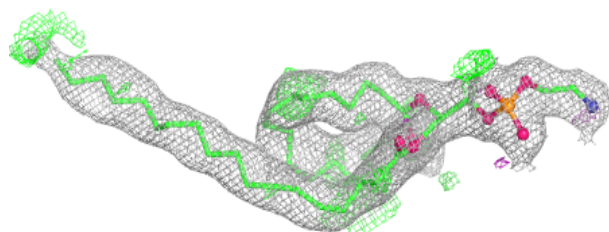
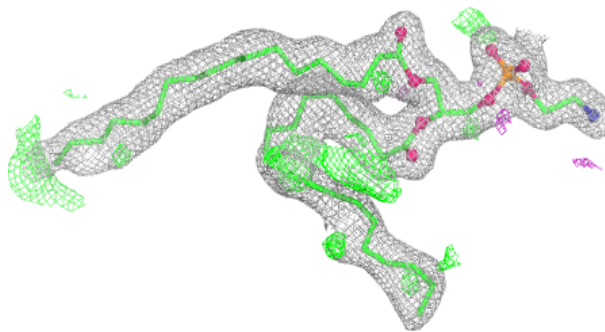
**Electron density around CHD P 304:**

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

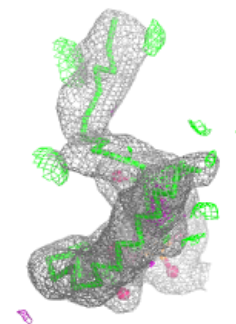
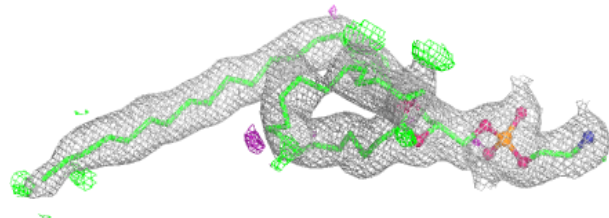
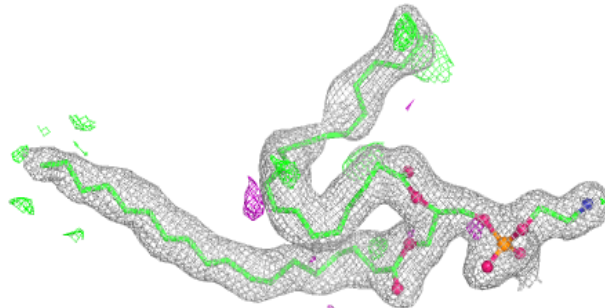


**Electron density around PEK C 309:**

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

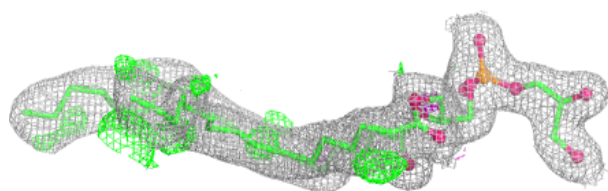
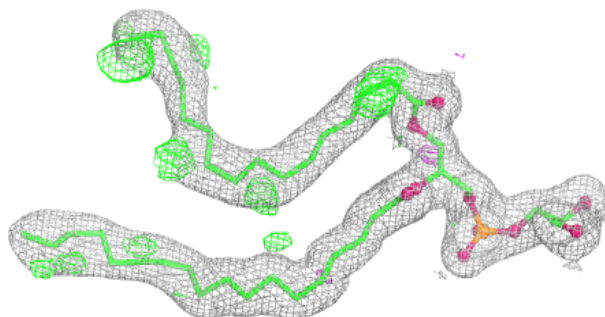
**Electron density around PEK P 308:**

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

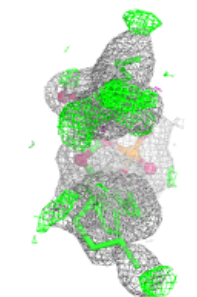
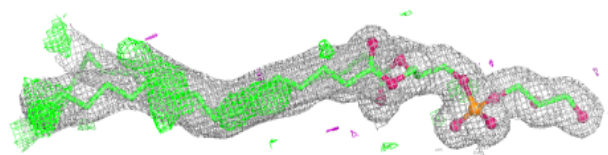
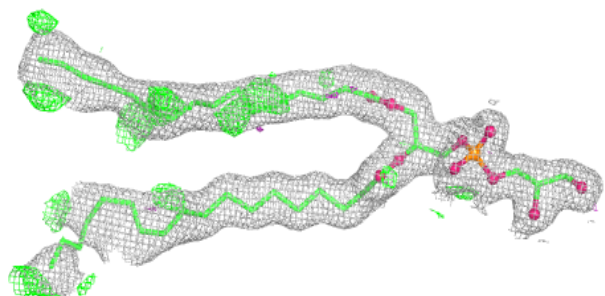


**Electron density around PGV N 607:**

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

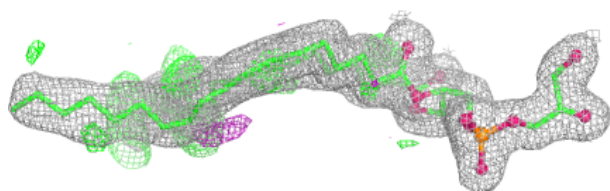
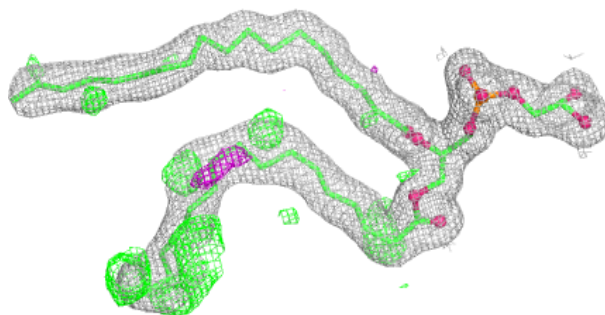
**Electron density around PGV C 310:**

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

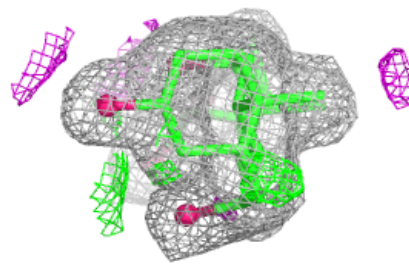
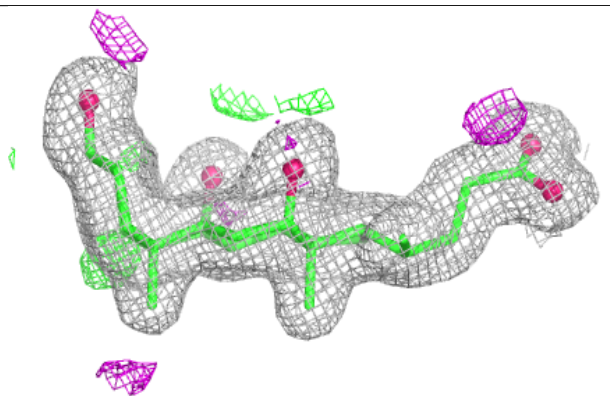
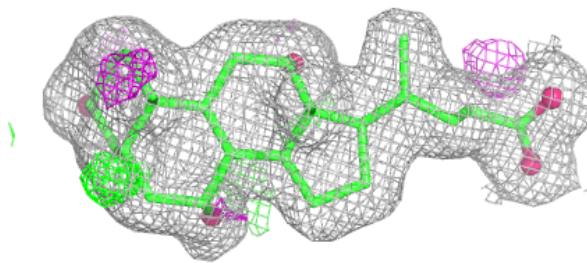


**Electron density around PGV A 608:**

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

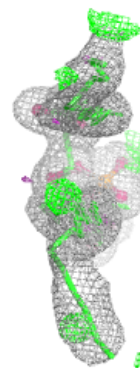
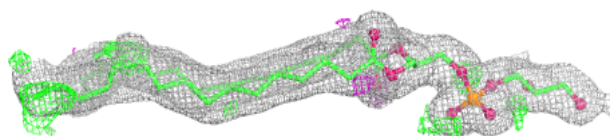
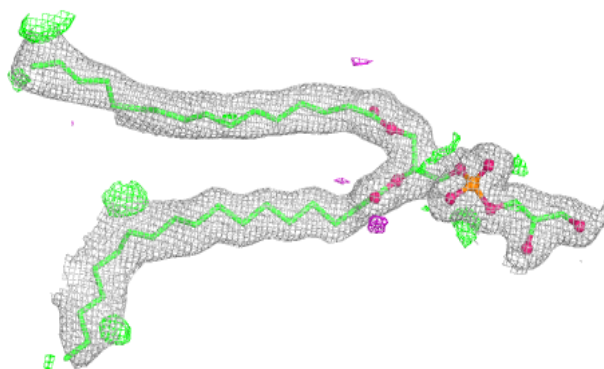
**Electron density around CHD T 101:**

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

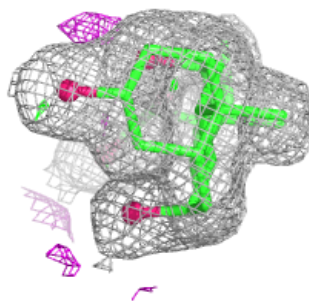
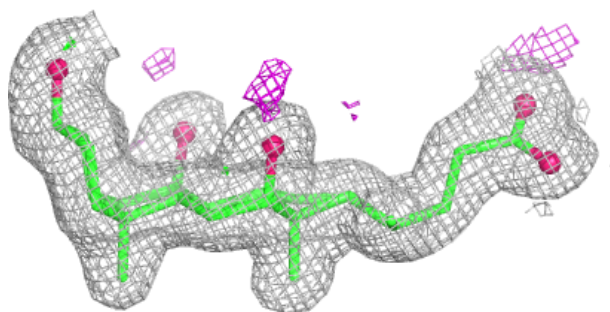
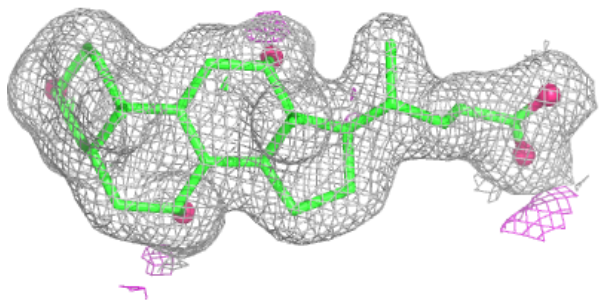


**Electron density around PGV P 309:**

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

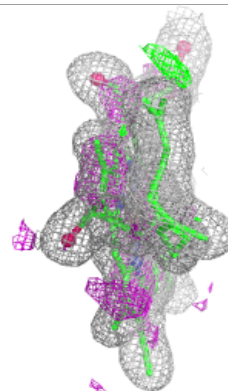
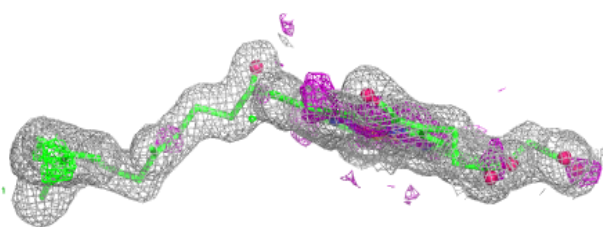
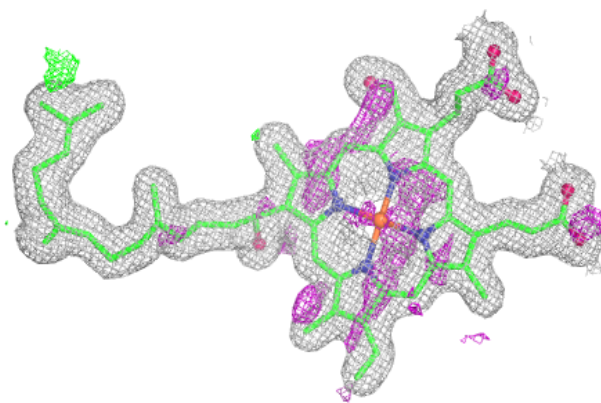
**Electron density around CHD G 101:**

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

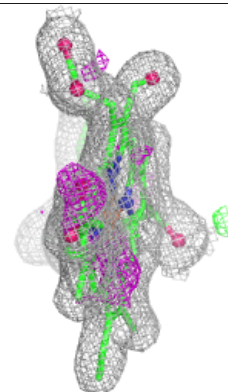
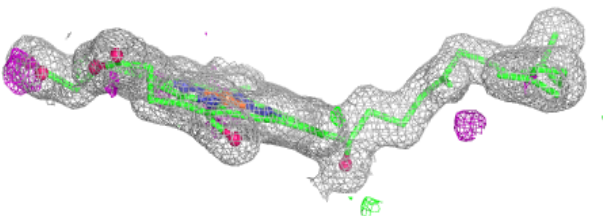
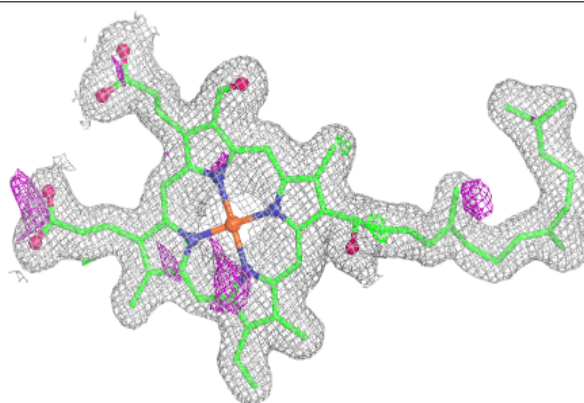


**Electron density around HEA A 602:**

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

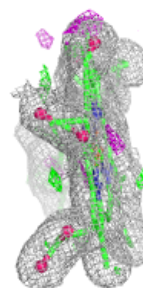
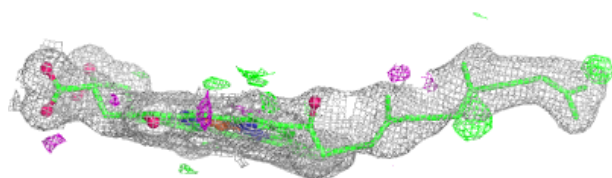
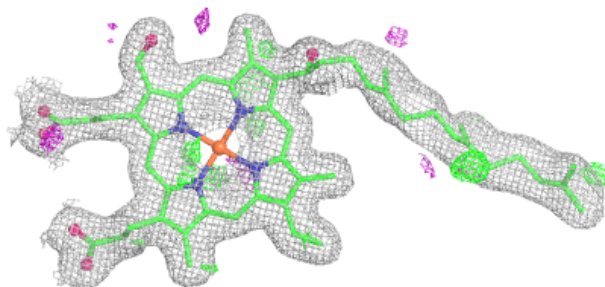
**Electron density around HEA N 602:**

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

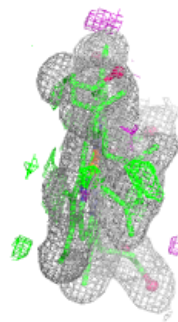
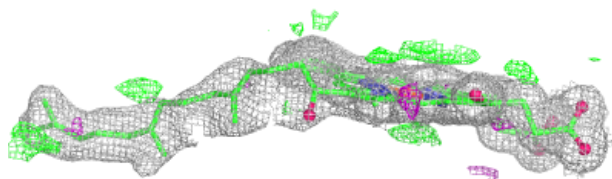
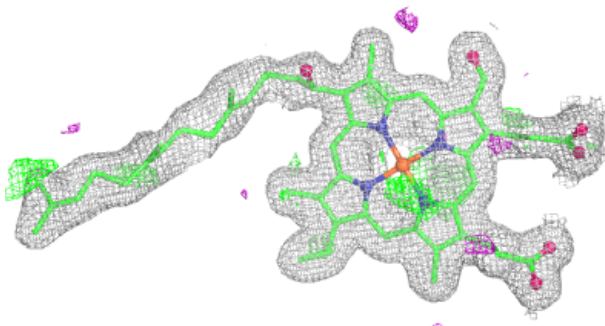


**Electron density around HEA N 601 (B):**

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

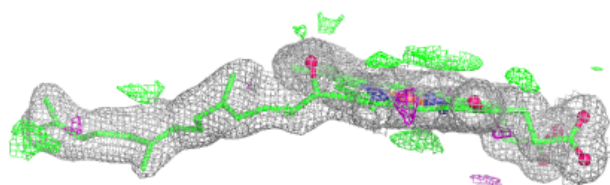
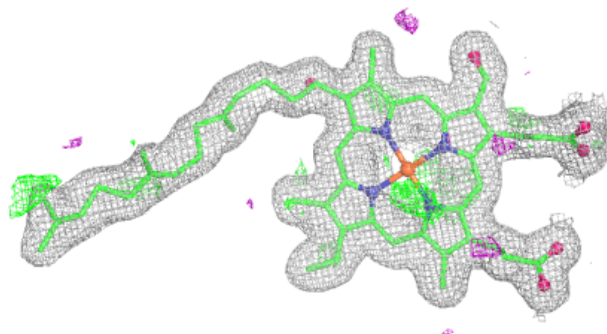
**Electron density around HEA A 601 (B):**

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

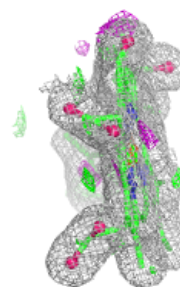
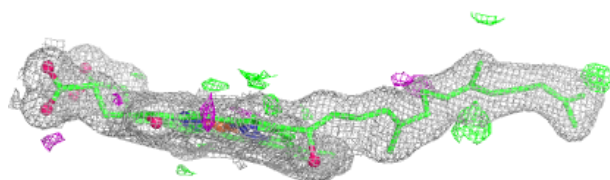
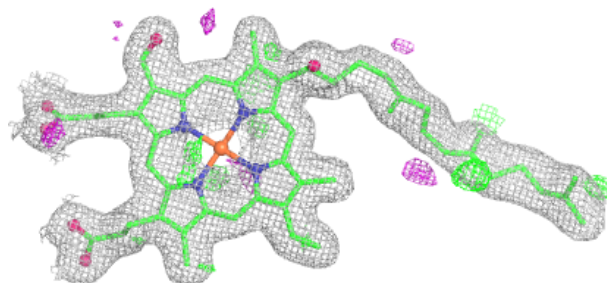


**Electron density around HEA A 601 (A):**

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

**Electron density around HEA N 601 (A):**

$2mF_o-DF_c$  (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.