



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:59 AM JST

PDB ID : 5B1A / pdb\_00005b1a  
Title : Bovine heart cytochrome c oxidase in the fully oxidized state at 1.5 angstrom resolution  
Authors : Yano, N.; Muramoto, K.; Shimada, A.; Takemura, S.; Baba, J.; Fujisawa, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2015-12-01  
Resolution : 1.50 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](#) ①) were used in the production of this report:

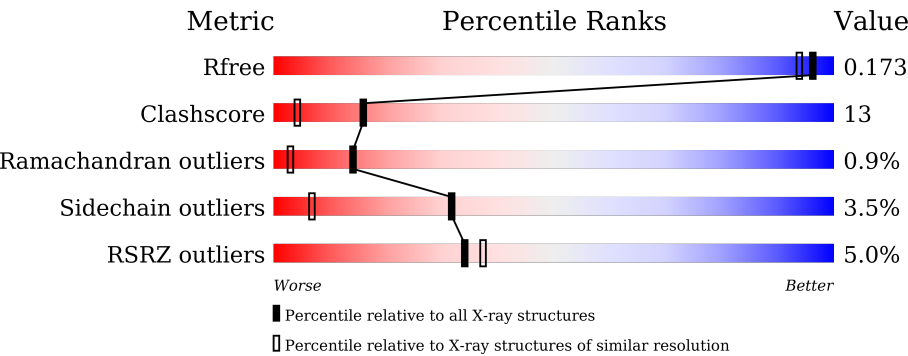
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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 1.50 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.



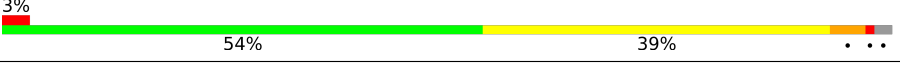
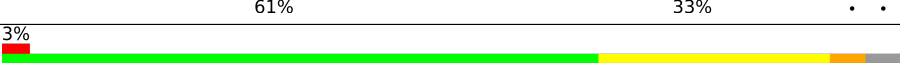
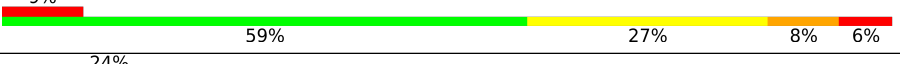
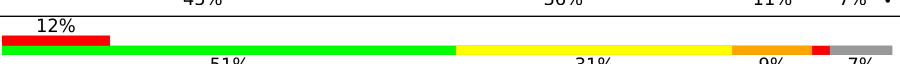
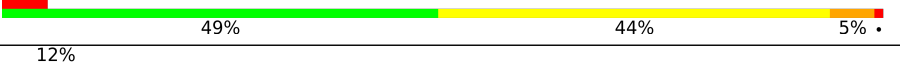
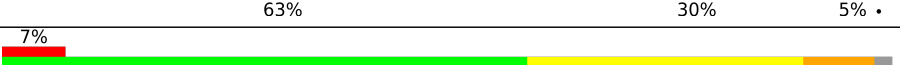
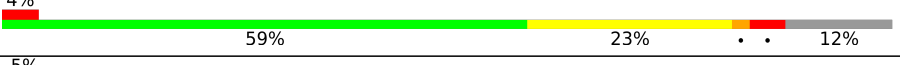
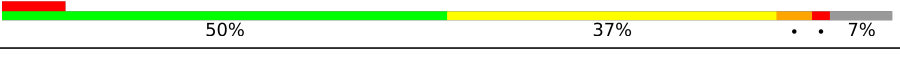
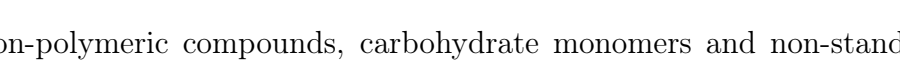
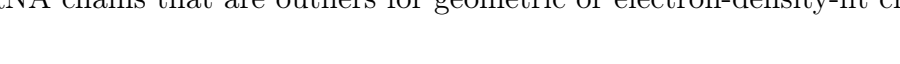
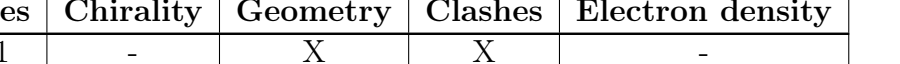
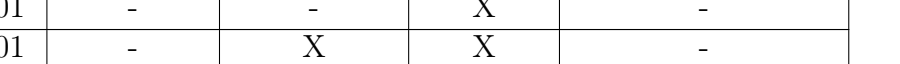
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 4037 (1.50-1.50)                                      |
| Clashscore            | 190562                      | 4235 (1.50-1.50)                                      |
| Ramachandran outliers | 187476                      | 4153 (1.50-1.50)                                      |
| Sidechain outliers    | 187428                      | 4150 (1.50-1.50)                                      |
| RSRZ outliers         | 180081                      | 4039 (1.50-1.50)                                      |

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><div></div><div></div><div></div><div></div></div><div>60%35%5%•</div></div>              |
| 1   | N     | 514    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>63%32%•</div></div>                |
| 2   | B     | 227    | <div><div>7%</div><div></div><div><div></div><div></div><div></div><div></div></div><div>55%37%7%•</div></div> |
| 2   | O     | 227    | <div><div>5%</div><div></div><div><div></div><div></div><div></div><div></div></div><div>60%33%5%•</div></div> |
| 3   | C     | 261    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>59%35%5%•</div></div>              |
| 3   | P     | 261    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>61%33%5%•</div></div>              |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | D     | 147    |    |
| 4   | Q     | 147    |    |
| 5   | E     | 109    |    |
| 5   | R     | 109    |    |
| 6   | F     | 98     |    |
| 6   | S     | 98     |    |
| 7   | G     | 85     |    |
| 7   | T     | 85     |    |
| 8   | H     | 85     |    |
| 8   | U     | 85     |   |
| 9   | I     | 73     |  |
| 9   | V     | 73     |  |
| 10  | J     | 59     |  |
| 10  | W     | 59     |  |
| 11  | K     | 56     |  |
| 11  | X     | 56     |  |
| 12  | L     | 47     |  |
| 12  | Y     | 47     |  |
| 13  | M     | 46     |  |
| 13  | Z     | 46     |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | FME  | B     | 1   | -         | X        | X       | -                |
| 20  | TGL  | D     | 201 | -         | -        | X       | -                |
| 20  | TGL  | Y     | 101 | -         | X        | X       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CDL  | C     | 303 | -         | -        | X       | -                |
| 25  | CDL  | G     | 102 | -         | -        | X       | -                |
| 25  | CDL  | P     | 304 | -         | -        | X       | -                |
| 25  | CDL  | T     | 103 | -         | -        | X       | -                |
| 9   | SAC  | V     | 1   | -         | X        | -       | -                |

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 35054 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       | 18      | 0     |
|     |       |          | 4168  | 2778 | 645 | 704 | 41 |         |         |       |
| 1   | N     | 514      | Total | C    | N   | O   | S  | 0       | 16      | 0     |
|     |       |          | 4154  | 2771 | 643 | 699 | 41 |         |         |       |

- 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       | 9       | 0     |
|     |       |          | 1899  | 1234 | 292 | 353 | 20 |         |         |       |
| 2   | O     | 227      | Total | C    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 1870  | 1215 | 288 | 347 | 20 |         |         |       |

- 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       | 9       | 0     |
|     |       |          | 2185  | 1457 | 349 | 363 | 16 |         |         |       |
| 3   | P     | 259      | Total | C    | N   | O   | S  | 0       | 9       | 0     |
|     |       |          | 2185  | 1457 | 349 | 363 | 16 |         |         |       |

- 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       | 5       | 0     |
|     |       |          | 1242  | 809 | 206 | 223 | 4 |         |         |       |
| 4   | Q     | 144      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1224  | 797 | 202 | 221 | 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       | 1       | 0     |
|     |       |          | 863   | 550 | 148 | 163 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 98       | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 778   | 481 | 139 | 152 | 6 |         |         |       |
| 6   | S     | 98       | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 763   | 473 | 136 | 148 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |   |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|---|
| 7   | G     | 84       | Total<br>686 | C<br>440 | N<br>130 | O<br>114 | P<br>1 | S<br>1  | 0       | 1     | 0 |
| 7   | T     | 84       | Total<br>686 | C<br>440 | 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       | 1       | 0     |
|     |       |          | 469   | 302 | 79 | 85 | 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       | 1       | 0     |
|     |       |          | 391   | 255 | 66 | 68 | 2 |         |         |       |

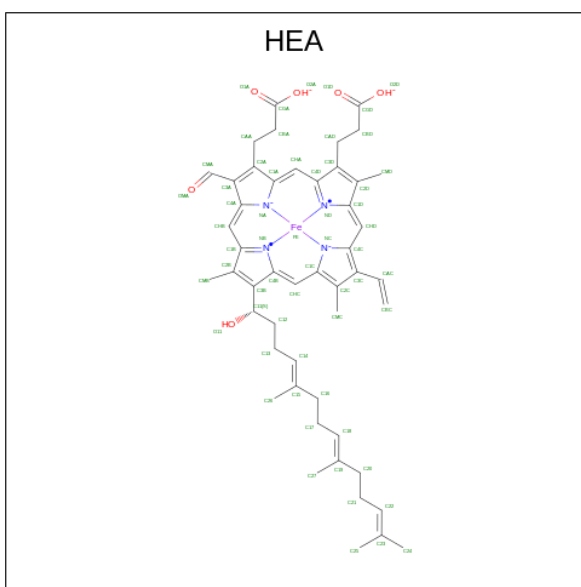
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

| 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       | 1       | 0     |
|     |       |          | 388   | 259 | 65 | 61 | 3 |         |         |       |

- 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     |
|     |       |          | 335   | 223 | 53 | 59 |         |         |       |
| 13  | Z     | 43       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 335   | 223 | 53 | 59 |         |         |       |

- 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>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6  | 0       | 0 |
| 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>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6  | 0       | 0 |
| 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  |         |         |

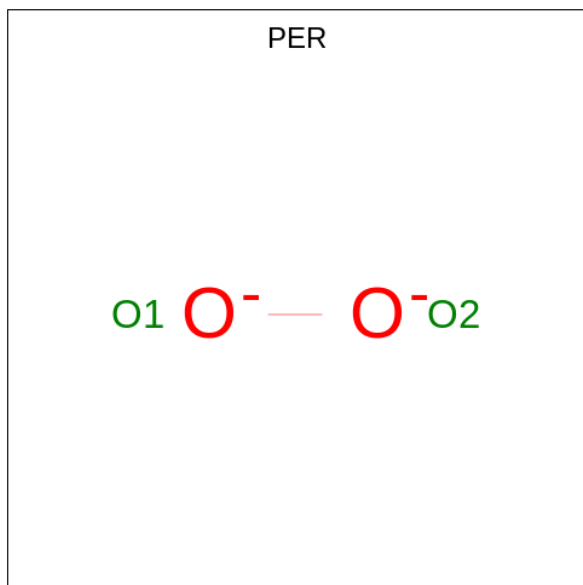
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| 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).

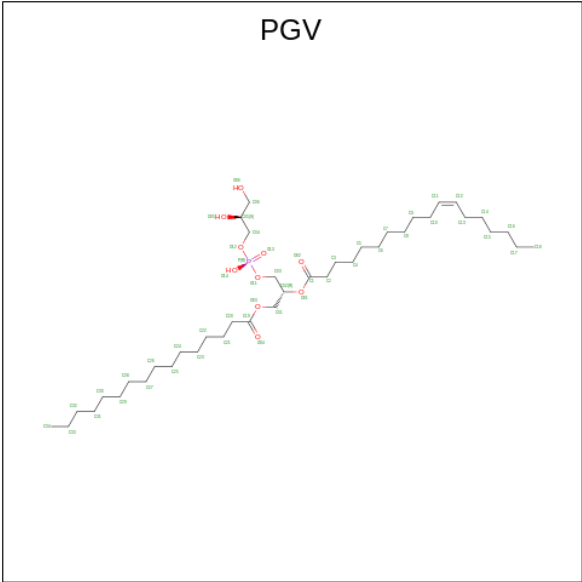
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17  | A     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 17  | N     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 18 is PEROXIDE ION (CCD ID: PER) (formula: O<sub>2</sub>).



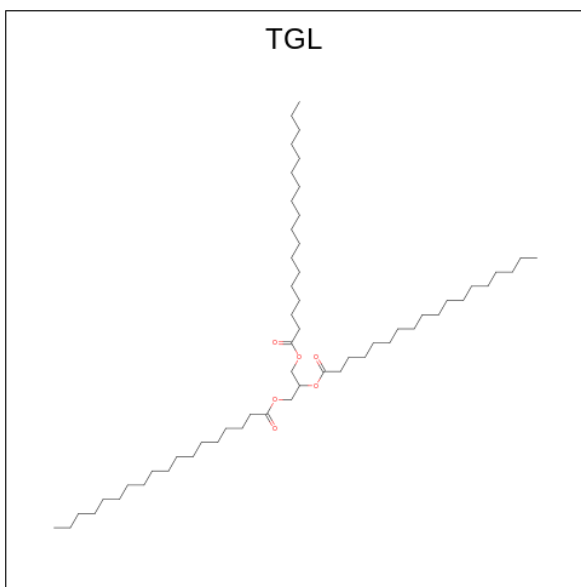
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 18  | A     | 1        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 18  | N     | 1        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |

- 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).



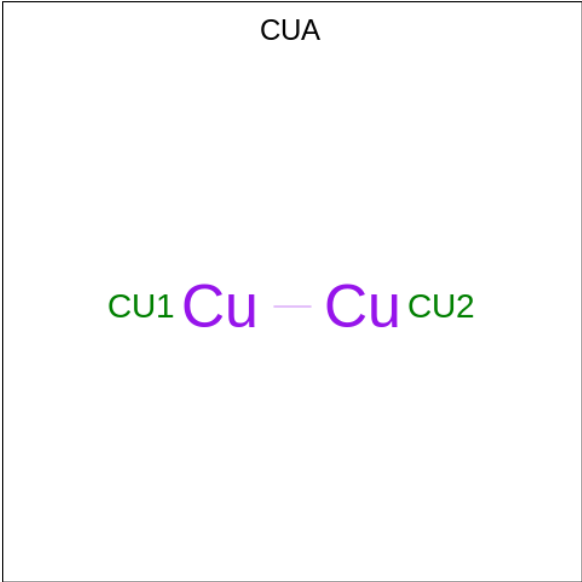
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | A     | 1       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

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



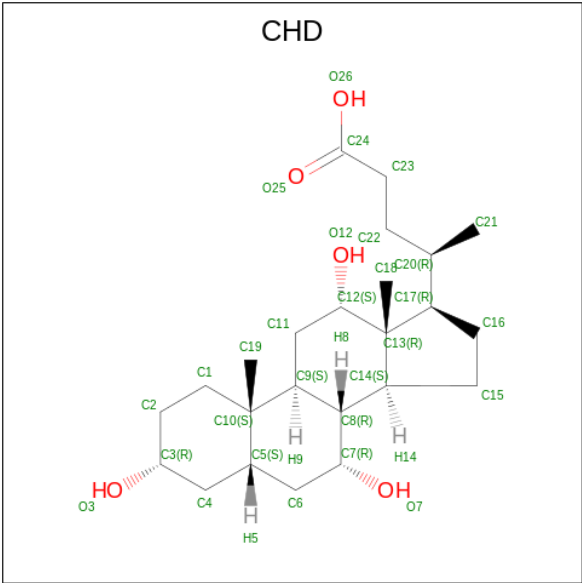
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 20  | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 20  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 20  | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 20  | N     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 20  | Q     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 20  | Y     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21  | B     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 21  | O     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



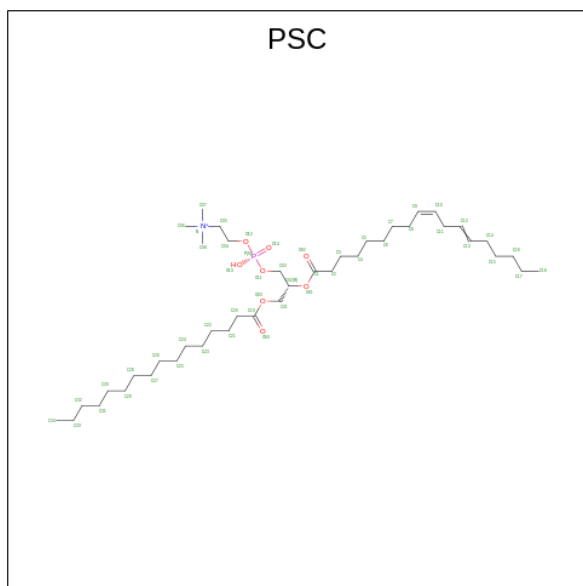
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 22  | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 22  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 22  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 22  | J     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 22  | O     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 22  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 22  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 22  | W     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)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).

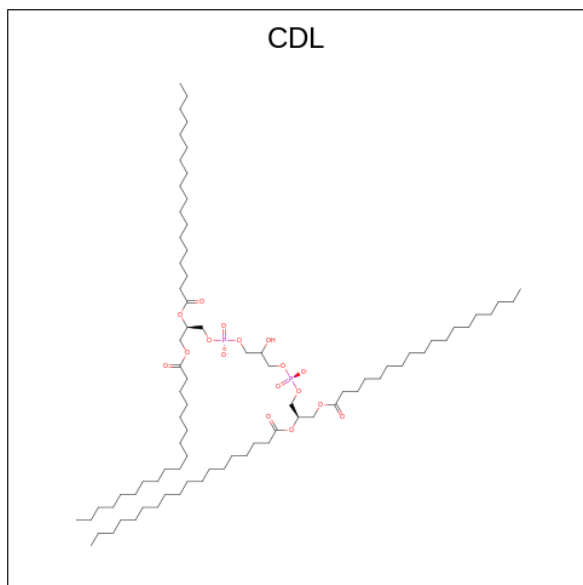


| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 23  | B     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |
| 23  | O     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |

- Molecule 24 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

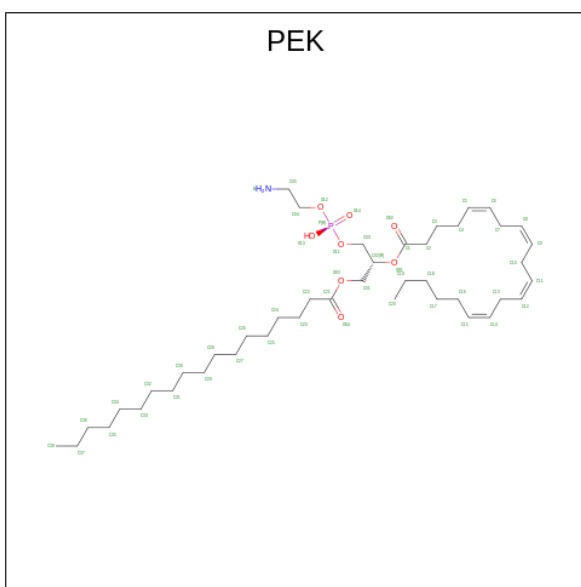
| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 24  | C     | 1        | Total X<br>1 1 | 0       | 0       |
| 24  | P     | 1        | Total X<br>1 1 | 0       | 0       |

- 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<br>100 81 17 2 | 0       | 0       |
| 25  | G     | 1        | Total C O P<br>100 81 17 2 | 0       | 0       |
| 25  | P     | 1        | Total C O P<br>100 81 17 2 | 0       | 0       |
| 25  | T     | 1        | Total C O P<br>100 81 17 2 | 0       | 0       |

- 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:  $C_{43}H_{78}NO_8P$ ).

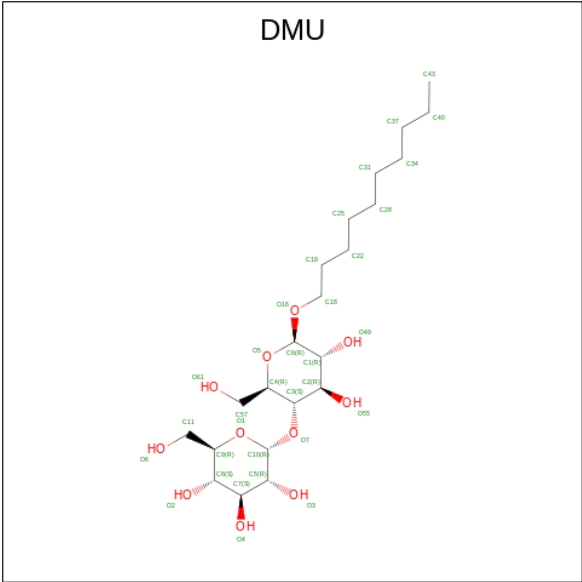


| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 26  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 26  | G     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 26  | G     | 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 |         |         |
| 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 DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 28  | J     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 28  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 28  | P     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 28  | Z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |

- Molecule 29 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 29  | A     | 297      | Total | O   | 0       | 0       |
|     |       |          | 297   | 297 |         |         |
| 29  | B     | 273      | Total | O   | 0       | 1       |
|     |       |          | 274   | 274 |         |         |
| 29  | C     | 176      | Total | O   | 0       | 0       |
|     |       |          | 176   | 176 |         |         |
| 29  | D     | 266      | Total | O   | 0       | 0       |
|     |       |          | 266   | 266 |         |         |
| 29  | E     | 178      | Total | O   | 0       | 0       |
|     |       |          | 178   | 178 |         |         |
| 29  | F     | 199      | Total | O   | 0       | 0       |
|     |       |          | 199   | 199 |         |         |
| 29  | G     | 100      | Total | O   | 0       | 0       |
|     |       |          | 100   | 100 |         |         |
| 29  | H     | 122      | Total | O   | 0       | 0       |
|     |       |          | 122   | 122 |         |         |

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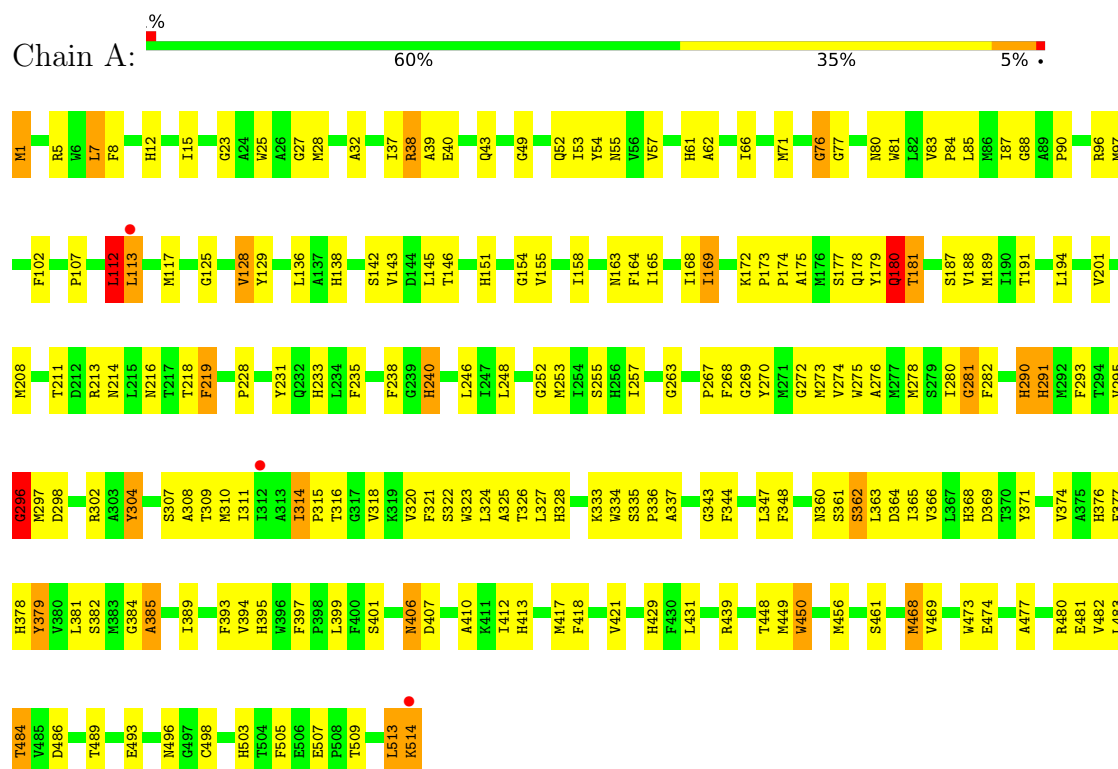
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 29  | I     | 88       | Total<br>88  | O<br>88  | 0       | 0       |
| 29  | J     | 63       | Total<br>63  | O<br>63  | 0       | 0       |
| 29  | K     | 69       | Total<br>69  | O<br>69  | 0       | 0       |
| 29  | L     | 48       | Total<br>48  | O<br>48  | 0       | 0       |
| 29  | M     | 47       | Total<br>47  | O<br>47  | 0       | 0       |
| 29  | N     | 290      | Total<br>290 | O<br>290 | 0       | 0       |
| 29  | O     | 242      | Total<br>243 | O<br>243 | 0       | 1       |
| 29  | P     | 173      | Total<br>173 | O<br>173 | 0       | 0       |
| 29  | Q     | 164      | Total<br>164 | O<br>164 | 0       | 0       |
| 29  | R     | 151      | Total<br>151 | O<br>151 | 0       | 0       |
| 29  | S     | 186      | Total<br>186 | O<br>186 | 0       | 0       |
| 29  | T     | 94       | Total<br>94  | O<br>94  | 0       | 0       |
| 29  | U     | 110      | Total<br>110 | O<br>110 | 0       | 0       |
| 29  | V     | 71       | Total<br>71  | O<br>71  | 0       | 0       |
| 29  | W     | 58       | Total<br>58  | O<br>58  | 0       | 0       |
| 29  | X     | 57       | Total<br>57  | O<br>57  | 0       | 0       |
| 29  | Y     | 40       | Total<br>40  | O<br>40  | 0       | 0       |
| 29  | Z     | 37       | Total<br>37  | O<br>37  | 0       | 0       |

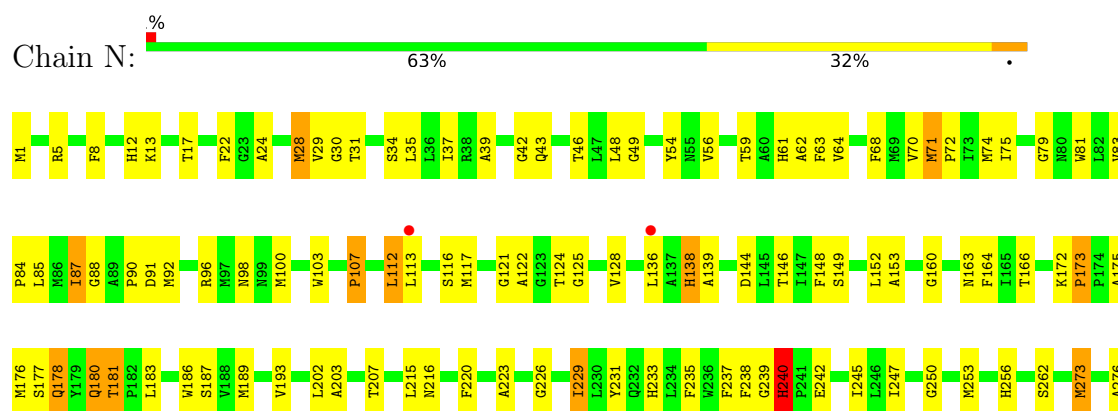
### 3 Residue-property plots [i](#)

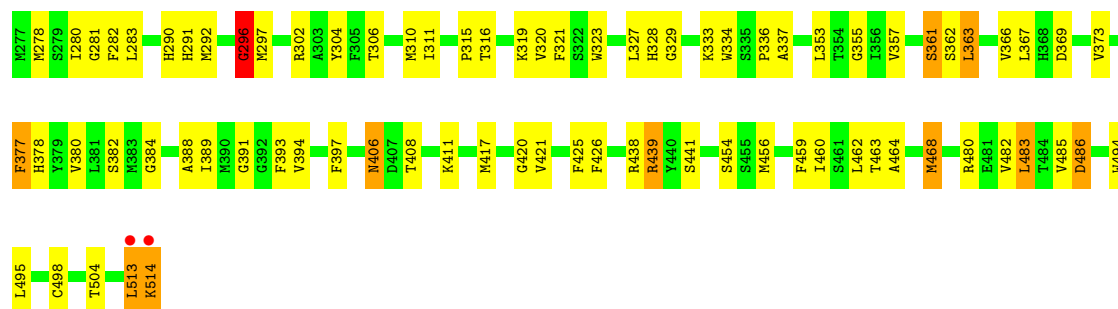
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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



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

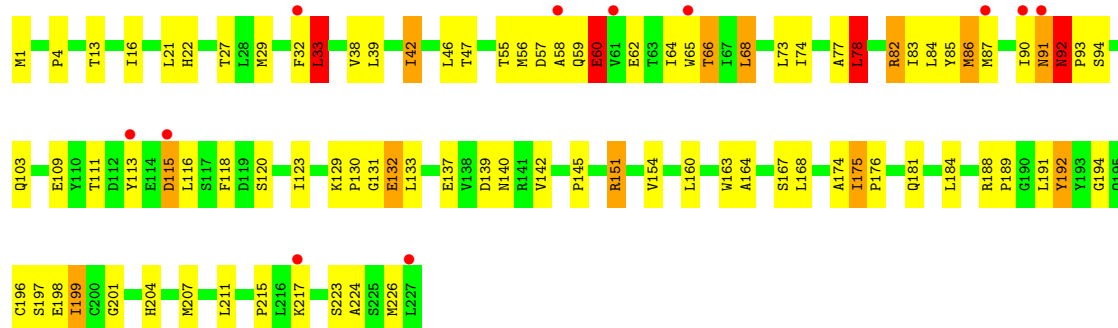




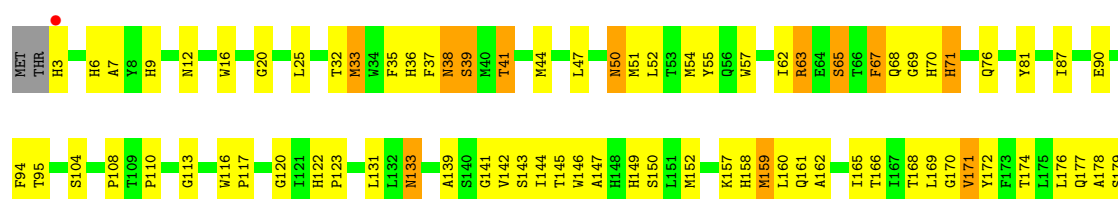
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

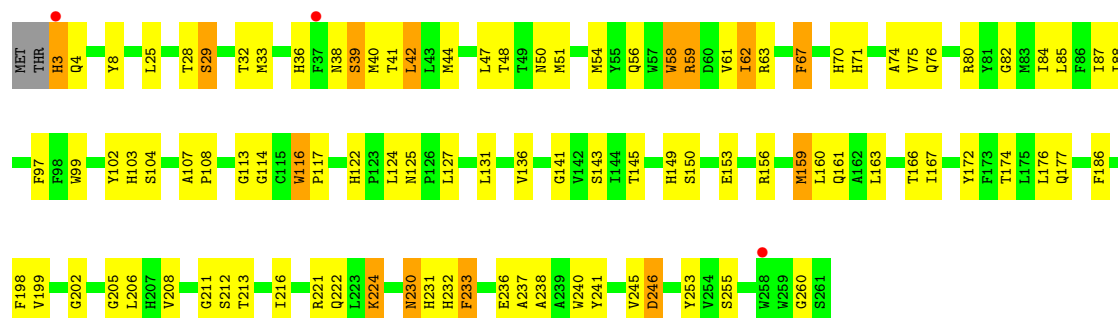


• Molecule 3: Cytochrome c oxidase subunit 3

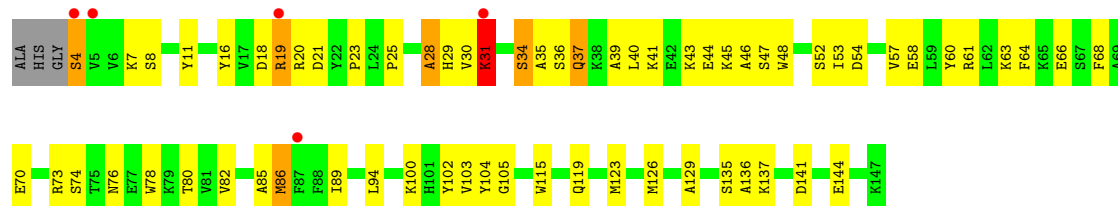




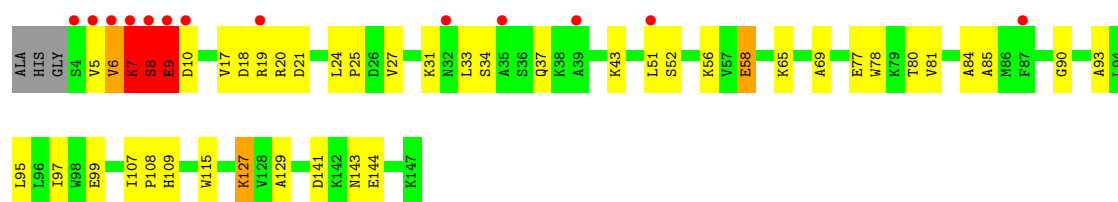
• Molecule 3: Cytochrome c oxidase subunit 3



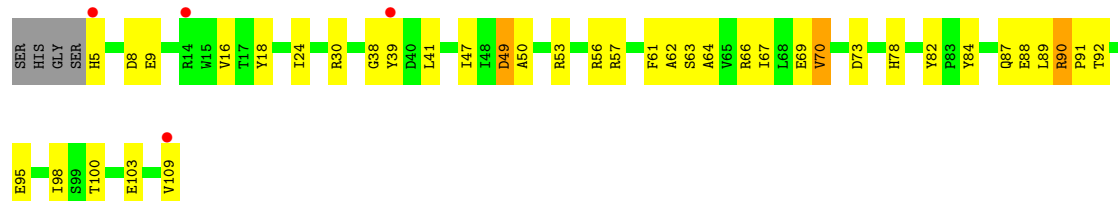
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



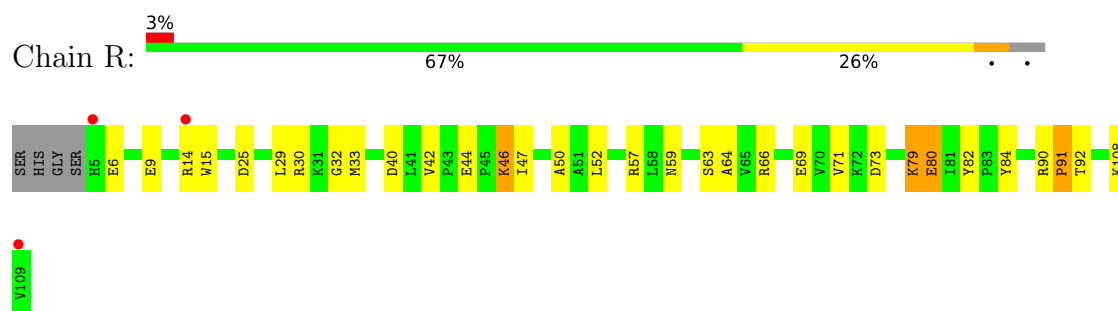
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



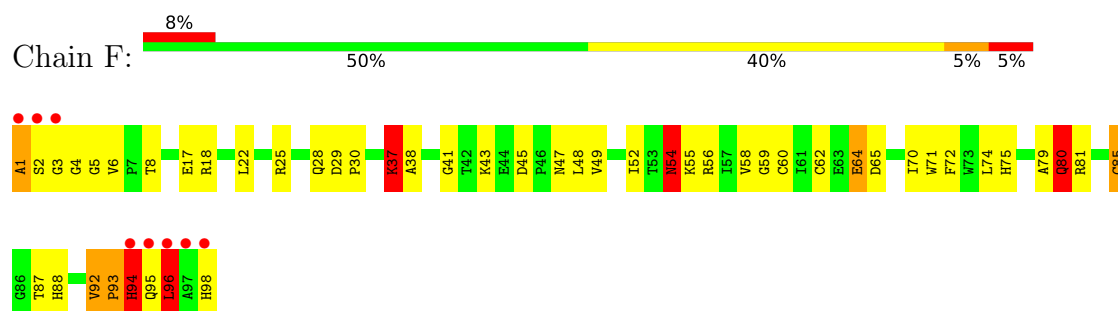
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



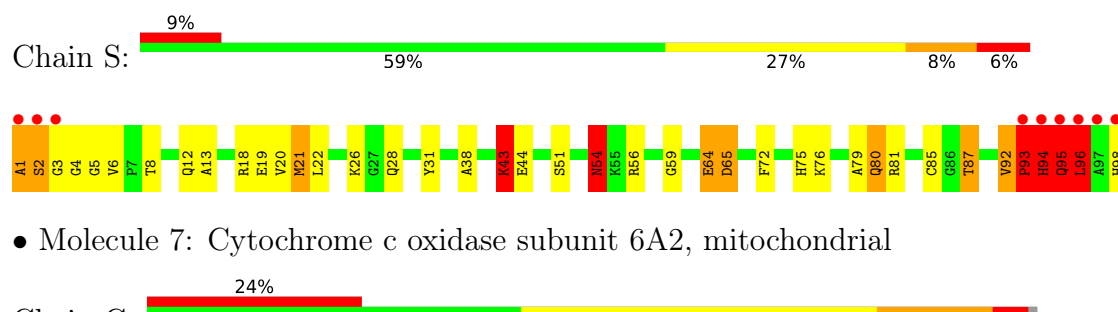
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



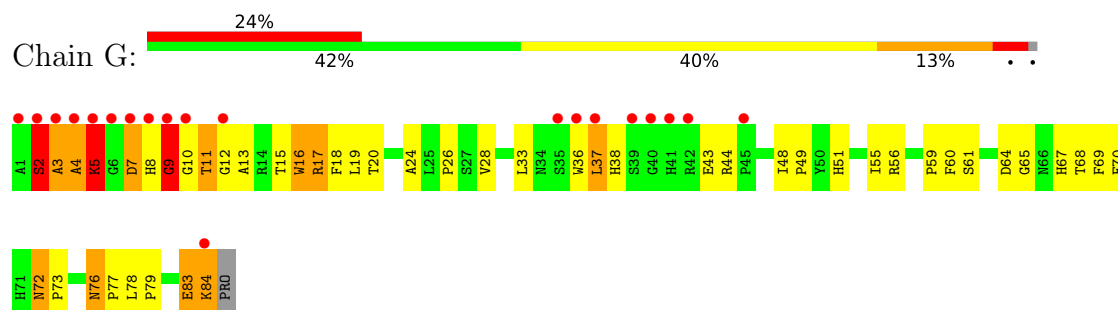
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



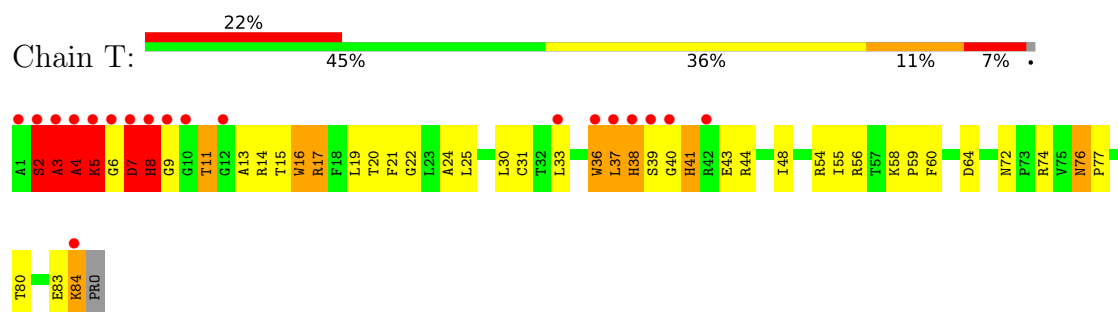
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



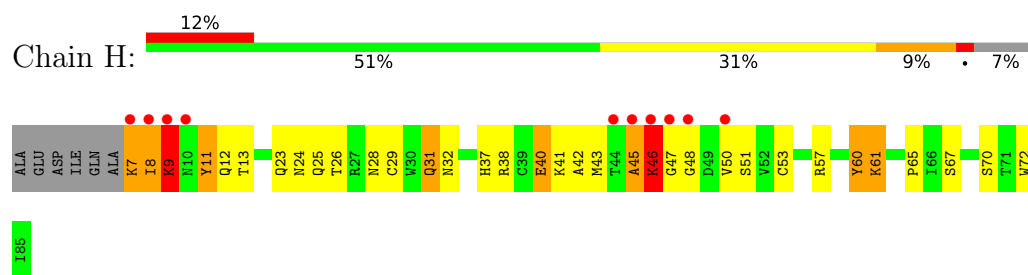
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



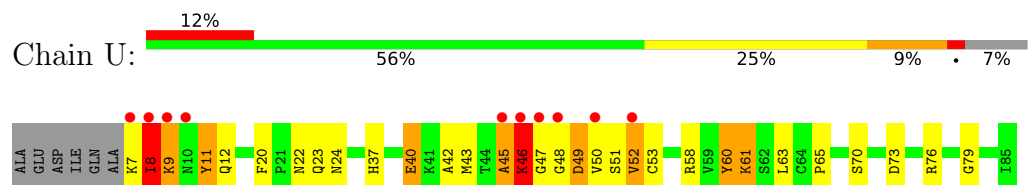
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



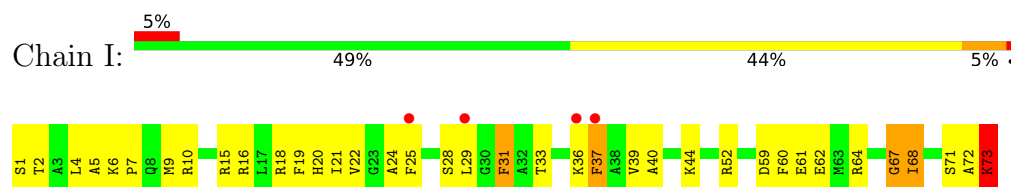
- Molecule 8: Cytochrome c oxidase subunit 6B1



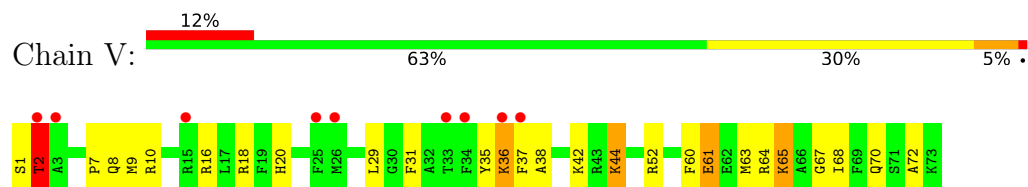
- Molecule 8: Cytochrome c oxidase subunit 6B1



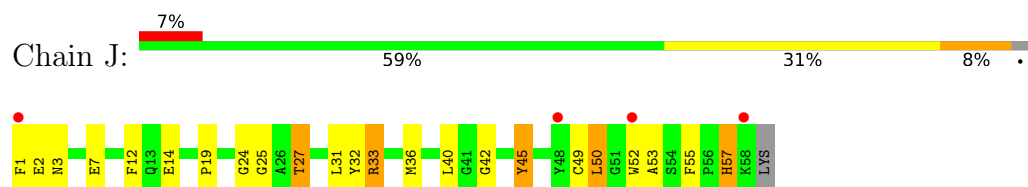
- Molecule 9: Cytochrome c oxidase subunit 6C



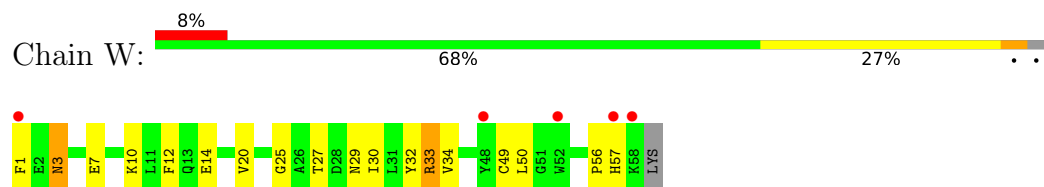
- Molecule 9: Cytochrome c oxidase subunit 6C



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



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



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

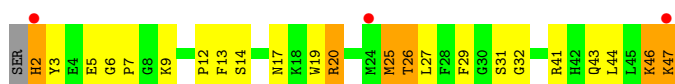




- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



- 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, $\alpha$ , $\beta$ , $\gamma$                | 181.94Å 204.40Å 177.90Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 40.00 – 1.50<br>40.00 – 1.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.3 (40.00-1.50)<br>98.3 (40.00-1.50)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.86 (at 1.40Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0103                                             | Depositor        |
| R, $R_{free}$                                                           | 0.149 , 0.172<br>0.151 , 0.173                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 63174 reflections (5.02%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 20.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.642                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 63.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | 0.001 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.98                                                        | EDS              |
| Total number of atoms                                                   | 35054                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 37.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: CHD, SAC, CU, CDL, TPO, DMU, FME, NA, UNX, MG, PGV, PER, HEA, PEK, ZN, PSC, TGL, CUA

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     | 2.24         | 132/4297 (3.1%)  | 2.09        | 111/5864 (1.9%)  |
| 1   | N     | 2.21         | 126/4283 (2.9%)  | 1.95        | 76/5845 (1.3%)   |
| 2   | B     | 2.30         | 77/1937 (4.0%)   | 1.91        | 36/2637 (1.4%)   |
| 2   | O     | 2.11         | 56/1908 (2.9%)   | 1.74        | 22/2597 (0.8%)   |
| 3   | C     | 2.20         | 71/2272 (3.1%)   | 1.96        | 40/3102 (1.3%)   |
| 3   | P     | 2.21         | 57/2272 (2.5%)   | 1.94        | 37/3102 (1.2%)   |
| 4   | D     | 2.25         | 45/1277 (3.5%)   | 2.00        | 39/1720 (2.3%)   |
| 4   | Q     | 2.01         | 28/1259 (2.2%)   | 1.73        | 15/1698 (0.9%)   |
| 5   | E     | 2.35         | 36/871 (4.1%)    | 2.22        | 29/1182 (2.5%)   |
| 5   | R     | 2.20         | 24/882 (2.7%)    | 1.77        | 14/1196 (1.2%)   |
| 6   | F     | 2.49         | 43/795 (5.4%)    | 2.08        | 26/1079 (2.4%)   |
| 6   | S     | 2.34         | 30/780 (3.8%)    | 2.01        | 28/1058 (2.6%)   |
| 7   | G     | 2.56         | 43/702 (6.1%)    | 2.14        | 31/953 (3.3%)    |
| 7   | T     | 2.41         | 36/702 (5.1%)    | 1.92        | 23/953 (2.4%)    |
| 8   | H     | 2.10         | 21/682 (3.1%)    | 1.80        | 11/921 (1.2%)    |
| 8   | U     | 2.03         | 23/682 (3.4%)    | 1.61        | 4/921 (0.4%)     |
| 9   | I     | 2.38         | 35/605 (5.8%)    | 1.88        | 13/802 (1.6%)    |
| 9   | V     | 2.04         | 16/605 (2.6%)    | 1.94        | 12/802 (1.5%)    |
| 10  | J     | 2.29         | 18/471 (3.8%)    | 1.88        | 6/636 (0.9%)     |
| 10  | W     | 1.94         | 6/480 (1.2%)     | 1.56        | 5/648 (0.8%)     |
| 11  | K     | 2.36         | 14/398 (3.5%)    | 1.86        | 9/546 (1.6%)     |
| 11  | X     | 1.83         | 5/405 (1.2%)     | 1.50        | 5/556 (0.9%)     |
| 12  | L     | 2.23         | 16/393 (4.1%)    | 1.95        | 7/526 (1.3%)     |
| 12  | Y     | 2.21         | 19/401 (4.7%)    | 1.73        | 5/536 (0.9%)     |
| 13  | M     | 2.11         | 7/345 (2.0%)     | 1.96        | 9/470 (1.9%)     |
| 13  | Z     | 2.14         | 14/345 (4.1%)    | 1.65        | 2/470 (0.4%)     |
| All | All   | 2.22         | 998/30049 (3.3%) | 1.93        | 615/40820 (1.5%) |

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                   | 4                   |
| 1   | N     | 0                   | 3                   |
| 2   | B     | 0                   | 3                   |
| 3   | C     | 0                   | 1                   |
| 4   | Q     | 0                   | 1                   |
| 5   | E     | 0                   | 2                   |
| 6   | F     | 0                   | 1                   |
| 6   | S     | 0                   | 2                   |
| 7   | G     | 0                   | 1                   |
| 7   | T     | 0                   | 1                   |
| 10  | J     | 0                   | 1                   |
| 11  | K     | 0                   | 1                   |
| 13  | M     | 0                   | 1                   |
| All | All   | 0                   | 22                  |

All (998) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 5   | R     | 90  | ARG  | NE-CZ  | 14.77  | 1.49        | 1.33     |
| 11  | K     | 47  | ARG  | CZ-NH2 | 14.29  | 1.52        | 1.33     |
| 11  | K     | 54  | ARG  | NE-CZ  | 13.20  | 1.47        | 1.33     |
| 7   | T     | 80  | THR  | C-O    | -12.38 | 1.07        | 1.24     |
| 11  | X     | 54  | ARG  | CZ-NH2 | 12.24  | 1.49        | 1.33     |
| 4   | Q     | 6   | VAL  | CA-C   | 11.62  | 1.66        | 1.52     |
| 6   | S     | 92  | VAL  | C-O    | -11.60 | 1.09        | 1.24     |
| 4   | Q     | 6   | VAL  | C-O    | 11.46  | 1.38        | 1.24     |
| 7   | G     | 5   | LYS  | CA-C   | 11.44  | 1.68        | 1.52     |
| 9   | I     | 4   | LEU  | CA-CB  | 11.31  | 1.70        | 1.53     |
| 1   | A     | 482 | VAL  | CA-CB  | 11.04  | 1.65        | 1.54     |
| 11  | K     | 17  | VAL  | N-CA   | 10.77  | 1.59        | 1.46     |
| 6   | F     | 3   | GLY  | CA-C   | 10.62  | 1.62        | 1.51     |
| 2   | O     | 65  | TRP  | CB-CG  | -10.43 | 1.18        | 1.50     |
| 4   | Q     | 6   | VAL  | CA-CB  | 10.32  | 1.66        | 1.54     |
| 12  | L     | 26  | THR  | CB-CG2 | -10.27 | 1.18        | 1.52     |
| 5   | E     | 9   | GLU  | CA-CB  | 10.20  | 1.69        | 1.53     |
| 7   | G     | 13  | ALA  | N-CA   | 10.13  | 1.58        | 1.46     |
| 10  | J     | 25  | GLY  | N-CA   | 10.06  | 1.56        | 1.44     |
| 2   | O     | 123 | ILE  | N-CA   | 10.03  | 1.58        | 1.46     |
| 2   | B     | 65  | TRP  | CB-CG  | -9.90  | 1.19        | 1.50     |
| 6   | S     | 64  | GLU  | CA-C   | 9.90   | 1.65        | 1.52     |
| 4   | Q     | 20  | ARG  | CD-NE  | -9.89  | 1.32        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | C     | 41  | THR  | C-O    | 9.67  | 1.35        | 1.24     |
| 7   | T     | 5   | LYS  | CA-C   | 9.67  | 1.65        | 1.52     |
| 4   | Q     | 18  | ASP  | N-CA   | 9.62  | 1.58        | 1.46     |
| 6   | F     | 62  | CYS  | N-CA   | 9.61  | 1.58        | 1.46     |
| 4   | Q     | 6   | VAL  | C-N    | 9.58  | 1.45        | 1.33     |
| 7   | T     | 17  | ARG  | CZ-NH2 | 9.54  | 1.45        | 1.33     |
| 2   | B     | 38  | VAL  | CA-CB  | 9.50  | 1.65        | 1.54     |
| 1   | N     | 173 | PRO  | CA-CB  | 9.44  | 1.62        | 1.53     |
| 6   | F     | 4   | GLY  | N-CA   | 9.43  | 1.59        | 1.45     |
| 4   | D     | 58  | GLU  | CD-OE1 | 9.36  | 1.43        | 1.25     |
| 2   | O     | 145 | PRO  | C-O    | 9.34  | 1.33        | 1.23     |
| 6   | F     | 1   | ALA  | C-O    | 9.29  | 1.42        | 1.23     |
| 1   | A     | 363 | LEU  | CB-CG  | -9.27 | 1.34        | 1.53     |
| 3   | P     | 224 | LYS  | CE-NZ  | 9.27  | 1.77        | 1.49     |
| 9   | I     | 7   | PRO  | CA-C   | -9.23 | 1.41        | 1.52     |
| 5   | E     | 95  | GLU  | CA-C   | 9.21  | 1.64        | 1.52     |
| 6   | S     | 4   | GLY  | N-CA   | 9.12  | 1.58        | 1.45     |
| 5   | E     | 91  | PRO  | CA-C   | 9.08  | 1.65        | 1.52     |
| 5   | R     | 32  | GLY  | N-CA   | 9.08  | 1.57        | 1.45     |
| 11  | K     | 47  | ARG  | CD-NE  | 9.06  | 1.58        | 1.46     |
| 6   | S     | 93  | PRO  | CA-CB  | 9.06  | 1.66        | 1.53     |
| 2   | B     | 14  | SER  | N-CA   | 9.04  | 1.53        | 1.45     |
| 1   | N     | 226 | GLY  | N-CA   | 9.04  | 1.56        | 1.45     |
| 5   | E     | 87  | GLN  | N-CA   | 9.01  | 1.56        | 1.46     |
| 9   | V     | 8   | GLN  | CG-CD  | -8.98 | 1.29        | 1.52     |
| 6   | S     | 3   | GLY  | CA-C   | 8.90  | 1.60        | 1.51     |
| 7   | G     | 3   | ALA  | N-CA   | 8.88  | 1.57        | 1.46     |
| 7   | G     | 3   | ALA  | CA-C   | 8.87  | 1.64        | 1.52     |
| 6   | S     | 3   | GLY  | N-CA   | 8.82  | 1.54        | 1.45     |
| 2   | B     | 59  | GLN  | CD-OE1 | 8.79  | 1.40        | 1.23     |
| 7   | T     | 55  | ILE  | CA-CB  | 8.76  | 1.64        | 1.54     |
| 7   | G     | 5   | LYS  | CA-CB  | 8.75  | 1.68        | 1.53     |
| 6   | F     | 2   | SER  | N-CA   | 8.71  | 1.58        | 1.46     |
| 7   | G     | 2   | SER  | CA-C   | 8.63  | 1.64        | 1.52     |
| 2   | O     | 21  | LEU  | CA-CB  | 8.63  | 1.66        | 1.53     |
| 5   | E     | 41  | LEU  | C-O    | 8.61  | 1.35        | 1.23     |
| 2   | B     | 55  | THR  | C-O    | 8.60  | 1.34        | 1.23     |
| 2   | B     | 21  | LEU  | CA-CB  | 8.58  | 1.66        | 1.53     |
| 1   | A     | 96  | ARG  | CZ-NH1 | 8.55  | 1.44        | 1.32     |
| 7   | G     | 16  | TRP  | CA-C   | 8.55  | 1.64        | 1.52     |
| 3   | C     | 63  | ARG  | CZ-NH2 | 8.48  | 1.44        | 1.33     |
| 5   | E     | 70  | VAL  | CA-CB  | 8.47  | 1.65        | 1.54     |

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| Mol | Chain | Res    | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 1   | A     | 173    | PRO  | CA-C   | -8.45 | 1.47        | 1.51     |
| 1   | A     | 214    | ASN  | C-O    | 8.44  | 1.34        | 1.24     |
| 4   | D     | 85     | ALA  | C-O    | 8.42  | 1.33        | 1.24     |
| 7   | T     | 4      | ALA  | C-O    | -8.42 | 1.13        | 1.24     |
| 1   | A     | 49     | GLY  | C-O    | 8.36  | 1.34        | 1.23     |
| 9   | I     | 72     | ALA  | CA-C   | -8.35 | 1.42        | 1.52     |
| 6   | F     | 70     | ILE  | N-CA   | 8.35  | 1.56        | 1.46     |
| 1   | A     | 448    | THR  | C-O    | 8.34  | 1.34        | 1.24     |
| 6   | S     | 1      | ALA  | C-O    | 8.29  | 1.40        | 1.23     |
| 2   | B     | 115    | ASP  | CB-CG  | 8.27  | 1.72        | 1.52     |
| 4   | Q     | 20     | ARG  | CZ-NH2 | -8.26 | 1.22        | 1.33     |
| 7   | T     | 20     | THR  | N-CA   | 8.25  | 1.56        | 1.46     |
| 1   | A     | 333    | LYS  | C-O    | 8.23  | 1.33        | 1.24     |
| 10  | J     | 19     | PRO  | CA-CB  | 8.21  | 1.65        | 1.53     |
| 1   | N     | 83     | VAL  | CA-CB  | 8.19  | 1.58        | 1.54     |
| 1   | A     | 83     | VAL  | CA-CB  | 8.18  | 1.58        | 1.54     |
| 1   | N     | 250    | GLY  | CA-C   | 8.16  | 1.60        | 1.52     |
| 1   | N     | 281    | GLY  | N-CA   | 8.13  | 1.55        | 1.45     |
| 5   | R     | 46     | LYS  | CE-NZ  | 8.12  | 1.73        | 1.49     |
| 8   | H     | 11     | TYR  | N-CA   | 8.12  | 1.56        | 1.46     |
| 3   | C     | 113    | GLY  | N-CA   | 8.11  | 1.56        | 1.45     |
| 7   | G     | 48     | ILE  | N-CA   | 8.08  | 1.52        | 1.45     |
| 9   | I     | 18     | ARG  | C-O    | 8.07  | 1.33        | 1.24     |
| 1   | A     | 498    | CYS  | C-O    | 8.07  | 1.32        | 1.25     |
| 1   | N     | 223    | ALA  | N-CA   | 8.06  | 1.56        | 1.46     |
| 1   | A     | 240    | HIS  | N-CA   | 8.04  | 1.53        | 1.46     |
| 1   | A     | 514    | LYS  | N-CA   | 8.02  | 1.61        | 1.46     |
| 6   | F     | 3      | GLY  | N-CA   | 7.99  | 1.53        | 1.45     |
| 1   | A     | 513    | LEU  | CA-C   | -7.98 | 1.43        | 1.52     |
| 3   | P     | 255    | SER  | C-O    | 7.97  | 1.33        | 1.24     |
| 7   | T     | 19     | LEU  | CA-C   | 7.95  | 1.63        | 1.52     |
| 2   | O     | 82     | ARG  | N-CA   | 7.94  | 1.55        | 1.46     |
| 3   | C     | 158    | HIS  | C-N    | 7.88  | 1.43        | 1.33     |
| 6   | F     | 43     | LYS  | CA-C   | 7.82  | 1.63        | 1.52     |
| 1   | N     | 49     | GLY  | C-O    | 7.82  | 1.34        | 1.23     |
| 5   | E     | 98     | ILE  | C-O    | 7.79  | 1.32        | 1.24     |
| 1   | N     | 468    | MET  | SD-CE  | 7.76  | 1.99        | 1.79     |
| 1   | A     | 113[A] | LEU  | CA-C   | 7.75  | 1.62        | 1.52     |
| 1   | A     | 113[B] | LEU  | CA-C   | 7.75  | 1.62        | 1.52     |
| 7   | T     | 36     | TRP  | CB-CG  | 7.75  | 1.74        | 1.50     |
| 2   | B     | 31     | VAL  | CA-CB  | 7.74  | 1.63        | 1.54     |
| 5   | E     | 69     | GLU  | CA-CB  | 7.70  | 1.66        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | D     | 28  | ALA  | C-O     | 7.70  | 1.33        | 1.23     |
| 1   | A     | 406 | ASN  | C-O     | 7.70  | 1.33        | 1.24     |
| 3   | P     | 107 | ALA  | CA-CB   | 7.68  | 1.62        | 1.53     |
| 1   | A     | 456 | MET  | N-CA    | 7.66  | 1.55        | 1.46     |
| 9   | I     | 68  | ILE  | CB-CG1  | -7.64 | 1.38        | 1.53     |
| 13  | Z     | 4   | LYS  | N-CA    | 7.64  | 1.57        | 1.45     |
| 7   | G     | 55  | ILE  | CA-CB   | 7.62  | 1.62        | 1.54     |
| 1   | A     | 37  | ILE  | N-CA    | 7.58  | 1.55        | 1.46     |
| 6   | F     | 85  | CYS  | C-O     | 7.57  | 1.33        | 1.24     |
| 8   | U     | 11  | TYR  | N-CA    | 7.56  | 1.55        | 1.46     |
| 1   | A     | 61  | HIS  | ND1-CE1 | 7.55  | 1.40        | 1.32     |
| 4   | D     | 34  | SER  | CA-C    | -7.54 | 1.42        | 1.53     |
| 6   | F     | 56  | ARG  | CZ-NH1  | 7.53  | 1.43        | 1.32     |
| 4   | D     | 40  | LEU  | C-O     | 7.52  | 1.33        | 1.24     |
| 1   | N     | 146 | THR  | N-CA    | 7.51  | 1.55        | 1.46     |
| 2   | O     | 60  | GLU  | CD-OE1  | 7.51  | 1.39        | 1.25     |
| 7   | G     | 69  | PHE  | C-O     | 7.50  | 1.32        | 1.24     |
| 2   | B     | 223 | SER  | CA-CB   | 7.50  | 1.65        | 1.53     |
| 4   | D     | 105 | GLY  | N-CA    | 7.49  | 1.54        | 1.44     |
| 3   | P     | 149 | HIS  | CD2-NE2 | 7.47  | 1.46        | 1.37     |
| 12  | Y     | 5   | GLU  | CA-C    | -7.47 | 1.43        | 1.52     |
| 1   | A     | 189 | MET  | CG-SD   | -7.45 | 1.62        | 1.80     |
| 1   | N     | 514 | LYS  | CA-CB   | 7.45  | 1.68        | 1.53     |
| 2   | O     | 33  | LEU  | N-CA    | 7.45  | 1.55        | 1.46     |
| 1   | A     | 324 | LEU  | N-CA    | 7.44  | 1.55        | 1.46     |
| 6   | S     | 18  | ARG  | CZ-NH1  | 7.43  | 1.43        | 1.32     |
| 1   | N     | 439 | ARG  | CZ-NH1  | 7.41  | 1.43        | 1.32     |
| 5   | E     | 38  | GLY  | N-CA    | 7.41  | 1.55        | 1.45     |
| 10  | J     | 50  | LEU  | N-CA    | 7.39  | 1.55        | 1.46     |
| 6   | F     | 2   | SER  | CA-C    | 7.38  | 1.62        | 1.52     |
| 6   | S     | 93  | PRO  | CA-C    | 7.38  | 1.62        | 1.52     |
| 5   | E     | 63  | SER  | CA-C    | 7.37  | 1.62        | 1.52     |
| 7   | T     | 8   | HIS  | N-CA    | 7.37  | 1.55        | 1.46     |
| 9   | V     | 9   | MET  | CA-C    | -7.37 | 1.43        | 1.52     |
| 1   | A     | 97  | MET  | CA-C    | 7.35  | 1.62        | 1.52     |
| 2   | O     | 167 | SER  | CB-OG   | -7.35 | 1.27        | 1.42     |
| 6   | F     | 49  | VAL  | C-O     | 7.33  | 1.32        | 1.24     |
| 6   | F     | 59  | GLY  | CA-C    | -7.25 | 1.47        | 1.52     |
| 7   | G     | 19  | LEU  | CA-C    | 7.25  | 1.62        | 1.52     |
| 5   | E     | 82  | TYR  | CA-CB   | 7.24  | 1.62        | 1.53     |
| 1   | N     | 514 | LYS  | N-CA    | 7.23  | 1.59        | 1.46     |
| 10  | W     | 25  | GLY  | N-CA    | 7.23  | 1.56        | 1.45     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | E     | 109 | VAL  | N-CA   | 7.23  | 1.59        | 1.46     |
| 5   | E     | 47  | ILE  | N-CA   | 7.22  | 1.55        | 1.46     |
| 4   | D     | 103 | VAL  | CA-CB  | 7.21  | 1.61        | 1.55     |
| 7   | G     | 49  | PRO  | CA-C   | 7.21  | 1.60        | 1.53     |
| 6   | F     | 5   | GLY  | C-N    | 7.21  | 1.39        | 1.32     |
| 2   | O     | 78  | LEU  | N-CA   | 7.20  | 1.52        | 1.46     |
| 5   | E     | 90  | ARG  | CZ-NH1 | 7.19  | 1.42        | 1.32     |
| 1   | N     | 460 | ILE  | CA-CB  | 7.18  | 1.63        | 1.54     |
| 2   | B     | 103 | GLN  | C-O    | 7.17  | 1.32        | 1.24     |
| 10  | J     | 2   | GLU  | CA-C   | 7.17  | 1.61        | 1.52     |
| 2   | O     | 57  | ASP  | N-CA   | 7.16  | 1.55        | 1.46     |
| 7   | T     | 77  | PRO  | C-O    | 7.16  | 1.32        | 1.23     |
| 3   | P     | 221 | ARG  | N-CA   | 7.16  | 1.55        | 1.46     |
| 12  | Y     | 31  | SER  | CA-C   | 7.16  | 1.62        | 1.52     |
| 1   | A     | 382 | SER  | CA-CB  | 7.16  | 1.65        | 1.53     |
| 2   | O     | 55  | THR  | C-O    | 7.15  | 1.32        | 1.23     |
| 4   | D     | 141 | ASP  | N-CA   | 7.13  | 1.55        | 1.46     |
| 7   | T     | 5   | LYS  | CA-CB  | 7.13  | 1.65        | 1.53     |
| 10  | J     | 33  | ARG  | CA-CB  | 7.13  | 1.64        | 1.53     |
| 10  | J     | 25  | GLY  | C-O    | 7.12  | 1.31        | 1.24     |
| 10  | W     | 33  | ARG  | CA-CB  | 7.12  | 1.64        | 1.53     |
| 3   | C     | 230 | ASN  | CB-CG  | -7.12 | 1.34        | 1.52     |
| 4   | Q     | 99  | GLU  | C-O    | -7.11 | 1.15        | 1.24     |
| 3   | C     | 157 | LYS  | N-CA   | 7.10  | 1.54        | 1.46     |
| 2   | B     | 174 | ALA  | C-N    | 7.09  | 1.38        | 1.33     |
| 7   | T     | 48  | ILE  | CA-C   | 7.09  | 1.60        | 1.52     |
| 1   | N     | 203 | ALA  | C-O    | 7.07  | 1.32        | 1.24     |
| 1   | N     | 56  | VAL  | N-CA   | 7.07  | 1.54        | 1.46     |
| 1   | A     | 321 | PHE  | N-CA   | 7.06  | 1.55        | 1.46     |
| 4   | Q     | 25  | PRO  | N-CA   | 7.04  | 1.55        | 1.47     |
| 3   | C     | 199 | VAL  | N-CA   | 7.03  | 1.54        | 1.46     |
| 1   | A     | 52  | GLN  | CA-CB  | 7.03  | 1.64        | 1.53     |
| 4   | Q     | 9   | GLU  | N-CA   | 7.02  | 1.55        | 1.46     |
| 9   | I     | 59  | ASP  | CA-C   | 7.01  | 1.61        | 1.52     |
| 4   | D     | 35  | ALA  | CA-C   | 7.01  | 1.62        | 1.52     |
| 9   | V     | 7   | PRO  | CA-C   | -7.01 | 1.43        | 1.52     |
| 2   | B     | 51  | THR  | C-O    | 7.00  | 1.32        | 1.23     |
| 10  | J     | 33  | ARG  | N-CA   | 6.99  | 1.54        | 1.46     |
| 3   | P     | 76  | GLN  | CB-CG  | -6.99 | 1.31        | 1.52     |
| 6   | S     | 3   | GLY  | C-O    | 6.99  | 1.33        | 1.23     |
| 9   | I     | 25  | PHE  | C-O    | 6.98  | 1.32        | 1.24     |
| 1   | A     | 43  | GLN  | CA-CB  | -6.96 | 1.44        | 1.53     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 3   | P     | 122    | HIS  | C-O     | 6.96  | 1.31        | 1.24     |
| 1   | A     | 281    | GLY  | N-CA    | 6.95  | 1.54        | 1.45     |
| 7   | T     | 2      | SER  | CA-C    | 6.94  | 1.61        | 1.52     |
| 2   | B     | 65     | TRP  | N-CA    | -6.93 | 1.36        | 1.46     |
| 6   | F     | 80     | GLN  | CD-OE1  | 6.92  | 1.36        | 1.23     |
| 1   | N     | 363    | LEU  | CB-CG   | -6.92 | 1.39        | 1.53     |
| 9   | I     | 62     | GLU  | C-O     | 6.92  | 1.32        | 1.24     |
| 2   | B     | 152    | MET  | CB-CG   | -6.92 | 1.31        | 1.52     |
| 3   | C     | 232    | HIS  | ND1-CE1 | 6.90  | 1.39        | 1.32     |
| 11  | X     | 47     | ARG  | NE-CZ   | 6.90  | 1.40        | 1.33     |
| 11  | X     | 33     | ALA  | N-CA    | 6.89  | 1.55        | 1.46     |
| 1   | N     | 411    | LYS  | CA-CB   | 6.89  | 1.64        | 1.53     |
| 8   | U     | 8      | ILE  | CA-CB   | 6.89  | 1.63        | 1.54     |
| 8   | U     | 63     | LEU  | CA-CB   | 6.89  | 1.64        | 1.53     |
| 1   | N     | 175    | ALA  | N-CA    | 6.88  | 1.55        | 1.46     |
| 1   | A     | 298[A] | ASP  | C-N     | 6.87  | 1.42        | 1.34     |
| 1   | A     | 298[B] | ASP  | C-N     | 6.87  | 1.42        | 1.34     |
| 3   | C     | 65     | SER  | CA-CB   | 6.86  | 1.63        | 1.53     |
| 3   | P     | 87     | ILE  | N-CA    | 6.85  | 1.54        | 1.46     |
| 5   | E     | 16     | VAL  | CA-CB   | 6.85  | 1.63        | 1.54     |
| 6   | F     | 1      | ALA  | C-N     | 6.84  | 1.43        | 1.33     |
| 8   | U     | 46     | LYS  | CA-C    | 6.83  | 1.61        | 1.52     |
| 1   | N     | 513    | LEU  | C-O     | 6.83  | 1.33        | 1.23     |
| 1   | N     | 98     | ASN  | N-CA    | 6.83  | 1.54        | 1.46     |
| 9   | V     | 72     | ALA  | CA-C    | -6.83 | 1.45        | 1.52     |
| 2   | O     | 191    | LEU  | N-CA    | 6.81  | 1.54        | 1.46     |
| 7   | G     | 20     | THR  | N-CA    | 6.80  | 1.54        | 1.46     |
| 7   | G     | 83     | GLU  | N-CA    | 6.79  | 1.54        | 1.46     |
| 1   | N     | 121    | GLY  | N-CA    | 6.78  | 1.52        | 1.45     |
| 1   | A     | 401    | SER  | CA-CB   | 6.76  | 1.63        | 1.54     |
| 7   | G     | 36     | TRP  | CB-CG   | 6.76  | 1.71        | 1.50     |
| 1   | A     | 164    | PHE  | CA-CB   | 6.75  | 1.64        | 1.53     |
| 3   | C     | 120    | GLY  | N-CA    | 6.73  | 1.55        | 1.45     |
| 12  | Y     | 26     | THR  | CB-CG2  | -6.73 | 1.30        | 1.52     |
| 1   | A     | 407    | ASP  | N-CA    | 6.73  | 1.54        | 1.46     |
| 2   | B     | 175    | ILE  | CA-C    | -6.72 | 1.47        | 1.52     |
| 1   | N     | 48     | LEU  | C-O     | -6.72 | 1.15        | 1.23     |
| 2   | O     | 60     | GLU  | CA-CB   | 6.72  | 1.64        | 1.53     |
| 4   | Q     | 8      | SER  | CA-C    | 6.72  | 1.61        | 1.52     |
| 1   | N     | 122    | ALA  | CA-CB   | 6.71  | 1.61        | 1.53     |
| 10  | J     | 27     | THR  | CA-C    | -6.71 | 1.43        | 1.52     |
| 4   | Q     | 90     | GLY  | N-CA    | 6.71  | 1.54        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 509 | THR  | C-O     | 6.71  | 1.33        | 1.23     |
| 4   | Q     | 129 | ALA  | CA-C    | 6.70  | 1.60        | 1.53     |
| 1   | A     | 228 | PRO  | CA-CB   | 6.70  | 1.63        | 1.53     |
| 5   | R     | 66  | ARG  | CA-CB   | 6.70  | 1.63        | 1.53     |
| 8   | H     | 53  | CYS  | C-O     | 6.69  | 1.32        | 1.24     |
| 1   | A     | 233 | HIS  | N-CA    | 6.68  | 1.54        | 1.46     |
| 5   | E     | 56  | ARG  | CZ-NH2  | 6.68  | 1.42        | 1.33     |
| 2   | B     | 5   | MET  | N-CA    | 6.68  | 1.55        | 1.46     |
| 3   | C     | 169 | LEU  | CA-CB   | 6.68  | 1.64        | 1.53     |
| 6   | F     | 18  | ARG  | CZ-NH2  | 6.68  | 1.42        | 1.33     |
| 11  | K     | 50  | PRO  | C-O     | 6.68  | 1.31        | 1.23     |
| 7   | G     | 17  | ARG  | CZ-NH2  | 6.67  | 1.42        | 1.33     |
| 4   | D     | 115 | TRP  | CA-C    | 6.67  | 1.61        | 1.52     |
| 8   | H     | 67  | SER  | N-CA    | 6.67  | 1.54        | 1.46     |
| 9   | I     | 15  | ARG  | C-O     | 6.67  | 1.31        | 1.24     |
| 2   | O     | 66  | THR  | CB-OG1  | 6.66  | 1.54        | 1.43     |
| 7   | T     | 56  | ARG  | CA-CB   | 6.66  | 1.62        | 1.52     |
| 4   | D     | 61  | ARG  | CZ-NH2  | 6.66  | 1.42        | 1.33     |
| 4   | D     | 54  | ASP  | C-O     | 6.65  | 1.31        | 1.24     |
| 1   | N     | 406 | ASN  | N-CA    | -6.64 | 1.38        | 1.46     |
| 2   | O     | 65  | TRP  | CD2-CE3 | 6.64  | 1.50        | 1.40     |
| 1   | N     | 486 | ASP  | CG-OD1  | 6.63  | 1.38        | 1.25     |
| 7   | T     | 60  | PHE  | C-O     | 6.62  | 1.32        | 1.23     |
| 1   | A     | 267 | PRO  | C-O     | 6.61  | 1.31        | 1.23     |
| 2   | B     | 184 | LEU  | CB-CG   | -6.61 | 1.40        | 1.53     |
| 13  | M     | 41  | LYS  | N-CA    | 6.61  | 1.54        | 1.46     |
| 4   | D     | 53  | ILE  | CA-C    | 6.61  | 1.60        | 1.52     |
| 1   | N     | 71  | MET  | SD-CE   | -6.60 | 1.63        | 1.79     |
| 7   | G     | 48  | ILE  | CB-CG1  | 6.59  | 1.66        | 1.53     |
| 1   | A     | 218 | THR  | C-O     | -6.58 | 1.16        | 1.24     |
| 9   | I     | 4   | LEU  | N-CA    | -6.57 | 1.37        | 1.46     |
| 7   | T     | 13  | ALA  | N-CA    | 6.57  | 1.54        | 1.46     |
| 1   | N     | 438 | ARG  | CA-CB   | 6.56  | 1.64        | 1.53     |
| 1   | N     | 220 | PHE  | CA-C    | -6.55 | 1.44        | 1.52     |
| 4   | D     | 29  | HIS  | C-O     | 6.55  | 1.31        | 1.24     |
| 6   | S     | 44  | GLU  | C-O     | 6.55  | 1.32        | 1.24     |
| 3   | P     | 241 | TYR  | CA-C    | 6.55  | 1.61        | 1.52     |
| 8   | U     | 20  | PHE  | CA-CB   | 6.54  | 1.60        | 1.53     |
| 3   | P     | 167 | ILE  | N-CA    | 6.53  | 1.54        | 1.46     |
| 1   | N     | 193 | VAL  | C-O     | 6.53  | 1.31        | 1.24     |
| 6   | S     | 6   | VAL  | N-CA    | 6.53  | 1.53        | 1.46     |
| 6   | F     | 29  | ASP  | CA-CB   | 6.52  | 1.60        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 325 | ALA  | N-CA    | 6.52  | 1.54        | 1.46     |
| 13  | Z     | 35  | TYR  | CA-C    | 6.51  | 1.61        | 1.52     |
| 1   | N     | 8   | PHE  | N-CA    | 6.51  | 1.53        | 1.46     |
| 1   | A     | 96  | ARG  | CA-CB   | 6.51  | 1.63        | 1.53     |
| 1   | A     | 410 | ALA  | CA-CB   | 6.51  | 1.64        | 1.53     |
| 2   | B     | 71  | ILE  | C-O     | 6.50  | 1.31        | 1.24     |
| 4   | D     | 44  | GLU  | CD-OE1  | 6.50  | 1.37        | 1.25     |
| 1   | N     | 87  | ILE  | CA-CB   | 6.50  | 1.62        | 1.54     |
| 2   | O     | 86  | MET  | N-CA    | 6.49  | 1.54        | 1.46     |
| 3   | P     | 231 | HIS  | ND1-CE1 | 6.49  | 1.39        | 1.32     |
| 12  | Y     | 30  | GLY  | CA-C    | 6.49  | 1.59        | 1.52     |
| 7   | G     | 77  | PRO  | C-O     | 6.48  | 1.31        | 1.23     |
| 3   | P     | 260 | GLY  | N-CA    | 6.48  | 1.53        | 1.45     |
| 1   | N     | 482 | VAL  | CA-CB   | 6.47  | 1.61        | 1.54     |
| 8   | U     | 50  | VAL  | N-CA    | 6.47  | 1.54        | 1.46     |
| 8   | U     | 12  | GLN  | N-CA    | -6.46 | 1.39        | 1.46     |
| 8   | H     | 70  | SER  | N-CA    | -6.45 | 1.38        | 1.46     |
| 1   | N     | 242 | GLU  | CA-CB   | 6.44  | 1.63        | 1.53     |
| 12  | Y     | 2   | HIS  | N-CA    | 6.44  | 1.58        | 1.46     |
| 1   | A     | 12  | HIS  | N-CA    | 6.43  | 1.54        | 1.46     |
| 1   | N     | 406 | ASN  | CA-CB   | 6.43  | 1.61        | 1.53     |
| 5   | R     | 80  | GLU  | CA-C    | 6.43  | 1.61        | 1.52     |
| 2   | B     | 82  | ARG  | CZ-NH1  | 6.43  | 1.41        | 1.32     |
| 4   | D     | 135 | SER  | CA-CB   | 6.43  | 1.64        | 1.53     |
| 2   | O     | 103 | GLN  | C-O     | 6.42  | 1.31        | 1.24     |
| 11  | K     | 47  | ARG  | NE-CZ   | 6.42  | 1.40        | 1.33     |
| 1   | A     | 505 | PHE  | C-O     | 6.41  | 1.31        | 1.23     |
| 2   | O     | 118 | PHE  | C-O     | 6.41  | 1.31        | 1.23     |
| 1   | N     | 61  | HIS  | ND1-CE1 | 6.40  | 1.39        | 1.32     |
| 1   | A     | 343 | GLY  | N-CA    | 6.40  | 1.53        | 1.45     |
| 2   | O     | 188 | ARG  | N-CA    | 6.40  | 1.54        | 1.45     |
| 1   | N     | 85  | LEU  | N-CA    | 6.39  | 1.54        | 1.46     |
| 1   | A     | 480 | ARG  | CZ-NH2  | 6.39  | 1.41        | 1.33     |
| 1   | N     | 384 | GLY  | N-CA    | 6.39  | 1.54        | 1.45     |
| 9   | V     | 18  | ARG  | N-CA    | 6.39  | 1.53        | 1.46     |
| 13  | Z     | 16  | ALA  | N-CA    | -6.37 | 1.38        | 1.46     |
| 4   | D     | 43  | LYS  | C-O     | 6.37  | 1.32        | 1.24     |
| 10  | J     | 3   | ASN  | N-CA    | 6.37  | 1.54        | 1.46     |
| 1   | N     | 39  | ALA  | N-CA    | 6.36  | 1.54        | 1.46     |
| 3   | P     | 39  | SER  | C-O     | 6.36  | 1.31        | 1.23     |
| 4   | D     | 7   | LYS  | C-O     | 6.36  | 1.31        | 1.23     |
| 8   | U     | 22  | ASN  | CG-OD1  | 6.35  | 1.35        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 189 | PRO  | CA-CB   | 6.35  | 1.62        | 1.53     |
| 1   | N     | 46  | THR  | C-O     | 6.35  | 1.31        | 1.24     |
| 2   | B     | 82  | ARG  | N-CA    | 6.34  | 1.54        | 1.46     |
| 10  | J     | 42  | GLY  | CA-C    | 6.34  | 1.59        | 1.51     |
| 1   | N     | 49  | GLY  | N-CA    | 6.34  | 1.51        | 1.45     |
| 7   | G     | 51  | HIS  | ND1-CE1 | 6.33  | 1.38        | 1.32     |
| 2   | B     | 214 | VAL  | CA-CB   | 6.33  | 1.62        | 1.54     |
| 2   | B     | 59  | GLN  | CG-CD   | 6.33  | 1.67        | 1.52     |
| 4   | D     | 94  | LEU  | CA-C    | -6.33 | 1.44        | 1.52     |
| 1   | A     | 145 | LEU  | CA-C    | 6.32  | 1.60        | 1.52     |
| 9   | I     | 9   | MET  | N-CA    | 6.32  | 1.54        | 1.45     |
| 1   | N     | 153 | ALA  | N-CA    | 6.30  | 1.53        | 1.46     |
| 1   | A     | 322 | SER  | CA-CB   | 6.29  | 1.63        | 1.53     |
| 2   | B     | 115 | ASP  | CA-C    | 6.29  | 1.60        | 1.52     |
| 5   | E     | 41  | LEU  | N-CA    | 6.27  | 1.54        | 1.46     |
| 1   | A     | 8   | PHE  | N-CA    | 6.26  | 1.53        | 1.46     |
| 3   | P     | 104 | SER  | CB-OG   | 6.26  | 1.54        | 1.42     |
| 2   | O     | 151 | ARG  | CA-C    | 6.26  | 1.60        | 1.52     |
| 1   | A     | 296 | GLY  | N-CA    | 6.26  | 1.54        | 1.45     |
| 3   | P     | 125 | ASN  | CA-C    | 6.25  | 1.59        | 1.52     |
| 9   | V     | 65  | LYS  | N-CA    | 6.25  | 1.54        | 1.46     |
| 7   | G     | 60  | PHE  | C-O     | 6.25  | 1.31        | 1.23     |
| 3   | P     | 58  | TRP  | C-O     | 6.23  | 1.31        | 1.24     |
| 4   | D     | 47  | SER  | CA-CB   | 6.23  | 1.63        | 1.53     |
| 1   | N     | 81  | TRP  | N-CA    | 6.23  | 1.53        | 1.46     |
| 1   | N     | 485 | VAL  | CA-CB   | 6.23  | 1.65        | 1.54     |
| 6   | F     | 47  | ASN  | N-CA    | 6.22  | 1.53        | 1.46     |
| 6   | F     | 56  | ARG  | N-CA    | 6.22  | 1.53        | 1.45     |
| 1   | A     | 315 | PRO  | C-N     | 6.22  | 1.42        | 1.33     |
| 8   | U     | 42  | ALA  | N-CA    | 6.22  | 1.53        | 1.46     |
| 3   | C     | 123 | PRO  | C-O     | 6.21  | 1.31        | 1.23     |
| 1   | A     | 238 | PHE  | CA-CB   | 6.21  | 1.63        | 1.53     |
| 3   | P     | 113 | GLY  | N-CA    | 6.21  | 1.53        | 1.45     |
| 10  | W     | 3   | ASN  | N-CA    | 6.20  | 1.54        | 1.46     |
| 1   | N     | 13  | LYS  | CA-CB   | 6.20  | 1.63        | 1.53     |
| 5   | R     | 9   | GLU  | CA-C    | 6.20  | 1.60        | 1.52     |
| 7   | T     | 64  | ASP  | CG-OD1  | 6.20  | 1.37        | 1.25     |
| 3   | P     | 41  | THR  | CA-C    | 6.20  | 1.60        | 1.52     |
| 3   | P     | 108 | PRO  | C-O     | 6.20  | 1.30        | 1.23     |
| 2   | B     | 44  | LEU  | C-O     | 6.19  | 1.31        | 1.24     |
| 12  | L     | 32  | GLY  | N-CA    | 6.19  | 1.53        | 1.45     |
| 4   | D     | 52  | SER  | CA-C    | -6.19 | 1.44        | 1.53     |

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| Mol | Chain | Res   | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|---------|-------|-------------|----------|
| 7   | G     | 48    | ILE  | CA-CB   | -6.19 | 1.49        | 1.54     |
| 3   | P     | 122   | HIS  | N-CA    | 6.19  | 1.53        | 1.46     |
| 6   | F     | 45    | ASP  | C-O     | 6.18  | 1.30        | 1.23     |
| 9   | I     | 4     | LEU  | C-O     | 6.18  | 1.31        | 1.23     |
| 10  | J     | 55    | PHE  | CA-C    | -6.18 | 1.45        | 1.52     |
| 1   | A     | 77    | GLY  | N-CA    | 6.17  | 1.54        | 1.45     |
| 3   | P     | 141   | GLY  | N-CA    | 6.17  | 1.53        | 1.45     |
| 2   | B     | 149   | THR  | CA-C    | 6.17  | 1.61        | 1.52     |
| 6   | S     | 93    | PRO  | C-O     | 6.17  | 1.31        | 1.24     |
| 2   | B     | 204   | HIS  | CE1-NE2 | 6.17  | 1.38        | 1.32     |
| 12  | L     | 6     | GLY  | CA-C    | 6.17  | 1.60        | 1.51     |
| 1   | N     | 310   | MET  | SD-CE   | -6.16 | 1.64        | 1.79     |
| 2   | B     | 82    | ARG  | C-O     | 6.15  | 1.31        | 1.24     |
| 1   | N     | 138   | HIS  | ND1-CE1 | 6.15  | 1.38        | 1.32     |
| 1   | A     | 87    | ILE  | CA-C    | -6.15 | 1.44        | 1.52     |
| 6   | F     | 96    | LEU  | N-CA    | 6.14  | 1.54        | 1.46     |
| 1   | A     | 468   | MET  | SD-CE   | 6.14  | 1.95        | 1.79     |
| 1   | A     | 397   | PHE  | CA-CB   | 6.14  | 1.62        | 1.53     |
| 9   | I     | 37    | PHE  | CA-CB   | 6.14  | 1.63        | 1.53     |
| 6   | F     | 17    | GLU  | CA-CB   | 6.14  | 1.62        | 1.53     |
| 1   | A     | 474   | GLU  | N-CA    | 6.13  | 1.53        | 1.46     |
| 1   | N     | 5     | ARG  | CA-C    | 6.13  | 1.60        | 1.52     |
| 7   | G     | 56    | ARG  | CZ-NH1  | 6.12  | 1.41        | 1.32     |
| 2   | B     | 140   | ASN  | N-CA    | 6.12  | 1.53        | 1.46     |
| 10  | W     | 34    | VAL  | N-CA    | 6.12  | 1.53        | 1.46     |
| 4   | Q     | 141   | ASP  | N-CA    | 6.11  | 1.54        | 1.46     |
| 4   | D     | 102   | TYR  | C-O     | 6.11  | 1.31        | 1.23     |
| 6   | S     | 2     | SER  | N-CA    | 6.11  | 1.54        | 1.46     |
| 1   | N     | 253   | MET  | N-CA    | 6.10  | 1.53        | 1.46     |
| 9   | V     | 42    | LYS  | N-CA    | -6.10 | 1.39        | 1.46     |
| 6   | F     | 54[A] | ASN  | C-O     | 6.09  | 1.32        | 1.24     |
| 6   | F     | 54[B] | ASN  | C-O     | 6.09  | 1.32        | 1.24     |
| 5   | R     | 59    | ASN  | CA-C    | -6.09 | 1.45        | 1.53     |
| 1   | A     | 252   | GLY  | C-O     | 6.09  | 1.31        | 1.23     |
| 2   | B     | 14    | SER  | CA-C    | 6.09  | 1.58        | 1.52     |
| 13  | M     | 9     | PRO  | N-CA    | 6.09  | 1.54        | 1.47     |
| 2   | B     | 78    | LEU  | N-CA    | 6.08  | 1.52        | 1.46     |
| 12  | Y     | 8     | GLY  | N-CA    | 6.08  | 1.54        | 1.45     |
| 11  | K     | 38    | ILE  | CA-CB   | 6.08  | 1.60        | 1.54     |
| 1   | N     | 12    | HIS  | N-CA    | 6.07  | 1.53        | 1.46     |
| 5   | R     | 73    | ASP  | CG-OD2  | -6.07 | 1.13        | 1.25     |
| 1   | N     | 103   | TRP  | CA-CB   | 6.07  | 1.64        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | N     | 373 | VAL  | CA-CB   | -6.06 | 1.46        | 1.54     |
| 3   | P     | 82  | GLY  | CA-C    | 6.06  | 1.58        | 1.52     |
| 5   | E     | 78  | HIS  | C-O     | 6.06  | 1.30        | 1.23     |
| 3   | P     | 199 | VAL  | N-CA    | 6.05  | 1.53        | 1.46     |
| 2   | B     | 188 | ARG  | N-CA    | 6.05  | 1.51        | 1.45     |
| 4   | D     | 137 | LYS  | N-CA    | 6.05  | 1.54        | 1.46     |
| 1   | N     | 328 | HIS  | N-CA    | 6.05  | 1.53        | 1.46     |
| 3   | C     | 196 | THR  | N-CA    | 6.05  | 1.53        | 1.46     |
| 2   | B     | 65  | TRP  | CD2-CE3 | 6.04  | 1.50        | 1.40     |
| 6   | S     | 64  | GLU  | C-N     | -6.04 | 1.25        | 1.33     |
| 7   | T     | 13  | ALA  | CA-C    | -6.04 | 1.45        | 1.52     |
| 1   | N     | 64  | VAL  | N-CA    | 6.04  | 1.53        | 1.46     |
| 7   | T     | 17  | ARG  | CZ-NH1  | 6.04  | 1.41        | 1.32     |
| 12  | Y     | 10  | ASN  | CA-CB   | 6.03  | 1.61        | 1.53     |
| 3   | C     | 145 | THR  | N-CA    | 6.03  | 1.53        | 1.46     |
| 2   | B     | 86  | MET  | N-CA    | 6.02  | 1.53        | 1.46     |
| 3   | C     | 71  | HIS  | CE1-NE2 | 6.02  | 1.38        | 1.32     |
| 3   | C     | 94  | PHE  | C-O     | 6.02  | 1.31        | 1.24     |
| 5   | E     | 24  | ILE  | N-CA    | 6.02  | 1.53        | 1.46     |
| 1   | N     | 306 | THR  | C-O     | 6.02  | 1.31        | 1.24     |
| 1   | N     | 84  | PRO  | CA-CB   | 6.02  | 1.62        | 1.53     |
| 3   | P     | 71  | HIS  | ND1-CE1 | 6.02  | 1.38        | 1.32     |
| 1   | N     | 166 | THR  | CA-CB   | 6.01  | 1.62        | 1.53     |
| 4   | D     | 23  | PRO  | CA-CB   | 6.01  | 1.62        | 1.53     |
| 2   | O     | 4   | PRO  | N-CA    | 6.01  | 1.54        | 1.47     |
| 7   | G     | 68  | THR  | C-O     | 6.01  | 1.31        | 1.23     |
| 1   | A     | 371 | TYR  | CA-C    | 6.01  | 1.60        | 1.52     |
| 5   | R     | 63  | SER  | CA-C    | 6.01  | 1.60        | 1.52     |
| 6   | F     | 64  | GLU  | C-N     | -6.00 | 1.25        | 1.33     |
| 4   | D     | 8   | SER  | C-O     | -6.00 | 1.17        | 1.24     |
| 1   | N     | 463 | THR  | N-CA    | 6.00  | 1.53        | 1.46     |
| 8   | H     | 41  | LYS  | CA-C    | 6.00  | 1.60        | 1.52     |
| 8   | H     | 75  | ARG  | NE-CZ   | 5.99  | 1.39        | 1.33     |
| 3   | P     | 213 | THR  | N-CA    | 5.99  | 1.53        | 1.46     |
| 13  | Z     | 9   | PRO  | CA-CB   | 5.98  | 1.61        | 1.53     |
| 1   | A     | 248 | LEU  | N-CA    | 5.98  | 1.52        | 1.46     |
| 1   | N     | 494 | TRP  | N-CA    | 5.98  | 1.53        | 1.46     |
| 7   | T     | 77  | PRO  | N-CA    | 5.98  | 1.53        | 1.46     |
| 1   | A     | 151 | HIS  | CD2-NE2 | 5.98  | 1.44        | 1.37     |
| 2   | B     | 133 | LEU  | CB-CG   | 5.98  | 1.65        | 1.53     |
| 2   | B     | 115 | ASP  | CG-OD1  | 5.97  | 1.36        | 1.25     |
| 6   | S     | 54  | ASN  | CG-ND2  | -5.97 | 1.20        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | L     | 19  | TRP  | CA-CB   | 5.97  | 1.62        | 1.53     |
| 1   | N     | 256 | HIS  | ND1-CE1 | 5.97  | 1.38        | 1.32     |
| 9   | V     | 68  | ILE  | CA-CB   | -5.97 | 1.46        | 1.54     |
| 3   | C     | 182 | TYR  | CZ-OH   | -5.97 | 1.25        | 1.38     |
| 3   | C     | 104 | SER  | CB-OG   | 5.96  | 1.54        | 1.42     |
| 1   | N     | 421 | VAL  | CA-CB   | 5.96  | 1.62        | 1.54     |
| 12  | L     | 12  | PRO  | N-CA    | 5.96  | 1.53        | 1.47     |
| 12  | Y     | 7   | PRO  | C-O     | 5.96  | 1.30        | 1.23     |
| 3   | C     | 162 | ALA  | C-N     | 5.96  | 1.42        | 1.33     |
| 6   | F     | 92  | VAL  | CA-CB   | 5.96  | 1.61        | 1.54     |
| 1   | N     | 494 | TRP  | CA-C    | -5.96 | 1.44        | 1.52     |
| 9   | I     | 31  | PHE  | CA-C    | 5.96  | 1.60        | 1.52     |
| 1   | A     | 267 | PRO  | CA-CB   | 5.95  | 1.61        | 1.53     |
| 6   | S     | 12  | GLN  | CA-CB   | 5.95  | 1.62        | 1.54     |
| 9   | I     | 33  | THR  | N-CA    | 5.94  | 1.53        | 1.46     |
| 4   | D     | 64  | PHE  | N-CA    | -5.93 | 1.38        | 1.45     |
| 7   | T     | 3   | ALA  | N-CA    | 5.93  | 1.53        | 1.46     |
| 1   | A     | 327 | LEU  | CA-CB   | 5.93  | 1.63        | 1.53     |
| 1   | N     | 397 | PHE  | C-O     | 5.92  | 1.30        | 1.24     |
| 1   | A     | 368 | HIS  | CE1-NE2 | 5.91  | 1.38        | 1.32     |
| 1   | N     | 441 | SER  | CA-CB   | 5.91  | 1.64        | 1.53     |
| 2   | O     | 223 | SER  | N-CA    | 5.91  | 1.53        | 1.46     |
| 1   | A     | 365 | ILE  | C-O     | 5.91  | 1.31        | 1.24     |
| 13  | M     | 37  | LEU  | CB-CG   | -5.91 | 1.41        | 1.53     |
| 3   | P     | 116 | TRP  | CA-CB   | 5.91  | 1.63        | 1.53     |
| 3   | C     | 70  | HIS  | CD2-NE2 | 5.90  | 1.44        | 1.37     |
| 4   | D     | 35  | ALA  | N-CA    | -5.90 | 1.39        | 1.46     |
| 10  | J     | 14  | GLU  | N-CA    | 5.90  | 1.53        | 1.46     |
| 1   | N     | 189 | MET  | C-N     | 5.90  | 1.41        | 1.33     |
| 1   | A     | 347 | LEU  | N-CA    | 5.89  | 1.53        | 1.46     |
| 1   | N     | 181 | THR  | CB-OG1  | -5.89 | 1.34        | 1.43     |
| 9   | V     | 68  | ILE  | CB-CG1  | -5.89 | 1.41        | 1.53     |
| 6   | F     | 72  | PHE  | CA-CB   | 5.89  | 1.63        | 1.53     |
| 10  | J     | 31  | LEU  | CA-C    | 5.88  | 1.60        | 1.52     |
| 1   | N     | 54  | TYR  | N-CA    | 5.88  | 1.53        | 1.46     |
| 10  | J     | 27  | THR  | N-CA    | 5.88  | 1.53        | 1.46     |
| 1   | N     | 160 | GLY  | N-CA    | 5.87  | 1.53        | 1.45     |
| 6   | S     | 18  | ARG  | CD-NE   | 5.87  | 1.54        | 1.46     |
| 8   | U     | 49  | ASP  | CA-C    | 5.87  | 1.59        | 1.52     |
| 2   | O     | 59  | GLN  | N-CA    | 5.87  | 1.53        | 1.46     |
| 2   | B     | 66  | THR  | N-CA    | 5.87  | 1.53        | 1.46     |
| 7   | G     | 15  | THR  | CA-CB   | 5.86  | 1.62        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | C     | 20  | GLY  | CA-C    | 5.86  | 1.58        | 1.52     |
| 2   | B     | 48  | THR  | N-CA    | 5.86  | 1.53        | 1.46     |
| 1   | A     | 181 | THR  | CB-OG1  | -5.85 | 1.34        | 1.43     |
| 4   | D     | 64  | PHE  | CA-CB   | 5.85  | 1.66        | 1.54     |
| 6   | F     | 58  | VAL  | C-N     | 5.85  | 1.38        | 1.33     |
| 1   | N     | 96  | ARG  | CZ-NH1  | 5.85  | 1.41        | 1.32     |
| 1   | A     | 90  | PRO  | N-CD    | 5.84  | 1.55        | 1.47     |
| 5   | R     | 44  | GLU  | N-CA    | 5.84  | 1.53        | 1.45     |
| 5   | E     | 103 | GLU  | CA-C    | 5.84  | 1.60        | 1.52     |
| 1   | A     | 290 | HIS  | CE1-NE2 | 5.83  | 1.38        | 1.32     |
| 2   | B     | 79  | PRO  | N-CA    | 5.83  | 1.55        | 1.47     |
| 10  | J     | 45  | TYR  | N-CA    | 5.83  | 1.53        | 1.46     |
| 12  | L     | 25  | MET  | C-O     | 5.82  | 1.31        | 1.24     |
| 6   | S     | 1   | ALA  | C-N     | 5.82  | 1.41        | 1.33     |
| 6   | S     | 43  | LYS  | CG-CD   | 5.82  | 1.70        | 1.52     |
| 9   | I     | 6   | LYS  | CA-C    | -5.82 | 1.45        | 1.52     |
| 12  | Y     | 44  | LEU  | C-O     | 5.82  | 1.31        | 1.24     |
| 1   | A     | 154 | GLY  | N-CA    | 5.82  | 1.53        | 1.45     |
| 8   | U     | 52  | VAL  | CA-CB   | 5.82  | 1.62        | 1.54     |
| 2   | B     | 101 | GLY  | CA-C    | 5.82  | 1.59        | 1.52     |
| 7   | T     | 22  | GLY  | N-CA    | 5.81  | 1.53        | 1.45     |
| 5   | R     | 9   | GLU  | CA-CB   | 5.81  | 1.62        | 1.53     |
| 1   | A     | 395 | HIS  | CG-ND1  | 5.80  | 1.44        | 1.38     |
| 9   | I     | 71  | SER  | N-CA    | 5.80  | 1.53        | 1.46     |
| 4   | Q     | 5   | VAL  | CA-C    | 5.80  | 1.60        | 1.52     |
| 2   | O     | 198 | GLU  | C-O     | 5.80  | 1.30        | 1.23     |
| 3   | P     | 59  | ARG  | CZ-NH1  | 5.80  | 1.40        | 1.32     |
| 1   | A     | 368 | HIS  | ND1-CE1 | 5.80  | 1.38        | 1.32     |
| 3   | C     | 108 | PRO  | N-CA    | 5.80  | 1.54        | 1.47     |
| 1   | N     | 28  | MET  | N-CA    | 5.80  | 1.53        | 1.46     |
| 2   | O     | 38  | VAL  | CA-CB   | 5.80  | 1.61        | 1.54     |
| 3   | P     | 211 | GLY  | N-CA    | 5.80  | 1.52        | 1.45     |
| 7   | T     | 14  | ARG  | CZ-NH1  | 5.80  | 1.40        | 1.32     |
| 10  | W     | 33  | ARG  | N-CA    | 5.79  | 1.53        | 1.46     |
| 13  | Z     | 13  | LYS  | CA-C    | 5.79  | 1.60        | 1.52     |
| 1   | N     | 238 | PHE  | CA-CB   | 5.78  | 1.62        | 1.53     |
| 2   | O     | 175 | ILE  | CA-CB   | 5.78  | 1.58        | 1.54     |
| 2   | B     | 211 | LEU  | N-CA    | 5.78  | 1.53        | 1.46     |
| 1   | A     | 213 | ARG  | CZ-NH2  | 5.78  | 1.41        | 1.33     |
| 1   | N     | 420 | GLY  | N-CA    | 5.77  | 1.53        | 1.45     |
| 7   | G     | 36  | TRP  | CA-C    | -5.77 | 1.46        | 1.53     |
| 1   | N     | 149 | SER  | CA-C    | 5.76  | 1.60        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | Q     | 25  | PRO  | C-O     | 5.76  | 1.30        | 1.23     |
| 2   | B     | 68  | LEU  | N-CA    | 5.76  | 1.54        | 1.46     |
| 3   | C     | 172 | TYR  | CG-CD1  | 5.76  | 1.51        | 1.39     |
| 7   | G     | 26  | PRO  | C-O     | 5.76  | 1.31        | 1.24     |
| 6   | S     | 72  | PHE  | N-CA    | 5.75  | 1.53        | 1.46     |
| 3   | C     | 243 | HIS  | ND1-CE1 | 5.75  | 1.38        | 1.32     |
| 1   | N     | 71  | MET  | CG-SD   | 5.75  | 1.95        | 1.80     |
| 1   | A     | 496 | ASN  | CA-CB   | 5.75  | 1.62        | 1.53     |
| 1   | N     | 242 | GLU  | CD-OE1  | 5.74  | 1.36        | 1.25     |
| 1   | A     | 484 | THR  | CB-OG1  | -5.74 | 1.34        | 1.43     |
| 1   | N     | 183 | LEU  | CA-C    | 5.74  | 1.60        | 1.52     |
| 8   | H     | 40  | GLU  | CD-OE2  | 5.74  | 1.36        | 1.25     |
| 4   | Q     | 144 | GLU  | CA-C    | 5.73  | 1.59        | 1.52     |
| 3   | C     | 35  | PHE  | N-CA    | 5.73  | 1.53        | 1.46     |
| 5   | E     | 39  | TYR  | CG-CD2  | -5.73 | 1.27        | 1.39     |
| 11  | K     | 53  | TRP  | CA-CB   | 5.73  | 1.63        | 1.54     |
| 3   | P     | 70  | HIS  | C-N     | 5.72  | 1.41        | 1.33     |
| 7   | T     | 25  | LEU  | N-CA    | 5.72  | 1.54        | 1.46     |
| 1   | A     | 412 | ILE  | N-CA    | 5.72  | 1.53        | 1.46     |
| 3   | C     | 260 | GLY  | N-CA    | 5.72  | 1.52        | 1.45     |
| 4   | D     | 25  | PRO  | N-CA    | 5.72  | 1.54        | 1.47     |
| 10  | J     | 33  | ARG  | CA-C    | -5.72 | 1.45        | 1.52     |
| 7   | T     | 7   | ASP  | N-CA    | 5.72  | 1.53        | 1.46     |
| 2   | B     | 21  | LEU  | CA-C    | 5.72  | 1.60        | 1.52     |
| 3   | C     | 52  | LEU  | CB-CG   | 5.72  | 1.64        | 1.53     |
| 1   | N     | 100 | MET  | SD-CE   | -5.72 | 1.65        | 1.79     |
| 1   | A     | 498 | CYS  | CA-C    | -5.71 | 1.46        | 1.52     |
| 7   | G     | 12  | GLY  | CA-C    | 5.71  | 1.62        | 1.52     |
| 4   | Q     | 27  | VAL  | CA-CB   | 5.71  | 1.63        | 1.54     |
| 4   | Q     | 81  | VAL  | C-O     | 5.71  | 1.30        | 1.24     |
| 2   | B     | 74  | ILE  | N-CA    | 5.70  | 1.53        | 1.46     |
| 12  | Y     | 27  | LEU  | N-CA    | 5.70  | 1.53        | 1.46     |
| 1   | A     | 253 | MET  | N-CA    | 5.69  | 1.53        | 1.46     |
| 3   | C     | 6   | HIS  | CA-CB   | 5.69  | 1.62        | 1.53     |
| 9   | I     | 29  | LEU  | N-CA    | 5.69  | 1.53        | 1.46     |
| 7   | G     | 67  | HIS  | CA-C    | 5.68  | 1.59        | 1.52     |
| 1   | A     | 88  | GLY  | N-CA    | 5.68  | 1.53        | 1.45     |
| 2   | O     | 111 | THR  | C-O     | 5.68  | 1.31        | 1.24     |
| 9   | I     | 64  | ARG  | CA-CB   | 5.68  | 1.62        | 1.53     |
| 4   | D     | 18  | ASP  | N-CA    | 5.68  | 1.54        | 1.46     |
| 2   | O     | 59  | GLN  | C-O     | 5.68  | 1.30        | 1.24     |
| 12  | Y     | 21  | LEU  | C-O     | 5.68  | 1.30        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | O     | 68  | LEU  | N-CA   | 5.67  | 1.54        | 1.46     |
| 2   | B     | 55  | THR  | CB-CG2 | 5.67  | 1.71        | 1.52     |
| 12  | L     | 44  | LEU  | N-CA   | 5.67  | 1.53        | 1.46     |
| 3   | P     | 99  | TRP  | N-CA   | 5.67  | 1.53        | 1.46     |
| 3   | C     | 206 | LEU  | C-O    | 5.67  | 1.30        | 1.24     |
| 6   | F     | 62  | CYS  | C-O    | 5.67  | 1.30        | 1.24     |
| 1   | A     | 142 | SER  | N-CA   | 5.66  | 1.53        | 1.46     |
| 2   | B     | 164 | ALA  | N-CA   | 5.66  | 1.53        | 1.46     |
| 3   | C     | 166 | THR  | C-N    | 5.66  | 1.41        | 1.33     |
| 5   | E     | 89  | LEU  | CA-CB  | 5.66  | 1.63        | 1.53     |
| 12  | Y     | 20  | ARG  | NE-CZ  | 5.66  | 1.39        | 1.33     |
| 5   | E     | 8   | ASP  | C-O    | 5.66  | 1.30        | 1.24     |
| 2   | O     | 133 | LEU  | CA-C   | 5.66  | 1.59        | 1.52     |
| 5   | R     | 91  | PRO  | CA-C   | 5.66  | 1.60        | 1.52     |
| 12  | L     | 5   | GLU  | CD-OE2 | -5.65 | 1.14        | 1.25     |
| 4   | Q     | 77  | GLU  | N-CA   | 5.65  | 1.53        | 1.46     |
| 1   | A     | 76  | GLY  | N-CA   | 5.65  | 1.53        | 1.45     |
| 2   | B     | 89  | GLU  | CA-C   | 5.65  | 1.60        | 1.52     |
| 3   | P     | 237 | ALA  | C-N    | 5.65  | 1.41        | 1.34     |
| 7   | T     | 59  | PRO  | N-CA   | 5.65  | 1.53        | 1.47     |
| 8   | H     | 38  | ARG  | C-O    | 5.64  | 1.30        | 1.24     |
| 4   | D     | 141 | ASP  | CA-C   | -5.64 | 1.45        | 1.52     |
| 9   | I     | 59  | ASP  | C-O    | 5.64  | 1.30        | 1.24     |
| 1   | A     | 84  | PRO  | CA-CB  | 5.64  | 1.62        | 1.53     |
| 3   | C     | 141 | GLY  | N-CA   | 5.63  | 1.52        | 1.45     |
| 2   | O     | 109 | GLU  | N-CA   | 5.63  | 1.53        | 1.46     |
| 8   | U     | 53  | CYS  | C-O    | 5.63  | 1.31        | 1.23     |
| 2   | O     | 68  | LEU  | CA-C   | 5.62  | 1.59        | 1.52     |
| 2   | O     | 160 | LEU  | N-CA   | 5.62  | 1.52        | 1.46     |
| 8   | U     | 60  | TYR  | C-O    | 5.62  | 1.30        | 1.24     |
| 1   | N     | 273 | MET  | C-O    | -5.61 | 1.17        | 1.24     |
| 12  | L     | 17  | ASN  | CG-ND2 | 5.61  | 1.45        | 1.33     |
| 4   | D     | 37  | GLN  | CD-OE1 | 5.61  | 1.34        | 1.23     |
| 2   | O     | 90  | ILE  | CA-C   | 5.61  | 1.59        | 1.52     |
| 4   | Q     | 24  | LEU  | CB-CG  | 5.60  | 1.64        | 1.53     |
| 1   | A     | 335 | SER  | N-CA   | 5.60  | 1.53        | 1.45     |
| 6   | S     | 81  | ARG  | NE-CZ  | 5.60  | 1.39        | 1.33     |
| 3   | P     | 143 | SER  | CA-CB  | 5.59  | 1.62        | 1.53     |
| 9   | I     | 4   | LEU  | CA-C   | -5.59 | 1.45        | 1.52     |
| 1   | A     | 71  | MET  | CG-SD  | 5.58  | 1.94        | 1.80     |
| 8   | H     | 40  | GLU  | N-CA   | -5.58 | 1.39        | 1.46     |
| 1   | N     | 355 | GLY  | N-CA   | 5.58  | 1.53        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | T     | 16  | TRP  | CA-C    | 5.58  | 1.60        | 1.52     |
| 10  | J     | 53  | ALA  | N-CA    | 5.57  | 1.53        | 1.46     |
| 2   | B     | 67  | ILE  | CA-C    | 5.57  | 1.60        | 1.52     |
| 1   | N     | 187 | SER  | CA-CB   | 5.57  | 1.62        | 1.53     |
| 6   | S     | 26  | LYS  | CA-C    | 5.57  | 1.60        | 1.52     |
| 3   | C     | 143 | SER  | CA-CB   | 5.56  | 1.62        | 1.53     |
| 3   | C     | 176 | LEU  | CA-CB   | 5.56  | 1.61        | 1.53     |
| 1   | A     | 483 | LEU  | CA-C    | 5.56  | 1.55        | 1.52     |
| 8   | H     | 24  | ASN  | N-CA    | -5.55 | 1.39        | 1.46     |
| 4   | Q     | 27  | VAL  | CA-C    | -5.55 | 1.46        | 1.52     |
| 13  | M     | 30  | ALA  | N-CA    | 5.55  | 1.53        | 1.46     |
| 5   | R     | 40  | ASP  | C-O     | 5.55  | 1.29        | 1.23     |
| 9   | V     | 44  | LYS  | CA-C    | 5.55  | 1.59        | 1.52     |
| 2   | B     | 59  | GLN  | N-CA    | 5.55  | 1.53        | 1.46     |
| 1   | A     | 378 | HIS  | ND1-CE1 | 5.54  | 1.38        | 1.32     |
| 1   | N     | 367 | LEU  | CA-C    | 5.54  | 1.59        | 1.52     |
| 12  | Y     | 17  | ASN  | CA-CB   | 5.54  | 1.62        | 1.53     |
| 4   | D     | 63  | LYS  | C-O     | 5.54  | 1.30        | 1.24     |
| 4   | D     | 74  | SER  | N-CA    | 5.54  | 1.52        | 1.45     |
| 3   | P     | 198 | PHE  | CA-CB   | 5.54  | 1.62        | 1.53     |
| 4   | D     | 36  | SER  | C-O     | 5.53  | 1.31        | 1.24     |
| 3   | P     | 71  | HIS  | CE1-NE2 | 5.53  | 1.38        | 1.32     |
| 1   | N     | 189 | MET  | CG-SD   | -5.53 | 1.67        | 1.80     |
| 1   | A     | 23  | GLY  | N-CA    | 5.53  | 1.52        | 1.45     |
| 1   | A     | 71  | MET  | SD-CE   | -5.52 | 1.65        | 1.79     |
| 3   | C     | 87  | ILE  | N-CA    | 5.52  | 1.53        | 1.46     |
| 2   | B     | 147 | GLU  | N-CA    | 5.52  | 1.54        | 1.46     |
| 13  | M     | 31  | GLY  | N-CA    | 5.52  | 1.52        | 1.45     |
| 1   | N     | 319 | LYS  | CA-CB   | 5.52  | 1.62        | 1.53     |
| 11  | K     | 27  | ALA  | N-CA    | 5.52  | 1.53        | 1.46     |
| 1   | A     | 314 | ILE  | N-CA    | 5.51  | 1.53        | 1.46     |
| 3   | C     | 149 | HIS  | CD2-NE2 | 5.51  | 1.44        | 1.37     |
| 2   | O     | 78  | LEU  | CA-C    | 5.51  | 1.58        | 1.52     |
| 2   | O     | 189 | PRO  | CA-CB   | 5.51  | 1.61        | 1.53     |
| 3   | P     | 253 | TYR  | CA-CB   | 5.51  | 1.62        | 1.53     |
| 7   | G     | 55  | ILE  | CA-C    | -5.51 | 1.46        | 1.52     |
| 3   | P     | 176 | LEU  | C-O     | 5.51  | 1.30        | 1.24     |
| 12  | Y     | 30  | GLY  | C-O     | 5.51  | 1.30        | 1.23     |
| 2   | B     | 69  | PRO  | CA-CB   | 5.50  | 1.61        | 1.53     |
| 8   | H     | 29  | CYS  | CA-CB   | 5.50  | 1.61        | 1.53     |
| 1   | N     | 233 | HIS  | N-CA    | 5.50  | 1.53        | 1.46     |
| 3   | P     | 159 | MET  | CA-CB   | 5.50  | 1.61        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8   | U     | 40  | GLU  | CD-OE2  | 5.50  | 1.35        | 1.25     |
| 12  | Y     | 4   | GLU  | CD-OE1  | 5.50  | 1.35        | 1.25     |
| 1   | A     | 163 | ASN  | CG-ND2  | 5.50  | 1.44        | 1.33     |
| 1   | N     | 96  | ARG  | CA-CB   | 5.50  | 1.62        | 1.53     |
| 1   | N     | 283 | LEU  | CA-C    | 5.50  | 1.60        | 1.52     |
| 13  | Z     | 32  | TRP  | N-CA    | 5.50  | 1.52        | 1.46     |
| 6   | F     | 64  | GLU  | N-CA    | -5.50 | 1.39        | 1.46     |
| 1   | N     | 229 | ILE  | N-CA    | 5.49  | 1.53        | 1.46     |
| 1   | A     | 165 | ILE  | CA-CB   | 5.49  | 1.61        | 1.54     |
| 7   | G     | 2   | SER  | N-CA    | 5.49  | 1.53        | 1.46     |
| 9   | I     | 40  | ALA  | C-O     | 5.49  | 1.30        | 1.24     |
| 13  | Z     | 24  | LEU  | N-CA    | 5.49  | 1.53        | 1.46     |
| 4   | D     | 61  | ARG  | C-O     | 5.49  | 1.31        | 1.24     |
| 1   | N     | 239 | GLY  | N-CA    | 5.49  | 1.52        | 1.45     |
| 7   | G     | 73  | PRO  | C-O     | 5.48  | 1.31        | 1.24     |
| 3   | C     | 39  | SER  | C-O     | 5.48  | 1.30        | 1.23     |
| 3   | C     | 90  | GLU  | CD-OE1  | 5.48  | 1.35        | 1.25     |
| 2   | B     | 145 | PRO  | CA-CB   | 5.48  | 1.60        | 1.53     |
| 1   | A     | 328 | HIS  | N-CA    | 5.48  | 1.53        | 1.46     |
| 12  | L     | 43  | GLN  | N-CA    | 5.48  | 1.53        | 1.46     |
| 2   | B     | 167 | SER  | CA-CB   | -5.47 | 1.44        | 1.53     |
| 1   | N     | 290 | HIS  | CE1-NE2 | 5.47  | 1.38        | 1.32     |
| 5   | R     | 52  | LEU  | CA-CB   | 5.47  | 1.61        | 1.53     |
| 6   | S     | 96  | LEU  | N-CA    | 5.47  | 1.53        | 1.46     |
| 8   | H     | 50  | VAL  | N-CA    | 5.47  | 1.53        | 1.46     |
| 9   | I     | 28  | SER  | N-CA    | 5.47  | 1.52        | 1.46     |
| 1   | A     | 379 | TYR  | N-CA    | 5.47  | 1.52        | 1.46     |
| 3   | C     | 186 | PHE  | N-CA    | 5.47  | 1.52        | 1.45     |
| 7   | T     | 8   | HIS  | CA-C    | 5.47  | 1.60        | 1.52     |
| 1   | N     | 92  | MET  | CB-CG   | 5.46  | 1.68        | 1.52     |
| 3   | C     | 9   | HIS  | CE1-NE2 | 5.46  | 1.38        | 1.32     |
| 13  | M     | 37  | LEU  | CA-C    | -5.46 | 1.45        | 1.52     |
| 5   | R     | 71  | VAL  | CA-C    | 5.46  | 1.59        | 1.52     |
| 1   | A     | 344 | PHE  | CA-CB   | 5.46  | 1.61        | 1.53     |
| 1   | A     | 418 | PHE  | CA-CB   | 5.46  | 1.61        | 1.53     |
| 9   | V     | 8   | GLN  | CD-OE1  | 5.45  | 1.33        | 1.23     |
| 3   | C     | 244 | PHE  | CD1-CE1 | 5.45  | 1.55        | 1.38     |
| 3   | C     | 122 | HIS  | C-O     | 5.44  | 1.30        | 1.24     |
| 2   | O     | 39  | LEU  | C-O     | 5.44  | 1.30        | 1.24     |
| 2   | B     | 193 | TYR  | N-CA    | 5.44  | 1.52        | 1.45     |
| 4   | Q     | 69  | ALA  | N-CA    | 5.44  | 1.52        | 1.46     |
| 8   | U     | 9   | LYS  | N-CA    | 5.44  | 1.53        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | L     | 29  | PHE  | CD2-CE2 | -5.43 | 1.22        | 1.38     |
| 2   | O     | 73  | LEU  | N-CA    | 5.43  | 1.52        | 1.46     |
| 5   | E     | 18  | TYR  | N-CA    | 5.43  | 1.52        | 1.46     |
| 12  | Y     | 20  | ARG  | CZ-NH1  | 5.43  | 1.40        | 1.32     |
| 1   | A     | 327 | LEU  | N-CA    | 5.43  | 1.53        | 1.46     |
| 12  | L     | 2   | HIS  | CA-C    | 5.43  | 1.64        | 1.52     |
| 1   | N     | 215 | LEU  | CA-CB   | 5.43  | 1.60        | 1.53     |
| 1   | A     | 318 | VAL  | C-N     | 5.43  | 1.41        | 1.33     |
| 3   | P     | 230 | ASN  | CB-CG   | -5.43 | 1.38        | 1.52     |
| 1   | N     | 17  | THR  | CA-C    | 5.42  | 1.59        | 1.52     |
| 2   | B     | 143 | VAL  | N-CA    | 5.42  | 1.52        | 1.46     |
| 1   | N     | 176 | MET  | CA-CB   | 5.42  | 1.60        | 1.53     |
| 9   | I     | 28  | SER  | CB-OG   | 5.42  | 1.52        | 1.42     |
| 5   | E     | 62  | ALA  | CA-CB   | 5.42  | 1.61        | 1.53     |
| 5   | E     | 73  | ASP  | CA-CB   | 5.42  | 1.61        | 1.53     |
| 2   | B     | 68  | LEU  | CA-C    | 5.42  | 1.59        | 1.52     |
| 3   | C     | 12  | ASN  | N-CA    | 5.42  | 1.53        | 1.45     |
| 11  | K     | 54  | ARG  | CZ-NH2  | 5.42  | 1.40        | 1.33     |
| 7   | G     | 78  | LEU  | CA-C    | 5.41  | 1.59        | 1.52     |
| 1   | N     | 163 | ASN  | CG-ND2  | 5.41  | 1.44        | 1.33     |
| 3   | P     | 206 | LEU  | C-O     | 5.41  | 1.30        | 1.24     |
| 1   | N     | 480 | ARG  | CD-NE   | 5.41  | 1.53        | 1.46     |
| 2   | B     | 65  | TRP  | CZ2-CH2 | 5.41  | 1.47        | 1.37     |
| 2   | O     | 103 | GLN  | CA-CB   | -5.41 | 1.46        | 1.53     |
| 2   | B     | 209 | ILE  | N-CA    | 5.40  | 1.52        | 1.46     |
| 5   | E     | 53  | ARG  | CA-CB   | 5.40  | 1.62        | 1.53     |
| 2   | B     | 118 | PHE  | CA-C    | -5.40 | 1.46        | 1.52     |
| 6   | F     | 43  | LYS  | N-CA    | -5.40 | 1.39        | 1.46     |
| 12  | Y     | 40  | VAL  | CA-CB   | 5.40  | 1.61        | 1.54     |
| 1   | N     | 100 | MET  | CA-C    | 5.40  | 1.60        | 1.52     |
| 8   | H     | 80  | THR  | N-CA    | 5.39  | 1.52        | 1.46     |
| 6   | S     | 43  | LYS  | CB-CG   | 5.39  | 1.68        | 1.52     |
| 10  | W     | 1   | PHE  | N-CA    | 5.39  | 1.56        | 1.46     |
| 1   | A     | 507 | GLU  | CA-C    | 5.39  | 1.59        | 1.52     |
| 2   | B     | 155 | SER  | CA-C    | 5.39  | 1.59        | 1.52     |
| 3   | P     | 232 | HIS  | N-CA    | 5.39  | 1.53        | 1.46     |
| 1   | A     | 378 | HIS  | CE1-NE2 | 5.38  | 1.38        | 1.32     |
| 1   | A     | 477 | ALA  | C-O     | 5.38  | 1.30        | 1.24     |
| 5   | R     | 30  | ARG  | CA-CB   | 5.38  | 1.61        | 1.53     |
| 13  | Z     | 2   | THR  | CA-C    | -5.38 | 1.46        | 1.52     |
| 12  | L     | 27  | LEU  | N-CA    | 5.38  | 1.52        | 1.46     |
| 1   | A     | 66  | ILE  | CA-CB   | 5.38  | 1.61        | 1.54     |

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| Mol | Chain | Res   | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|---------|-------|-------------|----------|
| 1   | A     | 381   | LEU  | C-O     | 5.38  | 1.30        | 1.23     |
| 3   | C     | 165   | ILE  | C-N     | 5.38  | 1.40        | 1.33     |
| 6   | S     | 20    | VAL  | N-CA    | 5.38  | 1.52        | 1.46     |
| 8   | U     | 61    | LYS  | C-O     | 5.38  | 1.30        | 1.24     |
| 1   | A     | 307   | SER  | N-CA    | 5.37  | 1.52        | 1.46     |
| 3   | C     | 33[A] | MET  | N-CA    | 5.37  | 1.52        | 1.46     |
| 3   | C     | 33[B] | MET  | N-CA    | 5.37  | 1.52        | 1.46     |
| 9   | I     | 33    | THR  | CA-C    | -5.37 | 1.45        | 1.52     |
| 2   | O     | 154   | VAL  | C-O     | 5.37  | 1.29        | 1.24     |
| 4   | Q     | 56    | LYS  | N-CA    | 5.37  | 1.52        | 1.46     |
| 1   | N     | 12    | HIS  | CD2-NE2 | 5.37  | 1.43        | 1.37     |
| 1   | N     | 59    | THR  | C-O     | 5.37  | 1.30        | 1.24     |
| 1   | N     | 72    | PRO  | CA-CB   | 5.37  | 1.61        | 1.53     |
| 8   | U     | 73    | ASP  | N-CA    | 5.37  | 1.52        | 1.46     |
| 2   | B     | 114   | GLU  | CA-C    | 5.37  | 1.59        | 1.52     |
| 5   | E     | 90    | ARG  | CA-C    | 5.37  | 1.59        | 1.52     |
| 6   | F     | 18    | ARG  | CZ-NH1  | 5.37  | 1.40        | 1.32     |
| 5   | E     | 73    | ASP  | CB-CG   | 5.36  | 1.65        | 1.52     |
| 6   | S     | 81    | ARG  | CA-C    | -5.36 | 1.46        | 1.52     |
| 7   | T     | 21    | PHE  | CG-CD1  | -5.36 | 1.27        | 1.38     |
| 2   | B     | 199   | ILE  | CA-CB   | 5.36  | 1.60        | 1.54     |
| 3   | C     | 63    | ARG  | N-CA    | 5.36  | 1.52        | 1.46     |
| 3   | C     | 255   | SER  | CA-CB   | 5.36  | 1.62        | 1.53     |
| 5   | E     | 64    | ALA  | N-CA    | 5.36  | 1.52        | 1.46     |
| 2   | O     | 66    | THR  | CA-C    | 5.36  | 1.58        | 1.52     |
| 1   | N     | 92    | MET  | N-CA    | 5.35  | 1.52        | 1.45     |
| 5   | R     | 46    | LYS  | N-CA    | 5.35  | 1.52        | 1.46     |
| 9   | V     | 70    | GLN  | CD-NE2  | 5.35  | 1.44        | 1.33     |
| 7   | G     | 56    | ARG  | CA-CB   | 5.35  | 1.60        | 1.52     |
| 3   | C     | 215   | LEU  | CA-CB   | 5.35  | 1.61        | 1.53     |
| 9   | I     | 67    | GLY  | N-CA    | 5.35  | 1.53        | 1.45     |
| 9   | V     | 10    | ARG  | CZ-NH1  | 5.35  | 1.40        | 1.32     |
| 2   | B     | 132   | GLU  | CD-OE2  | 5.34  | 1.35        | 1.25     |
| 6   | F     | 37    | LYS  | CA-C    | 5.34  | 1.59        | 1.52     |
| 11  | K     | 47    | ARG  | CG-CD   | 5.34  | 1.68        | 1.52     |
| 3   | P     | 240   | TRP  | C-O     | 5.34  | 1.30        | 1.24     |
| 7   | G     | 67    | HIS  | ND1-CE1 | 5.33  | 1.37        | 1.32     |
| 1   | N     | 164   | PHE  | C-N     | 5.33  | 1.40        | 1.33     |
| 7   | T     | 59    | PRO  | C-O     | 5.33  | 1.29        | 1.23     |
| 7   | G     | 44    | ARG  | CA-CB   | -5.33 | 1.45        | 1.53     |
| 12  | Y     | 17    | ASN  | N-CA    | 5.33  | 1.52        | 1.46     |
| 1   | A     | 216   | ASN  | CA-CB   | 5.33  | 1.61        | 1.53     |

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| Mol | Chain | Res    | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|-------|-------------|----------|
| 1   | A     | 320    | VAL  | C-O    | 5.33  | 1.30        | 1.24     |
| 6   | F     | 93     | PRO  | C-O    | 5.33  | 1.29        | 1.23     |
| 4   | D     | 16     | TYR  | N-CA   | 5.32  | 1.52        | 1.46     |
| 6   | F     | 48     | LEU  | CA-CB  | 5.32  | 1.60        | 1.53     |
| 13  | Z     | 37     | LEU  | CA-C   | -5.32 | 1.45        | 1.52     |
| 7   | T     | 83     | GLU  | N-CA   | 5.32  | 1.52        | 1.46     |
| 3   | C     | 76     | GLN  | CB-CG  | -5.32 | 1.36        | 1.52     |
| 3   | C     | 32     | THR  | CA-C   | 5.31  | 1.59        | 1.52     |
| 8   | U     | 79     | GLY  | N-CA   | 5.31  | 1.52        | 1.45     |
| 2   | B     | 170    | LEU  | CA-CB  | 5.31  | 1.61        | 1.53     |
| 1   | N     | 438    | ARG  | NE-CZ  | 5.31  | 1.38        | 1.33     |
| 6   | F     | 18     | ARG  | CD-NE  | 5.31  | 1.53        | 1.46     |
| 1   | A     | 39     | ALA  | N-CA   | 5.30  | 1.52        | 1.46     |
| 1   | A     | 211    | THR  | C-O    | 5.30  | 1.30        | 1.24     |
| 9   | I     | 33     | THR  | CA-CB  | 5.30  | 1.61        | 1.53     |
| 2   | O     | 163    | TRP  | CA-CB  | 5.30  | 1.60        | 1.53     |
| 2   | B     | 68     | LEU  | CB-CG  | 5.29  | 1.64        | 1.53     |
| 3   | C     | 230    | ASN  | CA-CB  | -5.29 | 1.46        | 1.54     |
| 3   | P     | 145    | THR  | C-O    | 5.29  | 1.30        | 1.24     |
| 5   | R     | 29     | LEU  | N-CA   | 5.29  | 1.52        | 1.46     |
| 5   | R     | 84     | TYR  | CG-CD1 | 5.29  | 1.50        | 1.39     |
| 2   | O     | 140    | ASN  | C-O    | 5.29  | 1.29        | 1.24     |
| 1   | A     | 298[A] | ASP  | CA-C   | 5.29  | 1.59        | 1.52     |
| 1   | A     | 298[B] | ASP  | CA-C   | 5.29  | 1.59        | 1.52     |
| 1   | N     | 454    | SER  | CA-CB  | 5.29  | 1.61        | 1.53     |
| 3   | P     | 38     | ASN  | CA-C   | 5.29  | 1.59        | 1.53     |
| 5   | R     | 50     | ALA  | CA-CB  | 5.29  | 1.61        | 1.53     |
| 4   | D     | 48     | TRP  | C-N    | 5.29  | 1.41        | 1.33     |
| 7   | G     | 59     | PRO  | CA-CB  | 5.28  | 1.61        | 1.53     |
| 12  | L     | 26     | THR  | N-CA   | 5.28  | 1.52        | 1.46     |
| 2   | B     | 78     | LEU  | CA-C   | 5.28  | 1.58        | 1.52     |
| 1   | N     | 253    | MET  | SD-CE  | -5.28 | 1.66        | 1.79     |
| 4   | Q     | 97     | ILE  | C-O    | 5.28  | 1.30        | 1.24     |
| 9   | I     | 64     | ARG  | NE-CZ  | 5.28  | 1.38        | 1.33     |
| 7   | T     | 15     | THR  | CA-CB  | 5.27  | 1.61        | 1.53     |
| 3   | P     | 172    | TYR  | CG-CD1 | 5.27  | 1.50        | 1.39     |
| 2   | B     | 65     | TRP  | C-O    | -5.27 | 1.17        | 1.24     |
| 4   | D     | 39     | ALA  | CA-C   | 5.27  | 1.59        | 1.52     |
| 3   | P     | 102    | TYR  | CG-CD1 | -5.27 | 1.28        | 1.39     |
| 4   | Q     | 85     | ALA  | C-O    | 5.27  | 1.30        | 1.24     |
| 2   | B     | 59     | GLN  | CD-NE2 | 5.27  | 1.44        | 1.33     |
| 2   | O     | 197    | SER  | CB-OG  | 5.27  | 1.52        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | I     | 10  | ARG  | N-CA    | 5.27  | 1.52        | 1.46     |
| 12  | Y     | 36  | PRO  | CA-C    | 5.26  | 1.60        | 1.52     |
| 9   | V     | 63  | MET  | C-O     | 5.26  | 1.30        | 1.24     |
| 1   | A     | 421 | VAL  | CA-CB   | 5.26  | 1.61        | 1.54     |
| 2   | O     | 192 | TYR  | C-O     | -5.26 | 1.18        | 1.24     |
| 2   | B     | 82  | ARG  | CZ-NH2  | 5.25  | 1.40        | 1.33     |
| 3   | C     | 52  | LEU  | CA-C    | 5.25  | 1.59        | 1.52     |
| 3   | C     | 36  | HIS  | N-CA    | 5.25  | 1.52        | 1.45     |
| 1   | A     | 326 | THR  | CA-CB   | 5.25  | 1.61        | 1.53     |
| 7   | G     | 7   | ASP  | CA-C    | 5.25  | 1.59        | 1.52     |
| 3   | P     | 236 | GLU  | N-CA    | 5.25  | 1.52        | 1.46     |
| 8   | H     | 25  | GLN  | CA-CB   | 5.25  | 1.60        | 1.53     |
| 1   | N     | 483 | LEU  | C-O     | 5.25  | 1.30        | 1.23     |
| 4   | D     | 144 | GLU  | CA-C    | 5.24  | 1.58        | 1.52     |
| 8   | H     | 26  | THR  | C-O     | 5.24  | 1.30        | 1.24     |
| 8   | U     | 52  | VAL  | CA-C    | 5.24  | 1.59        | 1.52     |
| 7   | T     | 56  | ARG  | CZ-NH1  | 5.24  | 1.40        | 1.32     |
| 1   | A     | 255 | SER  | C-O     | 5.24  | 1.30        | 1.24     |
| 3   | C     | 67  | PHE  | N-CA    | 5.24  | 1.52        | 1.46     |
| 8   | H     | 31  | GLN  | N-CA    | -5.24 | 1.40        | 1.46     |
| 1   | A     | 481 | GLU  | C-N     | 5.24  | 1.40        | 1.33     |
| 7   | T     | 5   | LYS  | N-CA    | 5.24  | 1.52        | 1.46     |
| 5   | E     | 100 | THR  | CA-C    | 5.24  | 1.59        | 1.52     |
| 1   | N     | 382 | SER  | CB-OG   | -5.24 | 1.31        | 1.42     |
| 3   | P     | 84  | ILE  | N-CA    | 5.24  | 1.52        | 1.46     |
| 3   | C     | 152 | MET  | SD-CE   | -5.24 | 1.66        | 1.79     |
| 5   | R     | 57  | ARG  | CZ-NH1  | 5.24  | 1.40        | 1.32     |
| 3   | P     | 166 | THR  | N-CA    | -5.23 | 1.40        | 1.46     |
| 6   | S     | 79  | ALA  | N-CA    | 5.23  | 1.52        | 1.46     |
| 12  | L     | 41  | ARG  | C-O     | 5.23  | 1.30        | 1.24     |
| 9   | V     | 10  | ARG  | CD-NE   | -5.23 | 1.39        | 1.46     |
| 2   | O     | 60  | GLU  | CD-OE2  | 5.23  | 1.35        | 1.25     |
| 3   | C     | 205 | GLY  | N-CA    | 5.23  | 1.52        | 1.45     |
| 2   | O     | 74  | ILE  | N-CA    | 5.23  | 1.52        | 1.46     |
| 8   | U     | 76  | ARG  | CZ-NH1  | 5.23  | 1.40        | 1.32     |
| 1   | A     | 413 | HIS  | ND1-CE1 | 5.22  | 1.37        | 1.32     |
| 13  | Z     | 8   | THR  | C-O     | 5.22  | 1.30        | 1.24     |
| 8   | U     | 65  | PRO  | CA-C    | -5.22 | 1.46        | 1.52     |
| 5   | E     | 56  | ARG  | CA-CB   | 5.22  | 1.61        | 1.53     |
| 8   | H     | 46  | LYS  | N-CA    | 5.21  | 1.52        | 1.46     |
| 1   | N     | 92  | MET  | CG-SD   | -5.21 | 1.67        | 1.80     |
| 1   | N     | 280 | ILE  | N-CA    | 5.21  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | C     | 62  | ILE  | N-CA    | 5.21  | 1.52        | 1.46     |
| 2   | B     | 223 | SER  | C-O     | 5.21  | 1.30        | 1.24     |
| 1   | N     | 391 | GLY  | N-CA    | 5.21  | 1.52        | 1.45     |
| 7   | T     | 3   | ALA  | CA-C    | 5.20  | 1.59        | 1.52     |
| 1   | A     | 469 | VAL  | CA-C    | 5.20  | 1.59        | 1.52     |
| 5   | R     | 25  | ASP  | C-O     | 5.20  | 1.30        | 1.23     |
| 1   | A     | 85  | LEU  | N-CA    | 5.20  | 1.52        | 1.46     |
| 3   | C     | 232 | HIS  | CG-CD2  | 5.19  | 1.41        | 1.35     |
| 2   | O     | 120 | SER  | CA-C    | 5.19  | 1.58        | 1.53     |
| 1   | N     | 43  | GLN  | CA-C    | 5.19  | 1.58        | 1.52     |
| 5   | E     | 57  | ARG  | CZ-NH1  | 5.19  | 1.40        | 1.32     |
| 3   | P     | 56  | GLN  | CA-C    | 5.19  | 1.59        | 1.52     |
| 1   | A     | 168 | ILE  | N-CA    | 5.18  | 1.52        | 1.46     |
| 3   | C     | 245 | VAL  | N-CA    | 5.18  | 1.52        | 1.46     |
| 2   | O     | 142 | VAL  | CA-C    | 5.18  | 1.58        | 1.53     |
| 6   | F     | 49  | VAL  | CA-C    | -5.18 | 1.48        | 1.53     |
| 2   | B     | 184 | LEU  | C-O     | 5.18  | 1.30        | 1.23     |
| 3   | C     | 142 | VAL  | C-N     | 5.18  | 1.41        | 1.34     |
| 3   | P     | 36  | HIS  | N-CA    | 5.18  | 1.52        | 1.45     |
| 11  | X     | 52  | GLU  | CD-OE1  | 5.18  | 1.35        | 1.25     |
| 9   | I     | 61  | GLU  | CD-OE1  | -5.17 | 1.15        | 1.25     |
| 1   | N     | 90  | PRO  | CA-CB   | 5.17  | 1.61        | 1.53     |
| 1   | A     | 429 | HIS  | ND1-CE1 | 5.17  | 1.37        | 1.32     |
| 3   | C     | 177 | GLN  | CB-CG   | -5.17 | 1.36        | 1.52     |
| 11  | K     | 30  | VAL  | N-CA    | 5.17  | 1.52        | 1.46     |
| 1   | N     | 480 | ARG  | NE-CZ   | 5.17  | 1.38        | 1.33     |
| 2   | O     | 139 | ASP  | N-CA    | 5.17  | 1.52        | 1.46     |
| 13  | Z     | 40  | TYR  | CE1-CZ  | 5.17  | 1.50        | 1.38     |
| 1   | A     | 54  | TYR  | N-CA    | 5.17  | 1.52        | 1.46     |
| 4   | Q     | 43  | LYS  | C-O     | 5.17  | 1.30        | 1.24     |
| 9   | I     | 22  | VAL  | C-O     | 5.16  | 1.29        | 1.24     |
| 1   | N     | 464 | ALA  | N-CA    | 5.16  | 1.52        | 1.46     |
| 5   | E     | 84  | TYR  | N-CA    | 5.16  | 1.52        | 1.46     |
| 6   | F     | 49  | VAL  | N-CA    | 5.16  | 1.50        | 1.46     |
| 10  | J     | 24  | GLY  | N-CA    | 5.16  | 1.52        | 1.45     |
| 13  | M     | 23  | PHE  | C-O     | 5.16  | 1.30        | 1.24     |
| 8   | H     | 65  | PRO  | CA-C    | -5.16 | 1.46        | 1.52     |
| 8   | H     | 31  | GLN  | CA-C    | -5.15 | 1.46        | 1.52     |
| 2   | B     | 54  | SER  | C-O     | 5.15  | 1.30        | 1.23     |
| 3   | P     | 186 | PHE  | CA-CB   | 5.15  | 1.63        | 1.53     |
| 5   | E     | 30  | ARG  | CA-CB   | 5.15  | 1.61        | 1.53     |
| 6   | F     | 79  | ALA  | CA-C    | 5.15  | 1.59        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | G     | 7   | ASP  | N-CA    | 5.15  | 1.52        | 1.46     |
| 1   | N     | 81  | TRP  | CA-CB   | 5.15  | 1.61        | 1.53     |
| 7   | G     | 65  | GLY  | N-CA    | 5.15  | 1.52        | 1.45     |
| 1   | A     | 175 | ALA  | C-O     | 5.14  | 1.30        | 1.24     |
| 8   | H     | 72  | TRP  | N-CA    | 5.14  | 1.52        | 1.46     |
| 13  | Z     | 22  | THR  | N-CA    | 5.14  | 1.52        | 1.46     |
| 1   | N     | 90  | PRO  | N-CD    | 5.14  | 1.54        | 1.47     |
| 9   | V     | 8   | GLN  | CA-C    | 5.14  | 1.59        | 1.52     |
| 2   | B     | 153 | LEU  | N-CA    | 5.14  | 1.52        | 1.46     |
| 3   | P     | 260 | GLY  | CA-C    | 5.14  | 1.58        | 1.51     |
| 4   | D     | 126 | MET  | SD-CE   | -5.13 | 1.66        | 1.79     |
| 6   | F     | 88  | HIS  | C-O     | 5.13  | 1.30        | 1.23     |
| 2   | O     | 211 | LEU  | N-CA    | 5.13  | 1.51        | 1.45     |
| 2   | O     | 151 | ARG  | N-CA    | 5.13  | 1.52        | 1.46     |
| 8   | U     | 70  | SER  | CA-C    | 5.12  | 1.59        | 1.52     |
| 1   | A     | 158 | ILE  | CA-CB   | 5.12  | 1.60        | 1.54     |
| 9   | I     | 24  | ALA  | CA-CB   | 5.12  | 1.61        | 1.53     |
| 3   | C     | 226 | HIS  | CE1-NE2 | 5.12  | 1.37        | 1.32     |
| 11  | K     | 52  | GLU  | C-O     | 5.11  | 1.30        | 1.23     |
| 1   | A     | 503 | HIS  | C-O     | 5.11  | 1.30        | 1.24     |
| 4   | Q     | 7   | LYS  | CA-C    | 5.11  | 1.58        | 1.52     |
| 5   | R     | 69  | GLU  | CA-CB   | 5.10  | 1.61        | 1.53     |
| 1   | A     | 219 | PHE  | N-CA    | 5.10  | 1.52        | 1.46     |
| 3   | C     | 16  | TRP  | CA-CB   | 5.10  | 1.61        | 1.53     |
| 3   | C     | 139 | ALA  | CA-CB   | 5.10  | 1.61        | 1.53     |
| 3   | C     | 179 | SER  | N-CA    | 5.10  | 1.52        | 1.46     |
| 1   | N     | 68  | PHE  | C-N     | 5.10  | 1.40        | 1.33     |
| 3   | P     | 62  | ILE  | N-CA    | 5.10  | 1.52        | 1.46     |
| 2   | B     | 210 | VAL  | N-CA    | 5.09  | 1.52        | 1.46     |
| 7   | G     | 17  | ARG  | N-CA    | 5.09  | 1.52        | 1.46     |
| 1   | A     | 275 | TRP  | NE1-CE2 | 5.09  | 1.43        | 1.37     |
| 3   | C     | 178 | ALA  | N-CA    | 5.09  | 1.52        | 1.46     |
| 7   | G     | 72  | ASN  | CA-CB   | 5.09  | 1.59        | 1.53     |
| 3   | P     | 32  | THR  | CA-C    | 5.09  | 1.59        | 1.52     |
| 1   | A     | 263 | GLY  | C-O     | 5.09  | 1.30        | 1.24     |
| 1   | A     | 174 | PRO  | CA-CB   | 5.08  | 1.60        | 1.53     |
| 1   | N     | 46  | THR  | CA-C    | -5.08 | 1.46        | 1.52     |
| 1   | A     | 382 | SER  | C-O     | 5.08  | 1.30        | 1.24     |
| 7   | G     | 16  | TRP  | CZ3-CH2 | 5.08  | 1.53        | 1.40     |
| 4   | D     | 136 | ALA  | N-CA    | 5.08  | 1.52        | 1.46     |
| 9   | I     | 60  | PHE  | CG-CD2  | 5.08  | 1.49        | 1.38     |
| 3   | P     | 136 | VAL  | N-CA    | 5.08  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 5   | ARG  | CZ-NH1 | 5.07  | 1.39        | 1.32     |
| 1   | A     | 40  | GLU  | CA-C   | 5.07  | 1.59        | 1.52     |
| 6   | F     | 22  | LEU  | CB-CG  | 5.06  | 1.63        | 1.53     |
| 7   | T     | 64  | ASP  | CG-OD2 | -5.06 | 1.15        | 1.25     |
| 12  | L     | 13  | PHE  | CA-C   | 5.05  | 1.58        | 1.52     |
| 13  | Z     | 14  | GLU  | CA-CB  | 5.05  | 1.61        | 1.53     |
| 2   | B     | 43  | SER  | N-CA   | -5.05 | 1.40        | 1.46     |
| 1   | A     | 15  | ILE  | N-CA   | 5.05  | 1.52        | 1.46     |
| 1   | A     | 81  | TRP  | N-CA   | 5.05  | 1.52        | 1.46     |
| 5   | R     | 33  | MET  | N-CA   | 5.05  | 1.52        | 1.46     |
| 4   | D     | 58  | GLU  | N-CA   | 5.04  | 1.52        | 1.46     |
| 9   | I     | 20  | HIS  | CA-CB  | 5.04  | 1.61        | 1.53     |
| 3   | P     | 153 | GLU  | CA-CB  | 5.04  | 1.62        | 1.53     |
| 8   | H     | 13  | THR  | C-O    | 5.04  | 1.29        | 1.23     |
| 3   | C     | 68  | GLN  | CD-OE1 | 5.04  | 1.33        | 1.23     |
| 2   | O     | 39  | LEU  | N-CA   | -5.04 | 1.40        | 1.46     |
| 2   | O     | 201 | GLY  | CA-C   | 5.04  | 1.58        | 1.51     |
| 3   | P     | 74  | ALA  | N-CA   | 5.04  | 1.52        | 1.46     |
| 6   | S     | 2   | SER  | CA-C   | 5.04  | 1.59        | 1.52     |
| 1   | N     | 42  | GLY  | C-O    | 5.04  | 1.30        | 1.23     |
| 1   | N     | 320 | VAL  | C-O    | 5.04  | 1.30        | 1.24     |
| 2   | O     | 140 | ASN  | CA-CB  | 5.04  | 1.61        | 1.53     |
| 2   | B     | 11  | ASP  | CA-CB  | 5.03  | 1.61        | 1.53     |
| 3   | C     | 147 | ALA  | C-O    | 5.03  | 1.30        | 1.24     |
| 8   | U     | 65  | PRO  | N-CA   | 5.03  | 1.53        | 1.47     |
| 1   | A     | 169 | ILE  | CA-CB  | 5.03  | 1.60        | 1.54     |
| 1   | N     | 353 | LEU  | CA-CB  | 5.03  | 1.61        | 1.53     |
| 6   | F     | 60  | CYS  | C-O    | 5.02  | 1.29        | 1.24     |
| 3   | C     | 81  | TYR  | N-CA   | 5.02  | 1.52        | 1.46     |
| 11  | K     | 46  | GLY  | N-CA   | 5.02  | 1.52        | 1.45     |
| 4   | D     | 119 | GLN  | CA-C   | 5.02  | 1.59        | 1.52     |
| 13  | Z     | 4   | LYS  | C-N    | 5.02  | 1.39        | 1.33     |
| 11  | X     | 30  | VAL  | N-CA   | 5.02  | 1.52        | 1.46     |
| 3   | C     | 166 | THR  | CA-CB  | 5.01  | 1.61        | 1.53     |
| 4   | D     | 129 | ALA  | C-N    | -5.01 | 1.28        | 1.34     |
| 3   | C     | 221 | ARG  | CZ-NH2 | 5.01  | 1.40        | 1.33     |
| 2   | B     | 171 | LYS  | C-O    | 5.01  | 1.29        | 1.23     |
| 1   | N     | 292 | MET  | CA-CB  | 5.01  | 1.62        | 1.53     |
| 1   | A     | 269 | GLY  | CA-C   | 5.01  | 1.58        | 1.51     |
| 1   | N     | 125 | GLY  | CA-C   | 5.01  | 1.57        | 1.51     |
| 1   | N     | 231 | TYR  | CA-CB  | 5.01  | 1.61        | 1.53     |
| 5   | E     | 92  | THR  | N-CA   | 5.01  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 7   | G     | 76  | ASN  | CG-OD1 | 5.01 | 1.33        | 1.23     |
| 9   | I     | 39  | VAL  | C-O    | 5.01 | 1.30        | 1.24     |
| 1   | N     | 29  | VAL  | CA-C   | 5.01 | 1.59        | 1.52     |
| 1   | N     | 139 | ALA  | CA-CB  | 5.01 | 1.61        | 1.53     |
| 1   | N     | 193 | VAL  | N-CA   | 5.01 | 1.52        | 1.46     |
| 6   | S     | 95  | GLN  | CA-C   | 5.01 | 1.59        | 1.52     |
| 1   | A     | 187 | SER  | N-CA   | 5.00 | 1.52        | 1.46     |
| 1   | N     | 30  | GLY  | N-CA   | 5.00 | 1.52        | 1.45     |
| 2   | O     | 115 | ASP  | CB-CG  | 5.00 | 1.64        | 1.52     |

All (615) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 5   | E     | 90  | ARG  | NE-CZ-NH1  | 16.55  | 138.05      | 121.50   |
| 4   | Q     | 20  | ARG  | NE-CZ-NH2  | -16.36 | 104.48      | 119.20   |
| 9   | V     | 8   | GLN  | CB-CG-CD   | -16.31 | 84.88       | 112.60   |
| 4   | Q     | 20  | ARG  | NE-CZ-NH1  | 15.27  | 136.77      | 121.50   |
| 9   | V     | 8   | GLN  | CB-CA-C    | 13.21  | 131.02      | 109.89   |
| 1   | N     | 189 | MET  | CG-SD-CE   | -12.67 | 73.03       | 100.90   |
| 5   | E     | 90  | ARG  | NE-CZ-NH2  | -12.63 | 107.83      | 119.20   |
| 6   | F     | 1   | ALA  | CA-C-N     | 11.41  | 140.91      | 122.53   |
| 6   | F     | 1   | ALA  | C-N-CA     | 11.41  | 140.91      | 122.53   |
| 9   | V     | 68  | ILE  | CB-CG1-CD1 | -11.37 | 89.91       | 113.80   |
| 6   | S     | 43  | LYS  | CB-CG-CD   | 11.34  | 137.38      | 111.30   |
| 1   | A     | 240 | HIS  | CA-CB-CG   | -11.28 | 102.53      | 113.80   |
| 11  | K     | 47  | ARG  | NE-CZ-NH1  | -11.05 | 110.45      | 121.50   |
| 9   | V     | 10  | ARG  | NE-CZ-NH2  | -10.62 | 109.64      | 119.20   |
| 1   | A     | 189 | MET  | CG-SD-CE   | -10.62 | 77.54       | 100.90   |
| 1   | N     | 240 | HIS  | CA-CB-CG   | -10.52 | 103.28      | 113.80   |
| 6   | F     | 3   | GLY  | N-CA-C     | -10.21 | 98.80       | 110.96   |
| 8   | H     | 25  | GLN  | CA-C-O     | 10.17  | 131.95      | 119.95   |
| 11  | K     | 47  | ARG  | CG-CD-NE   | 9.93   | 133.85      | 112.00   |
| 1   | N     | 513 | LEU  | CA-C-N     | -9.79  | 104.08      | 121.70   |
| 1   | N     | 513 | LEU  | C-N-CA     | -9.79  | 104.08      | 121.70   |
| 10  | J     | 27  | THR  | N-CA-C     | 9.65   | 123.01      | 111.33   |
| 1   | A     | 448 | THR  | CA-C-O     | -9.49  | 110.36      | 120.42   |
| 5   | E     | 90  | ARG  | CD-NE-CZ   | 9.48   | 137.68      | 124.40   |
| 11  | K     | 47  | ARG  | NE-CZ-NH2  | 9.45   | 127.70      | 119.20   |
| 6   | S     | 1   | ALA  | CA-C-N     | 9.41   | 137.07      | 122.11   |
| 6   | S     | 1   | ALA  | C-N-CA     | 9.41   | 137.07      | 122.11   |
| 9   | V     | 10  | ARG  | NE-CZ-NH1  | 9.34   | 130.84      | 121.50   |
| 7   | G     | 48  | ILE  | CA-C-O     | -9.12  | 115.20      | 119.94   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 5   | E     | 70     | VAL  | CA-CB-CG1  | -9.04 | 95.04       | 110.40   |
| 4   | Q     | 8      | SER  | N-CA-C     | 9.02  | 130.02      | 110.80   |
| 6   | S     | 92     | VAL  | CA-C-N     | -8.99 | 108.60      | 119.84   |
| 6   | S     | 92     | VAL  | C-N-CA     | -8.99 | 108.60      | 119.84   |
| 1   | N     | 71     | MET  | CG-SD-CE   | -8.87 | 81.38       | 100.90   |
| 4   | Q     | 6      | VAL  | CB-CA-C    | 8.79  | 124.62      | 111.26   |
| 7   | T     | 83     | GLU  | N-CA-C     | 8.76  | 122.27      | 110.35   |
| 1   | A     | 477    | ALA  | CA-C-O     | -8.75 | 111.14      | 120.42   |
| 7   | G     | 24     | ALA  | CA-C-O     | -8.74 | 111.20      | 120.55   |
| 4   | D     | 74     | SER  | CA-CB-OG   | -8.65 | 93.80       | 111.10   |
| 11  | K     | 54     | ARG  | NE-CZ-NH1  | -8.63 | 112.87      | 121.50   |
| 1   | A     | 298[A] | ASP  | CA-C-O     | -8.52 | 112.52      | 121.55   |
| 1   | A     | 298[B] | ASP  | CA-C-O     | -8.52 | 112.52      | 121.55   |
| 7   | T     | 7      | ASP  | N-CA-C     | 8.51  | 128.92      | 110.80   |
| 10  | W     | 34     | VAL  | N-CA-C     | -8.48 | 102.27      | 110.42   |
| 11  | X     | 54     | ARG  | NE-CZ-NH1  | -8.46 | 113.04      | 121.50   |
| 6   | S     | 3      | GLY  | N-CA-C     | -8.44 | 99.08       | 110.56   |
| 4   | D     | 57     | VAL  | O-C-N      | 8.43  | 130.04      | 121.87   |
| 5   | E     | 103    | GLU  | O-C-N      | 8.35  | 133.62      | 122.43   |
| 12  | L     | 26     | THR  | CA-CB-OG1  | -8.34 | 97.09       | 109.60   |
| 7   | G     | 5      | LYS  | CB-CA-C    | 8.33  | 127.00      | 110.42   |
| 1   | A     | 213    | ARG  | NE-CZ-NH2  | -8.28 | 111.75      | 119.20   |
| 1   | A     | 513    | LEU  | CA-C-N     | -8.28 | 106.79      | 121.70   |
| 1   | A     | 513    | LEU  | C-N-CA     | -8.28 | 106.79      | 121.70   |
| 7   | T     | 24     | ALA  | CA-C-O     | -8.18 | 111.79      | 120.55   |
| 1   | A     | 309    | THR  | CA-C-O     | -8.17 | 111.76      | 120.42   |
| 2   | B     | 151    | ARG  | NE-CZ-NH1  | 8.16  | 129.66      | 121.50   |
| 4   | D     | 58     | GLU  | CB-CG-CD   | 8.16  | 126.47      | 112.60   |
| 4   | D     | 20     | ARG  | NE-CZ-NH1  | -8.14 | 113.36      | 121.50   |
| 2   | O     | 42     | ILE  | N-CA-C     | -8.10 | 102.65      | 110.42   |
| 1   | A     | 112    | LEU  | CD1-CG-CD2 | -8.04 | 93.12       | 110.80   |
| 4   | D     | 30     | VAL  | O-C-N      | 8.02  | 131.71      | 123.20   |
| 5   | E     | 70     | VAL  | CB-CA-C    | 7.89  | 122.80      | 112.14   |
| 4   | D     | 58     | GLU  | CG-CD-OE2  | -7.87 | 100.31      | 118.40   |
| 6   | S     | 94     | HIS  | N-CA-C     | 7.82  | 127.45      | 110.80   |
| 4   | D     | 60     | TYR  | O-C-N      | 7.81  | 130.40      | 122.12   |
| 3   | P     | 150    | SER  | O-C-N      | 7.79  | 130.38      | 122.12   |
| 1   | N     | 152    | LEU  | CD1-CG-CD2 | 7.72  | 127.79      | 110.80   |
| 4   | D     | 68     | PHE  | CA-C-O     | -7.71 | 112.38      | 120.55   |
| 4   | D     | 34     | SER  | O-C-N      | -7.71 | 112.03      | 122.36   |
| 7   | G     | 3      | ALA  | N-CA-C     | 7.70  | 127.19      | 110.80   |
| 5   | E     | 90     | ARG  | CB-CG-CD   | 7.68  | 128.96      | 111.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | C     | 150 | SER  | O-C-N     | 7.68  | 130.26      | 122.12   |
| 8   | H     | 12  | GLN  | N-CA-C    | -7.67 | 101.63      | 112.13   |
| 9   | I     | 52  | ARG  | CA-C-N    | -7.66 | 111.15      | 122.86   |
| 9   | I     | 52  | ARG  | C-N-CA    | -7.66 | 111.15      | 122.86   |
| 6   | F     | 6   | VAL  | CA-C-O    | 7.65  | 124.16      | 119.19   |
| 1   | A     | 38  | ARG  | NE-CZ-NH2 | -7.64 | 112.32      | 119.20   |
| 7   | T     | 41  | HIS  | N-CA-C    | 7.64  | 120.94      | 109.25   |
| 1   | A     | 316 | THR  | CA-C-O    | -7.60 | 112.37      | 120.42   |
| 4   | D     | 39  | ALA  | O-C-N     | 7.59  | 131.60      | 122.27   |
| 6   | F     | 64  | GLU  | CA-C-N    | -7.56 | 111.67      | 125.66   |
| 6   | F     | 64  | GLU  | C-N-CA    | -7.56 | 111.67      | 125.66   |
| 1   | A     | 327 | LEU  | CA-C-O    | -7.54 | 111.30      | 119.97   |
| 7   | T     | 2   | SER  | N-CA-C    | -7.54 | 103.65      | 114.12   |
| 13  | M     | 3   | ALA  | O-C-N     | 7.51  | 131.74      | 123.10   |
| 2   | O     | 174 | ALA  | CA-C-N    | -7.49 | 116.81      | 123.33   |
| 2   | O     | 174 | ALA  | C-N-CA    | -7.49 | 116.81      | 123.33   |
| 2   | B     | 139 | ASP  | N-CA-C    | 7.47  | 119.51      | 111.36   |
| 3   | C     | 76  | GLN  | CB-CG-CD  | 7.44  | 125.25      | 112.60   |
| 3   | C     | 147 | ALA  | CA-C-O    | -7.41 | 112.56      | 120.42   |
| 1   | N     | 100 | MET  | CA-C-N    | -7.40 | 110.36      | 120.28   |
| 1   | N     | 100 | MET  | C-N-CA    | -7.40 | 110.36      | 120.28   |
| 7   | T     | 44  | ARG  | CA-C-N    | 7.38  | 127.31      | 119.85   |
| 7   | T     | 44  | ARG  | C-N-CA    | 7.38  | 127.31      | 119.85   |
| 7   | G     | 56  | ARG  | NE-CZ-NH2 | 7.38  | 125.84      | 119.20   |
| 3   | P     | 84  | ILE  | N-CA-C    | -7.38 | 103.33      | 110.42   |
| 6   | F     | 17  | GLU  | O-C-N     | 7.38  | 129.76      | 122.09   |
| 5   | E     | 47  | ILE  | N-CA-C    | -7.34 | 103.63      | 110.53   |
| 1   | A     | 71  | MET  | CG-SD-CE  | -7.31 | 84.82       | 100.90   |
| 7   | G     | 44  | ARG  | N-CA-C    | 7.28  | 118.89      | 109.64   |
| 2   | O     | 65  | TRP  | CB-CA-C   | 7.27  | 123.93      | 110.11   |
| 1   | A     | 38  | ARG  | NE-CZ-NH1 | 7.27  | 128.77      | 121.50   |
| 7   | G     | 44  | ARG  | CA-C-N    | 7.26  | 127.18      | 119.85   |
| 7   | G     | 44  | ARG  | C-N-CA    | 7.26  | 127.18      | 119.85   |
| 12  | Y     | 27  | LEU  | N-CA-C    | -7.26 | 103.37      | 111.28   |
| 2   | B     | 44  | LEU  | N-CA-C    | -7.23 | 103.48      | 111.36   |
| 1   | A     | 270 | TYR  | CA-C-O    | -7.22 | 113.24      | 120.82   |
| 9   | I     | 5   | ALA  | N-CA-C    | 7.20  | 120.14      | 110.35   |
| 1   | A     | 295 | VAL  | O-C-N     | 7.19  | 130.46      | 122.12   |
| 1   | N     | 181 | THR  | CA-CB-OG1 | -7.19 | 98.81       | 109.60   |
| 4   | D     | 80  | THR  | N-CA-C    | -7.19 | 103.38      | 111.14   |
| 1   | N     | 216 | ASN  | CA-CB-CG  | -7.19 | 105.41      | 112.60   |
| 13  | M     | 8   | THR  | O-C-N     | -7.19 | 115.41      | 121.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | P     | 153 | GLU  | OE1-CD-OE2 | 7.17  | 140.12      | 122.90   |
| 5   | E     | 63  | SER  | O-C-N      | 7.16  | 131.07      | 122.27   |
| 5   | E     | 63  | SER  | CA-C-O     | -7.15 | 111.75      | 119.97   |
| 1   | A     | 102 | PHE  | CA-CB-CG   | -7.14 | 106.66      | 113.80   |
| 1   | A     | 365 | ILE  | CA-C-O     | -7.13 | 113.53      | 120.95   |
| 2   | B     | 91  | ASN  | N-CA-C     | 7.12  | 125.14      | 113.89   |
| 3   | C     | 181 | TYR  | CE1-CZ-CE2 | 7.07  | 134.45      | 120.30   |
| 2   | B     | 151 | ARG  | NE-CZ-NH2  | -7.07 | 112.84      | 119.20   |
| 6   | F     | 70  | ILE  | N-CA-CB    | -7.07 | 102.94      | 111.21   |
| 1   | A     | 323 | TRP  | CA-C-O     | -7.04 | 113.08      | 120.55   |
| 2   | B     | 59  | GLN  | N-CA-CB    | 7.02  | 120.44      | 110.12   |
| 7   | T     | 8   | HIS  | N-CA-C     | 7.01  | 125.74      | 110.80   |
| 3   | C     | 16  | TRP  | CA-C-N     | -7.01 | 111.27      | 119.05   |
| 3   | C     | 16  | TRP  | C-N-CA     | -7.01 | 111.27      | 119.05   |
| 1   | A     | 187 | SER  | CA-C-O     | -7.01 | 113.12      | 120.55   |
| 7   | G     | 2   | SER  | CA-CB-OG   | 6.99  | 125.07      | 111.10   |
| 1   | A     | 246 | LEU  | CA-C-O     | -6.97 | 111.95      | 119.97   |
| 7   | T     | 16  | TRP  | CA-C-O     | -6.96 | 110.67      | 119.31   |
| 4   | D     | 45  | LYS  | CG-CD-CE   | 6.96  | 127.30      | 111.30   |
| 7   | T     | 24  | ALA  | O-C-N      | 6.94  | 130.56      | 122.17   |
| 1   | A     | 450 | TRP  | CB-CG-CD1  | -6.91 | 116.54      | 126.90   |
| 2   | B     | 175 | ILE  | CA-C-O     | 6.89  | 123.78      | 119.51   |
| 1   | N     | 366 | VAL  | CG1-CB-CG2 | -6.88 | 95.66       | 110.80   |
| 4   | D     | 104 | TYR  | O-C-N      | 6.86  | 131.10      | 123.01   |
| 2   | B     | 184 | LEU  | N-CA-CB    | -6.85 | 98.60       | 111.00   |
| 9   | I     | 29  | LEU  | CA-C-N     | 6.85  | 127.54      | 119.94   |
| 9   | I     | 29  | LEU  | C-N-CA     | 6.85  | 127.54      | 119.94   |
| 1   | A     | 49  | GLY  | N-CA-C     | -6.83 | 101.38      | 110.74   |
| 6   | F     | 94  | HIS  | CA-C-N     | 6.82  | 134.56      | 121.54   |
| 6   | F     | 94  | HIS  | C-N-CA     | 6.82  | 134.56      | 121.54   |
| 6   | F     | 3   | GLY  | CA-C-N     | 6.80  | 134.74      | 121.41   |
| 6   | F     | 3   | GLY  | C-N-CA     | 6.80  | 134.74      | 121.41   |
| 9   | V     | 68  | ILE  | CA-CB-CG2  | 6.80  | 122.06      | 110.50   |
| 3   | P     | 222 | GLN  | CA-C-O     | -6.79 | 113.22      | 120.42   |
| 1   | N     | 125 | GLY  | N-CA-C     | -6.78 | 104.27      | 112.48   |
| 1   | N     | 245 | ILE  | N-CA-CB    | -6.77 | 101.33      | 110.54   |
| 7   | G     | 16  | TRP  | CA-C-O     | -6.77 | 111.06      | 119.38   |
| 1   | N     | 239 | GLY  | CA-C-O     | -6.76 | 112.87      | 120.30   |
| 5   | E     | 87  | GLN  | CA-C-O     | -6.74 | 113.66      | 121.07   |
| 1   | A     | 272 | GLY  | O-C-N      | 6.73  | 128.65      | 122.19   |
| 11  | K     | 47  | ARG  | CB-CG-CD   | 6.73  | 126.78      | 111.30   |
| 1   | A     | 32  | ALA  | O-C-N      | 6.72  | 129.24      | 122.12   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1   | A     | 180    | GLN  | CB-CG-CD   | 6.71  | 124.02      | 112.60   |
| 1   | A     | 481    | GLU  | CA-C-O     | 6.71  | 128.63      | 120.92   |
| 2   | B     | 175    | ILE  | N-CA-CB    | -6.71 | 105.26      | 112.37   |
| 1   | A     | 276    | ALA  | CA-C-O     | -6.68 | 113.34      | 120.42   |
| 2   | O     | 27     | THR  | N-CA-C     | -6.67 | 103.48      | 111.69   |
| 2   | B     | 81     | LEU  | CA-C-N     | -6.66 | 111.36      | 120.28   |
| 2   | B     | 81     | LEU  | C-N-CA     | -6.66 | 111.36      | 120.28   |
| 3   | C     | 178    | ALA  | N-CA-C     | -6.66 | 104.10      | 111.36   |
| 7   | G     | 2      | SER  | CA-C-N     | 6.65  | 134.25      | 121.54   |
| 7   | G     | 2      | SER  | C-N-CA     | 6.65  | 134.25      | 121.54   |
| 3   | C     | 94     | PHE  | CA-C-O     | -6.65 | 112.32      | 119.97   |
| 5   | R     | 64     | ALA  | N-CA-C     | -6.65 | 104.11      | 111.36   |
| 1   | N     | 377    | PHE  | CA-CB-CG   | 6.63  | 120.43      | 113.80   |
| 1   | A     | 235    | PHE  | CA-C-O     | -6.63 | 113.87      | 120.70   |
| 7   | G     | 16     | TRP  | O-C-N      | 6.62  | 131.30      | 122.43   |
| 1   | N     | 235    | PHE  | CA-CB-CG   | -6.62 | 107.18      | 113.80   |
| 1   | A     | 362[A] | SER  | CA-C-O     | 6.61  | 127.57      | 119.97   |
| 1   | A     | 362[B] | SER  | CA-C-O     | 6.61  | 127.57      | 119.97   |
| 9   | I     | 19     | PHE  | N-CA-C     | -6.60 | 104.01      | 111.07   |
| 11  | X     | 54     | ARG  | NE-CZ-NH2  | 6.59  | 125.13      | 119.20   |
| 4   | D     | 4      | SER  | N-CA-C     | 6.58  | 129.44      | 111.00   |
| 12  | L     | 46     | LYS  | CB-CG-CD   | -6.58 | 96.17       | 111.30   |
| 6   | F     | 1      | ALA  | O-C-N      | 6.58  | 133.52      | 123.00   |
| 1   | N     | 91     | ASP  | CA-CB-CG   | -6.57 | 106.03      | 112.60   |
| 11  | K     | 54     | ARG  | CA-C-O     | 6.57  | 131.96      | 120.80   |
| 4   | Q     | 31     | LYS  | CA-C-N     | -6.56 | 114.31      | 122.84   |
| 4   | Q     | 31     | LYS  | C-N-CA     | -6.56 | 114.31      | 122.84   |
| 3   | P     | 114    | GLY  | N-CA-C     | -6.55 | 104.99      | 115.08   |
| 1   | N     | 203    | ALA  | CA-C-O     | -6.55 | 113.61      | 120.55   |
| 2   | O     | 64     | ILE  | CB-CA-C    | -6.54 | 103.20      | 112.22   |
| 1   | A     | 113[A] | LEU  | O-C-N      | 6.53  | 128.80      | 122.07   |
| 1   | A     | 113[B] | LEU  | O-C-N      | 6.53  | 128.80      | 122.07   |
| 3   | P     | 131    | LEU  | N-CA-C     | -6.53 | 104.25      | 111.36   |
| 6   | F     | 3      | GLY  | CA-C-O     | -6.53 | 115.53      | 122.05   |
| 13  | M     | 21     | VAL  | N-CA-C     | -6.53 | 104.13      | 110.72   |
| 1   | A     | 194    | LEU  | CA-C-O     | -6.52 | 113.64      | 120.55   |
| 3   | P     | 88     | ILE  | CA-C-O     | -6.52 | 114.17      | 120.95   |
| 4   | Q     | 80     | THR  | N-CA-C     | -6.52 | 104.26      | 111.36   |
| 6   | F     | 62     | CYS  | N-CA-C     | -6.51 | 104.26      | 111.36   |
| 2   | B     | 168    | LEU  | CD1-CG-CD2 | -6.50 | 96.49       | 110.80   |
| 3   | C     | 150    | SER  | CA-C-O     | -6.49 | 113.67      | 120.55   |
| 1   | A     | 253    | MET  | CA-C-O     | -6.49 | 113.54      | 120.42   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 7   | G     | 28     | VAL  | CA-C-O     | -6.49 | 113.97      | 120.85   |
| 11  | X     | 39     | GLU  | CB-CA-C    | -6.48 | 100.42      | 111.31   |
| 3   | P     | 236    | GLU  | CA-CB-CG   | -6.46 | 101.17      | 114.10   |
| 2   | B     | 82     | ARG  | NE-CZ-NH2  | -6.46 | 113.39      | 119.20   |
| 1   | A     | 389    | ILE  | CA-C-O     | -6.45 | 114.33      | 121.17   |
| 1   | N     | 323    | TRP  | O-C-N      | 6.45  | 129.50      | 122.15   |
| 10  | J     | 27     | THR  | CB-CA-C    | 6.40  | 121.56      | 110.68   |
| 1   | N     | 98     | ASN  | OD1-CG-ND2 | 6.40  | 129.00      | 122.60   |
| 8   | U     | 8      | ILE  | CB-CA-C    | 6.39  | 121.77      | 111.29   |
| 2   | B     | 65     | TRP  | CB-CA-C    | 6.39  | 122.25      | 110.11   |
| 7   | G     | 56     | ARG  | NH1-CZ-NH2 | -6.39 | 111.00      | 119.30   |
| 1   | A     | 191    | THR  | O-C-N      | 6.38  | 128.89      | 122.12   |
| 1   | A     | 393    | PHE  | CA-CB-CG   | -6.38 | 107.42      | 113.80   |
| 1   | N     | 291    | HIS  | CA-CB-CG   | -6.37 | 107.43      | 113.80   |
| 1   | A     | 318    | VAL  | O-C-N      | -6.35 | 115.71      | 121.87   |
| 1   | N     | 98     | ASN  | N-CA-CB    | -6.35 | 100.78      | 110.12   |
| 1   | A     | 401    | SER  | CA-C-O     | -6.32 | 112.21      | 118.97   |
| 1   | N     | 237    | PHE  | CA-CB-CG   | -6.32 | 107.48      | 113.80   |
| 9   | V     | 52     | ARG  | CA-C-N     | -6.31 | 112.63      | 122.67   |
| 9   | V     | 52     | ARG  | C-N-CA     | -6.31 | 112.63      | 122.67   |
| 1   | N     | 100    | MET  | O-C-N      | 6.31  | 130.03      | 122.27   |
| 3   | P     | 61     | VAL  | N-CA-C     | -6.29 | 104.37      | 110.72   |
| 2   | O     | 184    | LEU  | N-CA-CB    | -6.27 | 99.95       | 110.80   |
| 2   | B     | 134    | ARG  | NE-CZ-NH2  | -6.26 | 113.57      | 119.20   |
| 1   | A     | 316    | THR  | O-C-N      | 6.25  | 129.28      | 122.15   |
| 1   | N     | 96     | ARG  | N-CA-CB    | -6.25 | 100.89      | 110.20   |
| 1   | N     | 296    | GLY  | O-C-N      | 6.24  | 130.81      | 122.70   |
| 3   | C     | 50     | ASN  | N-CA-C     | -6.23 | 104.41      | 111.14   |
| 4   | D     | 35     | ALA  | CA-C-O     | -6.22 | 114.24      | 120.90   |
| 1   | A     | 385    | ALA  | CA-C-O     | -6.21 | 114.25      | 120.90   |
| 1   | A     | 473    | TRP  | CA-C-O     | -6.18 | 113.87      | 120.42   |
| 9   | I     | 73     | LYS  | CG-CD-CE   | 6.18  | 125.51      | 111.30   |
| 7   | G     | 36     | TRP  | N-CA-CB    | 6.14  | 117.41      | 110.35   |
| 1   | N     | 124    | THR  | O-C-N      | 6.13  | 129.89      | 122.35   |
| 1   | A     | 27     | GLY  | CA-C-N     | -6.12 | 111.01      | 120.31   |
| 1   | A     | 27     | GLY  | C-N-CA     | -6.12 | 111.01      | 120.31   |
| 1   | A     | 304    | TYR  | CA-C-N     | -6.12 | 110.50      | 120.72   |
| 1   | A     | 304    | TYR  | C-N-CA     | -6.12 | 110.50      | 120.72   |
| 1   | A     | 298[A] | ASP  | CA-C-N     | 6.09  | 129.12      | 120.53   |
| 1   | A     | 298[A] | ASP  | C-N-CA     | 6.09  | 129.12      | 120.53   |
| 1   | A     | 298[B] | ASP  | CA-C-N     | 6.09  | 129.12      | 120.53   |
| 1   | A     | 298[B] | ASP  | C-N-CA     | 6.09  | 129.12      | 120.53   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | C     | 183 | GLU  | CA-C-N    | -6.09 | 111.84      | 120.49   |
| 3   | C     | 183 | GLU  | C-N-CA    | -6.09 | 111.84      | 120.49   |
| 3   | C     | 87  | ILE  | CA-C-O    | -6.08 | 114.62      | 120.95   |
| 13  | Z     | 5   | PRO  | CB-CA-C   | -6.08 | 102.99      | 110.95   |
| 6   | S     | 64  | GLU  | CA-C-N    | -6.07 | 114.43      | 125.66   |
| 6   | S     | 64  | GLU  | C-N-CA    | -6.07 | 114.43      | 125.66   |
| 2   | B     | 53  | THR  | CB-CA-C   | -6.06 | 100.26      | 110.44   |
| 5   | E     | 67  | ILE  | N-CA-C    | -6.05 | 104.61      | 110.72   |
| 1   | N     | 74  | MET  | CA-C-O    | -6.05 | 114.08      | 120.55   |
| 5   | R     | 82  | TYR  | CA-C-N    | -6.05 | 112.78      | 119.19   |
| 5   | R     | 82  | TYR  | C-N-CA    | -6.05 | 112.78      | 119.19   |
| 1   | A     | 252 | GLY  | CA-C-O    | -6.04 | 114.25      | 120.66   |
| 1   | A     | 327 | LEU  | O-C-N     | 6.04  | 129.70      | 122.27   |
| 1   | N     | 74  | MET  | CA-CB-CG  | -6.04 | 102.02      | 114.10   |
| 7   | G     | 44  | ARG  | CB-CG-CD  | -6.04 | 97.42       | 111.30   |
| 6   | S     | 5   | GLY  | CA-C-N    | -6.03 | 116.79      | 123.43   |
| 6   | S     | 5   | GLY  | C-N-CA    | -6.03 | 116.79      | 123.43   |
| 2   | B     | 59  | GLN  | CB-CG-CD  | 6.03  | 122.85      | 112.60   |
| 1   | A     | 173 | PRO  | CA-C-O    | 6.02  | 125.23      | 120.90   |
| 3   | C     | 198 | PHE  | CA-CB-CG  | -6.01 | 107.79      | 113.80   |
| 2   | B     | 103 | GLN  | CA-C-O    | -6.01 | 113.81      | 120.60   |
| 6   | F     | 95  | GLN  | N-CA-C    | 6.00  | 123.58      | 110.80   |
| 1   | A     | 469 | VAL  | O-C-N     | 6.00  | 127.69      | 121.87   |
| 3   | C     | 63  | ARG  | NE-CZ-NH2 | -5.99 | 113.81      | 119.20   |
| 1   | N     | 388 | ALA  | CA-C-O    | -5.99 | 114.07      | 120.42   |
| 1   | N     | 202 | LEU  | O-C-N     | 5.99  | 128.47      | 122.12   |
| 1   | A     | 397 | PHE  | CA-C-N    | -5.99 | 113.51      | 119.56   |
| 1   | A     | 397 | PHE  | C-N-CA    | -5.99 | 113.51      | 119.56   |
| 5   | E     | 61  | PHE  | CA-C-O    | 5.99  | 126.77      | 120.42   |
| 1   | A     | 216 | ASN  | CA-CB-CG  | -5.98 | 106.62      | 112.60   |
| 11  | K     | 39  | GLU  | CA-C-O    | 5.98  | 127.52      | 120.70   |
| 2   | O     | 131 | GLY  | N-CA-C    | -5.98 | 107.57      | 114.69   |
| 1   | N     | 79  | GLY  | CA-C-O    | -5.98 | 114.54      | 121.00   |
| 9   | I     | 22  | VAL  | CA-C-N    | 5.98  | 126.74      | 119.99   |
| 9   | I     | 22  | VAL  | C-N-CA    | 5.98  | 126.74      | 119.99   |
| 1   | N     | 329 | GLY  | CA-C-N    | -5.98 | 113.11      | 120.64   |
| 1   | N     | 329 | GLY  | C-N-CA    | -5.98 | 113.11      | 120.64   |
| 1   | N     | 425 | PHE  | CA-CB-CG  | -5.97 | 107.83      | 113.80   |
| 2   | O     | 82  | ARG  | NE-CZ-NH2 | -5.97 | 113.83      | 119.20   |
| 12  | L     | 20  | ARG  | NE-CZ-NH2 | -5.97 | 113.83      | 119.20   |
| 7   | T     | 19  | LEU  | O-C-N     | 5.96  | 128.44      | 122.12   |
| 4   | D     | 102 | TYR  | CA-C-N    | -5.95 | 117.14      | 122.97   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | D     | 102 | TYR  | C-N-CA     | -5.95 | 117.14      | 122.97   |
| 4   | D     | 119 | GLN  | CB-CG-CD   | -5.95 | 102.49      | 112.60   |
| 7   | G     | 7   | ASP  | N-CA-C     | 5.94  | 123.45      | 110.80   |
| 3   | C     | 159 | MET  | CA-C-N     | -5.93 | 111.74      | 120.28   |
| 3   | C     | 159 | MET  | C-N-CA     | -5.93 | 111.74      | 120.28   |
| 7   | G     | 2   | SER  | N-CA-C     | -5.92 | 106.05      | 113.28   |
| 1   | A     | 498 | CYS  | O-C-N      | -5.92 | 113.24      | 121.47   |
| 12  | L     | 31  | SER  | CA-C-O     | -5.92 | 114.15      | 120.42   |
| 2   | B     | 142 | VAL  | N-CA-CB    | -5.92 | 106.32      | 112.06   |
| 12  | Y     | 12  | PRO  | N-CA-C     | -5.91 | 107.88      | 114.92   |
| 3   | C     | 170 | GLY  | O-C-N      | 5.91  | 127.86      | 122.19   |
| 4   | D     | 74  | SER  | N-CA-CB    | -5.91 | 101.99      | 110.44   |
| 2   | O     | 92  | ASN  | N-CA-C     | 5.90  | 122.86      | 109.81   |
| 1   | N     | 74  | MET  | CB-CA-C    | -5.90 | 100.88      | 110.79   |
| 1   | A     | 145 | LEU  | O-C-N      | 5.90  | 128.37      | 122.12   |
| 3   | C     | 236 | GLU  | CA-CB-CG   | -5.90 | 102.31      | 114.10   |
| 3   | P     | 216 | ILE  | CA-C-O     | -5.90 | 114.60      | 120.85   |
| 3   | C     | 95  | THR  | OG1-CB-CG2 | -5.88 | 97.54       | 109.30   |
| 7   | T     | 15  | THR  | CA-CB-OG1  | -5.88 | 100.79      | 109.60   |
| 5   | E     | 66  | ARG  | NE-CZ-NH2  | -5.87 | 113.91      | 119.20   |
| 5   | E     | 18  | TYR  | N-CA-CB    | -5.87 | 101.50      | 110.01   |
| 9   | I     | 68  | ILE  | CA-CB-CG2  | 5.87  | 120.48      | 110.50   |
| 7   | G     | 36  | TRP  | CA-C-N     | 5.87  | 132.75      | 121.54   |
| 7   | G     | 36  | TRP  | C-N-CA     | 5.87  | 132.75      | 121.54   |
| 7   | T     | 2   | SER  | CA-C-N     | 5.87  | 132.75      | 121.54   |
| 7   | T     | 2   | SER  | C-N-CA     | 5.87  | 132.75      | 121.54   |
| 2   | O     | 85  | TYR  | N-CA-C     | 5.87  | 117.76      | 111.36   |
| 1   | N     | 112 | LEU  | CD1-CG-CD2 | -5.86 | 97.90       | 110.80   |
| 10  | W     | 12  | PHE  | CA-CB-CG   | -5.86 | 107.94      | 113.80   |
| 3   | P     | 212 | SER  | O-C-N      | 5.86  | 128.33      | 122.12   |
| 1   | A     | 253 | MET  | N-CA-C     | -5.85 | 104.99      | 111.36   |
| 1   | A     | 366 | VAL  | CG1-CB-CG2 | -5.84 | 97.94       | 110.80   |
| 4   | D     | 86  | MET  | N-CA-C     | -5.84 | 104.99      | 111.36   |
| 8   | H     | 32  | ASN  | N-CA-C     | 5.84  | 118.42      | 111.71   |
| 3   | C     | 233 | PHE  | CD1-CG-CD2 | 5.83  | 127.34      | 118.60   |
| 1   | N     | 70  | VAL  | N-CA-C     | -5.83 | 105.17      | 110.82   |
| 5   | R     | 63  | SER  | CA-C-O     | -5.83 | 113.52      | 120.10   |
| 1   | N     | 31  | THR  | N-CA-C     | -5.81 | 104.87      | 111.14   |
| 3   | C     | 170 | GLY  | CA-C-N     | -5.80 | 112.18      | 120.42   |
| 3   | C     | 170 | GLY  | C-N-CA     | -5.80 | 112.18      | 120.42   |
| 6   | S     | 92  | VAL  | CB-CA-C    | 5.80  | 121.92      | 111.36   |
| 2   | B     | 207 | MET  | O-C-N      | 5.79  | 125.92      | 121.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | N     | 262 | SER  | N-CA-C     | -5.79 | 106.07      | 113.02   |
| 11  | X     | 47  | ARG  | CD-NE-CZ   | 5.79  | 132.51      | 124.40   |
| 1   | A     | 57  | VAL  | CA-C-O     | -5.79 | 114.93      | 120.95   |
| 6   | S     | 59  | GLY  | O-C-N      | -5.78 | 118.48      | 123.80   |
| 13  | M     | 8   | THR  | CA-C-N     | 5.78  | 125.72      | 119.76   |
| 13  | M     | 8   | THR  | C-N-CA     | 5.78  | 125.72      | 119.76   |
| 5   | E     | 47  | ILE  | O-C-N      | 5.78  | 127.91      | 121.90   |
| 8   | U     | 12  | GLN  | N-CA-C     | -5.77 | 104.38      | 112.12   |
| 3   | P     | 163 | LEU  | CA-C-O     | -5.77 | 114.30      | 120.42   |
| 1   | A     | 145 | LEU  | CA-C-O     | -5.76 | 114.45      | 120.55   |
| 1   | N     | 323 | TRP  | CA-C-O     | -5.75 | 114.33      | 120.42   |
| 3   | P     | 29  | SER  | N-CA-C     | -5.75 | 105.10      | 111.71   |
| 3   | C     | 181 | TYR  | CB-CG-CD2  | -5.75 | 112.18      | 120.80   |
| 5   | R     | 90  | ARG  | NE-CZ-NH1  | -5.74 | 115.76      | 121.50   |
| 8   | U     | 9   | LYS  | N-CA-C     | 5.74  | 123.03      | 110.80   |
| 10  | W     | 57  | HIS  | N-CA-C     | 5.73  | 117.75      | 108.41   |
| 2   | B     | 143 | VAL  | N-CA-CB    | -5.73 | 104.28      | 110.53   |
| 3   | C     | 244 | PHE  | CD1-CE1-CZ | -5.73 | 109.69      | 120.00   |
| 4   | D     | 47  | SER  | N-CA-C     | 5.73  | 118.64      | 110.10   |
| 1   | N     | 247 | ILE  | CA-C-O     | -5.72 | 113.62      | 120.78   |
| 4   | D     | 35  | ALA  | O-C-N      | 5.72  | 128.04      | 122.09   |
| 4   | D     | 85  | ALA  | CA-C-O     | -5.72 | 114.48      | 120.55   |
| 5   | E     | 87  | GLN  | O-C-N      | 5.71  | 128.19      | 122.08   |
| 5   | R     | 69  | GLU  | CB-CA-C    | -5.71 | 101.14      | 110.85   |
| 1   | N     | 64  | VAL  | CA-C-O     | -5.71 | 115.12      | 121.17   |
| 6   | S     | 1   | ALA  | O-C-N      | 5.71  | 132.13      | 123.00   |
| 3   | C     | 171 | VAL  | O-C-N      | -5.70 | 115.96      | 121.83   |
| 7   | T     | 16  | TRP  | O-C-N      | 5.70  | 130.32      | 122.46   |
| 1   | A     | 27  | GLY  | O-C-N      | 5.70  | 128.28      | 122.24   |
| 1   | N     | 273 | MET  | O-C-N      | 5.69  | 128.63      | 122.15   |
| 1   | N     | 75  | ILE  | N-CA-C     | -5.68 | 106.16      | 111.45   |
| 1   | A     | 399 | LEU  | N-CA-C     | -5.67 | 105.02      | 111.14   |
| 5   | E     | 61  | PHE  | O-C-N      | -5.66 | 115.70      | 122.15   |
| 4   | Q     | 24  | LEU  | O-C-N      | 5.66  | 126.85      | 120.68   |
| 1   | N     | 70  | VAL  | CA-C-O     | -5.66 | 114.23      | 120.96   |
| 1   | A     | 401 | SER  | O-C-N      | 5.66  | 129.32      | 122.48   |
| 1   | A     | 397 | PHE  | O-C-N      | 5.65  | 126.29      | 120.70   |
| 5   | E     | 56  | ARG  | NE-CZ-NH1  | 5.65  | 127.15      | 121.50   |
| 1   | A     | 482 | VAL  | O-C-N      | 5.64  | 128.61      | 122.63   |
| 2   | B     | 92  | ASN  | CA-C-N     | -5.64 | 114.45      | 120.03   |
| 2   | B     | 92  | ASN  | C-N-CA     | -5.64 | 114.45      | 120.03   |
| 9   | V     | 10  | ARG  | CG-CD-NE   | -5.64 | 99.60       | 112.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 493 | GLU  | O-C-N     | 5.63  | 129.71      | 122.39   |
| 7   | G     | 61  | SER  | CA-CB-OG  | -5.63 | 99.84       | 111.10   |
| 4   | Q     | 6   | VAL  | N-CA-C    | -5.62 | 102.32      | 109.58   |
| 4   | D     | 73  | ARG  | CB-CG-CD  | -5.62 | 98.37       | 111.30   |
| 1   | A     | 496 | ASN  | CA-CB-CG  | -5.61 | 106.99      | 112.60   |
| 1   | A     | 128 | VAL  | CA-C-N    | -5.61 | 112.15      | 120.68   |
| 1   | A     | 128 | VAL  | C-N-CA    | -5.61 | 112.15      | 120.68   |
| 5   | R     | 32  | GLY  | N-CA-C    | -5.61 | 105.70      | 112.49   |
| 5   | E     | 49  | ASP  | CA-C-O    | -5.61 | 114.61      | 120.55   |
| 2   | B     | 90  | ILE  | CA-C-N    | -5.60 | 113.26      | 121.99   |
| 2   | B     | 90  | ILE  | C-N-CA    | -5.60 | 113.26      | 121.99   |
| 2   | B     | 151 | ARG  | CD-NE-CZ  | -5.58 | 116.59      | 124.40   |
| 5   | R     | 47  | ILE  | N-CA-C    | -5.58 | 105.29      | 110.53   |
| 2   | B     | 202 | SER  | N-CA-C    | 5.58  | 118.89      | 111.75   |
| 3   | P     | 85  | LEU  | N-CA-C    | -5.57 | 105.36      | 111.82   |
| 3   | P     | 246 | ASP  | CA-C-O    | -5.57 | 114.97      | 120.70   |
| 13  | M     | 37  | LEU  | CA-C-N    | -5.56 | 112.82      | 120.28   |
| 13  | M     | 37  | LEU  | C-N-CA    | -5.56 | 112.82      | 120.28   |
| 2   | O     | 132 | GLU  | CG-CD-OE1 | -5.56 | 105.61      | 118.40   |
| 3   | C     | 168 | THR  | CA-C-O    | 5.55  | 126.63      | 120.63   |
| 5   | E     | 56  | ARG  | NE-CZ-NH2 | -5.55 | 114.20      | 119.20   |
| 4   | D     | 46  | ALA  | CA-C-N    | -5.55 | 112.99      | 120.82   |
| 4   | D     | 46  | ALA  | C-N-CA    | -5.55 | 112.99      | 120.82   |
| 2   | O     | 224 | ALA  | N-CA-C    | -5.55 | 105.23      | 111.28   |
| 1   | N     | 361 | SER  | CA-C-O    | -5.54 | 114.43      | 120.41   |
| 10  | W     | 20  | VAL  | CA-C-O    | -5.54 | 114.64      | 120.57   |
| 9   | I     | 73  | LYS  | CA-CB-CG  | -5.53 | 103.05      | 114.10   |
| 3   | C     | 145 | THR  | O-C-N     | -5.52 | 115.86      | 122.15   |
| 6   | S     | 28  | GLN  | N-CA-C    | -5.52 | 101.59      | 110.14   |
| 1   | A     | 323 | TRP  | O-C-N     | 5.52  | 127.97      | 122.12   |
| 1   | A     | 371 | TYR  | CA-C-N    | -5.51 | 111.93      | 120.31   |
| 1   | A     | 371 | TYR  | C-N-CA    | -5.51 | 111.93      | 120.31   |
| 4   | Q     | 58  | GLU  | N-CA-CB   | 5.51  | 118.01      | 110.01   |
| 3   | P     | 97  | PHE  | CA-CB-CG  | -5.51 | 108.29      | 113.80   |
| 3   | P     | 150 | SER  | CA-C-O    | -5.51 | 114.71      | 120.55   |
| 2   | B     | 21  | LEU  | CB-CA-C   | -5.50 | 101.65      | 110.79   |
| 6   | S     | 56  | ARG  | CA-C-N    | -5.50 | 113.46      | 121.71   |
| 6   | S     | 56  | ARG  | C-N-CA    | -5.50 | 113.46      | 121.71   |
| 3   | P     | 56  | GLN  | CA-CB-CG  | -5.49 | 103.11      | 114.10   |
| 10  | J     | 12  | PHE  | CA-CB-CG  | -5.49 | 108.31      | 113.80   |
| 3   | P     | 246 | ASP  | N-CA-C    | -5.49 | 105.21      | 111.14   |
| 12  | Y     | 11  | ILE  | CB-CA-C   | -5.49 | 103.95      | 109.33   |

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| Mol | Chain | Res   | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 4   | D     | 66    | GLU  | O-C-N      | 5.49  | 129.41      | 123.10   |
| 3   | P     | 176   | LEU  | N-CA-C     | -5.49 | 105.21      | 111.14   |
| 1   | N     | 253   | MET  | CA-CB-CG   | -5.49 | 103.13      | 114.10   |
| 7   | G     | 36    | TRP  | N-CA-C     | -5.48 | 103.74      | 110.65   |
| 3   | P     | 3     | HIS  | CA-C-N     | -5.48 | 112.29      | 121.39   |
| 3   | P     | 3     | HIS  | C-N-CA     | -5.48 | 112.29      | 121.39   |
| 1   | A     | 88    | GLY  | CA-C-O     | -5.48 | 112.46      | 119.58   |
| 12  | L     | 12    | PRO  | N-CA-C     | -5.47 | 108.41      | 114.92   |
| 9   | I     | 5     | ALA  | CA-C-O     | -5.47 | 115.75      | 121.55   |
| 6   | S     | 3     | GLY  | CA-C-N     | 5.47  | 132.12      | 121.41   |
| 6   | S     | 3     | GLY  | C-N-CA     | 5.47  | 132.12      | 121.41   |
| 1   | N     | 421   | VAL  | CA-C-O     | -5.46 | 115.06      | 120.85   |
| 5   | E     | 67    | ILE  | CA-C-O     | -5.46 | 115.06      | 120.85   |
| 4   | D     | 136   | ALA  | N-CA-C     | -5.46 | 105.88      | 112.54   |
| 5   | R     | 42    | VAL  | N-CA-C     | -5.46 | 101.61      | 108.05   |
| 1   | A     | 376   | HIS  | CA-C-N     | -5.46 | 111.59      | 121.14   |
| 1   | A     | 376   | HIS  | C-N-CA     | -5.46 | 111.59      | 121.14   |
| 6   | F     | 88    | HIS  | O-C-N      | 5.46  | 129.49      | 123.16   |
| 1   | A     | 8     | PHE  | CB-CG-CD2  | -5.45 | 111.43      | 120.70   |
| 8   | H     | 32    | ASN  | CB-CG-ND2  | 5.45  | 124.57      | 116.40   |
| 1   | N     | 327   | LEU  | O-C-N      | 5.45  | 127.90      | 122.12   |
| 1   | N     | 393   | PHE  | CA-CB-CG   | -5.45 | 108.35      | 113.80   |
| 6   | F     | 94    | HIS  | O-C-N      | 5.44  | 129.83      | 122.59   |
| 3   | P     | 236   | GLU  | N-CA-C     | -5.44 | 105.35      | 111.28   |
| 5   | R     | 9     | GLU  | CB-CG-CD   | 5.44  | 121.85      | 112.60   |
| 1   | A     | 365   | ILE  | N-CA-C     | -5.44 | 105.07      | 110.62   |
| 2   | B     | 60    | GLU  | CA-C-O     | 5.44  | 126.30      | 120.70   |
| 2   | O     | 129   | LYS  | N-CA-C     | -5.44 | 102.30      | 110.24   |
| 8   | H     | 42    | ALA  | N-CA-C     | -5.43 | 105.25      | 111.07   |
| 7   | T     | 5     | LYS  | CB-CA-C    | 5.43  | 121.23      | 110.42   |
| 4   | D     | 31[A] | LYS  | CA-CB-CG   | 5.43  | 124.96      | 114.10   |
| 4   | D     | 31[B] | LYS  | CA-CB-CG   | 5.43  | 124.96      | 114.10   |
| 7   | G     | 64    | ASP  | CB-CG-OD2  | -5.43 | 105.91      | 118.40   |
| 2   | O     | 132   | GLU  | CG-CD-OE2  | 5.42  | 130.88      | 118.40   |
| 9   | V     | 38    | ALA  | N-CA-C     | 5.42  | 119.61      | 112.89   |
| 1   | A     | 377   | PHE  | CA-CB-CG   | 5.42  | 119.22      | 113.80   |
| 2   | B     | 48    | THR  | CA-CB-OG1  | -5.42 | 101.47      | 109.60   |
| 1   | N     | 320   | VAL  | CA-C-O     | -5.42 | 115.31      | 120.95   |
| 1   | A     | 181   | THR  | OG1-CB-CG2 | -5.42 | 98.46       | 109.30   |
| 4   | D     | 11    | TYR  | N-CA-C     | 5.42  | 117.94      | 111.71   |
| 1   | A     | 188   | VAL  | CA-C-O     | -5.41 | 115.11      | 120.85   |
| 6   | S     | 93    | PRO  | CB-CA-C    | 5.41  | 120.49      | 111.56   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 112 | ASP  | CA-C-O   | -5.41 | 113.75      | 119.97   |
| 6   | F     | 25  | ARG  | CB-CA-C  | -5.40 | 101.83      | 110.79   |
| 2   | O     | 204 | HIS  | N-CA-CB  | -5.40 | 102.18      | 110.12   |
| 1   | A     | 201 | VAL  | N-CA-C   | -5.40 | 105.12      | 111.00   |
| 1   | A     | 291 | HIS  | CA-CB-CG | -5.40 | 108.40      | 113.80   |
| 3   | P     | 233 | PHE  | CA-CB-CG | -5.39 | 108.41      | 113.80   |
| 5   | E     | 50  | ALA  | O-C-N    | 5.39  | 128.90      | 122.27   |
| 4   | Q     | 20  | ARG  | CD-NE-CZ | 5.39  | 131.94      | 124.40   |
| 1   | N     | 187 | SER  | O-C-N    | 5.39  | 128.52      | 122.22   |
| 13  | M     | 40  | TYR  | CA-C-O   | -5.38 | 114.71      | 120.42   |
| 11  | X     | 54  | ARG  | CA-C-O   | 5.38  | 129.95      | 120.80   |
| 7   | T     | 80  | THR  | N-CA-C   | 5.38  | 119.83      | 113.16   |
| 1   | A     | 194 | LEU  | O-C-N    | 5.36  | 127.80      | 122.12   |
| 1   | A     | 188 | VAL  | N-CA-C   | -5.36 | 105.31      | 110.72   |
| 8   | H     | 67  | SER  | O-C-N    | 5.35  | 128.85      | 122.27   |
| 10  | J     | 27  | THR  | N-CA-CB  | -5.35 | 102.03      | 110.06   |
| 1   | A     | 456 | MET  | N-CA-C   | -5.35 | 105.45      | 111.28   |
| 6   | F     | 81  | ARG  | CA-CB-CG | -5.35 | 103.40      | 114.10   |
| 1   | N     | 357 | VAL  | O-C-N    | 5.35  | 127.15      | 121.91   |
| 1   | A     | 461 | SER  | CA-CB-OG | -5.35 | 100.41      | 111.10   |
| 2   | B     | 204 | HIS  | N-CA-CB  | -5.35 | 102.04      | 110.06   |
| 3   | C     | 207 | HIS  | N-CA-C   | -5.35 | 105.53      | 111.36   |
| 6   | F     | 8   | THR  | CA-C-N   | -5.34 | 113.12      | 120.28   |
| 6   | F     | 8   | THR  | C-N-CA   | -5.34 | 113.12      | 120.28   |
| 1   | N     | 107 | PRO  | CB-CA-C  | -5.34 | 103.88      | 112.21   |
| 1   | N     | 315 | PRO  | CA-C-N   | -5.34 | 112.71      | 120.29   |
| 1   | N     | 315 | PRO  | C-N-CA   | -5.34 | 112.71      | 120.29   |
| 1   | A     | 304 | TYR  | O-C-N    | 5.33  | 127.78      | 122.12   |
| 1   | A     | 231 | TYR  | O-C-N    | 5.33  | 127.77      | 122.12   |
| 1   | A     | 348 | PHE  | CA-CB-CG | -5.33 | 108.47      | 113.80   |
| 2   | B     | 89  | GLU  | CA-C-N   | 5.33  | 127.72      | 120.63   |
| 2   | B     | 89  | GLU  | C-N-CA   | 5.33  | 127.72      | 120.63   |
| 6   | S     | 64  | GLU  | CA-CB-CG | -5.33 | 103.44      | 114.10   |
| 6   | F     | 28  | GLN  | CA-CB-CG | -5.32 | 103.46      | 114.10   |
| 2   | O     | 199 | ILE  | O-C-N    | 5.32  | 127.95      | 122.79   |
| 4   | Q     | 84  | ALA  | N-CA-C   | -5.32 | 105.56      | 111.36   |
| 1   | A     | 143 | VAL  | N-CA-C   | -5.32 | 104.44      | 111.09   |
| 3   | C     | 233 | PHE  | CA-CB-CG | -5.32 | 108.48      | 113.80   |
| 3   | P     | 67  | PHE  | CA-C-N   | -5.32 | 113.81      | 122.26   |
| 3   | P     | 67  | PHE  | C-N-CA   | -5.32 | 113.81      | 122.26   |
| 7   | G     | 13  | ALA  | CA-C-O   | -5.31 | 114.92      | 120.55   |
| 1   | N     | 63  | PHE  | CA-C-O   | -5.31 | 114.79      | 120.42   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | D     | 76  | ASN  | CA-CB-CG   | -5.30 | 107.30      | 112.60   |
| 7   | G     | 69  | PHE  | N-CA-C     | 5.30  | 117.27      | 111.50   |
| 3   | P     | 42  | LEU  | CB-CA-C    | -5.30 | 101.99      | 110.79   |
| 3   | C     | 252 | LEU  | CB-CA-C    | -5.29 | 101.85      | 110.85   |
| 2   | B     | 65  | TRP  | CA-CB-CG   | 5.29  | 123.65      | 113.60   |
| 1   | N     | 37  | ILE  | CB-CA-C    | -5.27 | 105.22      | 111.97   |
| 4   | Q     | 127 | LYS  | CD-CE-NZ   | 5.27  | 128.78      | 111.90   |
| 12  | Y     | 20  | ARG  | N-CA-C     | -5.27 | 105.53      | 111.28   |
| 1   | A     | 7   | LEU  | CD1-CG-CD2 | 5.27  | 122.39      | 110.80   |
| 8   | H     | 61  | LYS  | CA-CB-CG   | -5.26 | 103.57      | 114.10   |
| 1   | N     | 88  | GLY  | O-C-N      | 5.26  | 128.76      | 122.34   |
| 1   | A     | 55  | ASN  | CA-CB-CG   | -5.26 | 107.34      | 112.60   |
| 5   | R     | 63  | SER  | N-CA-C     | -5.25 | 105.67      | 111.71   |
| 7   | T     | 58  | LYS  | CA-C-O     | 5.25  | 124.38      | 119.13   |
| 1   | A     | 280 | ILE  | O-C-N      | 5.24  | 126.96      | 121.87   |
| 12  | L     | 20  | ARG  | CG-CD-NE   | -5.24 | 100.47      | 112.00   |
| 1   | A     | 146 | THR  | N-CA-CB    | -5.24 | 102.41      | 110.01   |
| 8   | H     | 57  | ARG  | CB-CA-C    | -5.24 | 102.65      | 110.88   |
| 4   | D     | 20  | ARG  | NE-CZ-NH2  | 5.24  | 123.92      | 119.20   |
| 1   | N     | 144 | ASP  | OD1-CG-OD2 | 5.24  | 135.47      | 122.90   |
| 3   | P     | 8   | TYR  | CA-C-N     | -5.24 | 115.72      | 123.05   |
| 3   | P     | 8   | TYR  | C-N-CA     | -5.24 | 115.72      | 123.05   |
| 4   | D     | 41  | LYS  | N-CA-C     | -5.24 | 105.75      | 111.82   |
| 3   | P     | 211 | GLY  | CA-C-O     | -5.23 | 115.11      | 120.66   |
| 1   | N     | 183 | LEU  | CA-C-N     | -5.23 | 113.27      | 120.28   |
| 1   | N     | 183 | LEU  | C-N-CA     | -5.23 | 113.27      | 120.28   |
| 1   | A     | 52  | GLN  | CA-C-O     | -5.23 | 115.32      | 120.70   |
| 7   | G     | 36  | TRP  | CB-CA-C    | 5.22  | 118.89      | 111.74   |
| 1   | N     | 316 | THR  | O-C-N      | 5.22  | 128.10      | 122.15   |
| 1   | A     | 155 | VAL  | CA-C-O     | -5.21 | 115.32      | 120.85   |
| 4   | D     | 89  | ILE  | N-CA-C     | -5.21 | 105.45      | 110.72   |
| 3   | C     | 57  | TRP  | N-CA-CB    | -5.21 | 102.51      | 110.07   |
| 3   | P     | 198 | PHE  | CA-CB-CG   | -5.21 | 108.59      | 113.80   |
| 10  | J     | 2   | GLU  | CA-C-N     | -5.21 | 115.49      | 122.42   |
| 10  | J     | 2   | GLU  | C-N-CA     | -5.21 | 115.49      | 122.42   |
| 7   | T     | 76  | ASN  | CA-C-N     | -5.21 | 115.21      | 120.31   |
| 7   | T     | 76  | ASN  | C-N-CA     | -5.21 | 115.21      | 120.31   |
| 7   | T     | 2   | SER  | CA-CB-OG   | 5.20  | 121.49      | 111.10   |
| 1   | A     | 449 | MET  | CA-CB-CG   | -5.19 | 103.72      | 114.10   |
| 1   | N     | 373 | VAL  | N-CA-C     | -5.19 | 105.48      | 110.72   |
| 7   | T     | 54  | ARG  | CA-C-N     | -5.19 | 113.70      | 120.91   |
| 7   | T     | 54  | ARG  | C-N-CA     | -5.19 | 113.70      | 120.91   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 5   | R     | 15  | TRP  | O-C-N      | -5.18 | 116.62      | 122.12   |
| 1   | N     | 163 | ASN  | O-C-N      | 5.18  | 127.41      | 122.07   |
| 8   | H     | 28  | ASN  | CB-CA-C    | 5.18  | 119.01      | 110.88   |
| 11  | K     | 51  | LYS  | CD-CE-NZ   | -5.18 | 95.32       | 111.90   |
| 3   | C     | 69  | GLY  | CA-C-N     | -5.17 | 111.59      | 121.94   |
| 3   | C     | 69  | GLY  | C-N-CA     | -5.17 | 111.59      | 121.94   |
| 1   | N     | 378 | HIS  | CA-CB-CG   | -5.17 | 108.63      | 113.80   |
| 2   | O     | 21  | LEU  | CB-CA-C    | -5.17 | 102.77      | 110.88   |
| 1   | N     | 189 | MET  | CB-CG-SD   | -5.16 | 97.21       | 112.70   |
| 5   | E     | 95  | GLU  | O-C-N      | 5.16  | 127.59      | 122.12   |
| 11  | K     | 7   | PRO  | CB-CA-C    | -5.16 | 104.81      | 111.46   |
| 5   | E     | 84  | TYR  | CZ-CE2-CD2 | -5.15 | 110.33      | 119.60   |
| 1   | N     | 276 | ALA  | CA-C-O     | -5.15 | 115.09      | 120.55   |
| 9   | V     | 67  | GLY  | CA-C-N     | -5.15 | 112.19      | 120.64   |
| 9   | V     | 67  | GLY  | C-N-CA     | -5.15 | 112.19      | 120.64   |
| 3   | C     | 244 | PHE  | CE1-CZ-CE2 | 5.14  | 129.25      | 120.00   |
| 1   | A     | 125 | GLY  | N-CA-C     | -5.14 | 106.26      | 112.48   |
| 7   | G     | 9   | GLY  | N-CA-C     | -5.13 | 101.01      | 113.18   |
| 1   | A     | 374 | VAL  | CA-C-O     | -5.13 | 115.08      | 120.57   |
| 5   | E     | 87  | GLN  | CB-CG-CD   | -5.13 | 103.88      | 112.60   |
| 1   | N     | 498 | CYS  | O-C-N      | 5.13  | 127.03      | 121.23   |
| 1   | N     | 389 | ILE  | CA-C-O     | -5.13 | 115.62      | 120.95   |
| 12  | Y     | 30  | GLY  | CA-C-O     | -5.13 | 115.47      | 120.75   |
| 10  | W     | 30  | ILE  | N-CA-C     | -5.13 | 105.50      | 110.42   |
| 1   | A     | 371 | TYR  | CA-C-O     | -5.12 | 112.39      | 119.05   |
| 2   | O     | 33  | LEU  | CB-CG-CD1  | 5.12  | 126.07      | 110.70   |
| 6   | S     | 81  | ARG  | CD-NE-CZ   | -5.12 | 117.23      | 124.40   |
| 5   | R     | 69  | GLU  | CB-CG-CD   | -5.12 | 103.90      | 112.60   |
| 13  | Z     | 4   | LYS  | CA-C-O     | 5.12  | 126.81      | 120.87   |
| 6   | F     | 56  | ARG  | CA-C-N     | -5.12 | 114.60      | 121.66   |
| 6   | F     | 56  | ARG  | C-N-CA     | -5.12 | 114.60      | 121.66   |
| 1   | A     | 15  | ILE  | CA-C-O     | -5.11 | 115.43      | 120.85   |
| 4   | D     | 37  | GLN  | N-CA-C     | -5.11 | 105.79      | 111.36   |
| 2   | O     | 91  | ASN  | N-CA-C     | 5.11  | 120.25      | 112.54   |
| 1   | A     | 310 | MET  | CA-CB-CG   | -5.11 | 103.89      | 114.10   |
| 4   | D     | 80  | THR  | CA-C-O     | -5.11 | 115.44      | 120.70   |
| 2   | B     | 80  | SER  | N-CA-C     | 5.10  | 117.23      | 111.11   |
| 3   | C     | 113 | GLY  | N-CA-C     | -5.10 | 108.07      | 115.27   |
| 1   | A     | 129 | TYR  | CB-CG-CD1  | -5.10 | 113.15      | 120.80   |
| 3   | C     | 7   | ALA  | N-CA-CB    | -5.09 | 103.11      | 110.70   |
| 1   | N     | 456 | MET  | CA-CB-CG   | -5.09 | 103.91      | 114.10   |
| 3   | P     | 241 | TYR  | N-CA-C     | -5.09 | 105.81      | 111.36   |

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| Mol | Chain | Res   | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|-------|-------------|----------|
| 1   | A     | 364   | ASP  | CA-CB-CG   | -5.08 | 107.52      | 112.60   |
| 3   | C     | 216   | ILE  | N-CA-CB    | -5.08 | 103.63      | 110.54   |
| 6   | S     | 21[A] | MET  | CA-C-O     | 5.08  | 126.16      | 120.82   |
| 6   | S     | 21[B] | MET  | CA-C-O     | 5.08  | 126.16      | 120.82   |
| 3   | P     | 174   | THR  | CA-C-O     | -5.07 | 115.17      | 120.55   |
| 4   | Q     | 6     | VAL  | CA-CB-CG1  | 5.07  | 119.03      | 110.40   |
| 7   | G     | 64    | ASP  | CA-C-N     | -5.07 | 114.73      | 122.28   |
| 7   | G     | 64    | ASP  | C-N-CA     | -5.07 | 114.73      | 122.28   |
| 6   | S     | 65    | ASP  | CA-C-N     | -5.07 | 113.51      | 120.71   |
| 6   | S     | 65    | ASP  | C-N-CA     | -5.07 | 113.51      | 120.71   |
| 5   | E     | 100   | THR  | CA-CB-CG2  | -5.07 | 101.89      | 110.50   |
| 5   | E     | 98    | ILE  | O-C-N      | -5.06 | 116.76      | 122.94   |
| 5   | R     | 92    | THR  | N-CA-C     | -5.06 | 105.84      | 111.36   |
| 1   | N     | 193   | VAL  | N-CA-C     | -5.06 | 105.61      | 110.72   |
| 4   | D     | 70    | GLU  | O-C-N      | -5.05 | 116.39      | 122.15   |
| 5   | E     | 103   | GLU  | CA-C-O     | -5.05 | 113.17      | 119.38   |
| 8   | U     | 46    | LYS  | CB-CA-C    | 5.05  | 120.47      | 110.42   |
| 1   | N     | 276   | ALA  | O-C-N      | 5.05  | 127.47      | 122.12   |
| 2   | O     | 176   | PRO  | O-C-N      | 5.05  | 129.16      | 123.10   |
| 6   | S     | 8     | THR  | CA-C-N     | -5.04 | 113.52      | 120.28   |
| 6   | S     | 8     | THR  | C-N-CA     | -5.04 | 113.52      | 120.28   |
| 1   | N     | 207   | THR  | CA-C-O     | -5.04 | 115.08      | 120.42   |
| 1   | N     | 5     | ARG  | CA-CB-CG   | -5.04 | 104.02      | 114.10   |
| 2   | O     | 199   | ILE  | N-CA-C     | 5.04  | 115.90      | 109.30   |
| 4   | Q     | 95    | LEU  | CB-CA-C    | -5.04 | 102.29      | 110.85   |
| 8   | H     | 75    | ARG  | CA-CB-CG   | -5.04 | 104.03      | 114.10   |
| 9   | I     | 7     | PRO  | O-C-N      | -5.04 | 116.61      | 122.86   |
| 12  | L     | 27    | LEU  | N-CA-CB    | 5.03  | 117.61      | 110.16   |
| 13  | M     | 11    | SER  | N-CA-CB    | -5.03 | 103.34      | 110.04   |
| 4   | D     | 94    | LEU  | O-C-N      | -5.03 | 116.79      | 122.12   |
| 3   | P     | 124   | LEU  | N-CA-C     | -5.03 | 103.51      | 110.35   |
| 6   | F     | 96    | LEU  | N-CA-C     | 5.02  | 121.50      | 110.80   |
| 8   | H     | 9     | LYS  | N-CA-CB    | 5.02  | 118.97      | 110.49   |
| 7   | G     | 83    | GLU  | N-CA-C     | 5.02  | 117.51      | 110.23   |
| 3   | P     | 75    | VAL  | N-CA-C     | -5.01 | 105.66      | 110.72   |
| 1   | A     | 257   | ILE  | CA-C-O     | -5.00 | 115.49      | 121.05   |
| 3   | C     | 38    | ASN  | N-CA-C     | 5.00  | 118.34      | 111.54   |
| 3   | C     | 146   | TRP  | CG-CD2-CE3 | -5.00 | 128.90      | 133.90   |
| 3   | P     | 238   | ALA  | CA-C-N     | -5.00 | 112.70      | 120.31   |
| 3   | P     | 238   | ALA  | C-N-CA     | -5.00 | 112.70      | 120.31   |

There are no chirality outliers.

All (22) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 296 | GLY  | Mainchain |
| 1   | A     | 304 | TYR  | Sidechain |
| 1   | A     | 379 | TYR  | Sidechain |
| 1   | A     | 38  | ARG  | Sidechain |
| 2   | B     | 110 | TYR  | Sidechain |
| 2   | B     | 151 | ARG  | Sidechain |
| 2   | B     | 68  | LEU  | Mainchain |
| 3   | C     | 133 | ASN  | Sidechain |
| 5   | E     | 49  | ASP  | Sidechain |
| 5   | E     | 88  | GLU  | Sidechain |
| 6   | F     | 93  | PRO  | Peptide   |
| 7   | G     | 18  | PHE  | Sidechain |
| 10  | J     | 57  | HIS  | Peptide   |
| 11  | K     | 39  | GLU  | Mainchain |
| 13  | M     | 14  | GLU  | Sidechain |
| 1   | N     | 240 | HIS  | Sidechain |
| 1   | N     | 296 | GLY  | Mainchain |
| 1   | N     | 304 | TYR  | Sidechain |
| 4   | Q     | 8   | SER  | Peptide   |
| 6   | S     | 92  | VAL  | Mainchain |
| 6   | S     | 93  | PRO  | Peptide   |
| 7   | T     | 40  | GLY  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4168  | 0        | 4137     | 78      | 0            |
| 1   | N     | 4154  | 0        | 4129     | 84      | 0            |
| 2   | B     | 1899  | 0        | 1898     | 67      | 0            |
| 2   | O     | 1870  | 0        | 1868     | 42      | 0            |
| 3   | C     | 2185  | 0        | 2097     | 41      | 0            |
| 3   | P     | 2185  | 0        | 2097     | 52      | 0            |
| 4   | D     | 1242  | 0        | 1235     | 24      | 0            |
| 4   | Q     | 1224  | 0        | 1211     | 25      | 0            |
| 5   | E     | 852   | 0        | 845      | 1       | 0            |
| 5   | R     | 863   | 0        | 857      | 9       | 2            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | F     | 778   | 0        | 754      | 27      | 0            |
| 6   | S     | 763   | 0        | 742      | 40      | 0            |
| 7   | G     | 686   | 0        | 652      | 40      | 0            |
| 7   | T     | 686   | 0        | 651      | 45      | 0            |
| 8   | H     | 662   | 0        | 623      | 27      | 0            |
| 8   | U     | 662   | 0        | 623      | 18      | 0            |
| 9   | I     | 601   | 0        | 613      | 16      | 2            |
| 9   | V     | 601   | 0        | 613      | 13      | 0            |
| 10  | J     | 460   | 0        | 459      | 14      | 0            |
| 10  | W     | 469   | 0        | 464      | 10      | 0            |
| 11  | K     | 384   | 0        | 366      | 7       | 0            |
| 11  | X     | 391   | 0        | 374      | 4       | 0            |
| 12  | L     | 380   | 0        | 380      | 19      | 0            |
| 12  | Y     | 388   | 0        | 388      | 30      | 0            |
| 13  | M     | 335   | 0        | 352      | 8       | 0            |
| 13  | Z     | 335   | 0        | 352      | 6       | 0            |
| 14  | A     | 120   | 0        | 107      | 7       | 0            |
| 14  | N     | 120   | 0        | 107      | 12      | 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  | N     | 1     | 0        | 0        | 0       | 0            |
| 18  | A     | 2     | 0        | 0        | 1       | 0            |
| 18  | N     | 2     | 0        | 0        | 1       | 0            |
| 19  | A     | 102   | 0        | 152      | 11      | 0            |
| 19  | C     | 102   | 0        | 152      | 9       | 0            |
| 19  | N     | 51    | 0        | 76       | 1       | 0            |
| 19  | P     | 102   | 0        | 152      | 10      | 0            |
| 19  | Q     | 51    | 0        | 76       | 11      | 0            |
| 20  | B     | 63    | 0        | 109      | 3       | 0            |
| 20  | D     | 63    | 0        | 106      | 21      | 0            |
| 20  | L     | 63    | 0        | 110      | 19      | 0            |
| 20  | N     | 63    | 0        | 110      | 6       | 0            |
| 20  | Q     | 63    | 0        | 110      | 15      | 0            |
| 20  | Y     | 63    | 0        | 110      | 23      | 0            |
| 21  | B     | 2     | 0        | 0        | 0       | 0            |
| 21  | O     | 2     | 0        | 0        | 0       | 0            |
| 22  | B     | 29    | 0        | 39       | 0       | 0            |
| 22  | C     | 58    | 0        | 77       | 3       | 0            |
| 22  | J     | 29    | 0        | 37       | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | O     | 29    | 0        | 39       | 0       | 0            |
| 22  | P     | 58    | 0        | 77       | 7       | 0            |
| 22  | W     | 29    | 0        | 38       | 6       | 0            |
| 23  | B     | 52    | 0        | 80       | 13      | 0            |
| 23  | O     | 52    | 0        | 80       | 19      | 0            |
| 24  | C     | 1     | 0        | 0        | 0       | 0            |
| 24  | P     | 1     | 0        | 0        | 0       | 0            |
| 25  | C     | 100   | 0        | 154      | 26      | 0            |
| 25  | G     | 100   | 0        | 156      | 37      | 0            |
| 25  | P     | 100   | 0        | 156      | 24      | 0            |
| 25  | T     | 100   | 0        | 156      | 28      | 0            |
| 26  | C     | 53    | 0        | 77       | 13      | 0            |
| 26  | G     | 106   | 0        | 154      | 16      | 0            |
| 26  | P     | 53    | 0        | 77       | 14      | 0            |
| 26  | T     | 106   | 0        | 154      | 18      | 0            |
| 27  | F     | 1     | 0        | 0        | 0       | 0            |
| 27  | S     | 1     | 0        | 0        | 0       | 0            |
| 28  | J     | 33    | 0        | 42       | 5       | 0            |
| 28  | M     | 33    | 0        | 42       | 0       | 0            |
| 28  | P     | 33    | 0        | 42       | 10      | 0            |
| 28  | Z     | 33    | 0        | 42       | 0       | 0            |
| 29  | A     | 297   | 0        | 0        | 18      | 0            |
| 29  | B     | 274   | 0        | 0        | 13      | 0            |
| 29  | C     | 176   | 0        | 0        | 8       | 0            |
| 29  | D     | 266   | 0        | 0        | 5       | 0            |
| 29  | E     | 178   | 0        | 0        | 2       | 0            |
| 29  | F     | 199   | 0        | 0        | 9       | 0            |
| 29  | G     | 100   | 0        | 0        | 7       | 0            |
| 29  | H     | 122   | 0        | 0        | 8       | 0            |
| 29  | I     | 88    | 0        | 0        | 2       | 0            |
| 29  | J     | 63    | 0        | 0        | 2       | 0            |
| 29  | K     | 69    | 0        | 0        | 4       | 0            |
| 29  | L     | 48    | 0        | 0        | 2       | 0            |
| 29  | M     | 47    | 0        | 0        | 1       | 0            |
| 29  | N     | 290   | 0        | 0        | 12      | 0            |
| 29  | O     | 243   | 0        | 0        | 4       | 0            |
| 29  | P     | 173   | 0        | 0        | 8       | 0            |
| 29  | Q     | 164   | 0        | 0        | 8       | 0            |
| 29  | R     | 151   | 0        | 0        | 4       | 0            |
| 29  | S     | 186   | 0        | 0        | 9       | 0            |
| 29  | T     | 94    | 0        | 0        | 3       | 0            |
| 29  | U     | 110   | 0        | 0        | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | V     | 71    | 0        | 0        | 2       | 0            |
| 29  | W     | 58    | 0        | 0        | 1       | 0            |
| 29  | X     | 57    | 0        | 0        | 1       | 0            |
| 29  | Y     | 40    | 0        | 0        | 3       | 0            |
| 29  | Z     | 37    | 0        | 0        | 1       | 0            |
| All | All   | 35054 | 0        | 31976    | 839     | 2            |

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 13.

All (839) 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) |
|---------------------|--------------------|--------------------------|-------------------|
| 19:C:302:PGV:C21    | 19:C:302:PGV:C22   | 1.77                     | 1.62              |
| 26:T:101:PEK:C3     | 26:T:101:PEK:C2    | 1.76                     | 1.56              |
| 2:B:1:FME:CN        | 2:B:1:FME:N        | 1.70                     | 1.53              |
| 3:P:224:LYS:CE      | 3:P:224:LYS:NZ     | 1.77                     | 1.47              |
| 20:D:201:TGL:OG2    | 20:D:201:TGL:CB1   | 1.63                     | 1.47              |
| 1:N:302[B]:ARG:NH1  | 1:N:361:SER:CB     | 1.76                     | 1.47              |
| 1:N:302[B]:ARG:HH12 | 1:N:361:SER:CB     | 1.27                     | 1.45              |
| 5:R:46:LYS:CE       | 5:R:46:LYS:NZ      | 1.73                     | 1.45              |
| 12:Y:20:ARG:HH22    | 12:Y:24[B]:MET:CE  | 1.36                     | 1.37              |
| 12:Y:20:ARG:NH2     | 20:Y:101:TGL:HC32  | 1.35                     | 1.37              |
| 2:B:22[B]:HIS:CE1   | 9:I:44:LYS:HE3     | 1.65                     | 1.31              |
| 12:L:20:ARG:NH2     | 20:L:101:TGL:HC32  | 1.43                     | 1.31              |
| 26:C:306:PEK:H383   | 25:G:102:CDL:C27   | 1.62                     | 1.26              |
| 2:O:22[B]:HIS:CE1   | 9:V:44:LYS:HE2     | 1.70                     | 1.25              |
| 18:A:606:PER:O2     | 18:A:606:PER:O1    | 1.55                     | 1.24              |
| 2:B:115:ASP:HB3     | 29:B:601:HOH:O     | 1.34                     | 1.23              |
| 1:N:302[B]:ARG:NH1  | 1:N:361:SER:HB2    | 0.92                     | 1.22              |
| 6:S:76:LYS:CE       | 6:S:93:PRO:HG2     | 1.68                     | 1.22              |
| 18:N:606:PER:O2     | 18:N:606:PER:O1    | 1.55                     | 1.21              |
| 4:D:100[B]:LYS:HE2  | 29:D:401:HOH:O     | 1.40                     | 1.17              |
| 12:Y:20:ARG:NH2     | 12:Y:24[B]:MET:CE  | 2.07                     | 1.17              |
| 7:G:5:LYS:HG3       | 26:G:103:PEK:H371  | 1.28                     | 1.15              |
| 12:L:9:LYS:HE3      | 29:L:224:HOH:O     | 1.42                     | 1.15              |
| 2:B:1:FME:N         | 2:B:1:FME:O1       | 1.80                     | 1.14              |
| 29:P:436:HOH:O      | 6:S:1:ALA:HB2      | 1.45                     | 1.14              |
| 23:O:303:PSC:H12    | 23:O:303:PSC:C34   | 1.77                     | 1.13              |
| 6:S:85:CYS:SG       | 6:S:87[A]:THR:HG23 | 1.88                     | 1.13              |
| 20:Q:202:TGL:H362   | 9:V:20:HIS:HE1     | 1.12                     | 1.12              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 11:K:54:ARG:HD2     | 29:K:141:HOH:O     | 1.45                     | 1.12              |
| 8:H:9:LYS:CE        | 8:H:9:LYS:HA       | 1.79                     | 1.11              |
| 26:C:306:PEK:H383   | 25:G:102:CDL:H273  | 1.13                     | 1.11              |
| 26:P:308:PEK:H383   | 25:T:103:CDL:H273  | 1.21                     | 1.10              |
| 12:Y:20:ARG:NH2     | 12:Y:24[B]:MET:HE1 | 1.64                     | 1.10              |
| 7:G:84:LYS:H        | 7:G:84:LYS:HD2     | 1.11                     | 1.09              |
| 26:P:308:PEK:C38    | 25:T:103:CDL:H273  | 1.82                     | 1.09              |
| 1:A:136[B]:LEU:HD11 | 29:A:988:HOH:O     | 1.52                     | 1.09              |
| 20:D:201:TGL:OG2    | 20:D:201:TGL:CB2   | 2.01                     | 1.08              |
| 8:H:9:LYS:HA        | 8:H:9:LYS:HE2      | 1.33                     | 1.08              |
| 1:A:486[B]:ASP:OD2  | 4:D:19[B]:ARG:HD2  | 1.52                     | 1.08              |
| 6:S:19:GLU:HG2      | 29:S:314:HOH:O     | 1.54                     | 1.07              |
| 1:A:513:LEU:O       | 1:A:514:LYS:HB2    | 1.54                     | 1.06              |
| 1:N:513:LEU:O       | 1:N:514:LYS:HB2    | 1.52                     | 1.06              |
| 23:O:303:PSC:H12    | 23:O:303:PSC:H342  | 1.34                     | 1.06              |
| 26:T:102:PEK:H361   | 25:T:103:CDL:H872  | 1.32                     | 1.06              |
| 6:S:76:LYS:HE2      | 6:S:93:PRO:HG2     | 1.11                     | 1.05              |
| 26:C:306:PEK:C38    | 25:G:102:CDL:C27   | 2.33                     | 1.05              |
| 19:Q:201:PGV:C2     | 19:Q:201:PGV:H011  | 1.84                     | 1.05              |
| 2:B:22[B]:HIS:CE1   | 9:I:44:LYS:CE      | 2.40                     | 1.04              |
| 12:Y:24[B]:MET:SD   | 20:Y:101:TGL:HC21  | 1.97                     | 1.04              |
| 12:L:14:SER:H       | 20:L:101:TGL:HC31  | 1.17                     | 1.04              |
| 1:N:417[A]:MET:HE2  | 29:N:880:HOH:O     | 1.56                     | 1.04              |
| 12:Y:20:ARG:HH22    | 12:Y:24[B]:MET:HE1 | 0.86                     | 1.03              |
| 4:Q:9:GLU:HB3       | 29:Q:427:HOH:O     | 1.54                     | 1.03              |
| 20:Y:101:TGL:HC41   | 20:Y:101:TGL:OC1   | 1.21                     | 1.03              |
| 1:A:282:PHE:HA      | 7:T:4:ALA:HB3      | 1.41                     | 1.03              |
| 12:Y:20:ARG:HH21    | 20:Y:101:TGL:CC3   | 1.72                     | 1.02              |
| 19:A:608:PGV:H311   | 13:M:19:LEU:HD23   | 1.41                     | 1.02              |
| 1:N:483:LEU:HD13    | 4:Q:6:VAL:HB       | 1.39                     | 1.02              |
| 1:N:513:LEU:O       | 1:N:514:LYS:CB     | 2.04                     | 1.02              |
| 4:Q:65:LYS:HE3      | 29:Q:421:HOH:O     | 1.55                     | 1.02              |
| 12:Y:20:ARG:NH2     | 20:Y:101:TGL:CC3   | 2.23                     | 1.01              |
| 5:E:90:ARG:HD2      | 29:E:311:HOH:O     | 1.58                     | 1.01              |
| 26:P:308:PEK:C38    | 25:T:103:CDL:C27   | 2.39                     | 1.01              |
| 1:N:302[B]:ARG:HH11 | 1:N:361:SER:HB2    | 1.19                     | 1.01              |
| 20:Q:202:TGL:H362   | 9:V:20:HIS:CE1     | 1.97                     | 0.99              |
| 7:G:5:LYS:HB2       | 26:G:103:PEK:H351  | 1.45                     | 0.98              |
| 7:G:11:TPO:HG22     | 7:G:16:TRP:HE1     | 1.28                     | 0.98              |
| 29:A:964:HOH:O      | 20:D:201:TGL:HC31  | 1.62                     | 0.98              |
| 1:N:486:ASP:OD2     | 4:Q:19[B]:ARG:HD2  | 1.64                     | 0.97              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B:49:LYS:HE2     | 29:B:609:HOH:O    | 1.65                     | 0.97              |
| 12:Y:14:SER:H      | 20:Y:101:TGL:HC31 | 1.31                     | 0.95              |
| 6:F:1:ALA:HB3      | 6:S:65:ASP:OD1    | 1.67                     | 0.95              |
| 1:A:178[B]:GLN:NE2 | 29:A:701:HOH:O    | 1.97                     | 0.95              |
| 26:C:306:PEK:C38   | 25:G:102:CDL:H273 | 1.93                     | 0.94              |
| 25:G:102:CDL:C24   | 25:G:102:CDL:H541 | 1.96                     | 0.94              |
| 26:P:308:PEK:H382  | 25:T:103:CDL:C27  | 1.98                     | 0.94              |
| 7:G:4:ALA:CB       | 1:N:282:PHE:HA    | 1.98                     | 0.94              |
| 23:O:303:PSC:H342  | 23:O:303:PSC:C12  | 1.96                     | 0.94              |
| 26:P:308:PEK:H051  | 29:P:476:HOH:O    | 1.67                     | 0.93              |
| 6:S:76:LYS:HE2     | 6:S:93:PRO:CG     | 1.99                     | 0.93              |
| 3:C:67:PHE:HE1     | 25:C:303:CDL:H1   | 1.35                     | 0.92              |
| 12:L:20:ARG:HH22   | 20:L:101:TGL:CC3  | 1.81                     | 0.92              |
| 2:O:22[B]:HIS:HE1  | 9:V:44:LYS:HE2    | 1.27                     | 0.92              |
| 2:B:87[B]:MET:HE2  | 29:B:417:HOH:O    | 1.70                     | 0.92              |
| 3:C:51[B]:MET:HE2  | 25:C:303:CDL:H391 | 1.50                     | 0.92              |
| 1:N:178[B]:GLN:HG3 | 1:N:186:TRP:CZ2   | 2.04                     | 0.92              |
| 25:T:103:CDL:H242  | 25:T:103:CDL:H541 | 1.48                     | 0.92              |
| 2:B:22[B]:HIS:HE1  | 9:I:44:LYS:HE3    | 1.11                     | 0.91              |
| 2:B:56:MET:HA      | 23:B:304:PSC:H201 | 1.51                     | 0.91              |
| 3:C:180[B]:GLU:HG2 | 29:C:422:HOH:O    | 1.70                     | 0.91              |
| 19:Q:201:PGV:H011  | 19:Q:201:PGV:H22  | 1.51                     | 0.91              |
| 23:O:303:PSC:H71   | 29:V:170:HOH:O    | 1.69                     | 0.90              |
| 3:C:224:LYS:CD     | 25:C:303:CDL:HB31 | 2.00                     | 0.90              |
| 2:B:1:FME:CN       | 2:B:1:FME:CA      | 2.49                     | 0.90              |
| 1:A:282:PHE:HA     | 7:T:4:ALA:CB      | 2.01                     | 0.89              |
| 8:U:9:LYS:HG2      | 29:U:187:HOH:O    | 1.71                     | 0.89              |
| 1:A:486[B]:ASP:OD2 | 4:D:19[B]:ARG:CD  | 2.20                     | 0.89              |
| 7:G:72:ASN:H       | 7:G:76:ASN:HD22   | 1.17                     | 0.89              |
| 19:A:607:PGV:H343  | 26:G:101:PEK:H382 | 1.55                     | 0.88              |
| 12:L:20:ARG:HH22   | 20:L:101:TGL:HC32 | 1.12                     | 0.88              |
| 1:A:417[B]:MET:CE  | 29:A:816:HOH:O    | 2.21                     | 0.88              |
| 12:Y:20:ARG:NH2    | 12:Y:24[B]:MET:SD | 2.47                     | 0.88              |
| 23:B:304:PSC:H02   | 23:B:304:PSC:H212 | 1.54                     | 0.88              |
| 3:P:156:ARG:HE     | 22:P:305:CHD:H232 | 1.38                     | 0.88              |
| 3:P:67:PHE:HE1     | 25:P:304:CDL:H1   | 1.39                     | 0.87              |
| 4:D:19[A]:ARG:NH2  | 4:D:21:ASP:OD1    | 2.07                     | 0.87              |
| 20:Y:101:TGL:OC1   | 20:Y:101:TGL:CC4  | 2.17                     | 0.87              |
| 12:L:20:ARG:NH2    | 20:L:101:TGL:CC3  | 2.34                     | 0.86              |
| 4:Q:6:VAL:HG12     | 4:Q:10:ASP:OD2    | 1.74                     | 0.86              |
| 7:T:72:ASN:H       | 7:T:76:ASN:HD22   | 1.19                     | 0.86              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:Q:9:GLU:OE2       | 4:Q:9:GLU:HA       | 1.76                     | 0.86              |
| 2:B:22[B]:HIS:HE1   | 9:I:44:LYS:CE      | 1.79                     | 0.85              |
| 25:G:102:CDL:H212   | 1:N:311[A]:ILE:CD1 | 2.07                     | 0.85              |
| 23:O:303:PSC:H12    | 23:O:303:PSC:H343  | 1.58                     | 0.85              |
| 6:S:75:HIS:H        | 6:S:80:GLN:HE22    | 1.21                     | 0.85              |
| 1:A:178[B]:GLN:HG3  | 7:T:7:ASP:OD2      | 1.77                     | 0.85              |
| 10:J:49:CYS:HB3     | 28:J:101:DMU:H9    | 1.58                     | 0.84              |
| 6:S:94:HIS:CD2      | 6:S:95:GLN:H       | 1.93                     | 0.84              |
| 1:N:136[B]:LEU:HD11 | 29:N:976:HOH:O     | 1.77                     | 0.84              |
| 3:P:50:ASN:HD22     | 3:P:51[A]:MET:HE2  | 1.43                     | 0.84              |
| 7:G:84:LYS:H        | 7:G:84:LYS:CD      | 1.89                     | 0.84              |
| 2:O:29[B]:MET:SD    | 2:O:33:LEU:HD22    | 2.18                     | 0.83              |
| 7:G:4:ALA:HB1       | 1:N:282:PHE:HA     | 1.59                     | 0.83              |
| 1:N:417[A]:MET:CE   | 29:N:880:HOH:O     | 2.19                     | 0.83              |
| 6:F:75:HIS:H        | 6:F:80:GLN:HE22    | 1.26                     | 0.83              |
| 1:N:514:LYS:HA      | 6:S:38:ALA:HB3     | 1.61                     | 0.83              |
| 1:N:321:PHE:CD2     | 23:O:303:PSC:H341  | 2.12                     | 0.83              |
| 1:A:513:LEU:O       | 1:A:514:LYS:CB     | 2.27                     | 0.82              |
| 3:C:224:LYS:HE3     | 25:C:303:CDL:HB31  | 1.61                     | 0.82              |
| 12:Y:24[B]:MET:HG2  | 20:Y:101:TGL:HA22  | 1.61                     | 0.82              |
| 25:G:102:CDL:H352   | 2:O:78:LEU:HD12    | 1.59                     | 0.82              |
| 19:Q:201:PGV:H011   | 19:Q:201:PGV:H21   | 1.61                     | 0.82              |
| 1:N:28:MET:CE       | 14:N:601:HEA:H271  | 2.10                     | 0.81              |
| 1:A:178[B]:GLN:CD   | 1:A:178[B]:GLN:H   | 1.87                     | 0.81              |
| 25:G:102:CDL:H541   | 25:G:102:CDL:H241  | 1.61                     | 0.81              |
| 20:D:201:TGL:CB1    | 20:D:201:TGL:CG2   | 2.57                     | 0.81              |
| 26:P:308:PEK:H383   | 25:T:103:CDL:C27   | 2.04                     | 0.81              |
| 7:T:30:LEU:HD21     | 25:T:103:CDL:H471  | 1.61                     | 0.81              |
| 19:Q:201:PGV:H311   | 13:Z:19:LEU:HD23   | 1.63                     | 0.81              |
| 6:F:85:CYS:SG       | 6:F:87[A]:THR:HG23 | 2.21                     | 0.81              |
| 6:S:94:HIS:HA       | 29:S:318:HOH:O     | 1.81                     | 0.81              |
| 12:L:20:ARG:HH21    | 20:L:101:TGL:HC32  | 1.42                     | 0.81              |
| 3:P:63:ARG:HE       | 25:P:304:CDL:CA2   | 1.93                     | 0.80              |
| 8:H:9:LYS:CE        | 8:H:9:LYS:CA       | 2.53                     | 0.80              |
| 3:C:161[A]:GLN:HE22 | 26:C:306:PEK:C2    | 1.95                     | 0.80              |
| 2:B:16[B]:ILE:HG23  | 29:B:523:HOH:O     | 1.80                     | 0.79              |
| 25:T:103:CDL:H181   | 25:T:103:CDL:H511  | 1.61                     | 0.79              |
| 7:G:37:LEU:HD21     | 25:G:102:CDL:H361  | 1.65                     | 0.79              |
| 6:F:54[A]:ASN:HD22  | 6:F:54[A]:ASN:H    | 1.29                     | 0.79              |
| 20:Q:202:TGL:H352   | 9:V:16:ARG:HE      | 1.46                     | 0.79              |
| 26:P:308:PEK:H382   | 25:T:103:CDL:H272  | 1.64                     | 0.79              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:Q:19[A]:ARG:HG2   | 4:Q:21:ASP:OD1     | 1.81                     | 0.79              |
| 3:P:160:LEU:HD13    | 22:P:305:CHD:H181  | 1.65                     | 0.79              |
| 12:Y:20:ARG:HH21    | 20:Y:101:TGL:HC32  | 0.89                     | 0.79              |
| 3:C:67:PHE:CE1      | 25:C:303:CDL:H1    | 2.18                     | 0.78              |
| 12:Y:24[B]:MET:SD   | 20:Y:101:TGL:CC2   | 2.72                     | 0.78              |
| 3:C:224:LYS:CE      | 25:C:303:CDL:HB31  | 2.11                     | 0.78              |
| 3:P:156:ARG:HE      | 22:P:305:CHD:C23   | 1.96                     | 0.78              |
| 3:C:63:ARG:HE       | 25:C:303:CDL:CA2   | 1.96                     | 0.78              |
| 8:H:9:LYS:HE2       | 8:H:9:LYS:CA       | 2.13                     | 0.78              |
| 2:B:82:ARG:HD2      | 29:B:403:HOH:O     | 1.82                     | 0.78              |
| 26:P:308:PEK:N      | 26:P:308:PEK:O02   | 2.16                     | 0.78              |
| 26:C:306:PEK:H383   | 25:G:102:CDL:H271  | 1.63                     | 0.77              |
| 7:T:36:TRP:HE3      | 7:T:39:SER:HB3     | 1.47                     | 0.77              |
| 3:C:63:ARG:HE       | 25:C:303:CDL:HA21  | 1.48                     | 0.77              |
| 26:T:101:PEK:C3     | 26:T:101:PEK:C1    | 2.62                     | 0.77              |
| 1:N:28:MET:CE       | 14:N:601:HEA:C27   | 2.63                     | 0.77              |
| 4:D:34:SER:H        | 4:D:37:GLN:HE21    | 1.33                     | 0.77              |
| 19:C:302:PGV:C21    | 19:C:302:PGV:H221  | 2.12                     | 0.77              |
| 25:G:102:CDL:H332   | 29:O:488:HOH:O     | 1.85                     | 0.77              |
| 25:G:102:CDL:H342   | 25:G:102:CDL:OA7   | 1.84                     | 0.77              |
| 3:P:67:PHE:CE1      | 25:P:304:CDL:H1    | 2.20                     | 0.77              |
| 20:N:608:TGL:H281   | 20:N:608:TGL:HB91  | 1.68                     | 0.76              |
| 19:P:303:PGV:H172   | 25:P:304:CDL:H642  | 1.65                     | 0.76              |
| 23:O:303:PSC:C34    | 23:O:303:PSC:C12   | 2.59                     | 0.76              |
| 4:D:78:TRP:CA       | 20:D:201:TGL:HB21  | 2.15                     | 0.75              |
| 6:S:43:LYS:HD2      | 6:S:43:LYS:H       | 1.52                     | 0.75              |
| 2:B:74:ILE:O        | 2:B:78:LEU:HD13    | 1.85                     | 0.75              |
| 12:L:20:ARG:HH22    | 20:L:101:TGL:HC52  | 1.52                     | 0.75              |
| 1:A:53:ILE:HG13     | 29:A:980:HOH:O     | 1.87                     | 0.75              |
| 2:B:56:MET:HG2      | 23:B:304:PSC:H211  | 1.68                     | 0.75              |
| 20:L:101:TGL:H362   | 20:L:101:TGL:H312  | 1.67                     | 0.75              |
| 20:N:608:TGL:H281   | 20:N:608:TGL:CB9   | 2.17                     | 0.75              |
| 1:N:297[B]:MET:SD   | 1:N:302[B]:ARG:HG3 | 2.27                     | 0.74              |
| 1:A:514:LYS:HA      | 6:F:38:ALA:HB3     | 1.69                     | 0.74              |
| 2:B:53:THR:HG21     | 29:D:305:HOH:O     | 1.88                     | 0.74              |
| 26:P:308:PEK:H041   | 7:T:17:ARG:HH22    | 1.52                     | 0.74              |
| 3:C:224:LYS:HD2     | 25:C:303:CDL:HB31  | 1.68                     | 0.74              |
| 1:N:406:ASN:HD21    | 19:Q:201:PGV:H21   | 1.52                     | 0.73              |
| 3:C:33[B]:MET:HG2   | 3:C:39:SER:O       | 1.88                     | 0.73              |
| 3:C:161[A]:GLN:HE22 | 26:C:306:PEK:H22   | 1.50                     | 0.73              |
| 25:C:303:CDL:H522   | 25:C:303:CDL:OB9   | 1.88                     | 0.73              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 26:P:308:PEK:H042   | 6:S:1:ALA:H1        | 1.53                     | 0.73              |
| 25:T:103:CDL:H762   | 25:T:103:CDL:H562   | 1.69                     | 0.73              |
| 6:S:43:LYS:H        | 6:S:43:LYS:CD       | 2.00                     | 0.73              |
| 25:G:102:CDL:H212   | 1:N:311[A]:ILE:HD12 | 1.69                     | 0.73              |
| 3:P:33[A]:MET:HB2   | 28:P:306:DMU:H8     | 1.70                     | 0.73              |
| 25:G:102:CDL:H522   | 25:G:102:CDL:H201   | 1.71                     | 0.73              |
| 3:P:33[B]:MET:HE3   | 28:P:306:DMU:H6     | 1.70                     | 0.73              |
| 7:G:76:ASN:HD21     | 26:G:101:PEK:HN2    | 1.37                     | 0.72              |
| 23:O:303:PSC:H212   | 23:O:303:PSC:H02    | 1.71                     | 0.72              |
| 3:P:156:ARG:NE      | 22:P:305:CHD:H232   | 2.05                     | 0.72              |
| 7:T:11:TPO:HG22     | 7:T:16:TRP:HE1      | 1.55                     | 0.72              |
| 3:P:33[A]:MET:HB2   | 28:P:306:DMU:C19    | 2.20                     | 0.71              |
| 19:A:607:PGV:H183   | 26:G:101:PEK:H322   | 1.71                     | 0.71              |
| 2:O:60:GLU:CD       | 2:O:60:GLU:H        | 1.97                     | 0.71              |
| 12:L:20:ARG:HH22    | 20:L:101:TGL:CC5    | 2.03                     | 0.71              |
| 7:T:30:LEU:CD2      | 25:T:103:CDL:H471   | 2.20                     | 0.70              |
| 2:B:49:LYS:HD3      | 20:D:201:TGL:HC71   | 1.73                     | 0.70              |
| 7:T:36:TRP:CE3      | 7:T:39:SER:HB3      | 2.26                     | 0.70              |
| 8:U:45:ALA:O        | 8:U:47:GLY:N        | 2.25                     | 0.70              |
| 1:N:302[B]:ARG:HH12 | 1:N:361:SER:CA      | 2.04                     | 0.70              |
| 3:P:63:ARG:HE       | 25:P:304:CDL:HA22   | 1.54                     | 0.70              |
| 1:A:112:LEU:HG      | 29:A:937:HOH:O      | 1.90                     | 0.70              |
| 2:O:22[B]:HIS:CE1   | 9:V:44:LYS:CE       | 2.63                     | 0.70              |
| 1:N:178[B]:GLN:CG   | 1:N:186:TRP:CZ2     | 2.73                     | 0.70              |
| 4:Q:6:VAL:CG1       | 4:Q:10:ASP:OD2      | 2.40                     | 0.70              |
| 12:Y:14:SER:N       | 20:Y:101:TGL:HC31   | 2.06                     | 0.70              |
| 4:D:31[A]:LYS:CG    | 29:D:301:HOH:O      | 2.40                     | 0.70              |
| 25:G:102:CDL:H241   | 25:G:102:CDL:C54    | 2.21                     | 0.70              |
| 20:Q:202:TGL:H231   | 20:Q:202:TGL:CA9    | 2.21                     | 0.70              |
| 19:C:302:PGV:C21    | 19:C:302:PGV:H222   | 2.12                     | 0.70              |
| 1:N:28:MET:HE1      | 14:N:601:HEA:C27    | 2.22                     | 0.70              |
| 2:B:29[B]:MET:SD    | 2:B:33:LEU:HD22     | 2.32                     | 0.69              |
| 2:O:87[B]:MET:HE2   | 29:O:411:HOH:O      | 1.90                     | 0.69              |
| 1:A:406:ASN:HD21    | 19:A:608:PGV:H22    | 1.56                     | 0.69              |
| 10:J:33:ARG:HG2     | 22:J:102:CHD:H152   | 1.75                     | 0.69              |
| 1:A:28:MET:CE       | 14:A:601:HEA:C27    | 2.71                     | 0.69              |
| 2:O:56:MET:HG2      | 23:O:303:PSC:H211   | 1.75                     | 0.69              |
| 3:P:127:LEU:HD13    | 25:T:103:CDL:OB3    | 1.92                     | 0.69              |
| 7:T:76:ASN:HD21     | 26:T:101:PEK:HN2    | 1.36                     | 0.69              |
| 11:K:47:ARG:HD3     | 29:K:160:HOH:O      | 1.91                     | 0.69              |
| 1:A:177:SER:H       | 1:A:180:GLN:HE21    | 1.40                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:P:301:PGV:H32   | 29:P:523:HOH:O     | 1.91                     | 0.69              |
| 5:R:80:GLU:H       | 5:R:80:GLU:CD      | 2.00                     | 0.68              |
| 6:S:94:HIS:HD2     | 6:S:95:GLN:O       | 1.76                     | 0.68              |
| 25:T:103:CDL:H511  | 25:T:103:CDL:C18   | 2.23                     | 0.68              |
| 26:P:308:PEK:H042  | 6:S:1:ALA:N        | 2.08                     | 0.68              |
| 6:F:92:VAL:HG21    | 29:F:387:HOH:O     | 1.94                     | 0.68              |
| 1:N:178[B]:GLN:HG3 | 1:N:186:TRP:CE2    | 2.29                     | 0.67              |
| 3:P:63:ARG:HE      | 25:P:304:CDL:HA21  | 1.59                     | 0.67              |
| 10:W:10:LYS:O      | 10:W:14[B]:GLU:HG3 | 1.94                     | 0.67              |
| 7:T:38:HIS:HD2     | 29:T:210:HOH:O     | 1.76                     | 0.67              |
| 25:P:304:CDL:OB9   | 25:P:304:CDL:H522  | 1.94                     | 0.67              |
| 1:A:484:THR:HG22   | 29:A:972:HOH:O     | 1.94                     | 0.67              |
| 1:N:28:MET:HE1     | 14:N:601:HEA:H271  | 1.76                     | 0.67              |
| 8:U:48:GLY:HA2     | 29:U:176:HOH:O     | 1.94                     | 0.67              |
| 14:N:602:HEA:HBC1  | 14:N:602:HEA:HMC1  | 1.77                     | 0.67              |
| 1:N:302[B]:ARG:NH1 | 1:N:361:SER:OG     | 2.28                     | 0.67              |
| 19:P:303:PGV:H172  | 25:P:304:CDL:C64   | 2.25                     | 0.67              |
| 1:A:273:MET:HE2    | 29:A:888:HOH:O     | 1.94                     | 0.66              |
| 7:G:72:ASN:H       | 7:G:76:ASN:ND2     | 1.93                     | 0.66              |
| 25:P:304:CDL:HB21  | 25:P:304:CDL:OB6   | 1.95                     | 0.66              |
| 7:T:5:LYS:HG3      | 26:T:102:PEK:H351  | 1.76                     | 0.66              |
| 2:B:33:LEU:HD13    | 9:I:31:PHE:CD1     | 2.30                     | 0.66              |
| 7:G:11:TPO:HG21    | 29:G:280:HOH:O     | 1.96                     | 0.66              |
| 8:H:23:GLN:HG3     | 29:H:166:HOH:O     | 1.95                     | 0.66              |
| 10:W:33:ARG:HG2    | 22:W:101:CHD:H182  | 1.76                     | 0.66              |
| 12:L:14:SER:N      | 20:L:101:TGL:HC31  | 2.01                     | 0.66              |
| 6:S:43:LYS:HE2     | 29:S:342:HOH:O     | 1.95                     | 0.66              |
| 3:P:4:GLN:N        | 29:P:401:HOH:O     | 2.29                     | 0.66              |
| 7:T:37:LEU:HD23    | 25:T:103:CDL:H361  | 1.77                     | 0.66              |
| 29:C:541:HOH:O     | 10:J:1:PHE:HE2     | 1.79                     | 0.65              |
| 23:O:303:PSC:H212  | 23:O:303:PSC:C02   | 2.26                     | 0.65              |
| 4:Q:78:TRP:N       | 20:Q:202:TGL:HB21  | 2.11                     | 0.65              |
| 4:D:31[A]:LYS:HG2  | 29:D:301:HOH:O     | 1.95                     | 0.65              |
| 7:G:3:ALA:HB3      | 26:G:103:PEK:H362  | 1.79                     | 0.65              |
| 2:O:29[B]:MET:SD   | 2:O:33:LEU:CD2     | 2.84                     | 0.65              |
| 6:S:94:HIS:CD2     | 6:S:95:GLN:N       | 2.64                     | 0.65              |
| 26:T:102:PEK:C36   | 25:T:103:CDL:H872  | 2.20                     | 0.65              |
| 12:Y:20:ARG:CZ     | 12:Y:24[B]:MET:CE  | 2.75                     | 0.65              |
| 7:G:3:ALA:CB       | 26:G:103:PEK:H383  | 2.27                     | 0.64              |
| 29:N:703:HOH:O     | 4:Q:6:VAL:HG11     | 1.97                     | 0.64              |
| 10:J:32:TYR:OH     | 22:J:102:CHD:H213  | 1.97                     | 0.64              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:R:46:LYS:NZ       | 5:R:46:LYS:CD      | 2.56                     | 0.64              |
| 6:F:41:GLY:HA3      | 6:F:87[B]:THR:HG22 | 1.80                     | 0.64              |
| 7:G:5:LYS:CG        | 26:G:103:PEK:H371  | 2.17                     | 0.64              |
| 23:O:303:PSC:C28    | 23:O:303:PSC:H322  | 2.27                     | 0.64              |
| 1:A:468:MET:HG3     | 29:A:957:HOH:O     | 1.97                     | 0.64              |
| 1:N:302[B]:ARG:HH11 | 1:N:361:SER:CB     | 1.87                     | 0.64              |
| 4:D:28:ALA:H        | 4:D:31[B]:LYS:NZ   | 1.95                     | 0.63              |
| 8:H:47:GLY:HA2      | 29:H:180:HOH:O     | 1.97                     | 0.63              |
| 1:N:177:SER:H       | 1:N:180:GLN:HE21   | 1.46                     | 0.63              |
| 1:N:297[B]:MET:HB3  | 1:N:302[B]:ARG:HD2 | 1.79                     | 0.63              |
| 2:O:22[B]:HIS:HE1   | 9:V:44:LYS:CE      | 2.06                     | 0.63              |
| 19:A:608:PGV:H061   | 19:A:608:PGV:O11   | 1.99                     | 0.63              |
| 7:G:3:ALA:HB1       | 26:G:103:PEK:H383  | 1.79                     | 0.63              |
| 7:T:84:LYS:H        | 7:T:84:LYS:NZ      | 1.96                     | 0.63              |
| 2:B:83:ILE:O        | 2:B:87[A]:MET:HG3  | 1.99                     | 0.62              |
| 14:N:601:HEA:HBC1   | 14:N:601:HEA:HMC1  | 1.81                     | 0.62              |
| 13:M:39:ASN:O       | 13:M:43:SER:HB3    | 1.99                     | 0.62              |
| 7:T:72:ASN:H        | 7:T:76:ASN:ND2     | 1.94                     | 0.62              |
| 2:B:1:FME:HCN       | 2:B:193:TYR:H      | 1.64                     | 0.62              |
| 6:S:22:LEU:HD12     | 29:S:329:HOH:O     | 1.99                     | 0.62              |
| 7:T:84:LYS:H        | 7:T:84:LYS:HZ3     | 1.47                     | 0.62              |
| 20:Q:202:TGL:H231   | 20:Q:202:TGL:HA92  | 1.81                     | 0.62              |
| 13:Z:42:LYS:O       | 13:Z:42:LYS:HG3    | 1.99                     | 0.62              |
| 2:O:92:ASN:HB3      | 29:U:128:HOH:O     | 1.99                     | 0.62              |
| 7:T:11:TPO:CG2      | 7:T:11:TPO:O       | 2.48                     | 0.62              |
| 20:D:201:TGL:CB1    | 20:D:201:TGL:CG3   | 2.77                     | 0.62              |
| 25:G:102:CDL:H541   | 25:G:102:CDL:H242  | 1.80                     | 0.62              |
| 1:A:281:GLY:C       | 7:T:4:ALA:HB1      | 2.25                     | 0.61              |
| 20:N:608:TGL:HB91   | 20:N:608:TGL:C28   | 2.30                     | 0.61              |
| 6:S:94:HIS:CG       | 6:S:95:GLN:H       | 2.14                     | 0.61              |
| 1:A:334:TRP:CH2     | 2:B:46:LEU:HD13    | 2.35                     | 0.61              |
| 2:O:47:THR:HB       | 20:Q:202:TGL:H181  | 1.81                     | 0.61              |
| 2:B:32[B]:PHE:CD2   | 9:I:31:PHE:CZ      | 2.89                     | 0.61              |
| 4:Q:78:TRP:HB3      | 20:Q:202:TGL:HB22  | 1.83                     | 0.61              |
| 6:S:43:LYS:HD3      | 29:S:251:HOH:O     | 1.99                     | 0.61              |
| 20:Y:101:TGL:HG31   | 29:Y:221:HOH:O     | 2.00                     | 0.61              |
| 23:B:304:PSC:H212   | 23:B:304:PSC:C02   | 2.28                     | 0.61              |
| 20:D:201:TGL:HC32   | 20:D:201:TGL:HG12  | 1.82                     | 0.60              |
| 5:R:46:LYS:NZ       | 29:R:202:HOH:O     | 2.34                     | 0.60              |
| 6:S:76:LYS:NZ       | 6:S:93:PRO:HG2     | 2.15                     | 0.60              |
| 1:A:28:MET:HE1      | 14:A:601:HEA:C27   | 2.31                     | 0.60              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:B:183[A]:THR:HG22 | 29:B:462:HOH:O     | 2.00                     | 0.60              |
| 26:G:101:PEK:C12    | 26:G:101:PEK:H161  | 2.30                     | 0.60              |
| 19:A:608:PGV:H311   | 13:M:19:LEU:CD2    | 2.26                     | 0.60              |
| 1:A:417[B]:MET:HE2  | 29:A:816:HOH:O     | 1.97                     | 0.60              |
| 19:C:302:PGV:H12    | 19:C:302:PGV:H161  | 1.84                     | 0.60              |
| 6:F:94:HIS:CE1      | 29:F:203:HOH:O     | 2.53                     | 0.60              |
| 1:N:468:MET:HG3     | 29:N:943:HOH:O     | 2.00                     | 0.60              |
| 20:D:201:TGL:H231   | 20:D:201:TGL:HA91  | 1.84                     | 0.60              |
| 1:A:278[B]:MET:CE   | 7:T:5:LYS:HB3      | 2.31                     | 0.60              |
| 6:S:19:GLU:OE1      | 6:S:31:TYR:OH      | 2.17                     | 0.60              |
| 7:T:38:HIS:CD2      | 29:T:210:HOH:O     | 2.50                     | 0.60              |
| 7:T:3:ALA:O         | 7:T:4:ALA:HB2      | 2.02                     | 0.59              |
| 8:U:43:MET:CE       | 8:U:49:ASP:H       | 2.15                     | 0.59              |
| 1:A:514:LYS:HD2     | 29:F:252:HOH:O     | 2.02                     | 0.59              |
| 13:M:41:LYS:NZ      | 29:M:201:HOH:O     | 2.34                     | 0.59              |
| 2:B:52:HIS:HE1      | 23:B:304:PSC:H212  | 1.66                     | 0.59              |
| 6:F:54[A]:ASN:H     | 6:F:54[A]:ASN:ND2  | 1.99                     | 0.59              |
| 1:N:334:TRP:CH2     | 2:O:46:LEU:HD13    | 2.37                     | 0.59              |
| 3:P:224:LYS:CD      | 25:P:304:CDL:HB32  | 2.32                     | 0.59              |
| 6:S:43:LYS:CE       | 29:S:342:HOH:O     | 2.48                     | 0.59              |
| 3:C:161[A]:GLN:HE22 | 26:C:306:PEK:H21   | 1.66                     | 0.59              |
| 4:D:78:TRP:HA       | 20:D:201:TGL:HB21  | 1.84                     | 0.59              |
| 26:C:306:PEK:H382   | 25:G:102:CDL:C27   | 2.29                     | 0.59              |
| 3:C:224:LYS:CD      | 25:C:303:CDL:CB3   | 2.77                     | 0.58              |
| 6:F:54[A]:ASN:HD22  | 6:F:54[A]:ASN:N    | 2.00                     | 0.58              |
| 2:B:52:HIS:CE1      | 23:B:304:PSC:H211  | 2.38                     | 0.58              |
| 29:C:541:HOH:O      | 10:J:1:PHE:CE2     | 2.52                     | 0.58              |
| 6:F:30:PRO:O        | 6:F:96:LEU:HD11    | 2.02                     | 0.58              |
| 25:G:102:CDL:HA21   | 25:G:102:CDL:H111  | 1.86                     | 0.58              |
| 20:Y:101:TGL:CG3    | 29:Y:221:HOH:O     | 2.52                     | 0.58              |
| 23:O:303:PSC:H012   | 23:O:303:PSC:P     | 2.43                     | 0.58              |
| 7:T:31:CYS:SG       | 25:T:103:CDL:H532  | 2.43                     | 0.58              |
| 12:Y:24[B]:MET:CG   | 20:Y:101:TGL:HA22  | 2.32                     | 0.58              |
| 3:C:51[B]:MET:CE    | 25:C:303:CDL:H391  | 2.29                     | 0.58              |
| 1:N:273:MET:HE2     | 29:N:749:HOH:O     | 2.03                     | 0.58              |
| 4:D:78:TRP:N        | 20:D:201:TGL:HB21  | 2.17                     | 0.58              |
| 12:L:2:HIS:CG       | 12:L:3:TYR:H       | 2.21                     | 0.58              |
| 8:U:43:MET:HE3      | 8:U:49:ASP:N       | 2.18                     | 0.58              |
| 1:A:113[B]:LEU:HD11 | 1:A:117[B]:MET:SD  | 2.43                     | 0.58              |
| 7:G:4:ALA:HB1       | 1:N:282:PHE:CA     | 2.32                     | 0.58              |
| 1:N:302[B]:ARG:HH11 | 1:N:302[B]:ARG:HG2 | 1.66                     | 0.58              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:C:55:TYR:CE1      | 25:C:303:CDL:H532  | 2.38                     | 0.58              |
| 7:G:84:LYS:HD2      | 7:G:84:LYS:N       | 1.97                     | 0.58              |
| 1:A:302[B]:ARG:NE   | 1:A:361[B]:SER:OG  | 2.35                     | 0.58              |
| 7:G:4:ALA:HB3       | 1:N:282:PHE:HA     | 1.81                     | 0.58              |
| 7:T:2:SER:OG        | 26:T:102:PEK:H302  | 2.04                     | 0.58              |
| 6:F:87[A]:THR:HG21  | 29:F:324:HOH:O     | 2.03                     | 0.57              |
| 2:B:70:ALA:HB1      | 25:T:103:CDL:H461  | 1.86                     | 0.57              |
| 10:J:50:LEU:HB2     | 28:J:101:DMU:H20   | 1.86                     | 0.57              |
| 19:P:301:PGV:H062   | 8:U:24:ASN:HB3     | 1.86                     | 0.57              |
| 2:B:1:FME:CN        | 2:B:1:FME:HA       | 2.35                     | 0.57              |
| 2:O:42:ILE:HG21     | 20:Q:202:TGL:H232  | 1.86                     | 0.57              |
| 19:A:607:PGV:C18    | 26:G:101:PEK:H322  | 2.34                     | 0.57              |
| 25:G:102:CDL:HA31   | 29:G:267:HOH:O     | 2.04                     | 0.57              |
| 1:N:35:LEU:HD11     | 1:N:462:LEU:HB2    | 1.87                     | 0.57              |
| 7:G:9:GLY:HA3       | 29:N:797:HOH:O     | 2.05                     | 0.57              |
| 3:C:224:LYS:HE3     | 25:C:303:CDL:CB3   | 2.32                     | 0.57              |
| 20:Y:101:TGL:HC42   | 29:Y:225:HOH:O     | 2.04                     | 0.56              |
| 1:A:177:SER:H       | 1:A:180:GLN:NE2    | 2.03                     | 0.56              |
| 12:L:46:LYS:HA      | 29:L:217:HOH:O     | 2.04                     | 0.56              |
| 3:C:63:ARG:HE       | 25:C:303:CDL:HA22  | 1.69                     | 0.56              |
| 6:F:94:HIS:HE1      | 29:F:203:HOH:O     | 1.85                     | 0.56              |
| 1:N:116:SER:HB3     | 29:N:931:HOH:O     | 2.05                     | 0.56              |
| 1:A:302[B]:ARG:NE   | 2:B:84:LEU:HD11    | 2.20                     | 0.56              |
| 3:C:174:THR:HG21    | 25:C:303:CDL:H861  | 1.88                     | 0.56              |
| 1:N:177:SER:H       | 1:N:180:GLN:NE2    | 2.04                     | 0.56              |
| 2:B:52:HIS:HE1      | 23:B:304:PSC:C21   | 2.18                     | 0.56              |
| 6:F:54[B]:ASN:ND2   | 29:F:203:HOH:O     | 2.39                     | 0.56              |
| 20:N:608:TGL:H281   | 20:N:608:TGL:HB92  | 1.88                     | 0.56              |
| 1:N:136[B]:LEU:CD1  | 29:N:976:HOH:O     | 2.47                     | 0.56              |
| 23:B:304:PSC:H032   | 29:E:275:HOH:O     | 2.05                     | 0.56              |
| 25:G:102:CDL:H511   | 25:G:102:CDL:H182  | 1.87                     | 0.56              |
| 26:T:101:PEK:C2     | 26:T:101:PEK:H32   | 2.19                     | 0.55              |
| 2:B:29[B]:MET:SD    | 2:B:33:LEU:CD2     | 2.93                     | 0.55              |
| 4:D:34:SER:H        | 4:D:37:GLN:NE2     | 2.03                     | 0.55              |
| 7:G:5:LYS:HD3       | 1:N:278[B]:MET:HE3 | 1.89                     | 0.55              |
| 8:H:8:ILE:O         | 8:H:8:ILE:HG22     | 2.06                     | 0.55              |
| 1:A:311[B]:ILE:HG13 | 1:A:314:ILE:HD12   | 1.87                     | 0.55              |
| 10:J:27:THR:HG22    | 29:J:205:HOH:O     | 2.06                     | 0.55              |
| 2:O:132:GLU:HB3     | 2:O:137:GLU:HG3    | 1.88                     | 0.55              |
| 1:A:282:PHE:CA      | 7:T:4:ALA:HB3      | 2.24                     | 0.55              |
| 2:B:49:LYS:HD3      | 20:D:201:TGL:CC7   | 2.36                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:D:100[B]:LYS:CE  | 29:D:401:HOH:O      | 2.18                     | 0.55              |
| 1:N:112:LEU:HD23   | 1:N:112:LEU:C       | 2.32                     | 0.55              |
| 3:C:51[B]:MET:HE2  | 25:C:303:CDL:C39    | 2.33                     | 0.55              |
| 6:S:94:HIS:N       | 29:S:204:HOH:O      | 2.38                     | 0.55              |
| 1:A:172:LYS:NZ     | 1:A:178[A]:GLN:HE22 | 2.05                     | 0.55              |
| 6:S:94:HIS:CD2     | 6:S:95:GLN:O        | 2.59                     | 0.55              |
| 12:Y:20:ARG:CZ     | 12:Y:24[B]:MET:HE1  | 2.34                     | 0.55              |
| 23:B:304:PSC:H21   | 23:B:304:PSC:H011   | 1.88                     | 0.55              |
| 3:P:246:ASP:HB2    | 29:P:522:HOH:O      | 2.06                     | 0.54              |
| 6:S:54:ASN:HD22    | 6:S:54:ASN:C        | 2.15                     | 0.54              |
| 8:U:9:LYS:HA       | 29:U:129:HOH:O      | 2.07                     | 0.54              |
| 7:T:5:LYS:HB2      | 26:T:102:PEK:H331   | 1.88                     | 0.54              |
| 25:G:102:CDL:H632  | 29:G:258:HOH:O      | 2.07                     | 0.54              |
| 19:P:303:PGV:H182  | 25:P:304:CDL:H662   | 1.89                     | 0.54              |
| 7:T:5:LYS:HG3      | 26:T:102:PEK:H371   | 1.88                     | 0.54              |
| 2:B:83:ILE:O       | 2:B:87[B]:MET:HB2   | 2.07                     | 0.54              |
| 14:A:602:HEA:HBC1  | 14:A:602:HEA:HMC3   | 1.90                     | 0.54              |
| 2:B:227:LEU:HD21   | 29:B:548:HOH:O      | 2.06                     | 0.54              |
| 19:N:607:PGV:H61   | 3:P:54[A]:MET:HG2   | 1.89                     | 0.54              |
| 23:O:303:PSC:H22   | 23:O:303:PSC:H201   | 1.89                     | 0.54              |
| 2:B:217:LYS:HD3    | 29:B:615:HOH:O      | 2.08                     | 0.54              |
| 19:C:302:PGV:C22   | 19:C:302:PGV:H211   | 2.17                     | 0.54              |
| 1:A:28:MET:CE      | 14:A:601:HEA:H271   | 2.35                     | 0.54              |
| 2:O:58:ALA:O       | 2:O:62:GLU:HG3      | 2.08                     | 0.54              |
| 4:Q:17[A]:VAL:CG1  | 29:Q:419:HOH:O      | 2.56                     | 0.54              |
| 25:C:303:CDL:H811  | 25:C:303:CDL:H672   | 1.89                     | 0.53              |
| 3:P:29:SER:HB2     | 28:P:306:DMU:H21    | 1.90                     | 0.53              |
| 2:B:16[A]:ILE:HD12 | 2:B:87[A]:MET:HG2   | 1.89                     | 0.53              |
| 4:D:82:VAL:HG12    | 4:D:86:MET:HE2      | 1.90                     | 0.53              |
| 1:A:1:FME:HE2      | 1:A:1:FME:HA        | 1.91                     | 0.53              |
| 2:B:52:HIS:CE1     | 23:B:304:PSC:C21    | 2.91                     | 0.53              |
| 4:Q:19[B]:ARG:NH2  | 29:Q:302:HOH:O      | 2.39                     | 0.53              |
| 1:A:28:MET:CE      | 14:A:601:HEA:H273   | 2.38                     | 0.53              |
| 1:A:28:MET:HE2     | 14:A:601:HEA:H273   | 1.90                     | 0.53              |
| 1:A:278[B]:MET:HE1 | 7:T:5:LYS:HB3       | 1.90                     | 0.53              |
| 8:H:43:MET:HE1     | 8:U:43:MET:HE1      | 1.90                     | 0.53              |
| 1:N:172:LYS:NZ     | 1:N:178[A]:GLN:HE22 | 2.06                     | 0.53              |
| 1:N:459:PHE:HE2    | 29:Q:311:HOH:O      | 1.92                     | 0.53              |
| 26:T:101:PEK:C1    | 26:T:101:PEK:H31    | 2.36                     | 0.53              |
| 1:A:334:TRP:CZ3    | 20:D:201:TGL:HA52   | 2.43                     | 0.53              |
| 20:B:301:TGL:HC22  | 29:I:173:HOH:O      | 2.08                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:F:41:GLY:HA3      | 6:F:87[B]:THR:CG2   | 2.38                     | 0.53              |
| 25:P:304:CDL:OB9    | 25:P:304:CDL:HB4    | 2.09                     | 0.53              |
| 2:B:183[A]:THR:HG23 | 29:B:622:HOH:O      | 2.08                     | 0.53              |
| 3:C:33[B]:MET:HE1   | 10:J:45:TYR:OH      | 2.09                     | 0.53              |
| 3:P:161[A]:GLN:HE22 | 26:P:308:PEK:H21    | 1.74                     | 0.53              |
| 19:Q:201:PGV:C2     | 19:Q:201:PGV:C01    | 2.67                     | 0.53              |
| 6:S:76:LYS:CE       | 6:S:93:PRO:CG       | 2.62                     | 0.53              |
| 6:F:1:ALA:HA        | 7:G:17:ARG:NH1      | 2.24                     | 0.53              |
| 7:G:2:SER:OG        | 26:G:103:PEK:C29    | 2.56                     | 0.53              |
| 1:A:514:LYS:HE2     | 29:F:223:HOH:O      | 2.09                     | 0.53              |
| 3:C:171:VAL:HG22    | 25:C:303:CDL:H851   | 1.90                     | 0.53              |
| 3:C:246:ASP:HB2     | 29:C:531:HOH:O      | 2.09                     | 0.53              |
| 25:G:102:CDL:H761   | 1:N:282:PHE:HZ      | 1.74                     | 0.53              |
| 19:Q:201:PGV:H162   | 19:Q:201:PGV:H321   | 1.91                     | 0.53              |
| 1:A:25:TRP:CE3      | 20:L:101:TGL:HB92   | 2.44                     | 0.53              |
| 23:O:303:PSC:H22    | 23:O:303:PSC:H231   | 1.91                     | 0.53              |
| 19:P:303:PGV:H11    | 19:P:303:PGV:C15    | 2.40                     | 0.52              |
| 7:T:8:HIS:O         | 7:T:9:GLY:C         | 2.51                     | 0.52              |
| 2:B:41[B]:ILE:HD11  | 9:I:21:ILE:HD13     | 1.90                     | 0.52              |
| 7:G:5:LYS:HB3       | 1:N:278[B]:MET:HE1  | 1.91                     | 0.52              |
| 1:N:28:MET:CE       | 14:N:601:HEA:H273   | 2.40                     | 0.52              |
| 3:P:33[A]:MET:HB2   | 28:P:306:DMU:H9     | 1.91                     | 0.52              |
| 4:Q:93:ALA:HB3      | 11:X:28[B]:VAL:HG12 | 1.91                     | 0.52              |
| 7:T:2:SER:OG        | 26:T:102:PEK:H291   | 2.09                     | 0.52              |
| 9:I:67:GLY:HA3      | 11:K:54:ARG:HD3     | 1.91                     | 0.52              |
| 25:G:102:CDL:H611   | 25:G:102:CDL:H652   | 1.92                     | 0.52              |
| 3:P:3:HIS:C         | 29:P:401:HOH:O      | 2.52                     | 0.52              |
| 28:P:306:DMU:H11    | 10:W:49:CYS:HB3     | 1.91                     | 0.52              |
| 2:B:22[B]:HIS:CE1   | 9:I:44:LYS:HE2      | 2.41                     | 0.52              |
| 25:C:303:CDL:OB6    | 25:C:303:CDL:HB22   | 2.10                     | 0.52              |
| 20:B:301:TGL:HC21   | 29:B:589:HOH:O      | 2.10                     | 0.52              |
| 3:P:80[A]:ARG:HG2   | 3:P:233:PHE:CE2     | 2.45                     | 0.52              |
| 12:Y:20:ARG:NH1     | 12:Y:24[B]:MET:CE   | 2.73                     | 0.52              |
| 6:F:1:ALA:CB        | 6:S:65:ASP:OD1      | 2.50                     | 0.52              |
| 25:G:102:CDL:H511   | 25:G:102:CDL:C18    | 2.40                     | 0.52              |
| 8:U:9:LYS:HG3       | 8:U:11:TYR:H        | 1.76                     | 0.52              |
| 1:A:486[A]:ASP:OD1  | 4:D:19[A]:ARG:HD2   | 2.10                     | 0.51              |
| 8:U:7:LYS:O         | 8:U:8:ILE:HB        | 2.10                     | 0.51              |
| 1:A:281:GLY:O       | 7:T:4:ALA:HB1       | 2.10                     | 0.51              |
| 19:Q:201:PGV:H301   | 19:Q:201:PGV:H142   | 1.92                     | 0.51              |
| 12:L:20:ARG:HH22    | 20:L:101:TGL:CC4    | 2.22                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:240:HIS:C      | 1:A:240:HIS:CD2    | 2.88                     | 0.51              |
| 7:G:5:LYS:CB       | 26:G:103:PEK:H351  | 2.31                     | 0.51              |
| 8:H:9:LYS:HD3      | 8:H:11:TYR:H       | 1.75                     | 0.51              |
| 2:O:60:GLU:CD      | 2:O:60:GLU:N       | 2.68                     | 0.51              |
| 4:D:100[B]:LYS:HD2 | 4:D:100[B]:LYS:O   | 2.10                     | 0.51              |
| 5:R:14[B]:ARG:HG2  | 29:R:228:HOH:O     | 2.11                     | 0.51              |
| 12:Y:24[B]:MET:SD  | 20:Y:101:TGL:CC3   | 2.99                     | 0.51              |
| 20:Y:101:TGL:H162  | 20:Y:101:TGL:OA1   | 2.11                     | 0.51              |
| 20:L:101:TGL:H102  | 20:L:101:TGL:H292  | 1.92                     | 0.51              |
| 1:N:28:MET:HE2     | 14:N:601:HEA:H273  | 1.93                     | 0.51              |
| 7:G:11:TPO:CG2     | 7:G:16:TRP:HE1     | 2.12                     | 0.51              |
| 19:Q:201:PGV:H22   | 19:Q:201:PGV:C01   | 2.32                     | 0.51              |
| 10:W:33:ARG:HG2    | 22:W:101:CHD:C18   | 2.39                     | 0.51              |
| 2:O:113:TYR:HD1    | 8:U:58:ARG:HH22    | 1.59                     | 0.51              |
| 12:Y:26:THR:HG23   | 13:Z:25:SER:CB     | 2.41                     | 0.50              |
| 3:P:40:MET:O       | 3:P:44[B]:MET:HG3  | 2.10                     | 0.50              |
| 7:T:5:LYS:HB2      | 26:T:102:PEK:H351  | 1.94                     | 0.50              |
| 1:A:514:LYS:HA     | 6:F:38:ALA:CB      | 2.39                     | 0.50              |
| 29:O:571:HOH:O     | 20:Q:202:TGL:HC61  | 2.12                     | 0.50              |
| 4:Q:33:LEU:HD22    | 4:Q:37:GLN:HB3     | 1.94                     | 0.50              |
| 12:Y:20:ARG:HH12   | 12:Y:24[B]:MET:CE  | 2.23                     | 0.50              |
| 2:O:113:TYR:HD1    | 8:U:58:ARG:NH2     | 2.10                     | 0.50              |
| 2:O:196:CYS:HB2    | 2:O:207:MET:HG3    | 1.93                     | 0.50              |
| 3:P:54[A]:MET:HB3  | 3:P:58:TRP:CZ3     | 2.46                     | 0.50              |
| 4:Q:7:LYS:N        | 4:Q:10:ASP:OD2     | 2.44                     | 0.50              |
| 10:W:32:TYR:OH     | 22:W:101:CHD:H213  | 2.11                     | 0.50              |
| 12:Y:20:ARG:NH2    | 12:Y:24[A]:MET:HG3 | 2.27                     | 0.50              |
| 12:Y:20:ARG:NH1    | 12:Y:24[B]:MET:HE2 | 2.27                     | 0.50              |
| 23:O:303:PSC:H201  | 23:O:303:PSC:C2    | 2.42                     | 0.50              |
| 2:B:86:MET:HE1     | 29:B:403:HOH:O     | 2.11                     | 0.50              |
| 1:N:240:HIS:C      | 1:N:240:HIS:CD2    | 2.90                     | 0.50              |
| 1:N:296:GLY:HA2    | 8:U:23:GLN:OE1     | 2.11                     | 0.50              |
| 12:Y:24[B]:MET:HG2 | 20:Y:101:TGL:CA2   | 2.39                     | 0.50              |
| 12:L:26:THR:HG23   | 13:M:25:SER:HB3    | 1.92                     | 0.50              |
| 3:P:116:TRP:HA     | 3:P:117:PRO:C      | 2.37                     | 0.50              |
| 4:Q:34:SER:H       | 4:Q:37:GLN:NE2     | 2.10                     | 0.50              |
| 6:S:64:GLU:O       | 6:S:65:ASP:HB2     | 2.11                     | 0.50              |
| 19:P:303:PGV:H11   | 19:P:303:PGV:H151  | 1.94                     | 0.49              |
| 7:G:37:LEU:HD21    | 25:G:102:CDL:C36   | 2.37                     | 0.49              |
| 2:O:116:LEU:HD13   | 2:O:226:MET:HG2    | 1.94                     | 0.49              |
| 4:Q:78:TRP:CA      | 20:Q:202:TGL:HB21  | 2.43                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 20:N:608:TGL:CB9   | 20:N:608:TGL:C28    | 2.86                     | 0.49              |
| 20:D:201:TGL:H342  | 9:I:16:ARG:HH21     | 1.76                     | 0.49              |
| 7:G:11:TPO:HG22    | 7:G:16:TRP:NE1      | 2.12                     | 0.49              |
| 20:L:101:TGL:H362  | 20:L:101:TGL:C31    | 2.39                     | 0.49              |
| 25:P:304:CDL:H392  | 25:P:304:CDL:H271   | 1.95                     | 0.49              |
| 6:S:85:CYS:SG      | 6:S:87[A]:THR:CG2   | 2.82                     | 0.49              |
| 8:U:43:MET:HE3     | 8:U:49:ASP:H        | 1.76                     | 0.49              |
| 1:A:107:PRO:HB3    | 3:C:25:LEU:HB2      | 1.95                     | 0.49              |
| 11:X:42:PRO:O      | 11:X:47:ARG:NH2     | 2.45                     | 0.49              |
| 2:B:16[B]:ILE:HG13 | 2:B:17:MET:N        | 2.27                     | 0.49              |
| 8:H:9:LYS:NZ       | 29:H:103:HOH:O      | 2.45                     | 0.49              |
| 1:N:178[B]:GLN:HA  | 1:N:181:THR:HG23    | 1.95                     | 0.49              |
| 22:P:307:CHD:H212  | 22:P:307:CHD:H12    | 1.95                     | 0.48              |
| 1:A:417[B]:MET:HE3 | 29:A:816:HOH:O      | 2.04                     | 0.48              |
| 2:B:41[A]:ILE:HD13 | 23:B:304:PSC:H342   | 1.94                     | 0.48              |
| 8:H:8:ILE:O        | 8:H:9:LYS:HE2       | 2.13                     | 0.48              |
| 8:H:8:ILE:C        | 8:H:9:LYS:HE2       | 2.38                     | 0.48              |
| 8:H:9:LYS:HE2      | 8:H:9:LYS:N         | 2.28                     | 0.48              |
| 12:L:47:LYS:NZ     | 12:L:47:LYS:HB3     | 2.28                     | 0.48              |
| 2:O:82:ARG:HH11    | 2:O:86:MET:HE1      | 1.79                     | 0.48              |
| 3:P:33[B]:MET:HA   | 28:P:306:DMU:H9     | 1.96                     | 0.48              |
| 3:P:59:ARG:HA      | 25:P:304:CDL:H512   | 1.94                     | 0.48              |
| 6:S:1:ALA:HA       | 7:T:17:ARG:NH1      | 2.29                     | 0.48              |
| 19:C:302:PGV:C22   | 19:C:302:PGV:H212   | 2.17                     | 0.48              |
| 7:G:70[B]:PHE:HB2  | 26:G:101:PEK:H041   | 1.94                     | 0.48              |
| 8:H:9:LYS:CE       | 29:H:103:HOH:O      | 2.60                     | 0.48              |
| 1:N:172:LYS:HZ2    | 1:N:178[A]:GLN:HE22 | 1.61                     | 0.48              |
| 1:N:362[B]:SER:O   | 2:O:87[B]:MET:HE1   | 2.14                     | 0.48              |
| 1:A:278[B]:MET:HE3 | 7:T:5:LYS:HB3       | 1.95                     | 0.48              |
| 2:B:196:CYS:HB2    | 2:B:207:MET:HG3     | 1.94                     | 0.48              |
| 8:H:43:MET:HE3     | 8:H:48:GLY:HA3      | 1.95                     | 0.48              |
| 10:W:56:PRO:HG3    | 12:Y:47:LYS:HE2     | 1.96                     | 0.48              |
| 4:D:78:TRP:HB3     | 20:D:201:TGL:CB2    | 2.44                     | 0.48              |
| 2:O:29[A]:MET:HB2  | 9:V:35:TYR:CE2      | 2.49                     | 0.48              |
| 20:D:201:TGL:OG2   | 20:D:201:TGL:CB3    | 2.61                     | 0.48              |
| 25:G:102:CDL:C33   | 29:O:488:HOH:O      | 2.50                     | 0.48              |
| 1:A:486[B]:ASP:OD2 | 4:D:19[B]:ARG:HD3   | 2.12                     | 0.48              |
| 8:H:45:ALA:O       | 8:H:47:GLY:N        | 2.47                     | 0.48              |
| 1:A:112:LEU:C      | 1:A:112:LEU:HD23    | 2.38                     | 0.47              |
| 6:F:64:GLU:O       | 6:F:65:ASP:HB2      | 2.15                     | 0.47              |
| 2:O:83:ILE:O       | 2:O:87[A]:MET:HG3   | 2.13                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:S:94:HIS:HD2      | 6:S:95:GLN:N        | 2.10                     | 0.47              |
| 8:H:37:HIS:HE1      | 29:H:111:HOH:O      | 1.96                     | 0.47              |
| 3:P:33[A]:MET:CB    | 28:P:306:DMU:H9     | 2.44                     | 0.47              |
| 1:N:408:THR:HB      | 19:Q:201:PGV:H51    | 1.96                     | 0.47              |
| 4:Q:52:SER:HB2      | 29:Q:316:HOH:O      | 2.12                     | 0.47              |
| 22:C:305:CHD:H212   | 22:C:305:CHD:H12    | 1.95                     | 0.47              |
| 20:Q:202:TGL:H231   | 20:Q:202:TGL:HA91   | 1.95                     | 0.47              |
| 2:B:41[A]:ILE:O     | 2:B:42:ILE:C        | 2.56                     | 0.47              |
| 3:C:3:HIS:N         | 29:C:406:HOH:O      | 2.46                     | 0.47              |
| 1:N:22:PHE:HA       | 20:Y:101:TGL:HB61   | 1.95                     | 0.47              |
| 5:R:79:LYS:HD2      | 5:R:79:LYS:HA       | 1.71                     | 0.47              |
| 2:B:1:FME:CN        | 2:B:193:TYR:H       | 2.27                     | 0.47              |
| 2:B:41[B]:ILE:HD11  | 9:I:21:ILE:CD1      | 2.44                     | 0.47              |
| 26:C:306:PEK:H382   | 25:G:102:CDL:H272   | 1.97                     | 0.47              |
| 1:N:113[A]:LEU:HD12 | 20:Y:101:TGL:C13    | 2.44                     | 0.47              |
| 1:N:337:ALA:HB2     | 1:N:394[A]:VAL:HG23 | 1.96                     | 0.47              |
| 3:P:33[A]:MET:HE2   | 3:P:42:LEU:H        | 1.80                     | 0.47              |
| 3:P:62:ILE:HD12     | 25:P:304:CDL:H511   | 1.97                     | 0.47              |
| 19:A:608:PGV:H231   | 13:M:12:PRO:HG3     | 1.97                     | 0.47              |
| 11:K:47:ARG:HG2     | 11:K:48:VAL:HG23    | 1.95                     | 0.47              |
| 1:N:513:LEU:O       | 1:N:514:LYS:CG      | 2.63                     | 0.47              |
| 25:P:304:CDL:H452   | 25:P:304:CDL:H411   | 1.96                     | 0.47              |
| 12:Y:20:ARG:CZ      | 12:Y:24[B]:MET:HE2  | 2.44                     | 0.47              |
| 7:G:5:LYS:HB3       | 1:N:278[B]:MET:CE   | 2.44                     | 0.47              |
| 3:P:205:GLY:HA3     | 26:T:101:PEK:H181   | 1.95                     | 0.47              |
| 25:P:304:CDL:H652   | 25:P:304:CDL:H242   | 1.96                     | 0.47              |
| 20:Y:101:TGL:HC52   | 20:Y:101:TGL:HC22   | 1.45                     | 0.47              |
| 3:C:47:LEU:O        | 3:C:51[A]:MET:HG2   | 2.15                     | 0.47              |
| 6:F:87[A]:THR:HG21  | 29:F:223:HOH:O      | 2.14                     | 0.47              |
| 25:G:102:CDL:H201   | 25:G:102:CDL:C52    | 2.42                     | 0.47              |
| 10:J:40:LEU:HD12    | 22:J:102:CHD:O12    | 2.15                     | 0.47              |
| 1:A:513:LEU:HD23    | 1:A:513:LEU:HA      | 1.82                     | 0.47              |
| 19:A:607:PGV:H343   | 26:G:101:PEK:C38    | 2.36                     | 0.47              |
| 2:B:58:ALA:O        | 2:B:62:GLU:HG3      | 2.15                     | 0.47              |
| 25:G:102:CDL:C44    | 1:N:311[B]:ILE:HG22 | 2.45                     | 0.46              |
| 8:H:9:LYS:CA        | 8:H:9:LYS:HE3       | 2.42                     | 0.46              |
| 25:T:103:CDL:H561   | 25:T:103:CDL:H592   | 1.52                     | 0.46              |
| 1:A:308:ALA:O       | 1:A:311[B]:ILE:HG22 | 2.16                     | 0.46              |
| 2:B:42:ILE:HG21     | 20:D:201:TGL:H232   | 1.97                     | 0.46              |
| 2:B:104:TRP:CG      | 2:B:203:ASN:HB2     | 2.50                     | 0.46              |
| 3:P:224:LYS:CE      | 25:P:304:CDL:HB32   | 2.45                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:A:282:PHE:CA     | 7:T:4:ALA:CB        | 2.85                     | 0.46              |
| 23:B:304:PSC:H221  | 23:B:304:PSC:H251   | 1.36                     | 0.46              |
| 4:D:28:ALA:H       | 4:D:31[B]:LYS:HZ3   | 1.63                     | 0.46              |
| 4:D:78:TRP:CB      | 20:D:201:TGL:HB21   | 2.45                     | 0.46              |
| 1:N:112:LEU:HG     | 29:N:921:HOH:O      | 2.15                     | 0.46              |
| 6:S:2:SER:HB2      | 29:S:309:HOH:O      | 2.16                     | 0.46              |
| 25:T:103:CDL:H362  | 25:T:103:CDL:H142   | 1.98                     | 0.46              |
| 9:I:73:LYS:HA      | 9:I:73:LYS:HD3      | 1.54                     | 0.46              |
| 11:K:39:GLU:HB3    | 29:K:112:HOH:O      | 2.14                     | 0.46              |
| 3:P:156:ARG:HE     | 22:P:305:CHD:C24    | 2.28                     | 0.46              |
| 1:N:148:PHE:HB3    | 3:P:28:THR:HB       | 1.98                     | 0.46              |
| 1:N:229:ILE:HD11   | 2:O:175:ILE:HD13    | 1.98                     | 0.46              |
| 3:P:3:HIS:HD2      | 29:P:534:HOH:O      | 1.97                     | 0.46              |
| 1:A:172:LYS:HZ2    | 1:A:178[A]:GLN:HE22 | 1.63                     | 0.46              |
| 7:G:3:ALA:O        | 7:G:4:ALA:CB        | 2.64                     | 0.46              |
| 8:H:7:LYS:HG3      | 8:H:8:ILE:HD12      | 1.97                     | 0.46              |
| 1:A:136[B]:LEU:CD1 | 29:A:988:HOH:O      | 2.33                     | 0.46              |
| 3:C:116:TRP:HA     | 3:C:117:PRO:C       | 2.40                     | 0.46              |
| 10:J:36:MET:HB3    | 22:J:102:CHD:H183   | 1.97                     | 0.46              |
| 1:N:34:SER:HB2     | 14:N:601:HEA:C2B    | 2.46                     | 0.46              |
| 2:O:116:LEU:HD13   | 2:O:226:MET:CG      | 2.46                     | 0.46              |
| 4:D:86:MET:HE1     | 11:K:22:ALA:HB2     | 1.98                     | 0.46              |
| 3:P:50:ASN:ND2     | 3:P:54[A]:MET:HE2   | 2.30                     | 0.46              |
| 19:A:608:PGV:H061  | 19:A:608:PGV:P      | 2.55                     | 0.46              |
| 3:C:133:ASN:ND2    | 29:C:402:HOH:O      | 2.39                     | 0.46              |
| 3:P:103:HIS:HA     | 19:P:301:PGV:H012   | 1.98                     | 0.46              |
| 19:P:303:PGV:C18   | 25:P:304:CDL:H662   | 2.46                     | 0.46              |
| 12:Y:12:PRO:HB2    | 20:Y:101:TGL:HG2    | 1.97                     | 0.46              |
| 3:C:160:LEU:HD13   | 22:C:304:CHD:H181   | 1.96                     | 0.45              |
| 3:P:208:VAL:HG22   | 3:P:245:VAL:CG1     | 2.46                     | 0.45              |
| 5:R:108:LYS:NZ     | 29:R:203:HOH:O      | 2.48                     | 0.45              |
| 1:A:337:ALA:HB2    | 1:A:394[A]:VAL:HG23 | 1.98                     | 0.45              |
| 29:A:703:HOH:O     | 6:F:37:LYS:HE2      | 2.17                     | 0.45              |
| 7:G:33:LEU:O       | 7:G:37:LEU:HB2      | 2.15                     | 0.45              |
| 3:P:33[B]:MET:HG2  | 3:P:39:SER:O        | 2.14                     | 0.45              |
| 7:T:3:ALA:O        | 7:T:4:ALA:CB        | 2.63                     | 0.45              |
| 9:V:61:GLU:OE1     | 9:V:64:ARG:NE       | 2.46                     | 0.45              |
| 10:J:49:CYS:HB3    | 28:J:101:DMU:C19    | 2.40                     | 0.45              |
| 1:A:290:HIS:CD2    | 1:A:291:HIS:CD2     | 3.04                     | 0.45              |
| 1:A:297[A]:MET:HG2 | 29:A:933:HOH:O      | 2.15                     | 0.45              |
| 7:T:31:CYS:SG      | 25:T:103:CDL:H551   | 2.56                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:O:82:ARG:HG2      | 2:O:86:MET:HE3      | 1.98                     | 0.45              |
| 3:C:50:ASN:ND2      | 3:C:54[A]:MET:HE2   | 2.31                     | 0.45              |
| 25:C:303:CDL:OB6    | 25:C:303:CDL:CB2    | 2.65                     | 0.45              |
| 4:D:78:TRP:HB3      | 20:D:201:TGL:HB21   | 1.98                     | 0.45              |
| 1:N:136[B]:LEU:HD11 | 29:T:280:HOH:O      | 2.16                     | 0.45              |
| 2:B:1:FME:HE3       | 4:D:123:MET:HE3     | 1.99                     | 0.45              |
| 8:H:31:GLN:NE2      | 29:H:101:HOH:O      | 2.37                     | 0.45              |
| 20:L:101:TGL:HA91   | 20:L:101:TGL:H222   | 1.63                     | 0.45              |
| 26:C:306:PEK:H331   | 26:C:306:PEK:H362   | 1.72                     | 0.45              |
| 6:F:87[B]:THR:HG21  | 29:F:304:HOH:O      | 2.16                     | 0.45              |
| 8:H:9:LYS:HD3       | 8:H:11:TYR:HB2      | 1.98                     | 0.45              |
| 2:O:32[B]:PHE:CD2   | 9:V:31:PHE:CZ       | 3.05                     | 0.45              |
| 8:U:43:MET:HE3      | 8:U:48:GLY:HA3      | 1.99                     | 0.45              |
| 2:B:22[B]:HIS:CE1   | 29:B:461:HOH:O      | 2.69                     | 0.45              |
| 22:C:304:CHD:H162   | 22:C:304:CHD:H231   | 1.98                     | 0.45              |
| 2:B:116:LEU:HD11    | 2:B:226:MET:HB3     | 1.99                     | 0.45              |
| 12:L:20:ARG:NH2     | 20:L:101:TGL:HC52   | 2.27                     | 0.45              |
| 3:P:33[A]:MET:CB    | 28:P:306:DMU:C19    | 2.94                     | 0.45              |
| 3:P:33[A]:MET:HE3   | 3:P:39:SER:OG       | 2.17                     | 0.45              |
| 1:A:178[B]:GLN:HG2  | 1:A:179:TYR:CE2     | 2.52                     | 0.44              |
| 2:O:92:ASN:HA       | 2:O:93:PRO:HD2      | 1.72                     | 0.44              |
| 25:T:103:CDL:H672   | 25:T:103:CDL:H612   | 1.99                     | 0.44              |
| 9:V:36:LYS:NZ       | 9:V:36:LYS:HB2      | 2.32                     | 0.44              |
| 2:B:78:LEU:N        | 2:B:78:LEU:CD1      | 2.81                     | 0.44              |
| 8:H:37:HIS:HD2      | 8:H:40:GLU:OE2      | 2.00                     | 0.44              |
| 3:P:47:LEU:O        | 3:P:51[A]:MET:HG2   | 2.18                     | 0.44              |
| 26:T:101:PEK:H203   | 26:T:101:PEK:H171   | 1.71                     | 0.44              |
| 7:G:2:SER:OG        | 26:G:103:PEK:H292   | 2.17                     | 0.44              |
| 10:J:7:GLU:HG3      | 29:J:238:HOH:O      | 2.16                     | 0.44              |
| 20:L:101:TGL:H312   | 20:L:101:TGL:C36    | 2.43                     | 0.44              |
| 1:N:336:PRO:HB2     | 1:N:394[B]:VAL:HG11 | 2.00                     | 0.44              |
| 1:N:483:LEU:HD21    | 13:Z:4:LYS:HE3      | 1.99                     | 0.44              |
| 10:J:52:TRP:O       | 10:J:57:HIS:HE1     | 2.00                     | 0.44              |
| 1:N:178[B]:GLN:HG3  | 1:N:178[B]:GLN:O    | 2.18                     | 0.44              |
| 3:P:33[B]:MET:CE    | 28:P:306:DMU:H6     | 2.43                     | 0.44              |
| 3:P:80[A]:ARG:HH11  | 3:P:80[A]:ARG:HD3   | 1.49                     | 0.44              |
| 7:T:37:LEU:HD12     | 7:T:37:LEU:HA       | 1.89                     | 0.44              |
| 25:T:103:CDL:H382   | 25:T:103:CDL:H161   | 1.98                     | 0.44              |
| 1:A:362[B]:SER:O    | 2:B:87[B]:MET:HE1   | 2.18                     | 0.44              |
| 23:O:303:PSC:H272   | 23:O:303:PSC:H242   | 1.66                     | 0.44              |
| 25:P:304:CDL:OA6    | 25:P:304:CDL:H132   | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:T:38:HIS:CE1     | 25:T:103:CDL:H122  | 2.52                     | 0.44              |
| 12:Y:26:THR:HG23   | 13:Z:25:SER:HB3    | 1.99                     | 0.44              |
| 7:G:38:HIS:CD2     | 29:G:209:HOH:O     | 2.71                     | 0.44              |
| 7:G:84:LYS:CD      | 7:G:84:LYS:N       | 2.69                     | 0.44              |
| 26:P:308:PEK:C04   | 6:S:1:ALA:N        | 2.78                     | 0.44              |
| 7:T:11:TPO:HG22    | 7:T:11:TPO:O       | 2.18                     | 0.44              |
| 29:A:703:HOH:O     | 6:F:37:LYS:HG3     | 2.17                     | 0.44              |
| 2:B:164:ALA:O      | 2:B:194:GLY:HA3    | 2.18                     | 0.44              |
| 20:B:301:TGL:H252  | 20:B:301:TGL:H221  | 1.76                     | 0.44              |
| 25:P:304:CDL:H672  | 25:P:304:CDL:H261  | 1.99                     | 0.44              |
| 5:R:6:GLU:HA       | 29:R:308:HOH:O     | 2.17                     | 0.44              |
| 11:K:6:ALA:N       | 29:K:103:HOH:O     | 2.51                     | 0.44              |
| 4:Q:6:VAL:HG13     | 29:Q:446:HOH:O     | 2.18                     | 0.44              |
| 1:A:302[B]:ARG:NH1 | 29:A:705:HOH:O     | 2.51                     | 0.43              |
| 2:B:32[B]:PHE:CE2  | 9:I:31:PHE:CZ      | 3.06                     | 0.43              |
| 20:Y:101:TGL:H252  | 20:Y:101:TGL:H283  | 1.53                     | 0.43              |
| 13:Z:41:LYS:NZ     | 29:Z:201:HOH:O     | 2.50                     | 0.43              |
| 25:C:303:CDL:H671  | 25:C:303:CDL:H641  | 1.87                     | 0.43              |
| 3:C:55:TYR:CD1     | 25:C:303:CDL:H532  | 2.54                     | 0.43              |
| 1:A:274:VAL:HG12   | 1:A:278[A]:MET:HE2 | 2.00                     | 0.43              |
| 19:C:302:PGV:H172  | 25:C:303:CDL:C65   | 2.48                     | 0.43              |
| 12:L:26:THR:HG23   | 13:M:25:SER:CB     | 2.47                     | 0.43              |
| 1:N:514:LYS:HG2    | 6:S:38:ALA:CB      | 2.48                     | 0.43              |
| 14:N:601:HEA:HHC   | 14:N:601:HEA:H122  | 2.01                     | 0.43              |
| 2:O:215:PRO:HD3    | 9:V:60:PHE:CD2     | 2.53                     | 0.43              |
| 7:T:8:HIS:O        | 7:T:8:HIS:CD2      | 2.71                     | 0.43              |
| 1:A:334:TRP:HB2    | 20:D:201:TGL:HG11  | 2.00                     | 0.43              |
| 2:B:41[B]:ILE:HD13 | 2:B:41[B]:ILE:HA   | 1.72                     | 0.43              |
| 7:G:83:GLU:OE2     | 29:G:201:HOH:O     | 2.21                     | 0.43              |
| 10:J:32:TYR:CE2    | 22:J:102:CHD:H213  | 2.54                     | 0.43              |
| 1:N:426:PHE:HZ     | 20:N:608:TGL:HA42  | 1.83                     | 0.43              |
| 2:O:151:ARG:HD3    | 2:O:181:GLN:HE21   | 1.84                     | 0.43              |
| 26:P:308:PEK:C1    | 29:P:441:HOH:O     | 2.67                     | 0.43              |
| 6:S:87[A]:THR:HG21 | 29:S:266:HOH:O     | 2.19                     | 0.43              |
| 7:T:5:LYS:CG       | 26:T:102:PEK:H351  | 2.46                     | 0.43              |
| 1:A:62:ALA:HB2     | 14:A:601:HEA:HBD1  | 2.00                     | 0.43              |
| 7:G:10:GLY:HA3     | 29:G:272:HOH:O     | 2.19                     | 0.43              |
| 1:N:377:PHE:HA     | 1:N:380:VAL:HG22   | 2.00                     | 0.43              |
| 1:N:514:LYS:NZ     | 29:N:704:HOH:O     | 2.50                     | 0.43              |
| 23:O:303:PSC:H322  | 23:O:303:PSC:H281  | 1.99                     | 0.43              |
| 3:P:63:ARG:NE      | 25:P:304:CDL:HA22  | 2.29                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 29:C:401:HOH:O      | 6:F:52:ILE:HD11     | 2.18                     | 0.43              |
| 4:D:19[A]:ARG:HH22  | 4:D:21:ASP:CG       | 2.27                     | 0.43              |
| 25:G:102:CDL:H441   | 1:N:311[B]:ILE:HG22 | 2.01                     | 0.43              |
| 4:Q:17[B]:VAL:HG22  | 4:Q:19[B]:ARG:HG3   | 2.00                     | 0.43              |
| 5:R:80:GLU:CD       | 5:R:80:GLU:N        | 2.74                     | 0.43              |
| 25:G:102:CDL:H401   | 2:O:77:ALA:CB       | 2.48                     | 0.43              |
| 10:W:27:THR:HG22    | 29:W:208:HOH:O      | 2.18                     | 0.43              |
| 29:A:763:HOH:O      | 12:L:7:PRO:HG3      | 2.19                     | 0.43              |
| 1:N:24:ALA:HB2      | 14:N:601:HEA:H253   | 2.01                     | 0.43              |
| 23:O:303:PSC:H262   | 23:O:303:PSC:H292   | 1.04                     | 0.43              |
| 20:Q:202:TGL:CA9    | 20:Q:202:TGL:C23    | 2.95                     | 0.43              |
| 25:T:103:CDL:H661   | 25:T:103:CDL:H631   | 1.77                     | 0.43              |
| 12:Y:20:ARG:NH2     | 12:Y:24[B]:MET:HE2  | 2.20                     | 0.43              |
| 23:O:303:PSC:H261   | 23:O:303:PSC:H291   | 0.86                     | 0.42              |
| 1:A:431:LEU:HD21    | 1:A:450:TRP:HB2     | 2.01                     | 0.42              |
| 3:C:41:THR:HA       | 3:C:44[B]:MET:HE2   | 2.01                     | 0.42              |
| 1:A:76:GLY:O        | 1:A:80:ASN:HB2      | 2.20                     | 0.42              |
| 26:C:306:PEK:C38    | 25:G:102:CDL:H271   | 2.30                     | 0.42              |
| 7:G:3:ALA:O         | 7:G:4:ALA:HB2       | 2.19                     | 0.42              |
| 6:S:51:SER:O        | 6:S:93:PRO:HA       | 2.19                     | 0.42              |
| 22:W:101:CHD:H111   | 22:W:101:CHD:H12A   | 1.90                     | 0.42              |
| 12:L:25:MET:HG2     | 20:L:101:TGL:HA62   | 2.01                     | 0.42              |
| 1:N:117[A]:MET:HB3  | 1:N:117[A]:MET:HE2  | 1.79                     | 0.42              |
| 19:Q:201:PGV:H22    | 19:Q:201:PGV:H202   | 2.01                     | 0.42              |
| 25:T:103:CDL:H541   | 25:T:103:CDL:C24    | 2.34                     | 0.42              |
| 3:C:37:PHE:CG       | 28:J:101:DMU:H6     | 2.54                     | 0.42              |
| 2:B:16[A]:ILE:HD11  | 2:B:86:MET:HG2      | 2.00                     | 0.42              |
| 3:C:33[A]:MET:HB2   | 28:J:101:DMU:C22    | 2.49                     | 0.42              |
| 1:N:302[B]:ARG:NH1  | 1:N:302[B]:ARG:HG2  | 2.35                     | 0.42              |
| 2:O:116:LEU:CD1     | 2:O:226:MET:HG2     | 2.50                     | 0.42              |
| 2:B:151:ARG:HD3     | 2:B:181:GLN:HE21    | 1.85                     | 0.42              |
| 9:I:73:LYS:HD3      | 29:I:125:HOH:O      | 2.18                     | 0.42              |
| 1:N:87:ILE:O        | 1:N:173:PRO:HD3     | 2.20                     | 0.42              |
| 25:T:103:CDL:H111   | 25:T:103:CDL:HA21   | 2.02                     | 0.42              |
| 1:A:169:ILE:HD13    | 1:A:169:ILE:HA      | 1.87                     | 0.42              |
| 19:A:608:PGV:O06    | 29:A:702:HOH:O      | 2.18                     | 0.42              |
| 19:C:307:PGV:H72    | 19:C:307:PGV:H42    | 1.77                     | 0.42              |
| 3:P:177:GLN:OE1     | 3:P:177:GLN:HA      | 2.20                     | 0.42              |
| 10:W:32:TYR:CE2     | 22:W:101:CHD:H213   | 2.55                     | 0.42              |
| 1:A:172:LYS:HD2     | 1:A:181:THR:HG22    | 2.01                     | 0.41              |
| 3:C:144[B]:ILE:HD12 | 3:C:144[B]:ILE:HA   | 1.93                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:N:62:ALA:HB2    | 14:N:601:HEA:HBD1   | 2.01                     | 0.41              |
| 20:Q:202:TGL:HG31 | 20:Q:202:TGL:HC21   | 1.55                     | 0.41              |
| 12:Y:20:ARG:NH1   | 12:Y:24[B]:MET:HE1  | 2.35                     | 0.41              |
| 3:C:217:VAL:HG22  | 25:C:303:CDL:H732   | 2.02                     | 0.41              |
| 20:D:201:TGL:HB92 | 20:D:201:TGL:H132   | 2.02                     | 0.41              |
| 1:A:336:PRO:HB2   | 1:A:394[B]:VAL:HG11 | 2.02                     | 0.41              |
| 1:A:489:THR:HA    | 6:F:71:TRP:O        | 2.20                     | 0.41              |
| 2:O:16:ILE:HD12   | 2:O:87[A]:MET:HG2   | 2.03                     | 0.41              |
| 2:O:130:PRO:HA    | 4:Q:115:TRP:CZ3     | 2.55                     | 0.41              |
| 2:B:56:MET:HA     | 23:B:304:PSC:C20    | 2.37                     | 0.41              |
| 25:G:102:CDL:H371 | 2:O:78:LEU:CD1      | 2.51                     | 0.41              |
| 9:I:68:ILE:HG21   | 9:I:68:ILE:HD13     | 1.71                     | 0.41              |
| 25:G:102:CDL:H201 | 25:G:102:CDL:H511   | 2.03                     | 0.41              |
| 1:N:439:ARG:HD3   | 2:O:199:ILE:HB      | 2.03                     | 0.41              |
| 25:T:103:CDL:H581 | 25:T:103:CDL:H782   | 2.03                     | 0.41              |
| 10:W:3:ASN:OD1    | 10:W:3:ASN:C        | 2.62                     | 0.41              |
| 1:A:360:ASN:O     | 1:A:361[A]:SER:C    | 2.62                     | 0.41              |
| 3:C:51[A]:MET:HE1 | 19:C:302:PGV:H162   | 2.02                     | 0.41              |
| 3:C:65:SER:HB3    | 3:C:71:HIS:CE1      | 2.56                     | 0.41              |
| 6:F:55:LYS:HA     | 6:F:74:LEU:O        | 2.20                     | 0.41              |
| 1:N:333:LYS:CD    | 29:N:988:HOH:O      | 2.68                     | 0.41              |
| 25:G:102:CDL:H541 | 25:G:102:CDL:C23    | 2.47                     | 0.41              |
| 8:H:8:ILE:O       | 8:H:8:ILE:CG2       | 2.69                     | 0.41              |
| 13:M:32:TRP:CZ3   | 13:M:40:TYR:OH      | 2.74                     | 0.41              |
| 1:N:71:MET:HB3    | 1:N:71:MET:HE2      | 1.98                     | 0.41              |
| 1:N:107:PRO:HB3   | 3:P:25:LEU:HB2      | 2.01                     | 0.41              |
| 1:N:361:SER:OG    | 2:O:84:LEU:HD13     | 2.20                     | 0.41              |
| 7:T:38:HIS:ND1    | 7:T:38:HIS:N        | 2.69                     | 0.41              |
| 1:A:268:PHE:CZ    | 2:B:58:ALA:HA       | 2.55                     | 0.41              |
| 2:B:1:FME:HCN     | 2:B:193:TYR:HB2     | 2.02                     | 0.41              |
| 3:C:131:LEU:CD2   | 25:G:102:CDL:HB61   | 2.51                     | 0.41              |
| 22:J:102:CHD:H193 | 22:J:102:CHD:H111   | 1.60                     | 0.41              |
| 2:O:164:ALA:O     | 2:O:194:GLY:HA3     | 2.21                     | 0.41              |
| 22:P:305:CHD:H162 | 22:P:305:CHD:H222   | 1.50                     | 0.41              |
| 11:X:8:ASP:HB2    | 29:X:111:HOH:O      | 2.20                     | 0.41              |
| 11:X:24:PHE:O     | 11:X:28[A]:VAL:HG12 | 2.21                     | 0.41              |
| 8:H:46:LYS:HD2    | 29:U:155:HOH:O      | 2.20                     | 0.41              |
| 29:H:145:HOH:O    | 8:U:46:LYS:HD3      | 2.19                     | 0.41              |
| 4:Q:107:ILE:HB    | 4:Q:108:PRO:CD      | 2.51                     | 0.41              |
| 7:T:41:HIS:HB3    | 7:T:74:ARG:NH1      | 2.36                     | 0.41              |
| 8:U:37:HIS:HD2    | 8:U:40:GLU:OE2      | 2.04                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:F:54[A]:ASN:ND2  | 6:F:54[A]:ASN:N    | 2.65                     | 0.41              |
| 25:G:102:CDL:C24   | 25:G:102:CDL:C54   | 2.80                     | 0.41              |
| 2:O:13:THR:HG21    | 2:O:192:TYR:CZ     | 2.55                     | 0.41              |
| 4:Q:109:HIS:HD2    | 29:Q:401:HOH:O     | 2.03                     | 0.41              |
| 9:V:2:THR:HG22     | 29:V:137:HOH:O     | 2.19                     | 0.41              |
| 1:A:384:GLY:O      | 1:A:385:ALA:C      | 2.63                     | 0.40              |
| 2:B:48:THR:HB      | 9:I:16:ARG:CZ      | 2.51                     | 0.40              |
| 7:G:84:LYS:NZ      | 29:G:203:HOH:O     | 2.49                     | 0.40              |
| 8:H:60:TYR:CD1     | 8:H:60:TYR:C       | 2.99                     | 0.40              |
| 20:L:101:TGL:HB31  | 20:L:101:TGL:HB62  | 1.80                     | 0.40              |
| 3:P:54[A]:MET:HE1  | 19:P:303:PGV:H131  | 2.03                     | 0.40              |
| 3:P:202:GLY:HA3    | 26:T:101:PEK:H21   | 2.03                     | 0.40              |
| 1:A:439:ARG:HD3    | 2:B:199:ILE:HB     | 2.03                     | 0.40              |
| 8:H:46:LYS:HG2     | 29:H:171:HOH:O     | 2.20                     | 0.40              |
| 3:P:48:THR:HG23    | 25:P:304:CDL:H401  | 2.03                     | 0.40              |
| 6:S:94:HIS:CG      | 6:S:95:GLN:N       | 2.84                     | 0.40              |
| 1:A:208[B]:MET:HB3 | 1:A:219:PHE:CD1    | 2.57                     | 0.40              |
| 1:A:293:PHE:CE1    | 1:A:361[B]:SER:HB2 | 2.57                     | 0.40              |
| 1:A:361[A]:SER:OG  | 2:B:84:LEU:HD13    | 2.21                     | 0.40              |
| 2:O:13:THR:HB      | 2:O:168:LEU:HD23   | 2.03                     | 0.40              |
| 4:Q:78:TRP:CB      | 20:Q:202:TGL:HB22  | 2.50                     | 0.40              |
| 6:S:13:ALA:CB      | 6:S:21[B]:MET:HE1  | 2.51                     | 0.40              |
| 8:U:45:ALA:C       | 8:U:47:GLY:H       | 2.29                     | 0.40              |
| 1:A:296:GLY:HA2    | 8:H:23:GLN:OE1     | 2.22                     | 0.40              |
| 25:P:304:CDL:H631  | 25:P:304:CDL:H222  | 2.02                     | 0.40              |
| 7:T:5:LYS:CB       | 26:T:102:PEK:H351  | 2.51                     | 0.40              |
| 2:B:59:GLN:HG2     | 29:B:468:HOH:O     | 2.20                     | 0.40              |
| 3:C:38:ASN:HA      | 29:C:450:HOH:O     | 2.21                     | 0.40              |
| 25:C:303:CDL:H201  | 25:C:303:CDL:H621  | 2.03                     | 0.40              |
| 26:C:306:PEK:H041  | 7:G:17:ARG:HH22    | 1.87                     | 0.40              |
| 10:W:29:ASN:H      | 10:W:29:ASN:HD22   | 1.69                     | 0.40              |
| 22:W:101:CHD:H212  | 22:W:101:CHD:H162  | 1.82                     | 0.40              |

All (2) 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) |
|---------------|-----------------------|--------------------------|-------------------|
| 9:I:2:THR:CB  | 5:R:80:GLU:OE1[3_647] | 2.00                     | 0.20              |
| 9:I:2:THR:CG2 | 5:R:80:GLU:OE1[3_647] | 2.19                     | 0.01              |

## 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     | 530/514 (103%) | 515 (97%)  | 15 (3%) | 0        | 100         | 100 |
| 1   | N     | 528/514 (103%) | 511 (97%)  | 17 (3%) | 0        | 100         | 100 |
| 2   | B     | 234/227 (103%) | 230 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 2   | O     | 230/227 (101%) | 225 (98%)  | 4 (2%)  | 1 (0%)   | 30          | 12  |
| 3   | C     | 266/261 (102%) | 261 (98%)  | 4 (2%)  | 1 (0%)   | 30          | 12  |
| 3   | P     | 266/261 (102%) | 261 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 4   | D     | 147/147 (100%) | 143 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 4   | Q     | 145/147 (99%)  | 139 (96%)  | 5 (3%)  | 1 (1%)   | 18          | 5   |
| 5   | E     | 103/109 (94%)  | 102 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 5   | R     | 104/109 (95%)  | 104 (100%) | 0       | 0        | 100         | 100 |
| 6   | F     | 100/98 (102%)  | 95 (95%)   | 3 (3%)  | 2 (2%)   | 6           | 1   |
| 6   | S     | 98/98 (100%)   | 92 (94%)   | 2 (2%)  | 4 (4%)   | 2           | 0   |
| 7   | G     | 82/85 (96%)    | 68 (83%)   | 8 (10%) | 6 (7%)   | 1           | 0   |
| 7   | T     | 82/85 (96%)    | 71 (87%)   | 5 (6%)  | 6 (7%)   | 1           | 0   |
| 8   | H     | 77/85 (91%)    | 68 (88%)   | 6 (8%)  | 3 (4%)   | 2           | 0   |
| 8   | U     | 77/85 (91%)    | 68 (88%)   | 5 (6%)  | 4 (5%)   | 1           | 0   |
| 9   | I     | 71/73 (97%)    | 71 (100%)  | 0       | 0        | 100         | 100 |
| 9   | V     | 71/73 (97%)    | 69 (97%)   | 1 (1%)  | 1 (1%)   | 9           | 1   |
| 10  | J     | 56/59 (95%)    | 56 (100%)  | 0       | 0        | 100         | 100 |
| 10  | W     | 57/59 (97%)    | 57 (100%)  | 0       | 0        | 100         | 100 |
| 11  | K     | 47/56 (84%)    | 45 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 11  | X     | 48/56 (86%)    | 46 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 12  | L     | 44/47 (94%)    | 42 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 12  | Y     | 45/47 (96%)    | 43 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 13  | M     | 41/46 (89%)    | 39 (95%)   | 2 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|----------|----------|-------------|---|
| 13  | Z     | 41/46 (89%)     | 39 (95%)   | 1 (2%)   | 1 (2%)   | 4           | 0 |
| All | All   | 3590/3614 (99%) | 3460 (96%) | 100 (3%) | 30 (1%)  | 14          | 4 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 94  | HIS  |
| 6   | F     | 96  | LEU  |
| 7   | G     | 4   | ALA  |
| 7   | G     | 5   | LYS  |
| 7   | G     | 8   | HIS  |
| 8   | H     | 8   | ILE  |
| 8   | H     | 45  | ALA  |
| 4   | Q     | 8   | SER  |
| 6   | S     | 94  | HIS  |
| 6   | S     | 95  | GLN  |
| 7   | T     | 3   | ALA  |
| 7   | T     | 4   | ALA  |
| 7   | T     | 5   | LYS  |
| 7   | T     | 7   | ASP  |
| 7   | T     | 8   | HIS  |
| 8   | U     | 8   | ILE  |
| 8   | U     | 45  | ALA  |
| 8   | U     | 46  | LYS  |
| 8   | H     | 46  | LYS  |
| 6   | S     | 96  | LEU  |
| 9   | V     | 2   | THR  |
| 13  | Z     | 42  | LYS  |
| 7   | G     | 37  | LEU  |
| 7   | G     | 7   | ASP  |
| 8   | U     | 51  | SER  |
| 3   | C     | 232 | HIS  |
| 2   | O     | 92  | ASN  |
| 7   | T     | 6   | GLY  |
| 6   | S     | 93  | PRO  |
| 7   | G     | 9   | GLY  |

### 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     | 444/426 (104%)   | 438 (99%)  | 6 (1%)   | 59          | 33  |
| 1   | N     | 442/426 (104%)   | 433 (98%)  | 9 (2%)   | 48          | 20  |
| 2   | B     | 219/210 (104%)   | 211 (96%)  | 8 (4%)   | 30          | 6   |
| 2   | O     | 215/210 (102%)   | 206 (96%)  | 9 (4%)   | 26          | 4   |
| 3   | C     | 233/226 (103%)   | 230 (99%)  | 3 (1%)   | 61          | 35  |
| 3   | P     | 233/226 (103%)   | 231 (99%)  | 2 (1%)   | 70          | 49  |
| 4   | D     | 133/129 (103%)   | 128 (96%)  | 5 (4%)   | 29          | 6   |
| 4   | Q     | 131/129 (102%)   | 124 (95%)  | 7 (5%)   | 20          | 3   |
| 5   | E     | 92/95 (97%)      | 90 (98%)   | 2 (2%)   | 45          | 17  |
| 5   | R     | 93/95 (98%)      | 91 (98%)   | 2 (2%)   | 45          | 17  |
| 6   | F     | 85/81 (105%)     | 79 (93%)   | 6 (7%)   | 13          | 1   |
| 6   | S     | 83/81 (102%)     | 75 (90%)   | 8 (10%)  | 8           | 0   |
| 7   | G     | 68/68 (100%)     | 64 (94%)   | 4 (6%)   | 18          | 2   |
| 7   | T     | 68/68 (100%)     | 61 (90%)   | 7 (10%)  | 7           | 0   |
| 8   | H     | 71/75 (95%)      | 66 (93%)   | 5 (7%)   | 14          | 1   |
| 8   | U     | 71/75 (95%)      | 67 (94%)   | 4 (6%)   | 19          | 2   |
| 9   | I     | 57/57 (100%)     | 54 (95%)   | 3 (5%)   | 20          | 3   |
| 9   | V     | 57/57 (100%)     | 51 (90%)   | 6 (10%)  | 6           | 0   |
| 10  | J     | 49/50 (98%)      | 49 (100%)  | 0        | 100         | 100 |
| 10  | W     | 50/50 (100%)     | 48 (96%)   | 2 (4%)   | 28          | 5   |
| 11  | K     | 39/46 (85%)      | 38 (97%)   | 1 (3%)   | 40          | 13  |
| 11  | X     | 40/46 (87%)      | 40 (100%)  | 0        | 100         | 100 |
| 12  | L     | 39/40 (98%)      | 38 (97%)   | 1 (3%)   | 40          | 13  |
| 12  | Y     | 40/40 (100%)     | 37 (92%)   | 3 (8%)   | 12          | 1   |
| 13  | M     | 37/38 (97%)      | 34 (92%)   | 3 (8%)   | 11          | 1   |
| 13  | Z     | 37/38 (97%)      | 33 (89%)   | 4 (11%)  | 6           | 0   |
| All | All   | 3126/3082 (101%) | 3016 (96%) | 110 (4%) | 32          | 7   |

All (110) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 7     | LEU  |
| 1   | A     | 112   | LEU  |
| 1   | A     | 128   | VAL  |
| 1   | A     | 138   | HIS  |
| 1   | A     | 180   | GLN  |
| 1   | A     | 369   | ASP  |
| 2   | B     | 33    | LEU  |
| 2   | B     | 59    | GLN  |
| 2   | B     | 60    | GLU  |
| 2   | B     | 75    | LEU  |
| 2   | B     | 86    | MET  |
| 2   | B     | 91    | ASN  |
| 2   | B     | 115   | ASP  |
| 2   | B     | 217   | LYS  |
| 3   | C     | 110   | PRO  |
| 3   | C     | 159   | MET  |
| 3   | C     | 230   | ASN  |
| 4   | D     | 4     | SER  |
| 4   | D     | 19[A] | ARG  |
| 4   | D     | 19[B] | ARG  |
| 4   | D     | 31[A] | LYS  |
| 4   | D     | 31[B] | LYS  |
| 5   | E     | 5     | HIS  |
| 5   | E     | 70    | VAL  |
| 6   | F     | 37    | LYS  |
| 6   | F     | 54[A] | ASN  |
| 6   | F     | 54[B] | ASN  |
| 6   | F     | 80    | GLN  |
| 6   | F     | 94    | HIS  |
| 6   | F     | 98    | HIS  |
| 7   | G     | 2     | SER  |
| 7   | G     | 43    | GLU  |
| 7   | G     | 79    | PRO  |
| 7   | G     | 84    | LYS  |
| 8   | H     | 7     | LYS  |
| 8   | H     | 9     | LYS  |
| 8   | H     | 51    | SER  |
| 8   | H     | 60    | TYR  |
| 8   | H     | 61    | LYS  |
| 9   | I     | 36    | LYS  |
| 9   | I     | 37    | PHE  |
| 9   | I     | 73    | LYS  |
| 11  | K     | 47    | ARG  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 12  | L     | 47     | LYS  |
| 13  | M     | 39     | ASN  |
| 13  | M     | 42     | LYS  |
| 13  | M     | 43     | SER  |
| 1   | N     | 128    | VAL  |
| 1   | N     | 138    | HIS  |
| 1   | N     | 178[A] | GLN  |
| 1   | N     | 178[B] | GLN  |
| 1   | N     | 180    | GLN  |
| 1   | N     | 363    | LEU  |
| 1   | N     | 369    | ASP  |
| 1   | N     | 495    | LEU  |
| 1   | N     | 504    | THR  |
| 2   | O     | 33     | LEU  |
| 2   | O     | 60     | GLU  |
| 2   | O     | 66     | THR  |
| 2   | O     | 68     | LEU  |
| 2   | O     | 78     | LEU  |
| 2   | O     | 91     | ASN  |
| 2   | O     | 94     | SER  |
| 2   | O     | 115    | ASP  |
| 2   | O     | 217    | LYS  |
| 3   | P     | 159    | MET  |
| 3   | P     | 230    | ASN  |
| 4   | Q     | 7      | LYS  |
| 4   | Q     | 8      | SER  |
| 4   | Q     | 9      | GLU  |
| 4   | Q     | 51     | LEU  |
| 4   | Q     | 58     | GLU  |
| 4   | Q     | 127    | LYS  |
| 4   | Q     | 143    | ASN  |
| 5   | R     | 79     | LYS  |
| 5   | R     | 91     | PRO  |
| 6   | S     | 43     | LYS  |
| 6   | S     | 54     | ASN  |
| 6   | S     | 80     | GLN  |
| 6   | S     | 87[A]  | THR  |
| 6   | S     | 87[B]  | THR  |
| 6   | S     | 94     | HIS  |
| 6   | S     | 96     | LEU  |
| 6   | S     | 98     | HIS  |
| 7   | T     | 2      | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | T     | 7   | ASP  |
| 7   | T     | 33  | LEU  |
| 7   | T     | 37  | LEU  |
| 7   | T     | 38  | HIS  |
| 7   | T     | 43  | GLU  |
| 7   | T     | 84  | LYS  |
| 8   | U     | 8   | ILE  |
| 8   | U     | 52  | VAL  |
| 8   | U     | 60  | TYR  |
| 8   | U     | 61  | LYS  |
| 9   | V     | 2   | THR  |
| 9   | V     | 29  | LEU  |
| 9   | V     | 36  | LYS  |
| 9   | V     | 37  | PHE  |
| 9   | V     | 61  | GLU  |
| 9   | V     | 65  | LYS  |
| 10  | W     | 7   | GLU  |
| 10  | W     | 50  | LEU  |
| 12  | Y     | 2   | HIS  |
| 12  | Y     | 11  | ILE  |
| 12  | Y     | 20  | ARG  |
| 13  | Z     | 13  | LYS  |
| 13  | Z     | 38  | ASP  |
| 13  | Z     | 39  | ASN  |
| 13  | Z     | 42  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 55  | ASN  |
| 1   | A     | 170 | ASN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 422 | ASN  |
| 1   | A     | 503 | HIS  |
| 2   | B     | 52  | HIS  |
| 2   | B     | 59  | GLN  |
| 2   | B     | 140 | ASN  |
| 2   | B     | 181 | GLN  |
| 3   | C     | 50  | ASN  |
| 3   | C     | 68  | GLN  |
| 3   | C     | 76  | GLN  |
| 3   | C     | 230 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 29  | HIS  |
| 4   | D     | 37  | GLN  |
| 4   | D     | 76  | ASN  |
| 4   | D     | 119 | GLN  |
| 4   | D     | 143 | ASN  |
| 5   | E     | 94  | ASN  |
| 6   | F     | 80  | GLN  |
| 6   | F     | 95  | GLN  |
| 7   | G     | 76  | ASN  |
| 8   | H     | 31  | GLN  |
| 8   | H     | 32  | ASN  |
| 8   | H     | 37  | HIS  |
| 10  | J     | 57  | HIS  |
| 11  | K     | 35  | GLN  |
| 1   | N     | 55  | ASN  |
| 1   | N     | 170 | ASN  |
| 1   | N     | 180 | GLN  |
| 1   | N     | 422 | ASN  |
| 1   | N     | 503 | HIS  |
| 2   | O     | 91  | ASN  |
| 2   | O     | 181 | GLN  |
| 3   | P     | 50  | ASN  |
| 3   | P     | 68  | GLN  |
| 3   | P     | 76  | GLN  |
| 4   | Q     | 37  | GLN  |
| 4   | Q     | 101 | HIS  |
| 5   | R     | 94  | ASN  |
| 6   | S     | 54  | ASN  |
| 6   | S     | 80  | GLN  |
| 6   | S     | 94  | HIS  |
| 7   | T     | 8   | HIS  |
| 7   | T     | 76  | ASN  |
| 8   | U     | 31  | GLN  |
| 8   | U     | 37  | HIS  |
| 9   | V     | 20  | HIS  |
| 10  | W     | 57  | HIS  |
| 11  | X     | 35  | GLN  |

### 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 |
| 2   | FME  | B     | 1   | 2    | 8,9,10       | 5.84 | 6 (75%)  | 7,9,11      | 8.82 | 4 (57%)  |
| 7   | TPO  | G     | 11  | 7    | 8,10,11      | 2.10 | 4 (50%)  | 10,14,16    | 1.99 | 2 (20%)  |
| 1   | FME  | N     | 1   | 1    | 8,9,10       | 1.31 | 1 (12%)  | 7,9,11      | 1.73 | 2 (28%)  |
| 9   | SAC  | V     | 1   | 9    | 7,8,9        | 2.32 | 2 (28%)  | 8,9,11      | 3.04 | 4 (50%)  |
| 7   | TPO  | T     | 11  | 7    | 8,10,11      | 1.69 | 2 (25%)  | 10,14,16    | 1.24 | 1 (10%)  |
| 1   | FME  | A     | 1   | 1    | 8,9,10       | 1.69 | 2 (25%)  | 7,9,11      | 1.64 | 3 (42%)  |
| 9   | SAC  | I     | 1   | 9    | 7,8,9        | 2.70 | 3 (42%)  | 8,9,11      | 1.44 | 1 (12%)  |
| 2   | FME  | O     | 1   | 2    | 8,9,10       | 1.93 | 4 (50%)  | 7,9,11      | 2.34 | 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 |
|-----|------|-------|-----|------|---------|-----------|-------|
| 2   | FME  | B     | 1   | 2    | -       | 1/7/9/11  | -     |
| 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  | -     |
| 7   | TPO  | T     | 11  | 7    | -       | 4/9/11/13 | -     |
| 1   | FME  | A     | 1   | 1    | -       | 3/7/9/11  | -     |
| 9   | SAC  | I     | 1   | 9    | -       | 1/7/8/10  | -     |
| 2   | FME  | O     | 1   | 2    | -       | 0/7/9/11  | -     |

All (24) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 1   | FME  | CN-N  | 11.15 | 1.71        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 1   | FME  | O1-CN   | -8.94 | 0.95        | 1.22     |
| 9   | I     | 1   | SAC  | OAC-C1A | 5.36  | 1.35        | 1.23     |
| 9   | V     | 1   | SAC  | OAC-C1A | 4.57  | 1.33        | 1.23     |
| 2   | B     | 1   | FME  | CB-CA   | 4.52  | 1.61        | 1.53     |
| 2   | B     | 1   | FME  | CG-SD   | -4.20 | 1.59        | 1.81     |
| 9   | V     | 1   | SAC  | CA-N    | 3.84  | 1.51        | 1.46     |
| 2   | B     | 1   | FME  | CA-N    | 3.75  | 1.51        | 1.46     |
| 2   | B     | 1   | FME  | CB-CG   | 3.68  | 1.65        | 1.51     |
| 1   | A     | 1   | FME  | CA-N    | 3.41  | 1.51        | 1.46     |
| 7   | G     | 11  | TPO  | P-O1P   | 3.38  | 1.61        | 1.50     |
| 9   | I     | 1   | SAC  | CA-N    | 3.32  | 1.51        | 1.46     |
| 2   | O     | 1   | FME  | CG-SD   | -3.03 | 1.65        | 1.81     |
| 7   | T     | 11  | TPO  | P-O1P   | 2.97  | 1.60        | 1.50     |
| 2   | O     | 1   | FME  | CB-CA   | 2.87  | 1.58        | 1.53     |
| 1   | A     | 1   | FME  | O-C     | 2.85  | 1.31        | 1.19     |
| 7   | G     | 11  | TPO  | CG2-CB  | 2.60  | 1.57        | 1.51     |
| 9   | I     | 1   | SAC  | O-C     | 2.33  | 1.29        | 1.19     |
| 2   | O     | 1   | FME  | CN-N    | 2.24  | 1.40        | 1.33     |
| 2   | O     | 1   | FME  | CB-CG   | 2.22  | 1.60        | 1.51     |
| 1   | N     | 1   | FME  | CB-CG   | 2.17  | 1.59        | 1.51     |
| 7   | G     | 11  | TPO  | P-OG1   | 2.14  | 1.63        | 1.59     |
| 7   | T     | 11  | TPO  | P-OG1   | 2.08  | 1.63        | 1.59     |
| 7   | G     | 11  | TPO  | P-O2P   | 2.02  | 1.62        | 1.54     |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2   | B     | 1   | FME  | O1-CN-N   | -17.24 | 79.86       | 125.27   |
| 2   | B     | 1   | FME  | CA-N-CN   | -13.95 | 101.37      | 122.82   |
| 2   | B     | 1   | FME  | CG-CB-CA  | -5.63  | 97.31       | 112.95   |
| 7   | G     | 11  | TPO  | CG2-CB-CA | 5.16   | 123.35      | 113.16   |
| 9   | V     | 1   | SAC  | C-CA-N    | -5.02  | 100.67      | 109.73   |
| 2   | O     | 1   | FME  | CG-CB-CA  | -4.32  | 100.96      | 112.95   |
| 2   | B     | 1   | FME  | C-CA-N    | 4.25   | 117.40      | 109.73   |
| 9   | V     | 1   | SAC  | C2A-C1A-N | 3.90   | 122.70      | 116.10   |
| 9   | V     | 1   | SAC  | CA-N-C1A  | 3.83   | 130.21      | 123.15   |
| 9   | I     | 1   | SAC  | CB-CA-N   | 3.14   | 117.60      | 110.55   |
| 1   | N     | 1   | FME  | CE-SD-CG  | 3.13   | 111.16      | 100.40   |
| 9   | V     | 1   | SAC  | OAC-C1A-N | -3.10  | 116.26      | 121.95   |
| 2   | O     | 1   | FME  | C-CA-N    | -3.02  | 104.28      | 109.73   |
| 7   | T     | 11  | TPO  | O3P-P-OG1 | 2.99   | 119.39      | 105.99   |
| 1   | N     | 1   | FME  | O-C-CA    | -2.68  | 117.75      | 124.78   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | G     | 11  | TPO  | O-C-CA   | -2.68 | 117.75      | 124.78   |
| 2   | O     | 1   | FME  | CA-N-CN  | -2.62 | 118.79      | 122.82   |
| 1   | A     | 1   | FME  | O-C-CA   | -2.60 | 117.97      | 124.78   |
| 1   | A     | 1   | FME  | CE-SD-CG | 2.07  | 107.50      | 100.40   |
| 1   | A     | 1   | FME  | O1-CN-N  | -2.03 | 119.92      | 125.27   |

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 16 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 1   | FME  | 8       | 0            |
| 7   | G     | 11  | TPO  | 4       | 0            |
| 7   | T     | 11  | TPO  | 3       | 0            |
| 1   | A     | 1   | FME  | 1       | 0            |

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 46 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 |
| 25  | CDL  | C     | 303 | -     | 99,99,99     | 1.82 | 20 (20%) | 105,111,111 | 2.30 | 34 (32%) |
| 23  | PSC  | O     | 303 | -     | 51,51,51     | 1.45 | 3 (5%)   | 57,59,59    | 1.73 | 11 (19%) |
| 26  | PEK  | T     | 101 | -     | 52,52,52     | 1.60 | 4 (7%)   | 55,57,57    | 2.28 | 10 (18%) |
| 28  | DMU  | P     | 306 | -     | 34,34,34     | 0.87 | 1 (2%)   | 45,45,45    | 1.80 | 9 (20%)  |
| 22  | CHD  | P     | 307 | -     | 32,32,32     | 1.98 | 13 (40%) | 51,51,51    | 2.47 | 20 (39%) |
| 14  | HEA  | A     | 601 | 1     | 66,67,67     | 2.34 | 24 (36%) | 78,103,103  | 2.30 | 25 (32%) |
| 22  | CHD  | C     | 305 | -     | 32,32,32     | 2.46 | 15 (46%) | 51,51,51    | 2.68 | 20 (39%) |
| 26  | PEK  | G     | 101 | -     | 52,52,52     | 1.20 | 5 (9%)   | 55,57,57    | 1.66 | 12 (21%) |
| 19  | PGV  | P     | 301 | -     | 50,50,50     | 1.11 | 2 (4%)   | 53,56,56    | 1.68 | 10 (18%) |
| 20  | TGL  | N     | 608 | -     | 62,62,62     | 1.44 | 8 (12%)  | 65,65,65    | 2.18 | 14 (21%) |
| 26  | PEK  | P     | 308 | -     | 52,52,52     | 1.68 | 6 (11%)  | 55,57,57    | 1.92 | 14 (25%) |
| 22  | CHD  | O     | 302 | -     | 32,32,32     | 2.42 | 11 (34%) | 51,51,51    | 2.45 | 21 (41%) |
| 20  | TGL  | L     | 101 | -     | 62,62,62     | 2.10 | 13 (20%) | 65,65,65    | 2.84 | 27 (41%) |
| 19  | PGV  | A     | 608 | -     | 50,50,50     | 1.97 | 6 (12%)  | 53,56,56    | 2.43 | 14 (26%) |
| 25  | CDL  | P     | 304 | -     | 99,99,99     | 2.05 | 22 (22%) | 105,111,111 | 2.17 | 35 (33%) |
| 26  | PEK  | T     | 102 | -     | 52,52,52     | 1.30 | 2 (3%)   | 55,57,57    | 1.55 | 8 (14%)  |
| 23  | PSC  | B     | 304 | -     | 51,51,51     | 1.32 | 3 (5%)   | 57,59,59    | 1.77 | 12 (21%) |
| 21  | CUA  | O     | 301 | 2     | 0,1,1        | -    | -        | -           | -    | -        |
| 19  | PGV  | C     | 307 | -     | 50,50,50     | 1.29 | 4 (8%)   | 53,56,56    | 1.60 | 8 (15%)  |
| 22  | CHD  | W     | 101 | -     | 32,32,32     | 2.03 | 13 (40%) | 51,51,51    | 4.55 | 31 (60%) |
| 28  | DMU  | J     | 101 | -     | 34,34,34     | 1.00 | 1 (2%)   | 45,45,45    | 1.48 | 6 (13%)  |
| 18  | PER  | A     | 606 | 14,15 | 1,1,1        | 1.25 | 0        | -           | -    | -        |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | PGV  | A     | 607 | -     | 50,50,50     | 1.49 | 9 (18%)  | 53,56,56    | 1.54 | 11 (20%) |
| 20  | TGL  | Q     | 202 | -     | 62,62,62     | 2.36 | 11 (17%) | 65,65,65    | 2.77 | 14 (21%) |
| 20  | TGL  | D     | 201 | -     | 62,62,62     | 2.77 | 11 (17%) | 65,65,65    | 3.36 | 24 (36%) |
| 26  | PEK  | C     | 306 | -     | 52,52,52     | 1.61 | 5 (9%)   | 55,57,57    | 2.21 | 18 (32%) |
| 20  | TGL  | Y     | 101 | -     | 62,62,62     | 2.05 | 11 (17%) | 65,65,65    | 3.06 | 27 (41%) |
| 14  | HEA  | N     | 602 | 1,18  | 66,67,67     | 1.85 | 17 (25%) | 78,103,103  | 2.66 | 37 (47%) |
| 14  | HEA  | N     | 601 | 1     | 66,67,67     | 2.22 | 25 (37%) | 78,103,103  | 2.52 | 26 (33%) |
| 19  | PGV  | Q     | 201 | -     | 50,50,50     | 1.31 | 3 (6%)   | 53,56,56    | 1.74 | 10 (18%) |
| 25  | CDL  | T     | 103 | -     | 99,99,99     | 1.53 | 12 (12%) | 105,111,111 | 1.67 | 18 (17%) |
| 26  | PEK  | G     | 103 | -     | 52,52,52     | 1.29 | 3 (5%)   | 55,57,57    | 1.64 | 11 (20%) |
| 14  | HEA  | A     | 602 | 1,18  | 66,67,67     | 1.73 | 18 (27%) | 78,103,103  | 2.14 | 23 (29%) |
| 19  | PGV  | C     | 302 | -     | 50,50,50     | 1.41 | 5 (10%)  | 53,56,56    | 2.06 | 5 (9%)   |
| 22  | CHD  | P     | 305 | -     | 32,32,32     | 1.53 | 6 (18%)  | 51,51,51    | 3.52 | 29 (56%) |
| 22  | CHD  | B     | 303 | -     | 32,32,32     | 2.75 | 18 (56%) | 51,51,51    | 2.65 | 23 (45%) |
| 22  | CHD  | J     | 102 | -     | 32,32,32     | 1.86 | 9 (28%)  | 51,51,51    | 4.61 | 35 (68%) |
| 18  | PER  | N     | 606 | 14,15 | 1,1,1        | 1.24 | 0        | -           | -    | -        |
| 25  | CDL  | G     | 102 | -     | 99,99,99     | 1.49 | 13 (13%) | 105,111,111 | 1.82 | 22 (20%) |
| 19  | PGV  | P     | 303 | -     | 50,50,50     | 1.06 | 3 (6%)   | 53,56,56    | 1.51 | 13 (24%) |
| 20  | TGL  | B     | 301 | -     | 62,62,62     | 1.71 | 8 (12%)  | 65,65,65    | 2.82 | 21 (32%) |
| 28  | DMU  | Z     | 101 | -     | 34,34,34     | 1.26 | 5 (14%)  | 45,45,45    | 1.84 | 12 (26%) |
| 21  | CUA  | B     | 302 | 2     | 0,1,1        | -    | -        | -           | -    | -        |
| 28  | DMU  | M     | 101 | -     | 34,34,34     | 1.49 | 5 (14%)  | 45,45,45    | 2.24 | 16 (35%) |
| 22  | CHD  | C     | 304 | -     | 32,32,32     | 1.48 | 5 (15%)  | 51,51,51    | 3.85 | 30 (58%) |
| 19  | PGV  | N     | 607 | -     | 50,50,50     | 1.47 | 7 (14%)  | 53,56,56    | 1.50 | 11 (20%) |

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   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 25  | CDL  | C     | 303 | -    | -       | 57/110/110/110 | -       |
| 23  | PSC  | O     | 303 | -    | -       | 27/55/55/55    | -       |
| 26  | PEK  | T     | 101 | -    | -       | 21/56/56/56    | -       |
| 28  | DMU  | P     | 306 | -    | -       | 6/19/59/59     | 0/2/2/2 |
| 22  | CHD  | P     | 307 | -    | -       | 3/9/74/74      | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 14  | HEA  | A     | 601 | 1    | -       | 5/36/76/76     | -       |
| 22  | CHD  | C     | 305 | -    | -       | 2/9/74/74      | 0/4/4/4 |
| 26  | PEK  | G     | 101 | -    | -       | 16/56/56/56    | -       |
| 19  | PGV  | P     | 301 | -    | -       | 30/55/55/55    | -       |
| 20  | TGL  | N     | 608 | -    | -       | 43/65/65/65    | -       |
| 26  | PEK  | P     | 308 | -    | -       | 22/56/56/56    | -       |
| 22  | CHD  | O     | 302 | -    | -       | 2/9/74/74      | 0/4/4/4 |
| 20  | TGL  | L     | 101 | -    | -       | 34/65/65/65    | -       |
| 19  | PGV  | A     | 608 | -    | -       | 34/55/55/55    | -       |
| 25  | CDL  | P     | 304 | -    | -       | 62/110/110/110 | -       |
| 26  | PEK  | T     | 102 | -    | -       | 28/56/56/56    | -       |
| 23  | PSC  | B     | 304 | -    | -       | 31/55/55/55    | -       |
| 19  | PGV  | C     | 307 | -    | -       | 33/55/55/55    | -       |
| 22  | CHD  | W     | 101 | -    | -       | 9/9/74/74      | 0/4/4/4 |
| 28  | DMU  | J     | 101 | -    | -       | 6/19/59/59     | 0/2/2/2 |
| 19  | PGV  | A     | 607 | -    | -       | 8/55/55/55     | -       |
| 20  | TGL  | Q     | 202 | -    | -       | 36/65/65/65    | -       |
| 20  | TGL  | D     | 201 | -    | -       | 33/65/65/65    | -       |
| 26  | PEK  | C     | 306 | -    | -       | 34/56/56/56    | -       |
| 20  | TGL  | Y     | 101 | -    | -       | 41/65/65/65    | -       |
| 14  | HEA  | N     | 602 | 1,18 | -       | 4/36/76/76     | -       |
| 14  | HEA  | N     | 601 | 1    | -       | 6/36/76/76     | -       |
| 19  | PGV  | Q     | 201 | -    | -       | 31/55/55/55    | -       |
| 25  | CDL  | T     | 103 | -    | -       | 62/110/110/110 | -       |
| 26  | PEK  | G     | 103 | -    | -       | 22/56/56/56    | -       |
| 14  | HEA  | A     | 602 | 1,18 | -       | 4/36/76/76     | -       |
| 19  | PGV  | C     | 302 | -    | -       | 14/55/55/55    | -       |
| 22  | CHD  | P     | 305 | -    | -       | 7/9/74/74      | 0/4/4/4 |
| 22  | CHD  | B     | 303 | -    | -       | 2/9/74/74      | 0/4/4/4 |
| 22  | CHD  | J     | 102 | -    | -       | 7/9/74/74      | 0/4/4/4 |
| 25  | CDL  | G     | 102 | -    | -       | 59/110/110/110 | -       |
| 19  | PGV  | P     | 303 | -    | -       | 10/55/55/55    | -       |
| 20  | TGL  | B     | 301 | -    | -       | 31/65/65/65    | -       |
| 28  | DMU  | Z     | 101 | -    | -       | 5/19/59/59     | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 28  | DMU  | M     | 101 | -    | -       | 5/19/59/59 | 0/2/2/2 |
| 22  | CHD  | C     | 304 | -    | -       | 8/9/74/74  | 0/4/4/4 |
| 19  | PGV  | N     | 607 | -    | -       | 9/55/55/55 | -       |

All (385) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 20  | D     | 201 | TGL  | OB1-CB1 | 12.98 | 1.61        | 1.22     |
| 20  | Q     | 202 | TGL  | OB1-CB1 | 11.24 | 1.55        | 1.22     |
| 20  | D     | 201 | TGL  | OG2-CB1 | 10.44 | 1.63        | 1.34     |
| 20  | Q     | 202 | TGL  | OG2-CB1 | 9.46  | 1.60        | 1.34     |
| 14  | A     | 601 | HEA  | C18-C19 | -8.37 | 1.12        | 1.33     |
| 20  | L     | 101 | TGL  | OG2-CB1 | 8.31  | 1.57        | 1.34     |
| 20  | Y     | 101 | TGL  | OG2-CB1 | 7.74  | 1.56        | 1.34     |
| 19  | A     | 608 | PGV  | O02-C1  | 7.55  | 1.44        | 1.22     |
| 20  | B     | 301 | TGL  | OG1-CA1 | 7.27  | 1.54        | 1.33     |
| 25  | P     | 304 | CDL  | OB8-CB7 | 7.06  | 1.54        | 1.33     |
| 20  | Y     | 101 | TGL  | OG3-CC1 | 7.02  | 1.53        | 1.33     |
| 26  | P     | 308 | PEK  | O01-C1  | 7.01  | 1.54        | 1.34     |
| 19  | A     | 608 | PGV  | O03-C19 | 6.99  | 1.53        | 1.33     |
| 25  | P     | 304 | CDL  | PB2-OB3 | 6.75  | 1.74        | 1.50     |
| 26  | T     | 101 | PEK  | C3-C2   | 6.53  | 1.76        | 1.52     |
| 20  | D     | 201 | TGL  | OC1-CC1 | 6.49  | 1.41        | 1.22     |
| 26  | C     | 306 | PEK  | O01-C1  | 6.39  | 1.52        | 1.34     |
| 14  | N     | 601 | HEA  | C18-C19 | -6.29 | 1.17        | 1.33     |
| 14  | A     | 601 | HEA  | C16-C17 | -6.26 | 1.32        | 1.53     |
| 23  | O     | 303 | PSC  | O01-C1  | 6.22  | 1.51        | 1.34     |
| 25  | C     | 303 | CDL  | PB2-OB3 | 6.21  | 1.72        | 1.50     |
| 20  | Y     | 101 | TGL  | OG1-CA1 | 6.20  | 1.51        | 1.33     |
| 26  | P     | 308 | PEK  | O03-C21 | 6.20  | 1.51        | 1.33     |
| 26  | C     | 306 | PEK  | O03-C21 | 6.17  | 1.51        | 1.33     |
| 20  | B     | 301 | TGL  | OC1-CC1 | -6.16 | 1.04        | 1.22     |
| 25  | C     | 303 | CDL  | OB8-CB7 | 6.13  | 1.51        | 1.33     |
| 26  | G     | 103 | PEK  | O01-C1  | 6.06  | 1.51        | 1.34     |
| 25  | P     | 304 | CDL  | OA8-CA7 | 6.02  | 1.50        | 1.33     |
| 19  | Q     | 201 | PGV  | O03-C19 | 5.89  | 1.50        | 1.33     |
| 20  | L     | 101 | TGL  | OG3-CC1 | 5.87  | 1.50        | 1.33     |
| 25  | T     | 103 | CDL  | OB8-CB7 | 5.81  | 1.50        | 1.33     |
| 25  | P     | 304 | CDL  | OA6-CA5 | 5.78  | 1.50        | 1.34     |
| 25  | C     | 303 | CDL  | OA8-CA7 | 5.76  | 1.50        | 1.33     |
| 26  | T     | 101 | PEK  | C2-C1   | 5.74  | 1.67        | 1.50     |
| 20  | D     | 201 | TGL  | OG1-CA1 | 5.71  | 1.50        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | B     | 304 | PSC  | O01-C1  | 5.71  | 1.50        | 1.34     |
| 25  | T     | 103 | CDL  | OA6-CA5 | 5.66  | 1.50        | 1.34     |
| 26  | T     | 102 | PEK  | O01-C1  | 5.64  | 1.50        | 1.34     |
| 25  | P     | 304 | CDL  | O1-C1   | 5.59  | 1.60        | 1.43     |
| 22  | O     | 302 | CHD  | C10-C5  | -5.56 | 1.46        | 1.55     |
| 20  | N     | 608 | TGL  | OG1-CA1 | 5.50  | 1.49        | 1.33     |
| 26  | G     | 103 | PEK  | O03-C21 | 5.46  | 1.49        | 1.33     |
| 20  | L     | 101 | TGL  | OG1-CA1 | 5.44  | 1.49        | 1.33     |
| 25  | G     | 102 | CDL  | OB6-CB5 | 5.42  | 1.49        | 1.34     |
| 25  | G     | 102 | CDL  | OB8-CB7 | 5.38  | 1.49        | 1.33     |
| 26  | T     | 102 | PEK  | O03-C21 | 5.35  | 1.49        | 1.33     |
| 14  | N     | 601 | HEA  | O11-C11 | 5.28  | 1.54        | 1.42     |
| 25  | G     | 102 | CDL  | OA6-CA5 | 5.28  | 1.49        | 1.34     |
| 25  | T     | 103 | CDL  | OB6-CB5 | 5.27  | 1.49        | 1.34     |
| 25  | C     | 303 | CDL  | OA6-CA5 | 5.20  | 1.49        | 1.34     |
| 22  | C     | 305 | CHD  | C22-C20 | 5.19  | 1.67        | 1.54     |
| 22  | O     | 302 | CHD  | C19-C10 | 5.19  | 1.63        | 1.54     |
| 22  | B     | 303 | CHD  | C13-C14 | -5.14 | 1.46        | 1.55     |
| 20  | Q     | 202 | TGL  | OG3-CC1 | 5.10  | 1.48        | 1.33     |
| 22  | B     | 303 | CHD  | C19-C10 | 5.10  | 1.63        | 1.54     |
| 20  | Q     | 202 | TGL  | OG1-CA1 | 5.06  | 1.48        | 1.33     |
| 22  | O     | 302 | CHD  | C15-C14 | 4.93  | 1.64        | 1.54     |
| 14  | A     | 602 | HEA  | C18-C19 | 4.91  | 1.44        | 1.33     |
| 19  | C     | 307 | PGV  | O01-C1  | 4.85  | 1.48        | 1.34     |
| 19  | A     | 608 | PGV  | P-O13   | 4.82  | 1.68        | 1.50     |
| 25  | T     | 103 | CDL  | OA8-CA7 | 4.80  | 1.47        | 1.33     |
| 22  | P     | 307 | CHD  | C11-C12 | 4.79  | 1.61        | 1.53     |
| 19  | Q     | 201 | PGV  | O01-C1  | 4.75  | 1.47        | 1.34     |
| 25  | C     | 303 | CDL  | O1-C1   | 4.69  | 1.57        | 1.43     |
| 25  | P     | 304 | CDL  | CB2-C1  | 4.65  | 1.67        | 1.51     |
| 14  | N     | 601 | HEA  | CHC-C4B | 4.59  | 1.47        | 1.38     |
| 25  | G     | 102 | CDL  | OA8-CA7 | 4.58  | 1.46        | 1.33     |
| 19  | C     | 302 | PGV  | C22-C21 | 4.57  | 1.77        | 1.51     |
| 19  | P     | 301 | PGV  | O03-C19 | 4.55  | 1.46        | 1.33     |
| 20  | D     | 201 | TGL  | CC2-CC1 | 4.53  | 1.63        | 1.50     |
| 22  | J     | 102 | CHD  | C20-C17 | 4.51  | 1.62        | 1.54     |
| 22  | B     | 303 | CHD  | C4-C3   | 4.49  | 1.60        | 1.51     |
| 23  | B     | 304 | PSC  | O03-C19 | 4.42  | 1.46        | 1.33     |
| 14  | N     | 601 | HEA  | C16-C17 | -4.38 | 1.39        | 1.53     |
| 20  | D     | 201 | TGL  | OG3-CC1 | 4.36  | 1.46        | 1.33     |
| 19  | P     | 301 | PGV  | O01-C1  | 4.35  | 1.46        | 1.34     |
| 25  | P     | 304 | CDL  | OB8-CB6 | 4.32  | 1.55        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 20  | N     | 608 | TGL  | OG3-CC1 | 4.31  | 1.45        | 1.33     |
| 25  | C     | 303 | CDL  | CB2-C1  | 4.26  | 1.66        | 1.51     |
| 22  | W     | 101 | CHD  | C13-C17 | 4.23  | 1.62        | 1.55     |
| 19  | A     | 607 | PGV  | C01-C02 | 4.23  | 1.63        | 1.50     |
| 19  | C     | 302 | PGV  | C20-C19 | 4.22  | 1.63        | 1.50     |
| 20  | B     | 301 | TGL  | OG3-CC1 | 4.18  | 1.45        | 1.33     |
| 22  | B     | 303 | CHD  | C16-C17 | 4.16  | 1.63        | 1.54     |
| 23  | O     | 303 | PSC  | O03-C19 | 4.16  | 1.45        | 1.33     |
| 14  | N     | 602 | HEA  | C3A-C4A | -4.15 | 1.38        | 1.46     |
| 14  | N     | 601 | HEA  | CMC-C2C | 4.15  | 1.59        | 1.50     |
| 22  | O     | 302 | CHD  | C16-C17 | 4.10  | 1.62        | 1.54     |
| 20  | D     | 201 | TGL  | C10-CB9 | -4.08 | 1.28        | 1.51     |
| 23  | O     | 303 | PSC  | C13-C12 | 4.07  | 1.55        | 1.31     |
| 25  | C     | 303 | CDL  | C79-C78 | -4.05 | 1.28        | 1.51     |
| 14  | N     | 602 | HEA  | CBA-CGA | 4.05  | 1.60        | 1.50     |
| 19  | C     | 307 | PGV  | O03-C19 | 4.05  | 1.45        | 1.33     |
| 14  | N     | 602 | HEA  | FE-NB   | 4.04  | 2.07        | 1.94     |
| 22  | B     | 303 | CHD  | C4-C5   | 4.03  | 1.60        | 1.53     |
| 28  | J     | 101 | DMU  | O16-C6  | 4.03  | 1.47        | 1.40     |
| 22  | B     | 303 | CHD  | C15-C14 | 4.02  | 1.62        | 1.54     |
| 22  | B     | 303 | CHD  | C23-C24 | 4.00  | 1.59        | 1.50     |
| 25  | P     | 304 | CDL  | OB6-CB5 | 3.98  | 1.45        | 1.34     |
| 22  | C     | 305 | CHD  | C11-C12 | 3.96  | 1.59        | 1.53     |
| 23  | B     | 304 | PSC  | C13-C12 | 3.92  | 1.54        | 1.31     |
| 19  | N     | 607 | PGV  | C01-C02 | 3.90  | 1.62        | 1.50     |
| 22  | C     | 305 | CHD  | C4-C3   | 3.88  | 1.59        | 1.51     |
| 14  | A     | 601 | HEA  | C14-C15 | -3.87 | 1.23        | 1.33     |
| 22  | B     | 303 | CHD  | O7-C7   | 3.84  | 1.51        | 1.43     |
| 20  | B     | 301 | TGL  | CB2-CB1 | -3.83 | 1.39        | 1.50     |
| 22  | P     | 305 | CHD  | O25-C24 | 3.82  | 1.34        | 1.22     |
| 22  | W     | 101 | CHD  | C13-C12 | 3.81  | 1.60        | 1.54     |
| 19  | A     | 608 | PGV  | P-O12   | 3.79  | 1.74        | 1.59     |
| 22  | C     | 305 | CHD  | C6-C5   | 3.78  | 1.59        | 1.53     |
| 22  | O     | 302 | CHD  | C6-C7   | 3.78  | 1.59        | 1.52     |
| 19  | A     | 608 | PGV  | O01-C1  | 3.74  | 1.44        | 1.34     |
| 14  | N     | 601 | HEA  | CMB-C2B | 3.73  | 1.58        | 1.50     |
| 20  | L     | 101 | TGL  | CC2-CC1 | 3.72  | 1.61        | 1.50     |
| 14  | A     | 601 | HEA  | C16-C15 | 3.71  | 1.59        | 1.51     |
| 25  | T     | 103 | CDL  | C42-C41 | -3.70 | 1.30        | 1.51     |
| 20  | N     | 608 | TGL  | OG2-CB1 | 3.69  | 1.44        | 1.34     |
| 14  | A     | 601 | HEA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 28  | M     | 101 | DMU  | O7-C3   | 3.67  | 1.53        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | P     | 306 | DMU  | O16-C6  | 3.60  | 1.46        | 1.40     |
| 14  | A     | 602 | HEA  | FE-NB   | 3.58  | 2.05        | 1.94     |
| 22  | B     | 303 | CHD  | C10-C5  | -3.56 | 1.49        | 1.55     |
| 14  | N     | 601 | HEA  | C16-C15 | 3.52  | 1.58        | 1.51     |
| 20  | L     | 101 | TGL  | C20-CA9 | -3.52 | 1.31        | 1.51     |
| 22  | W     | 101 | CHD  | C8-C14  | 3.51  | 1.60        | 1.53     |
| 22  | C     | 305 | CHD  | C16-C17 | 3.48  | 1.61        | 1.54     |
| 22  | J     | 102 | CHD  | C8-C14  | 3.48  | 1.60        | 1.53     |
| 25  | P     | 304 | CDL  | C79-C78 | -3.46 | 1.32        | 1.51     |
| 25  | P     | 304 | CDL  | OB2-CB2 | 3.46  | 1.58        | 1.44     |
| 25  | P     | 304 | CDL  | C59-C58 | -3.45 | 1.32        | 1.51     |
| 22  | P     | 307 | CHD  | C22-C20 | 3.44  | 1.63        | 1.54     |
| 22  | P     | 307 | CHD  | C6-C7   | 3.41  | 1.58        | 1.52     |
| 22  | B     | 303 | CHD  | C6-C7   | 3.39  | 1.58        | 1.52     |
| 14  | A     | 601 | HEA  | CBD-CAD | 3.38  | 1.62        | 1.52     |
| 20  | L     | 101 | TGL  | C10-CB9 | -3.36 | 1.32        | 1.51     |
| 25  | G     | 102 | CDL  | C59-C58 | -3.36 | 1.32        | 1.51     |
| 19  | N     | 607 | PGV  | O01-C02 | -3.36 | 1.38        | 1.46     |
| 20  | L     | 101 | TGL  | CB2-CB1 | 3.35  | 1.60        | 1.50     |
| 22  | B     | 303 | CHD  | C6-C5   | 3.35  | 1.59        | 1.53     |
| 22  | C     | 305 | CHD  | O12-C12 | 3.33  | 1.49        | 1.43     |
| 14  | A     | 602 | HEA  | C24-C23 | 3.31  | 1.59        | 1.50     |
| 14  | A     | 601 | HEA  | CHA-C1A | 3.31  | 1.44        | 1.38     |
| 26  | T     | 101 | PEK  | O11-C03 | 3.31  | 1.57        | 1.44     |
| 25  | P     | 304 | CDL  | PB2-OB2 | 3.31  | 1.72        | 1.59     |
| 14  | N     | 602 | HEA  | C14-C15 | 3.30  | 1.40        | 1.33     |
| 14  | N     | 602 | HEA  | C20-C19 | 3.30  | 1.58        | 1.51     |
| 25  | C     | 303 | CDL  | PB2-OB2 | 3.29  | 1.72        | 1.59     |
| 22  | B     | 303 | CHD  | C18-C13 | 3.29  | 1.59        | 1.54     |
| 20  | Q     | 202 | TGL  | C10-CB9 | -3.28 | 1.33        | 1.51     |
| 26  | G     | 101 | PEK  | C23-C22 | -3.27 | 1.40        | 1.52     |
| 25  | G     | 102 | CDL  | C62-C61 | -3.27 | 1.33        | 1.51     |
| 14  | A     | 601 | HEA  | C4A-NA  | -3.25 | 1.33        | 1.39     |
| 22  | P     | 305 | CHD  | C11-C9  | 3.24  | 1.59        | 1.53     |
| 22  | P     | 307 | CHD  | C23-C24 | 3.24  | 1.58        | 1.50     |
| 25  | T     | 103 | CDL  | C62-C61 | -3.23 | 1.33        | 1.51     |
| 14  | N     | 602 | HEA  | O11-C11 | 3.22  | 1.49        | 1.42     |
| 20  | Y     | 101 | TGL  | C20-CA9 | -3.22 | 1.33        | 1.51     |
| 22  | W     | 101 | CHD  | C20-C17 | 3.21  | 1.60        | 1.54     |
| 22  | C     | 305 | CHD  | C13-C17 | 3.20  | 1.61        | 1.55     |
| 22  | C     | 304 | CHD  | C8-C9   | 3.20  | 1.60        | 1.53     |
| 14  | N     | 602 | HEA  | CBA-CAA | 3.18  | 1.62        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | N     | 607 | PGV  | O03-C01 | 3.18  | 1.52        | 1.45     |
| 22  | C     | 305 | CHD  | C2-C3   | 3.17  | 1.59        | 1.51     |
| 14  | N     | 602 | HEA  | CHA-C4D | 3.17  | 1.46        | 1.39     |
| 19  | N     | 607 | PGV  | C3-C2   | 3.17  | 1.63        | 1.52     |
| 14  | A     | 601 | HEA  | C3A-C4A | -3.16 | 1.40        | 1.46     |
| 20  | L     | 101 | TGL  | OG2-CG2 | 3.16  | 1.54        | 1.46     |
| 20  | N     | 608 | TGL  | OC1-CC1 | -3.14 | 1.13        | 1.22     |
| 22  | W     | 101 | CHD  | C8-C9   | 3.13  | 1.60        | 1.53     |
| 22  | J     | 102 | CHD  | C13-C17 | 3.13  | 1.60        | 1.55     |
| 14  | A     | 601 | HEA  | C4C-NC  | -3.12 | 1.33        | 1.39     |
| 20  | L     | 101 | TGL  | CG3-CG2 | 3.12  | 1.60        | 1.50     |
| 20  | Q     | 202 | TGL  | OC1-CC1 | 3.12  | 1.31        | 1.22     |
| 25  | P     | 304 | CDL  | C19-C18 | -3.12 | 1.34        | 1.51     |
| 22  | J     | 102 | CHD  | C8-C9   | 3.10  | 1.59        | 1.53     |
| 25  | P     | 304 | CDL  | C62-C61 | -3.10 | 1.34        | 1.51     |
| 25  | T     | 103 | CDL  | C22-C21 | -3.09 | 1.34        | 1.51     |
| 22  | P     | 307 | CHD  | C16-C15 | 3.09  | 1.62        | 1.54     |
| 25  | C     | 303 | CDL  | OB6-CB5 | 3.08  | 1.43        | 1.34     |
| 14  | A     | 602 | HEA  | C12-C11 | 3.08  | 1.58        | 1.52     |
| 19  | C     | 302 | PGV  | C21-C20 | 3.07  | 1.63        | 1.52     |
| 25  | G     | 102 | CDL  | C82-C81 | -3.07 | 1.34        | 1.51     |
| 22  | C     | 305 | CHD  | C16-C15 | 3.06  | 1.62        | 1.54     |
| 22  | P     | 305 | CHD  | C8-C9   | 3.06  | 1.59        | 1.53     |
| 14  | A     | 601 | HEA  | CMB-C2B | 3.06  | 1.57        | 1.50     |
| 26  | P     | 308 | PEK  | P-O11   | 3.04  | 1.71        | 1.59     |
| 25  | P     | 304 | CDL  | C22-C21 | -3.04 | 1.34        | 1.51     |
| 22  | O     | 302 | CHD  | C4-C3   | 3.03  | 1.57        | 1.51     |
| 20  | Y     | 101 | TGL  | C10-CB9 | -3.03 | 1.34        | 1.51     |
| 14  | N     | 601 | HEA  | CMD-C2D | 3.03  | 1.57        | 1.50     |
| 14  | A     | 601 | HEA  | C22-C23 | 3.02  | 1.41        | 1.32     |
| 25  | C     | 303 | CDL  | C82-C81 | -3.01 | 1.34        | 1.51     |
| 25  | T     | 103 | CDL  | C59-C58 | -3.00 | 1.34        | 1.51     |
| 22  | C     | 304 | CHD  | C10-C5  | 2.99  | 1.60        | 1.55     |
| 22  | O     | 302 | CHD  | C13-C12 | 2.99  | 1.59        | 1.54     |
| 22  | O     | 302 | CHD  | C8-C9   | 2.98  | 1.59        | 1.53     |
| 25  | C     | 303 | CDL  | C59-C58 | -2.97 | 1.34        | 1.51     |
| 26  | C     | 306 | PEK  | C22-C21 | 2.97  | 1.59        | 1.50     |
| 14  | N     | 602 | HEA  | CMB-C2B | 2.97  | 1.57        | 1.50     |
| 25  | C     | 303 | CDL  | C62-C61 | -2.95 | 1.35        | 1.51     |
| 22  | C     | 304 | CHD  | C8-C14  | 2.95  | 1.59        | 1.53     |
| 26  | P     | 308 | PEK  | C22-C21 | 2.94  | 1.59        | 1.50     |
| 25  | P     | 304 | CDL  | PA1-OA5 | 2.93  | 1.71        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | W     | 101 | CHD  | C13-C14 | 2.93  | 1.60        | 1.55     |
| 20  | N     | 608 | TGL  | C20-CA9 | -2.91 | 1.35        | 1.51     |
| 25  | T     | 103 | CDL  | C19-C18 | -2.91 | 1.35        | 1.51     |
| 22  | J     | 102 | CHD  | C8-C7   | 2.90  | 1.58        | 1.53     |
| 20  | L     | 101 | TGL  | OB1-CB1 | 2.89  | 1.31        | 1.22     |
| 20  | Y     | 101 | TGL  | CG3-CG2 | 2.88  | 1.59        | 1.50     |
| 19  | P     | 303 | PGV  | C20-C19 | 2.88  | 1.59        | 1.50     |
| 28  | Z     | 101 | DMU  | O55-C2  | 2.87  | 1.49        | 1.43     |
| 14  | A     | 601 | HEA  | CBA-CGA | 2.87  | 1.57        | 1.50     |
| 14  | A     | 601 | HEA  | CHB-C4A | 2.87  | 1.44        | 1.38     |
| 26  | C     | 306 | PEK  | P-O11   | 2.86  | 1.70        | 1.59     |
| 22  | B     | 303 | CHD  | C8-C7   | -2.86 | 1.48        | 1.53     |
| 14  | A     | 601 | HEA  | C12-C13 | 2.85  | 1.62        | 1.53     |
| 25  | T     | 103 | CDL  | C39-C38 | -2.85 | 1.35        | 1.51     |
| 14  | A     | 602 | HEA  | CHA-C1A | 2.85  | 1.43        | 1.38     |
| 25  | C     | 303 | CDL  | C19-C18 | -2.85 | 1.35        | 1.51     |
| 19  | N     | 607 | PGV  | O01-C1  | 2.84  | 1.42        | 1.34     |
| 19  | A     | 607 | PGV  | C3-C2   | 2.84  | 1.62        | 1.52     |
| 20  | B     | 301 | TGL  | C20-CA9 | -2.83 | 1.35        | 1.51     |
| 20  | N     | 608 | TGL  | C10-CB9 | -2.83 | 1.35        | 1.51     |
| 14  | N     | 601 | HEA  | C4A-NA  | -2.80 | 1.34        | 1.39     |
| 20  | D     | 201 | TGL  | C15-CC9 | -2.80 | 1.35        | 1.51     |
| 20  | Y     | 101 | TGL  | CC3-CC2 | 2.80  | 1.62        | 1.52     |
| 19  | N     | 607 | PGV  | C03-C02 | 2.80  | 1.59        | 1.50     |
| 25  | P     | 304 | CDL  | C39-C38 | -2.79 | 1.35        | 1.51     |
| 22  | C     | 305 | CHD  | C10-C9  | 2.79  | 1.61        | 1.56     |
| 25  | C     | 303 | CDL  | OB8-CB6 | 2.79  | 1.51        | 1.45     |
| 14  | N     | 601 | HEA  | C12-C13 | 2.78  | 1.62        | 1.53     |
| 26  | G     | 101 | PEK  | O01-C02 | 2.78  | 1.53        | 1.46     |
| 14  | A     | 602 | HEA  | CBD-CGD | 2.77  | 1.57        | 1.50     |
| 14  | N     | 602 | HEA  | CHB-C4A | 2.77  | 1.43        | 1.38     |
| 14  | A     | 602 | HEA  | C12-C13 | 2.77  | 1.62        | 1.53     |
| 20  | D     | 201 | TGL  | C20-CA9 | -2.76 | 1.36        | 1.51     |
| 22  | P     | 307 | CHD  | C16-C17 | 2.76  | 1.60        | 1.54     |
| 14  | N     | 602 | HEA  | C12-C13 | 2.76  | 1.62        | 1.53     |
| 25  | G     | 102 | CDL  | C39-C38 | -2.75 | 1.36        | 1.51     |
| 14  | A     | 601 | HEA  | CBA-CAA | 2.74  | 1.60        | 1.52     |
| 26  | T     | 101 | PEK  | C23-C22 | -2.74 | 1.42        | 1.52     |
| 14  | N     | 601 | HEA  | O1A-CGA | 2.74  | 1.31        | 1.22     |
| 14  | A     | 602 | HEA  | CHD-C1D | 2.73  | 1.44        | 1.38     |
| 28  | M     | 101 | DMU  | C2-C1   | 2.73  | 1.59        | 1.52     |
| 22  | C     | 305 | CHD  | O25-C24 | 2.73  | 1.31        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 20  | Q     | 202 | TGL  | C20-CA9 | -2.72 | 1.36        | 1.51     |
| 25  | G     | 102 | CDL  | C19-C18 | -2.71 | 1.36        | 1.51     |
| 25  | C     | 303 | CDL  | OB2-CB2 | 2.71  | 1.55        | 1.44     |
| 25  | C     | 303 | CDL  | C22-C21 | -2.71 | 1.36        | 1.51     |
| 22  | W     | 101 | CHD  | C8-C7   | 2.71  | 1.58        | 1.53     |
| 22  | P     | 307 | CHD  | C6-C5   | 2.71  | 1.58        | 1.53     |
| 14  | N     | 602 | HEA  | C3B-C2B | 2.71  | 1.40        | 1.34     |
| 14  | N     | 602 | HEA  | C1B-C2B | 2.70  | 1.49        | 1.44     |
| 14  | N     | 601 | HEA  | C1C-NC  | 2.70  | 1.45        | 1.39     |
| 28  | M     | 101 | DMU  | O5-C4   | 2.70  | 1.50        | 1.44     |
| 20  | N     | 608 | TGL  | C15-CC9 | -2.68 | 1.36        | 1.51     |
| 26  | G     | 101 | PEK  | O11-C03 | 2.68  | 1.55        | 1.44     |
| 25  | P     | 304 | CDL  | C82-C81 | -2.68 | 1.36        | 1.51     |
| 14  | N     | 601 | HEA  | CHD-C1D | 2.68  | 1.44        | 1.38     |
| 22  | P     | 307 | CHD  | C22-C23 | -2.67 | 1.44        | 1.52     |
| 22  | C     | 305 | CHD  | C8-C7   | 2.66  | 1.58        | 1.53     |
| 14  | A     | 602 | HEA  | C1A-C2A | -2.66 | 1.40        | 1.45     |
| 14  | N     | 602 | HEA  | O1D-CGD | 2.65  | 1.30        | 1.22     |
| 22  | C     | 305 | CHD  | C13-C12 | -2.65 | 1.50        | 1.54     |
| 14  | A     | 602 | HEA  | CMC-C2C | 2.64  | 1.56        | 1.50     |
| 19  | A     | 607 | PGV  | O03-C01 | 2.63  | 1.51        | 1.45     |
| 20  | D     | 201 | TGL  | CG3-CG2 | 2.63  | 1.58        | 1.50     |
| 22  | B     | 303 | CHD  | C21-C20 | 2.63  | 1.59        | 1.53     |
| 14  | N     | 601 | HEA  | CBA-CGA | 2.63  | 1.56        | 1.50     |
| 22  | C     | 305 | CHD  | C11-C9  | 2.62  | 1.58        | 1.53     |
| 25  | C     | 303 | CDL  | PA1-OA5 | 2.61  | 1.69        | 1.59     |
| 19  | P     | 303 | PGV  | P-O14   | -2.61 | 1.43        | 1.55     |
| 22  | W     | 101 | CHD  | C11-C9  | 2.59  | 1.58        | 1.53     |
| 14  | A     | 602 | HEA  | C3A-C2A | 2.58  | 1.42        | 1.36     |
| 22  | P     | 307 | CHD  | C11-C9  | 2.58  | 1.58        | 1.53     |
| 20  | Y     | 101 | TGL  | C15-CC9 | -2.58 | 1.37        | 1.51     |
| 20  | Y     | 101 | TGL  | OG2-CG2 | 2.57  | 1.53        | 1.46     |
| 14  | N     | 601 | HEA  | C3A-C4A | -2.57 | 1.41        | 1.46     |
| 14  | A     | 601 | HEA  | C1A-C2A | -2.57 | 1.40        | 1.45     |
| 14  | A     | 602 | HEA  | C3B-C2B | 2.56  | 1.40        | 1.34     |
| 14  | A     | 601 | HEA  | CMC-C2C | 2.55  | 1.56        | 1.50     |
| 28  | M     | 101 | DMU  | O16-C6  | 2.54  | 1.44        | 1.40     |
| 14  | N     | 602 | HEA  | C12-C11 | 2.53  | 1.57        | 1.52     |
| 14  | N     | 602 | HEA  | C13-C14 | 2.53  | 1.58        | 1.50     |
| 22  | B     | 303 | CHD  | C10-C9  | -2.52 | 1.51        | 1.56     |
| 20  | Y     | 101 | TGL  | CB2-CB1 | 2.52  | 1.58        | 1.50     |
| 25  | T     | 103 | CDL  | C82-C81 | -2.52 | 1.37        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | Z     | 101 | DMU  | O7-C3   | 2.52  | 1.50        | 1.43     |
| 25  | C     | 303 | CDL  | C39-C38 | -2.52 | 1.37        | 1.51     |
| 25  | G     | 102 | CDL  | C79-C78 | -2.51 | 1.37        | 1.51     |
| 25  | C     | 303 | CDL  | C42-C41 | -2.51 | 1.37        | 1.51     |
| 14  | N     | 601 | HEA  | CHB-C4A | 2.51  | 1.43        | 1.38     |
| 14  | N     | 601 | HEA  | C1D-C2D | -2.50 | 1.39        | 1.44     |
| 22  | W     | 101 | CHD  | O26-C24 | -2.49 | 1.22        | 1.30     |
| 22  | P     | 305 | CHD  | C10-C5  | 2.48  | 1.59        | 1.55     |
| 20  | Y     | 101 | TGL  | CC2-CC1 | 2.48  | 1.58        | 1.50     |
| 14  | A     | 601 | HEA  | C1D-ND  | -2.47 | 1.36        | 1.40     |
| 25  | P     | 304 | CDL  | C42-C41 | -2.46 | 1.37        | 1.51     |
| 22  | O     | 302 | CHD  | C13-C14 | -2.46 | 1.51        | 1.55     |
| 22  | P     | 307 | CHD  | C2-C3   | 2.44  | 1.57        | 1.51     |
| 19  | A     | 607 | PGV  | O01-C1  | 2.43  | 1.41        | 1.34     |
| 25  | G     | 102 | CDL  | C42-C41 | -2.43 | 1.37        | 1.51     |
| 20  | Q     | 202 | TGL  | C15-CC9 | -2.42 | 1.38        | 1.51     |
| 25  | P     | 304 | CDL  | OA2-CA2 | -2.41 | 1.35        | 1.44     |
| 20  | B     | 301 | TGL  | C10-CB9 | -2.41 | 1.38        | 1.51     |
| 22  | B     | 303 | CHD  | C8-C9   | 2.40  | 1.58        | 1.53     |
| 14  | N     | 601 | HEA  | C14-C15 | -2.39 | 1.27        | 1.33     |
| 20  | L     | 101 | TGL  | C15-CC9 | -2.39 | 1.38        | 1.51     |
| 20  | Q     | 202 | TGL  | CB3-CB2 | 2.39  | 1.61        | 1.52     |
| 26  | C     | 306 | PEK  | O04-C21 | 2.38  | 1.29        | 1.22     |
| 20  | L     | 101 | TGL  | CG1-CG2 | 2.37  | 1.58        | 1.50     |
| 28  | Z     | 101 | DMU  | O16-C6  | 2.37  | 1.44        | 1.40     |
| 22  | J     | 102 | CHD  | C13-C12 | 2.37  | 1.58        | 1.54     |
| 14  | N     | 601 | HEA  | CBD-CAD | 2.35  | 1.59        | 1.52     |
| 19  | C     | 302 | PGV  | O06-C06 | 2.35  | 1.52        | 1.42     |
| 19  | C     | 307 | PGV  | P-O11   | 2.35  | 1.68        | 1.59     |
| 14  | N     | 601 | HEA  | O2A-CGA | -2.34 | 1.22        | 1.30     |
| 14  | N     | 601 | HEA  | CHA-C4D | 2.33  | 1.44        | 1.39     |
| 22  | C     | 305 | CHD  | C23-C24 | 2.32  | 1.56        | 1.50     |
| 14  | N     | 601 | HEA  | CHA-C1A | 2.32  | 1.42        | 1.38     |
| 19  | A     | 607 | PGV  | C29-C28 | 2.31  | 1.64        | 1.51     |
| 26  | P     | 308 | PEK  | P-O12   | 2.31  | 1.68        | 1.59     |
| 20  | L     | 101 | TGL  | CA6-CA5 | -2.31 | 1.38        | 1.51     |
| 22  | J     | 102 | CHD  | C23-C24 | 2.31  | 1.55        | 1.50     |
| 19  | A     | 608 | PGV  | C3-C2   | -2.29 | 1.43        | 1.52     |
| 25  | C     | 303 | CDL  | CA2-C1  | 2.29  | 1.59        | 1.51     |
| 14  | A     | 602 | HEA  | FE-ND   | 2.29  | 2.01        | 1.94     |
| 14  | A     | 601 | HEA  | CAD-C3D | 2.28  | 1.57        | 1.51     |
| 28  | Z     | 101 | DMU  | O1-C10  | 2.28  | 1.47        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 20  | B     | 301 | TGL  | C15-CC9 | -2.28 | 1.38        | 1.51     |
| 25  | G     | 102 | CDL  | C22-C21 | -2.28 | 1.38        | 1.51     |
| 22  | O     | 302 | CHD  | C4-C5   | 2.27  | 1.57        | 1.53     |
| 22  | B     | 303 | CHD  | O3-C3   | 2.27  | 1.50        | 1.43     |
| 22  | W     | 101 | CHD  | C23-C24 | 2.27  | 1.55        | 1.50     |
| 14  | N     | 601 | HEA  | C4B-NB  | -2.27 | 1.36        | 1.40     |
| 28  | M     | 101 | DMU  | C3-C4   | 2.26  | 1.58        | 1.52     |
| 25  | P     | 304 | CDL  | C31-CA7 | 2.26  | 1.57        | 1.50     |
| 19  | A     | 607 | PGV  | C8-C7   | 2.26  | 1.64        | 1.51     |
| 25  | T     | 103 | CDL  | C79-C78 | -2.26 | 1.38        | 1.51     |
| 19  | Q     | 201 | PGV  | C3-C2   | -2.25 | 1.43        | 1.52     |
| 19  | N     | 607 | PGV  | C8-C7   | 2.25  | 1.64        | 1.51     |
| 22  | P     | 305 | CHD  | C8-C14  | 2.24  | 1.58        | 1.53     |
| 20  | B     | 301 | TGL  | CG1-CG2 | 2.24  | 1.57        | 1.50     |
| 25  | G     | 102 | CDL  | CB6-CB4 | 2.23  | 1.57        | 1.50     |
| 14  | N     | 601 | HEA  | C4B-C3B | -2.23 | 1.40        | 1.44     |
| 14  | A     | 601 | HEA  | CBC-CAC | 2.22  | 1.41        | 1.30     |
| 22  | W     | 101 | CHD  | C16-C17 | 2.22  | 1.59        | 1.54     |
| 14  | A     | 602 | HEA  | C4A-NA  | -2.22 | 1.35        | 1.39     |
| 26  | P     | 308 | PEK  | C03-C02 | 2.21  | 1.57        | 1.50     |
| 14  | N     | 602 | HEA  | C4D-ND  | 2.20  | 1.43        | 1.38     |
| 20  | N     | 608 | TGL  | CG1-CG2 | 2.20  | 1.57        | 1.50     |
| 19  | A     | 607 | PGV  | C04-C05 | 2.20  | 1.58        | 1.51     |
| 22  | P     | 307 | CHD  | O25-C24 | 2.19  | 1.29        | 1.22     |
| 14  | A     | 602 | HEA  | C3C-C2C | -2.19 | 1.33        | 1.41     |
| 22  | W     | 101 | CHD  | O25-C24 | 2.19  | 1.29        | 1.22     |
| 19  | A     | 607 | PGV  | O06-C06 | 2.19  | 1.51        | 1.42     |
| 14  | A     | 601 | HEA  | CHB-C1B | 2.18  | 1.44        | 1.39     |
| 14  | A     | 601 | HEA  | C4B-NB  | -2.18 | 1.36        | 1.40     |
| 22  | J     | 102 | CHD  | C6-C7   | 2.17  | 1.56        | 1.52     |
| 22  | O     | 302 | CHD  | C23-C24 | 2.16  | 1.55        | 1.50     |
| 14  | A     | 601 | HEA  | CHC-C4B | 2.15  | 1.42        | 1.38     |
| 14  | N     | 601 | HEA  | C4C-NC  | -2.14 | 1.35        | 1.39     |
| 26  | G     | 101 | PEK  | C38-C37 | 2.14  | 1.67        | 1.49     |
| 22  | P     | 305 | CHD  | C13-C14 | 2.13  | 1.59        | 1.55     |
| 22  | B     | 303 | CHD  | C1-C10  | 2.12  | 1.57        | 1.54     |
| 19  | A     | 607 | PGV  | C25-C24 | 2.12  | 1.63        | 1.51     |
| 14  | A     | 602 | HEA  | C21-C22 | 2.11  | 1.57        | 1.50     |
| 28  | Z     | 101 | DMU  | O3-C5   | 2.11  | 1.47        | 1.43     |
| 22  | J     | 102 | CHD  | C6-C5   | 2.09  | 1.57        | 1.53     |
| 20  | Q     | 202 | TGL  | CC2-CC1 | 2.09  | 1.56        | 1.50     |
| 19  | C     | 307 | PGV  | C21-C20 | -2.08 | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | P     | 304 | CDL  | C11-CA5 | 2.08  | 1.56        | 1.50     |
| 26  | G     | 103 | PEK  | C01-C02 | 2.08  | 1.57        | 1.50     |
| 22  | C     | 304 | CHD  | C20-C17 | 2.08  | 1.58        | 1.54     |
| 22  | C     | 304 | CHD  | C11-C9  | 2.07  | 1.57        | 1.53     |
| 22  | P     | 307 | CHD  | C13-C17 | 2.05  | 1.59        | 1.55     |
| 14  | A     | 602 | HEA  | C4D-C3D | 2.04  | 1.48        | 1.45     |
| 22  | W     | 101 | CHD  | C6-C7   | 2.04  | 1.56        | 1.52     |
| 19  | C     | 302 | PGV  | O01-C02 | -2.04 | 1.41        | 1.46     |
| 22  | P     | 307 | CHD  | C8-C14  | 2.04  | 1.57        | 1.53     |
| 19  | P     | 303 | PGV  | C01-C02 | 2.03  | 1.56        | 1.50     |
| 20  | D     | 201 | TGL  | CB2-CB1 | 2.03  | 1.56        | 1.50     |
| 20  | Q     | 202 | TGL  | CC3-CC2 | 2.02  | 1.59        | 1.52     |
| 14  | A     | 602 | HEA  | C3A-C4A | -2.01 | 1.42        | 1.46     |
| 26  | G     | 101 | PEK  | P-O12   | -2.00 | 1.51        | 1.59     |

All (777) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 22  | W     | 101 | CHD  | C17-C13-C12 | 17.08  | 133.26      | 117.67   |
| 20  | D     | 201 | TGL  | OG2-CB1-CB2 | -15.65 | 77.78       | 111.50   |
| 22  | W     | 101 | CHD  | C18-C13-C12 | -13.78 | 95.04       | 109.07   |
| 22  | J     | 102 | CHD  | C17-C13-C12 | 13.68  | 130.16      | 117.67   |
| 20  | D     | 201 | TGL  | OG2-CB1-OB1 | 13.55  | 156.45      | 123.70   |
| 26  | T     | 101 | PEK  | C2-C3-C4    | 13.21  | 136.78      | 113.23   |
| 20  | Q     | 202 | TGL  | OG2-CB1-CB2 | -12.51 | 84.54       | 111.50   |
| 20  | Q     | 202 | TGL  | OG2-CB1-OB1 | 11.29  | 150.99      | 123.70   |
| 14  | N     | 601 | HEA  | C17-C18-C19 | 10.46  | 152.85      | 127.66   |
| 22  | P     | 305 | CHD  | C18-C13-C12 | -10.04 | 98.84       | 109.07   |
| 22  | J     | 102 | CHD  | C14-C8-C7   | 10.01  | 125.09      | 111.81   |
| 25  | C     | 303 | CDL  | C52-C51-CB5 | -9.90  | 77.62       | 113.62   |
| 20  | Y     | 101 | TGL  | CC4-CC3-CC2 | -9.74  | 78.17       | 113.19   |
| 22  | J     | 102 | CHD  | C15-C14-C8  | 9.67   | 131.85      | 118.33   |
| 22  | J     | 102 | CHD  | C13-C17-C20 | 9.58   | 130.94      | 119.50   |
| 20  | L     | 101 | TGL  | CC4-CC3-CC2 | -9.48  | 79.13       | 113.19   |
| 22  | W     | 101 | CHD  | C13-C17-C20 | 9.28   | 130.57      | 119.50   |
| 20  | B     | 301 | TGL  | OG2-CB1-CB2 | 9.24   | 131.43      | 111.50   |
| 22  | C     | 304 | CHD  | C18-C13-C12 | -9.23  | 99.66       | 109.07   |
| 20  | Y     | 101 | TGL  | OG2-CB1-CB2 | 8.94   | 130.76      | 111.50   |
| 22  | J     | 102 | CHD  | C10-C9-C8   | 8.70   | 121.16      | 111.82   |
| 25  | P     | 304 | CDL  | C52-C51-CB5 | -8.59  | 82.38       | 113.62   |
| 20  | L     | 101 | TGL  | CG2-OG2-CB1 | 8.35   | 138.36      | 117.79   |
| 19  | C     | 302 | PGV  | C23-C22-C21 | 8.33   | 156.69      | 114.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | A     | 601 | HEA  | C17-C18-C19 | 8.29  | 147.62      | 127.66   |
| 19  | C     | 302 | PGV  | C22-C21-C20 | 8.18  | 142.59      | 113.19   |
| 20  | Y     | 101 | TGL  | CG2-OG2-CB1 | 8.03  | 137.57      | 117.79   |
| 20  | B     | 301 | TGL  | CG3-OG3-CC1 | 7.99  | 146.69      | 117.12   |
| 14  | N     | 601 | HEA  | C27-C19-C18 | -7.84 | 103.56      | 123.68   |
| 22  | P     | 305 | CHD  | C6-C7-C8    | 7.71  | 119.71      | 111.48   |
| 20  | B     | 301 | TGL  | OG2-CG2-CG3 | 7.58  | 135.85      | 108.40   |
| 26  | C     | 306 | PEK  | C36-C35-C34 | -7.51 | 76.28       | 114.42   |
| 14  | A     | 601 | HEA  | C20-C19-C18 | 7.50  | 136.29      | 121.12   |
| 23  | O     | 303 | PSC  | O01-C1-C2   | 7.44  | 127.53      | 111.50   |
| 22  | C     | 304 | CHD  | C6-C7-C8    | 7.35  | 119.33      | 111.48   |
| 22  | C     | 304 | CHD  | C16-C17-C20 | 7.31  | 123.47      | 112.15   |
| 22  | W     | 101 | CHD  | O12-C12-C13 | 7.24  | 123.27      | 111.03   |
| 19  | A     | 608 | PGV  | C3-C2-C1    | 7.22  | 139.87      | 113.62   |
| 25  | G     | 102 | CDL  | OA6-CA5-C11 | 7.10  | 126.81      | 111.50   |
| 14  | N     | 601 | HEA  | C27-C19-C20 | 7.07  | 127.16      | 115.27   |
| 22  | C     | 305 | CHD  | C17-C13-C12 | -6.98 | 111.30      | 117.67   |
| 22  | W     | 101 | CHD  | C14-C8-C7   | 6.98  | 121.06      | 111.81   |
| 14  | N     | 602 | HEA  | C4B-NB-C1B  | 6.97  | 112.28      | 105.07   |
| 28  | M     | 101 | DMU  | C28-C25-C22 | -6.95 | 79.15       | 114.42   |
| 22  | P     | 305 | CHD  | C6-C5-C10   | 6.94  | 120.02      | 112.66   |
| 22  | P     | 307 | CHD  | C6-C7-C8    | -6.94 | 104.08      | 111.48   |
| 26  | G     | 103 | PEK  | O01-C1-C2   | 6.89  | 126.35      | 111.50   |
| 22  | P     | 305 | CHD  | C4-C3-C2    | 6.82  | 118.69      | 110.55   |
| 19  | A     | 608 | PGV  | O01-C1-C2   | -6.81 | 96.82       | 111.50   |
| 20  | Q     | 202 | TGL  | CB3-CB2-CB1 | 6.74  | 138.13      | 113.62   |
| 20  | L     | 101 | TGL  | OG3-CC1-CC2 | 6.68  | 132.86      | 111.91   |
| 22  | C     | 304 | CHD  | C14-C13-C12 | 6.67  | 113.61      | 107.40   |
| 20  | Y     | 101 | TGL  | C26-C25-C24 | -6.64 | 80.72       | 114.42   |
| 25  | G     | 102 | CDL  | OB6-CB5-C51 | 6.56  | 125.65      | 111.50   |
| 22  | W     | 101 | CHD  | C17-C13-C14 | -6.56 | 93.48       | 100.09   |
| 22  | B     | 303 | CHD  | C11-C12-C13 | -6.54 | 104.53      | 111.24   |
| 22  | C     | 304 | CHD  | C6-C5-C4    | -6.53 | 103.68      | 111.19   |
| 22  | J     | 102 | CHD  | C18-C13-C12 | -6.50 | 102.45      | 109.07   |
| 22  | W     | 101 | CHD  | C11-C12-C13 | 6.49  | 117.91      | 111.24   |
| 22  | J     | 102 | CHD  | C11-C12-C13 | 6.49  | 117.91      | 111.24   |
| 22  | C     | 304 | CHD  | C6-C5-C10   | 6.46  | 119.52      | 112.66   |
| 22  | C     | 304 | CHD  | C15-C14-C8  | 6.43  | 127.33      | 118.33   |
| 26  | T     | 102 | PEK  | O01-C1-C2   | 6.42  | 125.34      | 111.50   |
| 22  | C     | 304 | CHD  | C10-C9-C8   | 6.42  | 118.71      | 111.82   |
| 19  | P     | 301 | PGV  | O03-C19-C20 | 6.39  | 131.96      | 111.91   |
| 23  | B     | 304 | PSC  | O01-C1-C2   | 6.38  | 125.26      | 111.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | J     | 102 | CHD  | C5-C6-C7    | 6.37  | 121.49      | 114.46   |
| 20  | N     | 608 | TGL  | CG2-OG2-CB1 | 6.36  | 133.44      | 117.79   |
| 14  | A     | 602 | HEA  | C4B-NB-C1B  | 6.32  | 111.61      | 105.07   |
| 14  | A     | 602 | HEA  | C13-C12-C11 | -6.31 | 104.87      | 114.35   |
| 22  | C     | 305 | CHD  | C6-C7-C8    | -6.29 | 104.77      | 111.48   |
| 20  | D     | 201 | TGL  | CB3-CB2-CB1 | 6.15  | 136.00      | 113.62   |
| 20  | B     | 301 | TGL  | OG1-CA1-CA2 | 6.03  | 130.84      | 111.91   |
| 19  | C     | 307 | PGV  | O03-C19-C20 | 6.03  | 130.82      | 111.91   |
| 22  | J     | 102 | CHD  | C6-C5-C10   | 6.02  | 119.05      | 112.66   |
| 14  | N     | 602 | HEA  | CHB-C1B-NB  | 5.99  | 130.92      | 124.42   |
| 22  | C     | 304 | CHD  | C4-C5-C10   | 5.98  | 119.00      | 112.66   |
| 25  | P     | 304 | CDL  | OB8-CB7-C71 | 5.94  | 130.54      | 111.91   |
| 22  | P     | 305 | CHD  | O7-C7-C6    | -5.92 | 95.25       | 109.94   |
| 19  | A     | 608 | PGV  | O01-C1-O02  | 5.92  | 138.00      | 123.70   |
| 25  | P     | 304 | CDL  | OA6-CA5-C11 | 5.87  | 124.15      | 111.50   |
| 22  | C     | 304 | CHD  | O7-C7-C6    | -5.85 | 95.42       | 109.94   |
| 25  | C     | 303 | CDL  | OA6-CA5-C11 | 5.83  | 124.06      | 111.50   |
| 20  | N     | 608 | TGL  | OG2-CG2-CG3 | 5.81  | 129.44      | 108.40   |
| 22  | C     | 304 | CHD  | C19-C10-C1  | -5.79 | 98.93       | 108.26   |
| 20  | Q     | 202 | TGL  | CG3-CG2-CG1 | -5.77 | 98.15       | 111.79   |
| 22  | C     | 304 | CHD  | C22-C23-C24 | -5.75 | 97.24       | 112.51   |
| 19  | A     | 608 | PGV  | C02-O01-C1  | 5.74  | 131.93      | 117.79   |
| 20  | B     | 301 | TGL  | OG3-CG3-CG2 | -5.72 | 91.79       | 108.43   |
| 25  | T     | 103 | CDL  | OA6-CA5-C11 | 5.72  | 123.83      | 111.50   |
| 20  | Y     | 101 | TGL  | CB3-CB2-CB1 | 5.66  | 134.20      | 113.62   |
| 25  | C     | 303 | CDL  | OB8-CB7-C71 | 5.64  | 129.62      | 111.91   |
| 20  | N     | 608 | TGL  | CG3-OG3-CC1 | 5.64  | 138.02      | 117.12   |
| 22  | C     | 305 | CHD  | C22-C23-C24 | -5.63 | 97.56       | 112.51   |
| 14  | N     | 602 | HEA  | CAD-CBD-CGD | -5.61 | 101.53      | 113.60   |
| 20  | Y     | 101 | TGL  | OG3-CC1-CC2 | 5.55  | 129.34      | 111.91   |
| 20  | D     | 201 | TGL  | OC1-CC1-CC2 | 5.50  | 145.21      | 123.73   |
| 25  | P     | 304 | CDL  | CA4-OA6-CA5 | 5.48  | 131.29      | 117.79   |
| 20  | N     | 608 | TGL  | OG1-CA1-CA2 | 5.46  | 129.03      | 111.91   |
| 22  | P     | 307 | CHD  | C21-C20-C22 | -5.45 | 101.81      | 110.36   |
| 22  | C     | 305 | CHD  | C18-C13-C12 | 5.44  | 114.61      | 109.07   |
| 22  | C     | 305 | CHD  | C23-C22-C20 | -5.42 | 104.61      | 114.52   |
| 22  | B     | 303 | CHD  | C5-C4-C3    | -5.41 | 104.81      | 112.76   |
| 22  | C     | 304 | CHD  | C16-C17-C13 | 5.40  | 108.85      | 103.55   |
| 22  | P     | 307 | CHD  | C17-C13-C12 | -5.38 | 112.75      | 117.67   |
| 25  | T     | 103 | CDL  | OB6-CB5-C51 | 5.37  | 123.07      | 111.50   |
| 26  | P     | 308 | PEK  | O03-C21-C22 | 5.36  | 128.74      | 111.91   |
| 14  | A     | 602 | HEA  | C4C-NC-C1C  | -5.30 | 100.16      | 105.35   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | P     | 305 | CHD  | C15-C14-C13 | 5.28  | 108.74      | 103.55   |
| 22  | B     | 303 | CHD  | C19-C10-C1  | -5.26 | 99.79       | 108.26   |
| 22  | O     | 302 | CHD  | C5-C4-C3    | -5.23 | 105.08      | 112.76   |
| 14  | N     | 602 | HEA  | C4A-NA-C1A  | -5.22 | 100.24      | 105.35   |
| 22  | J     | 102 | CHD  | C9-C8-C7    | 5.20  | 118.10      | 111.88   |
| 28  | M     | 101 | DMU  | O5-C4-C3    | -5.20 | 98.79       | 109.75   |
| 26  | C     | 306 | PEK  | O03-C21-O04 | -5.16 | 110.58      | 123.59   |
| 20  | L     | 101 | TGL  | OG2-CB1-CB2 | 5.12  | 122.53      | 111.50   |
| 14  | A     | 601 | HEA  | C27-C19-C18 | -5.04 | 110.76      | 123.68   |
| 22  | P     | 305 | CHD  | C6-C5-C4    | -5.03 | 105.39      | 111.19   |
| 20  | D     | 201 | TGL  | C21-C20-CA9 | 5.03  | 139.94      | 114.42   |
| 22  | P     | 305 | CHD  | C10-C9-C8   | 4.97  | 117.16      | 111.82   |
| 14  | A     | 601 | HEA  | C1D-C2D-C3D | -4.97 | 101.73      | 106.96   |
| 22  | W     | 101 | CHD  | C4-C5-C10   | 4.96  | 117.93      | 112.66   |
| 22  | O     | 302 | CHD  | C6-C5-C4    | -4.94 | 105.50      | 111.19   |
| 20  | L     | 101 | TGL  | C22-C21-C20 | -4.93 | 89.39       | 114.42   |
| 14  | N     | 602 | HEA  | C13-C12-C11 | -4.93 | 106.94      | 114.35   |
| 22  | O     | 302 | CHD  | C2-C1-C10   | -4.92 | 104.34      | 112.78   |
| 19  | C     | 302 | PGV  | C30-C29-C28 | -4.86 | 89.77       | 114.42   |
| 22  | O     | 302 | CHD  | C15-C14-C8  | -4.85 | 111.55      | 118.33   |
| 20  | Y     | 101 | TGL  | OG3-CG3-CG2 | 4.81  | 122.43      | 108.43   |
| 20  | B     | 301 | TGL  | OG3-CC1-CC2 | 4.80  | 126.98      | 111.91   |
| 20  | D     | 201 | TGL  | CG1-OG1-CA1 | 4.79  | 134.88      | 117.12   |
| 26  | C     | 306 | PEK  | O01-C1-C2   | 4.78  | 121.80      | 111.50   |
| 20  | N     | 608 | TGL  | OG2-CB1-CB2 | 4.78  | 121.79      | 111.50   |
| 22  | P     | 305 | CHD  | C16-C17-C13 | 4.76  | 108.23      | 103.55   |
| 20  | L     | 101 | TGL  | OG3-CC1-OC1 | -4.74 | 111.62      | 123.59   |
| 20  | L     | 101 | TGL  | OG1-CG1-CG2 | 4.73  | 122.21      | 108.43   |
| 22  | O     | 302 | CHD  | C19-C10-C1  | -4.73 | 100.64      | 108.26   |
| 22  | P     | 305 | CHD  | C14-C8-C9   | -4.72 | 103.24      | 109.71   |
| 22  | P     | 307 | CHD  | C22-C23-C24 | -4.71 | 100.00      | 112.51   |
| 22  | P     | 307 | CHD  | C22-C20-C17 | -4.71 | 100.55      | 110.28   |
| 23  | O     | 303 | PSC  | C28-C27-C26 | -4.69 | 90.61       | 114.42   |
| 20  | B     | 301 | TGL  | CB3-CB2-CB1 | -4.68 | 96.59       | 113.62   |
| 22  | C     | 304 | CHD  | C17-C13-C14 | -4.68 | 95.37       | 100.09   |
| 22  | J     | 102 | CHD  | C1-C10-C9   | -4.68 | 104.00      | 111.35   |
| 14  | N     | 602 | HEA  | C3C-C4C-NC  | 4.67  | 113.12      | 110.25   |
| 22  | C     | 304 | CHD  | C5-C6-C7    | 4.67  | 119.61      | 114.46   |
| 14  | N     | 601 | HEA  | C3C-C4C-NC  | 4.63  | 113.10      | 110.25   |
| 20  | B     | 301 | TGL  | CG2-OG2-CB1 | 4.61  | 129.15      | 117.79   |
| 28  | Z     | 101 | DMU  | C28-C25-C22 | -4.60 | 91.06       | 114.42   |
| 25  | C     | 303 | CDL  | C53-C52-C51 | -4.59 | 96.69       | 113.19   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | Q     | 201 | PGV  | C5-C4-C3    | -4.58 | 91.17       | 114.42   |
| 22  | W     | 101 | CHD  | C15-C14-C8  | 4.58  | 124.73      | 118.33   |
| 20  | N     | 608 | TGL  | OG1-CA1-OA1 | -4.57 | 112.06      | 123.59   |
| 22  | B     | 303 | CHD  | C15-C14-C13 | 4.55  | 108.02      | 103.55   |
| 22  | P     | 305 | CHD  | C4-C5-C10   | 4.53  | 117.47      | 112.66   |
| 26  | P     | 308 | PEK  | C02-O01-C1  | 4.52  | 128.93      | 117.79   |
| 25  | C     | 303 | CDL  | OB6-CB5-C51 | 4.52  | 121.25      | 111.50   |
| 22  | J     | 102 | CHD  | O12-C12-C13 | 4.52  | 118.67      | 111.03   |
| 20  | D     | 201 | TGL  | CB5-CB4-CB3 | 4.52  | 137.35      | 114.42   |
| 14  | N     | 602 | HEA  | C3B-C4B-NB  | -4.52 | 104.49      | 109.84   |
| 20  | B     | 301 | TGL  | CB4-CB3-CB2 | -4.51 | 96.99       | 113.19   |
| 22  | P     | 307 | CHD  | C23-C22-C20 | -4.50 | 106.30      | 114.52   |
| 26  | P     | 308 | PEK  | O03-C21-O04 | -4.50 | 112.25      | 123.59   |
| 20  | L     | 101 | TGL  | CB3-CB2-CB1 | 4.48  | 129.92      | 113.62   |
| 22  | J     | 102 | CHD  | C2-C1-C10   | 4.47  | 120.45      | 112.78   |
| 26  | C     | 306 | PEK  | C24-C23-C22 | 4.47  | 129.26      | 113.19   |
| 25  | C     | 303 | CDL  | C76-C75-C74 | -4.46 | 91.79       | 114.42   |
| 14  | N     | 602 | HEA  | C3A-C2A-C1A | -4.45 | 102.83      | 107.08   |
| 22  | B     | 303 | CHD  | O3-C3-C4    | -4.43 | 101.03      | 109.85   |
| 25  | T     | 103 | CDL  | CA4-OA6-CA5 | 4.42  | 128.67      | 117.79   |
| 20  | D     | 201 | TGL  | OG3-CC1-OC1 | -4.41 | 112.46      | 123.59   |
| 14  | N     | 602 | HEA  | CHA-C4D-ND  | -4.41 | 119.63      | 124.42   |
| 22  | P     | 307 | CHD  | C1-C10-C5   | 4.39  | 114.26      | 107.77   |
| 25  | C     | 303 | CDL  | OB5-PB2-OB3 | 4.37  | 126.15      | 109.07   |
| 19  | C     | 307 | PGV  | O03-C01-C02 | 4.37  | 121.16      | 108.43   |
| 22  | J     | 102 | CHD  | C6-C5-C4    | -4.37 | 106.16      | 111.19   |
| 25  | C     | 303 | CDL  | CB6-CB4-CB3 | -4.36 | 101.46      | 111.79   |
| 22  | B     | 303 | CHD  | C2-C1-C10   | -4.35 | 105.31      | 112.78   |
| 22  | W     | 101 | CHD  | C10-C9-C8   | 4.35  | 116.49      | 111.82   |
| 22  | J     | 102 | CHD  | C9-C10-C5   | 4.34  | 114.68      | 108.58   |
| 22  | J     | 102 | CHD  | C14-C13-C12 | -4.33 | 103.37      | 107.40   |
| 22  | B     | 303 | CHD  | C6-C5-C4    | -4.33 | 106.20      | 111.19   |
| 14  | A     | 602 | HEA  | CAD-CBD-CGD | -4.31 | 104.32      | 113.60   |
| 22  | O     | 302 | CHD  | C17-C13-C14 | 4.31  | 104.44      | 100.09   |
| 14  | N     | 602 | HEA  | C1D-C2D-C3D | 4.31  | 111.48      | 106.96   |
| 22  | J     | 102 | CHD  | C5-C4-C3    | 4.30  | 119.07      | 112.76   |
| 14  | A     | 602 | HEA  | CHC-C4B-NB  | 4.29  | 129.67      | 124.37   |
| 25  | T     | 103 | CDL  | OB8-CB6-CB4 | 4.28  | 120.88      | 108.43   |
| 28  | J     | 101 | DMU  | O16-C6-C1   | 4.28  | 114.98      | 108.30   |
| 19  | C     | 302 | PGV  | C28-C27-C26 | -4.27 | 92.74       | 114.42   |
| 20  | N     | 608 | TGL  | CB3-CB2-CB1 | 4.27  | 129.15      | 113.62   |
| 22  | J     | 102 | CHD  | C1-C2-C3    | 4.25  | 115.93      | 110.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | G     | 101 | PEK  | C24-C23-C22 | -4.24 | 97.93       | 113.19   |
| 26  | G     | 101 | PEK  | O04-C21-C22 | 4.24  | 140.28      | 123.73   |
| 22  | J     | 102 | CHD  | C4-C3-C2    | 4.22  | 115.60      | 110.55   |
| 22  | J     | 102 | CHD  | C17-C13-C14 | -4.21 | 95.85       | 100.09   |
| 22  | B     | 303 | CHD  | C15-C14-C8  | -4.20 | 112.46      | 118.33   |
| 20  | B     | 301 | TGL  | OG3-CC1-OC1 | -4.20 | 113.00      | 123.59   |
| 20  | Y     | 101 | TGL  | CA4-CA3-CA2 | -4.19 | 98.13       | 113.19   |
| 28  | P     | 306 | DMU  | O1-C10-C5   | -4.17 | 101.52      | 110.35   |
| 22  | W     | 101 | CHD  | O26-C24-O25 | -4.17 | 112.91      | 123.30   |
| 14  | N     | 602 | HEA  | C2A-C1A-NA  | 4.16  | 114.37      | 110.32   |
| 20  | Y     | 101 | TGL  | CA8-CA7-CA6 | -4.16 | 93.33       | 114.42   |
| 26  | C     | 306 | PEK  | C02-O01-C1  | 4.15  | 128.01      | 117.79   |
| 22  | P     | 307 | CHD  | C14-C8-C7   | -4.13 | 106.33      | 111.81   |
| 26  | P     | 308 | PEK  | C24-C23-C22 | 4.13  | 128.02      | 113.19   |
| 22  | C     | 305 | CHD  | C22-C20-C17 | -4.12 | 101.77      | 110.28   |
| 19  | A     | 608 | PGV  | O03-C19-C20 | 4.12  | 124.83      | 111.91   |
| 25  | C     | 303 | CDL  | OB8-CB6-CB4 | -4.11 | 96.47       | 108.43   |
| 20  | Y     | 101 | TGL  | CG3-OG3-CC1 | 4.10  | 132.31      | 117.12   |
| 28  | M     | 101 | DMU  | C18-O16-C6  | -4.09 | 107.05      | 113.84   |
| 14  | A     | 602 | HEA  | CHB-C1B-NB  | 4.09  | 128.86      | 124.42   |
| 22  | W     | 101 | CHD  | C4-C3-C2    | 4.09  | 115.43      | 110.55   |
| 14  | A     | 602 | HEA  | C27-C19-C20 | 4.08  | 122.14      | 115.27   |
| 14  | N     | 601 | HEA  | C1D-ND-C4D  | -4.08 | 100.86      | 105.07   |
| 22  | C     | 305 | CHD  | C16-C17-C13 | -4.07 | 99.56       | 103.55   |
| 22  | C     | 305 | CHD  | C11-C9-C10  | -4.07 | 109.53      | 113.73   |
| 25  | T     | 103 | CDL  | OA8-CA7-C31 | 4.06  | 124.64      | 111.91   |
| 14  | A     | 601 | HEA  | C2D-C1D-ND  | 4.06  | 114.64      | 109.84   |
| 28  | M     | 101 | DMU  | O5-C6-O16   | -4.05 | 100.38      | 109.97   |
| 14  | A     | 602 | HEA  | C20-C19-C18 | -4.04 | 112.94      | 121.12   |
| 20  | L     | 101 | TGL  | C20-CA9-CA8 | -4.04 | 93.93       | 114.42   |
| 26  | C     | 306 | PEK  | C03-C02-C01 | -4.03 | 102.25      | 111.79   |
| 22  | W     | 101 | CHD  | C5-C4-C3    | 4.02  | 118.66      | 112.76   |
| 23  | B     | 304 | PSC  | C32-C31-C30 | -4.01 | 94.07       | 114.42   |
| 14  | N     | 602 | HEA  | CHC-C4B-NB  | 4.01  | 129.32      | 124.37   |
| 22  | B     | 303 | CHD  | C9-C11-C12  | 4.01  | 119.59      | 114.30   |
| 25  | G     | 102 | CDL  | OA6-CA5-OA7 | -4.00 | 114.03      | 123.70   |
| 20  | L     | 101 | TGL  | CA4-CA3-CA2 | -4.00 | 98.80       | 113.19   |
| 14  | N     | 602 | HEA  | O1A-CGA-CBA | -3.99 | 110.26      | 123.08   |
| 22  | J     | 102 | CHD  | C1-C10-C5   | 3.98  | 113.65      | 107.77   |
| 14  | N     | 601 | HEA  | CMB-C2B-C1B | -3.98 | 118.98      | 125.04   |
| 19  | Q     | 201 | PGV  | C8-C7-C6    | -3.97 | 94.25       | 114.42   |
| 14  | N     | 601 | HEA  | C20-C19-C18 | 3.97  | 129.15      | 121.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | W     | 101 | CHD  | C11-C9-C10  | 3.96  | 117.81      | 113.73   |
| 25  | G     | 102 | CDL  | OB8-CB6-CB4 | 3.95  | 119.94      | 108.43   |
| 28  | Z     | 101 | DMU  | O55-C2-C1   | -3.94 | 101.25      | 110.35   |
| 19  | Q     | 201 | PGV  | C3-C2-C1    | -3.93 | 99.31       | 113.62   |
| 22  | W     | 101 | CHD  | C22-C20-C17 | 3.93  | 118.40      | 110.28   |
| 22  | O     | 302 | CHD  | C16-C17-C13 | -3.91 | 99.71       | 103.55   |
| 26  | P     | 308 | PEK  | O01-C1-C2   | 3.91  | 119.94      | 111.50   |
| 22  | P     | 305 | CHD  | C19-C10-C9  | -3.91 | 105.80      | 111.18   |
| 20  | N     | 608 | TGL  | OG2-CB1-OB1 | -3.90 | 114.28      | 123.70   |
| 22  | J     | 102 | CHD  | C9-C11-C12  | -3.89 | 109.16      | 114.30   |
| 20  | Q     | 202 | TGL  | OG3-CC1-OC1 | -3.88 | 113.81      | 123.59   |
| 25  | G     | 102 | CDL  | OA8-CA7-C31 | 3.86  | 124.03      | 111.91   |
| 25  | C     | 303 | CDL  | C77-C76-C75 | -3.86 | 94.82       | 114.42   |
| 22  | J     | 102 | CHD  | C22-C20-C17 | 3.86  | 118.26      | 110.28   |
| 19  | Q     | 201 | PGV  | O01-C02-C01 | 3.86  | 122.37      | 108.40   |
| 28  | P     | 306 | DMU  | O1-C9-C8    | 3.86  | 116.69      | 109.69   |
| 22  | C     | 305 | CHD  | C14-C8-C7   | -3.85 | 106.70      | 111.81   |
| 20  | B     | 301 | TGL  | CB5-CB4-CB3 | -3.82 | 95.03       | 114.42   |
| 26  | T     | 101 | PEK  | C3-C2-C1    | -3.80 | 99.78       | 113.62   |
| 20  | L     | 101 | TGL  | CG3-OG3-CC1 | 3.80  | 131.20      | 117.12   |
| 19  | P     | 301 | PGV  | O04-C19-C20 | -3.79 | 108.94      | 123.73   |
| 25  | P     | 304 | CDL  | OA4-PA1-OA3 | 3.79  | 130.96      | 112.24   |
| 25  | C     | 303 | CDL  | C73-C72-C71 | -3.77 | 99.65       | 113.19   |
| 20  | Y     | 101 | TGL  | OG1-CA1-CA2 | 3.77  | 123.73      | 111.91   |
| 14  | N     | 602 | HEA  | CAA-CBA-CGA | -3.76 | 105.51      | 113.60   |
| 19  | A     | 607 | PGV  | C34-C33-C32 | -3.75 | 84.93       | 113.42   |
| 14  | N     | 601 | HEA  | C2D-C1D-ND  | 3.75  | 114.28      | 109.84   |
| 20  | L     | 101 | TGL  | C24-C23-C22 | -3.73 | 95.47       | 114.42   |
| 22  | C     | 304 | CHD  | O25-C24-C23 | -3.72 | 111.11      | 123.08   |
| 19  | A     | 608 | PGV  | O01-C02-C01 | 3.71  | 121.84      | 108.40   |
| 28  | P     | 306 | DMU  | O7-C10-C5   | 3.70  | 117.69      | 108.10   |
| 20  | B     | 301 | TGL  | OG2-CB1-OB1 | -3.70 | 114.76      | 123.70   |
| 26  | T     | 102 | PEK  | C2-C3-C4    | 3.69  | 119.81      | 113.23   |
| 22  | P     | 305 | CHD  | C19-C10-C1  | -3.69 | 102.31      | 108.26   |
| 25  | C     | 303 | CDL  | OB4-PB2-OB5 | -3.69 | 90.60       | 107.75   |
| 14  | N     | 601 | HEA  | C3A-C2A-C1A | -3.69 | 103.55      | 107.08   |
| 22  | W     | 101 | CHD  | C23-C22-C20 | 3.69  | 121.25      | 114.52   |
| 14  | A     | 602 | HEA  | C3C-C4C-NC  | 3.68  | 112.51      | 110.25   |
| 19  | A     | 608 | PGV  | C23-C22-C21 | -3.68 | 95.75       | 114.42   |
| 19  | Q     | 201 | PGV  | C01-O03-C19 | 3.67  | 130.72      | 117.12   |
| 25  | G     | 102 | CDL  | OA8-CA7-OA9 | -3.67 | 114.34      | 123.59   |
| 19  | A     | 608 | PGV  | C01-O03-C19 | 3.66  | 130.69      | 117.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | C     | 306 | PEK  | O03-C21-C22 | 3.65  | 123.37      | 111.91   |
| 26  | G     | 103 | PEK  | O03-C01-C02 | 3.64  | 119.02      | 108.43   |
| 25  | P     | 304 | CDL  | O1-C1-CB2   | 3.64  | 122.31      | 109.56   |
| 28  | M     | 101 | DMU  | C31-C28-C25 | -3.63 | 95.98       | 114.42   |
| 25  | C     | 303 | CDL  | OB6-CB5-OB7 | -3.63 | 114.92      | 123.70   |
| 14  | N     | 601 | HEA  | O1A-CGA-CBA | -3.63 | 111.41      | 123.08   |
| 14  | N     | 602 | HEA  | C1D-ND-C4D  | -3.63 | 101.32      | 105.07   |
| 22  | P     | 305 | CHD  | C14-C13-C12 | 3.63  | 110.78      | 107.40   |
| 20  | D     | 201 | TGL  | CG3-OG3-CC1 | 3.62  | 130.54      | 117.12   |
| 22  | B     | 303 | CHD  | O12-C12-C13 | -3.61 | 104.92      | 111.03   |
| 28  | Z     | 101 | DMU  | C6-C1-C2    | -3.60 | 102.49      | 110.00   |
| 20  | Y     | 101 | TGL  | CB5-CB4-CB3 | -3.60 | 96.17       | 114.42   |
| 20  | L     | 101 | TGL  | OG2-CG2-CG3 | 3.59  | 121.40      | 108.40   |
| 26  | C     | 306 | PEK  | C26-C25-C24 | 3.59  | 132.63      | 114.42   |
| 25  | C     | 303 | CDL  | C39-C38-C37 | 3.58  | 132.61      | 114.42   |
| 23  | B     | 304 | PSC  | C28-C27-C26 | -3.58 | 96.27       | 114.42   |
| 25  | P     | 304 | CDL  | C54-C53-C52 | 3.57  | 132.57      | 114.42   |
| 19  | Q     | 201 | PGV  | O01-C1-C2   | 3.57  | 119.20      | 111.50   |
| 20  | Y     | 101 | TGL  | CG1-OG1-CA1 | 3.57  | 130.34      | 117.12   |
| 22  | J     | 102 | CHD  | C14-C8-C9   | -3.57 | 104.82      | 109.71   |
| 22  | P     | 305 | CHD  | O3-C3-C4    | -3.57 | 102.75      | 109.85   |
| 22  | O     | 302 | CHD  | O3-C3-C4    | -3.54 | 102.81      | 109.85   |
| 20  | L     | 101 | TGL  | C26-C25-C24 | -3.54 | 96.47       | 114.42   |
| 22  | J     | 102 | CHD  | C6-C7-C8    | 3.53  | 115.24      | 111.48   |
| 22  | B     | 303 | CHD  | C14-C13-C12 | 3.52  | 110.68      | 107.40   |
| 26  | P     | 308 | PEK  | C36-C35-C34 | -3.52 | 96.55       | 114.42   |
| 22  | W     | 101 | CHD  | C1-C10-C5   | 3.52  | 112.97      | 107.77   |
| 14  | A     | 601 | HEA  | C13-C12-C11 | -3.50 | 109.09      | 114.35   |
| 28  | P     | 306 | DMU  | O3-C5-C10   | 3.50  | 118.54      | 110.05   |
| 28  | Z     | 101 | DMU  | C18-O16-C6  | -3.49 | 108.05      | 113.84   |
| 28  | Z     | 101 | DMU  | O49-C1-C6   | -3.46 | 101.63      | 110.05   |
| 22  | J     | 102 | CHD  | C23-C22-C20 | 3.46  | 120.84      | 114.52   |
| 20  | L     | 101 | TGL  | CA5-CA4-CA3 | -3.45 | 96.89       | 114.42   |
| 26  | P     | 308 | PEK  | C35-C34-C33 | 3.45  | 131.91      | 114.42   |
| 22  | C     | 305 | CHD  | C15-C14-C8  | -3.43 | 113.53      | 118.33   |
| 19  | P     | 301 | PGV  | C03-C02-C01 | -3.43 | 103.66      | 111.79   |
| 20  | B     | 301 | TGL  | OA1-CA1-CA2 | -3.43 | 110.35      | 123.73   |
| 25  | C     | 303 | CDL  | OB6-CB4-CB3 | -3.43 | 95.99       | 108.40   |
| 25  | G     | 102 | CDL  | CA4-OA6-CA5 | 3.42  | 126.20      | 117.79   |
| 19  | A     | 607 | PGV  | C30-C29-C28 | 3.41  | 131.76      | 114.42   |
| 14  | N     | 602 | HEA  | C3D-C4D-ND  | 3.41  | 113.66      | 110.36   |
| 20  | Y     | 101 | TGL  | OB1-CB1-CB2 | -3.41 | 110.44      | 123.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | P     | 306 | DMU  | O6-C11-C9   | -3.41 | 99.61       | 111.29   |
| 19  | N     | 607 | PGV  | O02-C1-C2   | 3.40  | 137.01      | 123.73   |
| 14  | N     | 601 | HEA  | OMA-CMA-C3A | -3.39 | 118.02      | 125.69   |
| 25  | G     | 102 | CDL  | C80-C79-C78 | 3.39  | 131.62      | 114.42   |
| 22  | O     | 302 | CHD  | C14-C8-C9   | -3.38 | 105.07      | 109.71   |
| 22  | W     | 101 | CHD  | C21-C20-C22 | 3.38  | 115.66      | 110.36   |
| 23  | B     | 304 | PSC  | C08-N-C07   | -3.37 | 100.31      | 108.97   |
| 28  | P     | 306 | DMU  | O16-C6-C1   | 3.37  | 113.56      | 108.30   |
| 20  | D     | 201 | TGL  | CA4-CA3-CA2 | 3.37  | 125.29      | 113.19   |
| 22  | P     | 305 | CHD  | C15-C14-C8  | 3.34  | 123.00      | 118.33   |
| 14  | A     | 602 | HEA  | C16-C15-C14 | -3.33 | 114.39      | 121.12   |
| 19  | P     | 301 | PGV  | C02-O01-C1  | 3.32  | 125.97      | 117.79   |
| 25  | P     | 304 | CDL  | OB2-PB2-OB3 | 3.31  | 122.00      | 109.07   |
| 25  | P     | 304 | CDL  | CB4-OB6-CB5 | -3.30 | 109.67      | 117.79   |
| 28  | Z     | 101 | DMU  | O5-C6-O16   | -3.30 | 102.17      | 109.97   |
| 22  | O     | 302 | CHD  | O7-C7-C8    | 3.29  | 116.77      | 109.43   |
| 23  | B     | 304 | PSC  | C29-C28-C27 | -3.29 | 97.74       | 114.42   |
| 14  | A     | 601 | HEA  | CHD-C1D-C2D | -3.28 | 117.61      | 126.73   |
| 19  | P     | 303 | PGV  | C27-C26-C25 | -3.28 | 97.78       | 114.42   |
| 22  | C     | 305 | CHD  | C9-C11-C12  | -3.27 | 109.98      | 114.30   |
| 19  | A     | 608 | PGV  | O04-C19-C20 | -3.27 | 110.96      | 123.73   |
| 28  | M     | 101 | DMU  | C22-C19-C18 | -3.27 | 99.01       | 113.49   |
| 22  | O     | 302 | CHD  | C14-C13-C12 | -3.26 | 104.36      | 107.40   |
| 22  | P     | 305 | CHD  | C5-C6-C7    | 3.25  | 118.05      | 114.46   |
| 22  | C     | 304 | CHD  | C4-C3-C2    | 3.25  | 114.43      | 110.55   |
| 20  | Q     | 202 | TGL  | C16-C15-CC9 | 3.25  | 130.91      | 114.42   |
| 14  | A     | 602 | HEA  | C3B-C4B-NB  | -3.24 | 106.00      | 109.84   |
| 22  | P     | 305 | CHD  | C21-C20-C22 | 3.24  | 115.44      | 110.36   |
| 25  | P     | 304 | CDL  | C78-C77-C76 | -3.22 | 98.07       | 114.42   |
| 22  | W     | 101 | CHD  | C13-C14-C8  | 3.22  | 118.85      | 114.74   |
| 22  | P     | 305 | CHD  | O12-C12-C13 | 3.21  | 116.46      | 111.03   |
| 14  | N     | 602 | HEA  | C26-C15-C16 | 3.20  | 120.66      | 115.27   |
| 14  | A     | 601 | HEA  | CAA-CBA-CGA | -3.20 | 106.71      | 113.60   |
| 25  | T     | 103 | CDL  | CB6-OB8-CB7 | 3.19  | 128.94      | 117.12   |
| 26  | P     | 308 | PEK  | C27-C26-C25 | 3.19  | 130.62      | 114.42   |
| 19  | P     | 303 | PGV  | C03-C02-C01 | -3.19 | 104.25      | 111.79   |
| 22  | P     | 307 | CHD  | C11-C12-C13 | -3.18 | 107.97      | 111.24   |
| 22  | B     | 303 | CHD  | C6-C7-C8    | 3.18  | 114.88      | 111.48   |
| 22  | P     | 307 | CHD  | O7-C7-C8    | 3.18  | 116.54      | 109.43   |
| 23  | O     | 303 | PSC  | C29-C28-C27 | -3.18 | 98.30       | 114.42   |
| 20  | Q     | 202 | TGL  | C21-C20-CA9 | 3.16  | 130.48      | 114.42   |
| 22  | B     | 303 | CHD  | C5-C6-C7    | -3.16 | 110.97      | 114.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | C     | 303 | CDL  | CA6-OA8-CA7 | 3.16  | 128.82      | 117.12   |
| 28  | J     | 101 | DMU  | C28-C25-C22 | 3.15  | 130.40      | 114.42   |
| 25  | G     | 102 | CDL  | C40-C39-C38 | 3.15  | 130.40      | 114.42   |
| 22  | P     | 305 | CHD  | C17-C13-C12 | 3.14  | 120.54      | 117.67   |
| 20  | B     | 301 | TGL  | C15-CC9-CC8 | 3.14  | 130.38      | 114.42   |
| 19  | A     | 608 | PGV  | O14-P-O11   | -3.14 | 93.15       | 107.75   |
| 25  | T     | 103 | CDL  | CA6-CA4-CA3 | -3.14 | 104.36      | 111.79   |
| 25  | G     | 102 | CDL  | CB6-OB8-CB7 | 3.13  | 128.73      | 117.12   |
| 14  | N     | 601 | HEA  | CAA-CBA-CGA | -3.13 | 106.88      | 113.60   |
| 19  | A     | 608 | PGV  | C27-C26-C25 | -3.13 | 98.56       | 114.42   |
| 25  | C     | 303 | CDL  | C42-C41-C40 | 3.12  | 130.28      | 114.42   |
| 25  | P     | 304 | CDL  | C32-C31-CA7 | 3.12  | 124.96      | 113.62   |
| 20  | D     | 201 | TGL  | OG3-CC1-CC2 | -3.12 | 102.12      | 111.91   |
| 26  | T     | 102 | PEK  | O03-C21-C22 | 3.12  | 121.69      | 111.91   |
| 20  | D     | 201 | TGL  | C14-C13-C12 | 3.12  | 130.25      | 114.42   |
| 25  | P     | 304 | CDL  | OA6-CA4-CA3 | 3.11  | 119.65      | 108.40   |
| 26  | G     | 103 | PEK  | C01-O03-C21 | 3.11  | 128.62      | 117.12   |
| 25  | T     | 103 | CDL  | C83-C82-C81 | 3.10  | 130.18      | 114.42   |
| 14  | A     | 601 | HEA  | C4B-NB-C1B  | -3.10 | 101.87      | 105.07   |
| 19  | Q     | 201 | PGV  | C4-C3-C2    | 3.10  | 124.34      | 113.19   |
| 14  | N     | 602 | HEA  | C4C-NC-C1C  | -3.09 | 102.32      | 105.35   |
| 23  | B     | 304 | PSC  | C31-C30-C29 | 3.09  | 130.13      | 114.42   |
| 26  | G     | 101 | PEK  | C30-C29-C28 | 3.09  | 130.13      | 114.42   |
| 25  | P     | 304 | CDL  | CA6-OA8-CA7 | 3.09  | 128.55      | 117.12   |
| 19  | C     | 307 | PGV  | O03-C19-O04 | -3.08 | 115.81      | 123.59   |
| 22  | W     | 101 | CHD  | O7-C7-C8    | 3.08  | 116.31      | 109.43   |
| 25  | P     | 304 | CDL  | OB8-CB7-OB9 | -3.08 | 115.82      | 123.59   |
| 25  | C     | 303 | CDL  | OB9-CB7-C71 | -3.08 | 111.72      | 123.73   |
| 20  | N     | 608 | TGL  | OG1-CG1-CG2 | 3.07  | 117.37      | 108.43   |
| 22  | C     | 305 | CHD  | C1-C10-C5   | 3.06  | 112.30      | 107.77   |
| 14  | N     | 601 | HEA  | C20-C21-C22 | 3.06  | 121.95      | 111.88   |
| 22  | C     | 304 | CHD  | C18-C13-C17 | 3.06  | 116.00      | 111.21   |
| 14  | N     | 602 | HEA  | CAD-C3D-C2D | 3.05  | 133.56      | 127.88   |
| 19  | P     | 301 | PGV  | O01-C1-C2   | 3.05  | 118.07      | 111.50   |
| 28  | M     | 101 | DMU  | O16-C6-C1   | -3.05 | 103.54      | 108.30   |
| 14  | A     | 601 | HEA  | C4A-C3A-C2A | 3.05  | 109.25      | 106.75   |
| 20  | L     | 101 | TGL  | C12-C11-C10 | -3.04 | 99.00       | 114.42   |
| 22  | P     | 305 | CHD  | C18-C13-C14 | 3.04  | 115.96      | 111.21   |
| 23  | B     | 304 | PSC  | C22-C21-C20 | 3.04  | 124.11      | 113.19   |
| 23  | B     | 304 | PSC  | C27-C26-C25 | -3.03 | 99.02       | 114.42   |
| 22  | P     | 305 | CHD  | C1-C10-C5   | 3.03  | 112.24      | 107.77   |
| 23  | O     | 303 | PSC  | O01-C02-C03 | 3.02  | 119.33      | 108.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | N     | 608 | TGL  | C11-C10-CB9 | 3.02  | 129.74      | 114.42   |
| 26  | G     | 101 | PEK  | O03-C21-C22 | -3.01 | 102.45      | 111.91   |
| 22  | W     | 101 | CHD  | C19-C10-C1  | -3.01 | 103.41      | 108.26   |
| 20  | D     | 201 | TGL  | OG1-CA1-CA2 | 3.01  | 121.36      | 111.91   |
| 25  | G     | 102 | CDL  | C23-C22-C21 | 3.01  | 129.70      | 114.42   |
| 22  | P     | 307 | CHD  | C13-C17-C20 | -3.01 | 115.91      | 119.50   |
| 25  | C     | 303 | CDL  | OA8-CA7-C31 | 3.00  | 121.33      | 111.91   |
| 25  | P     | 304 | CDL  | C72-C71-CB7 | 3.00  | 124.52      | 113.62   |
| 25  | P     | 304 | CDL  | C73-C72-C71 | -3.00 | 102.42      | 113.19   |
| 26  | P     | 308 | PEK  | O03-C01-C02 | 2.99  | 117.14      | 108.43   |
| 26  | T     | 101 | PEK  | O03-C21-C22 | 2.98  | 121.27      | 111.91   |
| 22  | C     | 305 | CHD  | C14-C8-C9   | -2.98 | 105.62      | 109.71   |
| 22  | P     | 305 | CHD  | O26-C24-C23 | -2.98 | 104.45      | 114.03   |
| 25  | P     | 304 | CDL  | OB6-CB4-CB3 | -2.98 | 97.63       | 108.40   |
| 14  | A     | 601 | HEA  | C3C-C4C-NC  | 2.97  | 112.08      | 110.25   |
| 20  | L     | 101 | TGL  | CC3-CC2-CC1 | 2.97  | 124.42      | 113.62   |
| 14  | A     | 601 | HEA  | C20-C21-C22 | -2.97 | 102.12      | 111.88   |
| 19  | P     | 301 | PGV  | C21-C20-C19 | -2.97 | 102.82      | 113.62   |
| 14  | A     | 601 | HEA  | C3B-C4B-NB  | 2.97  | 113.36      | 109.84   |
| 14  | N     | 602 | HEA  | C4D-C3D-C2D | -2.96 | 102.58      | 106.90   |
| 14  | A     | 601 | HEA  | CMB-C2B-C1B | -2.96 | 120.53      | 125.04   |
| 22  | B     | 303 | CHD  | C11-C9-C8   | -2.96 | 106.55      | 110.88   |
| 28  | Z     | 101 | DMU  | O16-C6-C1   | -2.95 | 103.70      | 108.30   |
| 23  | O     | 303 | PSC  | O01-C1-O02  | -2.95 | 116.58      | 123.70   |
| 20  | Q     | 202 | TGL  | OC1-CC1-CC2 | 2.94  | 135.21      | 123.73   |
| 22  | J     | 102 | CHD  | C4-C5-C10   | 2.94  | 115.78      | 112.66   |
| 14  | A     | 601 | HEA  | C27-C19-C20 | -2.94 | 110.33      | 115.27   |
| 20  | Y     | 101 | TGL  | C23-C22-C21 | -2.93 | 99.54       | 114.42   |
| 22  | C     | 304 | CHD  | O26-C24-O25 | 2.92  | 130.57      | 123.30   |
| 26  | T     | 101 | PEK  | O02-C1-C2   | 2.91  | 135.10      | 123.73   |
| 14  | N     | 602 | HEA  | C16-C15-C14 | -2.91 | 115.22      | 121.12   |
| 14  | A     | 602 | HEA  | CHB-C4A-C3A | -2.91 | 120.28      | 125.26   |
| 14  | N     | 602 | HEA  | C12-C13-C14 | -2.91 | 104.56      | 112.23   |
| 22  | J     | 102 | CHD  | C13-C14-C8  | -2.90 | 111.03      | 114.74   |
| 25  | P     | 304 | CDL  | C39-C38-C37 | 2.90  | 129.13      | 114.42   |
| 22  | B     | 303 | CHD  | O3-C3-C2    | 2.89  | 117.52      | 110.16   |
| 23  | O     | 303 | PSC  | C27-C26-C25 | -2.89 | 99.77       | 114.42   |
| 26  | G     | 103 | PEK  | C02-O01-C1  | 2.89  | 124.90      | 117.79   |
| 20  | L     | 101 | TGL  | C13-C12-C11 | 2.89  | 129.07      | 114.42   |
| 22  | O     | 302 | CHD  | C1-C10-C5   | 2.87  | 112.01      | 107.77   |
| 19  | Q     | 201 | PGV  | O03-C19-C20 | 2.87  | 120.91      | 111.91   |
| 22  | C     | 305 | CHD  | C1-C2-C3    | -2.86 | 106.79      | 110.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | Y     | 101 | TGL  | CC3-CC2-CC1 | 2.86  | 124.02      | 113.62   |
| 22  | B     | 303 | CHD  | C1-C10-C9   | 2.86  | 115.85      | 111.35   |
| 20  | B     | 301 | TGL  | OG1-CG1-CG2 | 2.86  | 116.75      | 108.43   |
| 22  | P     | 305 | CHD  | C13-C14-C8  | 2.85  | 118.38      | 114.74   |
| 26  | T     | 102 | PEK  | O01-C1-O02  | -2.85 | 116.80      | 123.70   |
| 14  | N     | 602 | HEA  | C2B-C1B-NB  | -2.85 | 106.47      | 109.88   |
| 23  | B     | 304 | PSC  | O01-C1-O02  | -2.85 | 116.82      | 123.70   |
| 25  | C     | 303 | CDL  | C75-C74-C73 | -2.85 | 99.98       | 114.42   |
| 25  | P     | 304 | CDL  | OA8-CA6-CA4 | 2.84  | 116.71      | 108.43   |
| 19  | A     | 607 | PGV  | C27-C26-C25 | 2.84  | 128.84      | 114.42   |
| 25  | C     | 303 | CDL  | OB4-PB2-OB2 | -2.84 | 94.58       | 107.75   |
| 19  | A     | 607 | PGV  | C31-C30-C29 | -2.83 | 100.04      | 114.42   |
| 25  | G     | 102 | CDL  | C19-C18-C17 | 2.83  | 128.81      | 114.42   |
| 26  | G     | 103 | PEK  | C14-C13-C12 | 2.83  | 125.97      | 112.02   |
| 22  | C     | 304 | CHD  | O7-C7-C8    | 2.83  | 115.76      | 109.43   |
| 20  | Y     | 101 | TGL  | OG2-CG2-CG3 | 2.83  | 118.64      | 108.40   |
| 14  | N     | 602 | HEA  | C4A-CHB-C1B | -2.83 | 119.96      | 126.06   |
| 22  | J     | 102 | CHD  | O7-C7-C8    | 2.82  | 115.73      | 109.43   |
| 25  | T     | 103 | CDL  | C76-C75-C74 | 2.82  | 128.72      | 114.42   |
| 20  | Q     | 202 | TGL  | CB5-CB4-CB3 | 2.81  | 128.72      | 114.42   |
| 20  | B     | 301 | TGL  | CB6-CB5-CB4 | -2.81 | 100.14      | 114.42   |
| 20  | N     | 608 | TGL  | C15-CC9-CC8 | 2.81  | 128.67      | 114.42   |
| 19  | N     | 607 | PGV  | C3-C2-C1    | -2.80 | 103.42      | 113.62   |
| 14  | N     | 602 | HEA  | CHB-C4A-C3A | -2.80 | 120.46      | 125.26   |
| 19  | N     | 607 | PGV  | O01-C1-C2   | -2.80 | 105.46      | 111.50   |
| 22  | P     | 305 | CHD  | C1-C2-C3    | 2.79  | 114.05      | 110.47   |
| 26  | C     | 306 | PEK  | C33-C32-C31 | -2.79 | 100.28      | 114.42   |
| 25  | P     | 304 | CDL  | OA8-CA7-C31 | 2.78  | 120.62      | 111.91   |
| 22  | C     | 304 | CHD  | C9-C11-C12  | -2.78 | 110.64      | 114.30   |
| 19  | N     | 607 | PGV  | C14-C13-C12 | -2.78 | 96.53       | 112.43   |
| 22  | C     | 305 | CHD  | C19-C10-C1  | -2.77 | 103.80      | 108.26   |
| 25  | T     | 103 | CDL  | C72-C71-CB7 | 2.77  | 123.69      | 113.62   |
| 20  | D     | 201 | TGL  | CG2-OG2-CB1 | -2.77 | 110.98      | 117.79   |
| 25  | P     | 304 | CDL  | C42-C41-C40 | 2.77  | 128.47      | 114.42   |
| 20  | N     | 608 | TGL  | OG3-CC1-OC1 | -2.77 | 116.61      | 123.59   |
| 28  | M     | 101 | DMU  | O49-C1-C2   | -2.76 | 103.96      | 110.35   |
| 25  | G     | 102 | CDL  | C72-C71-CB7 | 2.76  | 123.66      | 113.62   |
| 22  | W     | 101 | CHD  | C6-C7-C8    | 2.75  | 114.42      | 111.48   |
| 25  | C     | 303 | CDL  | CA4-OA6-CA5 | 2.75  | 124.57      | 117.79   |
| 14  | A     | 602 | HEA  | C2B-C1B-NB  | -2.75 | 106.59      | 109.88   |
| 22  | C     | 304 | CHD  | C14-C8-C7   | 2.75  | 115.46      | 111.81   |
| 28  | M     | 101 | DMU  | O1-C9-C8    | -2.75 | 104.70      | 109.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | G     | 102 | CDL  | C43-C42-C41 | -2.75 | 100.46      | 114.42   |
| 26  | T     | 101 | PEK  | O01-C1-C2   | -2.75 | 105.58      | 111.50   |
| 22  | C     | 304 | CHD  | C1-C10-C5   | 2.74  | 111.82      | 107.77   |
| 14  | A     | 601 | HEA  | C4A-CHB-C1B | -2.73 | 120.17      | 126.06   |
| 28  | M     | 101 | DMU  | O7-C3-C4    | -2.73 | 101.97      | 109.45   |
| 14  | N     | 601 | HEA  | C25-C23-C22 | -2.73 | 114.77      | 122.65   |
| 26  | G     | 101 | PEK  | C02-O01-C1  | -2.72 | 111.09      | 117.79   |
| 20  | B     | 301 | TGL  | OB1-CB1-CB2 | -2.72 | 113.13      | 123.73   |
| 28  | M     | 101 | DMU  | C6-C1-C2    | -2.71 | 104.34      | 110.00   |
| 25  | C     | 303 | CDL  | PA1-OA2-CA2 | 2.71  | 137.59      | 121.68   |
| 19  | C     | 307 | PGV  | O04-C19-C20 | -2.71 | 113.15      | 123.73   |
| 19  | N     | 607 | PGV  | O03-C19-O04 | -2.71 | 116.76      | 123.59   |
| 23  | O     | 303 | PSC  | C02-O01-C1  | 2.71  | 124.45      | 117.79   |
| 22  | P     | 305 | CHD  | C11-C9-C8   | 2.70  | 114.84      | 110.88   |
| 22  | P     | 307 | CHD  | C16-C17-C20 | -2.70 | 107.97      | 112.15   |
| 22  | P     | 307 | CHD  | C10-C9-C8   | -2.70 | 108.92      | 111.82   |
| 20  | B     | 301 | TGL  | CB8-CB7-CB6 | -2.69 | 100.76      | 114.42   |
| 22  | O     | 302 | CHD  | C18-C13-C12 | -2.69 | 106.33      | 109.07   |
| 22  | P     | 305 | CHD  | C2-C1-C10   | 2.69  | 117.39      | 112.78   |
| 19  | P     | 303 | PGV  | C24-C23-C22 | -2.69 | 100.77      | 114.42   |
| 28  | P     | 306 | DMU  | O16-C18-C19 | 2.68  | 118.97      | 109.56   |
| 14  | A     | 601 | HEA  | CHD-C1D-ND  | 2.68  | 127.68      | 124.37   |
| 20  | Q     | 202 | TGL  | C10-CB9-CB8 | 2.68  | 128.03      | 114.42   |
| 25  | G     | 102 | CDL  | C83-C82-C81 | 2.68  | 128.03      | 114.42   |
| 26  | T     | 101 | PEK  | C24-C23-C22 | -2.67 | 103.59      | 113.19   |
| 14  | A     | 602 | HEA  | C2A-C1A-NA  | 2.67  | 112.92      | 110.32   |
| 26  | T     | 102 | PEK  | O03-C01-C02 | 2.66  | 116.19      | 108.43   |
| 26  | T     | 101 | PEK  | C25-C24-C23 | 2.65  | 127.89      | 114.42   |
| 22  | C     | 305 | CHD  | C11-C9-C8   | 2.65  | 114.76      | 110.88   |
| 25  | T     | 103 | CDL  | OA6-CA5-OA7 | -2.65 | 117.30      | 123.70   |
| 19  | Q     | 201 | PGV  | C32-C31-C30 | 2.65  | 127.86      | 114.42   |
| 20  | Y     | 101 | TGL  | OC1-CC1-CC2 | -2.65 | 113.41      | 123.73   |
| 22  | J     | 102 | CHD  | C21-C20-C22 | 2.63  | 114.49      | 110.36   |
| 20  | Y     | 101 | TGL  | CA7-CA6-CA5 | -2.63 | 101.08      | 114.42   |
| 22  | B     | 303 | CHD  | O26-C24-O25 | 2.63  | 129.85      | 123.30   |
| 25  | T     | 103 | CDL  | CB2-C1-CA2  | -2.63 | 105.06      | 112.79   |
| 22  | P     | 307 | CHD  | C16-C17-C13 | -2.63 | 100.98      | 103.55   |
| 22  | W     | 101 | CHD  | C19-C10-C5  | -2.62 | 105.91      | 110.36   |
| 20  | L     | 101 | TGL  | OG1-CA1-CA2 | 2.62  | 120.14      | 111.91   |
| 20  | L     | 101 | TGL  | OB1-CB1-CB2 | -2.62 | 113.50      | 123.73   |
| 22  | B     | 303 | CHD  | C4-C3-C2    | 2.62  | 113.68      | 110.55   |
| 22  | W     | 101 | CHD  | C15-C14-C13 | 2.62  | 106.12      | 103.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | O     | 302 | CHD  | O26-C24-O25 | 2.62  | 129.83      | 123.30   |
| 28  | Z     | 101 | DMU  | O61-C57-C4  | -2.62 | 102.32      | 111.29   |
| 20  | Q     | 202 | TGL  | OG3-CG3-CG2 | -2.61 | 100.82      | 108.43   |
| 14  | N     | 602 | HEA  | CHC-C1C-C2C | -2.61 | 119.86      | 127.24   |
| 19  | P     | 303 | PGV  | C21-C20-C19 | -2.61 | 104.12      | 113.62   |
| 19  | Q     | 201 | PGV  | C7-C6-C5    | 2.61  | 127.69      | 114.42   |
| 25  | C     | 303 | CDL  | OA8-CA6-CA4 | 2.61  | 116.03      | 108.43   |
| 19  | N     | 607 | PGV  | O01-C1-O02  | -2.61 | 117.40      | 123.70   |
| 14  | N     | 601 | HEA  | C4C-NC-C1C  | -2.61 | 102.80      | 105.35   |
| 19  | A     | 607 | PGV  | O01-C1-O02  | -2.61 | 117.40      | 123.70   |
| 25  | G     | 102 | CDL  | C84-C83-C82 | 2.60  | 127.63      | 114.42   |
| 19  | C     | 302 | PGV  | C15-C14-C13 | 2.60  | 125.12      | 113.79   |
| 14  | A     | 602 | HEA  | C12-C13-C14 | -2.60 | 105.38      | 112.23   |
| 14  | A     | 602 | HEA  | C4A-NA-C1A  | -2.60 | 102.81      | 105.35   |
| 25  | G     | 102 | CDL  | C44-C43-C42 | 2.59  | 127.58      | 114.42   |
| 14  | A     | 601 | HEA  | O1A-CGA-CBA | -2.59 | 114.76      | 123.08   |
| 14  | A     | 601 | HEA  | O2A-CGA-CBA | 2.59  | 122.35      | 114.03   |
| 25  | P     | 304 | CDL  | OB9-CB7-C71 | -2.59 | 113.64      | 123.73   |
| 28  | M     | 101 | DMU  | O2-C8-C9    | -2.59 | 102.88      | 109.30   |
| 25  | P     | 304 | CDL  | C83-C82-C81 | 2.58  | 127.54      | 114.42   |
| 14  | N     | 601 | HEA  | C3B-C4B-NB  | 2.58  | 112.90      | 109.84   |
| 14  | N     | 602 | HEA  | C4B-C3B-C2B | 2.58  | 111.82      | 107.41   |
| 14  | N     | 601 | HEA  | C4B-NB-C1B  | -2.58 | 102.41      | 105.07   |
| 26  | C     | 306 | PEK  | C29-C28-C27 | 2.57  | 127.48      | 114.42   |
| 19  | A     | 608 | PGV  | C8-C9-C10   | -2.57 | 102.60      | 113.79   |
| 14  | N     | 602 | HEA  | C1C-CHC-C4B | -2.56 | 120.26      | 126.34   |
| 19  | P     | 303 | PGV  | C32-C31-C30 | 2.56  | 127.42      | 114.42   |
| 26  | T     | 102 | PEK  | C02-O01-C1  | 2.56  | 124.08      | 117.79   |
| 20  | B     | 301 | TGL  | C14-C13-C12 | -2.55 | 101.45      | 114.42   |
| 20  | D     | 201 | TGL  | C20-CA9-CA8 | 2.55  | 127.39      | 114.42   |
| 26  | G     | 101 | PEK  | O03-C21-O04 | -2.55 | 117.15      | 123.59   |
| 14  | N     | 602 | HEA  | C25-C23-C24 | 2.55  | 120.24      | 114.60   |
| 19  | A     | 608 | PGV  | O12-P-O13   | 2.55  | 119.03      | 109.07   |
| 14  | N     | 601 | HEA  | O2A-CGA-CBA | 2.54  | 122.19      | 114.03   |
| 25  | G     | 102 | CDL  | C79-C78-C77 | 2.54  | 127.31      | 114.42   |
| 22  | P     | 305 | CHD  | C9-C10-C5   | 2.54  | 112.14      | 108.58   |
| 25  | P     | 304 | CDL  | CB6-CB4-CB3 | 2.53  | 117.78      | 111.79   |
| 20  | Y     | 101 | TGL  | CC7-CC6-CC5 | 2.53  | 127.25      | 114.42   |
| 22  | C     | 304 | CHD  | C15-C14-C13 | 2.53  | 106.03      | 103.55   |
| 14  | N     | 601 | HEA  | C4A-C3A-C2A | 2.52  | 108.83      | 106.75   |
| 20  | Y     | 101 | TGL  | OG3-CC1-OC1 | -2.52 | 117.22      | 123.59   |
| 19  | C     | 307 | PGV  | O01-C1-C2   | 2.51  | 116.92      | 111.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | P     | 308 | PEK  | C26-C25-C24 | 2.51  | 127.19      | 114.42   |
| 22  | B     | 303 | CHD  | C16-C15-C14 | -2.51 | 100.15      | 105.13   |
| 26  | G     | 103 | PEK  | O02-C1-C2   | -2.51 | 113.94      | 123.73   |
| 26  | G     | 101 | PEK  | O01-C02-C01 | -2.51 | 99.31       | 108.40   |
| 14  | N     | 601 | HEA  | CHD-C1D-C2D | -2.51 | 119.76      | 126.73   |
| 14  | A     | 602 | HEA  | C13-C14-C15 | -2.51 | 121.62      | 127.66   |
| 25  | T     | 103 | CDL  | C19-C18-C17 | 2.51  | 127.15      | 114.42   |
| 25  | P     | 304 | CDL  | C82-C81-C80 | 2.50  | 127.12      | 114.42   |
| 19  | P     | 303 | PGV  | O03-C01-C02 | -2.50 | 101.16      | 108.43   |
| 22  | O     | 302 | CHD  | C1-C10-C9   | 2.49  | 115.27      | 111.35   |
| 22  | W     | 101 | CHD  | O25-C24-C23 | 2.49  | 131.07      | 123.08   |
| 28  | P     | 306 | DMU  | C1-C2-C3    | 2.48  | 115.35      | 109.68   |
| 26  | T     | 101 | PEK  | O01-C1-O02  | -2.48 | 117.71      | 123.70   |
| 26  | P     | 308 | PEK  | C29-C28-C27 | 2.48  | 127.01      | 114.42   |
| 19  | P     | 303 | PGV  | C15-C14-C13 | 2.48  | 124.58      | 113.79   |
| 25  | P     | 304 | CDL  | OA8-CA7-OA9 | -2.47 | 117.36      | 123.59   |
| 22  | C     | 305 | CHD  | O3-C3-C2    | -2.46 | 103.90      | 110.16   |
| 25  | C     | 303 | CDL  | C57-C56-C55 | 2.46  | 126.91      | 114.42   |
| 22  | P     | 307 | CHD  | C4-C5-C10   | -2.45 | 110.05      | 112.66   |
| 19  | P     | 303 | PGV  | O03-C19-C20 | -2.45 | 104.21      | 111.91   |
| 25  | P     | 304 | CDL  | C56-C55-C54 | 2.45  | 126.85      | 114.42   |
| 26  | C     | 306 | PEK  | O03-C01-C02 | 2.45  | 115.56      | 108.43   |
| 26  | C     | 306 | PEK  | O12-P-O14   | -2.45 | 99.51       | 109.07   |
| 26  | T     | 102 | PEK  | C01-O03-C21 | 2.45  | 126.18      | 117.12   |
| 26  | G     | 103 | PEK  | C24-C23-C22 | -2.45 | 104.40      | 113.19   |
| 22  | B     | 303 | CHD  | C18-C13-C12 | -2.44 | 106.58      | 109.07   |
| 14  | A     | 602 | HEA  | CHC-C1C-C2C | -2.43 | 120.36      | 127.24   |
| 22  | C     | 305 | CHD  | C4-C5-C10   | -2.43 | 110.08      | 112.66   |
| 25  | P     | 304 | CDL  | C76-C75-C74 | -2.43 | 102.09      | 114.42   |
| 19  | A     | 607 | PGV  | O02-C1-C2   | 2.43  | 133.21      | 123.73   |
| 20  | D     | 201 | TGL  | C12-C11-C10 | -2.42 | 102.14      | 114.42   |
| 28  | Z     | 101 | DMU  | O5-C4-C57   | 2.42  | 112.45      | 106.44   |
| 25  | P     | 304 | CDL  | CA6-CA4-CA3 | -2.42 | 106.07      | 111.79   |
| 14  | A     | 601 | HEA  | CHB-C1B-C2B | -2.41 | 121.21      | 124.98   |
| 19  | A     | 607 | PGV  | C4-C3-C2    | -2.41 | 104.52      | 113.19   |
| 22  | O     | 302 | CHD  | C4-C3-C2    | 2.41  | 113.43      | 110.55   |
| 14  | N     | 602 | HEA  | CBA-CAA-C2A | -2.41 | 105.94      | 112.63   |
| 22  | C     | 304 | CHD  | C21-C20-C22 | -2.41 | 106.59      | 110.36   |
| 25  | T     | 103 | CDL  | OB7-CB5-C51 | -2.41 | 114.35      | 123.73   |
| 23  | O     | 303 | PSC  | C21-C20-C19 | -2.40 | 104.88      | 113.62   |
| 22  | C     | 304 | CHD  | C19-C10-C9  | -2.40 | 107.88      | 111.18   |
| 22  | W     | 101 | CHD  | C9-C8-C7    | -2.40 | 109.01      | 111.88   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | Z     | 101 | DMU  | O49-C1-C2   | -2.39 | 104.82      | 110.35   |
| 20  | Y     | 101 | TGL  | C22-C21-C20 | -2.39 | 102.30      | 114.42   |
| 25  | C     | 303 | CDL  | C58-C57-C56 | 2.39  | 126.54      | 114.42   |
| 19  | C     | 307 | PGV  | P-O11-C03   | 2.39  | 135.67      | 121.68   |
| 25  | C     | 303 | CDL  | C87-C86-C85 | 2.38  | 131.51      | 113.42   |
| 25  | T     | 103 | CDL  | C23-C22-C21 | 2.38  | 126.52      | 114.42   |
| 26  | P     | 308 | PEK  | C3-C2-C1    | 2.38  | 122.28      | 113.62   |
| 22  | O     | 302 | CHD  | C16-C15-C14 | -2.38 | 100.42      | 105.13   |
| 22  | B     | 303 | CHD  | C9-C8-C7    | -2.38 | 109.03      | 111.88   |
| 20  | L     | 101 | TGL  | C15-CC9-CC8 | 2.37  | 126.47      | 114.42   |
| 14  | A     | 602 | HEA  | C21-C20-C19 | 2.37  | 120.78      | 112.98   |
| 26  | P     | 308 | PEK  | P-O11-C03   | 2.37  | 135.58      | 121.68   |
| 26  | G     | 103 | PEK  | C2-C3-C4    | -2.37 | 109.00      | 113.23   |
| 14  | A     | 602 | HEA  | C2C-C1C-NC  | 2.37  | 113.69      | 110.08   |
| 20  | Y     | 101 | TGL  | C15-CC9-CC8 | 2.37  | 126.44      | 114.42   |
| 23  | B     | 304 | PSC  | C07-N-C06   | 2.36  | 115.05      | 108.97   |
| 20  | Q     | 202 | TGL  | C15-CC9-CC8 | 2.36  | 126.39      | 114.42   |
| 26  | G     | 101 | PEK  | C03-C02-C01 | 2.36  | 117.36      | 111.79   |
| 26  | G     | 101 | PEK  | C38-C37-C36 | 2.35  | 131.26      | 113.42   |
| 26  | C     | 306 | PEK  | C34-C33-C32 | 2.35  | 126.35      | 114.42   |
| 22  | J     | 102 | CHD  | O26-C24-C23 | 2.35  | 121.57      | 114.03   |
| 20  | D     | 201 | TGL  | CC3-CC2-CC1 | -2.35 | 105.08      | 113.62   |
| 26  | G     | 103 | PEK  | C11-C10-C9  | 2.35  | 123.58      | 112.02   |
| 22  | W     | 101 | CHD  | C11-C9-C8   | 2.34  | 114.31      | 110.88   |
| 19  | P     | 301 | PGV  | P-O11-C03   | 2.34  | 135.40      | 121.68   |
| 25  | C     | 303 | CDL  | C22-C21-C20 | 2.34  | 126.30      | 114.42   |
| 28  | J     | 101 | DMU  | C18-O16-C6  | -2.33 | 109.97      | 113.84   |
| 20  | D     | 201 | TGL  | C16-C15-CC9 | 2.33  | 126.26      | 114.42   |
| 20  | L     | 101 | TGL  | CC6-CC5-CC4 | 2.33  | 126.26      | 114.42   |
| 25  | T     | 103 | CDL  | OA6-CA4-CA6 | 2.33  | 116.83      | 108.40   |
| 14  | A     | 601 | HEA  | C3A-C2A-C1A | -2.33 | 104.85      | 107.08   |
| 26  | C     | 306 | PEK  | O02-C1-C2   | -2.33 | 114.66      | 123.73   |
| 28  | P     | 306 | DMU  | O5-C6-O16   | 2.32  | 115.46      | 109.97   |
| 25  | C     | 303 | CDL  | OB2-PB2-OB3 | 2.32  | 118.12      | 109.07   |
| 28  | M     | 101 | DMU  | O4-C7-C5    | -2.31 | 105.00      | 110.35   |
| 28  | J     | 101 | DMU  | O1-C10-C5   | -2.31 | 105.46      | 110.35   |
| 22  | C     | 304 | CHD  | O3-C3-C4    | -2.31 | 105.26      | 109.85   |
| 22  | O     | 302 | CHD  | C13-C17-C20 | -2.30 | 116.75      | 119.50   |
| 19  | P     | 303 | PGV  | C26-C25-C24 | 2.30  | 126.10      | 114.42   |
| 22  | W     | 101 | CHD  | C16-C17-C13 | 2.30  | 105.81      | 103.55   |
| 26  | G     | 103 | PEK  | O03-C21-C22 | 2.29  | 119.11      | 111.91   |
| 19  | A     | 607 | PGV  | C32-C31-C30 | 2.29  | 126.05      | 114.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | Y     | 101 | TGL  | OG2-CB1-OB1 | -2.28 | 118.19      | 123.70   |
| 22  | P     | 307 | CHD  | C18-C13-C12 | 2.28  | 111.39      | 109.07   |
| 28  | Z     | 101 | DMU  | O3-C5-C7    | 2.28  | 115.62      | 110.35   |
| 14  | N     | 602 | HEA  | CHC-C1C-NC  | 2.28  | 128.03      | 123.85   |
| 22  | O     | 302 | CHD  | C17-C13-C12 | -2.27 | 115.59      | 117.67   |
| 20  | D     | 201 | TGL  | OG1-CA1-OA1 | -2.27 | 117.86      | 123.59   |
| 25  | G     | 102 | CDL  | C22-C21-C20 | 2.27  | 125.96      | 114.42   |
| 19  | N     | 607 | PGV  | C03-C02-C01 | -2.27 | 106.42      | 111.79   |
| 26  | C     | 306 | PEK  | C3-C2-C1    | 2.27  | 121.87      | 113.62   |
| 28  | J     | 101 | DMU  | O16-C18-C19 | 2.27  | 117.51      | 109.56   |
| 22  | C     | 305 | CHD  | C16-C15-C14 | -2.26 | 100.66      | 105.13   |
| 19  | C     | 307 | PGV  | C25-C24-C23 | 2.26  | 125.88      | 114.42   |
| 23  | O     | 303 | PSC  | C08-N-C06   | -2.25 | 103.19      | 108.97   |
| 22  | J     | 102 | CHD  | O26-C24-O25 | -2.25 | 117.70      | 123.30   |
| 20  | D     | 201 | TGL  | C11-C10-CB9 | 2.24  | 125.82      | 114.42   |
| 14  | N     | 602 | HEA  | C21-C20-C19 | 2.24  | 120.36      | 112.98   |
| 20  | Y     | 101 | TGL  | C30-C29-C14 | 2.24  | 125.82      | 114.42   |
| 20  | D     | 201 | TGL  | CB7-CB6-CB5 | -2.24 | 103.05      | 114.42   |
| 19  | P     | 301 | PGV  | C24-C23-C22 | 2.24  | 125.79      | 114.42   |
| 22  | C     | 304 | CHD  | C18-C13-C14 | 2.23  | 114.70      | 111.21   |
| 28  | M     | 101 | DMU  | C25-C22-C19 | -2.22 | 103.13      | 114.42   |
| 26  | T     | 101 | PEK  | O11-P-O14   | -2.22 | 100.40      | 109.07   |
| 20  | L     | 101 | TGL  | C25-C24-C23 | -2.22 | 103.16      | 114.42   |
| 23  | B     | 304 | PSC  | C26-C25-C24 | -2.21 | 103.19      | 114.42   |
| 25  | P     | 304 | CDL  | C63-C62-C61 | 2.21  | 125.66      | 114.42   |
| 14  | N     | 601 | HEA  | CHB-C4A-C3A | -2.21 | 121.48      | 125.26   |
| 19  | A     | 607 | PGV  | O01-C02-C01 | -2.21 | 100.41      | 108.40   |
| 25  | C     | 303 | CDL  | CA6-CA4-CA3 | -2.21 | 106.57      | 111.79   |
| 22  | P     | 307 | CHD  | C19-C10-C1  | -2.20 | 104.71      | 108.26   |
| 20  | Q     | 202 | TGL  | CG2-OG2-CB1 | 2.20  | 123.22      | 117.79   |
| 22  | C     | 305 | CHD  | C2-C1-C10   | 2.20  | 116.56      | 112.78   |
| 19  | P     | 301 | PGV  | C15-C14-C13 | 2.20  | 123.38      | 113.79   |
| 25  | T     | 103 | CDL  | OA9-CA7-C31 | -2.20 | 115.15      | 123.73   |
| 22  | W     | 101 | CHD  | C18-C13-C14 | 2.20  | 114.65      | 111.21   |
| 14  | A     | 601 | HEA  | CHB-C1B-NB  | 2.20  | 126.81      | 124.42   |
| 14  | N     | 602 | HEA  | OMA-CMA-C3A | -2.19 | 120.72      | 125.69   |
| 19  | N     | 607 | PGV  | O03-C19-C20 | 2.19  | 118.79      | 111.91   |
| 22  | C     | 304 | CHD  | C22-C20-C17 | 2.19  | 114.82      | 110.28   |
| 19  | A     | 607 | PGV  | C01-O03-C19 | -2.19 | 109.00      | 117.12   |
| 26  | C     | 306 | PEK  | O13-P-O11   | 2.19  | 117.91      | 107.75   |
| 20  | Y     | 101 | TGL  | CB8-CB7-CB6 | -2.18 | 103.33      | 114.42   |
| 14  | A     | 601 | HEA  | C4C-CHD-C1D | -2.18 | 121.16      | 126.34   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | P     | 303 | PGV  | C33-C32-C31 | 2.18  | 135.59      | 115.30   |
| 25  | G     | 102 | CDL  | OB7-CB5-C51 | -2.18 | 115.22      | 123.73   |
| 19  | P     | 303 | PGV  | C10-C11-C12 | -2.18 | 107.98      | 124.73   |
| 22  | O     | 302 | CHD  | C19-C10-C9  | -2.18 | 108.18      | 111.18   |
| 28  | Z     | 101 | DMU  | C11-C9-C8   | 2.18  | 118.11      | 113.00   |
| 26  | C     | 306 | PEK  | P-O11-C03   | 2.18  | 134.47      | 121.68   |
| 19  | C     | 307 | PGV  | C26-C25-C24 | 2.18  | 125.50      | 114.42   |
| 26  | P     | 308 | PEK  | C01-O03-C21 | 2.18  | 125.20      | 117.12   |
| 19  | A     | 607 | PGV  | C5-C4-C3    | -2.18 | 103.36      | 114.42   |
| 20  | B     | 301 | TGL  | C27-C26-C25 | -2.18 | 95.07       | 115.30   |
| 14  | A     | 602 | HEA  | C3A-C2A-C1A | -2.18 | 105.00      | 107.08   |
| 14  | N     | 602 | HEA  | O2A-CGA-O1A | 2.17  | 128.72      | 123.30   |
| 14  | N     | 601 | HEA  | CMB-C2B-C3B | 2.17  | 134.48      | 130.34   |
| 20  | L     | 101 | TGL  | CC7-CC6-CC5 | 2.17  | 125.44      | 114.42   |
| 20  | B     | 301 | TGL  | CG3-CG2-CG1 | -2.17 | 106.66      | 111.79   |
| 19  | P     | 303 | PGV  | C9-C10-C11  | 2.17  | 124.85      | 112.43   |
| 25  | G     | 102 | CDL  | C39-C38-C37 | 2.16  | 125.40      | 114.42   |
| 25  | P     | 304 | CDL  | OA6-CA5-OA7 | -2.16 | 118.48      | 123.70   |
| 14  | N     | 602 | HEA  | C1B-C2B-C3B | -2.16 | 104.22      | 106.80   |
| 26  | G     | 101 | PEK  | C25-C24-C23 | -2.16 | 103.47      | 114.42   |
| 19  | A     | 608 | PGV  | C10-C11-C12 | -2.16 | 108.17      | 124.73   |
| 25  | P     | 304 | CDL  | PA1-OA2-CA2 | 2.16  | 134.32      | 121.68   |
| 22  | P     | 305 | CHD  | C11-C12-C13 | -2.15 | 109.03      | 111.24   |
| 14  | N     | 601 | HEA  | C4A-CHB-C1B | -2.15 | 121.42      | 126.06   |
| 25  | C     | 303 | CDL  | OA4-PA1-OA3 | 2.15  | 122.86      | 112.24   |
| 14  | A     | 601 | HEA  | CAD-CBD-CGD | -2.15 | 108.98      | 113.60   |
| 26  | T     | 101 | PEK  | C3-C4-C5    | 2.15  | 124.73      | 112.43   |
| 20  | L     | 101 | TGL  | OG3-CG3-CG2 | 2.15  | 114.68      | 108.43   |
| 19  | N     | 607 | PGV  | C18-C17-C16 | -2.14 | 97.19       | 113.42   |
| 26  | G     | 101 | PEK  | C11-C10-C9  | 2.13  | 122.53      | 112.02   |
| 14  | N     | 602 | HEA  | C13-C14-C15 | -2.12 | 122.54      | 127.66   |
| 25  | C     | 303 | CDL  | C59-C58-C57 | 2.12  | 125.19      | 114.42   |
| 14  | N     | 601 | HEA  | CHB-C4A-NA  | 2.12  | 126.73      | 124.44   |
| 14  | A     | 602 | HEA  | C4A-CHB-C1B | -2.12 | 121.49      | 126.06   |
| 22  | W     | 101 | CHD  | C6-C5-C4    | -2.11 | 108.76      | 111.19   |
| 25  | G     | 102 | CDL  | C61-C60-C59 | -2.11 | 103.71      | 114.42   |
| 20  | D     | 201 | TGL  | C22-C21-C20 | 2.11  | 125.14      | 114.42   |
| 20  | L     | 101 | TGL  | OC1-CC1-CC2 | -2.11 | 115.51      | 123.73   |
| 20  | D     | 201 | TGL  | OG3-CG3-CG2 | -2.10 | 102.32      | 108.43   |
| 26  | C     | 306 | PEK  | C31-C30-C29 | 2.10  | 125.07      | 114.42   |
| 25  | P     | 304 | CDL  | C43-C42-C41 | 2.09  | 125.05      | 114.42   |
| 22  | P     | 307 | CHD  | C14-C8-C9   | -2.09 | 106.84      | 109.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | J     | 102 | CHD  | C15-C14-C13 | 2.09  | 105.60      | 103.55   |
| 25  | T     | 103 | CDL  | C22-C21-C20 | 2.09  | 125.02      | 114.42   |
| 19  | N     | 607 | PGV  | C32-C31-C30 | -2.08 | 103.86      | 114.42   |
| 22  | B     | 303 | CHD  | C18-C13-C17 | -2.08 | 107.96      | 111.21   |
| 22  | O     | 302 | CHD  | O12-C12-C13 | -2.08 | 107.52      | 111.03   |
| 26  | T     | 102 | PEK  | C11-C10-C9  | 2.07  | 122.23      | 112.02   |
| 22  | J     | 102 | CHD  | C18-C13-C17 | 2.07  | 114.45      | 111.21   |
| 14  | N     | 601 | HEA  | CHC-C1C-NC  | 2.06  | 127.64      | 123.85   |
| 28  | J     | 101 | DMU  | O1-C9-C8    | 2.06  | 113.44      | 109.69   |
| 23  | O     | 303 | PSC  | C04-C05-N   | 2.06  | 122.66      | 115.78   |
| 20  | Q     | 202 | TGL  | CG1-OG1-CA1 | 2.06  | 124.74      | 117.12   |
| 20  | N     | 608 | TGL  | C20-CA9-CA8 | 2.06  | 124.88      | 114.42   |
| 26  | G     | 103 | PEK  | O01-C02-C01 | 2.06  | 115.85      | 108.40   |
| 19  | P     | 301 | PGV  | C25-C24-C23 | 2.06  | 124.87      | 114.42   |
| 14  | N     | 602 | HEA  | C25-C23-C22 | -2.05 | 116.71      | 122.65   |
| 25  | P     | 304 | CDL  | C19-C18-C17 | 2.05  | 124.85      | 114.42   |
| 14  | N     | 601 | HEA  | C21-C20-C19 | -2.04 | 106.27      | 112.98   |
| 23  | B     | 304 | PSC  | C16-C15-C14 | 2.04  | 122.67      | 113.79   |
| 28  | M     | 101 | DMU  | O4-C7-C8    | 2.04  | 115.06      | 110.35   |
| 20  | N     | 608 | TGL  | C30-C29-C14 | 2.04  | 124.77      | 114.42   |
| 19  | P     | 303 | PGV  | C22-C21-C20 | -2.04 | 105.87      | 113.19   |
| 28  | M     | 101 | DMU  | O3-C5-C10   | -2.04 | 105.10      | 110.05   |
| 14  | A     | 601 | HEA  | CBA-CAA-C2A | -2.03 | 106.98      | 112.63   |
| 20  | D     | 201 | TGL  | CC6-CC5-CC4 | -2.03 | 104.10      | 114.42   |
| 22  | W     | 101 | CHD  | C14-C8-C9   | 2.03  | 112.50      | 109.71   |
| 22  | C     | 304 | CHD  | C19-C10-C5  | 2.03  | 113.81      | 110.36   |
| 25  | P     | 304 | CDL  | OA5-PA1-OA3 | -2.03 | 101.14      | 109.07   |
| 26  | G     | 101 | PEK  | C32-C31-C30 | -2.02 | 104.16      | 114.42   |
| 14  | A     | 602 | HEA  | C1C-CHC-C4B | -2.02 | 121.55      | 126.34   |
| 22  | J     | 102 | CHD  | C21-C20-C17 | 2.01  | 116.01      | 112.92   |
| 23  | O     | 303 | PSC  | O02-C1-C2   | -2.01 | 115.89      | 123.73   |
| 20  | Y     | 101 | TGL  | CG3-CG2-CG1 | -2.01 | 107.03      | 111.79   |
| 25  | C     | 303 | CDL  | O1-C1-CB2   | 2.01  | 116.59      | 109.56   |
| 22  | B     | 303 | CHD  | O7-C7-C8    | 2.01  | 113.91      | 109.43   |
| 22  | P     | 307 | CHD  | C15-C14-C8  | -2.01 | 115.53      | 118.33   |
| 19  | N     | 607 | PGV  | C4-C3-C2    | -2.00 | 105.98      | 113.19   |
| 20  | L     | 101 | TGL  | C16-C15-CC9 | 2.00  | 124.58      | 114.42   |
| 22  | P     | 307 | CHD  | O25-C24-C23 | 2.00  | 129.51      | 123.08   |
| 25  | C     | 303 | CDL  | C45-C44-C43 | 2.00  | 124.58      | 114.42   |

There are no chirality outliers.

All (909) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 608 | PGV  | C03-O11-P-O13   |
| 19  | A     | 608 | PGV  | C03-O11-P-O14   |
| 19  | A     | 608 | PGV  | C04-O12-P-O13   |
| 19  | A     | 608 | PGV  | C04-O12-P-O14   |
| 19  | A     | 608 | PGV  | O02-C1-O01-C02  |
| 19  | A     | 608 | PGV  | C2-C1-O01-C02   |
| 19  | C     | 307 | PGV  | C03-O11-P-O13   |
| 19  | C     | 307 | PGV  | C04-O12-P-O11   |
| 19  | C     | 307 | PGV  | C02-C03-O11-P   |
| 19  | P     | 301 | PGV  | C02-C03-O11-P   |
| 19  | P     | 301 | PGV  | C12-C13-C14-C15 |
| 19  | Q     | 201 | PGV  | C04-O12-P-O14   |
| 19  | Q     | 201 | PGV  | C02-C03-O11-P   |
| 19  | Q     | 201 | PGV  | C04-C05-C06-O06 |
| 19  | Q     | 201 | PGV  | O02-C1-O01-C02  |
| 19  | Q     | 201 | PGV  | C2-C1-O01-C02   |
| 20  | Q     | 202 | TGL  | CC2-CC1-OG3-CG3 |
| 20  | Q     | 202 | TGL  | OC1-CC1-OG3-CG3 |
| 20  | Y     | 101 | TGL  | CB2-CB1-OG2-CG2 |
| 22  | J     | 102 | CHD  | C13-C17-C20-C22 |
| 22  | J     | 102 | CHD  | C16-C17-C20-C21 |
| 22  | W     | 101 | CHD  | C13-C17-C20-C22 |
| 23  | B     | 304 | PSC  | C03-O11-P-O14   |
| 23  | B     | 304 | PSC  | O12-C04-C05-N   |
| 23  | B     | 304 | PSC  | C2-C1-O01-C02   |
| 23  | O     | 303 | PSC  | C03-O11-P-O13   |
| 23  | O     | 303 | PSC  | C03-O11-P-O14   |
| 23  | O     | 303 | PSC  | C2-C1-O01-C02   |
| 23  | O     | 303 | PSC  | C11-C12-C13-C14 |
| 25  | C     | 303 | CDL  | CA3-OA5-PA1-OA3 |
| 25  | C     | 303 | CDL  | C11-CA5-OA6-CA4 |
| 25  | C     | 303 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | C     | 303 | CDL  | C51-CB5-OB6-CB4 |
| 25  | G     | 102 | CDL  | CA2-OA2-PA1-OA3 |
| 25  | G     | 102 | CDL  | CA2-OA2-PA1-OA4 |
| 25  | G     | 102 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | G     | 102 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | G     | 102 | CDL  | C1-CB2-OB2-PB2  |
| 25  | G     | 102 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | G     | 102 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | G     | 102 | CDL  | CB3-OB5-PB2-OB3 |
| 25  | G     | 102 | CDL  | CB3-OB5-PB2-OB4 |
| 25  | P     | 304 | CDL  | CB2-C1-CA2-OA2  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | P     | 304 | CDL  | CA2-OA2-PA1-OA4 |
| 25  | P     | 304 | CDL  | CA3-OA5-PA1-OA3 |
| 25  | P     | 304 | CDL  | CB2-OB2-PB2-OB3 |
| 25  | P     | 304 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | P     | 304 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | P     | 304 | CDL  | CB3-OB5-PB2-OB3 |
| 25  | P     | 304 | CDL  | CB3-OB5-PB2-OB4 |
| 25  | P     | 304 | CDL  | C51-CB5-OB6-CB4 |
| 25  | T     | 103 | CDL  | CA2-C1-CB2-OB2  |
| 25  | T     | 103 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | T     | 103 | CDL  | OA9-CA7-OA8-CA6 |
| 25  | T     | 103 | CDL  | C31-CA7-OA8-CA6 |
| 25  | T     | 103 | CDL  | C1-CB2-OB2-PB2  |
| 25  | T     | 103 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | T     | 103 | CDL  | CB3-OB5-PB2-OB3 |
| 25  | T     | 103 | CDL  | CB3-OB5-PB2-OB4 |
| 26  | C     | 306 | PEK  | C04-O12-P-O14   |
| 26  | C     | 306 | PEK  | C2-C1-O01-C02   |
| 26  | C     | 306 | PEK  | C6-C7-C8-C9     |
| 26  | C     | 306 | PEK  | C9-C10-C11-C12  |
| 26  | C     | 306 | PEK  | C11-C12-C13-C14 |
| 26  | G     | 103 | PEK  | C03-O11-P-O14   |
| 26  | G     | 103 | PEK  | O12-C04-C05-N   |
| 26  | G     | 103 | PEK  | C2-C1-O01-C02   |
| 26  | G     | 103 | PEK  | C11-C12-C13-C14 |
| 26  | P     | 308 | PEK  | O02-C1-O01-C02  |
| 26  | P     | 308 | PEK  | C2-C1-O01-C02   |
| 26  | T     | 101 | PEK  | C11-C12-C13-C14 |
| 26  | T     | 101 | PEK  | C12-C13-C14-C15 |
| 26  | T     | 102 | PEK  | C04-O12-P-O14   |
| 26  | T     | 102 | PEK  | O12-C04-C05-N   |
| 28  | P     | 306 | DMU  | C1-C6-O16-C18   |
| 28  | P     | 306 | DMU  | O5-C6-O16-C18   |
| 19  | A     | 608 | PGV  | O04-C19-O03-C01 |
| 19  | Q     | 201 | PGV  | O04-C19-O03-C01 |
| 20  | D     | 201 | TGL  | OC1-CC1-OG3-CG3 |
| 20  | Y     | 101 | TGL  | OA1-CA1-OG1-CG1 |
| 19  | A     | 608 | PGV  | C20-C19-O03-C01 |
| 19  | Q     | 201 | PGV  | C20-C19-O03-C01 |
| 23  | O     | 303 | PSC  | C20-C19-O03-C01 |
| 23  | O     | 303 | PSC  | O04-C19-O03-C01 |
| 25  | G     | 102 | CDL  | OA9-CA7-OA8-CA6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | J     | 102 | CHD  | C13-C17-C20-C21 |
| 22  | W     | 101 | CHD  | C13-C17-C20-C21 |
| 19  | P     | 301 | PGV  | O02-C1-O01-C02  |
| 20  | L     | 101 | TGL  | OB1-CB1-OG2-CG2 |
| 20  | Y     | 101 | TGL  | OB1-CB1-OG2-CG2 |
| 23  | B     | 304 | PSC  | O02-C1-O01-C02  |
| 25  | C     | 303 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | C     | 303 | CDL  | OB7-CB5-OB6-CB4 |
| 26  | C     | 306 | PEK  | O02-C1-O01-C02  |
| 26  | T     | 102 | PEK  | O02-C1-O01-C02  |
| 20  | D     | 201 | TGL  | CC2-CC1-OG3-CG3 |
| 20  | Y     | 101 | TGL  | CA2-CA1-OG1-CG1 |
| 19  | P     | 301 | PGV  | C2-C1-O01-C02   |
| 25  | G     | 102 | CDL  | C11-CA5-OA6-CA4 |
| 26  | T     | 102 | PEK  | C2-C1-O01-C02   |
| 22  | C     | 304 | CHD  | C13-C17-C20-C21 |
| 22  | J     | 102 | CHD  | C16-C17-C20-C22 |
| 22  | C     | 304 | CHD  | C13-C17-C20-C22 |
| 22  | P     | 305 | CHD  | C13-C17-C20-C22 |
| 22  | W     | 101 | CHD  | C20-C22-C23-C24 |
| 23  | B     | 304 | PSC  | C20-C21-C22-C23 |
| 23  | B     | 304 | PSC  | C20-C19-O03-C01 |
| 25  | G     | 102 | CDL  | C31-CA7-OA8-CA6 |
| 19  | A     | 608 | PGV  | C10-C11-C12-C13 |
| 19  | C     | 307 | PGV  | C10-C11-C12-C13 |
| 26  | T     | 101 | PEK  | C7-C8-C9-C10    |
| 23  | O     | 303 | PSC  | O02-C1-O01-C02  |
| 26  | G     | 103 | PEK  | O02-C1-O01-C02  |
| 23  | B     | 304 | PSC  | O04-C19-O03-C01 |
| 22  | P     | 305 | CHD  | C16-C17-C20-C22 |
| 19  | P     | 301 | PGV  | O12-C04-C05-O05 |
| 25  | G     | 102 | CDL  | O1-C1-CA2-OA2   |
| 25  | T     | 103 | CDL  | O1-C1-CB2-OB2   |
| 23  | B     | 304 | PSC  | C22-C23-C24-C25 |
| 25  | T     | 103 | CDL  | C11-CA5-OA6-CA4 |
| 20  | B     | 301 | TGL  | CA1-CA2-CA3-CA4 |
| 26  | P     | 308 | PEK  | C33-C34-C35-C36 |
| 20  | D     | 201 | TGL  | CA9-C20-C21-C22 |
| 20  | Y     | 101 | TGL  | CC5-CC6-CC7-CC8 |
| 23  | O     | 303 | PSC  | C26-C27-C28-C29 |
| 25  | C     | 303 | CDL  | C76-C77-C78-C79 |
| 25  | T     | 103 | CDL  | C79-C80-C81-C82 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | P     | 306 | DMU  | O6-C11-C9-O1    |
| 22  | P     | 305 | CHD  | C16-C17-C20-C21 |
| 19  | P     | 303 | PGV  | C12-C13-C14-C15 |
| 25  | P     | 304 | CDL  | CA5-C11-C12-C13 |
| 19  | C     | 307 | PGV  | C20-C21-C22-C23 |
| 20  | B     | 301 | TGL  | OB1-CB1-OG2-CG2 |
| 23  | O     | 303 | PSC  | C20-C21-C22-C23 |
| 25  | C     | 303 | CDL  | CA4-CA3-OA5-PA1 |
| 23  | O     | 303 | PSC  | C24-C25-C26-C27 |
| 20  | D     | 201 | TGL  | C20-C21-C22-C23 |
| 22  | W     | 101 | CHD  | C16-C17-C20-C21 |
| 25  | T     | 103 | CDL  | C56-C57-C58-C59 |
| 20  | L     | 101 | TGL  | CC1-CC2-CC3-CC4 |
| 19  | A     | 608 | PGV  | O12-C04-C05-C06 |
| 25  | C     | 303 | CDL  | CB2-C1-CA2-OA2  |
| 25  | G     | 102 | CDL  | CB2-C1-CA2-OA2  |
| 25  | P     | 304 | CDL  | OB7-CB5-OB6-CB4 |
| 20  | B     | 301 | TGL  | CA2-CA1-OG1-CG1 |
| 20  | L     | 101 | TGL  | CA2-CA1-OG1-CG1 |
| 25  | T     | 103 | CDL  | C63-C64-C65-C66 |
| 28  | P     | 306 | DMU  | O6-C11-C9-C8    |
| 19  | A     | 608 | PGV  | O12-C04-C05-O05 |
| 19  | C     | 307 | PGV  | O12-C04-C05-O05 |
| 25  | P     | 304 | CDL  | O1-C1-CA2-OA2   |
| 25  | P     | 304 | CDL  | O1-C1-CB2-OB2   |
| 19  | C     | 307 | PGV  | C1-C2-C3-C4     |
| 20  | Q     | 202 | TGL  | OG1-CG1-CG2-OG2 |
| 19  | P     | 303 | PGV  | C30-C31-C32-C33 |
| 20  | Q     | 202 | TGL  | CA9-C20-C21-C22 |
| 20  | Y     | 101 | TGL  | CA9-C20-C21-C22 |
| 20  | B     | 301 | TGL  | CA9-C20-C21-C22 |
| 26  | G     | 103 | PEK  | C21-C22-C23-C24 |
| 22  | W     | 101 | CHD  | C17-C20-C22-C23 |
| 20  | N     | 608 | TGL  | CC7-CC8-CC9-C15 |
| 19  | A     | 608 | PGV  | C1-C2-C3-C4     |
| 23  | B     | 304 | PSC  | C1-C2-C3-C4     |
| 22  | C     | 304 | CHD  | C16-C17-C20-C21 |
| 26  | P     | 308 | PEK  | C2-C3-C4-C5     |
| 26  | T     | 101 | PEK  | C1-C2-C3-C4     |
| 19  | P     | 301 | PGV  | C1-C2-C3-C4     |
| 19  | Q     | 201 | PGV  | C19-C20-C21-C22 |
| 20  | B     | 301 | TGL  | OA1-CA1-OG1-CG1 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | T     | 103 | CDL  | C73-C74-C75-C76 |
| 20  | L     | 101 | TGL  | OA1-CA1-OG1-CG1 |
| 14  | A     | 601 | HEA  | C15-C16-C17-C18 |
| 14  | N     | 601 | HEA  | C19-C20-C21-C22 |
| 20  | N     | 608 | TGL  | C22-C23-C24-C25 |
| 25  | C     | 303 | CDL  | O1-C1-CA2-OA2   |
| 25  | G     | 102 | CDL  | O1-C1-CB2-OB2   |
| 20  | L     | 101 | TGL  | CB3-CB4-CB5-CB6 |
| 22  | W     | 101 | CHD  | C16-C17-C20-C22 |
| 26  | C     | 306 | PEK  | C1-C2-C3-C4     |
| 26  | C     | 306 | PEK  | C4-C5-C6-C7     |
| 26  | P     | 308 | PEK  | C10-C11-C12-C13 |
| 26  | T     | 101 | PEK  | C13-C14-C15-C16 |
| 19  | A     | 608 | PGV  | C03-O11-P-O12   |
| 19  | A     | 608 | PGV  | C04-O12-P-O11   |
| 19  | Q     | 201 | PGV  | C03-O11-P-O12   |
| 19  | Q     | 201 | PGV  | C04-O12-P-O11   |
| 23  | B     | 304 | PSC  | C03-O11-P-O12   |
| 23  | O     | 303 | PSC  | C03-O11-P-O12   |
| 25  | C     | 303 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | C     | 303 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | G     | 102 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | P     | 304 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | P     | 304 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | T     | 103 | CDL  | CB3-OB5-PB2-OB2 |
| 26  | P     | 308 | PEK  | C04-O12-P-O11   |
| 25  | T     | 103 | CDL  | CB5-C51-C52-C53 |
| 20  | Q     | 202 | TGL  | CB9-C10-C11-C12 |
| 20  | Q     | 202 | TGL  | CB1-CB2-CB3-CB4 |
| 19  | C     | 307 | PGV  | O12-C04-C05-C06 |
| 25  | G     | 102 | CDL  | CA2-C1-CB2-OB2  |
| 20  | N     | 608 | TGL  | OB1-CB1-OG2-CG2 |
| 26  | T     | 101 | PEK  | C2-C3-C4-C5     |
| 19  | P     | 301 | PGV  | C22-C23-C24-C25 |
| 20  | N     | 608 | TGL  | CB4-CB5-CB6-CB7 |
| 25  | C     | 303 | CDL  | C12-C13-C14-C15 |
| 25  | G     | 102 | CDL  | C23-C24-C25-C26 |
| 20  | B     | 301 | TGL  | CB2-CB1-OG2-CG2 |
| 20  | L     | 101 | TGL  | CB2-CB1-OG2-CG2 |
| 14  | A     | 601 | HEA  | C16-C17-C18-C19 |
| 19  | C     | 302 | PGV  | C14-C15-C16-C17 |
| 19  | C     | 307 | PGV  | C3-C4-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | C     | 307 | PGV  | C22-C23-C24-C25 |
| 20  | B     | 301 | TGL  | CA5-CA6-CA7-CA8 |
| 20  | L     | 101 | TGL  | CC6-CC7-CC8-CC9 |
| 20  | N     | 608 | TGL  | C13-C14-C29-C30 |
| 20  | Q     | 202 | TGL  | CC9-C15-C16-C17 |
| 20  | Y     | 101 | TGL  | C23-C24-C25-C26 |
| 25  | T     | 103 | CDL  | C18-C19-C20-C21 |
| 19  | A     | 608 | PGV  | C23-C24-C25-C26 |
| 20  | N     | 608 | TGL  | CA3-CA4-CA5-CA6 |
| 20  | Y     | 101 | TGL  | C10-C11-C12-C13 |
| 25  | C     | 303 | CDL  | C72-C73-C74-C75 |
| 25  | G     | 102 | CDL  | C19-C20-C21-C22 |
| 25  | G     | 102 | CDL  | C59-C60-C61-C62 |
| 25  | P     | 304 | CDL  | C38-C39-C40-C41 |
| 26  | G     | 101 | PEK  | C26-C27-C28-C29 |
| 26  | T     | 101 | PEK  | C30-C31-C32-C33 |
| 26  | T     | 102 | PEK  | C28-C29-C30-C31 |
| 19  | A     | 608 | PGV  | C03-C02-O01-C1  |
| 19  | Q     | 201 | PGV  | C01-C02-O01-C1  |
| 20  | Q     | 202 | TGL  | CG3-CG2-OG2-CB1 |
| 23  | O     | 303 | PSC  | C01-C02-O01-C1  |
| 26  | G     | 103 | PEK  | C01-C02-O01-C1  |
| 19  | A     | 608 | PGV  | C19-C20-C21-C22 |
| 20  | D     | 201 | TGL  | CC9-C15-C16-C17 |
| 25  | G     | 102 | CDL  | C82-C83-C84-C85 |
| 28  | M     | 101 | DMU  | C19-C22-C25-C28 |
| 25  | G     | 102 | CDL  | CB4-CB3-OB5-PB2 |
| 26  | P     | 308 | PEK  | C4-C5-C6-C7     |
| 26  | T     | 101 | PEK  | C10-C11-C12-C13 |
| 26  | T     | 102 | PEK  | C13-C14-C15-C16 |
| 19  | C     | 307 | PGV  | C28-C29-C30-C31 |
| 20  | N     | 608 | TGL  | CA2-CA3-CA4-CA5 |
| 19  | P     | 301 | PGV  | C5-C6-C7-C8     |
| 19  | P     | 301 | PGV  | C23-C24-C25-C26 |
| 19  | P     | 303 | PGV  | C7-C8-C9-C10    |
| 20  | B     | 301 | TGL  | C11-C12-C13-C14 |
| 20  | L     | 101 | TGL  | CB6-CB7-CB8-CB9 |
| 20  | L     | 101 | TGL  | C17-C18-C19-C33 |
| 20  | Q     | 202 | TGL  | C11-C10-CB9-CB8 |
| 20  | Q     | 202 | TGL  | C19-C33-C34-C35 |
| 25  | G     | 102 | CDL  | C35-C36-C37-C38 |
| 25  | T     | 103 | CDL  | C72-C73-C74-C75 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 608 | PGV  | C22-C23-C24-C25 |
| 19  | C     | 302 | PGV  | C7-C8-C9-C10    |
| 19  | C     | 307 | PGV  | C30-C31-C32-C33 |
| 25  | G     | 102 | CDL  | C72-C73-C74-C75 |
| 25  | P     | 304 | CDL  | C36-C37-C38-C39 |
| 28  | Z     | 101 | DMU  | C22-C25-C28-C31 |
| 19  | N     | 607 | PGV  | C14-C15-C16-C17 |
| 19  | P     | 301 | PGV  | C24-C25-C26-C27 |
| 20  | B     | 301 | TGL  | CB4-CB5-CB6-CB7 |
| 20  | Y     | 101 | TGL  | CA3-CA4-CA5-CA6 |
| 23  | O     | 303 | PSC  | C5-C6-C7-C8     |
| 25  | C     | 303 | CDL  | C63-C64-C65-C66 |
| 19  | P     | 301 | PGV  | C19-C20-C21-C22 |
| 19  | P     | 303 | PGV  | C24-C25-C26-C27 |
| 20  | B     | 301 | TGL  | CC4-CC5-CC6-CC7 |
| 20  | D     | 201 | TGL  | CA3-CA4-CA5-CA6 |
| 20  | D     | 201 | TGL  | C14-C29-C30-C31 |
| 20  | Q     | 202 | TGL  | C23-C24-C25-C26 |
| 20  | Y     | 101 | TGL  | CC6-CC7-CC8-CC9 |
| 20  | Y     | 101 | TGL  | C18-C19-C33-C34 |
| 25  | G     | 102 | CDL  | C38-C39-C40-C41 |
| 25  | G     | 102 | CDL  | C76-C77-C78-C79 |
| 25  | T     | 103 | CDL  | C71-C72-C73-C74 |
| 22  | P     | 305 | CHD  | C20-C22-C23-C24 |
| 20  | N     | 608 | TGL  | CA4-CA5-CA6-CA7 |
| 20  | N     | 608 | TGL  | CB6-CB7-CB8-CB9 |
| 20  | N     | 608 | TGL  | C19-C33-C34-C35 |
| 25  | T     | 103 | CDL  | C21-C22-C23-C24 |
| 19  | P     | 301 | PGV  | C04-C05-C06-O06 |
| 19  | P     | 301 | PGV  | C4-C5-C6-C7     |
| 20  | L     | 101 | TGL  | CB4-CB5-CB6-CB7 |
| 25  | C     | 303 | CDL  | C39-C40-C41-C42 |
| 25  | G     | 102 | CDL  | C54-C55-C56-C57 |
| 25  | P     | 304 | CDL  | C35-C36-C37-C38 |
| 25  | P     | 304 | CDL  | C60-C61-C62-C63 |
| 25  | T     | 103 | CDL  | C31-C32-C33-C34 |
| 19  | A     | 608 | PGV  | C12-C13-C14-C15 |
| 19  | N     | 607 | PGV  | C23-C24-C25-C26 |
| 20  | D     | 201 | TGL  | C16-C17-C18-C19 |
| 20  | L     | 101 | TGL  | CA5-CA6-CA7-CA8 |
| 20  | Q     | 202 | TGL  | CB5-CB6-CB7-CB8 |
| 23  | O     | 303 | PSC  | C3-C4-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | O     | 303 | PSC  | C4-C5-C6-C7     |
| 25  | C     | 303 | CDL  | C71-C72-C73-C74 |
| 25  | G     | 102 | CDL  | C41-C42-C43-C44 |
| 25  | P     | 304 | CDL  | C73-C74-C75-C76 |
| 25  | P     | 304 | CDL  | C79-C80-C81-C82 |
| 25  | T     | 103 | CDL  | C39-C40-C41-C42 |
| 26  | T     | 101 | PEK  | C26-C27-C28-C29 |
| 20  | Y     | 101 | TGL  | CA6-CA7-CA8-CA9 |
| 20  | Y     | 101 | TGL  | CC9-C15-C16-C17 |
| 25  | P     | 304 | CDL  | C59-C60-C61-C62 |
| 19  | P     | 301 | PGV  | C13-C14-C15-C16 |
| 20  | D     | 201 | TGL  | CA7-CA8-CA9-C20 |
| 20  | D     | 201 | TGL  | CB2-CB3-CB4-CB5 |
| 20  | L     | 101 | TGL  | C11-C12-C13-C14 |
| 20  | Q     | 202 | TGL  | CA5-CA6-CA7-CA8 |
| 25  | P     | 304 | CDL  | C40-C41-C42-C43 |
| 28  | Z     | 101 | DMU  | C25-C28-C31-C34 |
| 19  | C     | 302 | PGV  | C23-C24-C25-C26 |
| 23  | B     | 304 | PSC  | C24-C25-C26-C27 |
| 26  | G     | 101 | PEK  | C34-C35-C36-C37 |
| 25  | C     | 303 | CDL  | C31-CA7-OA8-CA6 |
| 20  | N     | 608 | TGL  | C12-C13-C14-C29 |
| 20  | N     | 608 | TGL  | CA9-C20-C21-C22 |
| 25  | G     | 102 | CDL  | C20-C21-C22-C23 |
| 19  | P     | 301 | PGV  | C6-C7-C8-C9     |
| 20  | N     | 608 | TGL  | CC5-CC6-CC7-CC8 |
| 23  | B     | 304 | PSC  | C27-C28-C29-C30 |
| 25  | C     | 303 | CDL  | C23-C24-C25-C26 |
| 25  | C     | 303 | CDL  | C31-C32-C33-C34 |
| 25  | T     | 103 | CDL  | C23-C24-C25-C26 |
| 26  | G     | 101 | PEK  | C28-C29-C30-C31 |
| 20  | N     | 608 | TGL  | OC1-CC1-OG3-CG3 |
| 19  | Q     | 201 | PGV  | C4-C5-C6-C7     |
| 25  | P     | 304 | CDL  | C20-C21-C22-C23 |
| 25  | T     | 103 | CDL  | C13-C14-C15-C16 |
| 25  | P     | 304 | CDL  | CA3-CA4-CA6-OA8 |
| 23  | B     | 304 | PSC  | C11-C12-C13-C14 |
| 26  | G     | 101 | PEK  | C10-C11-C12-C13 |
| 19  | A     | 607 | PGV  | C28-C29-C30-C31 |
| 20  | N     | 608 | TGL  | CB7-CB8-CB9-C10 |
| 25  | G     | 102 | CDL  | C33-C34-C35-C36 |
| 26  | G     | 101 | PEK  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | C     | 302 | PGV  | C27-C28-C29-C30 |
| 19  | C     | 307 | PGV  | C2-C1-O01-C02   |
| 20  | N     | 608 | TGL  | CB2-CB1-OG2-CG2 |
| 19  | Q     | 201 | PGV  | O05-C05-C06-O06 |
| 19  | C     | 307 | PGV  | C23-C24-C25-C26 |
| 19  | N     | 607 | PGV  | C29-C30-C31-C32 |
| 20  | N     | 608 | TGL  | CB5-CB6-CB7-CB8 |
| 20  | Q     | 202 | TGL  | C17-C18-C19-C33 |
| 26  | T     | 102 | PEK  | C25-C26-C27-C28 |
| 25  | C     | 303 | CDL  | OA9-CA7-OA8-CA6 |
| 25  | P     | 304 | CDL  | C16-C17-C18-C19 |
| 19  | P     | 301 | PGV  | C30-C31-C32-C33 |
| 25  | P     | 304 | CDL  | C43-C44-C45-C46 |
| 19  | Q     | 201 | PGV  | C14-C15-C16-C17 |
| 20  | L     | 101 | TGL  | C21-C20-CA9-CA8 |
| 25  | T     | 103 | CDL  | C61-C62-C63-C64 |
| 26  | G     | 101 | PEK  | C25-C26-C27-C28 |
| 19  | C     | 307 | PGV  | O02-C1-O01-C02  |
| 19  | Q     | 201 | PGV  | C2-C3-C4-C5     |
| 20  | B     | 301 | TGL  | C17-C18-C19-C33 |
| 20  | D     | 201 | TGL  | C11-C12-C13-C14 |
| 20  | Y     | 101 | TGL  | C16-C15-CC9-CC8 |
| 25  | P     | 304 | CDL  | C74-C75-C76-C77 |
| 28  | M     | 101 | DMU  | C22-C25-C28-C31 |
| 20  | D     | 201 | TGL  | CB9-C10-C11-C12 |
| 25  | G     | 102 | CDL  | C16-C17-C18-C19 |
| 20  | B     | 301 | TGL  | CC7-CC8-CC9-C15 |
| 28  | J     | 101 | DMU  | C19-C22-C25-C28 |
| 20  | N     | 608 | TGL  | CC2-CC1-OG3-CG3 |
| 20  | N     | 608 | TGL  | C21-C20-CA9-CA8 |
| 25  | T     | 103 | CDL  | C75-C76-C77-C78 |
| 19  | Q     | 201 | PGV  | C29-C30-C31-C32 |
| 20  | Q     | 202 | TGL  | CB2-CB3-CB4-CB5 |
| 23  | B     | 304 | PSC  | C30-C31-C32-C33 |
| 25  | T     | 103 | CDL  | C81-C82-C83-C84 |
| 26  | T     | 102 | PEK  | C33-C34-C35-C36 |
| 25  | P     | 304 | CDL  | C31-C32-C33-C34 |
| 26  | G     | 101 | PEK  | C7-C8-C9-C10    |
| 20  | Y     | 101 | TGL  | C25-C26-C27-C28 |
| 26  | G     | 103 | PEK  | C25-C26-C27-C28 |
| 23  | O     | 303 | PSC  | C6-C7-C8-C9     |
| 26  | C     | 306 | PEK  | C2-C3-C4-C5     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | G     | 101 | PEK  | C15-C16-C17-C18 |
| 26  | T     | 102 | PEK  | C2-C3-C4-C5     |
| 19  | C     | 307 | PGV  | C20-C19-O03-C01 |
| 20  | N     | 608 | TGL  | CA2-CA1-OG1-CG1 |
| 25  | G     | 102 | CDL  | C71-CB7-OB8-CB6 |
| 20  | N     | 608 | TGL  | C11-C10-CB9-CB8 |
| 25  | C     | 303 | CDL  | C18-C19-C20-C21 |
| 25  | G     | 102 | CDL  | C17-C18-C19-C20 |
| 25  | T     | 103 | CDL  | C83-C84-C85-C86 |
| 20  | D     | 201 | TGL  | CC6-CC7-CC8-CC9 |
| 25  | G     | 102 | CDL  | C13-C14-C15-C16 |
| 25  | G     | 102 | CDL  | C14-C15-C16-C17 |
| 25  | G     | 102 | CDL  | C22-C23-C24-C25 |
| 25  | G     | 102 | CDL  | C56-C57-C58-C59 |
| 25  | P     | 304 | CDL  | C58-C59-C60-C61 |
| 26  | C     | 306 | PEK  | C24-C25-C26-C27 |
| 26  | G     | 101 | PEK  | C16-C17-C18-C19 |
| 19  | A     | 608 | PGV  | C7-C8-C9-C10    |
| 20  | L     | 101 | TGL  | C18-C19-C33-C34 |
| 26  | P     | 308 | PEK  | C28-C29-C30-C31 |
| 20  | D     | 201 | TGL  | CA2-CA3-CA4-CA5 |
| 20  | N     | 608 | TGL  | CC4-CC5-CC6-CC7 |
| 19  | C     | 307 | PGV  | O01-C02-C03-O11 |
| 26  | T     | 102 | PEK  | O01-C02-C03-O11 |
| 19  | A     | 608 | PGV  | C20-C21-C22-C23 |
| 25  | C     | 303 | CDL  | C64-C65-C66-C67 |
| 20  | Y     | 101 | TGL  | CB7-CB8-CB9-C10 |
| 26  | P     | 308 | PEK  | C32-C33-C34-C35 |
| 28  | P     | 306 | DMU  | O16-C18-C19-C22 |
| 26  | C     | 306 | PEK  | C25-C26-C27-C28 |
| 20  | D     | 201 | TGL  | OG1-CG1-CG2-OG2 |
| 25  | T     | 103 | CDL  | OB6-CB4-CB6-OB8 |
| 20  | Q     | 202 | TGL  | CC5-CC6-CC7-CC8 |
| 25  | P     | 304 | CDL  | C57-C58-C59-C60 |
| 20  | Y     | 101 | TGL  | CB9-C10-C11-C12 |
| 25  | P     | 304 | CDL  | C72-C73-C74-C75 |
| 25  | T     | 103 | CDL  | C15-C16-C17-C18 |
| 26  | T     | 102 | PEK  | C32-C33-C34-C35 |
| 28  | Z     | 101 | DMU  | C19-C22-C25-C28 |
| 19  | P     | 301 | PGV  | C11-C10-C9-C8   |
| 20  | B     | 301 | TGL  | CB5-CB6-CB7-CB8 |
| 20  | B     | 301 | TGL  | C12-C13-C14-C29 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | B     | 301 | TGL  | C16-C17-C18-C19 |
| 25  | P     | 304 | CDL  | C37-C38-C39-C40 |
| 20  | D     | 201 | TGL  | C17-C18-C19-C33 |
| 20  | L     | 101 | TGL  | CB2-CB3-CB4-CB5 |
| 25  | C     | 303 | CDL  | C53-C54-C55-C56 |
| 25  | P     | 304 | CDL  | C12-C13-C14-C15 |
| 20  | N     | 608 | TGL  | C11-C12-C13-C14 |
| 20  | Y     | 101 | TGL  | CA2-CA3-CA4-CA5 |
| 25  | P     | 304 | CDL  | C80-C81-C82-C83 |
| 19  | C     | 307 | PGV  | C03-O11-P-O12   |
| 26  | G     | 103 | PEK  | C03-O11-P-O12   |
| 20  | Y     | 101 | TGL  | CC4-CC5-CC6-CC7 |
| 19  | A     | 608 | PGV  | C05-C04-O12-P   |
| 25  | P     | 304 | CDL  | C78-C79-C80-C81 |
| 19  | A     | 608 | PGV  | C01-C02-C03-O11 |
| 19  | C     | 307 | PGV  | C01-C02-C03-O11 |
| 19  | Q     | 201 | PGV  | C01-C02-C03-O11 |
| 25  | C     | 303 | CDL  | OA5-CA3-CA4-CA6 |
| 25  | P     | 304 | CDL  | OA5-CA3-CA4-CA6 |
| 23  | B     | 304 | PSC  | C26-C27-C28-C29 |
| 20  | D     | 201 | TGL  | C23-C24-C25-C26 |
| 20  | Q     | 202 | TGL  | CA6-CA7-CA8-CA9 |
| 20  | Y     | 101 | TGL  | C13-C14-C29-C30 |
| 25  | P     | 304 | CDL  | C23-C24-C25-C26 |
| 20  | Y     | 101 | TGL  | C22-C23-C24-C25 |
| 20  | Q     | 202 | TGL  | CC2-CC3-CC4-CC5 |
| 20  | Y     | 101 | TGL  | C11-C10-CB9-CB8 |
| 25  | G     | 102 | CDL  | C58-C59-C60-C61 |
| 19  | Q     | 201 | PGV  | O03-C01-C02-C03 |
| 20  | Q     | 202 | TGL  | CG1-CG2-CG3-OG3 |
| 23  | O     | 303 | PSC  | O03-C01-C02-C03 |
| 25  | G     | 102 | CDL  | CA3-CA4-CA6-OA8 |
| 25  | T     | 103 | CDL  | CB3-CB4-CB6-OB8 |
| 26  | T     | 102 | PEK  | C10-C11-C12-C13 |
| 25  | T     | 103 | CDL  | C64-C65-C66-C67 |
| 28  | J     | 101 | DMU  | C34-C37-C40-C43 |
| 20  | B     | 301 | TGL  | OC1-CC1-OG3-CG3 |
| 20  | N     | 608 | TGL  | OA1-CA1-OG1-CG1 |
| 19  | P     | 301 | PGV  | C15-C16-C17-C18 |
| 20  | B     | 301 | TGL  | C21-C20-CA9-CA8 |
| 20  | N     | 608 | TGL  | CC6-CC7-CC8-CC9 |
| 25  | C     | 303 | CDL  | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | N     | 608 | TGL  | CA1-CA2-CA3-CA4 |
| 19  | A     | 607 | PGV  | C31-C32-C33-C34 |
| 25  | T     | 103 | CDL  | C17-C18-C19-C20 |
| 20  | B     | 301 | TGL  | C29-C30-C31-C32 |
| 25  | C     | 303 | CDL  | C43-C44-C45-C46 |
| 20  | Q     | 202 | TGL  | C29-C30-C31-C32 |
| 25  | T     | 103 | CDL  | C22-C23-C24-C25 |
| 19  | A     | 608 | PGV  | C11-C10-C9-C8   |
| 19  | A     | 608 | PGV  | C31-C32-C33-C34 |
| 20  | L     | 101 | TGL  | CC3-CC4-CC5-CC6 |
| 19  | C     | 302 | PGV  | C15-C16-C17-C18 |
| 19  | Q     | 201 | PGV  | C31-C32-C33-C34 |
| 20  | Y     | 101 | TGL  | CB3-CB4-CB5-CB6 |
| 20  | Y     | 101 | TGL  | CC3-CC4-CC5-CC6 |
| 20  | D     | 201 | TGL  | CG3-CG2-OG2-CB1 |
| 23  | B     | 304 | PSC  | C01-C02-O01-C1  |
| 25  | P     | 304 | CDL  | CA3-CA4-OA6-CA5 |
| 25  | P     | 304 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | C     | 303 | CDL  | C14-C15-C16-C17 |
| 20  | B     | 301 | TGL  | CC2-CC1-OG3-CG3 |
| 19  | Q     | 201 | PGV  | C10-C11-C12-C13 |
| 26  | C     | 306 | PEK  | C7-C8-C9-C10    |
| 26  | T     | 101 | PEK  | C4-C5-C6-C7     |
| 25  | G     | 102 | CDL  | CA5-C11-C12-C13 |
| 23  | O     | 303 | PSC  | C2-C3-C4-C5     |
| 26  | P     | 308 | PEK  | C35-C36-C37-C38 |
| 22  | P     | 305 | CHD  | C13-C17-C20-C21 |
| 25  | C     | 303 | CDL  | C61-C62-C63-C64 |
| 25  | G     | 102 | CDL  | C11-C12-C13-C14 |
| 28  | P     | 306 | DMU  | C22-C25-C28-C31 |
| 20  | N     | 608 | TGL  | OG1-CG1-CG2-OG2 |
| 20  | N     | 608 | TGL  | CB9-C10-C11-C12 |
| 25  | G     | 102 | CDL  | C77-C78-C79-C80 |
| 26  | G     | 101 | PEK  | C35-C36-C37-C38 |
| 25  | G     | 102 | CDL  | OB9-CB7-OB8-CB6 |
| 25  | T     | 103 | CDL  | C36-C37-C38-C39 |
| 25  | G     | 102 | CDL  | C12-C13-C14-C15 |
| 20  | L     | 101 | TGL  | CC2-CC3-CC4-CC5 |
| 26  | C     | 306 | PEK  | C35-C36-C37-C38 |
| 19  | P     | 301 | PGV  | O12-C04-C05-C06 |
| 19  | C     | 307 | PGV  | C21-C22-C23-C24 |
| 25  | G     | 102 | CDL  | C79-C80-C81-C82 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | C     | 302 | PGV  | C10-C11-C12-C13 |
| 19  | Q     | 201 | PGV  | C27-C28-C29-C30 |
| 20  | Q     | 202 | TGL  | CB4-CB5-CB6-CB7 |
| 25  | C     | 303 | CDL  | C73-C74-C75-C76 |
| 19  | A     | 607 | PGV  | C30-C31-C32-C33 |
| 20  | D     | 201 | TGL  | CC5-CC6-CC7-CC8 |
| 26  | T     | 102 | PEK  | C01-C02-C03-O11 |
| 20  | D     | 201 | TGL  | C22-C23-C24-C25 |
| 25  | T     | 103 | CDL  | C12-C13-C14-C15 |
| 19  | C     | 307 | PGV  | C25-C26-C27-C28 |
| 19  | N     | 607 | PGV  | C13-C14-C15-C16 |
| 23  | B     | 304 | PSC  | C14-C15-C16-C17 |
| 26  | G     | 103 | PEK  | C23-C24-C25-C26 |
| 14  | N     | 601 | HEA  | C16-C17-C18-C19 |
| 20  | D     | 201 | TGL  | C13-C14-C29-C30 |
| 23  | O     | 303 | PSC  | C02-C03-O11-P   |
| 25  | P     | 304 | CDL  | CA4-CA3-OA5-PA1 |
| 19  | P     | 303 | PGV  | C28-C29-C30-C31 |
| 26  | C     | 306 | PEK  | C32-C33-C34-C35 |
| 23  | B     | 304 | PSC  | C2-C3-C4-C5     |
| 26  | G     | 103 | PEK  | C30-C31-C32-C33 |
| 19  | A     | 608 | PGV  | O03-C01-C02-C03 |
| 20  | B     | 301 | TGL  | OG1-CG1-CG2-CG3 |
| 23  | B     | 304 | PSC  | O03-C01-C02-C03 |
| 25  | C     | 303 | CDL  | CB3-CB4-CB6-OB8 |
| 25  | T     | 103 | CDL  | CA3-CA4-CA6-OA8 |
| 20  | Q     | 202 | TGL  | C15-C16-C17-C18 |
| 19  | P     | 301 | PGV  | C10-C11-C12-C13 |
| 23  | O     | 303 | PSC  | C11-C10-C9-C8   |
| 26  | G     | 103 | PEK  | C10-C11-C12-C13 |
| 26  | P     | 308 | PEK  | C7-C8-C9-C10    |
| 20  | D     | 201 | TGL  | CB4-CB5-CB6-CB7 |
| 23  | B     | 304 | PSC  | C29-C30-C31-C32 |
| 25  | T     | 103 | CDL  | C55-C56-C57-C58 |
| 28  | J     | 101 | DMU  | C28-C31-C34-C37 |
| 28  | J     | 101 | DMU  | C18-C19-C22-C25 |
| 20  | L     | 101 | TGL  | CC4-CC5-CC6-CC7 |
| 20  | Y     | 101 | TGL  | C11-C12-C13-C14 |
| 25  | T     | 103 | CDL  | C11-C12-C13-C14 |
| 25  | T     | 103 | CDL  | C43-C44-C45-C46 |
| 23  | B     | 304 | PSC  | C9-C10-C11-C12  |
| 23  | O     | 303 | PSC  | C9-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | O     | 303 | PSC  | C10-C11-C12-C13 |
| 26  | C     | 306 | PEK  | C5-C6-C7-C8     |
| 26  | C     | 306 | PEK  | C11-C10-C9-C8   |
| 26  | G     | 101 | PEK  | C9-C10-C11-C12  |
| 26  | G     | 103 | PEK  | C11-C10-C9-C8   |
| 26  | G     | 103 | PEK  | C9-C10-C11-C12  |
| 26  | G     | 103 | PEK  | C12-C13-C14-C15 |
| 26  | P     | 308 | PEK  | C5-C6-C7-C8     |
| 26  | P     | 308 | PEK  | C6-C7-C8-C9     |
| 26  | T     | 101 | PEK  | C11-C10-C9-C8   |
| 26  | T     | 102 | PEK  | C11-C10-C9-C8   |
| 26  | T     | 102 | PEK  | C9-C10-C11-C12  |
| 26  | T     | 102 | PEK  | C12-C13-C14-C15 |
| 25  | G     | 102 | CDL  | CB5-C51-C52-C53 |
| 23  | B     | 304 | PSC  | C3-C4-C5-C6     |
| 25  | T     | 103 | CDL  | C84-C85-C86-C87 |
| 19  | Q     | 201 | PGV  | O01-C02-C03-O11 |
| 25  | C     | 303 | CDL  | OA5-CA3-CA4-OA6 |
| 25  | P     | 304 | CDL  | OA5-CA3-CA4-OA6 |
| 25  | P     | 304 | CDL  | OB5-CB3-CB4-OB6 |
| 25  | T     | 103 | CDL  | OA5-CA3-CA4-OA6 |
| 25  | C     | 303 | CDL  | CB7-C71-C72-C73 |
| 19  | Q     | 201 | PGV  | C5-C6-C7-C8     |
| 19  | A     | 608 | PGV  | C15-C16-C17-C18 |
| 20  | N     | 608 | TGL  | C20-C21-C22-C23 |
| 19  | C     | 307 | PGV  | O03-C01-C02-O01 |
| 20  | B     | 301 | TGL  | OG1-CG1-CG2-OG2 |
| 20  | L     | 101 | TGL  | OG2-CG2-CG3-OG3 |
| 25  | T     | 103 | CDL  | OA6-CA4-CA6-OA8 |
| 26  | G     | 103 | PEK  | O03-C01-C02-O01 |
| 26  | T     | 102 | PEK  | O03-C01-C02-O01 |
| 20  | Q     | 202 | TGL  | C25-C26-C27-C28 |
| 14  | N     | 601 | HEA  | C15-C16-C17-C18 |
| 26  | C     | 306 | PEK  | C29-C30-C31-C32 |
| 22  | J     | 102 | CHD  | C17-C20-C22-C23 |
| 20  | Q     | 202 | TGL  | C20-C21-C22-C23 |
| 25  | T     | 103 | CDL  | C52-C53-C54-C55 |
| 20  | D     | 201 | TGL  | CC3-CC4-CC5-CC6 |
| 26  | T     | 101 | PEK  | C34-C35-C36-C37 |
| 19  | P     | 303 | PGV  | C02-C03-O11-P   |
| 26  | C     | 306 | PEK  | C02-C03-O11-P   |
| 26  | P     | 308 | PEK  | C02-C03-O11-P   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | P     | 301 | PGV  | C31-C32-C33-C34 |
| 20  | D     | 201 | TGL  | CC7-CC8-CC9-C15 |
| 28  | M     | 101 | DMU  | C25-C28-C31-C34 |
| 25  | G     | 102 | CDL  | C71-C72-C73-C74 |
| 19  | A     | 608 | PGV  | C11-C12-C13-C14 |
| 25  | P     | 304 | CDL  | C84-C85-C86-C87 |
| 25  | T     | 103 | CDL  | C14-C15-C16-C17 |
| 25  | P     | 304 | CDL  | C11-CA5-OA6-CA4 |
| 25  | C     | 303 | CDL  | C84-C85-C86-C87 |
| 19  | P     | 303 | PGV  | C22-C23-C24-C25 |
| 26  | C     | 306 | PEK  | C01-C02-C03-O11 |
| 19  | Q     | 201 | PGV  | C7-C8-C9-C10    |
| 20  | B     | 301 | TGL  | C24-C25-C26-C27 |
| 20  | L     | 101 | TGL  | C13-C14-C29-C30 |
| 23  | B     | 304 | PSC  | C23-C24-C25-C26 |
| 25  | C     | 303 | CDL  | C58-C59-C60-C61 |
| 20  | L     | 101 | TGL  | C12-C13-C14-C29 |
| 19  | C     | 307 | PGV  | O04-C19-O03-C01 |
| 19  | P     | 301 | PGV  | C29-C30-C31-C32 |
| 19  | C     | 302 | PGV  | C24-C25-C26-C27 |
| 20  | L     | 101 | TGL  | C10-C11-C12-C13 |
| 26  | C     | 306 | PEK  | C22-C21-O03-C01 |
| 25  | T     | 103 | CDL  | C54-C55-C56-C57 |
| 25  | T     | 103 | CDL  | C60-C61-C62-C63 |
| 26  | G     | 101 | PEK  | C22-C23-C24-C25 |
| 19  | C     | 302 | PGV  | C02-C03-O11-P   |
| 19  | C     | 307 | PGV  | O03-C01-C02-C03 |
| 20  | L     | 101 | TGL  | CG1-CG2-CG3-OG3 |
| 20  | N     | 608 | TGL  | OG1-CG1-CG2-CG3 |
| 20  | Q     | 202 | TGL  | OG1-CG1-CG2-CG3 |
| 25  | T     | 103 | CDL  | CB4-CB3-OB5-PB2 |
| 26  | G     | 103 | PEK  | C3-C4-C5-C6     |
| 25  | G     | 102 | CDL  | OB7-CB5-OB6-CB4 |
| 25  | C     | 303 | CDL  | C77-C78-C79-C80 |
| 25  | P     | 304 | CDL  | C11-C12-C13-C14 |
| 26  | C     | 306 | PEK  | O04-C21-O03-C01 |
| 19  | Q     | 201 | PGV  | O03-C01-C02-O01 |
| 20  | Y     | 101 | TGL  | OG2-CG2-CG3-OG3 |
| 23  | O     | 303 | PSC  | O03-C01-C02-O01 |
| 20  | B     | 301 | TGL  | C18-C19-C33-C34 |
| 25  | T     | 103 | CDL  | C16-C17-C18-C19 |
| 25  | P     | 304 | CDL  | CB4-CB6-OB8-CB7 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | C     | 302 | PGV  | C20-C21-C22-C23 |
| 25  | G     | 102 | CDL  | C64-C65-C66-C67 |
| 25  | P     | 304 | CDL  | C63-C64-C65-C66 |
| 19  | P     | 303 | PGV  | C15-C16-C17-C18 |
| 20  | D     | 201 | TGL  | CB5-CB6-CB7-CB8 |
| 20  | B     | 301 | TGL  | CA4-CA5-CA6-CA7 |
| 26  | C     | 306 | PEK  | C10-C11-C12-C13 |
| 22  | C     | 304 | CHD  | C16-C17-C20-C22 |
| 26  | T     | 101 | PEK  | C17-C18-C19-C20 |
| 26  | C     | 306 | PEK  | C26-C27-C28-C29 |
| 25  | G     | 102 | CDL  | C51-CB5-OB6-CB4 |
| 23  | B     | 304 | PSC  | C15-C16-C17-C18 |
| 20  | N     | 608 | TGL  | C10-C11-C12-C13 |
| 23  | B     | 304 | PSC  | C13-C14-C15-C16 |
| 23  | B     | 304 | PSC  | C04-O12-P-O11   |
| 25  | P     | 304 | CDL  | CA3-OA5-PA1-OA2 |
| 26  | C     | 306 | PEK  | C04-O12-P-O11   |
| 26  | T     | 102 | PEK  | C04-O12-P-O11   |
| 25  | P     | 304 | CDL  | C44-C45-C46-C47 |
| 28  | Z     | 101 | DMU  | C34-C37-C40-C43 |
| 20  | Q     | 202 | TGL  | C16-C17-C18-C19 |
| 19  | A     | 608 | PGV  | C02-C03-O11-P   |
| 25  | T     | 103 | CDL  | CA4-CA3-OA5-PA1 |
| 26  | C     | 306 | PEK  | C23-C24-C25-C26 |
| 19  | C     | 307 | PGV  | C04-O12-P-O14   |
| 19  | Q     | 201 | PGV  | C03-O11-P-O13   |
| 19  | Q     | 201 | PGV  | C04-O12-P-O13   |
| 23  | B     | 304 | PSC  | C03-O11-P-O13   |
| 25  | C     | 303 | CDL  | CB2-OB2-PB2-OB3 |
| 26  | P     | 308 | PEK  | C04-O12-P-O14   |
| 26  | T     | 102 | PEK  | C04-O12-P-O13   |
| 20  | Y     | 101 | TGL  | CB2-CB3-CB4-CB5 |
| 25  | T     | 103 | CDL  | C62-C63-C64-C65 |
| 26  | G     | 101 | PEK  | O12-C04-C05-N   |
| 20  | Y     | 101 | TGL  | C24-C25-C26-C27 |
| 19  | C     | 307 | PGV  | C24-C25-C26-C27 |
| 20  | L     | 101 | TGL  | C20-C21-C22-C23 |
| 20  | Y     | 101 | TGL  | C33-C34-C35-C36 |
| 26  | T     | 102 | PEK  | C7-C8-C9-C10    |
| 19  | Q     | 201 | PGV  | C21-C22-C23-C24 |
| 23  | B     | 304 | PSC  | C05-C04-O12-P   |
| 20  | L     | 101 | TGL  | OG1-CA1-CA2-CA3 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | Y     | 101 | TGL  | C15-C16-C17-C18 |
| 25  | T     | 103 | CDL  | CA7-C31-C32-C33 |
| 20  | Q     | 202 | TGL  | CA3-CA4-CA5-CA6 |
| 19  | A     | 608 | PGV  | O01-C02-C03-O11 |
| 26  | C     | 306 | PEK  | O01-C02-C03-O11 |
| 19  | N     | 607 | PGV  | C31-C32-C33-C34 |
| 25  | C     | 303 | CDL  | C44-C45-C46-C47 |
| 28  | M     | 101 | DMU  | C18-C19-C22-C25 |
| 20  | N     | 608 | TGL  | C29-C30-C31-C32 |
| 20  | N     | 608 | TGL  | CA5-CA6-CA7-CA8 |
| 19  | C     | 307 | PGV  | C27-C28-C29-C30 |
| 20  | D     | 201 | TGL  | C24-C25-C26-C27 |
| 25  | G     | 102 | CDL  | C31-C32-C33-C34 |
| 20  | D     | 201 | TGL  | OG1-CG1-CG2-CG3 |
| 20  | Q     | 202 | TGL  | CC3-CC4-CC5-CC6 |
| 23  | O     | 303 | PSC  | O12-C04-C05-N   |
| 26  | G     | 103 | PEK  | O03-C01-C02-C03 |
| 26  | T     | 102 | PEK  | O03-C01-C02-C03 |
| 20  | Q     | 202 | TGL  | OG2-CG2-CG3-OG3 |
| 23  | B     | 304 | PSC  | O03-C01-C02-O01 |
| 20  | D     | 201 | TGL  | C18-C19-C33-C34 |
| 20  | Q     | 202 | TGL  | CA4-CA5-CA6-CA7 |
| 25  | C     | 303 | CDL  | C17-C18-C19-C20 |
| 25  | T     | 103 | CDL  | C82-C83-C84-C85 |
| 25  | C     | 303 | CDL  | C20-C21-C22-C23 |
| 28  | Z     | 101 | DMU  | C28-C31-C34-C37 |
| 25  | T     | 103 | CDL  | C58-C59-C60-C61 |
| 25  | C     | 303 | CDL  | C19-C20-C21-C22 |
| 25  | C     | 303 | CDL  | C51-C52-C53-C54 |
| 26  | C     | 306 | PEK  | C28-C29-C30-C31 |
| 20  | Y     | 101 | TGL  | OG1-CA1-CA2-CA3 |
| 26  | P     | 308 | PEK  | O04-C21-O03-C01 |
| 20  | Y     | 101 | TGL  | OG2-CB1-CB2-CB3 |
| 25  | T     | 103 | CDL  | C35-C36-C37-C38 |
| 19  | C     | 307 | PGV  | C15-C16-C17-C18 |
| 20  | D     | 201 | TGL  | OB1-CB1-OG2-CG2 |
| 19  | A     | 608 | PGV  | C14-C15-C16-C17 |
| 25  | C     | 303 | CDL  | C22-C23-C24-C25 |
| 25  | P     | 304 | CDL  | C18-C19-C20-C21 |
| 25  | C     | 303 | CDL  | C78-C79-C80-C81 |
| 19  | P     | 301 | PGV  | C21-C22-C23-C24 |
| 23  | O     | 303 | PSC  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | G     | 102 | CDL  | C37-C38-C39-C40 |
| 25  | P     | 304 | CDL  | C22-C23-C24-C25 |
| 26  | G     | 101 | PEK  | C17-C18-C19-C20 |
| 26  | P     | 308 | PEK  | C3-C4-C5-C6     |
| 25  | G     | 102 | CDL  | OA6-CA4-CA6-OA8 |
| 25  | P     | 304 | CDL  | OA6-CA4-CA6-OA8 |
| 19  | P     | 301 | PGV  | C03-O11-P-O12   |
| 19  | P     | 301 | PGV  | C04-O12-P-O11   |
| 23  | O     | 303 | PSC  | C04-O12-P-O11   |
| 25  | C     | 303 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | C     | 303 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | G     | 102 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | J     | 101 | DMU  | O1-C10-O7-C3    |
| 20  | N     | 608 | TGL  | C14-C29-C30-C31 |
| 20  | D     | 201 | TGL  | C21-C20-CA9-CA8 |
| 20  | Y     | 101 | TGL  | CG1-CG2-CG3-OG3 |
| 25  | P     | 304 | CDL  | CB3-CB4-CB6-OB8 |
| 19  | C     | 307 | PGV  | C13-C14-C15-C16 |
| 20  | L     | 101 | TGL  | CB5-CB6-CB7-CB8 |
| 22  | W     | 101 | CHD  | C21-C20-C22-C23 |
| 19  | C     | 302 | PGV  | C12-C13-C14-C15 |
| 19  | P     | 303 | PGV  | C05-C04-O12-P   |
| 25  | C     | 303 | CDL  | C13-C14-C15-C16 |
| 25  | C     | 303 | CDL  | OB9-CB7-OB8-CB6 |
| 25  | P     | 304 | CDL  | CA2-C1-CB2-OB2  |
| 20  | Q     | 202 | TGL  | OG2-CB1-CB2-CB3 |
| 26  | P     | 308 | PEK  | C22-C21-O03-C01 |
| 22  | C     | 304 | CHD  | C21-C20-C22-C23 |
| 25  | P     | 304 | CDL  | C53-C54-C55-C56 |
| 26  | G     | 103 | PEK  | C13-C14-C15-C16 |
| 26  | T     | 101 | PEK  | O03-C21-C22-C23 |
| 20  | B     | 301 | TGL  | CA2-CA3-CA4-CA5 |
| 22  | P     | 307 | CHD  | C16-C17-C20-C22 |
| 19  | A     | 608 | PGV  | C13-C14-C15-C16 |
| 19  | Q     | 201 | PGV  | C15-C16-C17-C18 |
| 28  | M     | 101 | DMU  | C28-C31-C34-C37 |
| 20  | L     | 101 | TGL  | C11-C10-CB9-CB8 |
| 26  | G     | 103 | PEK  | C27-C28-C29-C30 |
| 22  | C     | 304 | CHD  | C22-C23-C24-O25 |
| 20  | N     | 608 | TGL  | C33-C34-C35-C36 |
| 22  | B     | 303 | CHD  | C22-C23-C24-O25 |
| 22  | O     | 302 | CHD  | C22-C23-C24-O25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | N     | 608 | TGL  | CB3-CB4-CB5-CB6 |
| 20  | N     | 608 | TGL  | C21-C22-C23-C24 |
| 19  | C     | 302 | PGV  | C05-C04-O12-P   |
| 26  | G     | 103 | PEK  | C29-C30-C31-C32 |
| 22  | C     | 304 | CHD  | C22-C23-C24-O26 |
| 20  | Y     | 101 | TGL  | C16-C17-C18-C19 |
| 26  | P     | 308 | PEK  | C22-C23-C24-C25 |
| 22  | B     | 303 | CHD  | C22-C23-C24-O26 |
| 20  | L     | 101 | TGL  | C24-C25-C26-C27 |
| 25  | T     | 103 | CDL  | C59-C60-C61-C62 |
| 20  | L     | 101 | TGL  | C23-C24-C25-C26 |
| 14  | A     | 602 | HEA  | CAA-CBA-CGA-O1A |
| 22  | J     | 102 | CHD  | C22-C23-C24-O25 |
| 22  | W     | 101 | CHD  | C22-C23-C24-O25 |
| 25  | P     | 304 | CDL  | C81-C82-C83-C84 |
| 25  | C     | 303 | CDL  | O1-C1-CB2-OB2   |
| 14  | N     | 601 | HEA  | CAD-CBD-CGD-O1D |
| 20  | D     | 201 | TGL  | CC4-CC5-CC6-CC7 |
| 25  | C     | 303 | CDL  | CA7-C31-C32-C33 |
| 20  | N     | 608 | TGL  | CA7-CA8-CA9-C20 |
| 22  | J     | 102 | CHD  | C22-C23-C24-O26 |
| 26  | T     | 101 | PEK  | O02-C1-O01-C02  |
| 23  | O     | 303 | PSC  | C12-C13-C14-C15 |
| 14  | A     | 601 | HEA  | CAD-CBD-CGD-O2D |
| 14  | N     | 601 | HEA  | CAD-CBD-CGD-O2D |
| 14  | N     | 602 | HEA  | CAA-CBA-CGA-O2A |
| 25  | T     | 103 | CDL  | C19-C20-C21-C22 |
| 26  | P     | 308 | PEK  | C11-C10-C9-C8   |
| 26  | P     | 308 | PEK  | C9-C10-C11-C12  |
| 26  | T     | 102 | PEK  | C11-C12-C13-C14 |
| 20  | N     | 608 | TGL  | CB2-CB3-CB4-CB5 |
| 20  | L     | 101 | TGL  | CA4-CA5-CA6-CA7 |
| 25  | P     | 304 | CDL  | C1-CA2-OA2-PA1  |
| 19  | P     | 301 | PGV  | O01-C02-C03-O11 |
| 26  | G     | 101 | PEK  | C13-C14-C15-C16 |
| 26  | T     | 101 | PEK  | C35-C36-C37-C38 |
| 19  | P     | 301 | PGV  | C01-C02-C03-O11 |
| 25  | T     | 103 | CDL  | OA5-CA3-CA4-CA6 |
| 19  | C     | 302 | PGV  | C11-C12-C13-C14 |
| 20  | B     | 301 | TGL  | C16-C15-CC9-CC8 |
| 25  | T     | 103 | CDL  | C80-C81-C82-C83 |
| 14  | A     | 602 | HEA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | O     | 302 | CHD  | C22-C23-C24-O26 |
| 20  | Y     | 101 | TGL  | CC1-CC2-CC3-CC4 |
| 26  | G     | 101 | PEK  | C27-C28-C29-C30 |
| 14  | N     | 602 | HEA  | CAD-CBD-CGD-O2D |
| 19  | P     | 303 | PGV  | C31-C32-C33-C34 |
| 25  | G     | 102 | CDL  | CA7-C31-C32-C33 |
| 20  | D     | 201 | TGL  | C19-C33-C34-C35 |
| 26  | C     | 306 | PEK  | C13-C14-C15-C16 |
| 25  | C     | 303 | CDL  | C60-C61-C62-C63 |
| 25  | T     | 103 | CDL  | C24-C25-C26-C27 |
| 25  | C     | 303 | CDL  | C71-CB7-OB8-CB6 |
| 19  | Q     | 201 | PGV  | C28-C29-C30-C31 |
| 26  | T     | 102 | PEK  | C3-C4-C5-C6     |
| 19  | C     | 302 | PGV  | C13-C14-C15-C16 |
| 19  | C     | 307 | PGV  | C31-C32-C33-C34 |
| 19  | A     | 607 | PGV  | C26-C27-C28-C29 |
| 19  | P     | 301 | PGV  | C25-C26-C27-C28 |
| 26  | C     | 306 | PEK  | C33-C34-C35-C36 |
| 14  | A     | 601 | HEA  | CAD-CBD-CGD-O1D |
| 25  | P     | 304 | CDL  | C21-C22-C23-C24 |
| 25  | G     | 102 | CDL  | C62-C63-C64-C65 |
| 19  | A     | 608 | PGV  | C9-C10-C11-C12  |
| 22  | C     | 304 | CHD  | C17-C20-C22-C23 |
| 14  | N     | 602 | HEA  | CAD-CBD-CGD-O1D |
| 14  | A     | 602 | HEA  | CAD-CBD-CGD-O1D |
| 20  | Y     | 101 | TGL  | CB4-CB5-CB6-CB7 |
| 19  | C     | 307 | PGV  | O05-C05-C06-O06 |
| 20  | Y     | 101 | TGL  | OB1-CB1-CB2-CB3 |
| 14  | A     | 602 | HEA  | CAD-CBD-CGD-O2D |
| 20  | B     | 301 | TGL  | C11-C10-CB9-CB8 |
| 20  | Q     | 202 | TGL  | OG3-CC1-CC2-CC3 |
| 19  | C     | 307 | PGV  | C4-C5-C6-C7     |
| 20  | D     | 201 | TGL  | C10-C11-C12-C13 |
| 25  | T     | 103 | CDL  | C40-C41-C42-C43 |
| 25  | P     | 304 | CDL  | C62-C63-C64-C65 |
| 26  | T     | 102 | PEK  | O03-C21-C22-C23 |
| 20  | Y     | 101 | TGL  | C21-C22-C23-C24 |
| 23  | B     | 304 | PSC  | C25-C26-C27-C28 |
| 19  | P     | 301 | PGV  | C11-C12-C13-C14 |
| 26  | C     | 306 | PEK  | C3-C4-C5-C6     |
| 20  | Y     | 101 | TGL  | C17-C18-C19-C33 |
| 14  | N     | 602 | HEA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | P     | 304 | CDL  | C71-C72-C73-C74 |
| 20  | N     | 608 | TGL  | CB1-CB2-CB3-CB4 |
| 19  | C     | 302 | PGV  | C28-C29-C30-C31 |
| 19  | A     | 607 | PGV  | O03-C19-C20-C21 |
| 26  | C     | 306 | PEK  | O01-C1-C2-C3    |
| 19  | A     | 607 | PGV  | C11-C12-C13-C14 |
| 19  | A     | 607 | PGV  | C11-C10-C9-C8   |
| 20  | Y     | 101 | TGL  | C12-C13-C14-C29 |
| 22  | P     | 305 | CHD  | C22-C23-C24-O25 |
| 26  | T     | 101 | PEK  | O01-C1-C2-C3    |
| 20  | L     | 101 | TGL  | CA6-CA7-CA8-CA9 |
| 22  | C     | 305 | CHD  | C22-C23-C24-O25 |
| 25  | G     | 102 | CDL  | C61-C62-C63-C64 |
| 26  | P     | 308 | PEK  | C29-C30-C31-C32 |
| 22  | P     | 307 | CHD  | C22-C23-C24-O25 |
| 22  | P     | 307 | CHD  | C22-C23-C24-O26 |
| 20  | Q     | 202 | TGL  | CC4-CC5-CC6-CC7 |
| 20  | Y     | 101 | TGL  | C29-C30-C31-C32 |
| 20  | B     | 301 | TGL  | OG1-CA1-CA2-CA3 |
| 19  | Q     | 201 | PGV  | C20-C21-C22-C23 |
| 22  | W     | 101 | CHD  | C22-C23-C24-O26 |
| 20  | B     | 301 | TGL  | OG3-CC1-CC2-CC3 |
| 20  | Q     | 202 | TGL  | CB6-CB7-CB8-CB9 |
| 19  | P     | 301 | PGV  | O05-C05-C06-O06 |
| 26  | T     | 102 | PEK  | C26-C27-C28-C29 |
| 14  | N     | 601 | HEA  | CAA-CBA-CGA-O2A |
| 22  | C     | 305 | CHD  | C22-C23-C24-O26 |
| 22  | P     | 305 | CHD  | C22-C23-C24-O26 |
| 20  | L     | 101 | TGL  | CC9-C15-C16-C17 |
| 25  | C     | 303 | CDL  | C21-C22-C23-C24 |
| 19  | N     | 607 | PGV  | C12-C13-C14-C15 |
| 26  | T     | 102 | PEK  | O04-C21-C22-C23 |
| 26  | T     | 101 | PEK  | C23-C24-C25-C26 |
| 26  | C     | 306 | PEK  | O02-C1-C2-C3    |
| 25  | C     | 303 | CDL  | C62-C63-C64-C65 |
| 19  | N     | 607 | PGV  | C11-C12-C13-C14 |
| 20  | B     | 301 | TGL  | OA1-CA1-CA2-CA3 |
| 20  | Q     | 202 | TGL  | OC1-CC1-CC2-CC3 |
| 25  | C     | 303 | CDL  | C74-C75-C76-C77 |
| 20  | L     | 101 | TGL  | OG1-CG1-CG2-CG3 |
| 20  | N     | 608 | TGL  | CG1-CG2-CG3-OG3 |
| 19  | N     | 607 | PGV  | O03-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 607 | PGV  | C27-C28-C29-C30 |
| 25  | P     | 304 | CDL  | C82-C83-C84-C85 |
| 19  | C     | 307 | PGV  | C03-O11-P-O14   |
| 25  | G     | 102 | CDL  | CA3-OA5-PA1-OA3 |
| 25  | T     | 103 | CDL  | CA3-OA5-PA1-OA3 |
| 26  | C     | 306 | PEK  | C03-O11-P-O13   |
| 26  | G     | 103 | PEK  | C03-O11-P-O13   |
| 26  | T     | 102 | PEK  | C03-O11-P-O14   |
| 20  | N     | 608 | TGL  | C18-C19-C33-C34 |
| 25  | G     | 102 | CDL  | C18-C19-C20-C21 |
| 26  | T     | 101 | PEK  | O12-C04-C05-N   |
| 25  | C     | 303 | CDL  | C59-C60-C61-C62 |
| 20  | L     | 101 | TGL  | OG2-CB1-CB2-CB3 |
| 25  | C     | 303 | CDL  | C11-C12-C13-C14 |
| 23  | B     | 304 | PSC  | C12-C13-C14-C15 |
| 19  | A     | 608 | PGV  | C24-C25-C26-C27 |
| 20  | Q     | 202 | TGL  | CC6-CC7-CC8-CC9 |
| 20  | N     | 608 | TGL  | CA6-CA7-CA8-CA9 |
| 14  | A     | 601 | HEA  | CAA-CBA-CGA-O2A |
| 19  | N     | 607 | PGV  | C24-C25-C26-C27 |
| 26  | C     | 306 | PEK  | C27-C28-C29-C30 |
| 26  | T     | 102 | PEK  | C21-C22-C23-C24 |
| 20  | B     | 301 | TGL  | OC1-CC1-CC2-CC3 |
| 26  | T     | 101 | PEK  | O02-C1-C2-C3    |
| 28  | J     | 101 | DMU  | C22-C25-C28-C31 |
| 26  | T     | 101 | PEK  | C3-C4-C5-C6     |

There are no ring outliers.

40 monomers are involved in 370 short contacts:

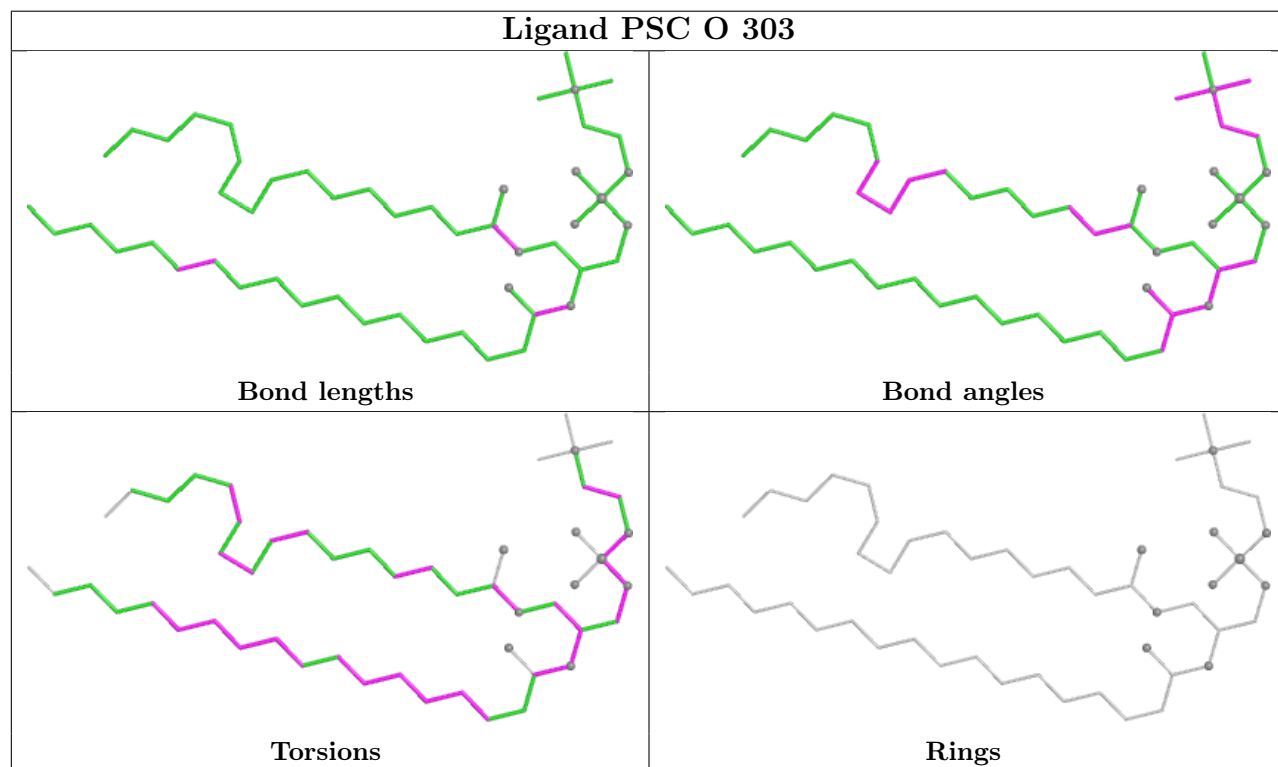
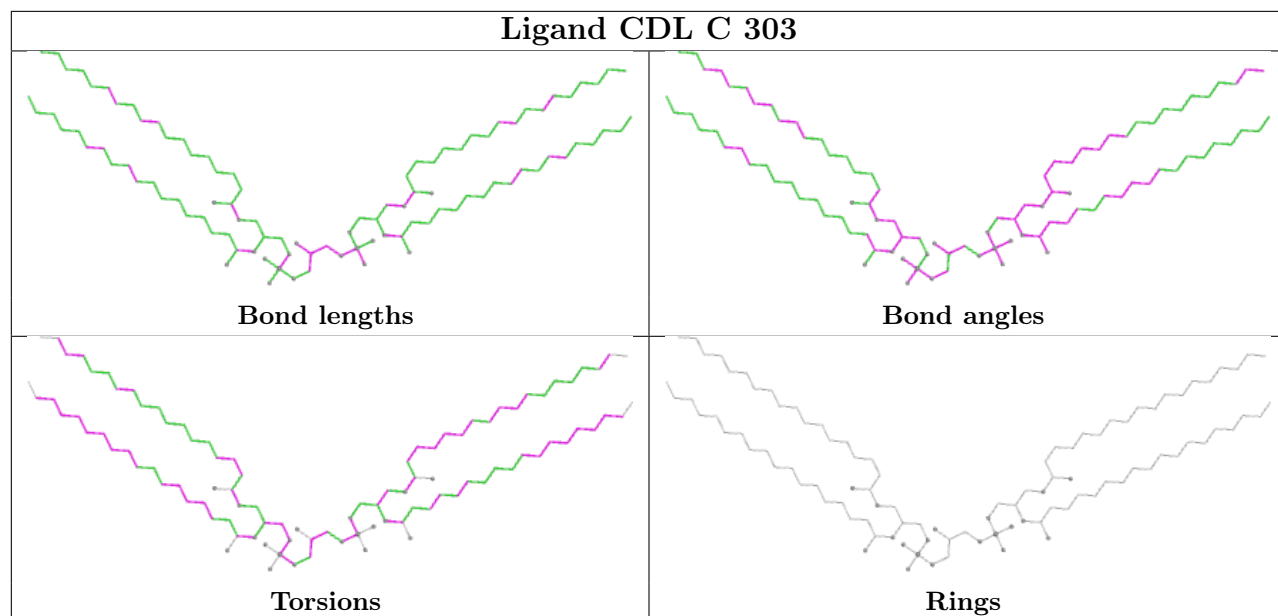
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | C     | 303 | CDL  | 26      | 0            |
| 23  | O     | 303 | PSC  | 19      | 0            |
| 26  | T     | 101 | PEK  | 8       | 0            |
| 28  | P     | 306 | DMU  | 10      | 0            |
| 22  | P     | 307 | CHD  | 1       | 0            |
| 14  | A     | 601 | HEA  | 6       | 0            |
| 22  | C     | 305 | CHD  | 1       | 0            |
| 26  | G     | 101 | PEK  | 7       | 0            |
| 19  | P     | 301 | PGV  | 3       | 0            |
| 20  | N     | 608 | TGL  | 6       | 0            |
| 26  | P     | 308 | PEK  | 14      | 0            |

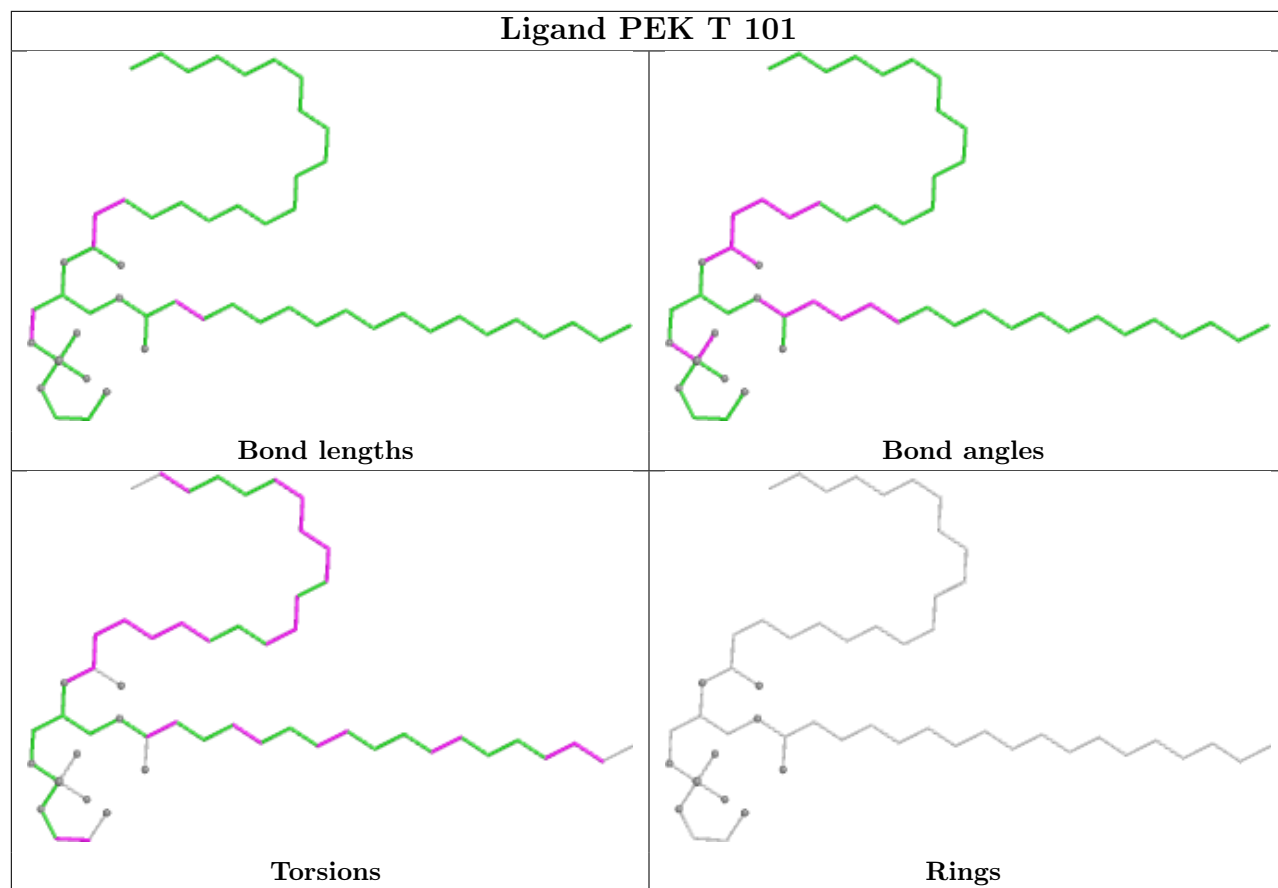
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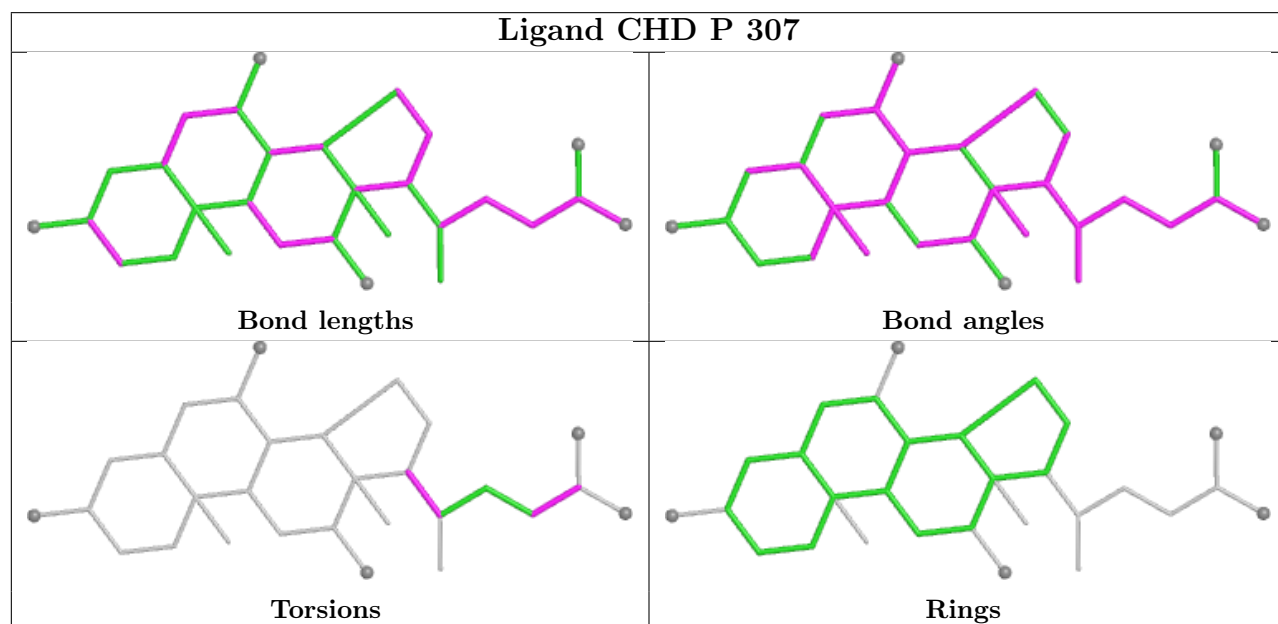
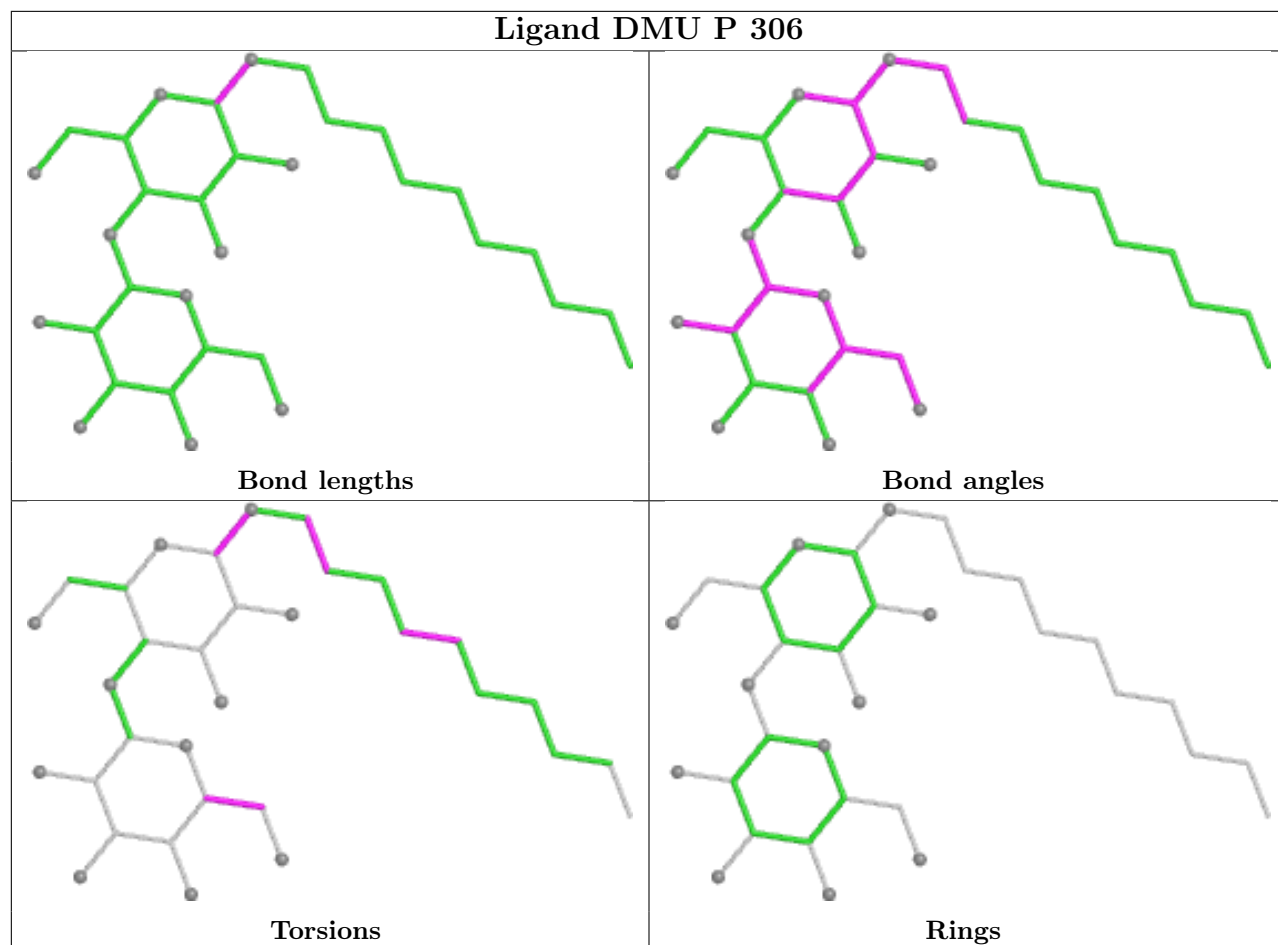
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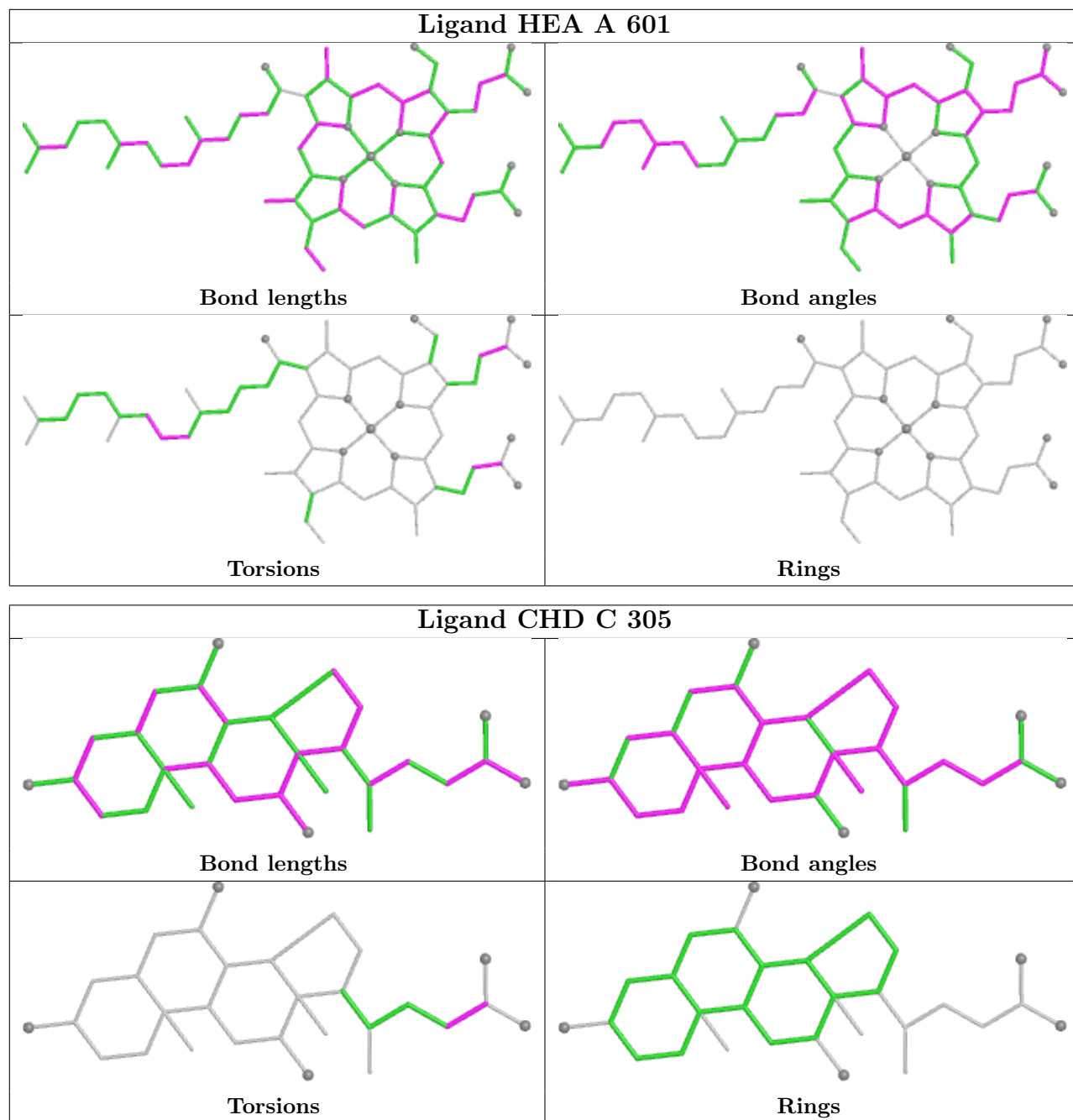
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 20  | L     | 101 | TGL  | 19      | 0            |
| 19  | A     | 608 | PGV  | 7       | 0            |
| 25  | P     | 304 | CDL  | 24      | 0            |
| 26  | T     | 102 | PEK  | 10      | 0            |
| 23  | B     | 304 | PSC  | 13      | 0            |
| 19  | C     | 307 | PGV  | 1       | 0            |
| 22  | W     | 101 | CHD  | 6       | 0            |
| 28  | J     | 101 | DMU  | 5       | 0            |
| 18  | A     | 606 | PER  | 1       | 0            |
| 19  | A     | 607 | PGV  | 4       | 0            |
| 20  | Q     | 202 | TGL  | 15      | 0            |
| 20  | D     | 201 | TGL  | 21      | 0            |
| 26  | C     | 306 | PEK  | 13      | 0            |
| 20  | Y     | 101 | TGL  | 23      | 0            |
| 14  | N     | 602 | HEA  | 1       | 0            |
| 14  | N     | 601 | HEA  | 11      | 0            |
| 19  | Q     | 201 | PGV  | 11      | 0            |
| 25  | T     | 103 | CDL  | 28      | 0            |
| 26  | G     | 103 | PEK  | 9       | 0            |
| 14  | A     | 602 | HEA  | 1       | 0            |
| 19  | C     | 302 | PGV  | 8       | 0            |
| 22  | P     | 305 | CHD  | 6       | 0            |
| 22  | J     | 102 | CHD  | 6       | 0            |
| 18  | N     | 606 | PER  | 1       | 0            |
| 25  | G     | 102 | CDL  | 37      | 0            |
| 19  | P     | 303 | PGV  | 7       | 0            |
| 20  | B     | 301 | TGL  | 3       | 0            |
| 22  | C     | 304 | CHD  | 2       | 0            |
| 19  | N     | 607 | PGV  | 1       | 0            |

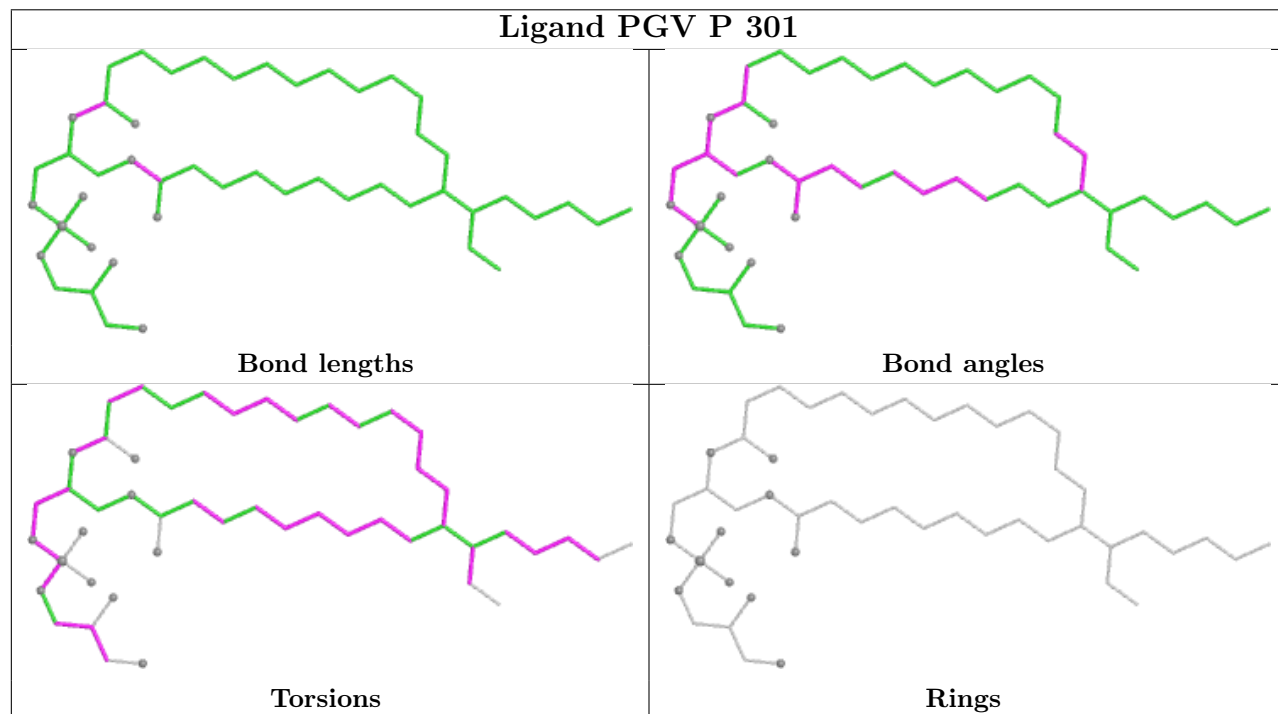
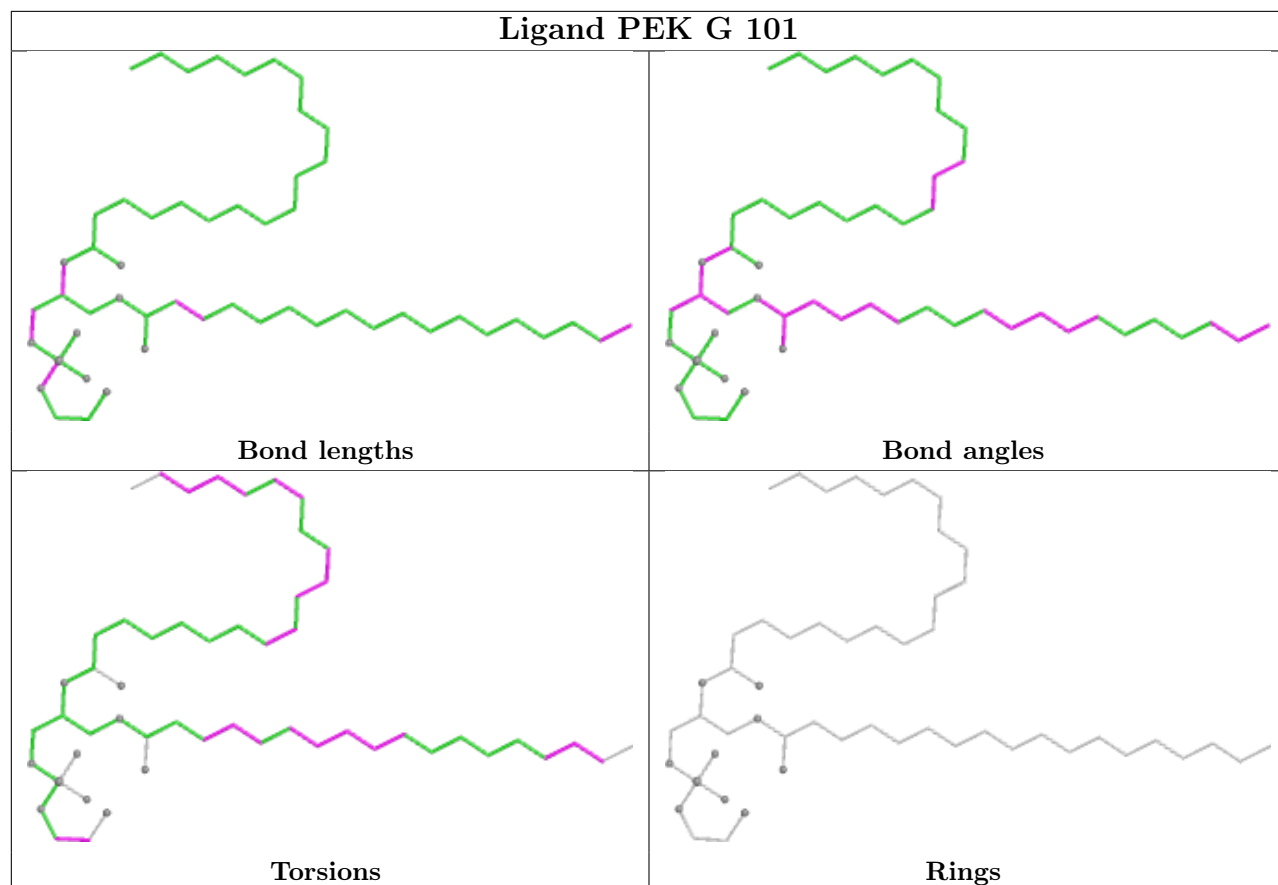
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

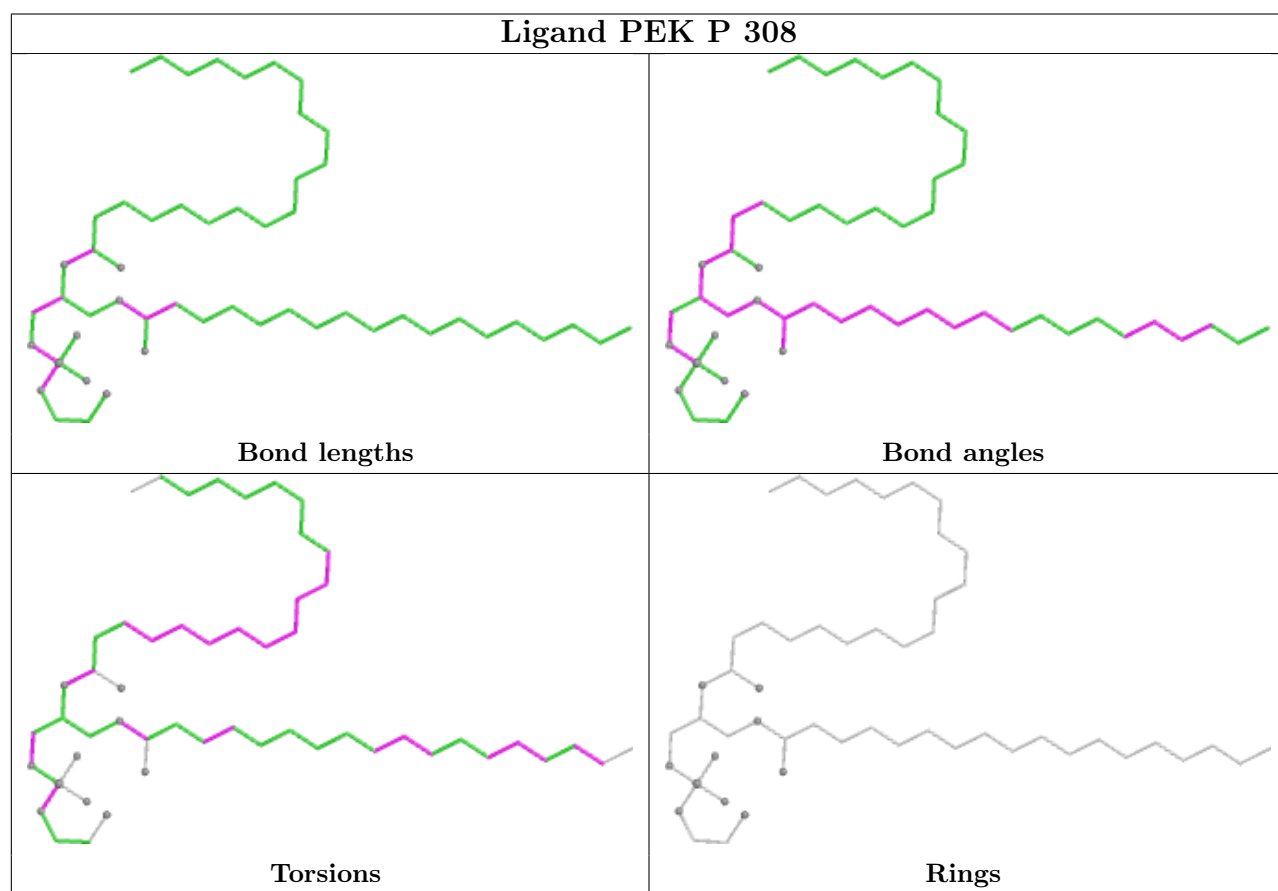
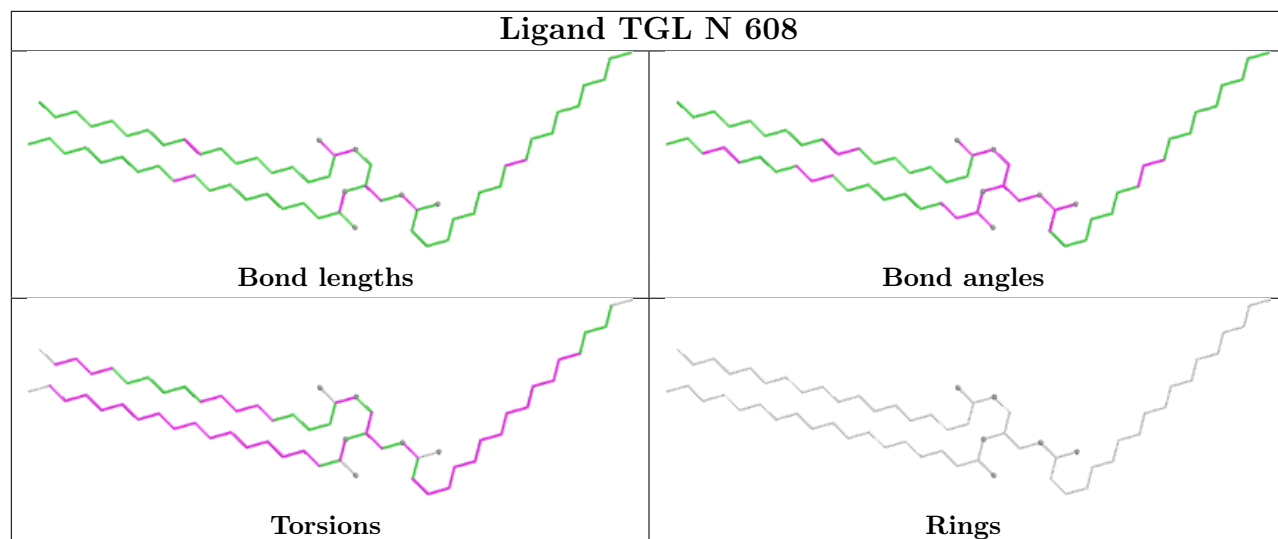


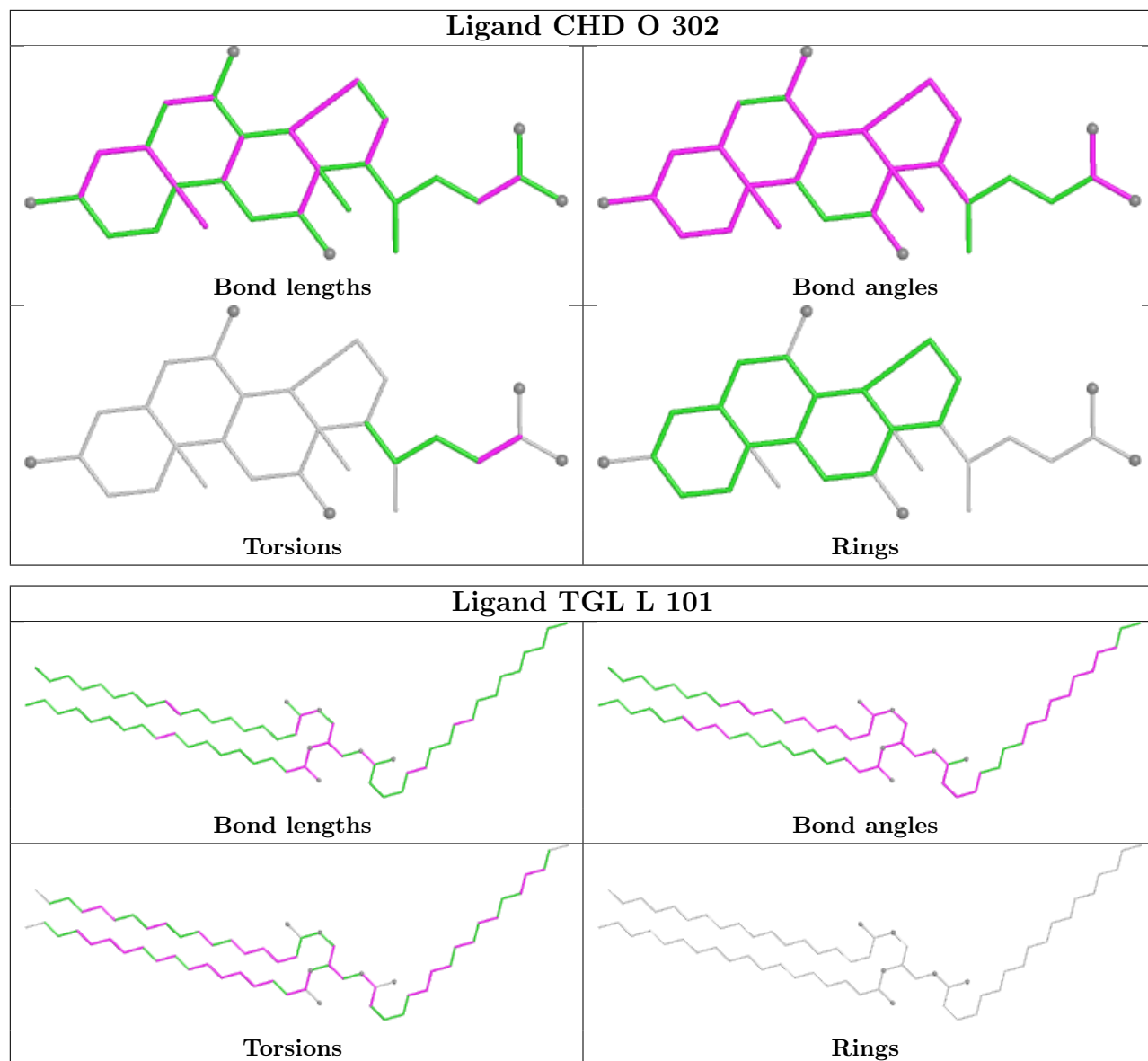


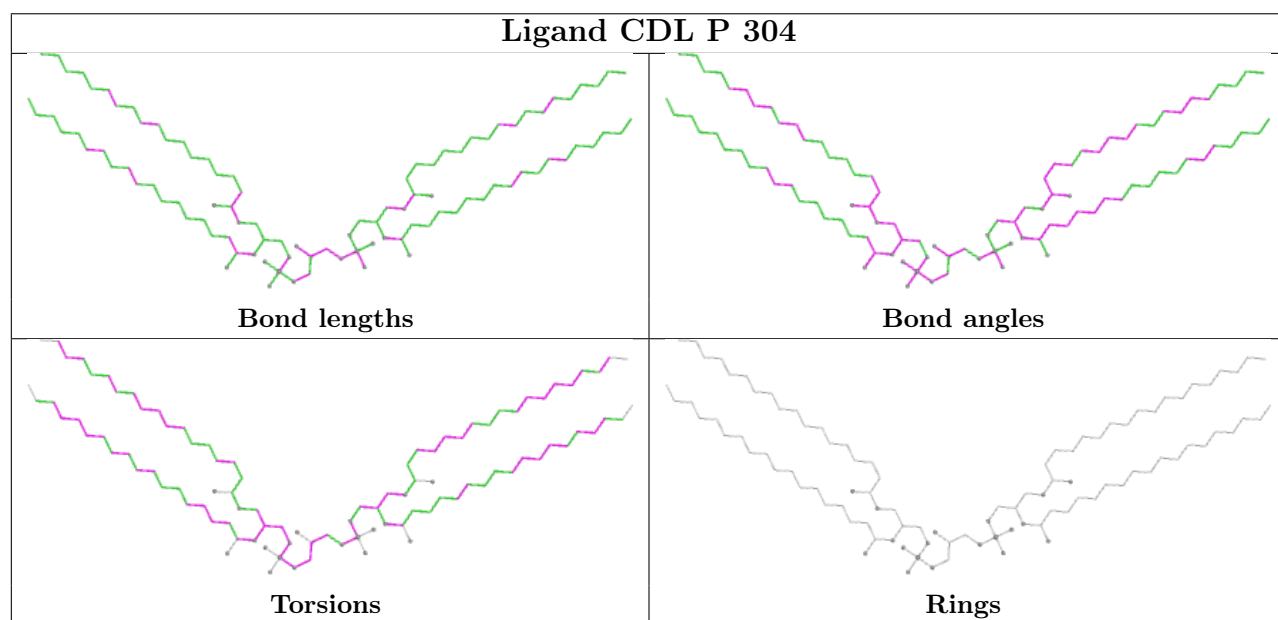
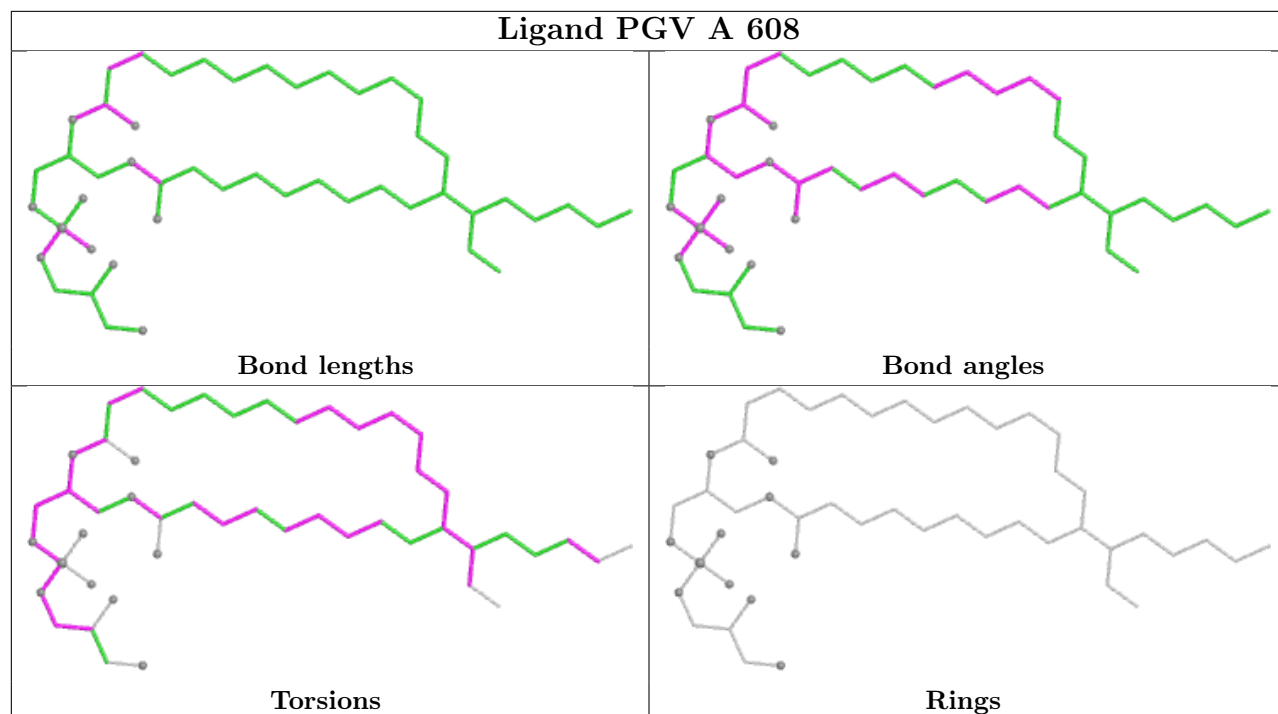




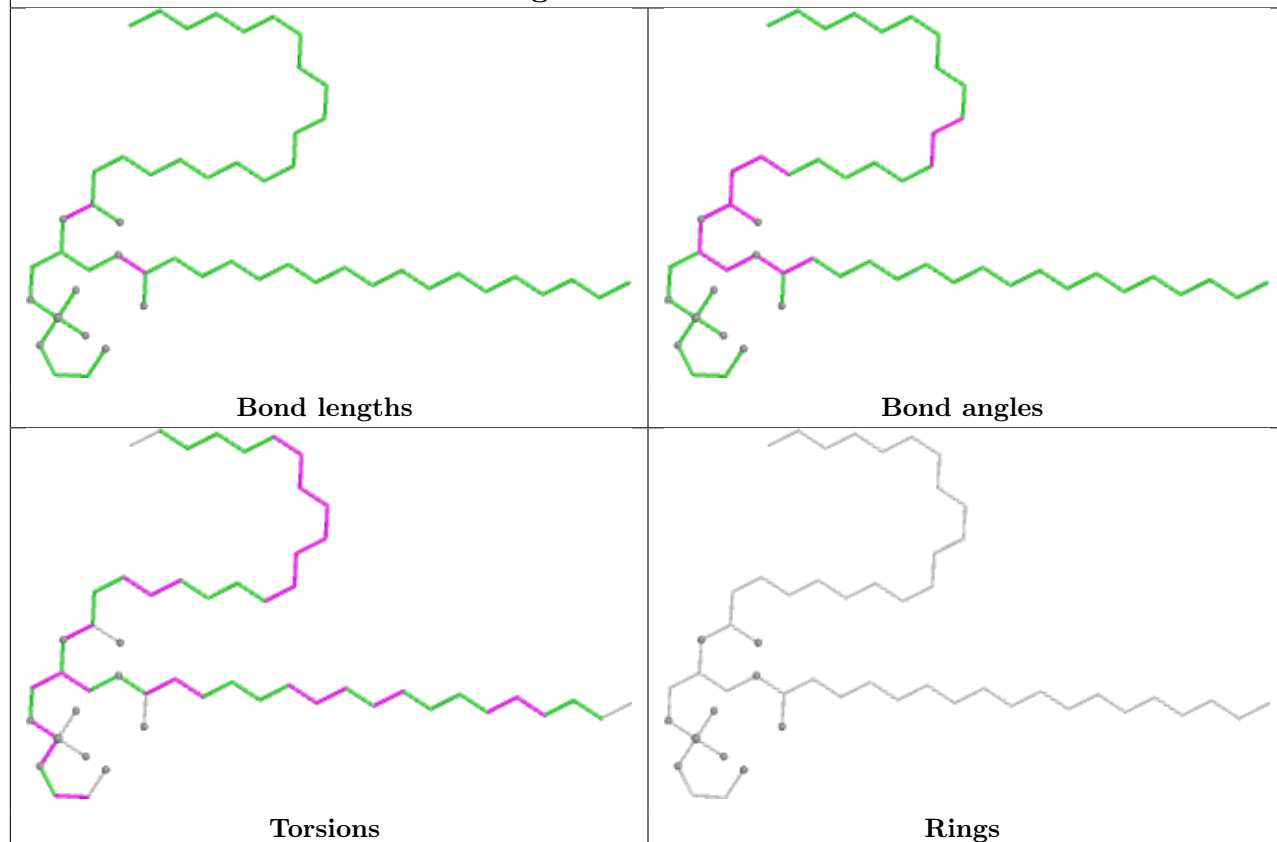




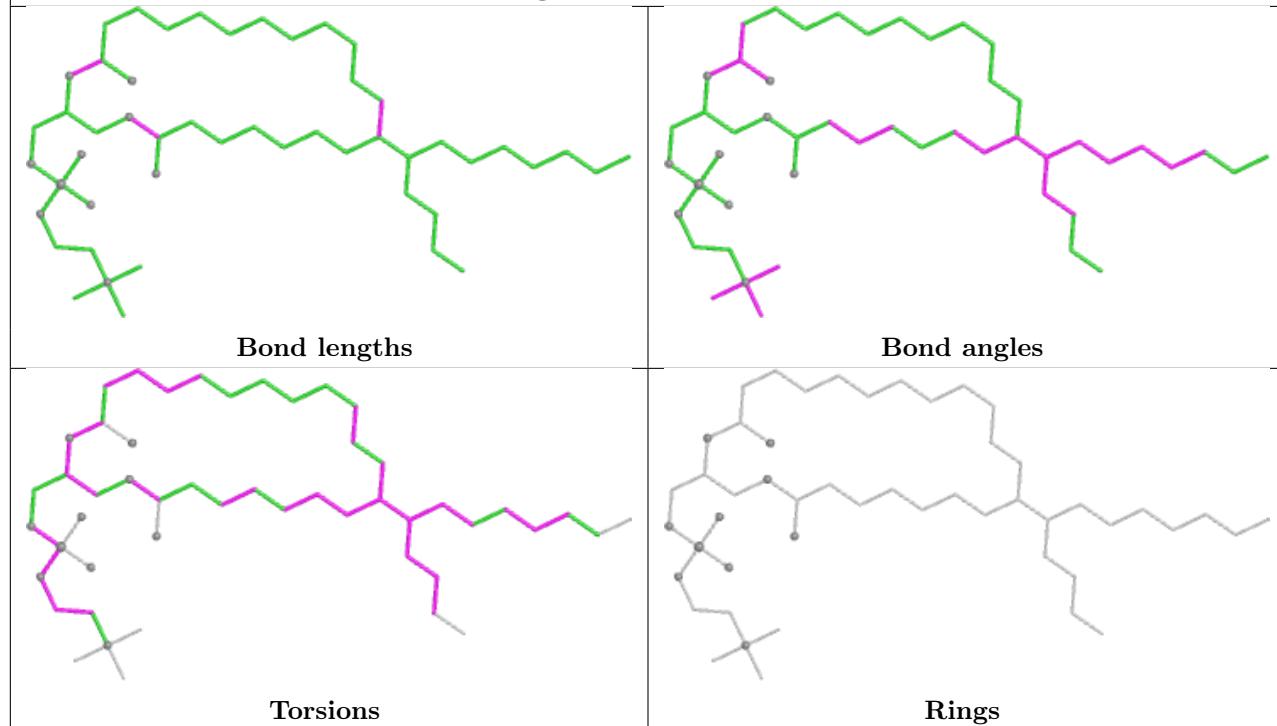


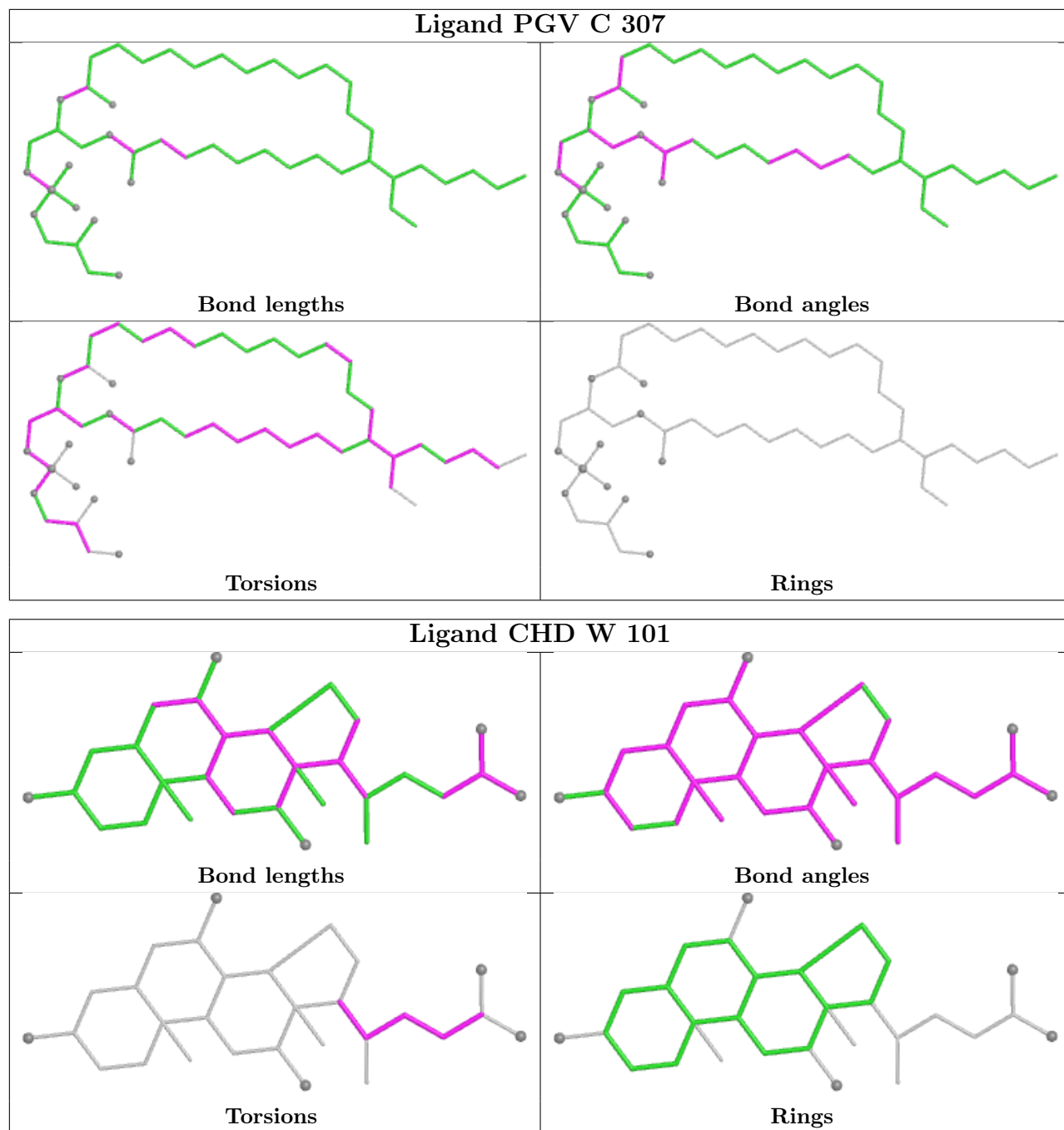


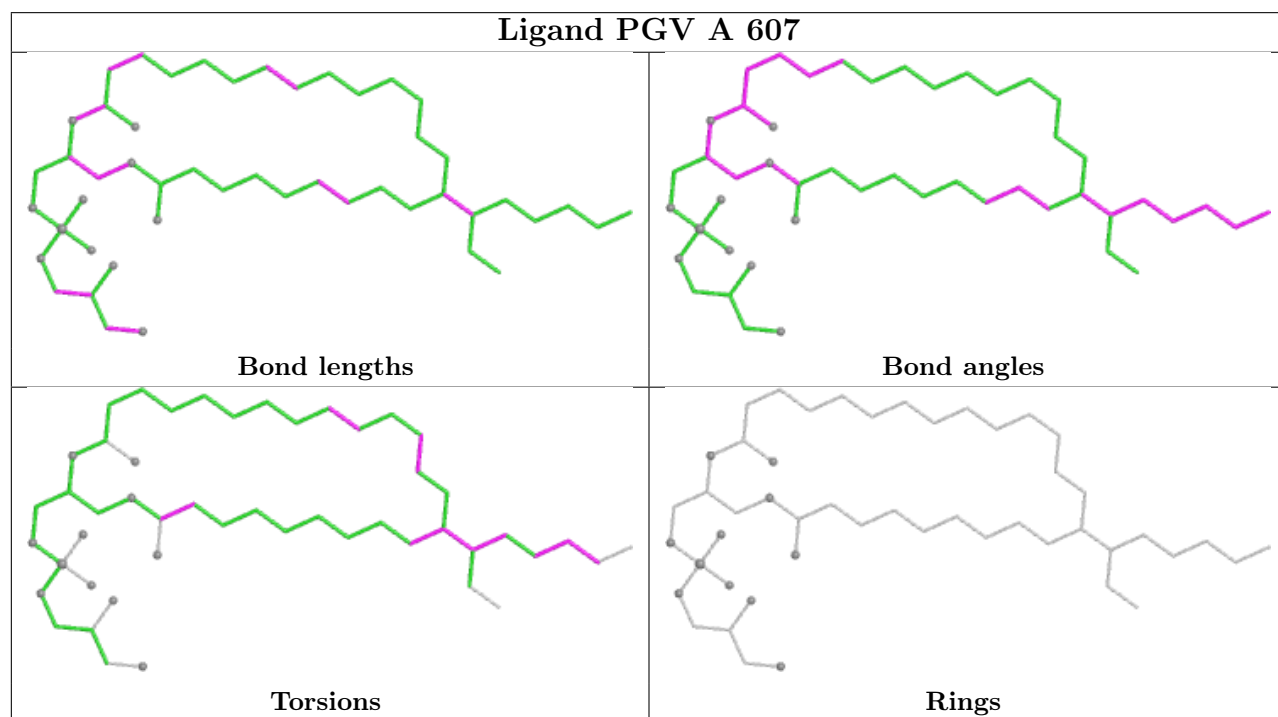
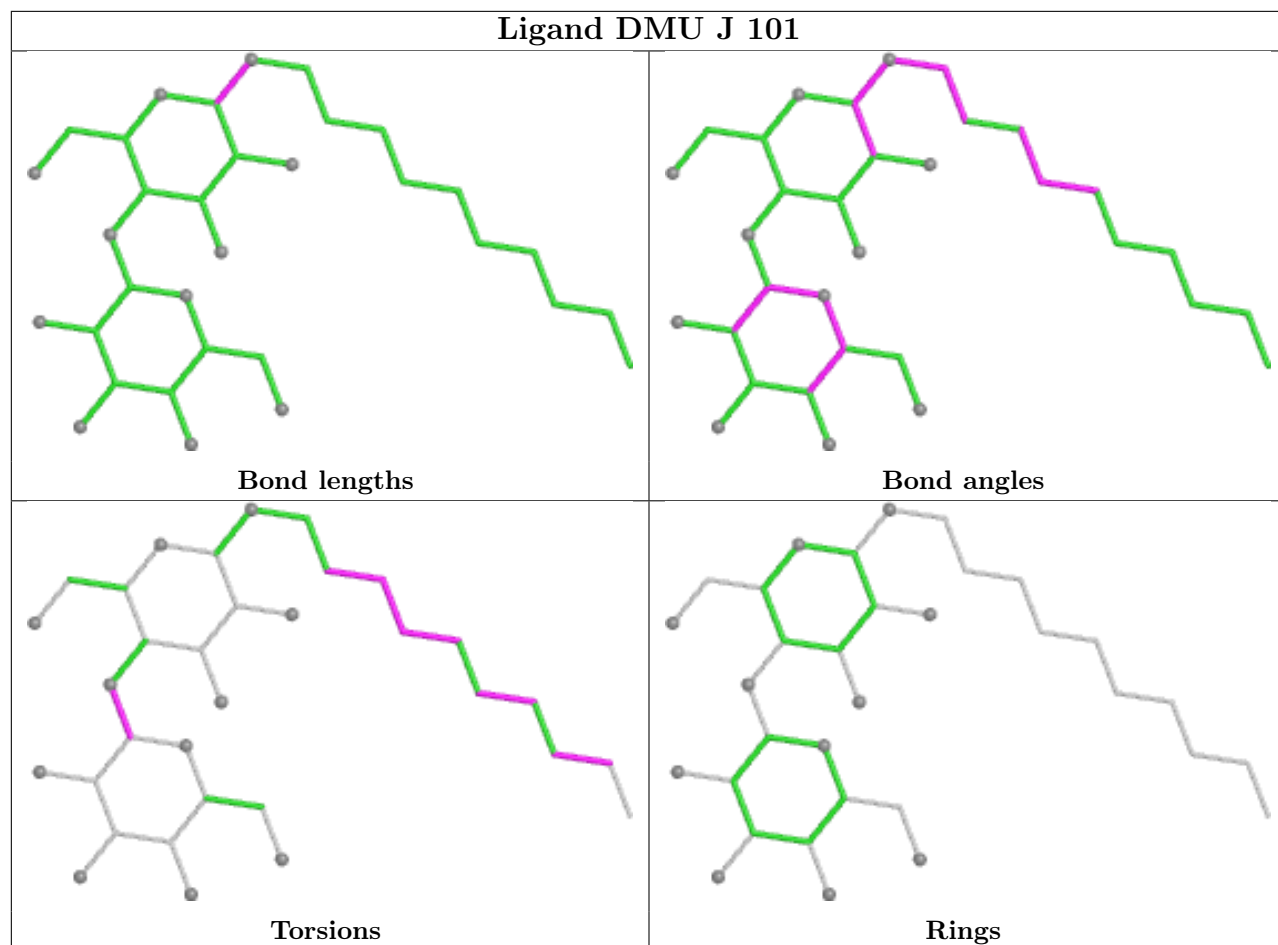
## Ligand PEK T 102

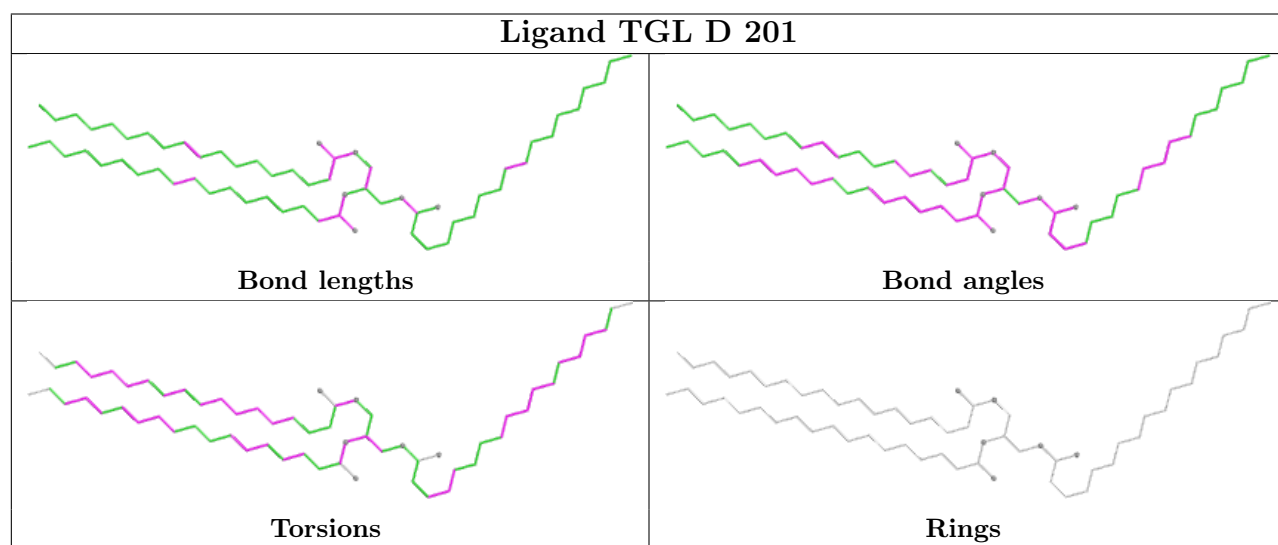
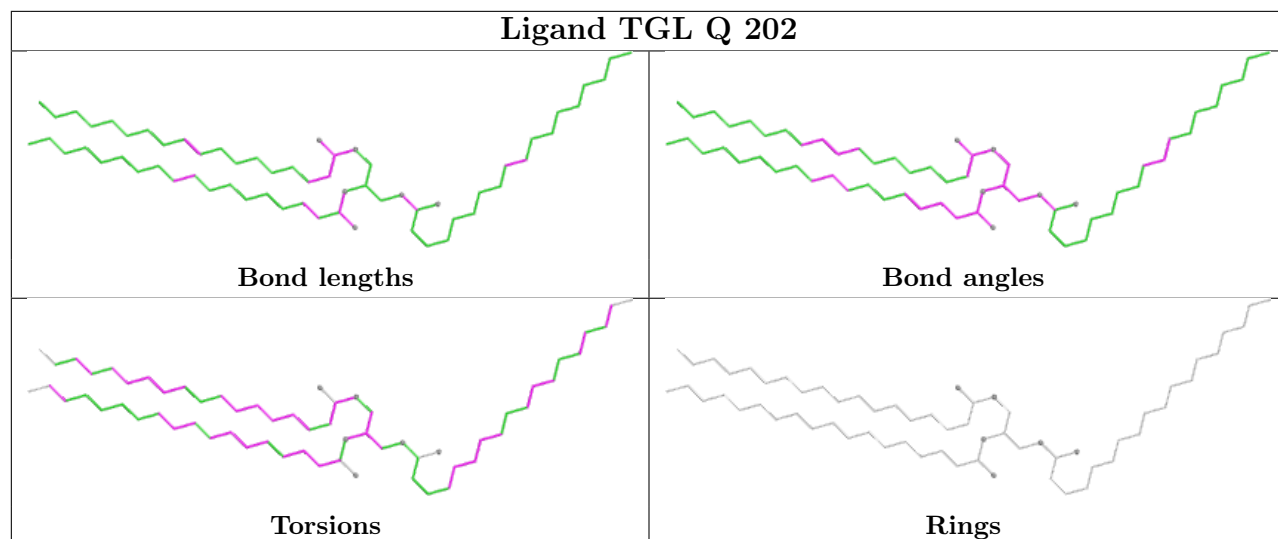


## Ligand PSC B 304

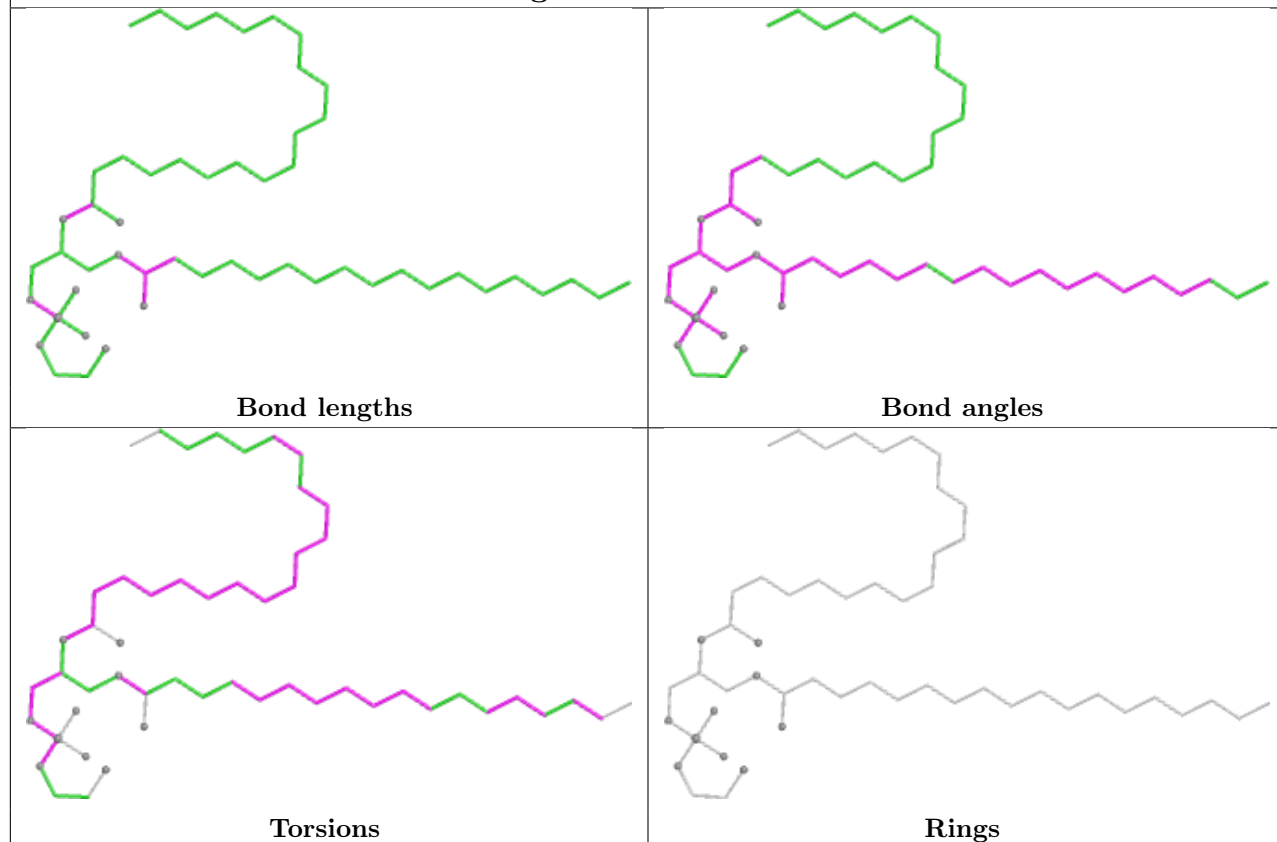




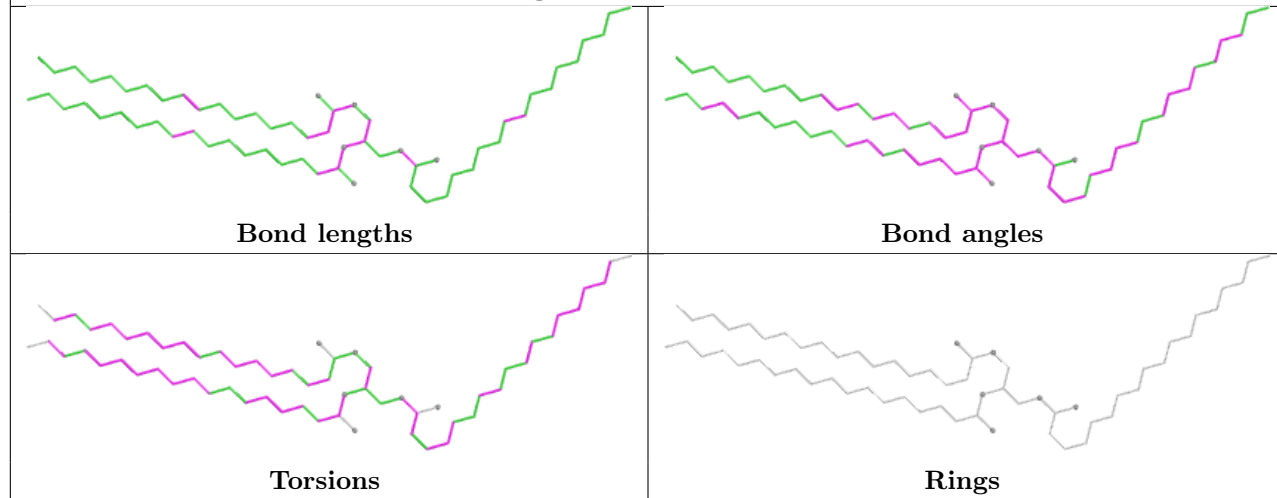


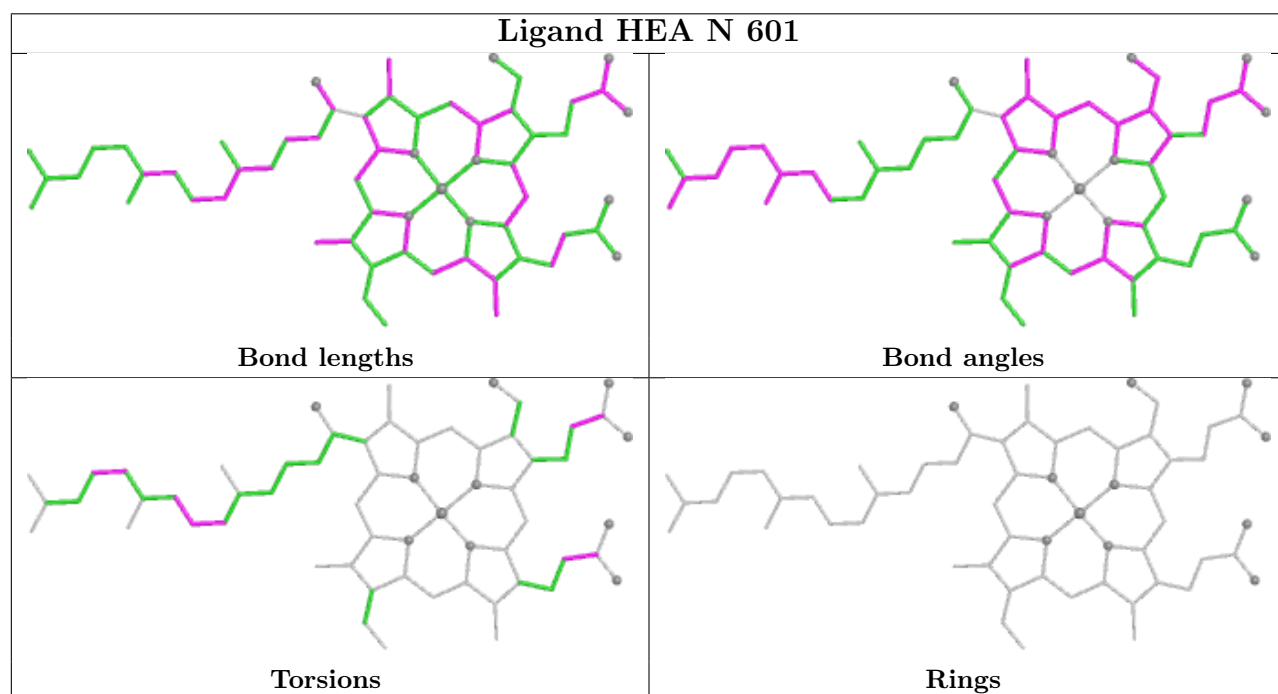
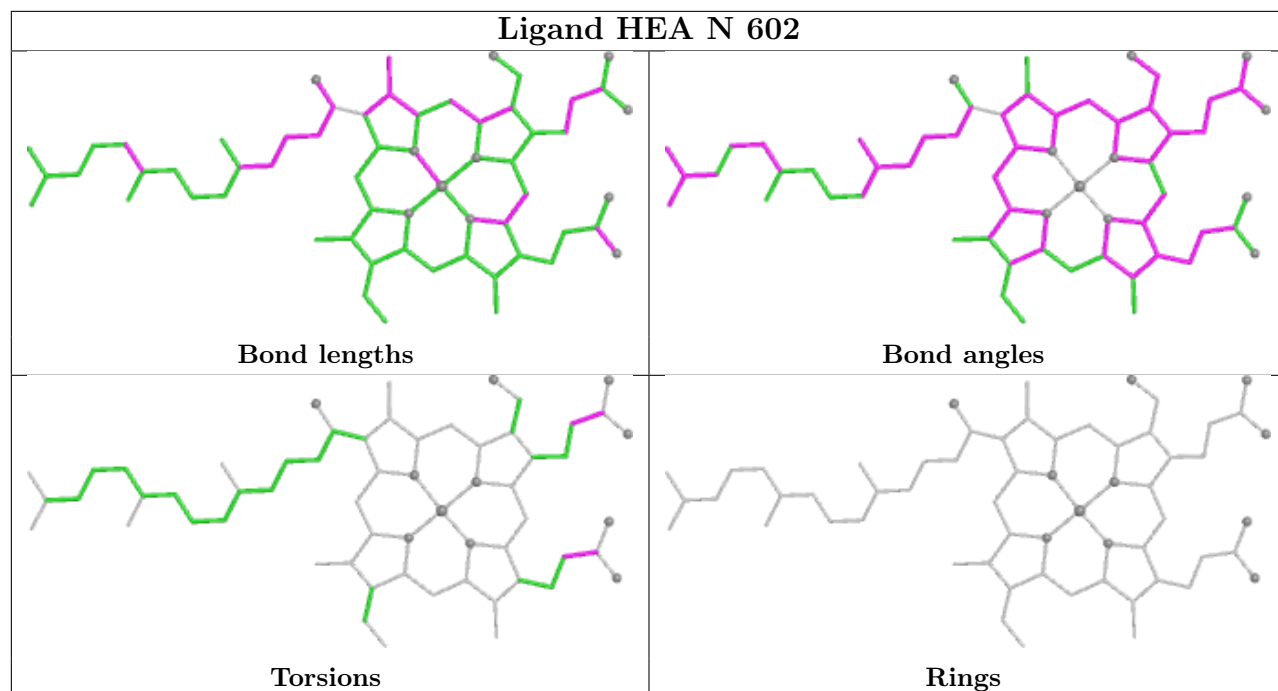


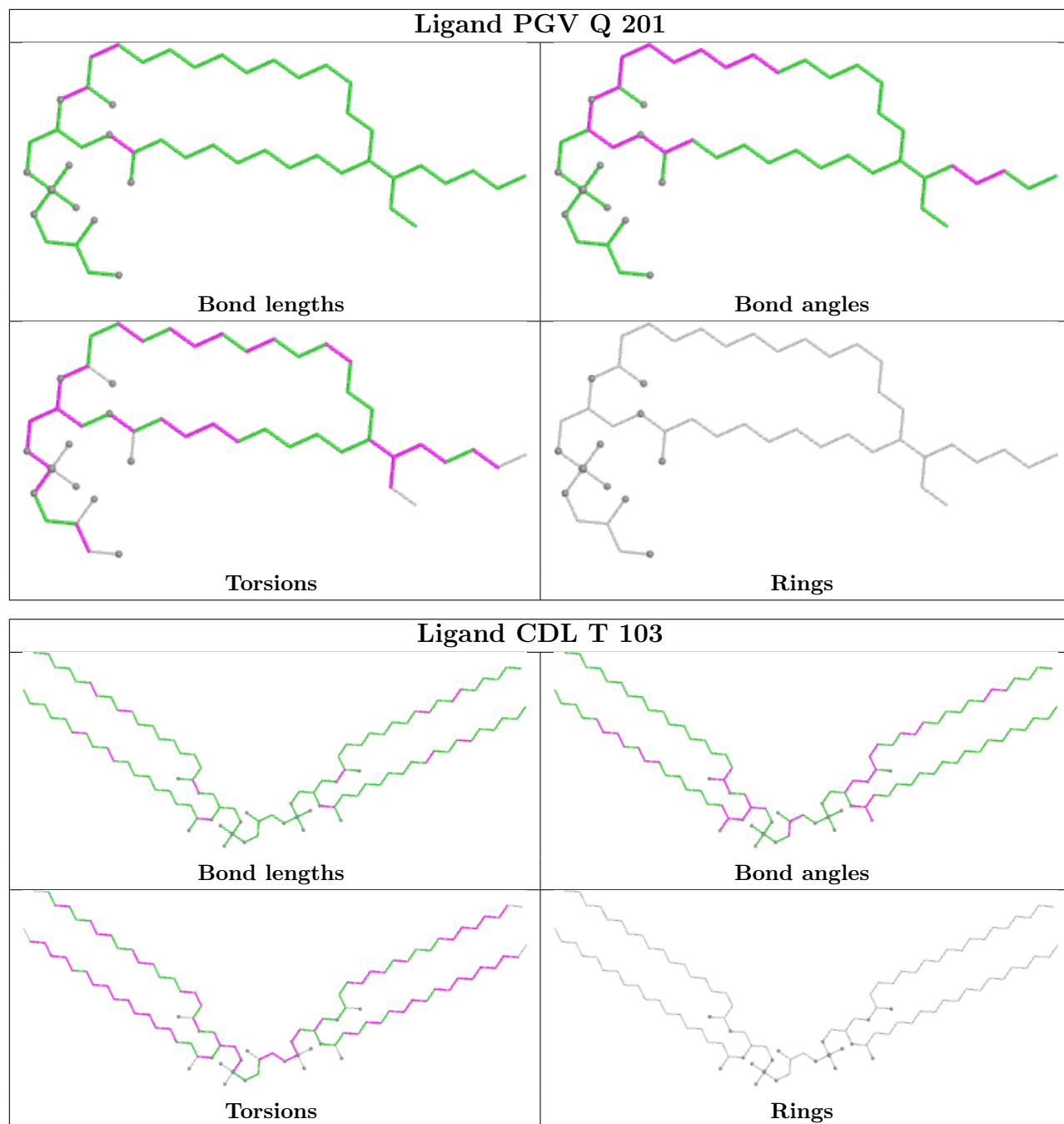
## Ligand PEK C 306

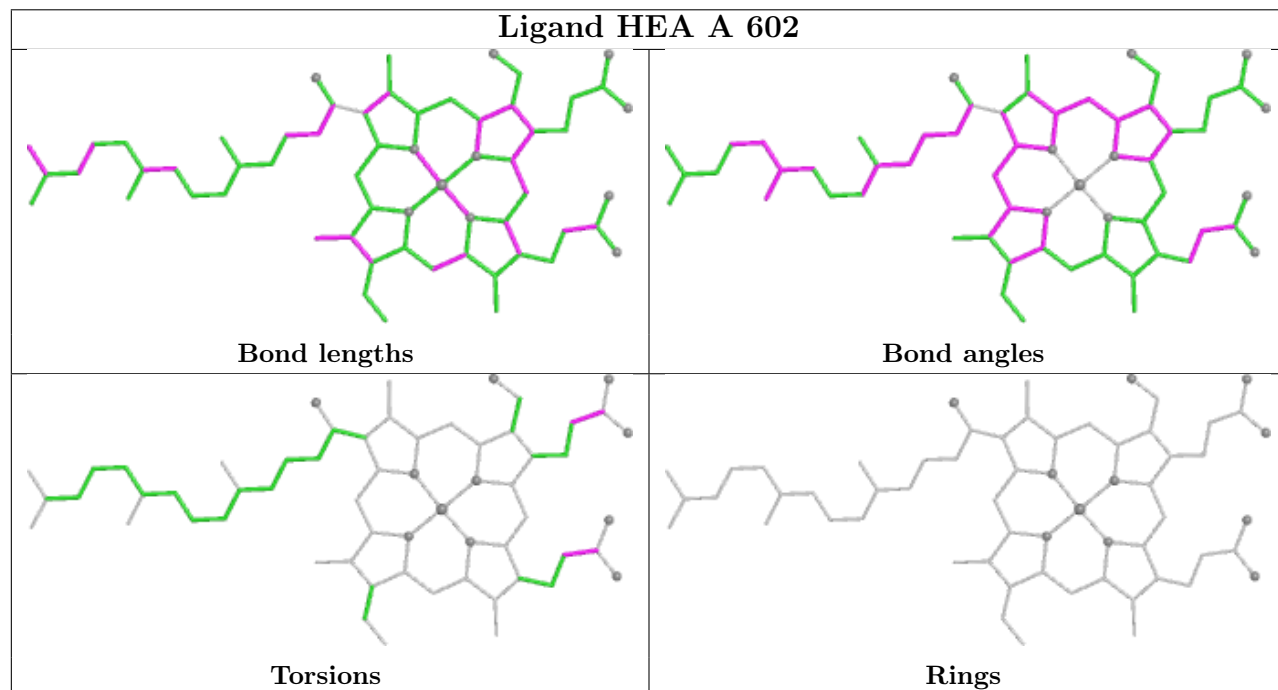
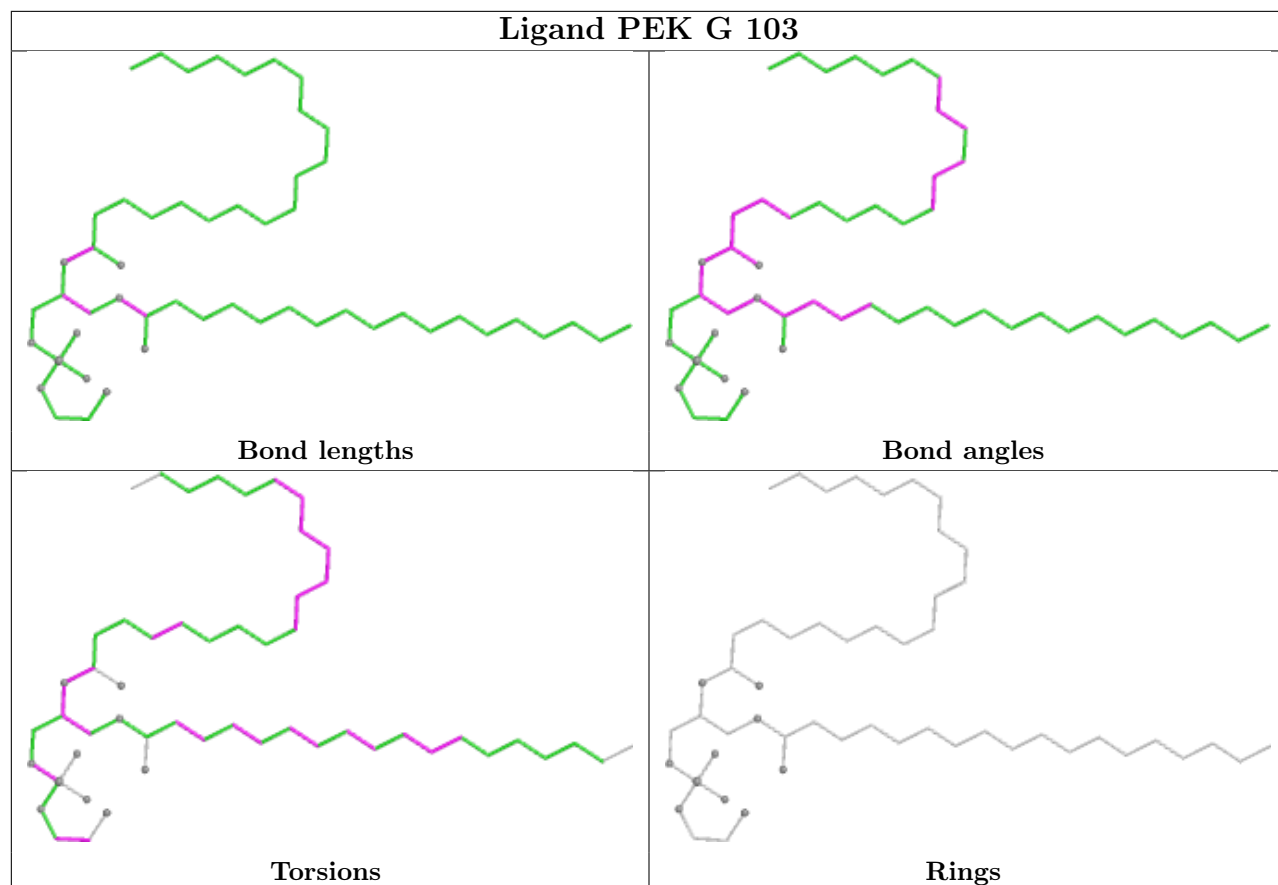


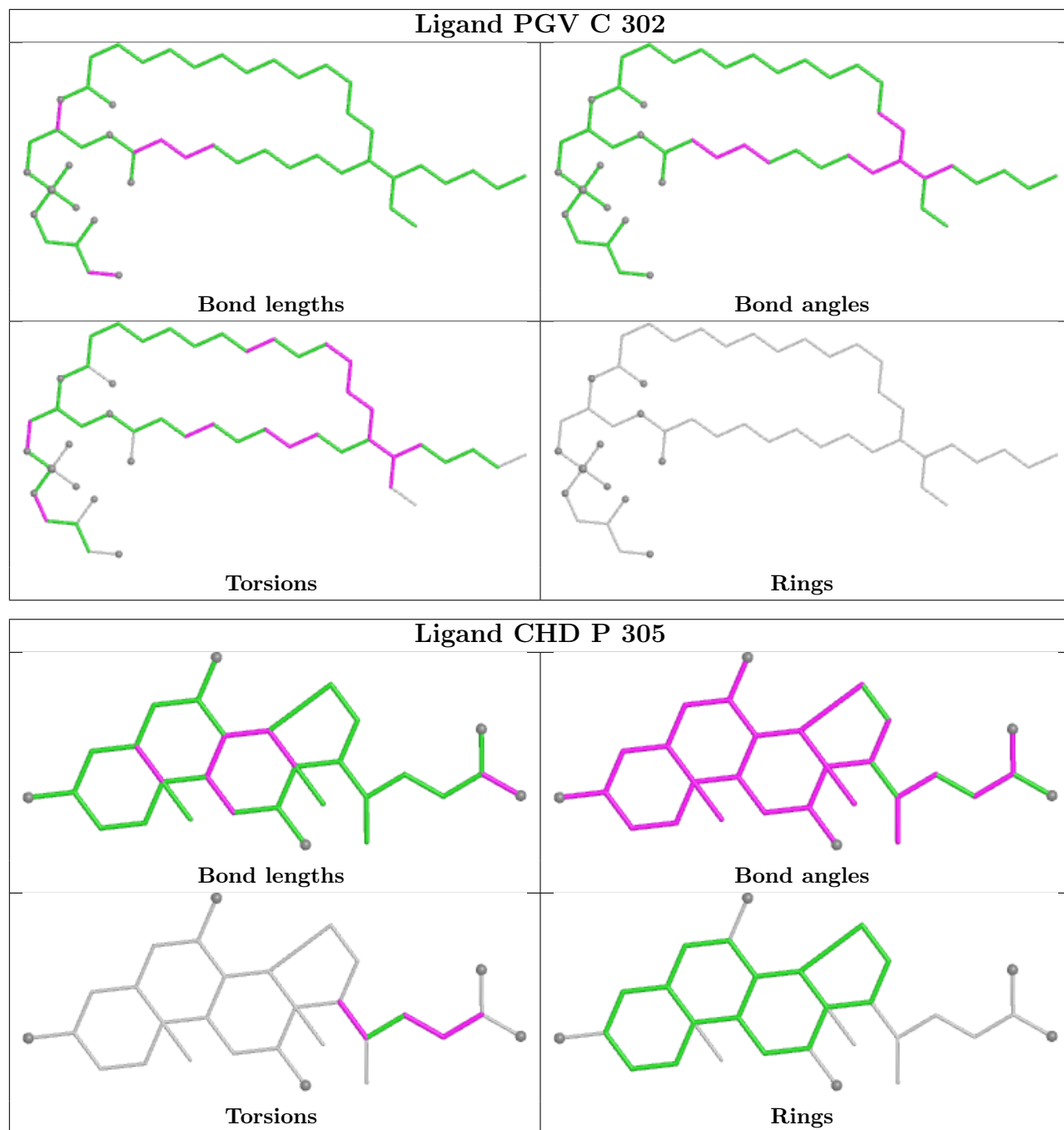
## Ligand TGL Y 101

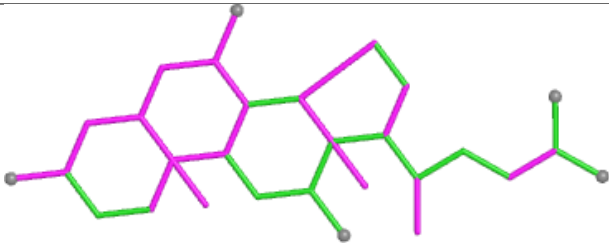
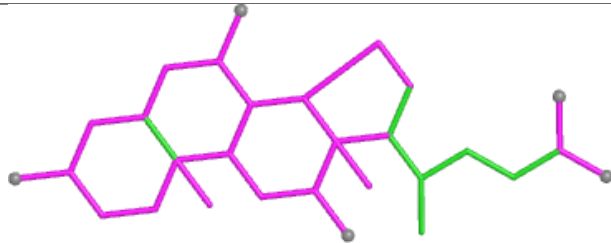
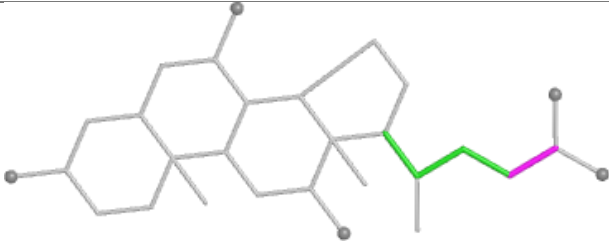
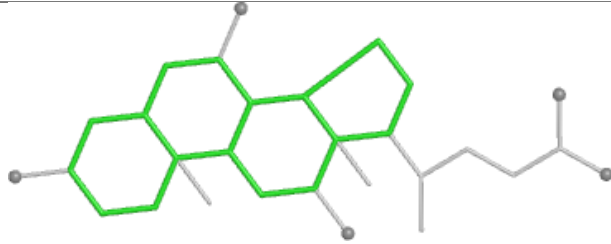


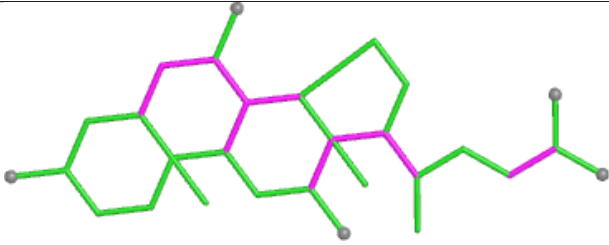
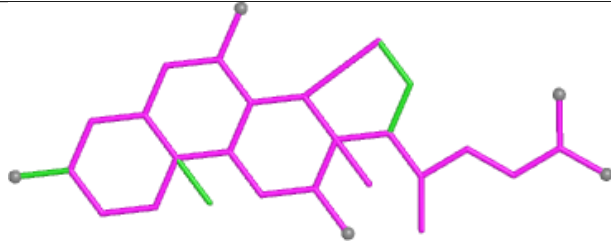
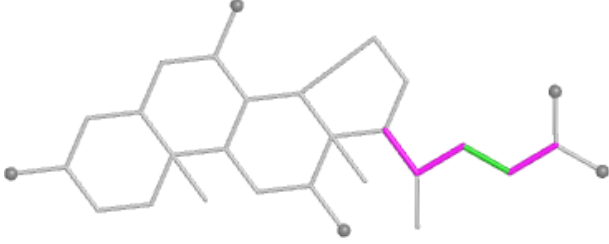
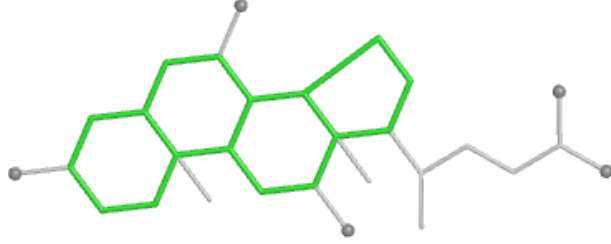


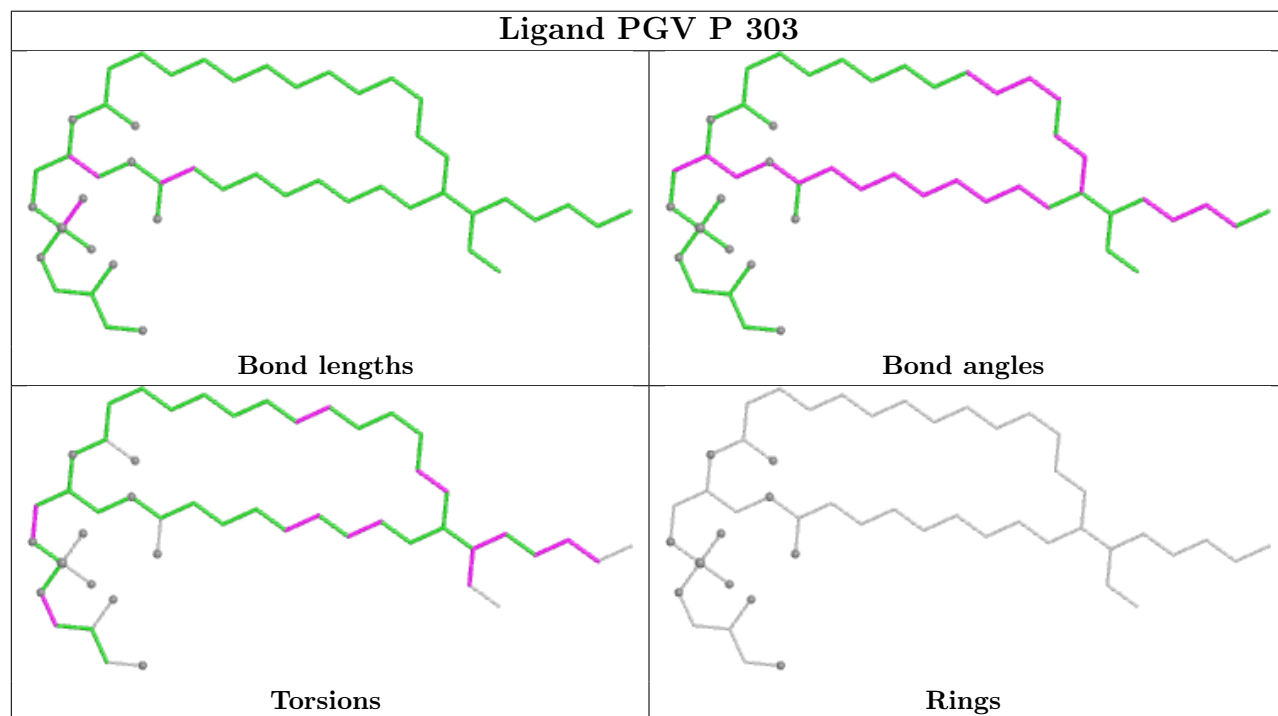
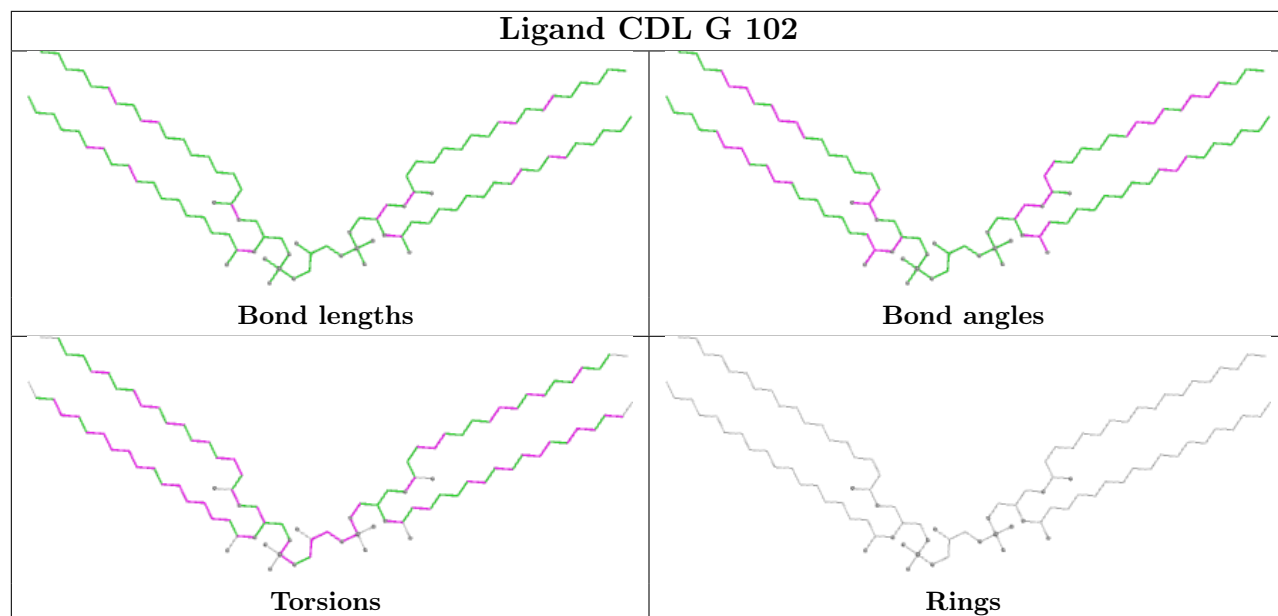


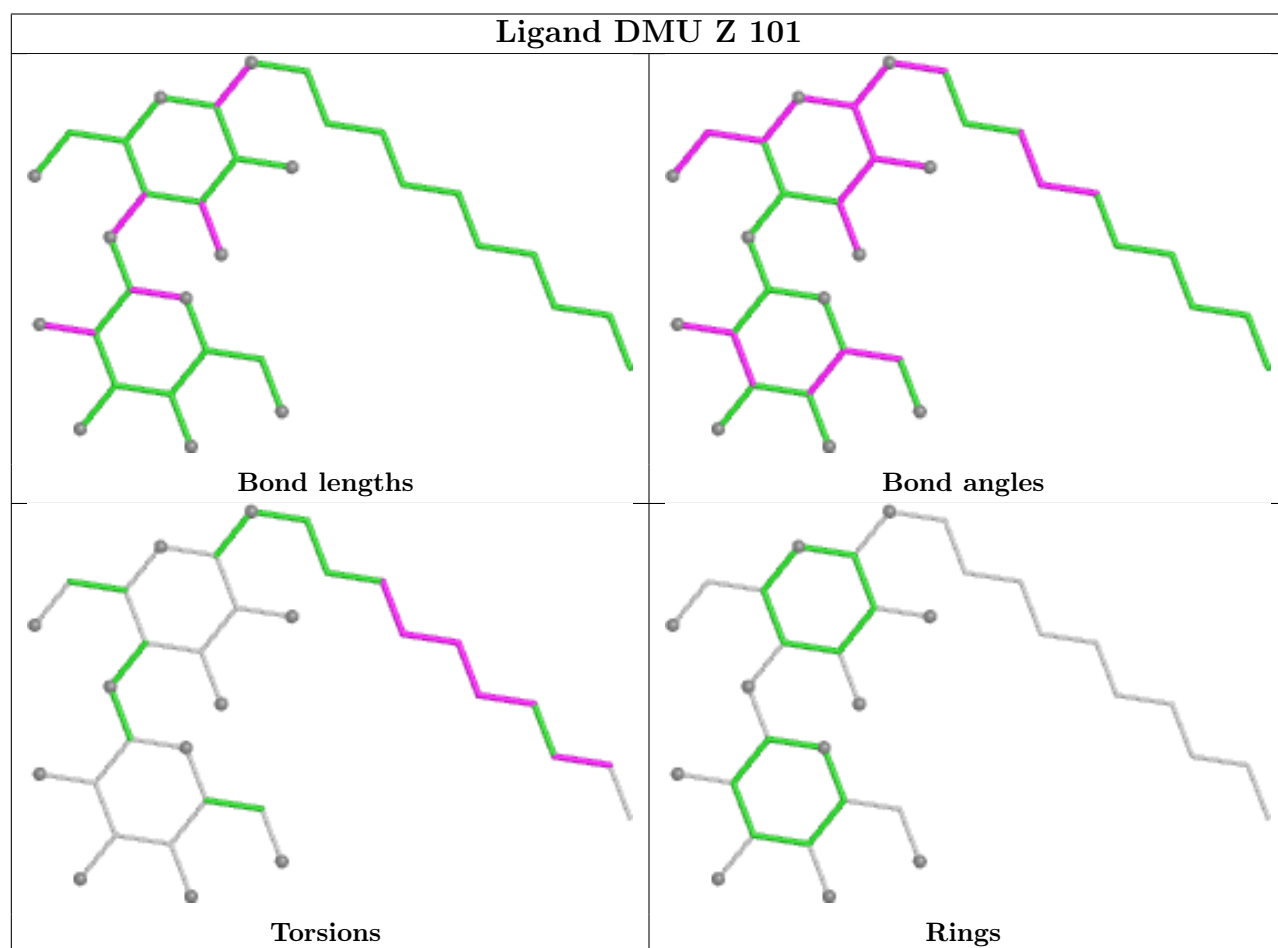
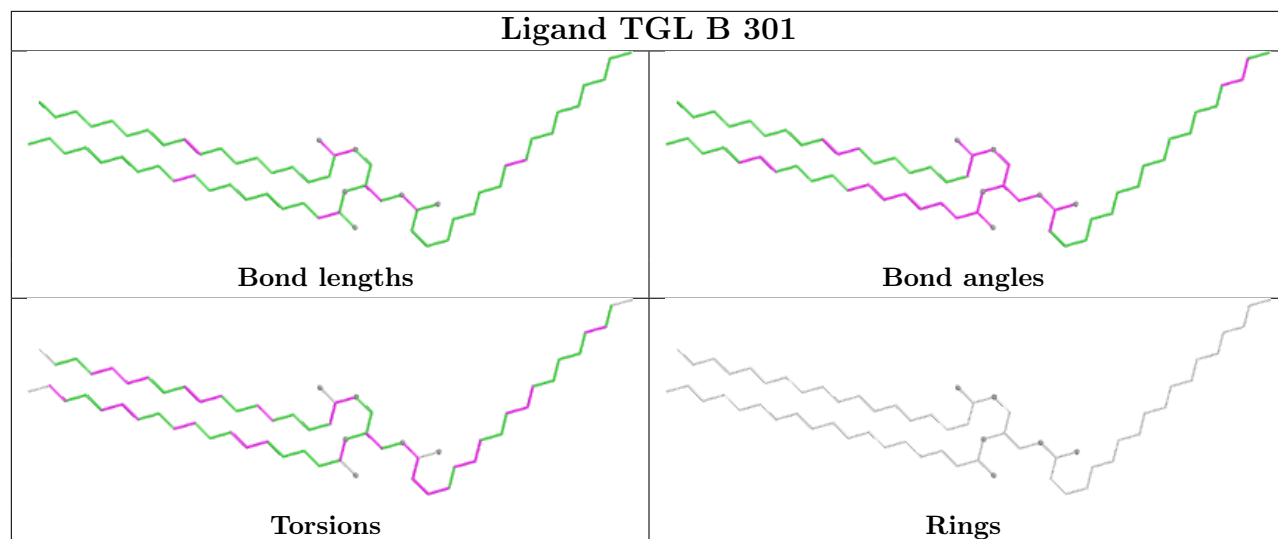




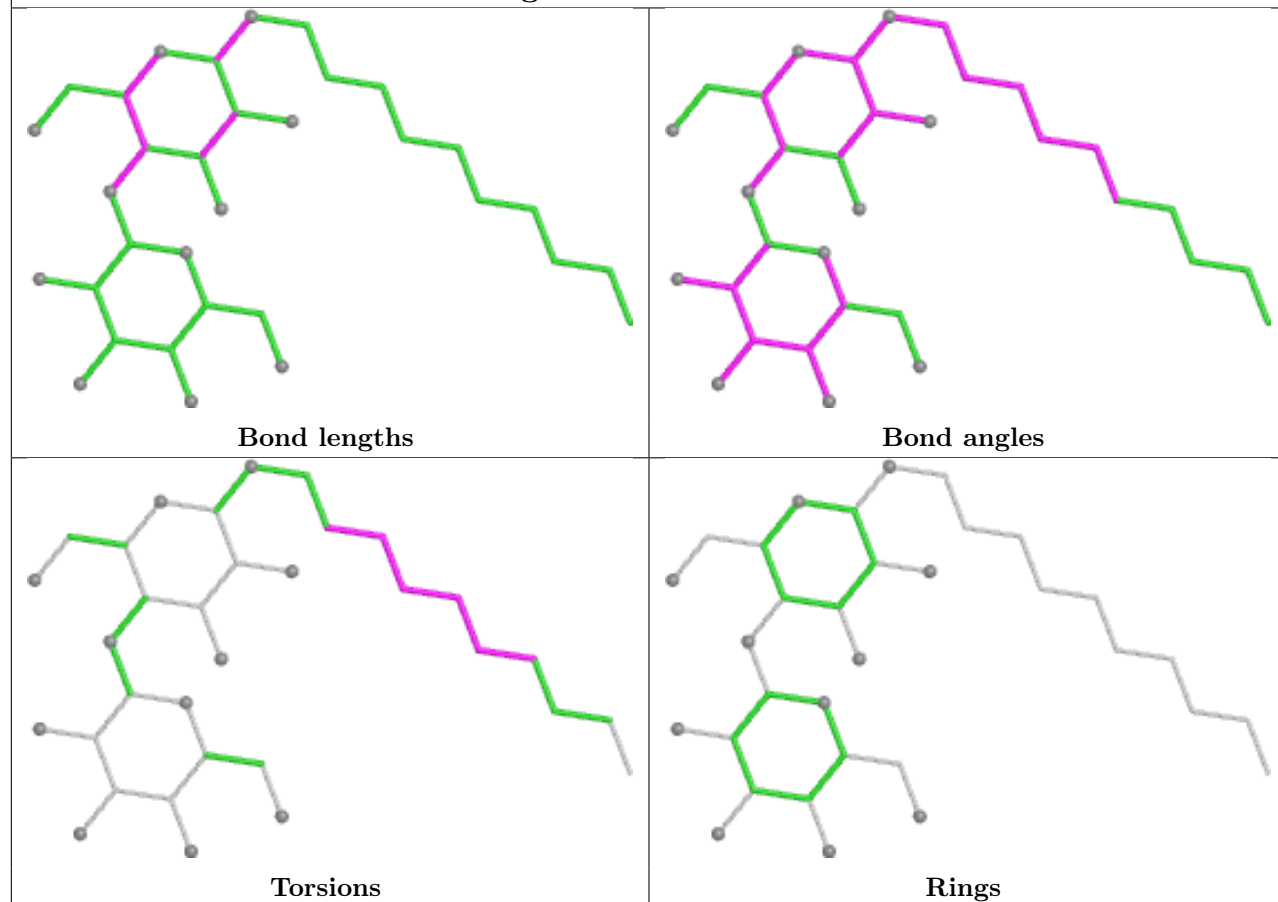
| Ligand CHD B 303                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CHD J 102                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

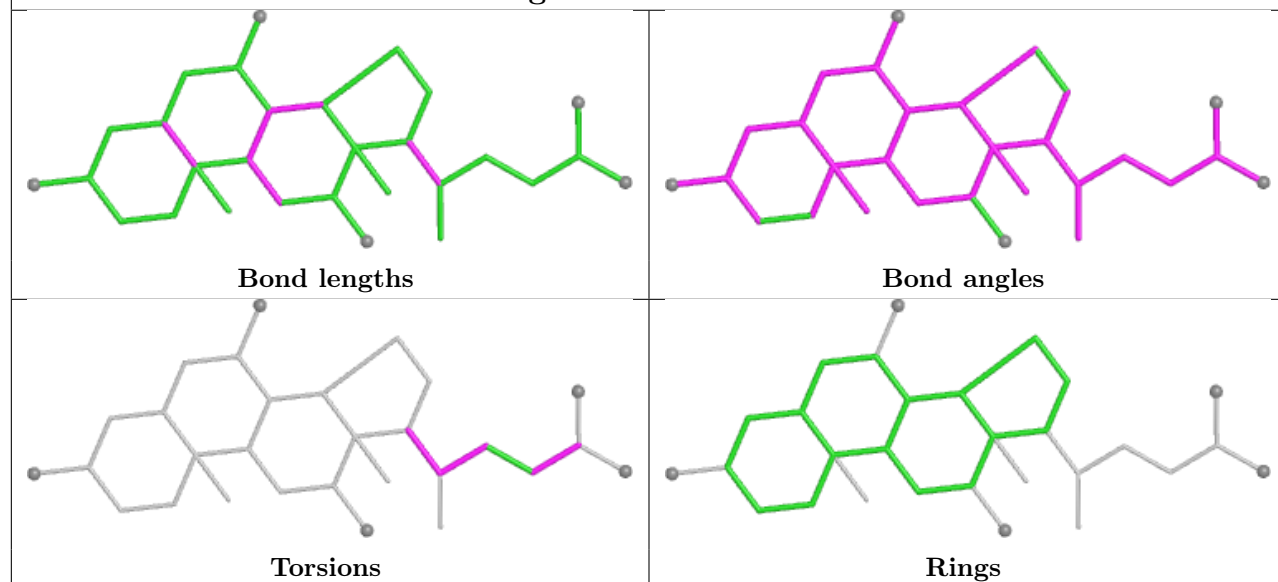


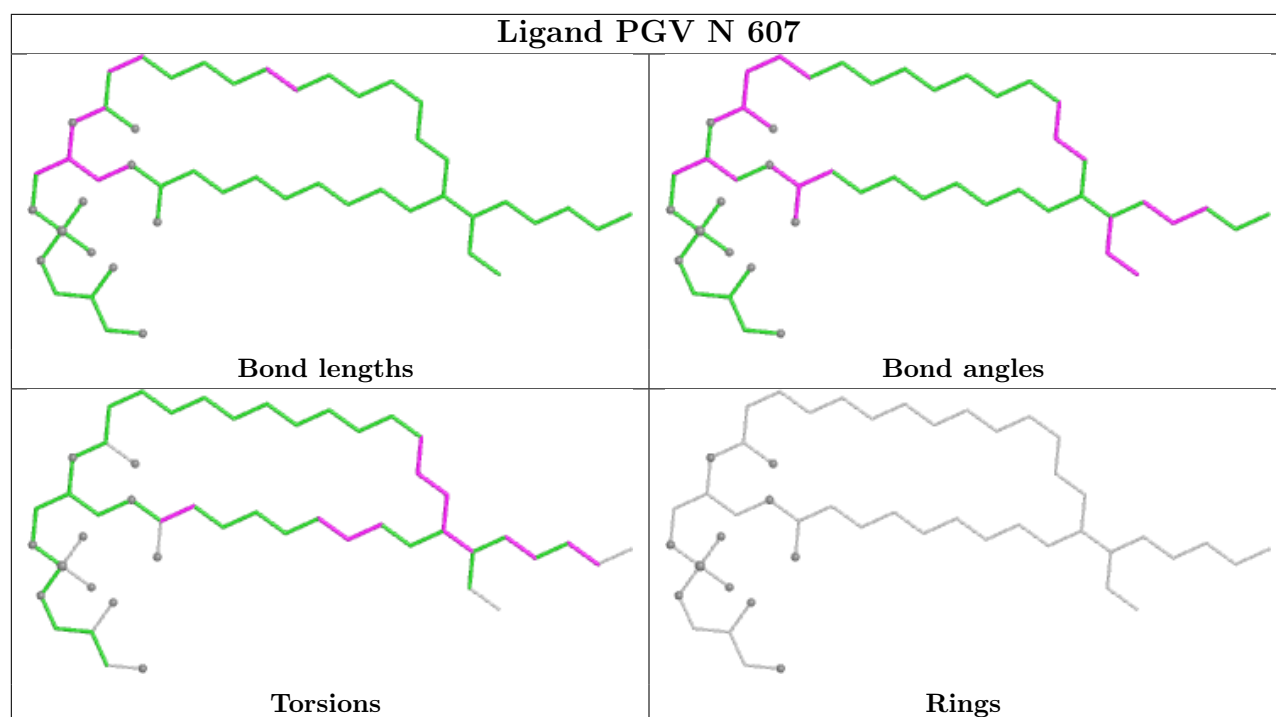


## Ligand DMU M 101



## Ligand CHD C 304





## 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%) | -0.45  | 3 (0%) 85 88  | 10, 21, 28, 68        | 18 (3%) |
| 1   | N     | 513/514 (99%) | -0.35  | 4 (0%) 82 86  | 11, 24, 33, 63        | 16 (3%) |
| 2   | B     | 226/227 (99%) | 0.04   | 15 (6%) 24 26 | 13, 27, 47, 71        | 9 (3%)  |
| 2   | O     | 226/227 (99%) | 0.16   | 11 (4%) 35 38 | 16, 34, 60, 90        | 5 (2%)  |
| 3   | C     | 259/261 (99%) | -0.25  | 2 (0%) 82 86  | 10, 24, 37, 77        | 9 (3%)  |
| 3   | P     | 259/261 (99%) | -0.22  | 3 (1%) 76 80  | 10, 26, 39, 70        | 9 (3%)  |
| 4   | D     | 144/147 (97%) | -0.01  | 5 (3%) 47 51  | 13, 29, 44, 76        | 5 (3%)  |
| 4   | Q     | 144/147 (97%) | 0.68   | 13 (9%) 15 16 | 17, 43, 76, 153       | 3 (2%)  |
| 5   | E     | 105/109 (96%) | -0.01  | 4 (3%) 44 48  | 23, 30, 53, 136       | 0       |
| 5   | R     | 105/109 (96%) | 0.22   | 3 (2%) 53 58  | 22, 37, 61, 149       | 1 (0%)  |
| 6   | F     | 98/98 (100%)  | 0.36   | 8 (8%) 17 19  | 14, 31, 94, 141       | 4 (4%)  |
| 6   | S     | 98/98 (100%)  | 0.57   | 9 (9%) 14 15  | 15, 30, 80, 126       | 2 (2%)  |
| 7   | G     | 83/85 (97%)   | 1.02   | 20 (24%) 2 2  | 14, 32, 110, 158      | 1 (1%)  |
| 7   | T     | 83/85 (97%)   | 1.09   | 19 (22%) 2 2  | 16, 36, 112, 154      | 1 (1%)  |
| 8   | H     | 79/85 (92%)   | 0.47   | 10 (12%) 8 8  | 25, 36, 92, 133       | 0       |
| 8   | U     | 79/85 (92%)   | 0.46   | 10 (12%) 8 8  | 31, 40, 103, 127      | 0       |
| 9   | I     | 72/73 (98%)   | 0.45   | 4 (5%) 30 33  | 27, 41, 63, 82        | 0       |
| 9   | V     | 72/73 (98%)   | 0.64   | 9 (12%) 8 8   | 27, 47, 69, 143       | 0       |
| 10  | J     | 58/59 (98%)   | 0.35   | 4 (6%) 23 25  | 25, 35, 65, 134       | 0       |
| 10  | W     | 58/59 (98%)   | 0.43   | 5 (8%) 16 17  | 19, 37, 69, 158       | 1 (1%)  |
| 11  | K     | 49/56 (87%)   | 0.12   | 2 (4%) 41 45  | 28, 35, 49, 58        | 0       |
| 11  | X     | 49/56 (87%)   | 0.48   | 3 (6%) 27 29  | 19, 47, 68, 81        | 1 (2%)  |
| 12  | L     | 46/47 (97%)   | -0.00  | 3 (6%) 25 27  | 22, 27, 53, 95        | 0       |
| 12  | Y     | 46/47 (97%)   | 0.25   | 4 (8%) 16 17  | 19, 33, 58, 125       | 1 (2%)  |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|----------------|-----------------------|---------|
| 13  | M     | 43/46 (93%)     | 0.17   | 3 (6%) 22 24   | 24, 28, 64, 118       | 0       |
| 13  | Z     | 43/46 (93%)     | 0.38   | 3 (6%) 22 24   | 31, 38, 79, 145       | 0       |
| All | All   | 3550/3614 (98%) | 0.05   | 179 (5%) 34 37 | 10, 28, 61, 158       | 86 (2%) |

All (179) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 6   | S     | 97  | ALA  | 12.1 |
| 6   | F     | 1   | ALA  | 12.0 |
| 4   | Q     | 5   | VAL  | 9.6  |
| 8   | H     | 8   | ILE  | 8.9  |
| 4   | Q     | 6   | VAL  | 8.6  |
| 7   | G     | 36  | TRP  | 8.6  |
| 6   | S     | 96  | LEU  | 8.6  |
| 7   | T     | 36  | TRP  | 8.6  |
| 7   | G     | 3   | ALA  | 8.1  |
| 6   | S     | 1   | ALA  | 8.0  |
| 8   | U     | 8   | ILE  | 7.7  |
| 5   | R     | 109 | VAL  | 7.6  |
| 7   | T     | 9   | GLY  | 7.5  |
| 6   | S     | 94  | HIS  | 7.3  |
| 7   | T     | 3   | ALA  | 6.9  |
| 7   | G     | 7   | ASP  | 6.6  |
| 3   | P     | 3   | HIS  | 6.4  |
| 6   | F     | 97  | ALA  | 6.3  |
| 7   | G     | 1   | ALA  | 6.3  |
| 9   | V     | 37  | PHE  | 6.2  |
| 10  | J     | 1   | PHE  | 6.1  |
| 7   | T     | 7   | ASP  | 6.0  |
| 7   | T     | 2   | SER  | 6.0  |
| 6   | S     | 98  | HIS  | 5.9  |
| 6   | F     | 96  | LEU  | 5.9  |
| 7   | G     | 4   | ALA  | 5.8  |
| 10  | W     | 1   | PHE  | 5.8  |
| 7   | T     | 10  | GLY  | 5.8  |
| 4   | Q     | 8   | SER  | 5.8  |
| 7   | T     | 5   | LYS  | 5.7  |
| 7   | T     | 8   | HIS  | 5.6  |
| 7   | G     | 8   | HIS  | 5.5  |
| 4   | Q     | 7   | LYS  | 5.4  |
| 7   | T     | 1   | ALA  | 5.4  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 7   | G     | 5      | LYS  | 5.0  |
| 6   | F     | 94     | HIS  | 5.0  |
| 1   | N     | 113[A] | LEU  | 5.0  |
| 6   | F     | 2      | SER  | 4.9  |
| 7   | T     | 6      | GLY  | 4.9  |
| 8   | H     | 46     | LYS  | 4.9  |
| 6   | S     | 95     | GLN  | 4.9  |
| 7   | G     | 2      | SER  | 4.8  |
| 8   | U     | 46     | LYS  | 4.7  |
| 6   | S     | 93     | PRO  | 4.7  |
| 1   | A     | 113[A] | LEU  | 4.6  |
| 7   | G     | 10     | GLY  | 4.6  |
| 7   | G     | 9      | GLY  | 4.5  |
| 4   | D     | 4      | SER  | 4.5  |
| 6   | S     | 3      | GLY  | 4.5  |
| 12  | Y     | 2      | HIS  | 4.4  |
| 4   | D     | 87[A]  | PHE  | 4.4  |
| 9   | I     | 37     | PHE  | 4.4  |
| 7   | G     | 6      | GLY  | 4.4  |
| 11  | X     | 6      | ALA  | 4.4  |
| 2   | O     | 113    | TYR  | 4.4  |
| 10  | W     | 58     | LYS  | 4.4  |
| 13  | M     | 40     | TYR  | 4.3  |
| 4   | Q     | 87[A]  | PHE  | 4.3  |
| 4   | Q     | 4      | SER  | 4.3  |
| 7   | T     | 4      | ALA  | 4.3  |
| 9   | V     | 2      | THR  | 4.0  |
| 12  | L     | 2      | HIS  | 4.0  |
| 7   | T     | 84     | LYS  | 4.0  |
| 3   | P     | 37     | PHE  | 3.9  |
| 6   | F     | 3      | GLY  | 3.9  |
| 5   | E     | 109    | VAL  | 3.9  |
| 6   | S     | 2      | SER  | 3.7  |
| 8   | U     | 47     | GLY  | 3.7  |
| 8   | H     | 47     | GLY  | 3.7  |
| 13  | M     | 42     | LYS  | 3.6  |
| 7   | G     | 37     | LEU  | 3.6  |
| 5   | R     | 14[A]  | ARG  | 3.6  |
| 5   | E     | 5      | HIS  | 3.6  |
| 13  | Z     | 43     | SER  | 3.5  |
| 2   | O     | 65     | TRP  | 3.5  |
| 10  | J     | 58     | LYS  | 3.5  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 6   | F     | 98     | HIS  | 3.5  |
| 12  | L     | 47     | LYS  | 3.5  |
| 7   | T     | 37     | LEU  | 3.5  |
| 1   | N     | 514    | LYS  | 3.4  |
| 10  | W     | 48     | TYR  | 3.4  |
| 2   | B     | 59     | GLN  | 3.4  |
| 2   | O     | 32[A]  | PHE  | 3.3  |
| 8   | U     | 45     | ALA  | 3.3  |
| 7   | G     | 84     | LYS  | 3.3  |
| 8   | H     | 44     | THR  | 3.3  |
| 3   | C     | 3      | HIS  | 3.2  |
| 4   | D     | 31[A]  | LYS  | 3.2  |
| 2   | B     | 90     | ILE  | 3.2  |
| 2   | B     | 65     | TRP  | 3.2  |
| 4   | D     | 5      | VAL  | 3.2  |
| 4   | Q     | 39     | ALA  | 3.1  |
| 11  | X     | 47     | ARG  | 3.1  |
| 1   | N     | 136[A] | LEU  | 3.1  |
| 13  | Z     | 40     | TYR  | 3.1  |
| 8   | H     | 48     | GLY  | 3.1  |
| 2   | B     | 32[A]  | PHE  | 3.0  |
| 9   | V     | 3      | ALA  | 3.0  |
| 8   | H     | 7      | LYS  | 3.0  |
| 2   | B     | 61     | VAL  | 3.0  |
| 2   | B     | 113    | TYR  | 3.0  |
| 7   | G     | 42     | ARG  | 2.9  |
| 5   | R     | 5      | HIS  | 2.9  |
| 2   | O     | 227    | LEU  | 2.9  |
| 10  | W     | 57     | HIS  | 2.8  |
| 2   | B     | 66     | THR  | 2.8  |
| 9   | V     | 36     | LYS  | 2.8  |
| 4   | Q     | 10     | ASP  | 2.8  |
| 7   | T     | 42     | ARG  | 2.8  |
| 4   | Q     | 51     | LEU  | 2.8  |
| 9   | I     | 29     | LEU  | 2.8  |
| 11  | K     | 6      | ALA  | 2.7  |
| 2   | O     | 90     | ILE  | 2.7  |
| 7   | T     | 40     | GLY  | 2.7  |
| 1   | A     | 312[A] | ILE  | 2.7  |
| 2   | O     | 217    | LYS  | 2.7  |
| 10  | W     | 52     | TRP  | 2.7  |
| 8   | H     | 45     | ALA  | 2.6  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 7   | G     | 41    | HIS  | 2.6  |
| 4   | Q     | 35    | ALA  | 2.6  |
| 2   | B     | 88    | ASP  | 2.6  |
| 8   | U     | 7     | LYS  | 2.6  |
| 9   | V     | 25    | PHE  | 2.6  |
| 2   | B     | 55    | THR  | 2.5  |
| 12  | Y     | 47    | LYS  | 2.5  |
| 11  | K     | 47    | ARG  | 2.5  |
| 7   | G     | 39    | SER  | 2.5  |
| 2   | B     | 60    | GLU  | 2.5  |
| 13  | Z     | 42    | LYS  | 2.5  |
| 8   | U     | 48    | GLY  | 2.5  |
| 1   | N     | 513   | LEU  | 2.5  |
| 11  | X     | 13    | TYR  | 2.5  |
| 8   | U     | 10    | ASN  | 2.5  |
| 7   | T     | 33    | LEU  | 2.4  |
| 2   | O     | 58    | ALA  | 2.4  |
| 9   | I     | 36    | LYS  | 2.4  |
| 4   | D     | 19[A] | ARG  | 2.4  |
| 4   | Q     | 19[A] | ARG  | 2.4  |
| 8   | U     | 52    | VAL  | 2.4  |
| 12  | L     | 24    | MET  | 2.4  |
| 7   | T     | 12    | GLY  | 2.4  |
| 3   | C     | 258   | TRP  | 2.3  |
| 5   | E     | 14    | ARG  | 2.3  |
| 1   | A     | 514   | LYS  | 2.3  |
| 9   | V     | 26    | MET  | 2.3  |
| 4   | Q     | 9     | GLU  | 2.3  |
| 4   | Q     | 32    | ASN  | 2.3  |
| 7   | T     | 38    | HIS  | 2.3  |
| 10  | J     | 48    | TYR  | 2.3  |
| 2   | B     | 58    | ALA  | 2.3  |
| 2   | B     | 87[A] | MET  | 2.3  |
| 7   | G     | 35    | SER  | 2.3  |
| 8   | H     | 50    | VAL  | 2.3  |
| 3   | P     | 258   | TRP  | 2.3  |
| 2   | B     | 67    | ILE  | 2.3  |
| 9   | V     | 15    | ARG  | 2.2  |
| 5   | E     | 39    | TYR  | 2.2  |
| 2   | O     | 115   | ASP  | 2.2  |
| 9   | V     | 34    | PHE  | 2.2  |
| 2   | B     | 56    | MET  | 2.2  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 7   | G     | 12    | GLY  | 2.2  |
| 8   | U     | 50    | VAL  | 2.2  |
| 8   | H     | 9     | LYS  | 2.2  |
| 7   | T     | 39    | SER  | 2.1  |
| 12  | Y     | 20    | ARG  | 2.1  |
| 13  | M     | 43    | SER  | 2.1  |
| 2   | O     | 87[A] | MET  | 2.1  |
| 7   | G     | 45    | PRO  | 2.1  |
| 9   | V     | 33    | THR  | 2.1  |
| 2   | O     | 61    | VAL  | 2.1  |
| 6   | F     | 95    | GLN  | 2.1  |
| 10  | J     | 52    | TRP  | 2.1  |
| 7   | G     | 40    | GLY  | 2.1  |
| 8   | U     | 9     | LYS  | 2.0  |
| 2   | B     | 16[A] | ILE  | 2.0  |
| 2   | O     | 91    | ASN  | 2.0  |
| 9   | I     | 25    | PHE  | 2.0  |
| 12  | Y     | 24[A] | MET  | 2.0  |
| 8   | H     | 10    | ASN  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 9   | SAC  | V     | 1   | 9/10  | 0.51 | 0.19 | 114,126,154,162            | 0     |
| 7   | TPO  | T     | 11  | 11/12 | 0.73 | 0.25 | 75,96,179,187              | 0     |
| 7   | TPO  | G     | 11  | 11/12 | 0.77 | 0.26 | 61,102,165,180             | 0     |
| 9   | SAC  | I     | 1   | 9/10  | 0.77 | 0.18 | 54,70,75,82                | 0     |
| 1   | FME  | A     | 1   | 10/11 | 0.94 | 0.11 | 31,39,64,89                | 0     |
| 1   | FME  | N     | 1   | 10/11 | 0.95 | 0.11 | 33,40,72,74                | 0     |
| 2   | FME  | B     | 1   | 10/11 | 0.97 | 0.09 | 22,27,48,55                | 0     |
| 2   | FME  | O     | 1   | 10/11 | 0.97 | 0.08 | 29,34,48,59                | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms   | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|---------|------|------|-----------------------------|-------|
| 22  | CHD  | W     | 101 | 29/29   | 0.68 | 0.25 | 59,136,161,164              | 0     |
| 22  | CHD  | J     | 102 | 29/29   | 0.71 | 0.25 | 57,133,165,172              | 0     |
| 22  | CHD  | P     | 305 | 29/29   | 0.75 | 0.20 | 47,91,109,111               | 0     |
| 19  | PGV  | C     | 307 | 51/51   | 0.78 | 0.25 | 47,85,169,181               | 0     |
| 28  | DMU  | J     | 101 | 33/33   | 0.78 | 0.19 | 44,65,156,176               | 0     |
| 26  | PEK  | T     | 102 | 53/53   | 0.79 | 0.26 | 44,95,159,176               | 0     |
| 22  | CHD  | C     | 304 | 29/29   | 0.80 | 0.20 | 46,96,116,118               | 0     |
| 26  | PEK  | C     | 306 | 53/53   | 0.80 | 0.21 | 34,78,128,158               | 0     |
| 23  | PSC  | O     | 303 | 52/52   | 0.81 | 0.26 | 37,75,191,211               | 0     |
| 20  | TGL  | N     | 608 | 63/63   | 0.81 | 0.27 | 47,76,120,136               | 0     |
| 26  | PEK  | G     | 103 | 53/53   | 0.82 | 0.24 | 46,93,150,158               | 0     |
| 25  | CDL  | T     | 103 | 100/100 | 0.82 | 0.25 | 50,91,168,202               | 0     |
| 19  | PGV  | P     | 301 | 51/51   | 0.82 | 0.23 | 45,85,147,177               | 0     |
| 20  | TGL  | B     | 301 | 63/63   | 0.83 | 0.22 | 40,65,90,103                | 0     |
| 20  | TGL  | Q     | 202 | 63/63   | 0.83 | 0.23 | 40,62,99,110                | 0     |
| 23  | PSC  | B     | 304 | 52/52   | 0.83 | 0.22 | 39,107,190,207              | 0     |
| 19  | PGV  | Q     | 201 | 51/51   | 0.84 | 0.21 | 42,79,161,191               | 0     |
| 20  | TGL  | D     | 201 | 63/63   | 0.84 | 0.19 | 30,55,90,101                | 0     |
| 24  | UNX  | C     | 301 | 1/1     | 0.84 | 0.30 | 39,39,39,39                 | 0     |
| 25  | CDL  | G     | 102 | 100/100 | 0.84 | 0.24 | 51,96,162,187               | 0     |
| 25  | CDL  | P     | 304 | 100/100 | 0.84 | 0.23 | 32,78,140,149               | 0     |
| 28  | DMU  | P     | 306 | 33/33   | 0.84 | 0.18 | 36,105,192,198              | 0     |
| 26  | PEK  | P     | 308 | 53/53   | 0.85 | 0.21 | 38,79,120,144               | 0     |
| 20  | TGL  | Y     | 101 | 63/63   | 0.85 | 0.21 | 37,64,106,120               | 0     |
| 19  | PGV  | A     | 608 | 51/51   | 0.86 | 0.22 | 31,68,107,120               | 0     |
| 20  | TGL  | L     | 101 | 63/63   | 0.86 | 0.21 | 30,58,96,101                | 0     |
| 25  | CDL  | C     | 303 | 100/100 | 0.86 | 0.19 | 29,72,127,137               | 0     |
| 24  | UNX  | P     | 302 | 1/1     | 0.87 | 0.36 | 38,38,38,38                 | 0     |
| 28  | DMU  | Z     | 101 | 33/33   | 0.91 | 0.11 | 41,47,61,63                 | 0     |
| 28  | DMU  | M     | 101 | 33/33   | 0.94 | 0.09 | 33,38,51,53                 | 0     |
| 26  | PEK  | T     | 101 | 53/53   | 0.95 | 0.14 | 26,42,83,92                 | 0     |
| 22  | CHD  | C     | 305 | 29/29   | 0.95 | 0.08 | 26,28,31,34                 | 0     |
| 22  | CHD  | O     | 302 | 29/29   | 0.96 | 0.07 | 23,26,29,34                 | 0     |
| 26  | PEK  | G     | 101 | 53/53   | 0.96 | 0.13 | 23,40,82,96                 | 0     |
| 22  | CHD  | B     | 303 | 29/29   | 0.96 | 0.07 | 24,26,29,37                 | 0     |
| 22  | CHD  | P     | 307 | 29/29   | 0.96 | 0.07 | 25,29,32,35                 | 0     |
| 18  | PER  | N     | 606 | 2/2     | 0.96 | 0.11 | 20,20,20,26                 | 0     |

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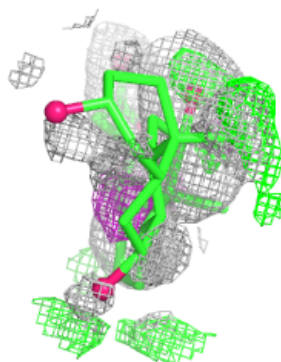
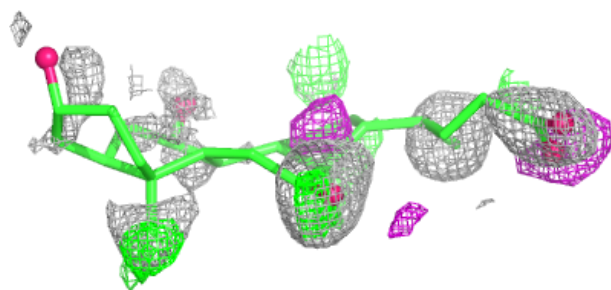
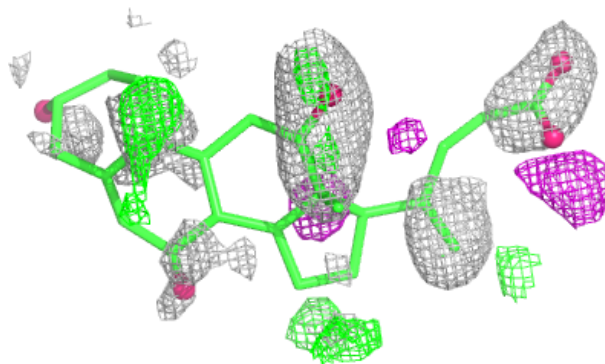
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 19  | PGV  | A     | 607 | 51/51 | 0.97 | 0.10 | 20,29,56,65                 | 0     |
| 19  | PGV  | N     | 607 | 51/51 | 0.97 | 0.11 | 22,32,67,68                 | 0     |
| 18  | PER  | A     | 606 | 2/2   | 0.97 | 0.09 | 17,17,17,22                 | 0     |
| 19  | PGV  | C     | 302 | 51/51 | 0.97 | 0.11 | 22,29,81,98                 | 0     |
| 19  | PGV  | P     | 303 | 51/51 | 0.98 | 0.09 | 21,30,71,79                 | 0     |
| 16  | MG   | N     | 604 | 1/1   | 0.98 | 0.04 | 25,25,25,25                 | 0     |
| 14  | HEA  | A     | 602 | 60/60 | 0.99 | 0.05 | 17,18,25,30                 | 0     |
| 14  | HEA  | N     | 601 | 60/60 | 0.99 | 0.06 | 21,23,43,51                 | 0     |
| 14  | HEA  | N     | 602 | 60/60 | 0.99 | 0.05 | 19,21,28,31                 | 0     |
| 16  | MG   | A     | 604 | 1/1   | 0.99 | 0.05 | 19,19,19,19                 | 0     |
| 14  | HEA  | A     | 601 | 60/60 | 0.99 | 0.06 | 17,19,37,48                 | 0     |
| 17  | NA   | A     | 605 | 1/1   | 0.99 | 0.06 | 23,23,23,23                 | 0     |
| 17  | NA   | N     | 605 | 1/1   | 1.00 | 0.03 | 30,30,30,30                 | 0     |
| 27  | ZN   | F     | 101 | 1/1   | 1.00 | 0.02 | 26,26,26,26                 | 0     |
| 27  | ZN   | S     | 101 | 1/1   | 1.00 | 0.02 | 26,26,26,26                 | 0     |
| 15  | CU   | N     | 603 | 1/1   | 1.00 | 0.01 | 21,21,21,21                 | 0     |
| 21  | CUA  | B     | 302 | 2/2   | 1.00 | 0.01 | 21,21,21,21                 | 0     |
| 21  | CUA  | O     | 301 | 2/2   | 1.00 | 0.02 | 27,27,27,27                 | 0     |
| 15  | CU   | A     | 603 | 1/1   | 1.00 | 0.01 | 19,19,19,19                 | 0     |

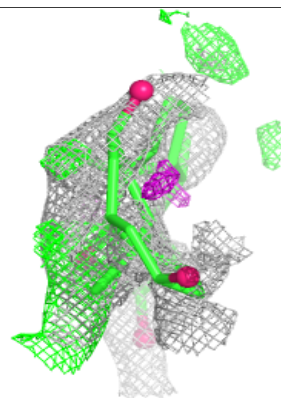
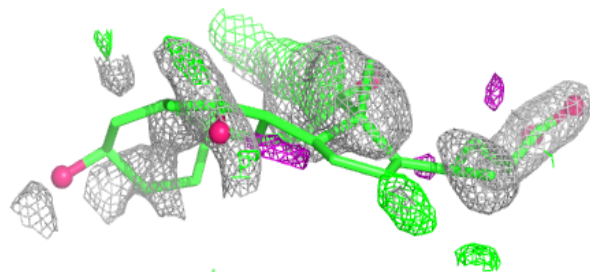
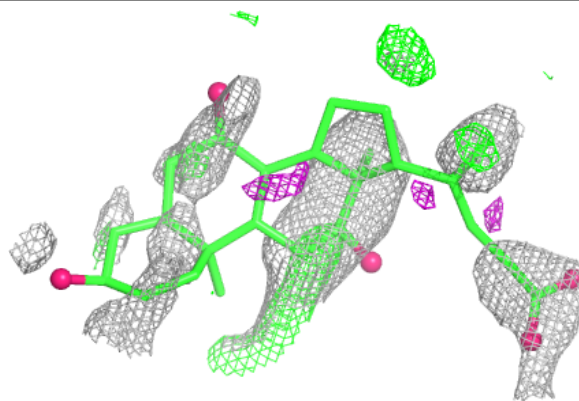
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CHD 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)

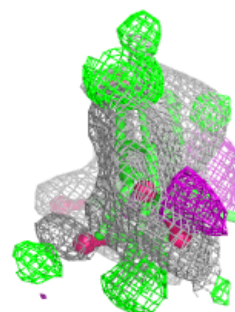
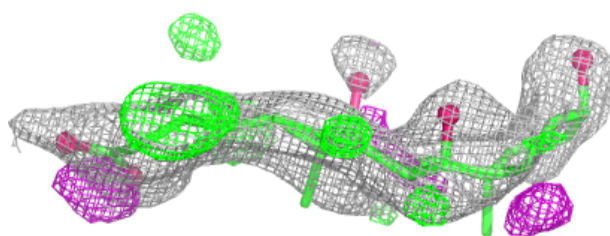
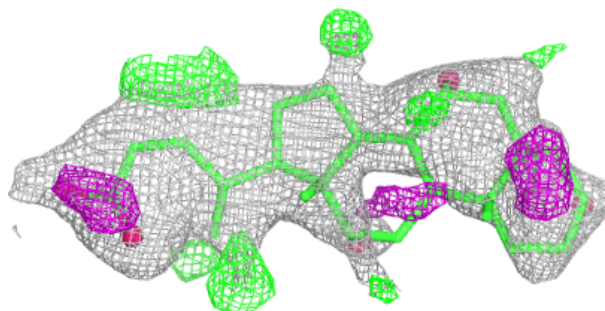
**Electron density around CHD J 102:**

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

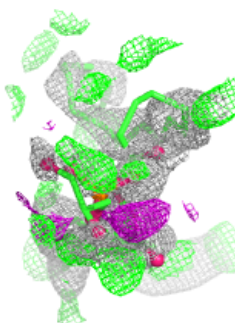
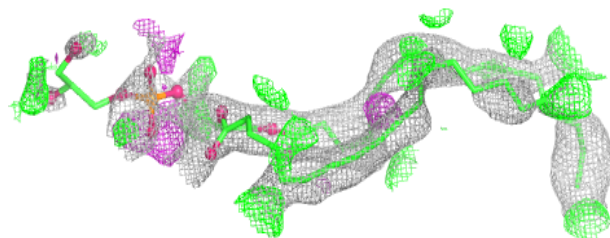
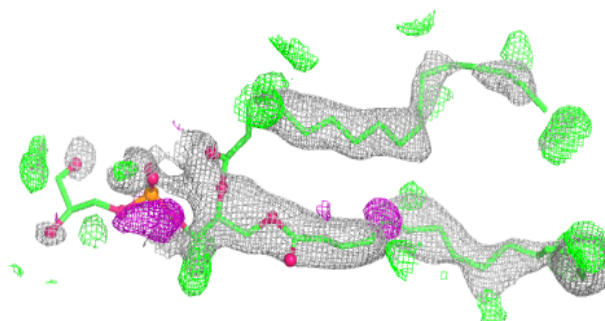


**Electron density around CHD P 305:**

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

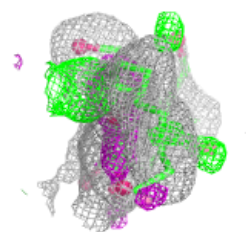
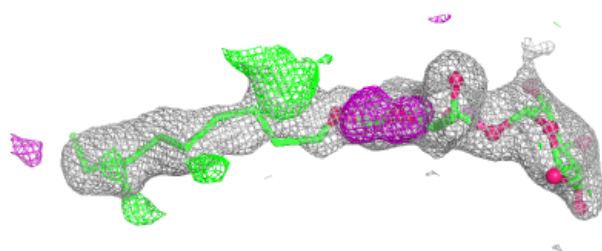
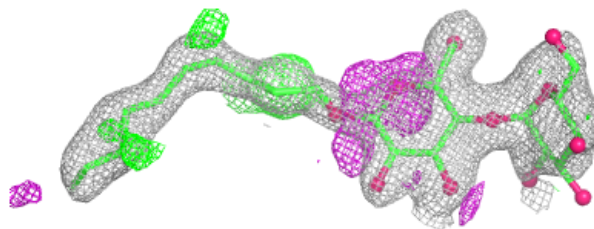
**Electron density around PGV C 307:**

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



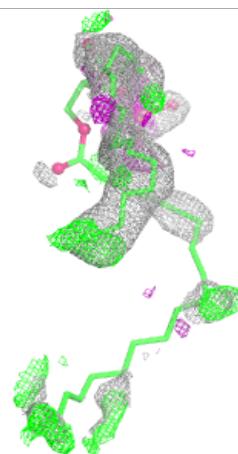
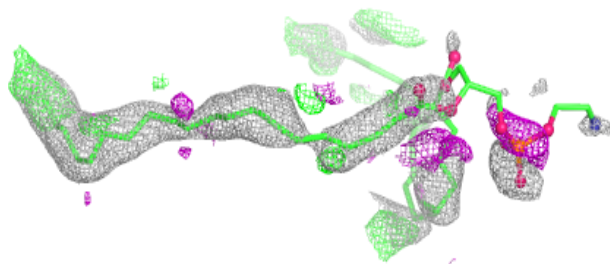
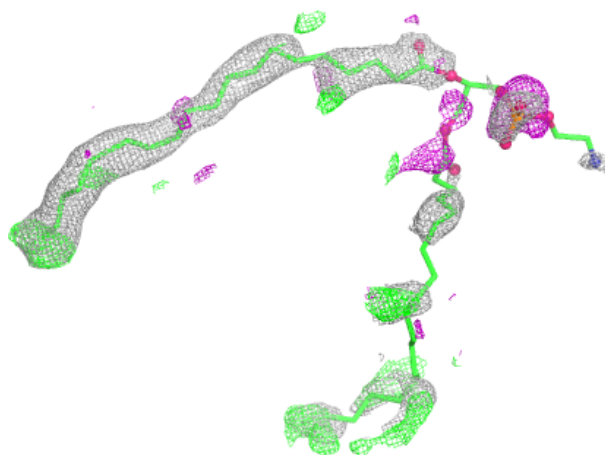
**Electron density around DMU J 101:**

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



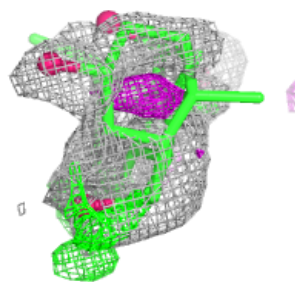
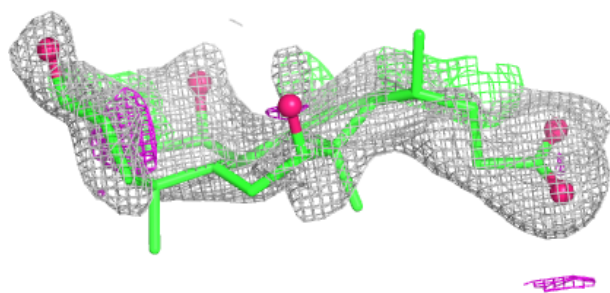
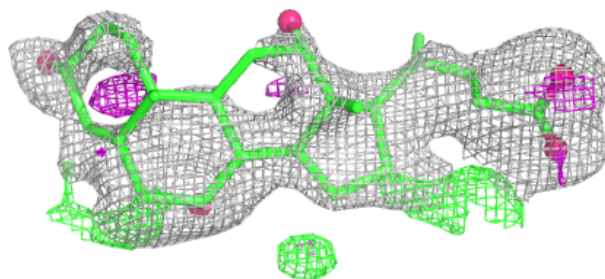
**Electron density around PEK T 102:**

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



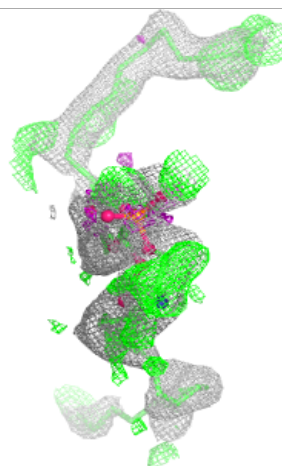
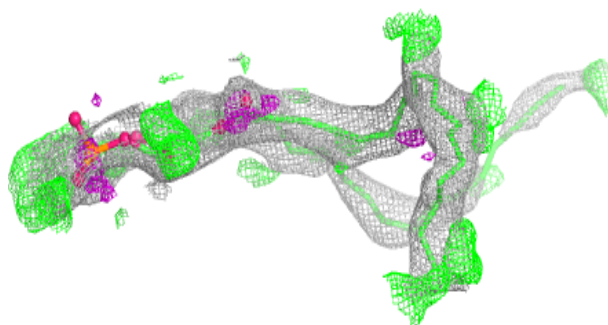
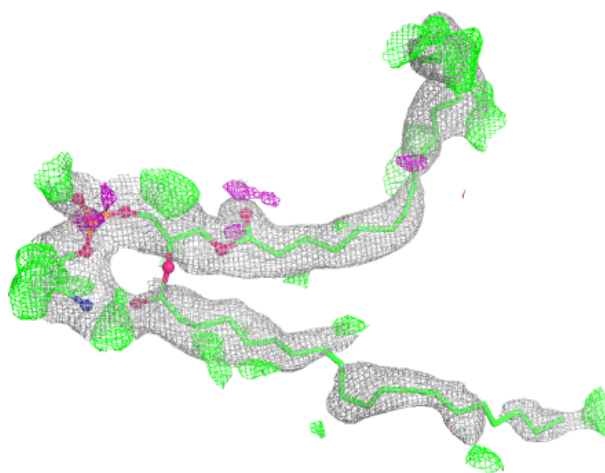
**Electron density around CHD C 304:**

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



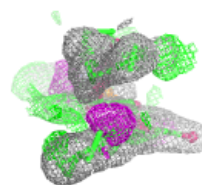
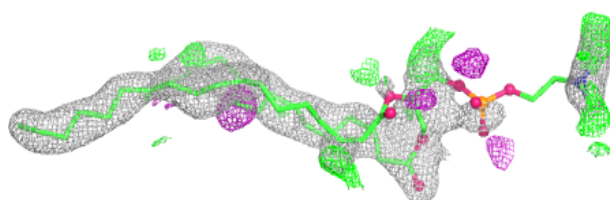
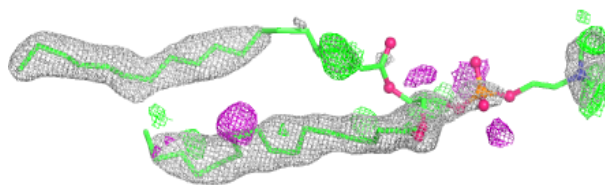
**Electron density around PEK C 306:**

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

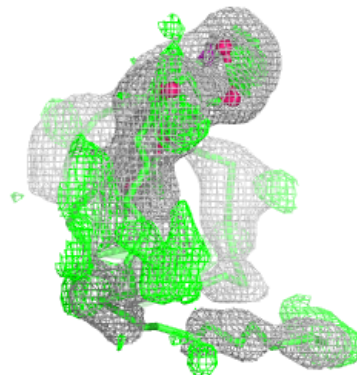
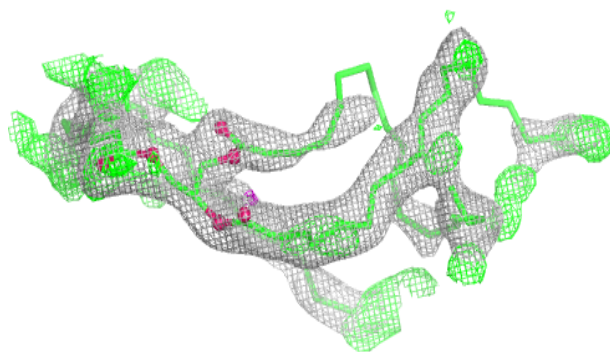
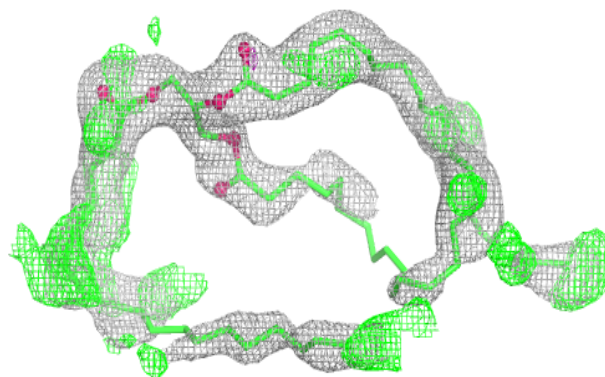


**Electron density around PSC O 303:**

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

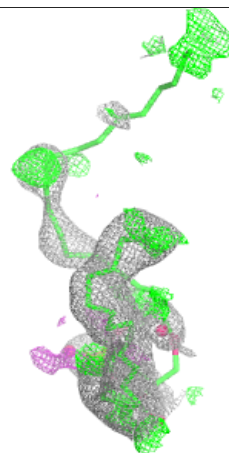
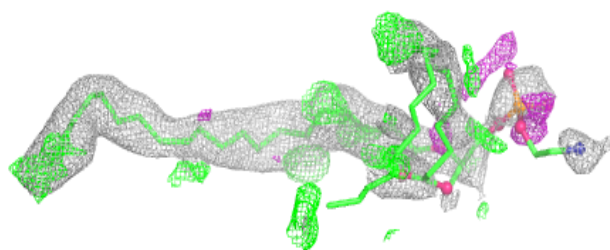
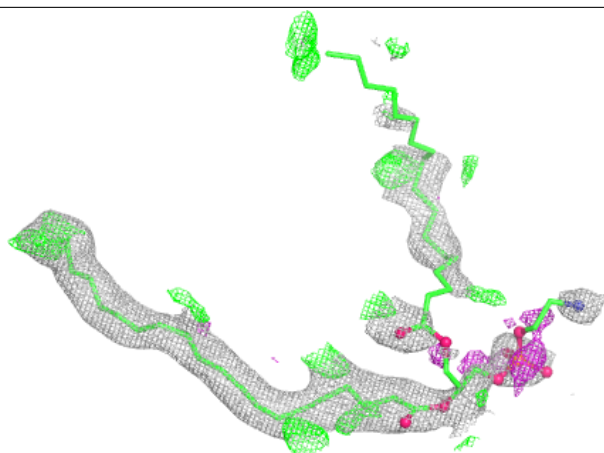
**Electron density around TGL N 608:**

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

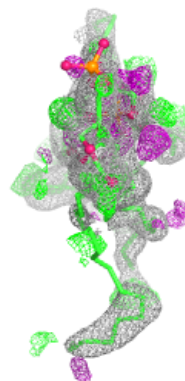
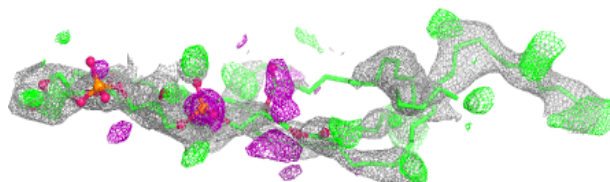
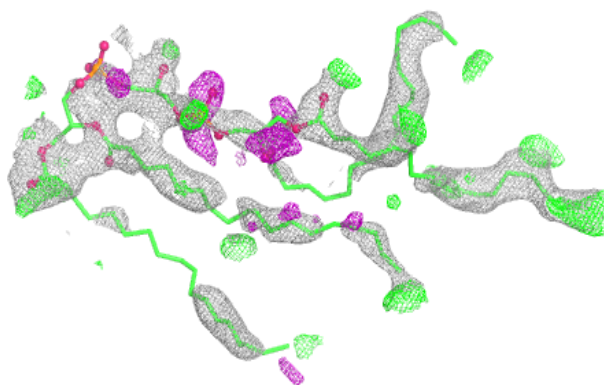


**Electron density around PEK G 103:**

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

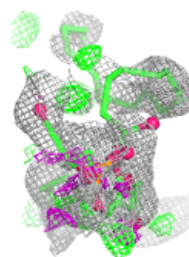
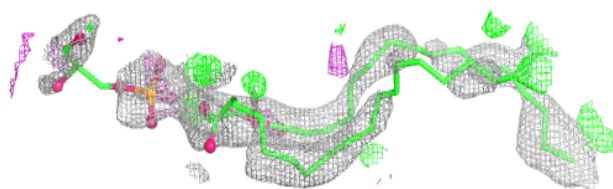
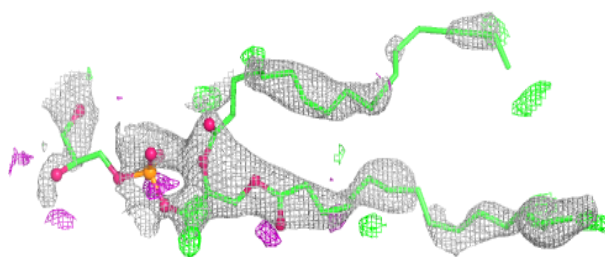
**Electron density around CDL T 103:**

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

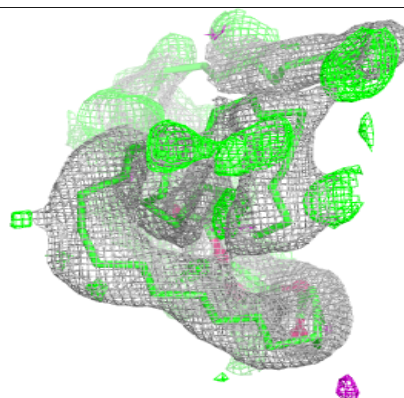
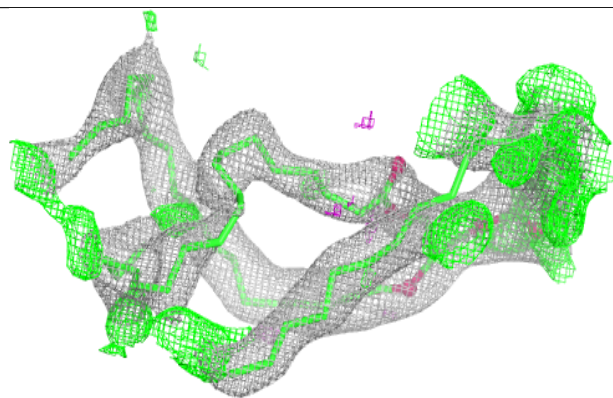
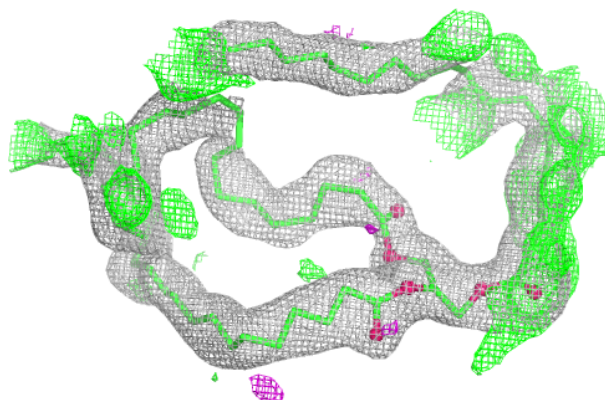


**Electron density around PGV P 301:**

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

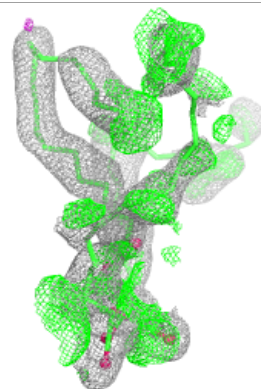
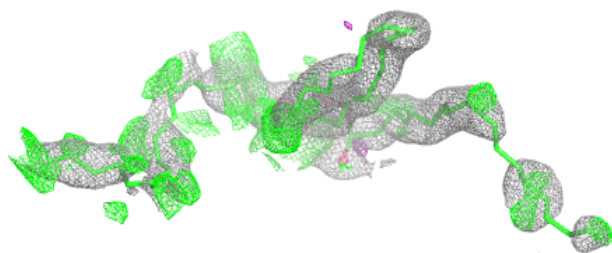
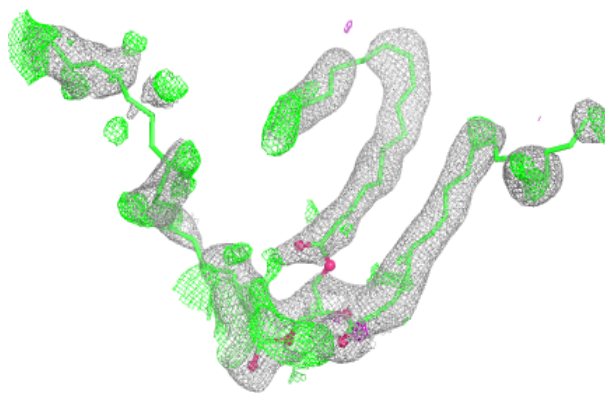
**Electron density around TGL B 301:**

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

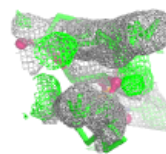
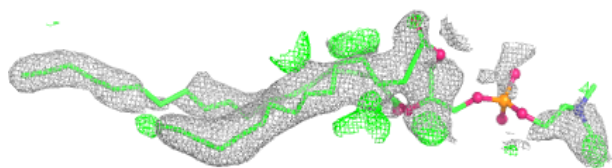
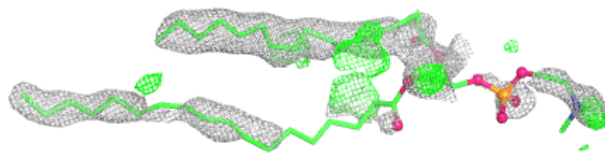


**Electron density around TGL Q 202:**

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

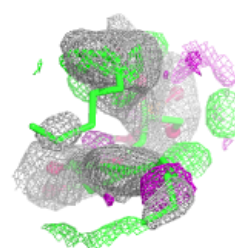
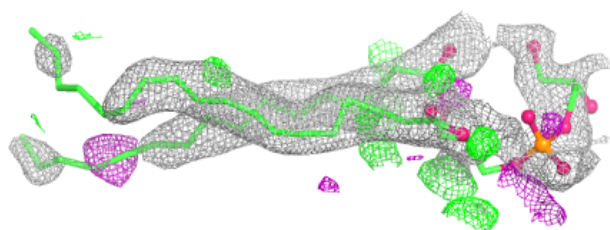
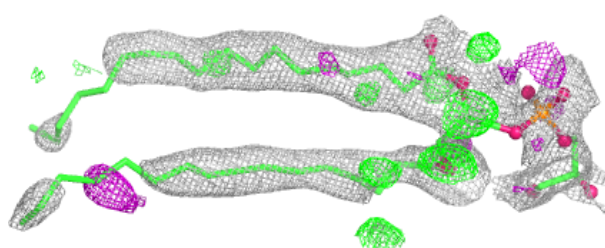
**Electron density around PSC B 304:**

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

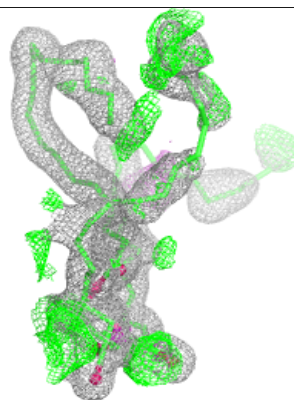
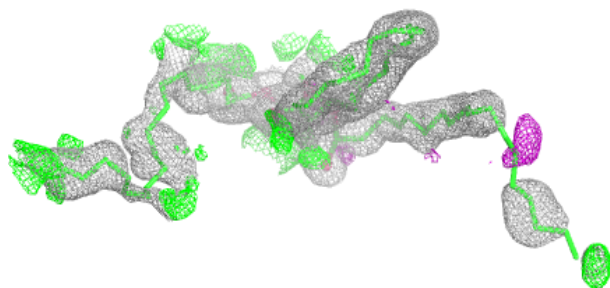
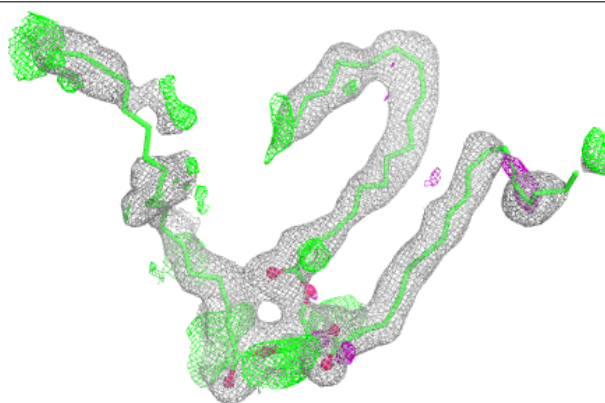


**Electron density around PGV Q 201:**

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

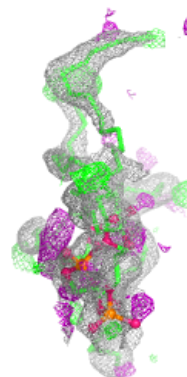
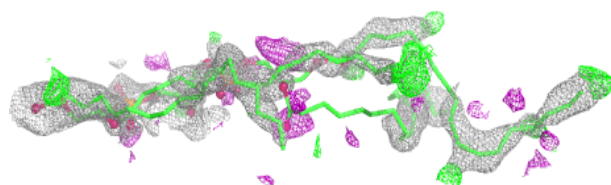
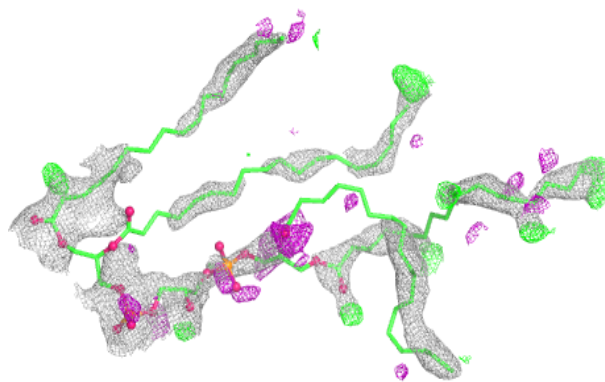
**Electron density around TGL D 201:**

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



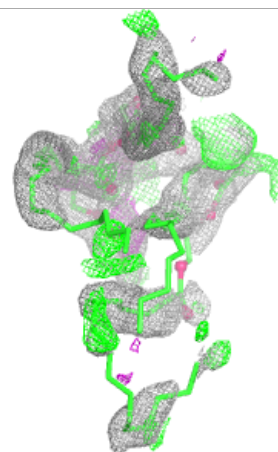
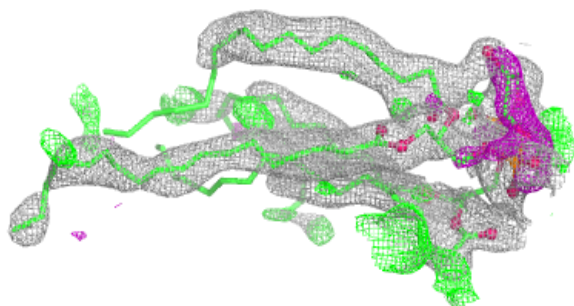
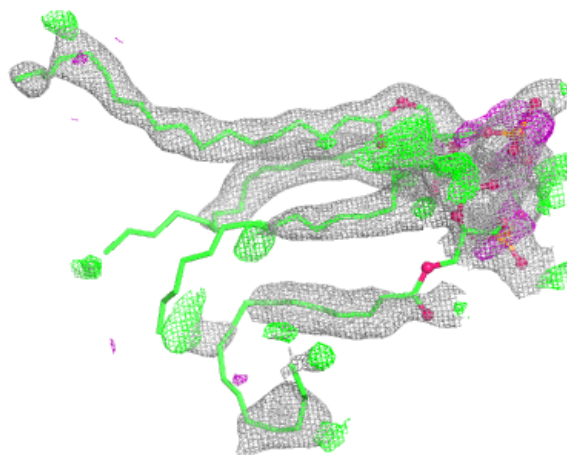
**Electron density around CDL G 102:**

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



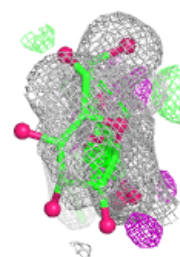
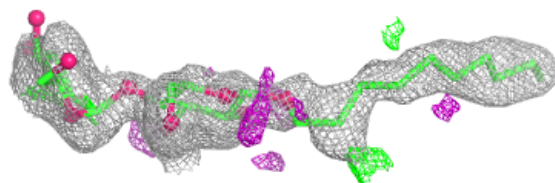
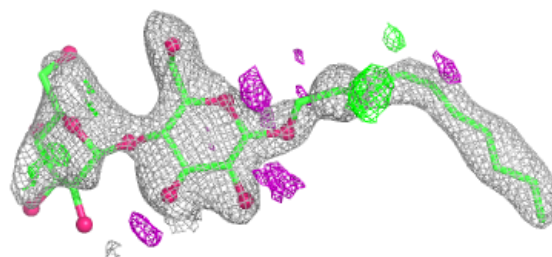
**Electron density around CDL P 304:**

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



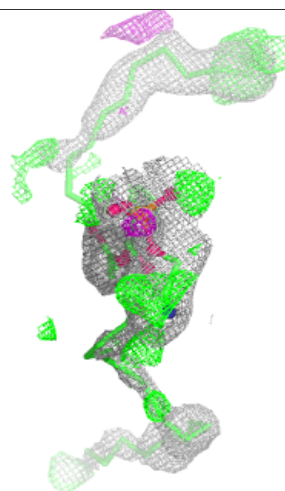
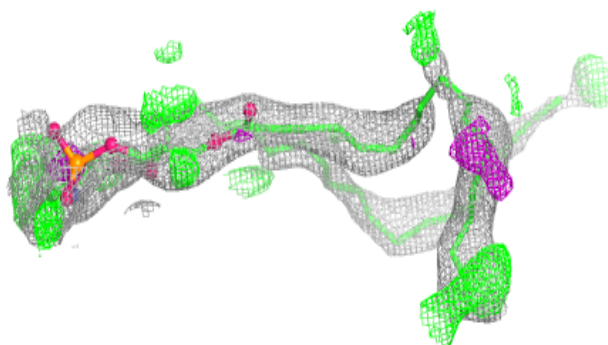
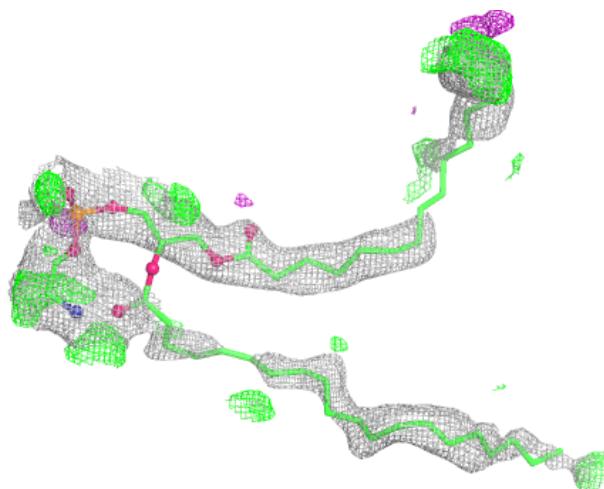
**Electron density around DMU P 306:**

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



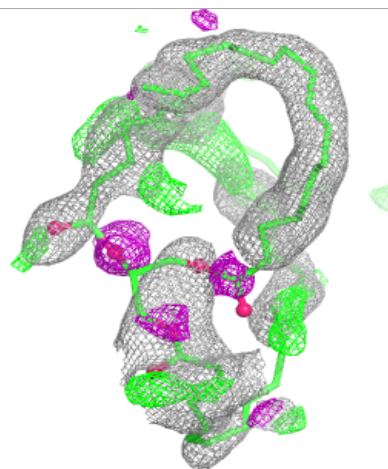
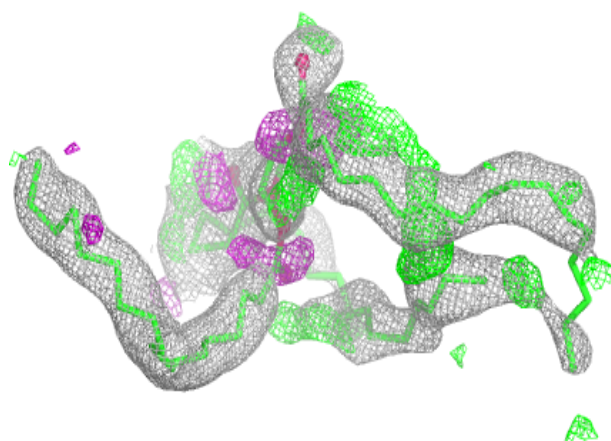
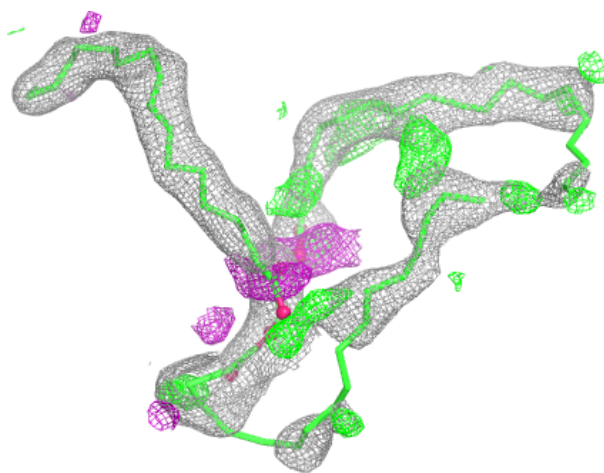
**Electron density around PEK P 308:**

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



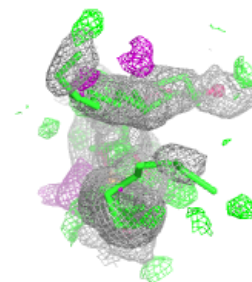
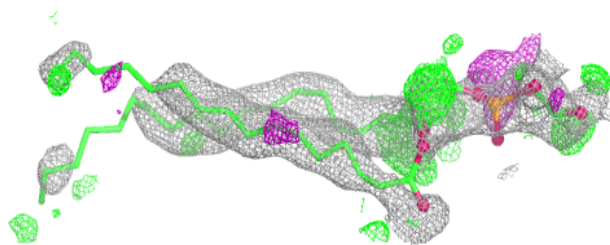
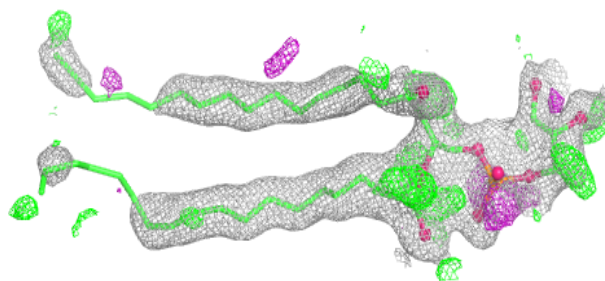
**Electron density around TGL Y 101:**

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



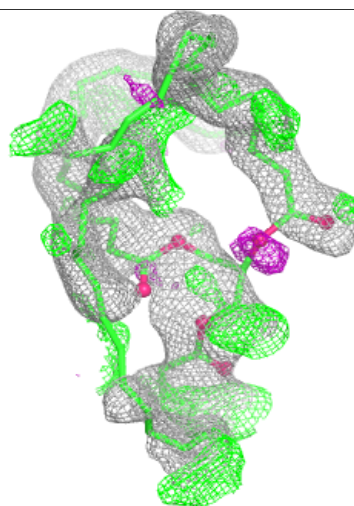
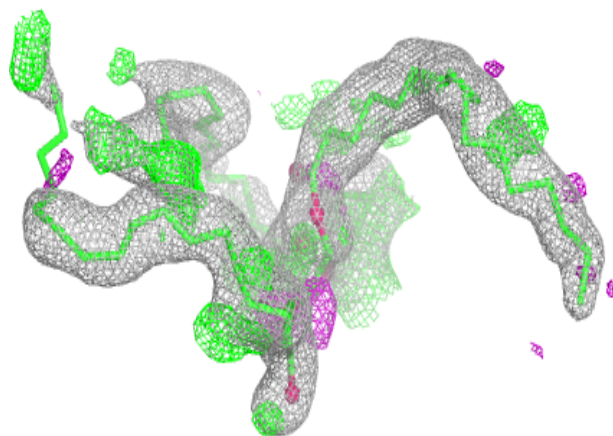
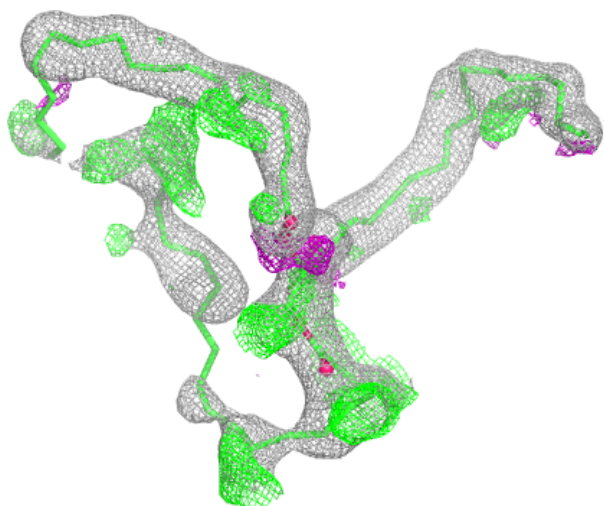
**Electron density around PGV A 608:**

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



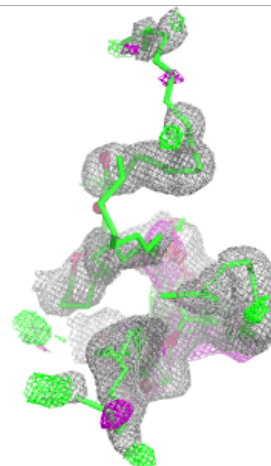
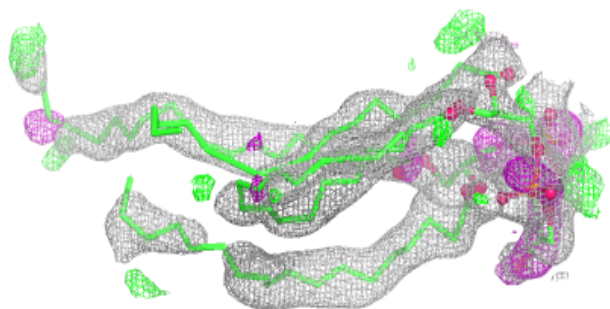
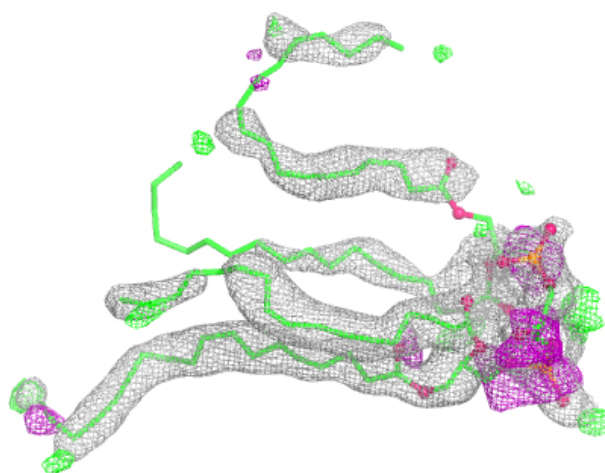
**Electron density around TGL L 101:**

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



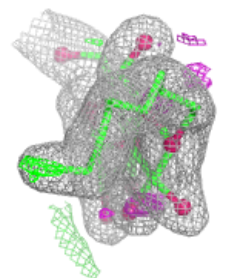
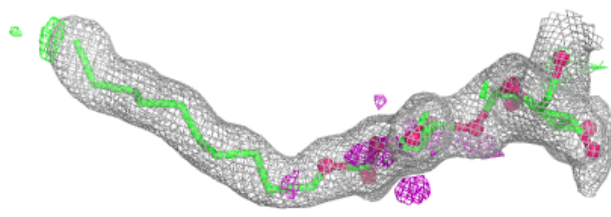
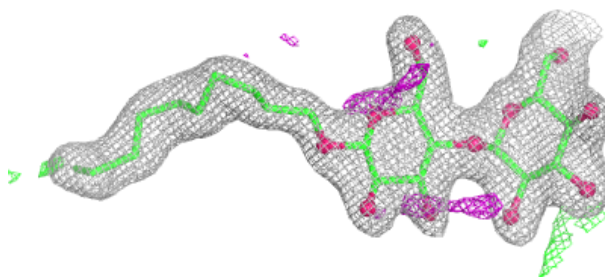
**Electron density around CDL C 303:**

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

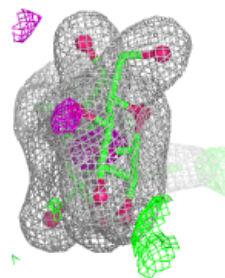
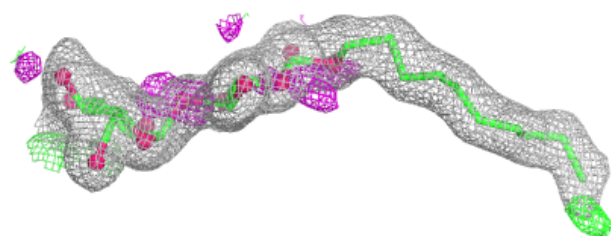
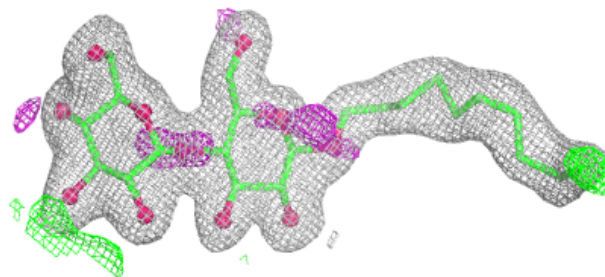


**Electron density around DMU Z 101:**

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

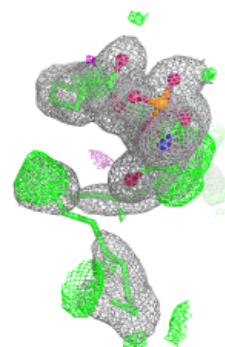
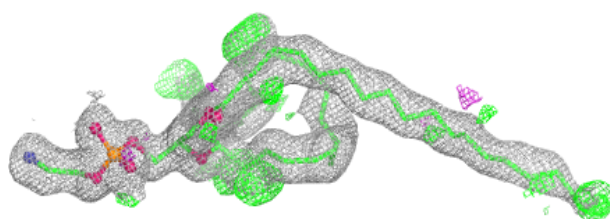
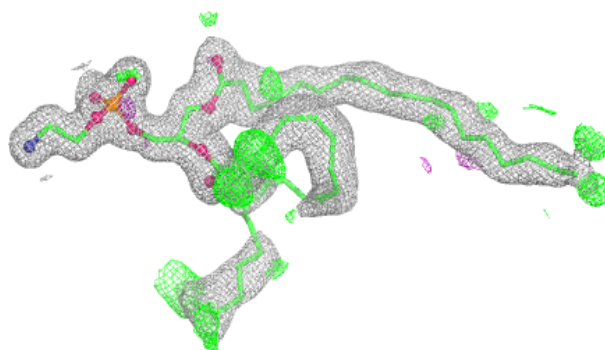
**Electron density around DMU M 101:**

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

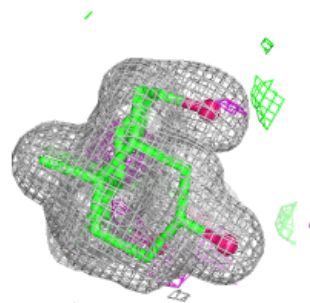
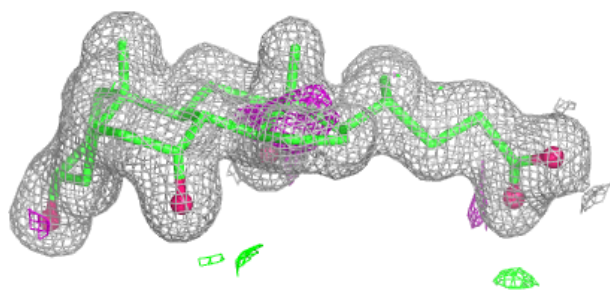
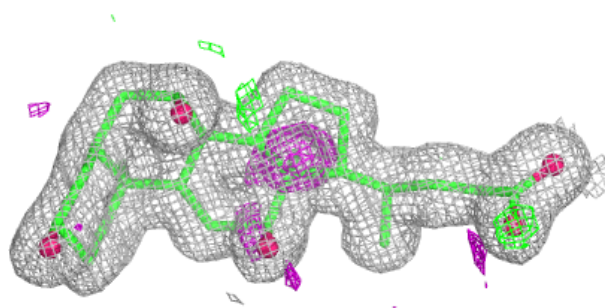


**Electron density around PEK T 101:**

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

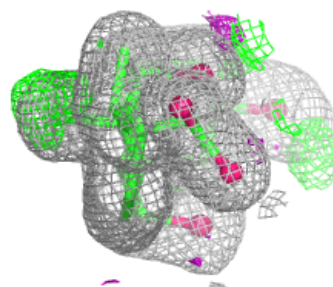
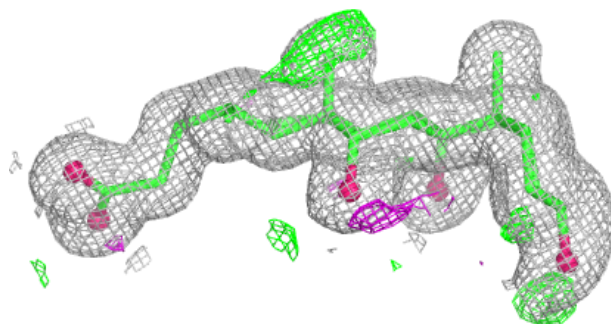
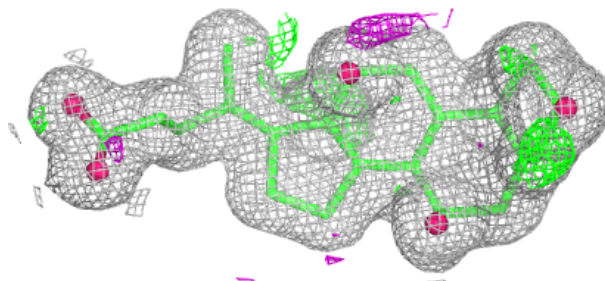
**Electron density around CHD C 305:**

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

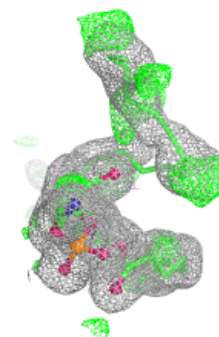
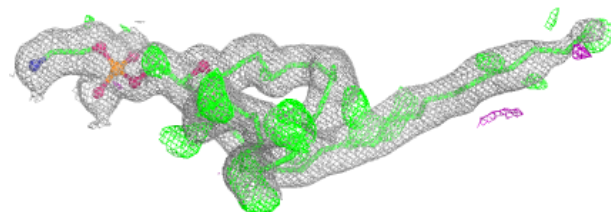
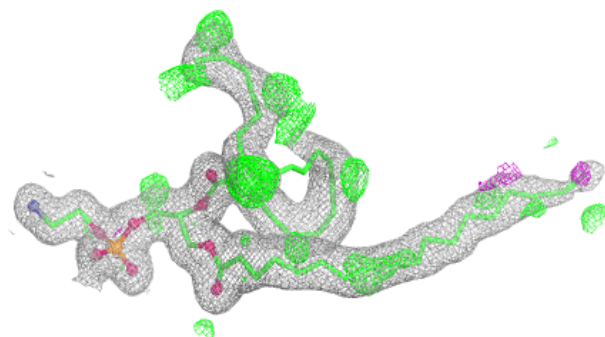


**Electron density around CHD O 302:**

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

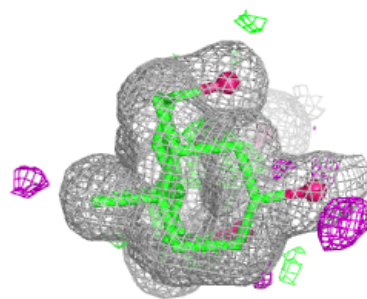
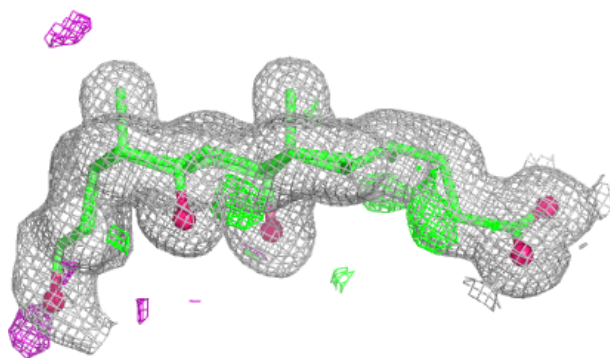
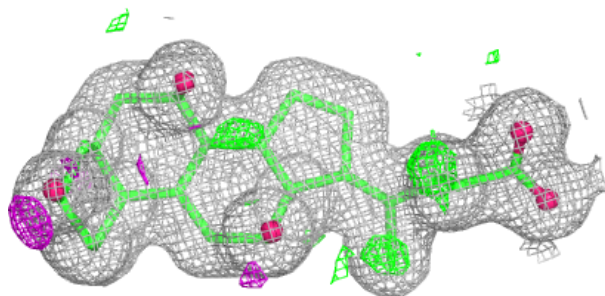
**Electron density around PEK G 101:**

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

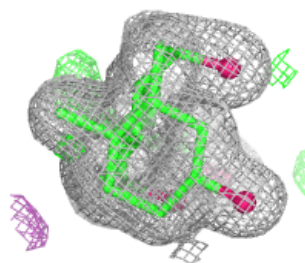
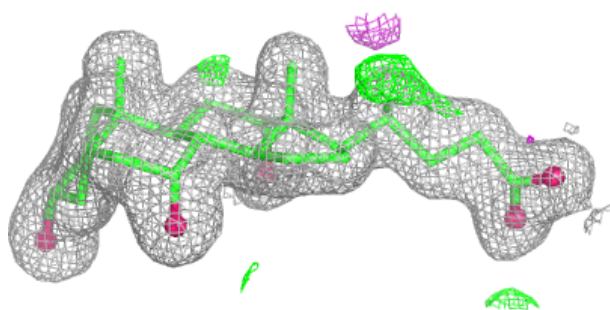
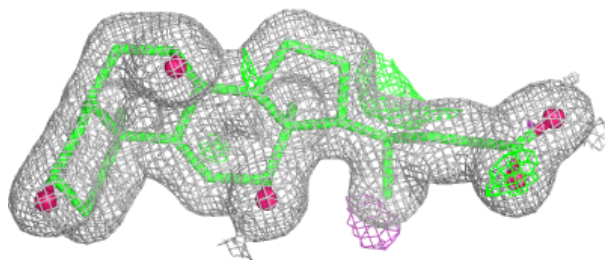


**Electron density around CHD B 303:**

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

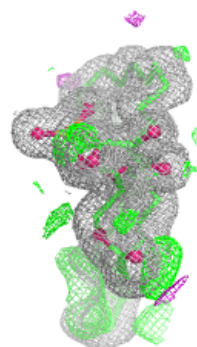
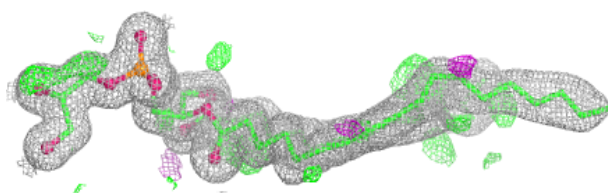
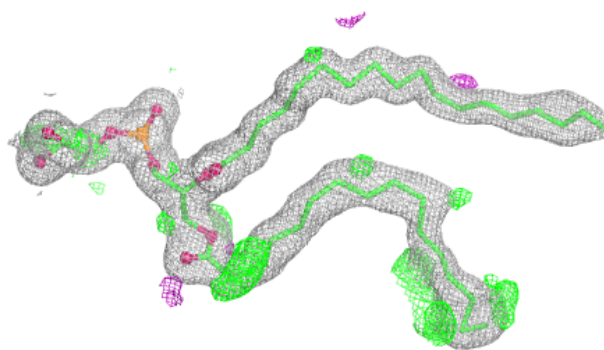
**Electron density around CHD P 307:**

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

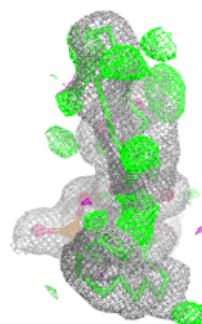
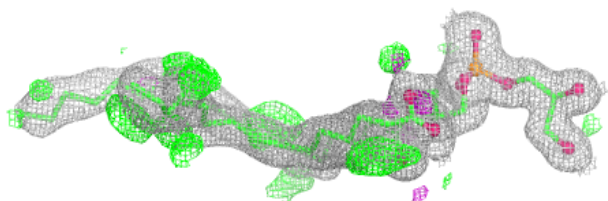
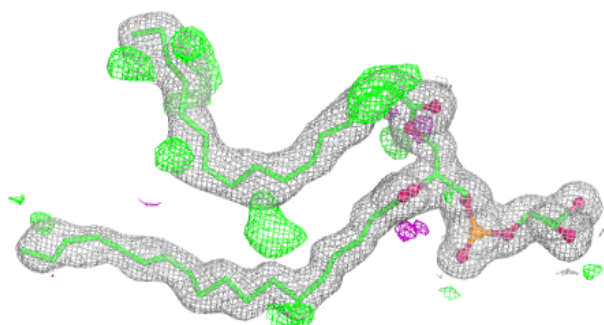


**Electron density around PGV A 607:**

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

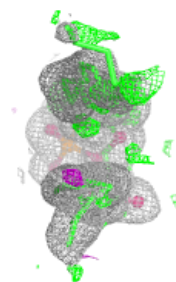
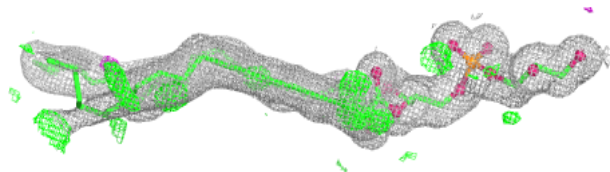
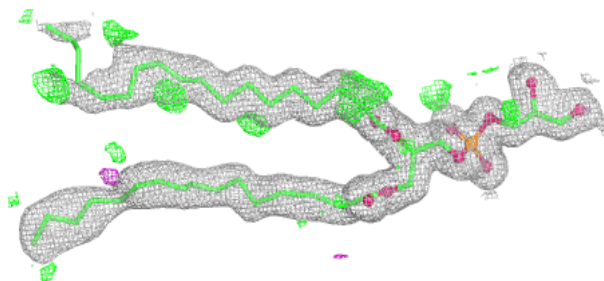
**Electron density around PGV N 607:**

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

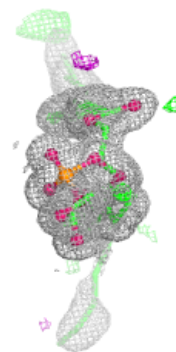
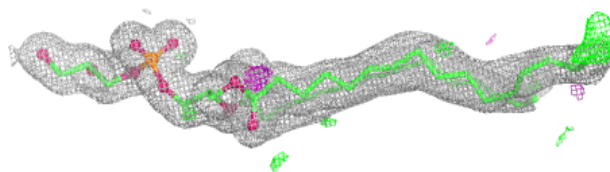
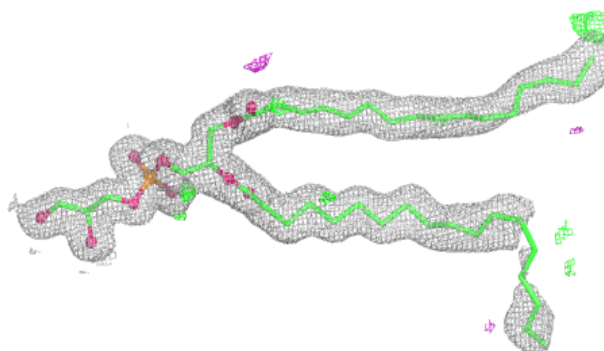


**Electron density around PGV C 302:**

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

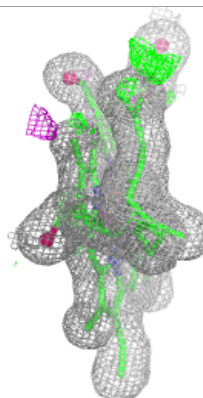
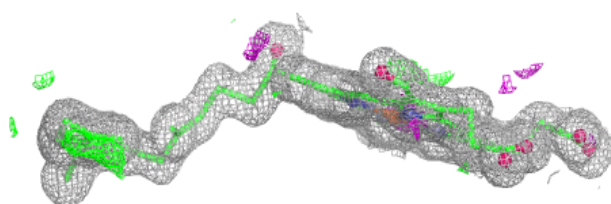
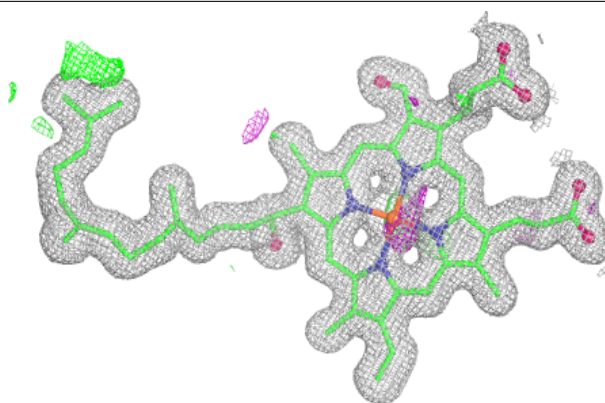
**Electron density around PGV P 303:**

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

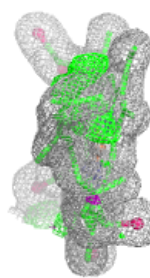
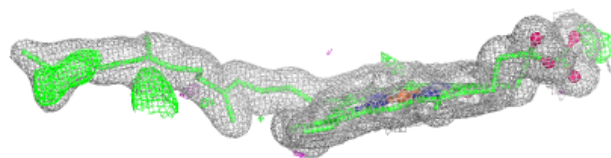
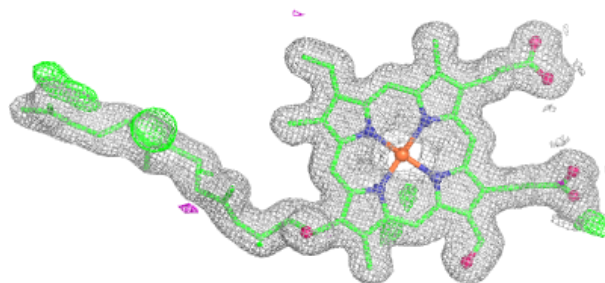


**Electron density around HEA A 602:**

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

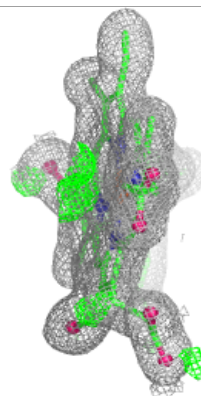
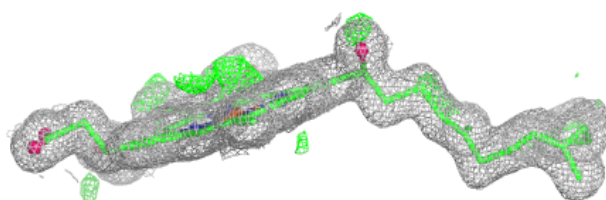
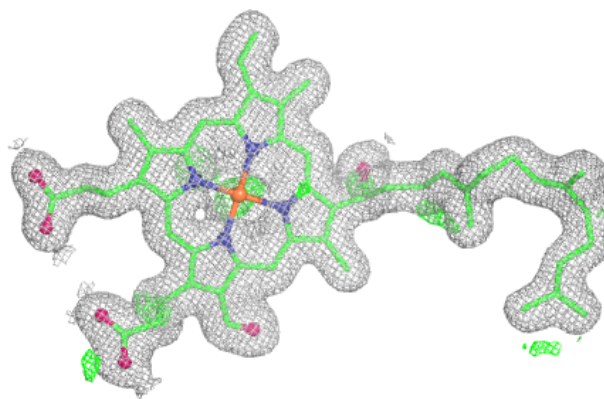
**Electron density around HEA N 601:**

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

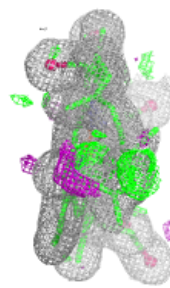
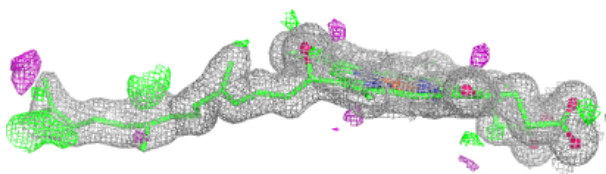
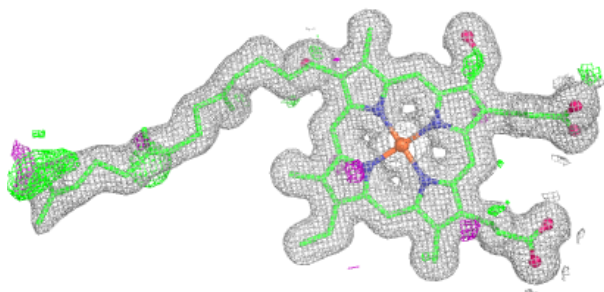


**Electron density around HEA N 602:**

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

**Electron density around HEA A 601:**

$2mF_o-DF_c$  (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.