



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:05 PM UTC

PDB ID : 1V55 / pdb\_00001v55  
Title : Bovine heart cytochrome c oxidase at the fully reduced state  
Authors : Tsukihara, T.; Shimokata, K.; Katayama, Y.; Shimada, H.; Muramoto, K.; Aoyama, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yao, M.; Ishimura, Y.; Yoshikawa, S.  
Deposited on : 2003-11-21  
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

**i**

## X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.

 $(\# \text{Entries, resolution range}(\text{\AA}))$ 

that have poor fit to the electron density. The numeric value is given above the bar.

### Quality of chain

| Company  | 100% Green (%) | 100% Yellow (%) | 100% Red (%) |
|----------|----------------|-----------------|--------------|
| Woolmark | 80%            | 18%             | 2%           |
| Woolmark | 77%            | 21%             | 2%           |
| Woolmark | 78%            | 18%             | 4%           |
| Woolmark | 71%            | 23%             | 6%           |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 261    |                  |
| 3   | P     | 261    |                  |
| 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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 1   | FME  | A     | 1    | -         | -        | X       | -                |
| 18  | TGL  | A     | 3522 | -         | -        | X       | -                |
| 18  | TGL  | N     | 4521 | -         | -        | X       | -                |
| 21  | CHD  | C     | 3271 | X         | -        | -       | -                |
| 21  | CHD  | J     | 3060 | X         | -        | -       | -                |
| 21  | CHD  | P     | 4271 | X         | -        | -       | -                |
| 21  | CHD  | W     | 4060 | X         | -        | -       | -                |
| 22  | CDL  | C     | 3270 | -         | -        | X       | -                |
| 27  | DMU  | M     | 3526 | X         | -        | -       | -                |
| 27  | DMU  | Z     | 4526 | X         | -        | -       | -                |

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32609 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 polypeptide I.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 514      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4027  | 2691 | 623 | 678 | 35 |         |         |       |
| 1   | N     | 514      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4027  | 2691 | 623 | 678 | 35 |         |         |       |

- Molecule 2 is a protein called Cytochrome c oxidase polypeptide II.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 227      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1824  | 1185 | 281 | 340 | 18 |         |         |       |
| 2   | O     | 227      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1824  | 1185 | 281 | 340 | 18 |         |         |       |

- Molecule 3 is a protein called Cytochrome c oxidase polypeptide III.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 259      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2110  | 1412 | 336 | 350 | 12 |         |         |       |
| 3   | P     | 259      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2110  | 1412 | 336 | 350 | 12 |         |         |       |

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

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

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

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

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide Vb.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 748   | 464 | 134 | 145 | 5 |         |         |       |
| 6   | S     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 748   | 464 | 134 | 145 | 5 |         |         |       |

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide VIa-heart.

| Mol | Chain | Residues | Atoms |     |     |     |   |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---|---------|---------|-------|
| 7   | G     | 84       | Total | C   | N   | O   | P | S | 0       | 0       | 0     |
|     |       |          | 675   | 431 | 129 | 113 | 1 | 1 |         |         |       |
| 7   | T     | 84       | Total | C   | N   | O   | P | S | 0       | 0       | 0     |
|     |       |          | 675   | 431 | 129 | 113 | 1 | 1 |         |         |       |

- Molecule 8 is a protein called Cytochrome c oxidase polypeptide VIb.

| 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 polypeptide VIc.

| 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 polypeptide VIIa-heart.

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

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

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide VIIb.

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

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide VIIc.

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

- Molecule 13 is a protein called Cytochrome c oxidase polypeptide VIII-heart.

| 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 COPPER (II) ION (CCD ID: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14  | A     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 14  | N     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

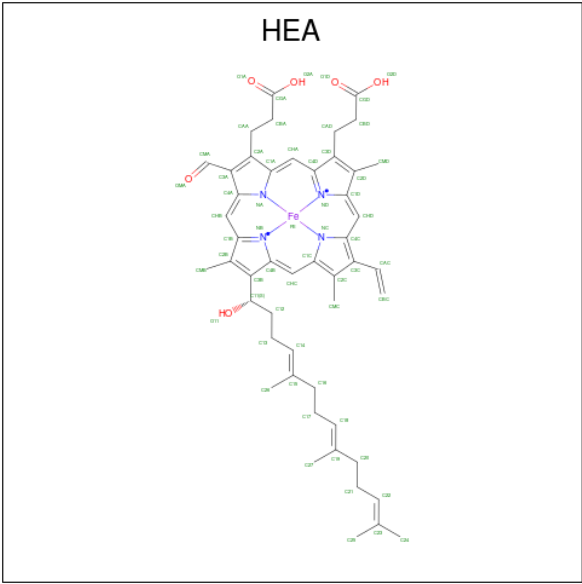
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

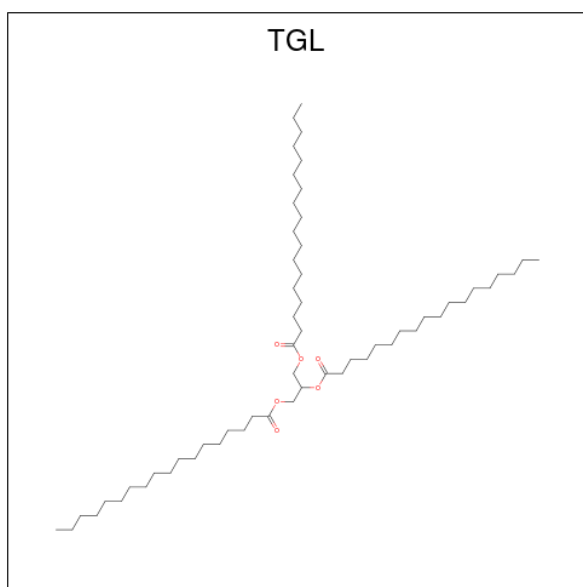
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16  | A     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | N     | 1        | Total | Na | 0       | 0       |
|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

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



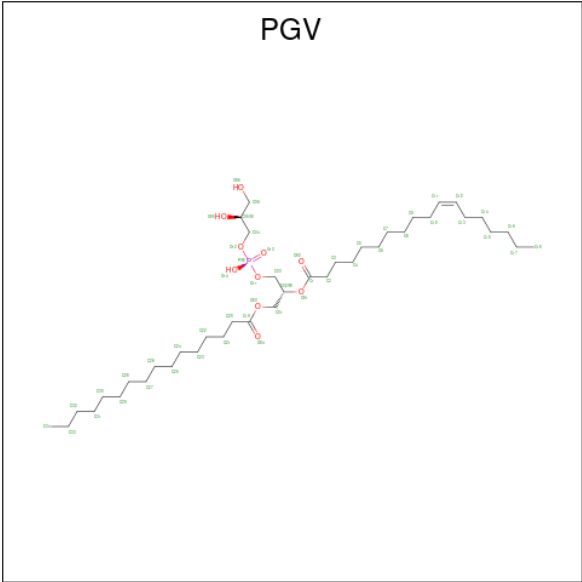
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17  | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |         |
| 17  | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |         |
| 17  | N     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |         |
| 17  | N     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |         |

- Molecule 18 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



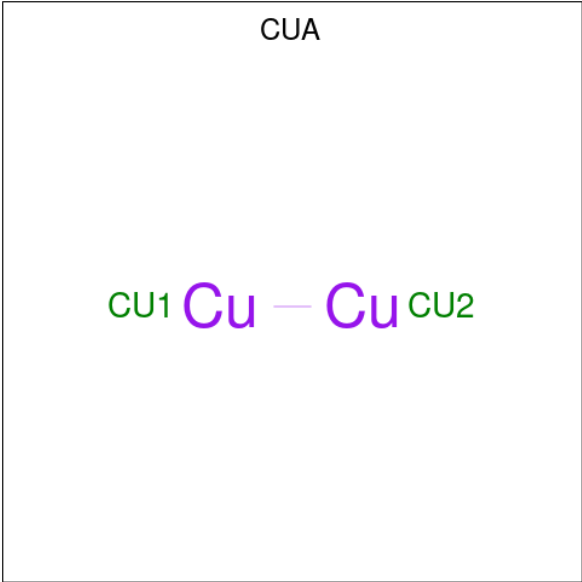
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 18  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 18  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 18  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 18  | N     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 18  | N     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 18  | Q     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |

- 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).



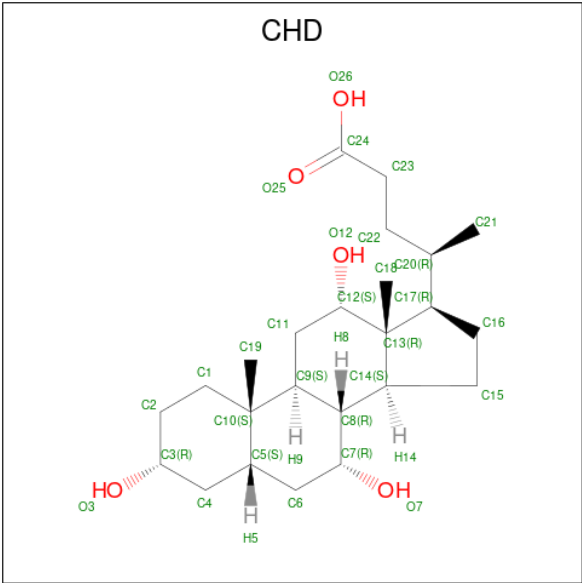
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | A     | 1       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

- Molecule 20 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 20  | B     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 20  | O     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 21 is CHOLIC ACID (CCD ID: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



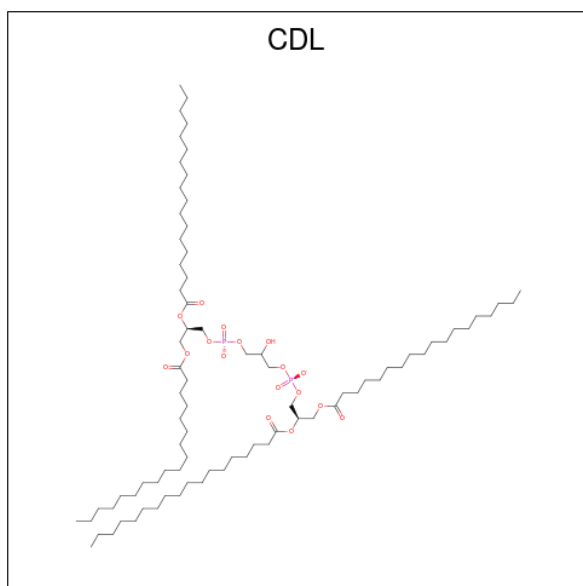
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21  | B     | 1        | Total | C  | O       | 0       |
|     |       |          | 29    | 24 | 5       |         |
| 21  | C     | 1        | Total | C  | O       | 0       |
|     |       |          | 29    | 24 | 5       |         |

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| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | J     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | O     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | W     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |

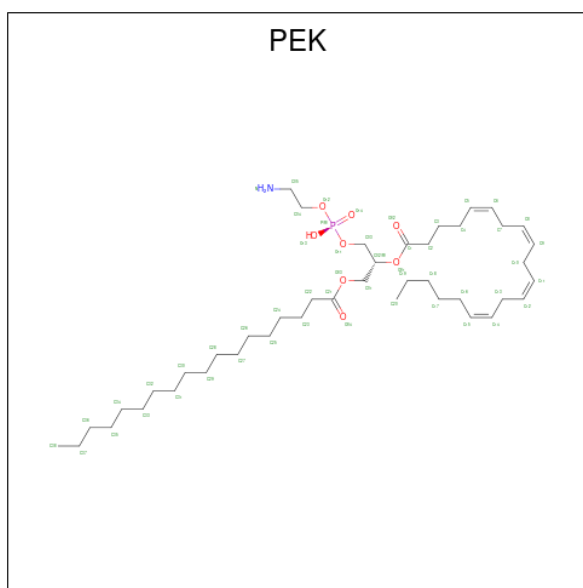
- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 22  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 22  | G     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 22  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 22  | T     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |

- Molecule 23 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE

(CCD ID: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).

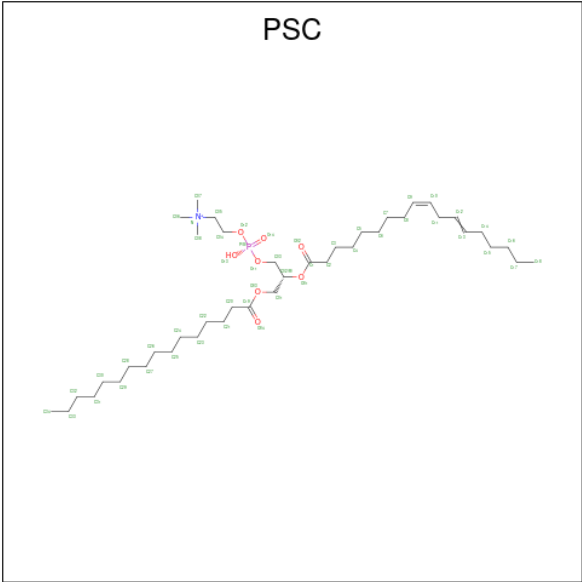


| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 23  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 23  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 23  | G     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 23  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 23  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 23  | T     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |

- Molecule 24 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

- Molecule 25 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).

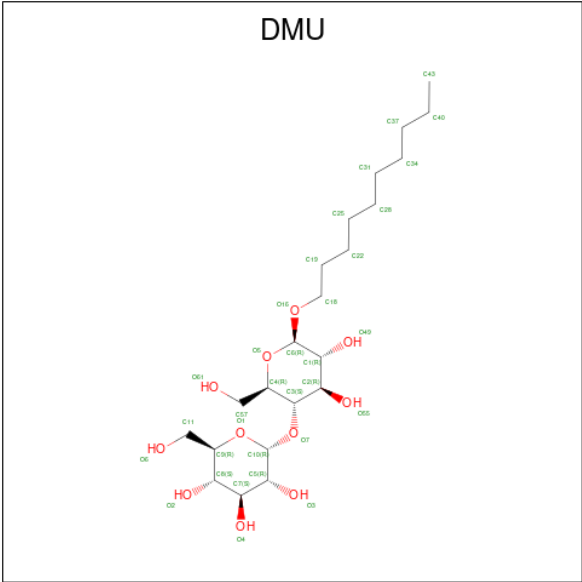


| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 25  | E     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |
| 25  | O     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 26  | F     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 26  | S     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 27 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 |
|-----|-------|----------|-------|----|----|---------|---------|
| 27  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 27  | Z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |

- Molecule 28 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 28  | A     | 229      | Total | O   | 0       | 0       |
|     |       |          | 229   | 229 |         |         |
| 28  | B     | 167      | Total | O   | 0       | 0       |
|     |       |          | 167   | 167 |         |         |
| 28  | C     | 107      | Total | O   | 0       | 0       |
|     |       |          | 107   | 107 |         |         |
| 28  | D     | 112      | Total | O   | 0       | 0       |
|     |       |          | 112   | 112 |         |         |
| 28  | E     | 90       | Total | O   | 0       | 0       |
|     |       |          | 90    | 90  |         |         |
| 28  | F     | 109      | Total | O   | 0       | 0       |
|     |       |          | 109   | 109 |         |         |
| 28  | G     | 54       | Total | O   | 0       | 0       |
|     |       |          | 54    | 54  |         |         |
| 28  | H     | 61       | Total | O   | 0       | 0       |
|     |       |          | 61    | 61  |         |         |
| 28  | I     | 50       | Total | O   | 0       | 0       |
|     |       |          | 50    | 50  |         |         |
| 28  | J     | 34       | Total | O   | 0       | 0       |
|     |       |          | 34    | 34  |         |         |

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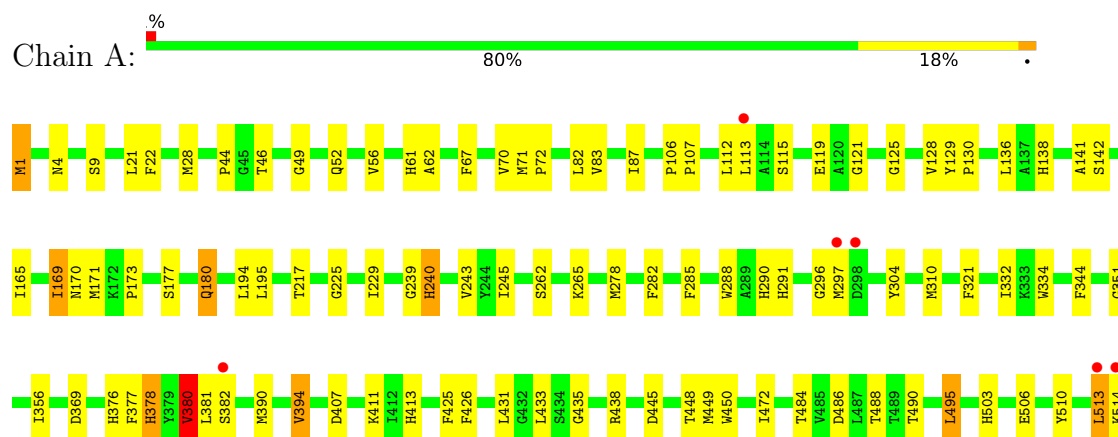
*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 28  | K     | 28       | Total<br>28  | O<br>28  | 0       | 0       |
| 28  | L     | 21       | Total<br>21  | O<br>21  | 0       | 0       |
| 28  | M     | 33       | Total<br>33  | O<br>33  | 0       | 0       |
| 28  | N     | 214      | Total<br>214 | O<br>214 | 0       | 0       |
| 28  | O     | 116      | Total<br>116 | O<br>116 | 0       | 0       |
| 28  | P     | 112      | Total<br>112 | O<br>112 | 0       | 0       |
| 28  | Q     | 72       | Total<br>72  | O<br>72  | 0       | 0       |
| 28  | R     | 48       | Total<br>48  | O<br>48  | 0       | 0       |
| 28  | S     | 77       | Total<br>77  | O<br>77  | 0       | 0       |
| 28  | T     | 48       | Total<br>48  | O<br>48  | 0       | 0       |
| 28  | U     | 54       | Total<br>54  | O<br>54  | 0       | 0       |
| 28  | V     | 32       | Total<br>32  | O<br>32  | 0       | 0       |
| 28  | W     | 20       | Total<br>20  | O<br>20  | 0       | 0       |
| 28  | X     | 20       | Total<br>20  | O<br>20  | 0       | 0       |
| 28  | Y     | 22       | Total<br>22  | O<br>22  | 0       | 0       |
| 28  | Z     | 13       | Total<br>13  | O<br>13  | 0       | 0       |

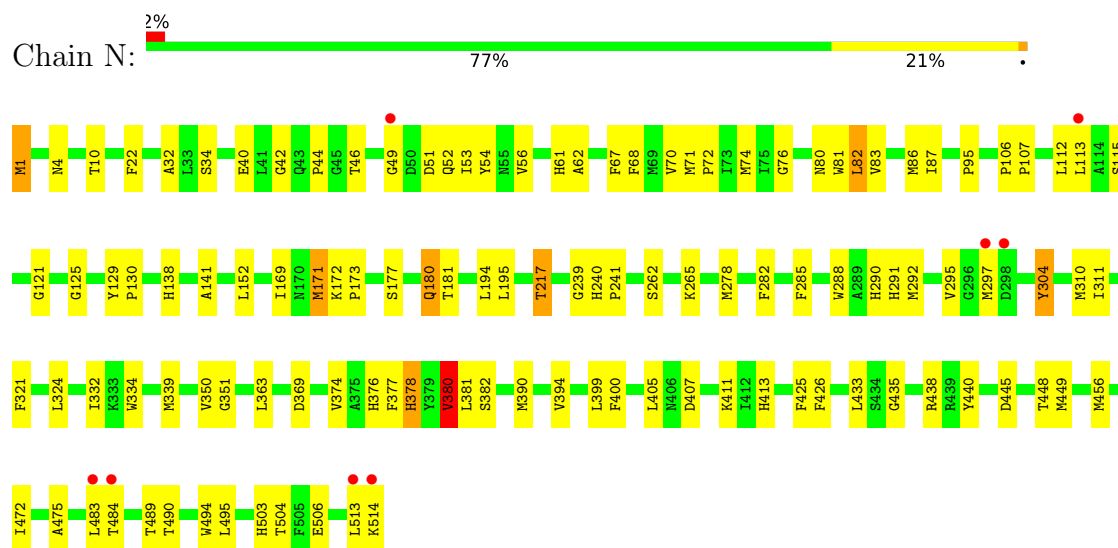
### 3 Residue-property plots

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

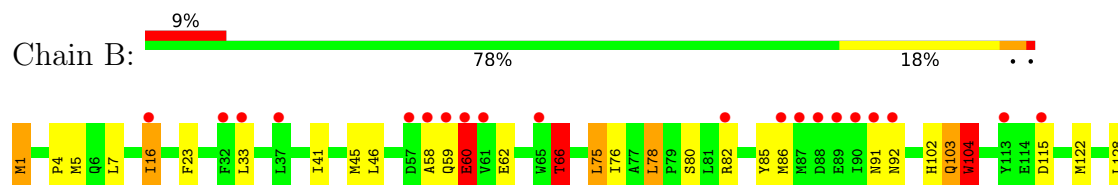
#### • Molecule 1: Cytochrome c oxidase polypeptide I



#### • Molecule 1: Cytochrome c oxidase polypeptide I

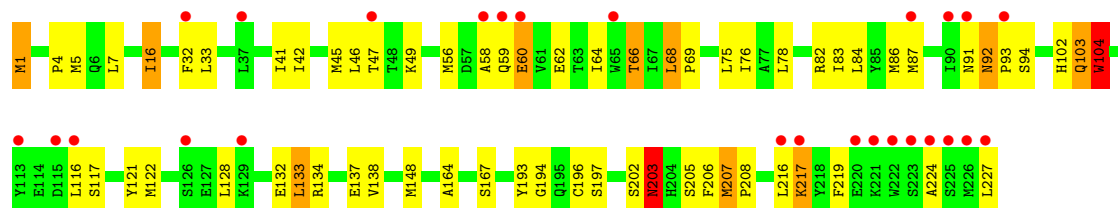


#### • Molecule 2: Cytochrome c oxidase polypeptide II

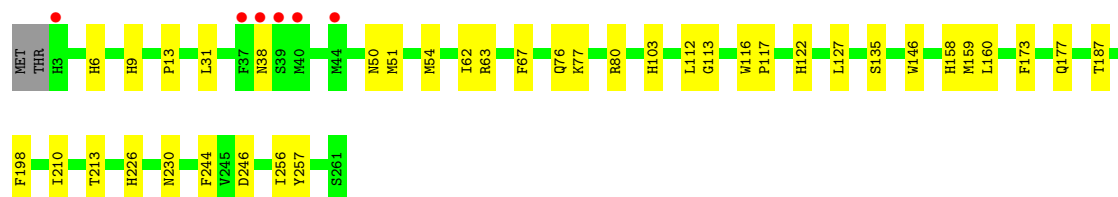
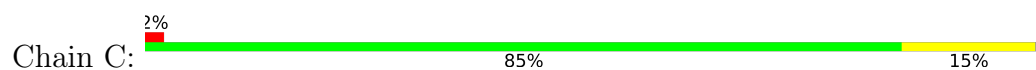




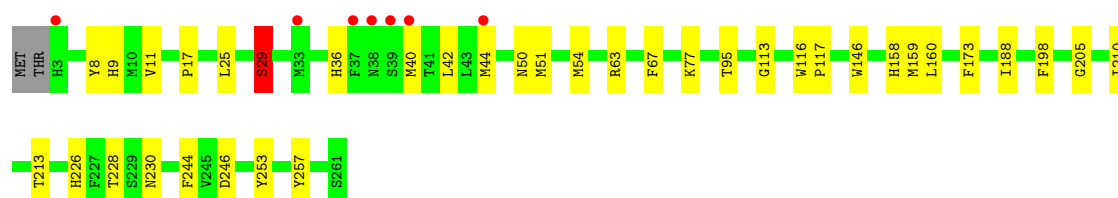
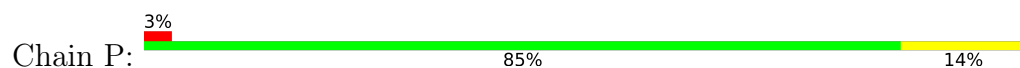
• Molecule 2: Cytochrome c oxidase polypeptide II



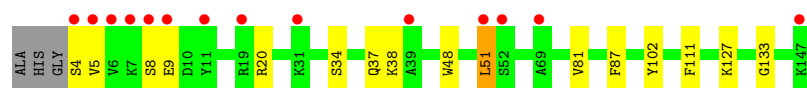
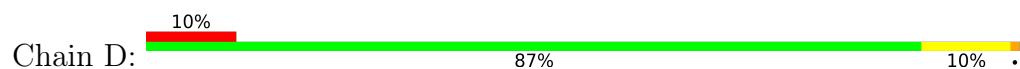
• Molecule 3: Cytochrome c oxidase polypeptide III



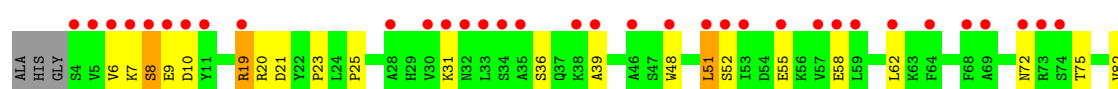
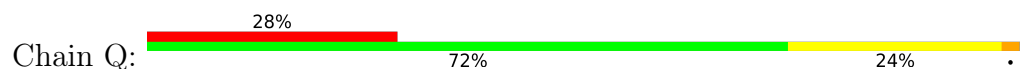
• Molecule 3: Cytochrome c oxidase polypeptide III

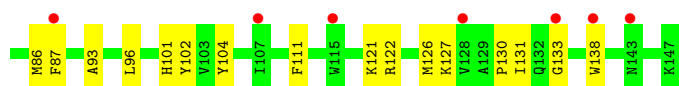


• Molecule 4: Cytochrome c oxidase subunit IV isoform 1

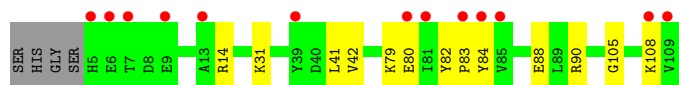
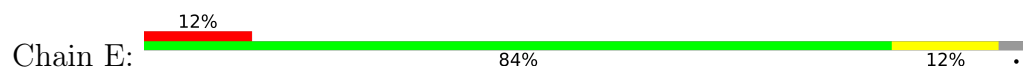


• Molecule 4: Cytochrome c oxidase subunit IV isoform 1

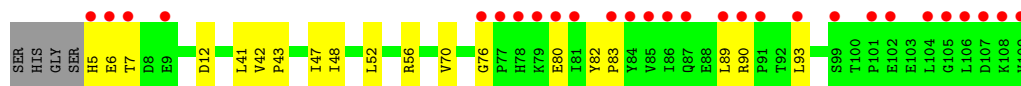
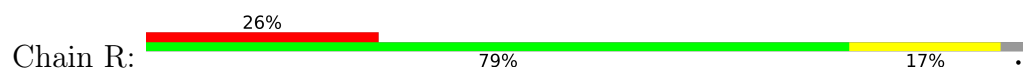




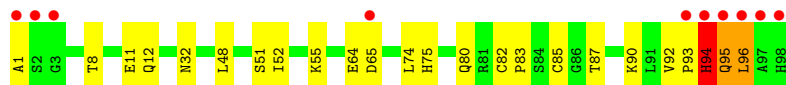
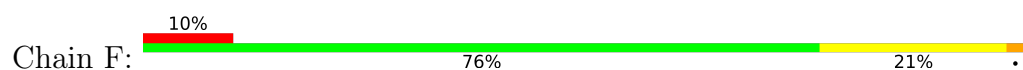
- Molecule 5: Cytochrome c oxidase polypeptide Va



- Molecule 5: Cytochrome c oxidase polypeptide Va



- Molecule 6: Cytochrome c oxidase polypeptide Vb



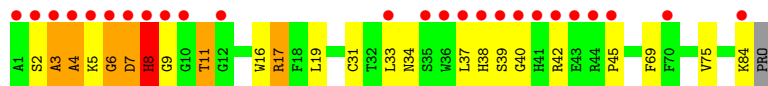
- Molecule 6: Cytochrome c oxidase polypeptide Vb



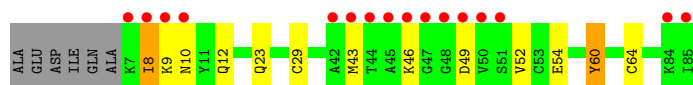
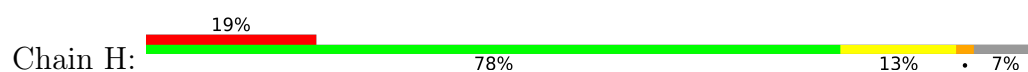
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



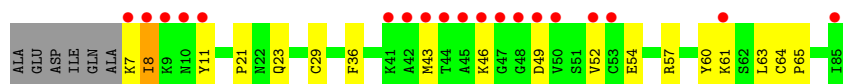
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



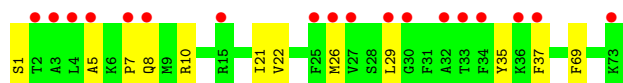
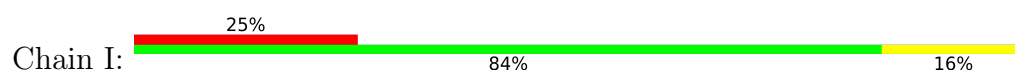
- Molecule 8: Cytochrome c oxidase polypeptide VIIb



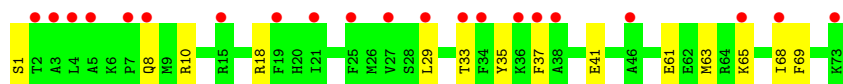
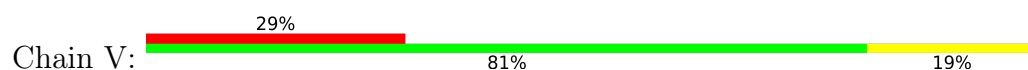
• Molecule 8: Cytochrome c oxidase polypeptide VIIb



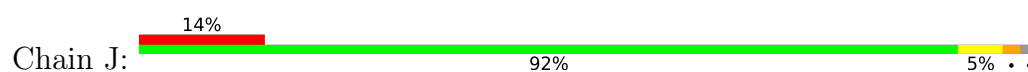
• Molecule 9: Cytochrome c oxidase polypeptide VIc



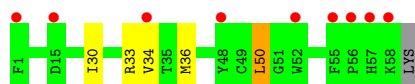
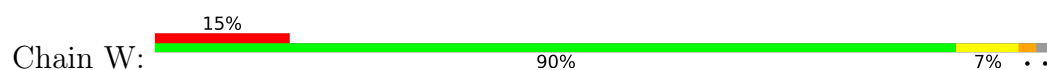
• Molecule 9: Cytochrome c oxidase polypeptide VIc



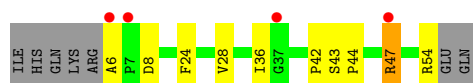
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



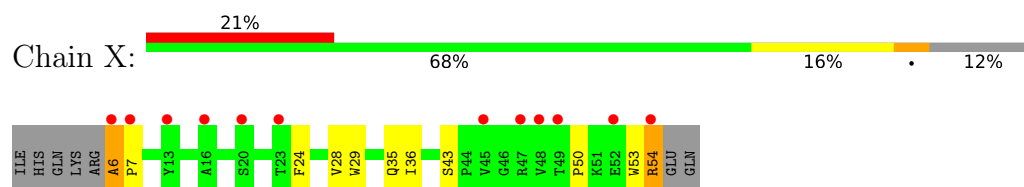
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



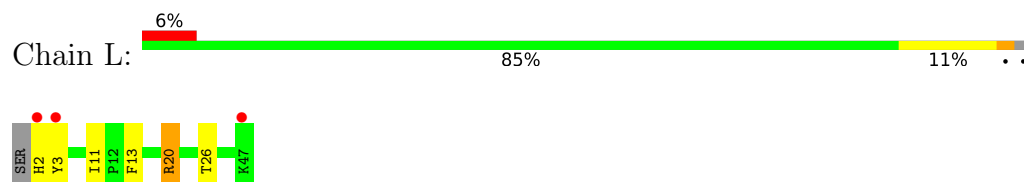
• Molecule 11: Cytochrome c oxidase polypeptide VIIb



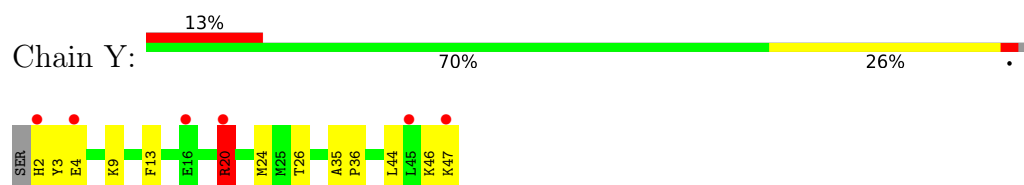
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



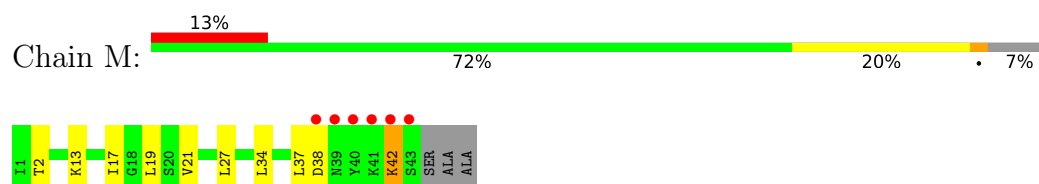
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



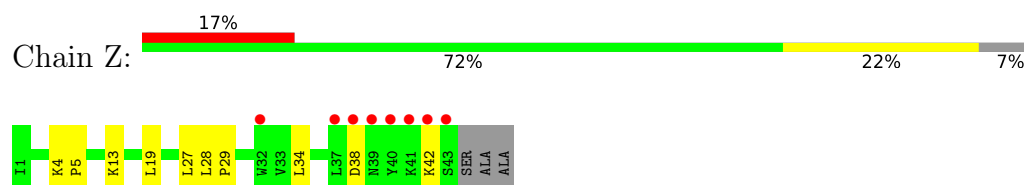
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 183.06Å 206.58Å 178.30Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 40.00 – 1.90<br>40.00 – 1.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (40.00-1.90)<br>98.7 (40.00-1.90)           | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.95 (at 1.90Å)                                             | Xtriage          |
| Refinement program                                                      | X-PLOR                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.203 , 0.230<br>0.205 , 0.206                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 26086 reflections (4.89%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 25.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.539                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 58.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | 0.007 for l,k,h                                             | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 32609                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 35.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: SAC, HEA, TGL, ZN, FME, DMU, TPO, UNX, CUA, CDL, PSC, MG, NA, PGV, PEK, CHD, CU

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 1   | A     | 0.69         | 3/4156 (0.1%)  | 1.09        | 33/5678 (0.6%)   |
| 1   | N     | 0.68         | 3/4156 (0.1%)  | 1.08        | 30/5678 (0.5%)   |
| 2   | B     | 0.64         | 0/1860         | 1.08        | 8/2534 (0.3%)    |
| 2   | O     | 0.64         | 0/1860         | 1.11        | 12/2534 (0.5%)   |
| 3   | C     | 0.59         | 0/2197         | 0.94        | 7/3005 (0.2%)    |
| 3   | P     | 0.59         | 0/2197         | 0.97        | 8/3005 (0.3%)    |
| 4   | D     | 0.58         | 0/1229         | 1.00        | 4/1658 (0.2%)    |
| 4   | Q     | 0.58         | 0/1229         | 1.01        | 2/1658 (0.1%)    |
| 5   | E     | 0.60         | 0/871          | 0.97        | 2/1182 (0.2%)    |
| 5   | R     | 0.59         | 0/871          | 1.08        | 3/1182 (0.3%)    |
| 6   | F     | 0.63         | 0/765          | 1.17        | 6/1038 (0.6%)    |
| 6   | S     | 0.62         | 0/765          | 1.17        | 6/1038 (0.6%)    |
| 7   | G     | 0.62         | 0/690          | 1.02        | 4/937 (0.4%)     |
| 7   | T     | 0.62         | 0/690          | 1.03        | 4/937 (0.4%)     |
| 8   | H     | 0.58         | 0/682          | 1.04        | 5/921 (0.5%)     |
| 8   | U     | 0.58         | 0/682          | 1.08        | 2/921 (0.2%)     |
| 9   | I     | 0.56         | 0/605          | 0.93        | 1/802 (0.1%)     |
| 9   | V     | 0.54         | 0/605          | 0.90        | 1/802 (0.1%)     |
| 10  | J     | 0.55         | 0/471          | 0.94        | 0/636            |
| 10  | W     | 0.53         | 0/471          | 0.96        | 0/636            |
| 11  | K     | 0.65         | 0/398          | 1.13        | 3/546 (0.5%)     |
| 11  | X     | 0.65         | 0/398          | 1.10        | 4/546 (0.7%)     |
| 12  | L     | 0.58         | 0/393          | 0.85        | 1/526 (0.2%)     |
| 12  | Y     | 0.55         | 0/393          | 0.92        | 1/526 (0.2%)     |
| 13  | M     | 0.60         | 0/345          | 0.94        | 1/470 (0.2%)     |
| 13  | Z     | 0.51         | 0/345          | 0.98        | 1/470 (0.2%)     |
| All | All   | 0.62         | 6/29324 (0.0%) | 1.04        | 149/39866 (0.4%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | N     | 0                   | 2                   |
| 2   | B     | 0                   | 2                   |
| 2   | O     | 0                   | 1                   |
| 8   | U     | 0                   | 1                   |
| All | All   | 0                   | 7                   |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | N     | 83  | VAL  | CA-CB   | 5.97 | 1.57        | 1.54     |
| 1   | A     | 130 | PRO  | CA-C    | 5.91 | 1.57        | 1.52     |
| 1   | N     | 378 | HIS  | ND1-CE1 | 5.48 | 1.38        | 1.32     |
| 1   | A     | 503 | HIS  | ND1-CE1 | 5.35 | 1.38        | 1.32     |
| 1   | N     | 503 | HIS  | ND1-CE1 | 5.31 | 1.37        | 1.32     |
| 1   | A     | 83  | VAL  | CA-CB   | 5.10 | 1.57        | 1.54     |

All (149) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | D     | 133 | GLY  | N-CA-C   | 13.09 | 128.33      | 112.49   |
| 4   | Q     | 133 | GLY  | N-CA-C   | 12.78 | 127.95      | 112.49   |
| 6   | F     | 93  | PRO  | N-CA-C   | 11.34 | 127.10      | 111.22   |
| 6   | S     | 93  | PRO  | N-CA-C   | 10.20 | 125.92      | 111.33   |
| 1   | N     | 378 | HIS  | CA-CB-CG | -9.69 | 104.11      | 113.80   |
| 1   | N     | 125 | GLY  | N-CA-C   | -9.59 | 100.88      | 112.48   |
| 1   | A     | 125 | GLY  | N-CA-C   | -9.38 | 101.13      | 112.48   |
| 5   | R     | 42  | VAL  | N-CA-C   | -8.80 | 97.91       | 107.77   |
| 1   | N     | 130 | PRO  | N-CA-C   | -8.35 | 100.52      | 110.70   |
| 6   | S     | 94  | HIS  | N-CA-C   | 7.94  | 127.71      | 110.80   |
| 6   | F     | 94  | HIS  | N-CA-C   | 7.67  | 127.14      | 110.80   |
| 5   | E     | 42  | VAL  | N-CA-C   | -7.60 | 99.26       | 107.77   |
| 1   | N     | 425 | PHE  | N-CA-C   | 7.57  | 122.65      | 113.41   |
| 2   | B     | 104 | TRP  | N-CA-C   | 7.54  | 126.85      | 110.80   |
| 8   | H     | 64  | CYS  | N-CA-C   | 7.33  | 118.88      | 109.65   |
| 1   | A     | 425 | PHE  | N-CA-C   | 7.32  | 122.34      | 113.41   |
| 1   | A     | 130 | PRO  | N-CA-C   | -7.31 | 101.78      | 110.70   |
| 8   | U     | 64  | CYS  | N-CA-C   | 7.15  | 118.65      | 109.65   |
| 11  | X     | 36  | ILE  | N-CA-C   | 7.14  | 119.00      | 112.43   |
| 1   | N     | 70  | VAL  | N-CA-C   | 7.13  | 117.22      | 110.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 61  | HIS  | ND1-CE1-NE2 | 7.12  | 115.52      | 108.40   |
| 12  | Y     | 20  | ARG  | N-CA-C      | -7.06 | 103.66      | 111.36   |
| 2   | B     | 197 | SER  | N-CA-C      | 7.05  | 121.57      | 112.26   |
| 2   | O     | 104 | TRP  | N-CA-C      | 7.03  | 125.77      | 110.80   |
| 1   | N     | 61  | HIS  | ND1-CE1-NE2 | 7.03  | 115.42      | 108.40   |
| 1   | N     | 61  | HIS  | CB-CG-CD2   | -6.98 | 122.13      | 131.20   |
| 5   | R     | 76  | GLY  | CA-C-N      | 6.92  | 127.51      | 120.04   |
| 5   | R     | 76  | GLY  | C-N-CA      | 6.92  | 127.51      | 120.04   |
| 1   | N     | 82  | LEU  | N-CA-C      | 6.88  | 122.01      | 112.45   |
| 1   | N     | 376 | HIS  | CB-CG-CD2   | -6.86 | 122.28      | 131.20   |
| 1   | N     | 262 | SER  | N-CA-C      | -6.85 | 104.67      | 113.16   |
| 2   | O     | 197 | SER  | N-CA-C      | 6.82  | 121.26      | 112.26   |
| 2   | B     | 103 | GLN  | CA-C-N      | 6.79  | 134.51      | 121.54   |
| 2   | B     | 103 | GLN  | C-N-CA      | 6.79  | 134.51      | 121.54   |
| 1   | N     | 288 | TRP  | N-CA-C      | 6.77  | 119.52      | 111.33   |
| 1   | A     | 262 | SER  | N-CA-C      | -6.73 | 104.69      | 113.17   |
| 13  | Z     | 27  | LEU  | N-CA-C      | 6.72  | 118.68      | 111.36   |
| 1   | A     | 169 | ILE  | CB-CA-C     | -6.70 | 103.27      | 112.04   |
| 1   | A     | 70  | VAL  | N-CA-C      | 6.67  | 116.77      | 110.30   |
| 11  | K     | 6   | ALA  | CA-C-N      | 6.64  | 127.00      | 119.83   |
| 11  | K     | 6   | ALA  | C-N-CA      | 6.64  | 127.00      | 119.83   |
| 1   | N     | 503 | HIS  | CB-CG-CD2   | -6.63 | 122.58      | 131.20   |
| 1   | A     | 503 | HIS  | CB-CG-CD2   | -6.59 | 122.64      | 131.20   |
| 1   | A     | 141 | ALA  | N-CA-C      | 6.58  | 120.57      | 112.54   |
| 1   | A     | 82  | LEU  | N-CA-C      | 6.56  | 121.56      | 112.45   |
| 1   | A     | 170 | ASN  | N-CA-C      | 6.42  | 121.19      | 113.23   |
| 6   | S     | 93  | PRO  | CA-C-N      | 6.37  | 133.70      | 121.54   |
| 6   | S     | 93  | PRO  | C-N-CA      | 6.37  | 133.70      | 121.54   |
| 3   | P     | 29  | SER  | N-CA-C      | -6.36 | 104.26      | 111.07   |
| 1   | A     | 288 | TRP  | N-CA-C      | 6.35  | 119.88      | 111.75   |
| 11  | K     | 36  | ILE  | N-CA-C      | 6.31  | 118.24      | 112.43   |
| 1   | N     | 445 | ASP  | N-CA-C      | 6.26  | 118.90      | 111.33   |
| 1   | N     | 448 | THR  | N-CA-C      | 6.23  | 117.73      | 111.07   |
| 1   | N     | 435 | GLY  | N-CA-C      | 6.17  | 124.64      | 115.64   |
| 1   | A     | 435 | GLY  | N-CA-C      | 6.08  | 124.53      | 115.64   |
| 3   | P     | 257 | TYR  | N-CA-C      | 6.06  | 117.68      | 111.14   |
| 1   | N     | 438 | ARG  | N-CA-C      | -6.04 | 102.74      | 110.53   |
| 4   | D     | 8   | SER  | N-CA-C      | 6.02  | 117.51      | 111.07   |
| 1   | A     | 445 | ASP  | N-CA-C      | 6.00  | 118.58      | 111.33   |
| 1   | A     | 438 | ARG  | N-CA-C      | -5.95 | 102.85      | 110.53   |
| 3   | P     | 113 | GLY  | N-CA-C      | -5.95 | 106.96      | 115.64   |
| 3   | C     | 198 | PHE  | N-CA-C      | 5.93  | 117.82      | 111.36   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 12  | L     | 20  | ARG  | N-CA-C    | -5.91 | 104.92      | 111.36   |
| 9   | V     | 69  | PHE  | N-CA-C    | 5.89  | 119.69      | 110.32   |
| 1   | A     | 171 | MET  | N-CA-C    | 5.89  | 120.17      | 111.87   |
| 3   | P     | 198 | PHE  | N-CA-C    | 5.87  | 117.76      | 111.36   |
| 8   | H     | 10  | ASN  | CA-C-N    | 5.85  | 129.07      | 120.82   |
| 8   | H     | 10  | ASN  | C-N-CA    | 5.85  | 129.07      | 120.82   |
| 1   | N     | 380 | VAL  | CB-CA-C   | -5.84 | 104.37      | 112.02   |
| 4   | D     | 5   | VAL  | N-CA-C    | 5.79  | 115.89      | 108.12   |
| 1   | A     | 239 | GLY  | N-CA-C    | 5.78  | 119.63      | 112.64   |
| 2   | B     | 66  | THR  | N-CA-C    | -5.77 | 105.51      | 113.18   |
| 1   | A     | 217 | THR  | N-CA-C    | -5.77 | 103.09      | 110.53   |
| 9   | I     | 69  | PHE  | N-CA-C    | 5.75  | 119.47      | 110.32   |
| 3   | C     | 113 | GLY  | N-CA-C    | -5.75 | 107.25      | 115.64   |
| 2   | O     | 58  | ALA  | N-CA-C    | 5.74  | 120.42      | 113.41   |
| 1   | A     | 506 | GLU  | N-CA-C    | -5.70 | 105.16      | 111.71   |
| 1   | N     | 332 | ILE  | N-CA-C    | 5.69  | 116.61      | 108.93   |
| 1   | N     | 171 | MET  | N-CA-C    | 5.67  | 119.86      | 111.87   |
| 1   | N     | 141 | ALA  | N-CA-C    | 5.66  | 119.45      | 112.54   |
| 6   | F     | 82  | CYS  | CA-C-N    | 5.65  | 125.49      | 119.28   |
| 6   | F     | 82  | CYS  | C-N-CA    | 5.65  | 125.49      | 119.28   |
| 6   | F     | 12  | GLN  | N-CA-C    | 5.60  | 121.90      | 114.12   |
| 13  | M     | 27  | LEU  | N-CA-C    | 5.59  | 118.56      | 111.69   |
| 1   | A     | 503 | HIS  | CB-CG-ND1 | 5.57  | 131.06      | 122.70   |
| 1   | N     | 503 | HIS  | CB-CG-ND1 | 5.57  | 131.06      | 122.70   |
| 2   | O     | 103 | GLN  | CA-C-N    | 5.57  | 132.17      | 121.54   |
| 2   | O     | 103 | GLN  | C-N-CA    | 5.57  | 132.17      | 121.54   |
| 1   | A     | 332 | ILE  | N-CA-C    | 5.55  | 116.42      | 108.93   |
| 1   | A     | 448 | THR  | N-CA-C    | 5.53  | 117.31      | 111.28   |
| 1   | A     | 9   | SER  | N-CA-C    | 5.50  | 117.83      | 110.35   |
| 1   | A     | 495 | LEU  | N-CA-C    | 5.49  | 119.60      | 113.01   |
| 3   | C     | 256 | ILE  | N-CA-C    | 5.49  | 116.15      | 110.82   |
| 1   | A     | 142 | SER  | N-CA-C    | 5.49  | 117.71      | 111.02   |
| 2   | B     | 133 | LEU  | N-CA-C    | 5.48  | 117.64      | 109.25   |
| 7   | G     | 69  | PHE  | N-CA-C    | 5.48  | 117.69      | 111.11   |
| 3   | P     | 159 | MET  | N-CA-C    | -5.45 | 105.25      | 111.14   |
| 3   | C     | 257 | TYR  | N-CA-C    | 5.45  | 117.30      | 111.36   |
| 2   | O     | 133 | LEU  | N-CA-C    | 5.42  | 117.54      | 109.25   |
| 2   | O     | 47  | THR  | N-CA-C    | 5.42  | 119.04      | 111.30   |
| 1   | A     | 129 | TYR  | N-CA-C    | 5.41  | 117.27      | 109.48   |
| 2   | O     | 203 | ASN  | N-CA-C    | 5.41  | 118.68      | 112.57   |
| 8   | H     | 54  | GLU  | N-CA-C    | 5.40  | 117.59      | 111.11   |
| 6   | S     | 49  | VAL  | N-CA-C    | 5.39  | 112.89      | 107.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 67  | PHE  | N-CA-C      | 5.39  | 119.02      | 112.23   |
| 1   | N     | 217 | THR  | N-CA-C      | -5.39 | 103.58      | 110.53   |
| 1   | N     | 129 | TYR  | N-CA-C      | 5.37  | 116.66      | 109.83   |
| 7   | T     | 75  | VAL  | N-CA-C      | 5.37  | 118.89      | 113.47   |
| 1   | A     | 378 | HIS  | CA-CB-CG    | -5.36 | 108.44      | 113.80   |
| 1   | N     | 495 | LEU  | N-CA-C      | 5.36  | 119.30      | 112.87   |
| 1   | A     | 380 | VAL  | CB-CA-C     | -5.36 | 104.83      | 112.22   |
| 4   | D     | 102 | TYR  | N-CA-C      | 5.33  | 120.06      | 113.50   |
| 3   | C     | 159 | MET  | N-CA-C      | -5.33 | 105.38      | 111.14   |
| 6   | F     | 32  | ASN  | N-CA-C      | 5.33  | 118.55      | 111.30   |
| 7   | G     | 75  | VAL  | N-CA-C      | 5.32  | 118.85      | 113.47   |
| 8   | H     | 12  | GLN  | N-CA-C      | -5.32 | 104.46      | 111.96   |
| 1   | N     | 74  | MET  | N-CA-C      | 5.32  | 116.88      | 111.14   |
| 1   | N     | 67  | PHE  | N-CA-C      | 5.31  | 118.92      | 112.23   |
| 4   | Q     | 8   | SER  | N-CA-C      | 5.31  | 117.48      | 111.11   |
| 8   | U     | 63  | LEU  | N-CA-C      | 5.28  | 119.79      | 112.45   |
| 1   | N     | 61  | HIS  | ND1-CG-CD2  | 5.28  | 111.38      | 106.10   |
| 5   | E     | 79  | LYS  | N-CA-C      | 5.25  | 119.17      | 112.87   |
| 6   | S     | 12  | GLN  | N-CA-C      | 5.25  | 121.08      | 114.31   |
| 3   | P     | 36  | HIS  | N-CA-C      | 5.25  | 120.55      | 114.04   |
| 3   | C     | 9   | HIS  | N-CA-C      | 5.24  | 117.29      | 108.96   |
| 1   | A     | 376 | HIS  | CB-CG-CD2   | -5.23 | 124.40      | 131.20   |
| 3   | P     | 9   | HIS  | N-CA-C      | 5.23  | 117.25      | 108.73   |
| 1   | N     | 239 | GLY  | N-CA-C      | 5.23  | 118.96      | 112.64   |
| 3   | P     | 228 | THR  | N-CA-C      | -5.18 | 102.39      | 110.42   |
| 2   | B     | 161 | HIS  | N-CA-C      | -5.18 | 101.56      | 108.86   |
| 7   | T     | 8   | HIS  | N-CA-C      | 5.16  | 121.80      | 110.80   |
| 1   | N     | 10  | THR  | N-CA-C      | -5.15 | 104.81      | 111.71   |
| 7   | G     | 6   | GLY  | N-CA-C      | 5.15  | 125.38      | 113.18   |
| 3   | C     | 6   | HIS  | N-CA-C      | -5.13 | 101.96      | 109.81   |
| 1   | A     | 438 | ARG  | CB-CA-C     | -5.10 | 99.84       | 110.40   |
| 1   | A     | 378 | HIS  | ND1-CE1-NE2 | 5.08  | 113.48      | 108.40   |
| 2   | O     | 64  | ILE  | CB-CA-C     | -5.08 | 105.47      | 111.81   |
| 2   | O     | 193 | TYR  | N-CA-C      | 5.07  | 118.00      | 110.14   |
| 1   | A     | 119 | GLU  | CB-CA-C     | -5.05 | 110.73      | 116.54   |
| 7   | G     | 8   | HIS  | N-CA-C      | 5.04  | 121.54      | 110.80   |
| 1   | N     | 506 | GLU  | N-CA-C      | -5.04 | 105.92      | 111.71   |
| 7   | T     | 69  | PHE  | N-CA-C      | 5.04  | 117.15      | 111.11   |
| 2   | B     | 58  | ALA  | N-CA-C      | 5.01  | 119.53      | 113.41   |
| 11  | X     | 35  | GLN  | N-CA-C      | 5.01  | 120.01      | 113.30   |
| 7   | T     | 6   | GLY  | N-CA-C      | 5.01  | 125.05      | 113.18   |
| 11  | X     | 6   | ALA  | CA-C-N      | 5.00  | 125.23      | 119.83   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 11  | X     | 6   | ALA  | C-N-CA | 5.00 | 125.23      | 119.83   |
| 2   | O     | 207 | MET  | CA-C-N | 5.00 | 125.01      | 120.21   |
| 2   | O     | 207 | MET  | C-N-CA | 5.00 | 125.01      | 120.21   |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 240 | HIS  | Sidechain |
| 2   | B     | 103 | GLN  | Mainchain |
| 2   | B     | 85  | TYR  | Sidechain |
| 1   | N     | 240 | HIS  | Sidechain |
| 1   | N     | 304 | TYR  | Sidechain |
| 2   | O     | 103 | GLN  | Mainchain |
| 8   | U     | 11  | TYR  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4027  | 0        | 4001     | 69      | 0            |
| 1   | N     | 4027  | 0        | 4001     | 83      | 0            |
| 2   | B     | 1824  | 0        | 1833     | 33      | 0            |
| 2   | O     | 1824  | 0        | 1833     | 47      | 0            |
| 3   | C     | 2110  | 0        | 2027     | 32      | 0            |
| 3   | P     | 2110  | 0        | 2027     | 30      | 0            |
| 4   | D     | 1195  | 0        | 1183     | 13      | 0            |
| 4   | Q     | 1195  | 0        | 1183     | 30      | 0            |
| 5   | E     | 852   | 0        | 845      | 7       | 0            |
| 5   | R     | 852   | 0        | 845      | 10      | 0            |
| 6   | F     | 748   | 0        | 728      | 13      | 0            |
| 6   | S     | 748   | 0        | 728      | 19      | 0            |
| 7   | G     | 675   | 0        | 644      | 26      | 0            |
| 7   | T     | 675   | 0        | 644      | 25      | 0            |
| 8   | H     | 662   | 0        | 623      | 5       | 0            |
| 8   | U     | 662   | 0        | 623      | 8       | 0            |
| 9   | I     | 601   | 0        | 613      | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | V     | 601   | 0        | 613      | 6       | 0            |
| 10  | J     | 460   | 0        | 459      | 4       | 0            |
| 10  | W     | 460   | 0        | 459      | 4       | 0            |
| 11  | K     | 384   | 0        | 366      | 5       | 0            |
| 11  | X     | 384   | 0        | 366      | 10      | 0            |
| 12  | L     | 380   | 0        | 380      | 14      | 0            |
| 12  | Y     | 380   | 0        | 380      | 11      | 0            |
| 13  | M     | 335   | 0        | 352      | 6       | 0            |
| 13  | Z     | 335   | 0        | 352      | 3       | 0            |
| 14  | A     | 1     | 0        | 0        | 0       | 0            |
| 14  | N     | 1     | 0        | 0        | 0       | 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     | 120   | 0        | 108      | 3       | 0            |
| 17  | N     | 120   | 0        | 108      | 3       | 0            |
| 18  | A     | 189   | 0        | 330      | 47      | 0            |
| 18  | N     | 126   | 0        | 220      | 41      | 0            |
| 18  | Q     | 63    | 0        | 110      | 6       | 0            |
| 19  | A     | 102   | 0        | 152      | 7       | 0            |
| 19  | C     | 102   | 0        | 152      | 10      | 0            |
| 19  | N     | 102   | 0        | 152      | 6       | 0            |
| 19  | P     | 102   | 0        | 152      | 7       | 0            |
| 20  | B     | 2     | 0        | 0        | 0       | 0            |
| 20  | O     | 2     | 0        | 0        | 0       | 0            |
| 21  | B     | 29    | 0        | 39       | 1       | 0            |
| 21  | C     | 58    | 0        | 78       | 4       | 0            |
| 21  | J     | 29    | 0        | 39       | 3       | 0            |
| 21  | O     | 29    | 0        | 39       | 0       | 0            |
| 21  | P     | 58    | 0        | 78       | 2       | 0            |
| 21  | W     | 29    | 0        | 39       | 3       | 0            |
| 22  | C     | 100   | 0        | 156      | 23      | 0            |
| 22  | G     | 100   | 0        | 156      | 17      | 0            |
| 22  | P     | 100   | 0        | 156      | 20      | 0            |
| 22  | T     | 100   | 0        | 156      | 20      | 0            |
| 23  | C     | 106   | 0        | 154      | 13      | 0            |
| 23  | G     | 53    | 0        | 77       | 6       | 0            |
| 23  | P     | 106   | 0        | 154      | 8       | 0            |
| 23  | T     | 53    | 0        | 77       | 8       | 0            |
| 24  | C     | 1     | 0        | 0        | 0       | 0            |
| 24  | P     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25  | E     | 52    | 0        | 80       | 12      | 0            |
| 25  | O     | 52    | 0        | 80       | 11      | 0            |
| 26  | F     | 1     | 0        | 0        | 0       | 0            |
| 26  | S     | 1     | 0        | 0        | 0       | 0            |
| 27  | M     | 33    | 0        | 37       | 0       | 0            |
| 27  | Z     | 33    | 0        | 37       | 0       | 0            |
| 28  | A     | 229   | 0        | 0        | 6       | 0            |
| 28  | B     | 167   | 0        | 0        | 2       | 0            |
| 28  | C     | 107   | 0        | 0        | 4       | 0            |
| 28  | D     | 112   | 0        | 0        | 3       | 0            |
| 28  | E     | 90    | 0        | 0        | 1       | 0            |
| 28  | F     | 109   | 0        | 0        | 1       | 0            |
| 28  | G     | 54    | 0        | 0        | 3       | 0            |
| 28  | H     | 61    | 0        | 0        | 2       | 0            |
| 28  | I     | 50    | 0        | 0        | 3       | 0            |
| 28  | J     | 34    | 0        | 0        | 2       | 0            |
| 28  | K     | 28    | 0        | 0        | 0       | 0            |
| 28  | L     | 21    | 0        | 0        | 1       | 0            |
| 28  | M     | 33    | 0        | 0        | 1       | 0            |
| 28  | N     | 214   | 0        | 0        | 3       | 0            |
| 28  | O     | 116   | 0        | 0        | 1       | 0            |
| 28  | P     | 112   | 0        | 0        | 4       | 0            |
| 28  | Q     | 72    | 0        | 0        | 3       | 0            |
| 28  | R     | 48    | 0        | 0        | 0       | 0            |
| 28  | S     | 77    | 0        | 0        | 3       | 0            |
| 28  | T     | 48    | 0        | 0        | 2       | 0            |
| 28  | U     | 54    | 0        | 0        | 1       | 0            |
| 28  | V     | 32    | 0        | 0        | 2       | 0            |
| 28  | W     | 20    | 0        | 0        | 0       | 0            |
| 28  | X     | 20    | 0        | 0        | 1       | 0            |
| 28  | Y     | 22    | 0        | 0        | 0       | 0            |
| 28  | Z     | 13    | 0        | 0        | 1       | 0            |
| All | All   | 32609 | 0        | 31224    | 600     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (600) 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) |
|----------------|--------------|--------------------------|-------------------|
| 7:T:84:LYS:HD2 | 7:T:84:LYS:H | 1.21                     | 1.03              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G:84:LYS:H       | 7:G:84:LYS:HD2     | 1.21                     | 1.03              |
| 10:W:33:ARG:HG2    | 21:W:4060:CHD:H152 | 1.42                     | 0.99              |
| 18:A:3522:TGL:HC32 | 12:L:20:ARG:HH22   | 1.29                     | 0.98              |
| 4:D:34:SER:H       | 4:D:37:GLN:HE21    | 1.14                     | 0.92              |
| 10:J:33:ARG:HG2    | 21:J:3060:CHD:H152 | 1.51                     | 0.92              |
| 22:C:3270:CDL:H242 | 22:C:3270:CDL:H661 | 1.54                     | 0.89              |
| 22:P:4270:CDL:H242 | 22:P:4270:CDL:H661 | 1.54                     | 0.89              |
| 6:S:94:HIS:CD2     | 6:S:95:GLN:H       | 1.89                     | 0.89              |
| 25:O:4230:PSC:H21  | 25:O:4230:PSC:H222 | 1.55                     | 0.88              |
| 18:A:3522:TGL:HC72 | 28:L:2344:HOH:O    | 1.73                     | 0.88              |
| 18:A:3522:TGL:HC61 | 12:L:20:ARG:HH12   | 1.39                     | 0.87              |
| 7:G:8:HIS:HD2      | 23:G:4263:PEK:H252 | 1.42                     | 0.85              |
| 18:N:4522:TGL:HC31 | 12:Y:13:PHE:HA     | 1.59                     | 0.85              |
| 25:E:3230:PSC:H222 | 25:E:3230:PSC:H21  | 1.59                     | 0.84              |
| 18:A:3522:TGL:CC6  | 12:L:20:ARG:HH12   | 1.91                     | 0.84              |
| 6:S:85:CYS:SG      | 6:S:87:THR:HG23    | 2.19                     | 0.82              |
| 8:H:23:GLN:HG3     | 28:H:2104:HOH:O    | 1.79                     | 0.81              |
| 2:O:41:ILE:HD13    | 25:O:4230:PSC:H342 | 1.62                     | 0.81              |
| 3:C:67:PHE:HE1     | 22:C:3270:CDL:H1   | 1.44                     | 0.80              |
| 3:C:63:ARG:HE      | 22:C:3270:CDL:HA22 | 1.43                     | 0.80              |
| 3:P:67:PHE:HE1     | 22:P:4270:CDL:H1   | 1.47                     | 0.80              |
| 1:N:1:FME:HCN      | 1:N:4:ASN:H        | 1.48                     | 0.79              |
| 6:S:94:HIS:CG      | 6:S:95:GLN:H       | 2.02                     | 0.78              |
| 3:P:63:ARG:HE      | 22:P:4270:CDL:HA22 | 1.47                     | 0.78              |
| 1:N:112:LEU:HG     | 28:N:1379:HOH:O    | 1.85                     | 0.76              |
| 18:A:3522:TGL:HC31 | 12:L:13:PHE:HA     | 1.66                     | 0.76              |
| 6:S:76:LYS:HE3     | 6:S:93:PRO:HG3     | 1.68                     | 0.76              |
| 23:P:4264:PEK:H102 | 23:P:4264:PEK:H161 | 1.68                     | 0.76              |
| 18:A:3521:TGL:HA91 | 18:A:3521:TGL:H241 | 1.68                     | 0.76              |
| 23:C:3264:PEK:H102 | 23:C:3264:PEK:H161 | 1.65                     | 0.75              |
| 1:A:229:ILE:HD11   | 2:B:175:ILE:HD13   | 1.66                     | 0.75              |
| 7:T:5:LYS:HD2      | 23:T:3263:PEK:H382 | 1.69                     | 0.75              |
| 3:C:210:ILE:HG23   | 19:C:3267:PGV:H102 | 1.68                     | 0.75              |
| 18:N:4522:TGL:HC62 | 18:N:4522:TGL:HC22 | 1.68                     | 0.74              |
| 7:G:5:LYS:HB3      | 1:N:278:MET:SD     | 2.27                     | 0.74              |
| 1:N:334:TRP:CZ3    | 18:Q:4523:TGL:HA42 | 2.23                     | 0.74              |
| 6:F:85:CYS:SG      | 6:F:87:THR:HG23    | 2.28                     | 0.73              |
| 1:N:68:PHE:HE2     | 1:N:112:LEU:HD13   | 1.50                     | 0.73              |
| 18:A:3522:TGL:HC22 | 18:A:3522:TGL:HC62 | 1.69                     | 0.73              |
| 3:C:160:LEU:HD13   | 21:C:3271:CHD:H181 | 1.69                     | 0.73              |
| 19:A:3524:PGV:H162 | 19:A:3524:PGV:H321 | 1.71                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:N:4524:PGV:H162 | 19:N:4524:PGV:H321 | 1.70                     | 0.72              |
| 3:P:210:ILE:HG23   | 19:P:4267:PGV:H102 | 1.72                     | 0.72              |
| 18:N:4521:TGL:HA91 | 18:N:4521:TGL:H241 | 1.70                     | 0.71              |
| 18:N:4521:TGL:HB91 | 2:O:32:PHE:CE2     | 2.25                     | 0.71              |
| 3:P:160:LEU:HD13   | 21:P:4271:CHD:H181 | 1.73                     | 0.70              |
| 13:M:42:LYS:HE3    | 13:M:42:LYS:HA     | 1.74                     | 0.70              |
| 23:G:4263:PEK:H9   | 3:P:244:PHE:HA     | 1.73                     | 0.70              |
| 5:E:82:TYR:HB3     | 5:E:83:PRO:HD3     | 1.74                     | 0.69              |
| 1:A:296:GLY:HA2    | 8:H:23:GLN:OE1     | 1.91                     | 0.69              |
| 1:N:426:PHE:CE1    | 18:N:4521:TGL:H282 | 2.28                     | 0.69              |
| 22:P:4270:CDL:H391 | 28:P:2645:HOH:O    | 1.91                     | 0.69              |
| 6:S:75:HIS:H       | 6:S:80:GLN:HE22    | 1.41                     | 0.68              |
| 1:A:1:FME:HE2      | 1:A:1:FME:HA       | 1.75                     | 0.68              |
| 3:P:29:SER:HB3     | 3:P:42:LEU:HD13    | 1.74                     | 0.68              |
| 7:T:31:CYS:SG      | 22:T:4269:CDL:H532 | 2.33                     | 0.68              |
| 1:A:282:PHE:HA     | 7:T:4:ALA:HB3      | 1.75                     | 0.68              |
| 1:N:113:LEU:HB3    | 28:N:2240:HOH:O    | 1.93                     | 0.68              |
| 19:A:3524:PGV:H032 | 28:A:3752:HOH:O    | 1.93                     | 0.67              |
| 1:A:278:MET:SD     | 7:T:5:LYS:HB3      | 2.35                     | 0.67              |
| 18:A:3522:TGL:HC61 | 12:L:20:ARG:NH1    | 2.09                     | 0.67              |
| 2:O:217:LYS:HA     | 2:O:217:LYS:HE2    | 1.76                     | 0.67              |
| 5:R:89:LEU:O       | 5:R:93:LEU:HG      | 1.94                     | 0.67              |
| 1:A:177:SER:H      | 1:A:180:GLN:HE21   | 1.43                     | 0.67              |
| 19:C:3267:PGV:H161 | 19:C:3267:PGV:H12  | 1.78                     | 0.66              |
| 1:N:456:MET:HG2    | 4:Q:96:LEU:HD13    | 1.78                     | 0.66              |
| 7:T:84:LYS:HD2     | 7:T:84:LYS:N       | 2.03                     | 0.66              |
| 4:D:34:SER:H       | 4:D:37:GLN:NE2     | 1.89                     | 0.66              |
| 3:C:244:PHE:HA     | 23:T:3263:PEK:H9   | 1.77                     | 0.66              |
| 23:P:4265:PEK:H383 | 22:T:4269:CDL:H272 | 1.77                     | 0.66              |
| 18:Q:4523:TGL:HC21 | 18:Q:4523:TGL:HG12 | 1.76                     | 0.66              |
| 2:O:56:MET:HA      | 25:O:4230:PSC:H202 | 1.78                     | 0.65              |
| 18:A:3522:TGL:HC32 | 12:L:20:ARG:NH2    | 2.09                     | 0.65              |
| 23:C:3264:PEK:H71  | 23:C:3264:PEK:H32  | 1.79                     | 0.65              |
| 3:C:50:ASN:HD22    | 3:C:51:MET:HE2     | 1.63                     | 0.64              |
| 6:F:8:THR:OG1      | 6:F:11:GLU:HG3     | 1.99                     | 0.63              |
| 7:G:36:TRP:HB3     | 28:G:628:HOH:O     | 1.97                     | 0.63              |
| 6:S:94:HIS:CD2     | 6:S:95:GLN:N       | 2.64                     | 0.63              |
| 18:A:3523:TGL:HC21 | 18:A:3523:TGL:HG12 | 1.79                     | 0.63              |
| 7:G:84:LYS:H       | 7:G:84:LYS:CD      | 2.02                     | 0.63              |
| 1:N:378:HIS:O      | 1:N:382:SER:HB2    | 1.99                     | 0.63              |
| 1:N:53:ILE:HG12    | 28:N:1382:HOH:O    | 1.98                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:63:ARG:HE      | 22:C:3270:CDL:CA2  | 2.11                     | 0.63              |
| 7:G:84:LYS:HD2     | 7:G:84:LYS:N       | 2.04                     | 0.62              |
| 23:C:3265:PEK:H383 | 22:G:3269:CDL:H272 | 1.82                     | 0.62              |
| 19:P:4267:PGV:H161 | 19:P:4267:PGV:H12  | 1.80                     | 0.62              |
| 1:A:426:PHE:CE1    | 18:A:3521:TGL:H282 | 2.34                     | 0.62              |
| 3:C:146:TRP:CZ2    | 7:G:17:ARG:HG3     | 2.34                     | 0.62              |
| 1:A:390:MET:HE2    | 1:A:413:HIS:HE1    | 1.64                     | 0.62              |
| 1:N:449:MET:SD     | 2:O:5:MET:HG2      | 2.39                     | 0.61              |
| 3:P:63:ARG:HE      | 22:P:4270:CDL:CA2  | 2.12                     | 0.61              |
| 1:N:433:LEU:HD11   | 18:N:4521:TGL:OB1  | 2.00                     | 0.61              |
| 25:O:4230:PSC:C07  | 9:V:10:ARG:HH21    | 2.13                     | 0.61              |
| 1:A:472:ILE:HG21   | 18:A:3522:TGL:HA81 | 1.81                     | 0.61              |
| 18:A:3523:TGL:HA81 | 18:A:3523:TGL:H242 | 1.80                     | 0.61              |
| 3:P:67:PHE:CE1     | 22:P:4270:CDL:H1   | 2.32                     | 0.61              |
| 22:C:3270:CDL:H312 | 22:C:3270:CDL:H151 | 1.81                     | 0.61              |
| 1:A:449:MET:SD     | 2:B:5:MET:HG2      | 2.41                     | 0.61              |
| 22:P:4270:CDL:H312 | 22:P:4270:CDL:H151 | 1.83                     | 0.61              |
| 2:B:62:GLU:O       | 2:B:66:THR:HB      | 2.00                     | 0.61              |
| 3:P:146:TRP:CZ2    | 7:T:17:ARG:HG3     | 2.36                     | 0.61              |
| 2:O:41:ILE:CD1     | 25:O:4230:PSC:H342 | 2.30                     | 0.60              |
| 3:P:246:ASP:HB2    | 28:P:1272:HOH:O    | 2.01                     | 0.60              |
| 1:N:472:ILE:HD13   | 18:N:4522:TGL:HA92 | 1.83                     | 0.60              |
| 18:A:3523:TGL:HC31 | 28:A:3753:HOH:O    | 2.02                     | 0.60              |
| 4:Q:58:GLU:O       | 4:Q:62:LEU:HG      | 2.02                     | 0.60              |
| 7:T:17:ARG:HD2     | 28:T:1509:HOH:O    | 2.02                     | 0.60              |
| 18:A:3522:TGL:H271 | 12:L:11:ILE:HG22   | 1.82                     | 0.60              |
| 19:A:3524:PGV:H311 | 13:M:19:LEU:HD23   | 1.83                     | 0.60              |
| 1:N:334:TRP:CH2    | 2:O:46:LEU:HD13    | 2.37                     | 0.60              |
| 2:O:104:TRP:CG     | 2:O:203:ASN:HB2    | 2.36                     | 0.60              |
| 18:Q:4523:TGL:HA81 | 18:Q:4523:TGL:H242 | 1.83                     | 0.59              |
| 9:V:63:MET:HB3     | 9:V:68:ILE:HD11    | 1.84                     | 0.59              |
| 3:C:213:THR:HG23   | 22:C:3270:CDL:H762 | 1.82                     | 0.59              |
| 8:U:49:ASP:O       | 8:U:52:VAL:HG22    | 2.03                     | 0.59              |
| 1:A:484:THR:HB     | 13:M:2:THR:OG1     | 2.02                     | 0.59              |
| 4:Q:127:LYS:O      | 4:Q:130:PRO:HD3    | 2.03                     | 0.59              |
| 7:G:31:CYS:SG      | 22:G:3269:CDL:H532 | 2.43                     | 0.59              |
| 1:A:1:FME:HE3      | 12:L:3:TYR:HE1     | 1.67                     | 0.59              |
| 11:K:24:PHE:O      | 11:K:28:VAL:HG12   | 2.02                     | 0.59              |
| 1:A:1:FME:HCN      | 1:A:4:ASN:H        | 1.68                     | 0.58              |
| 22:G:3269:CDL:HB32 | 1:N:304:TYR:HD1    | 1.68                     | 0.58              |
| 23:P:4264:PEK:H71  | 23:P:4264:PEK:H32  | 1.83                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:S:87:THR:HG21    | 28:S:1303:HOH:O    | 2.02                     | 0.58              |
| 7:T:38:HIS:NE2     | 22:T:4269:CDL:H111 | 2.18                     | 0.58              |
| 22:P:4270:CDL:H112 | 28:P:2598:HOH:O    | 2.03                     | 0.58              |
| 4:Q:82:VAL:O       | 4:Q:86:MET:HG3     | 2.03                     | 0.58              |
| 6:F:92:VAL:HG23    | 6:F:92:VAL:O       | 2.03                     | 0.58              |
| 1:A:177:SER:H      | 1:A:180:GLN:NE2    | 2.02                     | 0.58              |
| 7:G:45:PRO:HD2     | 28:G:132:HOH:O     | 2.03                     | 0.58              |
| 10:J:7:GLU:HG3     | 28:J:2487:HOH:O    | 2.03                     | 0.58              |
| 5:R:43:PRO:HB2     | 5:R:48:ILE:HD11    | 1.86                     | 0.58              |
| 8:H:43:MET:HE1     | 8:U:43:MET:HE1     | 1.86                     | 0.58              |
| 1:A:113:LEU:HD12   | 18:A:3522:TGL:H292 | 1.85                     | 0.57              |
| 7:T:45:PRO:HD2     | 28:T:1132:HOH:O    | 2.04                     | 0.57              |
| 19:N:4524:PGV:H141 | 4:Q:87:PHE:CE2     | 2.39                     | 0.57              |
| 19:A:3524:PGV:H141 | 4:D:87:PHE:CE2     | 2.39                     | 0.57              |
| 3:P:51:MET:HB3     | 22:P:4270:CDL:H622 | 1.87                     | 0.57              |
| 7:T:5:LYS:CD       | 23:T:3263:PEK:H382 | 2.33                     | 0.57              |
| 1:A:229:ILE:HD11   | 2:B:175:ILE:CD1    | 2.33                     | 0.57              |
| 1:N:350:VAL:HG11   | 18:N:4521:TGL:H281 | 1.87                     | 0.57              |
| 23:C:3265:PEK:H041 | 6:F:1:ALA:N        | 2.20                     | 0.56              |
| 1:N:68:PHE:CE2     | 1:N:112:LEU:HD13   | 2.37                     | 0.56              |
| 1:N:113:LEU:CD1    | 18:N:4522:TGL:H292 | 2.35                     | 0.56              |
| 18:N:4521:TGL:HB91 | 2:O:32:PHE:HE2     | 1.71                     | 0.56              |
| 3:C:51:MET:HB3     | 22:C:3270:CDL:H622 | 1.87                     | 0.56              |
| 6:S:22:LEU:HD12    | 28:S:2496:HOH:O    | 2.05                     | 0.56              |
| 2:O:196:CYS:HB2    | 2:O:207:MET:HG3    | 1.88                     | 0.56              |
| 2:O:224:ALA:O      | 2:O:227:LEU:HG     | 2.06                     | 0.56              |
| 1:N:113:LEU:HD12   | 18:N:4522:TGL:H292 | 1.88                     | 0.56              |
| 2:O:49:LYS:NZ      | 18:Q:4523:TGL:HC71 | 2.21                     | 0.56              |
| 3:C:246:ASP:HB2    | 28:C:3557:HOH:O    | 2.04                     | 0.56              |
| 3:P:25:LEU:O       | 3:P:29:SER:HB2     | 2.06                     | 0.56              |
| 3:P:226:HIS:CE1    | 22:P:4270:CDL:HB31 | 2.41                     | 0.56              |
| 25:E:3230:PSC:H072 | 9:I:10:ARG:HH21    | 1.70                     | 0.55              |
| 18:N:4521:TGL:H283 | 18:N:4521:TGL:H101 | 1.86                     | 0.55              |
| 2:O:84:LEU:HA      | 2:O:87:MET:HE2     | 1.88                     | 0.55              |
| 3:C:158:HIS:NE2    | 23:C:3265:PEK:H051 | 2.22                     | 0.55              |
| 22:C:3270:CDL:H662 | 19:C:3267:PGV:H182 | 1.88                     | 0.55              |
| 7:G:17:ARG:HD2     | 28:G:2008:HOH:O    | 2.06                     | 0.55              |
| 1:N:107:PRO:HB3    | 3:P:25:LEU:HB2     | 1.88                     | 0.55              |
| 1:A:136:LEU:HB2    | 28:A:3740:HOH:O    | 2.06                     | 0.55              |
| 2:B:139:ASP:HB2    | 28:B:4220:HOH:O    | 2.07                     | 0.55              |
| 18:N:4522:TGL:HG12 | 12:Y:13:PHE:HB3    | 1.88                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:377:PHE:O      | 1:A:381:LEU:HB3    | 2.07                     | 0.55              |
| 3:C:67:PHE:CE1     | 22:C:3270:CDL:H1   | 2.34                     | 0.55              |
| 2:O:83:ILE:O       | 2:O:87:MET:HG3     | 2.07                     | 0.55              |
| 9:V:65:LYS:O       | 11:X:54:ARG:NH1    | 2.36                     | 0.55              |
| 4:Q:20:ARG:HD2     | 4:Q:72:ASN:OD1     | 2.07                     | 0.54              |
| 2:O:59:GLN:O       | 2:O:59:GLN:HG3     | 2.08                     | 0.54              |
| 1:A:113:LEU:CD1    | 18:A:3522:TGL:H292 | 2.37                     | 0.54              |
| 18:A:3523:TGL:HB82 | 18:A:3523:TGL:H122 | 1.89                     | 0.54              |
| 1:N:52:GLN:O       | 1:N:56:VAL:HG23    | 2.07                     | 0.54              |
| 1:A:321:PHE:CD2    | 25:E:3230:PSC:H341 | 2.43                     | 0.54              |
| 7:G:8:HIS:CD2      | 23:G:4263:PEK:H252 | 2.32                     | 0.54              |
| 4:Q:19:ARG:HD2     | 4:Q:21:ASP:OD1     | 2.07                     | 0.54              |
| 18:A:3521:TGL:H283 | 18:A:3521:TGL:H101 | 1.89                     | 0.54              |
| 22:G:3269:CDL:H332 | 28:O:1358:HOH:O    | 2.08                     | 0.54              |
| 1:N:51:ASP:OD1     | 2:O:206:PHE:HE1    | 1.90                     | 0.54              |
| 2:B:196:CYS:HB2    | 2:B:207:MET:HG3    | 1.90                     | 0.53              |
| 22:P:4270:CDL:H121 | 28:P:2392:HOH:O    | 2.07                     | 0.53              |
| 1:N:177:SER:H      | 1:N:180:GLN:NE2    | 2.06                     | 0.53              |
| 18:N:4522:TGL:HC22 | 18:N:4522:TGL:CC6  | 2.37                     | 0.53              |
| 2:O:62:GLU:O       | 2:O:66:THR:HB      | 2.08                     | 0.53              |
| 7:T:38:HIS:CD2     | 22:T:4269:CDL:HA21 | 2.42                     | 0.53              |
| 18:A:3522:TGL:HC62 | 12:L:20:ARG:HH12   | 1.71                     | 0.53              |
| 1:N:194:LEU:HD22   | 1:N:285:PHE:HE2    | 1.72                     | 0.53              |
| 2:B:102:HIS:O      | 2:B:104:TRP:N      | 2.41                     | 0.53              |
| 1:N:334:TRP:HZ3    | 18:Q:4523:TGL:HA62 | 1.72                     | 0.53              |
| 3:P:213:THR:HG23   | 22:P:4270:CDL:H762 | 1.91                     | 0.53              |
| 9:I:8:GLN:HE22     | 9:I:10:ARG:H       | 1.57                     | 0.53              |
| 1:N:483:LEU:HD13   | 4:Q:6:VAL:HB       | 1.89                     | 0.53              |
| 4:D:20:ARG:HG3     | 28:D:168:HOH:O     | 2.09                     | 0.53              |
| 1:A:514:LYS:HE3    | 28:A:3750:HOH:O    | 2.08                     | 0.53              |
| 28:B:4144:HOH:O    | 22:T:4269:CDL:H332 | 2.09                     | 0.53              |
| 18:N:4522:TGL:CG1  | 12:Y:13:PHE:HB3    | 2.39                     | 0.53              |
| 18:N:4521:TGL:H101 | 18:N:4521:TGL:C28  | 2.39                     | 0.52              |
| 2:O:122:MET:HB2    | 2:O:208:PRO:HD2    | 1.92                     | 0.52              |
| 18:Q:4523:TGL:HB82 | 18:Q:4523:TGL:H122 | 1.90                     | 0.52              |
| 1:A:304:TYR:HD1    | 22:T:4269:CDL:HB32 | 1.75                     | 0.52              |
| 1:A:194:LEU:HD22   | 1:A:285:PHE:HE2    | 1.74                     | 0.52              |
| 2:B:164:ALA:O      | 2:B:194:GLY:HA3    | 2.09                     | 0.52              |
| 1:A:21:LEU:HD23    | 18:A:3522:TGL:H211 | 1.92                     | 0.52              |
| 2:O:49:LYS:O       | 4:Q:20:ARG:NH2     | 2.39                     | 0.52              |
| 1:A:28:MET:HE2     | 17:A:515:HEA:H271  | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:I:35:TYR:C       | 9:I:37:PHE:H       | 2.18                     | 0.52              |
| 2:B:104:TRP:CG     | 2:B:203:ASN:HB2    | 2.44                     | 0.52              |
| 7:T:3:ALA:O        | 7:T:4:ALA:HB2      | 2.10                     | 0.52              |
| 8:U:7:LYS:O        | 8:U:8:ILE:HG22     | 2.09                     | 0.52              |
| 7:T:11:TPO:HG22    | 7:T:16:TRP:HE1     | 1.74                     | 0.52              |
| 2:B:122:MET:HB2    | 2:B:208:PRO:HD2    | 1.92                     | 0.52              |
| 3:C:50:ASN:ND2     | 3:C:54:MET:HE2     | 2.25                     | 0.52              |
| 6:F:64:GLU:O       | 6:F:65:ASP:HB2     | 2.10                     | 0.52              |
| 23:P:4265:PEK:H041 | 6:S:1:ALA:N        | 2.24                     | 0.52              |
| 1:N:472:ILE:HG21   | 18:N:4522:TGL:HA81 | 1.91                     | 0.52              |
| 9:V:35:TYR:C       | 9:V:37:PHE:H       | 2.18                     | 0.52              |
| 18:A:3522:TGL:CC6  | 18:A:3522:TGL:HC22 | 2.37                     | 0.51              |
| 4:D:4:SER:N        | 28:D:257:HOH:O     | 2.44                     | 0.51              |
| 22:G:3269:CDL:H612 | 22:G:3269:CDL:H751 | 1.92                     | 0.51              |
| 6:S:92:VAL:O       | 6:S:92:VAL:HG23    | 2.11                     | 0.51              |
| 2:O:116:LEU:HD12   | 2:O:117:SER:N      | 2.26                     | 0.51              |
| 22:T:4269:CDL:H612 | 22:T:4269:CDL:H751 | 1.91                     | 0.51              |
| 1:A:87:ILE:O       | 1:A:173:PRO:HD3    | 2.11                     | 0.51              |
| 4:D:4:SER:HB2      | 28:D:257:HOH:O     | 2.09                     | 0.51              |
| 5:E:84:TYR:O       | 5:E:88:GLU:HG2     | 2.11                     | 0.51              |
| 6:F:75:HIS:H       | 6:F:80:GLN:HE22    | 1.58                     | 0.51              |
| 7:G:4:ALA:HB3      | 1:N:282:PHE:HA     | 1.93                     | 0.51              |
| 1:A:472:ILE:HD13   | 18:A:3522:TGL:HA92 | 1.93                     | 0.51              |
| 7:G:3:ALA:O        | 7:G:4:ALA:HB2      | 2.11                     | 0.51              |
| 1:N:22:PHE:HA      | 18:N:4522:TGL:HB72 | 1.93                     | 0.51              |
| 1:A:282:PHE:HA     | 7:T:4:ALA:CB       | 2.41                     | 0.51              |
| 23:P:4264:PEK:H102 | 23:P:4264:PEK:C16  | 2.40                     | 0.51              |
| 1:A:1:FME:HCN      | 1:A:4:ASN:HB2      | 1.92                     | 0.50              |
| 1:N:400:PHE:HB3    | 18:N:4522:TGL:H282 | 1.93                     | 0.50              |
| 1:N:514:LYS:HA     | 6:S:38:ALA:HB3     | 1.93                     | 0.50              |
| 4:Q:121:LYS:HG2    | 11:X:53:TRP:CD1    | 2.46                     | 0.50              |
| 18:A:3521:TGL:HC52 | 2:B:7:LEU:HD12     | 1.94                     | 0.50              |
| 6:S:51:SER:O       | 6:S:94:HIS:N       | 2.45                     | 0.50              |
| 3:C:103:HIS:HA     | 19:C:3268:PGV:H012 | 1.94                     | 0.50              |
| 1:N:106:PRO:HB2    | 1:N:107:PRO:HD3    | 1.94                     | 0.50              |
| 18:N:4521:TGL:H283 | 18:N:4521:TGL:CB9  | 2.42                     | 0.50              |
| 3:P:158:HIS:NE2    | 23:P:4265:PEK:H051 | 2.26                     | 0.50              |
| 18:A:3521:TGL:OB1  | 18:A:3521:TGL:HB42 | 2.11                     | 0.50              |
| 2:B:132:GLU:HB3    | 2:B:137:GLU:HG3    | 1.94                     | 0.50              |
| 13:M:17:ILE:O      | 13:M:21:VAL:HG23   | 2.12                     | 0.50              |
| 22:T:4269:CDL:H322 | 22:T:4269:CDL:HA62 | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:68:LEU:CB      | 2:O:69:PRO:HD3     | 2.42                     | 0.50              |
| 7:T:34:ASN:ND2     | 22:T:4269:CDL:H151 | 2.26                     | 0.50              |
| 13:Z:28:LEU:HB2    | 13:Z:29:PRO:HD3    | 1.93                     | 0.50              |
| 2:B:128:LEU:HD11   | 2:B:134:ARG:HA     | 1.94                     | 0.50              |
| 1:N:290:HIS:CD2    | 1:N:291:HIS:CD2    | 3.00                     | 0.50              |
| 22:C:3270:CDL:H192 | 22:C:3270:CDL:H372 | 1.94                     | 0.50              |
| 18:A:3521:TGL:HC22 | 28:I:346:HOH:O     | 2.12                     | 0.49              |
| 22:G:3269:CDL:HB32 | 1:N:304:TYR:CD1    | 2.47                     | 0.49              |
| 9:I:22:VAL:O       | 9:I:26:MET:HG2     | 2.12                     | 0.49              |
| 18:A:3521:TGL:H101 | 18:A:3521:TGL:C28  | 2.42                     | 0.49              |
| 2:O:82:ARG:NH1     | 2:O:86:MET:HE1     | 2.27                     | 0.49              |
| 25:E:3230:PSC:C07  | 9:I:10:ARG:HH21    | 2.25                     | 0.49              |
| 22:C:3270:CDL:H651 | 22:C:3270:CDL:H771 | 1.95                     | 0.49              |
| 23:C:3264:PEK:H102 | 23:C:3264:PEK:C16  | 2.38                     | 0.49              |
| 12:Y:20:ARG:HH21   | 12:Y:24:MET:HG3    | 1.78                     | 0.49              |
| 3:C:122:HIS:HD2    | 28:C:3562:HOH:O    | 1.95                     | 0.49              |
| 1:N:62:ALA:HB2     | 17:N:515:HEA:HBD1  | 1.93                     | 0.49              |
| 2:O:102:HIS:O      | 2:O:104:TRP:N      | 2.45                     | 0.49              |
| 1:A:52:GLN:O       | 1:A:56:VAL:HG23    | 2.12                     | 0.49              |
| 5:E:41:LEU:HA      | 28:I:301:HOH:O     | 2.12                     | 0.49              |
| 1:N:350:VAL:CG1    | 18:N:4521:TGL:H281 | 2.42                     | 0.49              |
| 1:N:472:ILE:HG21   | 18:N:4522:TGL:CA8  | 2.42                     | 0.49              |
| 7:T:2:SER:O        | 7:T:3:ALA:HB3      | 2.13                     | 0.49              |
| 1:N:42:GLY:HA3     | 4:Q:104:TYR:OH     | 2.12                     | 0.49              |
| 18:N:4521:TGL:OB1  | 18:N:4521:TGL:HB42 | 2.12                     | 0.49              |
| 18:N:4521:TGL:H283 | 18:N:4521:TGL:HB92 | 1.94                     | 0.49              |
| 22:P:4270:CDL:H231 | 22:P:4270:CDL:H641 | 1.95                     | 0.49              |
| 12:Y:46:LYS:O      | 12:Y:47:LYS:HB2    | 2.12                     | 0.49              |
| 2:B:172:THR:HG23   | 28:H:2574:HOH:O    | 2.12                     | 0.49              |
| 3:C:226:HIS:CE1    | 22:C:3270:CDL:HB31 | 2.48                     | 0.48              |
| 1:N:407:ASP:O      | 1:N:411:LYS:HG3    | 2.13                     | 0.48              |
| 22:P:4270:CDL:H372 | 22:P:4270:CDL:H192 | 1.93                     | 0.48              |
| 12:Y:2:HIS:ND1     | 12:Y:3:TYR:N       | 2.58                     | 0.48              |
| 28:A:3691:HOH:O    | 19:C:3268:PGV:H12  | 2.13                     | 0.48              |
| 6:F:92:VAL:O       | 6:F:92:VAL:CG2     | 2.61                     | 0.48              |
| 2:O:1:FME:HE1      | 2:O:133:LEU:HD22   | 1.95                     | 0.48              |
| 18:A:3521:TGL:H283 | 18:A:3521:TGL:HB92 | 1.95                     | 0.48              |
| 3:C:54:MET:HE1     | 19:C:3267:PGV:H141 | 1.95                     | 0.48              |
| 18:N:4522:TGL:HB52 | 18:N:4522:TGL:HB81 | 1.59                     | 0.48              |
| 1:A:472:ILE:HG21   | 18:A:3522:TGL:CA8  | 2.44                     | 0.48              |
| 1:N:87:ILE:O       | 1:N:173:PRO:HD3    | 2.13                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:164:ALA:O      | 2:O:194:GLY:HA3    | 2.13                     | 0.48              |
| 1:N:377:PHE:O      | 1:N:381:LEU:HB3    | 2.14                     | 0.48              |
| 18:N:4522:TGL:OA1  | 18:N:4522:TGL:H181 | 2.14                     | 0.48              |
| 22:P:4270:CDL:H651 | 22:P:4270:CDL:H771 | 1.95                     | 0.48              |
| 4:Q:23:PRO:O       | 4:Q:25:PRO:HD3     | 2.14                     | 0.48              |
| 4:Q:36:SER:O       | 4:Q:39:ALA:HB3     | 2.14                     | 0.48              |
| 10:W:30:ILE:O      | 10:W:34:VAL:HG23   | 2.13                     | 0.48              |
| 18:A:3521:TGL:H241 | 18:A:3521:TGL:CA9  | 2.43                     | 0.48              |
| 23:C:3265:PEK:H301 | 2:O:66:THR:CG2     | 2.44                     | 0.47              |
| 2:O:68:LEU:HD22    | 25:O:4230:PSC:H171 | 1.95                     | 0.47              |
| 1:A:390:MET:HE2    | 1:A:413:HIS:CE1    | 2.47                     | 0.47              |
| 18:A:3521:TGL:H283 | 18:A:3521:TGL:CB9  | 2.44                     | 0.47              |
| 18:A:3522:TGL:CG1  | 12:L:13:PHE:HB3    | 2.44                     | 0.47              |
| 3:C:177:GLN:HA     | 3:C:177:GLN:OE1    | 2.14                     | 0.47              |
| 7:G:5:LYS:HD2      | 23:G:4263:PEK:H382 | 1.95                     | 0.47              |
| 1:N:172:LYS:HD2    | 1:N:181:THR:CG2    | 2.44                     | 0.47              |
| 3:P:253:TYR:CE2    | 22:T:4269:CDL:H641 | 2.49                     | 0.47              |
| 4:D:9:GLU:CD       | 4:D:9:GLU:H        | 2.23                     | 0.47              |
| 22:G:3269:CDL:H172 | 22:G:3269:CDL:H511 | 1.97                     | 0.47              |
| 22:G:3269:CDL:H322 | 22:G:3269:CDL:HA62 | 1.95                     | 0.47              |
| 2:B:59:GLN:HG3     | 2:B:59:GLN:O       | 2.14                     | 0.47              |
| 5:E:14:ARG:HD2     | 28:E:3271:HOH:O    | 2.14                     | 0.47              |
| 6:F:90:LYS:HD2     | 28:F:187:HOH:O     | 2.14                     | 0.47              |
| 22:G:3269:CDL:H212 | 1:N:311:ILE:HD12   | 1.97                     | 0.47              |
| 2:O:203:ASN:N      | 2:O:203:ASN:HD22   | 2.12                     | 0.47              |
| 6:S:22:LEU:O       | 6:S:25:ARG:HB3     | 2.15                     | 0.47              |
| 1:A:378:HIS:O      | 1:A:382:SER:HB2    | 2.15                     | 0.47              |
| 1:N:115:SER:O      | 1:N:121:GLY:HA2    | 2.15                     | 0.47              |
| 1:N:351:GLY:C      | 1:N:380:VAL:HG13   | 2.40                     | 0.47              |
| 18:N:4521:TGL:HB91 | 2:O:32:PHE:CD2     | 2.49                     | 0.47              |
| 19:N:4524:PGV:H211 | 28:Z:2192:HOH:O    | 2.14                     | 0.47              |
| 2:O:202:SER:HB2    | 2:O:203:ASN:HD22   | 1.80                     | 0.47              |
| 4:Q:86:MET:HE1     | 28:X:2287:HOH:O    | 2.14                     | 0.47              |
| 11:X:24:PHE:O      | 11:X:28:VAL:HG12   | 2.14                     | 0.47              |
| 22:G:3269:CDL:H252 | 22:G:3269:CDL:H222 | 1.73                     | 0.47              |
| 2:O:128:LEU:HD11   | 2:O:134:ARG:HA     | 1.96                     | 0.47              |
| 25:O:4230:PSC:C14  | 25:O:4230:PSC:H343 | 2.45                     | 0.47              |
| 4:Q:101:HIS:HD2    | 4:Q:102:TYR:CE2    | 2.33                     | 0.47              |
| 23:C:3265:PEK:H232 | 7:G:21:PHE:CD2     | 2.49                     | 0.46              |
| 8:H:49:ASP:O       | 8:H:52:VAL:HG22    | 2.15                     | 0.46              |
| 1:N:76:GLY:O       | 1:N:80:ASN:HB2     | 2.14                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:T:8:HIS:CD2      | 23:T:3263:PEK:H231 | 2.50                     | 0.46              |
| 2:B:41:ILE:HD13    | 25:E:3230:PSC:H342 | 1.97                     | 0.46              |
| 1:N:177:SER:H      | 1:N:180:GLN:HE21   | 1.63                     | 0.46              |
| 11:X:54:ARG:NH2    | 11:X:54:ARG:HG3    | 2.29                     | 0.46              |
| 1:A:390:MET:O      | 1:A:394:VAL:HG13   | 2.15                     | 0.46              |
| 1:A:433:LEU:HD11   | 18:A:3521:TGL:OB1  | 2.15                     | 0.46              |
| 2:B:151:ARG:HD3    | 2:B:181:GLN:HE21   | 1.80                     | 0.46              |
| 7:G:50:TYR:HB3     | 7:G:52:HIS:CE1     | 2.50                     | 0.46              |
| 4:Q:131:ILE:HD12   | 4:Q:131:ILE:H      | 1.81                     | 0.46              |
| 11:X:54:ARG:HG3    | 11:X:54:ARG:HH21   | 1.80                     | 0.46              |
| 23:C:3265:PEK:H041 | 6:F:1:ALA:H2       | 1.80                     | 0.46              |
| 2:B:82:ARG:NH1     | 2:B:86:MET:HE1     | 2.30                     | 0.46              |
| 25:E:3230:PSC:C14  | 25:E:3230:PSC:H343 | 2.46                     | 0.46              |
| 1:N:95:PRO:HG2     | 3:P:11:VAL:CG2     | 2.46                     | 0.46              |
| 4:Q:75:THR:HG22    | 28:Q:1438:HOH:O    | 2.14                     | 0.46              |
| 22:C:3270:CDL:H652 | 22:C:3270:CDL:H621 | 1.59                     | 0.46              |
| 23:C:3265:PEK:H102 | 23:C:3265:PEK:H131 | 1.76                     | 0.46              |
| 1:N:426:PHE:CD1    | 18:N:4521:TGL:H282 | 2.50                     | 0.46              |
| 18:N:4521:TGL:H101 | 18:N:4521:TGL:C27  | 2.46                     | 0.46              |
| 13:Z:4:LYS:HB2     | 13:Z:5:PRO:CD      | 2.46                     | 0.46              |
| 1:A:195:LEU:HD23   | 1:A:245:ILE:HD13   | 1.97                     | 0.46              |
| 2:B:4:PRO:HB2      | 11:K:43:SER:HA     | 1.98                     | 0.46              |
| 22:T:4269:CDL:H172 | 22:T:4269:CDL:H511 | 1.96                     | 0.46              |
| 1:N:324:LEU:HD13   | 2:O:41:ILE:CG2     | 2.46                     | 0.46              |
| 4:Q:7:LYS:O        | 4:Q:10:ASP:HB2     | 2.15                     | 0.46              |
| 1:A:426:PHE:CD1    | 18:A:3521:TGL:H282 | 2.51                     | 0.46              |
| 1:A:1:FME:HA       | 1:A:1:FME:CE       | 2.45                     | 0.46              |
| 1:A:62:ALA:HB2     | 17:A:515:HEA:HBD1  | 1.98                     | 0.46              |
| 1:A:290:HIS:CD2    | 1:A:291:HIS:CD2    | 3.04                     | 0.46              |
| 4:Q:101:HIS:HD2    | 4:Q:102:TYR:CD2    | 2.34                     | 0.46              |
| 7:G:84:LYS:CD      | 7:G:84:LYS:N       | 2.74                     | 0.45              |
| 7:T:31:CYS:SG      | 22:T:4269:CDL:C53  | 3.03                     | 0.45              |
| 3:C:187:THR:HG22   | 23:C:3264:PEK:H052 | 1.97                     | 0.45              |
| 4:D:127:LYS:HD2    | 28:I:353:HOH:O     | 2.17                     | 0.45              |
| 7:G:7:ASP:O        | 1:N:169:ILE:HD12   | 2.15                     | 0.45              |
| 1:N:426:PHE:HE1    | 18:N:4521:TGL:H282 | 1.78                     | 0.45              |
| 22:P:4270:CDL:HB21 | 22:P:4270:CDL:CB3  | 2.47                     | 0.45              |
| 7:G:69:PHE:HD1     | 7:G:70:PHE:CE1     | 2.35                     | 0.45              |
| 4:Q:122:ARG:HG2    | 4:Q:126:MET:HE3    | 1.98                     | 0.45              |
| 7:T:7:ASP:O        | 7:T:9:GLY:N        | 2.48                     | 0.45              |
| 8:U:23:GLN:HG3     | 28:U:1462:HOH:O    | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:V:18:ARG:HD3     | 28:V:1387:HOH:O    | 2.16                     | 0.45              |
| 1:A:377:PHE:CD1    | 17:A:516:HEA:HAD1  | 2.52                     | 0.45              |
| 3:C:63:ARG:NE      | 22:C:3270:CDL:HA22 | 2.23                     | 0.45              |
| 1:A:334:TRP:CZ2    | 2:B:46:LEU:HB3     | 2.52                     | 0.45              |
| 1:N:82:LEU:O       | 1:N:86:MET:HG3     | 2.17                     | 0.45              |
| 1:N:265:LYS:HB2    | 1:N:490:THR:HG21   | 1.99                     | 0.45              |
| 11:X:54:ARG:HH21   | 11:X:54:ARG:CG     | 2.29                     | 0.45              |
| 1:A:22:PHE:HA      | 18:A:3522:TGL:HB72 | 1.99                     | 0.45              |
| 1:A:71:MET:HB2     | 1:A:72:PRO:HD3     | 1.99                     | 0.45              |
| 18:A:3522:TGL:HG12 | 12:L:13:PHE:HB3    | 1.98                     | 0.45              |
| 2:B:41:ILE:O       | 2:B:45:MET:HG2     | 2.17                     | 0.45              |
| 2:B:78:LEU:HD12    | 2:B:78:LEU:HA      | 1.78                     | 0.45              |
| 3:C:210:ILE:HD13   | 19:C:3267:PGV:H301 | 1.99                     | 0.45              |
| 22:C:3270:CDL:H632 | 22:C:3270:CDL:H602 | 1.64                     | 0.45              |
| 1:N:489:THR:HA     | 6:S:71:TRP:O       | 2.17                     | 0.45              |
| 1:A:225:GLY:HA3    | 3:C:112:LEU:HD21   | 1.98                     | 0.45              |
| 1:N:310:MET:HE1    | 2:O:76:ILE:HB      | 1.99                     | 0.45              |
| 7:T:84:LYS:H       | 7:T:84:LYS:CD      | 2.05                     | 0.45              |
| 18:N:4521:TGL:HA91 | 18:N:4521:TGL:H222 | 1.57                     | 0.45              |
| 1:A:165:ILE:O      | 1:A:169:ILE:HG12   | 2.15                     | 0.45              |
| 3:P:67:PHE:HE1     | 22:P:4270:CDL:C1   | 2.23                     | 0.45              |
| 1:A:106:PRO:HB2    | 1:A:107:PRO:HD3    | 1.99                     | 0.44              |
| 21:J:3060:CHD:H3   | 28:J:2631:HOH:O    | 2.17                     | 0.44              |
| 13:M:42:LYS:HA     | 13:M:42:LYS:CE     | 2.41                     | 0.44              |
| 18:N:4521:TGL:H101 | 18:N:4521:TGL:H271 | 1.98                     | 0.44              |
| 19:C:3268:PGV:H231 | 19:C:3268:PGV:H202 | 1.80                     | 0.44              |
| 1:N:71:MET:HE1     | 1:N:195:LEU:HD21   | 1.99                     | 0.44              |
| 2:O:4:PRO:HB2      | 11:X:43:SER:HA     | 1.99                     | 0.44              |
| 1:A:194:LEU:HD22   | 1:A:285:PHE:CE2    | 2.52                     | 0.44              |
| 18:A:3522:TGL:HB81 | 18:A:3522:TGL:HB52 | 1.60                     | 0.44              |
| 19:A:3524:PGV:H211 | 28:M:2318:HOH:O    | 2.17                     | 0.44              |
| 22:G:3269:CDL:H181 | 22:G:3269:CDL:H152 | 1.77                     | 0.44              |
| 5:R:80:GLU:C       | 5:R:83:PRO:HD2     | 2.42                     | 0.44              |
| 1:A:344:PHE:CD1    | 1:A:344:PHE:C      | 2.95                     | 0.44              |
| 1:A:431:LEU:HD21   | 1:A:450:TRP:HB2    | 1.99                     | 0.44              |
| 3:C:158:HIS:CE1    | 23:C:3265:PEK:H051 | 2.53                     | 0.44              |
| 1:N:44:PRO:HG2     | 4:Q:111:PHE:CZ     | 2.53                     | 0.44              |
| 1:N:171:MET:HG2    | 3:P:8:TYR:CE1      | 2.52                     | 0.44              |
| 1:N:378:HIS:CD2    | 1:N:382:SER:OG     | 2.71                     | 0.44              |
| 1:A:513:LEU:HD22   | 1:A:513:LEU:HA     | 1.75                     | 0.44              |
| 9:I:5:ALA:O        | 9:I:7:PRO:HD3      | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:216:LEU:O      | 2:O:219:PHE:HB3    | 2.18                     | 0.44              |
| 8:U:43:MET:HE2     | 8:U:52:VAL:HG21    | 1.99                     | 0.44              |
| 11:X:6:ALA:HA      | 11:X:7:PRO:HD2     | 1.89                     | 0.44              |
| 7:G:42:ARG:O       | 7:G:42:ARG:HD3     | 2.18                     | 0.44              |
| 1:N:390:MET:HE2    | 1:N:413:HIS:HE1    | 1.83                     | 0.44              |
| 3:P:116:TRP:HA     | 3:P:117:PRO:C      | 2.42                     | 0.44              |
| 5:R:5:HIS:HB3      | 5:R:6:GLU:H        | 1.63                     | 0.44              |
| 22:G:3269:CDL:H571 | 22:G:3269:CDL:H601 | 1.80                     | 0.44              |
| 19:P:4268:PGV:H231 | 19:P:4268:PGV:H202 | 1.82                     | 0.44              |
| 19:A:3524:PGV:H141 | 4:D:87:PHE:CD2     | 2.52                     | 0.44              |
| 22:T:4269:CDL:H252 | 22:T:4269:CDL:H222 | 1.73                     | 0.44              |
| 1:A:351:GLY:C      | 1:A:380:VAL:HG13   | 2.43                     | 0.43              |
| 2:O:92:ASN:HA      | 2:O:93:PRO:HD2     | 1.83                     | 0.43              |
| 3:P:50:ASN:ND2     | 3:P:54:MET:HE2     | 2.33                     | 0.43              |
| 22:C:3270:CDL:HB21 | 22:C:3270:CDL:CB3  | 2.48                     | 0.43              |
| 2:O:41:ILE:O       | 2:O:45:MET:HG2     | 2.17                     | 0.43              |
| 22:P:4270:CDL:H662 | 19:P:4267:PGV:H182 | 2.00                     | 0.43              |
| 1:A:407:ASP:O      | 1:A:411:LYS:HG3    | 2.19                     | 0.43              |
| 22:P:4270:CDL:H621 | 22:P:4270:CDL:H652 | 1.62                     | 0.43              |
| 18:A:3522:TGL:H271 | 12:L:11:ILE:CG2    | 2.49                     | 0.43              |
| 4:Q:48:TRP:O       | 4:Q:51:LEU:HB2     | 2.19                     | 0.43              |
| 5:R:12:ASP:HA      | 5:R:47:ILE:HD11    | 2.01                     | 0.43              |
| 12:Y:35:ALA:HB3    | 12:Y:36:PRO:HD3    | 2.00                     | 0.43              |
| 18:A:3521:TGL:HG11 | 2:B:7:LEU:HB3      | 2.00                     | 0.43              |
| 25:E:3230:PSC:H252 | 25:E:3230:PSC:H221 | 1.79                     | 0.43              |
| 1:N:440:TYR:CZ     | 2:O:205:SER:HA     | 2.53                     | 0.43              |
| 18:N:4522:TGL:H272 | 18:N:4522:TGL:H232 | 1.99                     | 0.43              |
| 18:A:3522:TGL:OA1  | 18:A:3522:TGL:H181 | 2.19                     | 0.43              |
| 22:C:3270:CDL:H231 | 22:C:3270:CDL:H641 | 2.00                     | 0.43              |
| 25:E:3230:PSC:H201 | 25:E:3230:PSC:H232 | 1.84                     | 0.43              |
| 7:G:25:LEU:HD23    | 7:G:25:LEU:HA      | 1.88                     | 0.43              |
| 6:S:94:HIS:CG      | 6:S:95:GLN:N       | 2.78                     | 0.43              |
| 12:Y:20:ARG:NH2    | 12:Y:24:MET:HG3    | 2.33                     | 0.43              |
| 1:A:334:TRP:CH2    | 2:B:46:LEU:HD13    | 2.54                     | 0.43              |
| 7:G:7:ASP:O        | 7:G:9:GLY:N        | 2.47                     | 0.43              |
| 1:N:32:ALA:HB3     | 12:Y:36:PRO:HG2    | 1.99                     | 0.43              |
| 1:N:363:LEU:HD23   | 1:N:363:LEU:HA     | 1.87                     | 0.43              |
| 19:N:4524:PGV:H141 | 4:Q:87:PHE:CD2     | 2.53                     | 0.43              |
| 10:W:50:LEU:O      | 10:W:50:LEU:HD22   | 2.18                     | 0.43              |
| 1:A:1:FME:HE3      | 12:L:3:TYR:CE1     | 2.51                     | 0.43              |
| 8:H:60:TYR:CD1     | 8:H:60:TYR:C       | 2.96                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:J:50:LEU:HD22   | 10:J:50:LEU:O      | 2.18                     | 0.43              |
| 5:R:48:ILE:O       | 5:R:52:LEU:HG      | 2.19                     | 0.43              |
| 21:C:3271:CHD:H161 | 28:C:3628:HOH:O    | 2.18                     | 0.43              |
| 21:C:3271:CHD:H222 | 21:C:3271:CHD:H162 | 1.72                     | 0.43              |
| 7:G:1:ALA:HB2      | 19:P:4268:PGV:H321 | 2.00                     | 0.43              |
| 22:G:3269:CDL:H522 | 22:G:3269:CDL:H202 | 2.01                     | 0.43              |
| 12:Y:4:GLU:HB3     | 12:Y:9:LYS:HB3     | 2.01                     | 0.43              |
| 1:A:115:SER:O      | 1:A:121:GLY:HA2    | 2.19                     | 0.43              |
| 1:A:240:HIS:O      | 1:A:243:VAL:HG22   | 2.19                     | 0.43              |
| 22:C:3270:CDL:H532 | 22:C:3270:CDL:H561 | 1.84                     | 0.43              |
| 4:D:48:TRP:HA      | 4:D:51:LEU:HD22    | 2.00                     | 0.43              |
| 18:N:4521:TGL:H283 | 18:N:4521:TGL:C10  | 2.49                     | 0.43              |
| 25:O:4230:PSC:H241 | 25:O:4230:PSC:H62  | 2.00                     | 0.43              |
| 7:T:5:LYS:HG3      | 23:T:3263:PEK:H382 | 2.01                     | 0.43              |
| 1:A:310:MET:HE2    | 1:A:356:ILE:HG23   | 2.01                     | 0.42              |
| 19:A:3524:PGV:H012 | 19:A:3524:PGV:C4   | 2.50                     | 0.42              |
| 25:E:3230:PSC:H62  | 25:E:3230:PSC:H241 | 2.01                     | 0.42              |
| 21:J:3060:CHD:H212 | 21:J:3060:CHD:H161 | 1.70                     | 0.42              |
| 1:N:399:LEU:HB2    | 1:N:494:TRP:CZ3    | 2.54                     | 0.42              |
| 2:O:5:MET:HE2      | 2:O:5:MET:HB3      | 1.88                     | 0.42              |
| 2:O:132:GLU:HB3    | 2:O:137:GLU:HG3    | 2.00                     | 0.42              |
| 25:O:4230:PSC:H231 | 25:O:4230:PSC:H42  | 2.01                     | 0.42              |
| 28:A:3743:HOH:O    | 11:K:8:ASP:HB2     | 2.19                     | 0.42              |
| 2:B:59:GLN:C       | 2:B:60:GLU:HG3     | 2.44                     | 0.42              |
| 3:C:135:SER:HB3    | 22:G:3269:CDL:H581 | 2.01                     | 0.42              |
| 18:N:4521:TGL:HG11 | 2:O:7:LEU:HB3      | 2.00                     | 0.42              |
| 4:Q:138:TRP:CH2    | 11:X:50:PRO:HG2    | 2.54                     | 0.42              |
| 7:T:8:HIS:ND1      | 23:T:3263:PEK:H311 | 2.34                     | 0.42              |
| 5:E:31:LYS:HE3     | 6:F:83:PRO:O       | 2.19                     | 0.42              |
| 5:E:80:GLU:H       | 5:E:80:GLU:CD      | 2.27                     | 0.42              |
| 1:N:426:PHE:CE1    | 18:N:4521:TGL:C28  | 3.01                     | 0.42              |
| 5:R:82:TYR:N       | 5:R:83:PRO:CD      | 2.82                     | 0.42              |
| 1:A:282:PHE:HZ     | 22:T:4269:CDL:H761 | 1.84                     | 0.42              |
| 22:P:4270:CDL:H522 | 22:P:4270:CDL:OB9  | 2.19                     | 0.42              |
| 4:Q:52:SER:OG      | 4:Q:55:GLU:HG3     | 2.20                     | 0.42              |
| 6:S:64:GLU:O       | 6:S:65:ASP:HB2     | 2.19                     | 0.42              |
| 1:A:310:MET:HE1    | 2:B:76:ILE:CG2     | 2.50                     | 0.42              |
| 18:A:3521:TGL:HA91 | 18:A:3521:TGL:H222 | 1.60                     | 0.42              |
| 3:C:146:TRP:CE2    | 7:G:17:ARG:HG3     | 2.54                     | 0.42              |
| 22:C:3270:CDL:PA1  | 22:C:3270:CDL:HB22 | 2.60                     | 0.42              |
| 11:K:42:PRO:HG2    | 11:K:47:ARG:HE     | 1.85                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:N:81:TRP:HZ2     | 18:N:4522:TGL:C28  | 2.33                     | 0.42              |
| 1:N:292:MET:O      | 1:N:295:VAL:HG22   | 2.20                     | 0.42              |
| 1:N:374:VAL:HA     | 1:N:377:PHE:CE1    | 2.55                     | 0.42              |
| 3:P:173:PHE:C      | 3:P:173:PHE:CD2    | 2.97                     | 0.42              |
| 18:A:3521:TGL:H101 | 18:A:3521:TGL:C27  | 2.49                     | 0.42              |
| 2:B:82:ARG:HH11    | 2:B:86:MET:HE1     | 1.85                     | 0.42              |
| 13:M:37:LEU:HA     | 13:M:37:LEU:HD23   | 1.72                     | 0.42              |
| 10:W:36:MET:HB3    | 21:W:4060:CHD:H181 | 2.01                     | 0.42              |
| 21:C:3271:CHD:H222 | 28:C:3628:HOH:O    | 2.19                     | 0.42              |
| 25:E:3230:PSC:H062 | 25:E:3230:PSC:H042 | 1.75                     | 0.42              |
| 9:I:21:ILE:HD13    | 9:I:21:ILE:HA      | 1.93                     | 0.42              |
| 8:U:36:PHE:CE1     | 8:U:57:ARG:HB2     | 2.54                     | 0.42              |
| 1:N:53:ILE:HD12    | 12:Y:44:LEU:HD23   | 2.01                     | 0.42              |
| 1:N:71:MET:HB2     | 1:N:72:PRO:HD3     | 2.02                     | 0.42              |
| 2:O:217:LYS:HE2    | 2:O:217:LYS:CA     | 2.49                     | 0.42              |
| 7:T:5:LYS:CG       | 23:T:3263:PEK:H382 | 2.50                     | 0.42              |
| 1:A:128:VAL:O      | 1:A:128:VAL:HG12   | 2.20                     | 0.42              |
| 22:C:3270:CDL:H812 | 19:C:3267:PGV:H181 | 2.02                     | 0.42              |
| 6:F:51:SER:O       | 6:F:94:HIS:N       | 2.53                     | 0.42              |
| 1:N:46:THR:OG1     | 1:N:49:GLY:HA2     | 2.20                     | 0.42              |
| 2:O:16:ILE:HD13    | 2:O:16:ILE:HA      | 1.96                     | 0.42              |
| 3:P:253:TYR:HE2    | 22:T:4269:CDL:H641 | 1.83                     | 0.42              |
| 4:Q:131:ILE:HD12   | 4:Q:131:ILE:N      | 2.34                     | 0.42              |
| 7:T:19:LEU:HD21    | 23:T:3263:PEK:H362 | 2.02                     | 0.42              |
| 22:T:4269:CDL:H432 | 22:T:4269:CDL:H402 | 1.78                     | 0.42              |
| 22:T:4269:CDL:H662 | 22:T:4269:CDL:H631 | 1.88                     | 0.42              |
| 21:W:4060:CHD:H161 | 21:W:4060:CHD:H212 | 1.71                     | 0.42              |
| 1:A:46:THR:OG1     | 1:A:49:GLY:HA2     | 2.20                     | 0.41              |
| 1:A:351:GLY:HA3    | 1:A:380:VAL:HG13   | 2.01                     | 0.41              |
| 18:A:3522:TGL:H272 | 18:A:3522:TGL:H232 | 2.02                     | 0.41              |
| 4:D:34:SER:O       | 4:D:38:LYS:HG3     | 2.20                     | 0.41              |
| 6:F:55:LYS:HA      | 6:F:74:LEU:O       | 2.19                     | 0.41              |
| 2:O:104:TRP:HA     | 2:O:207:MET:SD     | 2.60                     | 0.41              |
| 1:N:217:THR:HG22   | 3:P:188:ILE:HG12   | 2.01                     | 0.41              |
| 1:A:44:PRO:HG2     | 4:D:111:PHE:CZ     | 2.56                     | 0.41              |
| 25:E:3230:PSC:H343 | 25:E:3230:PSC:H141 | 2.02                     | 0.41              |
| 11:K:43:SER:HA     | 11:K:44:PRO:HD3    | 1.96                     | 0.41              |
| 2:B:16:ILE:HD13    | 2:B:16:ILE:HA      | 1.91                     | 0.41              |
| 3:C:31:LEU:HD23    | 3:C:31:LEU:HA      | 1.92                     | 0.41              |
| 1:N:40:GLU:HG2     | 1:N:54:TYR:CD2     | 2.55                     | 0.41              |
| 1:N:95:PRO:HG2     | 3:P:11:VAL:HG23    | 2.01                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:N:324:LEU:HD13   | 2:O:41:ILE:HG22    | 2.01                     | 0.41              |
| 19:N:4524:PGV:H311 | 13:Z:19:LEU:HD23   | 2.02                     | 0.41              |
| 6:S:13:ALA:O       | 6:S:18:ARG:HD2     | 2.19                     | 0.41              |
| 22:C:3270:CDL:OB9  | 22:C:3270:CDL:H522 | 2.21                     | 0.41              |
| 1:N:405:LEU:HD23   | 1:N:475:ALA:HB2    | 2.02                     | 0.41              |
| 18:N:4521:TGL:H281 | 18:N:4521:TGL:HB81 | 2.03                     | 0.41              |
| 3:P:40:MET:O       | 3:P:44:MET:HG2     | 2.20                     | 0.41              |
| 18:A:3521:TGL:H101 | 18:A:3521:TGL:H271 | 2.01                     | 0.41              |
| 22:G:3269:CDL:OA7  | 22:G:3269:CDL:H331 | 2.20                     | 0.41              |
| 10:J:44:LEU:HD23   | 10:J:44:LEU:HA     | 1.96                     | 0.41              |
| 1:N:339:MET:HE1    | 1:N:411:LYS:HD3    | 2.02                     | 0.41              |
| 18:N:4521:TGL:H241 | 18:N:4521:TGL:CA9  | 2.44                     | 0.41              |
| 21:P:4271:CHD:H162 | 21:P:4271:CHD:H222 | 1.71                     | 0.41              |
| 23:P:4265:PEK:H041 | 6:S:1:ALA:H2       | 1.83                     | 0.41              |
| 4:Q:93:ALA:HB2     | 11:X:29:TRP:CE2    | 2.55                     | 0.41              |
| 2:B:1:FME:HE1      | 2:B:133:LEU:HD22   | 2.03                     | 0.41              |
| 7:G:2:SER:OG       | 23:G:4263:PEK:H291 | 2.21                     | 0.41              |
| 22:G:3269:CDL:H402 | 22:G:3269:CDL:H432 | 1.76                     | 0.41              |
| 17:N:516:HEA:HHA   | 17:N:516:HEA:HAD2  | 1.88                     | 0.41              |
| 6:S:55:LYS:HA      | 6:S:74:LEU:O       | 2.21                     | 0.41              |
| 22:T:4269:CDL:H551 | 22:T:4269:CDL:H582 | 1.77                     | 0.41              |
| 3:C:62:ILE:HG13    | 19:C:3267:PGV:H21  | 2.02                     | 0.41              |
| 3:C:173:PHE:CD2    | 3:C:173:PHE:C      | 2.98                     | 0.41              |
| 1:N:68:PHE:HE2     | 1:N:112:LEU:CD1    | 2.27                     | 0.41              |
| 1:N:321:PHE:CD2    | 25:O:4230:PSC:H341 | 2.56                     | 0.41              |
| 2:O:42:ILE:O       | 2:O:46:LEU:HG      | 2.20                     | 0.41              |
| 2:O:121:TYR:O      | 2:O:138:VAL:HA     | 2.20                     | 0.41              |
| 1:A:334:TRP:CZ3    | 18:A:3523:TGL:HA62 | 2.55                     | 0.41              |
| 2:B:23:PHE:CZ      | 2:B:80:SER:HB2     | 2.56                     | 0.41              |
| 2:B:75:LEU:HA      | 2:B:75:LEU:HD12    | 1.79                     | 0.41              |
| 18:N:4521:TGL:HC22 | 28:Q:1346:HOH:O    | 2.21                     | 0.41              |
| 19:N:4524:PGV:H012 | 19:N:4524:PGV:C4   | 2.50                     | 0.41              |
| 3:P:205:GLY:HA3    | 23:P:4264:PEK:H181 | 2.02                     | 0.41              |
| 4:Q:48:TRP:CH2     | 5:R:56:ARG:HA      | 2.56                     | 0.41              |
| 4:Q:48:TRP:CD1     | 5:R:56:ARG:HH12    | 2.38                     | 0.41              |
| 5:R:41:LEU:HA      | 28:V:1301:HOH:O    | 2.21                     | 0.41              |
| 22:T:4269:CDL:H561 | 22:T:4269:CDL:H611 | 2.02                     | 0.41              |
| 3:C:67:PHE:HE1     | 22:C:3270:CDL:C1   | 2.25                     | 0.41              |
| 3:C:116:TRP:HA     | 3:C:117:PRO:C      | 2.46                     | 0.41              |
| 6:F:52:ILE:HA      | 6:F:94:HIS:HA      | 2.02                     | 0.41              |
| 1:N:34:SER:HB2     | 17:N:515:HEA:C2B   | 2.51                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:O:4230:PSC:H343 | 25:O:4230:PSC:H141 | 2.03                     | 0.41              |
| 8:U:8:ILE:HD12     | 8:U:8:ILE:HA       | 1.98                     | 0.41              |
| 8:U:54:GLU:CD      | 8:U:57:ARG:HH21    | 2.29                     | 0.41              |
| 2:B:155:SER:O      | 2:B:174:ALA:HB1    | 2.21                     | 0.40              |
| 21:B:4085:CHD:H12  | 21:B:4085:CHD:H212 | 2.03                     | 0.40              |
| 3:P:54:MET:HE1     | 19:P:4267:PGV:H141 | 2.02                     | 0.40              |
| 1:A:510:TYR:CD1    | 1:A:510:TYR:C      | 3.00                     | 0.40              |
| 18:A:3522:TGL:H291 | 18:A:3522:TGL:H122 | 1.90                     | 0.40              |
| 18:A:3523:TGL:HB51 | 4:D:81:VAL:HG11    | 2.03                     | 0.40              |
| 22:C:3270:CDL:HB22 | 22:C:3270:CDL:OA5  | 2.22                     | 0.40              |
| 7:G:19:LEU:HD21    | 23:G:4263:PEK:H362 | 2.03                     | 0.40              |
| 12:L:2:HIS:CG      | 12:L:3:TYR:H       | 2.39                     | 0.40              |
| 1:A:265:LYS:HB2    | 1:A:490:THR:HG21   | 2.02                     | 0.40              |
| 1:A:488:THR:HB     | 1:A:495:LEU:HD13   | 2.03                     | 0.40              |
| 22:T:4269:CDL:H601 | 22:T:4269:CDL:H571 | 1.76                     | 0.40              |
| 9:V:37:PHE:HA      | 9:V:41:GLU:HB2     | 2.03                     | 0.40              |
| 1:A:310:MET:HE1    | 2:B:76:ILE:HG21    | 2.04                     | 0.40              |
| 3:C:76:GLN:O       | 3:C:80:ARG:HG3     | 2.21                     | 0.40              |
| 1:N:514:LYS:HE2    | 28:S:1303:HOH:O    | 2.22                     | 0.40              |
| 4:Q:31:LYS:HB3     | 28:Q:2391:HOH:O    | 2.21                     | 0.40              |
| 23:C:3265:PEK:H383 | 22:G:3269:CDL:C27  | 2.50                     | 0.40              |
| 5:E:105:GLY:O      | 5:E:108:LYS:HG2    | 2.22                     | 0.40              |
| 25:E:3230:PSC:H231 | 25:E:3230:PSC:H42  | 2.03                     | 0.40              |
| 1:N:400:PHE:O      | 18:N:4522:TGL:H283 | 2.22                     | 0.40              |
| 3:P:95:THR:HG21    | 19:P:4268:PGV:H282 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 512/514 (100%) | 500 (98%) | 12 (2%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | N     | 512/514 (100%)  | 500 (98%)  | 12 (2%)  | 0        | 100         | 100 |
| 2   | B     | 225/227 (99%)   | 210 (93%)  | 12 (5%)  | 3 (1%)   | 9           | 3   |
| 2   | O     | 225/227 (99%)   | 208 (92%)  | 14 (6%)  | 3 (1%)   | 9           | 3   |
| 3   | C     | 257/261 (98%)   | 251 (98%)  | 5 (2%)   | 1 (0%)   | 30          | 22  |
| 3   | P     | 257/261 (98%)   | 251 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 4   | D     | 142/147 (97%)   | 139 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 4   | Q     | 142/147 (97%)   | 139 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 5   | E     | 103/109 (94%)   | 103 (100%) | 0        | 0        | 100         | 100 |
| 5   | R     | 103/109 (94%)   | 102 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 6   | F     | 96/98 (98%)     | 89 (93%)   | 4 (4%)   | 3 (3%)   | 3           | 0   |
| 6   | S     | 96/98 (98%)     | 91 (95%)   | 2 (2%)   | 3 (3%)   | 3           | 0   |
| 7   | G     | 81/85 (95%)     | 66 (82%)   | 8 (10%)  | 7 (9%)   | 0           | 0   |
| 7   | T     | 81/85 (95%)     | 65 (80%)   | 9 (11%)  | 7 (9%)   | 0           | 0   |
| 8   | H     | 77/85 (91%)     | 70 (91%)   | 4 (5%)   | 3 (4%)   | 2           | 0   |
| 8   | U     | 77/85 (91%)     | 70 (91%)   | 5 (6%)   | 2 (3%)   | 4           | 1   |
| 9   | I     | 71/73 (97%)     | 68 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 9   | V     | 71/73 (97%)     | 68 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 10  | J     | 56/59 (95%)     | 55 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 10  | W     | 56/59 (95%)     | 56 (100%)  | 0        | 0        | 100         | 100 |
| 11  | K     | 47/56 (84%)     | 47 (100%)  | 0        | 0        | 100         | 100 |
| 11  | X     | 47/56 (84%)     | 47 (100%)  | 0        | 0        | 100         | 100 |
| 12  | L     | 44/47 (94%)     | 42 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 12  | Y     | 44/47 (94%)     | 43 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 13  | M     | 41/46 (89%)     | 40 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 13  | Z     | 41/46 (89%)     | 40 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| All | All   | 3504/3614 (97%) | 3360 (96%) | 112 (3%) | 32 (1%)  | 14          | 6   |

All (32) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 95  | GLN  |
| 7   | G     | 4   | ALA  |
| 7   | G     | 7   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 8   | HIS  |
| 7   | G     | 39  | SER  |
| 6   | S     | 94  | HIS  |
| 6   | S     | 95  | GLN  |
| 7   | T     | 3   | ALA  |
| 7   | T     | 4   | ALA  |
| 7   | T     | 7   | ASP  |
| 7   | T     | 8   | HIS  |
| 7   | T     | 39  | SER  |
| 2   | B     | 104 | TRP  |
| 6   | F     | 94  | HIS  |
| 7   | G     | 3   | ALA  |
| 7   | G     | 40  | GLY  |
| 8   | H     | 8   | ILE  |
| 8   | H     | 46  | LYS  |
| 2   | O     | 104 | TRP  |
| 7   | T     | 40  | GLY  |
| 8   | U     | 8   | ILE  |
| 8   | U     | 46  | LYS  |
| 2   | B     | 60  | GLU  |
| 2   | O     | 60  | GLU  |
| 6   | F     | 96  | LEU  |
| 6   | S     | 96  | LEU  |
| 3   | C     | 38  | ASN  |
| 8   | H     | 9   | LYS  |
| 7   | G     | 6   | GLY  |
| 7   | T     | 6   | GLY  |
| 2   | B     | 92  | ASN  |
| 2   | O     | 92  | ASN  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |
|-----|-------|----------------|-----------|----------|-------------|
| 1   | A     | 426/426 (100%) | 417 (98%) | 9 (2%)   | 47 44       |
| 1   | N     | 426/426 (100%) | 415 (97%) | 11 (3%)  | 40 35       |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | B     | 210/210 (100%)  | 201 (96%)  | 9 (4%)   | 26          | 18 |
| 2   | O     | 210/210 (100%)  | 197 (94%)  | 13 (6%)  | 16          | 9  |
| 3   | C     | 224/226 (99%)   | 220 (98%)  | 4 (2%)   | 51          | 50 |
| 3   | P     | 224/226 (99%)   | 220 (98%)  | 4 (2%)   | 51          | 50 |
| 4   | D     | 128/129 (99%)   | 127 (99%)  | 1 (1%)   | 73          | 75 |
| 4   | Q     | 128/129 (99%)   | 124 (97%)  | 4 (3%)   | 35          | 29 |
| 5   | E     | 92/95 (97%)     | 91 (99%)   | 1 (1%)   | 65          | 67 |
| 5   | R     | 92/95 (97%)     | 89 (97%)   | 3 (3%)   | 33          | 26 |
| 6   | F     | 81/81 (100%)    | 78 (96%)   | 3 (4%)   | 30          | 22 |
| 6   | S     | 81/81 (100%)    | 77 (95%)   | 4 (5%)   | 22          | 14 |
| 7   | G     | 67/68 (98%)     | 63 (94%)   | 4 (6%)   | 17          | 9  |
| 7   | T     | 67/68 (98%)     | 63 (94%)   | 4 (6%)   | 17          | 9  |
| 8   | H     | 71/75 (95%)     | 68 (96%)   | 3 (4%)   | 26          | 19 |
| 8   | U     | 71/75 (95%)     | 66 (93%)   | 5 (7%)   | 14          | 7  |
| 9   | I     | 57/57 (100%)    | 56 (98%)   | 1 (2%)   | 51          | 50 |
| 9   | V     | 57/57 (100%)    | 53 (93%)   | 4 (7%)   | 14          | 7  |
| 10  | J     | 49/50 (98%)     | 48 (98%)   | 1 (2%)   | 48          | 46 |
| 10  | W     | 49/50 (98%)     | 48 (98%)   | 1 (2%)   | 48          | 46 |
| 11  | K     | 39/46 (85%)     | 37 (95%)   | 2 (5%)   | 21          | 13 |
| 11  | X     | 39/46 (85%)     | 38 (97%)   | 1 (3%)   | 40          | 35 |
| 12  | L     | 39/40 (98%)     | 38 (97%)   | 1 (3%)   | 40          | 35 |
| 12  | Y     | 39/40 (98%)     | 37 (95%)   | 2 (5%)   | 21          | 13 |
| 13  | M     | 37/38 (97%)     | 33 (89%)   | 4 (11%)  | 6           | 2  |
| 13  | Z     | 37/38 (97%)     | 33 (89%)   | 4 (11%)  | 6           | 2  |
| All | All   | 3040/3082 (99%) | 2937 (97%) | 103 (3%) | 32          | 25 |

All (103) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 112 | LEU  |
| 1   | A     | 138 | HIS  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 297 | MET  |
| 1   | A     | 369 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 380 | VAL  |
| 1   | A     | 394 | VAL  |
| 1   | A     | 486 | ASP  |
| 1   | A     | 513 | LEU  |
| 2   | B     | 16  | ILE  |
| 2   | B     | 33  | LEU  |
| 2   | B     | 60  | GLU  |
| 2   | B     | 66  | THR  |
| 2   | B     | 75  | LEU  |
| 2   | B     | 78  | LEU  |
| 2   | B     | 91  | ASN  |
| 2   | B     | 115 | ASP  |
| 2   | B     | 167 | SER  |
| 3   | C     | 13  | PRO  |
| 3   | C     | 77  | LYS  |
| 3   | C     | 127 | LEU  |
| 3   | C     | 230 | ASN  |
| 4   | D     | 51  | LEU  |
| 5   | E     | 90  | ARG  |
| 6   | F     | 48  | LEU  |
| 6   | F     | 95  | GLN  |
| 6   | F     | 96  | LEU  |
| 7   | G     | 17  | ARG  |
| 7   | G     | 36  | TRP  |
| 7   | G     | 42  | ARG  |
| 7   | G     | 84  | LYS  |
| 8   | H     | 8   | ILE  |
| 8   | H     | 29  | CYS  |
| 8   | H     | 60  | TYR  |
| 9   | I     | 29  | LEU  |
| 10  | J     | 50  | LEU  |
| 11  | K     | 47  | ARG  |
| 11  | K     | 54  | ARG  |
| 12  | L     | 26  | THR  |
| 13  | M     | 13  | LYS  |
| 13  | M     | 34  | LEU  |
| 13  | M     | 38  | ASP  |
| 13  | M     | 42  | LYS  |
| 1   | N     | 138 | HIS  |
| 1   | N     | 152 | LEU  |
| 1   | N     | 180 | GLN  |
| 1   | N     | 241 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 297 | MET  |
| 1   | N     | 369 | ASP  |
| 1   | N     | 380 | VAL  |
| 1   | N     | 394 | VAL  |
| 1   | N     | 484 | THR  |
| 1   | N     | 504 | THR  |
| 1   | N     | 513 | LEU  |
| 2   | O     | 16  | ILE  |
| 2   | O     | 33  | LEU  |
| 2   | O     | 60  | GLU  |
| 2   | O     | 66  | THR  |
| 2   | O     | 68  | LEU  |
| 2   | O     | 75  | LEU  |
| 2   | O     | 78  | LEU  |
| 2   | O     | 91  | ASN  |
| 2   | O     | 94  | SER  |
| 2   | O     | 148 | MET  |
| 2   | O     | 167 | SER  |
| 2   | O     | 203 | ASN  |
| 2   | O     | 217 | LYS  |
| 3   | P     | 17  | PRO  |
| 3   | P     | 29  | SER  |
| 3   | P     | 77  | LYS  |
| 3   | P     | 230 | ASN  |
| 4   | Q     | 8   | SER  |
| 4   | Q     | 9   | GLU  |
| 4   | Q     | 19  | ARG  |
| 4   | Q     | 51  | LEU  |
| 5   | R     | 7   | THR  |
| 5   | R     | 70  | VAL  |
| 5   | R     | 90  | ARG  |
| 6   | S     | 48  | LEU  |
| 6   | S     | 53  | THR  |
| 6   | S     | 54  | ASN  |
| 6   | S     | 80  | GLN  |
| 7   | T     | 17  | ARG  |
| 7   | T     | 33  | LEU  |
| 7   | T     | 37  | LEU  |
| 7   | T     | 42  | ARG  |
| 8   | U     | 21  | PRO  |
| 8   | U     | 29  | CYS  |
| 8   | U     | 60  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | U     | 61  | LYS  |
| 8   | U     | 65  | PRO  |
| 9   | V     | 8   | GLN  |
| 9   | V     | 29  | LEU  |
| 9   | V     | 33  | THR  |
| 9   | V     | 61  | GLU  |
| 10  | W     | 50  | LEU  |
| 11  | X     | 54  | ARG  |
| 12  | Y     | 20  | ARG  |
| 12  | Y     | 26  | THR  |
| 13  | Z     | 13  | LYS  |
| 13  | Z     | 34  | LEU  |
| 13  | Z     | 38  | ASP  |
| 13  | Z     | 42  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ASN  |
| 1   | A     | 80  | ASN  |
| 1   | A     | 98  | ASN  |
| 1   | A     | 151 | HIS  |
| 1   | A     | 170 | ASN  |
| 1   | A     | 178 | GLN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 360 | ASN  |
| 1   | A     | 422 | ASN  |
| 1   | A     | 503 | HIS  |
| 1   | A     | 512 | ASN  |
| 2   | B     | 10  | GLN  |
| 2   | B     | 91  | ASN  |
| 2   | B     | 92  | ASN  |
| 2   | B     | 140 | ASN  |
| 2   | B     | 181 | GLN  |
| 3   | C     | 50  | ASN  |
| 3   | C     | 68  | GLN  |
| 3   | C     | 76  | GLN  |
| 3   | C     | 161 | GLN  |
| 4   | D     | 32  | ASN  |
| 4   | D     | 37  | GLN  |
| 4   | D     | 119 | GLN  |
| 4   | D     | 143 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 94  | ASN  |
| 6   | F     | 80  | GLN  |
| 7   | G     | 8   | HIS  |
| 7   | G     | 34  | ASN  |
| 8   | H     | 31  | GLN  |
| 9   | I     | 8   | GLN  |
| 9   | I     | 53  | ASN  |
| 10  | J     | 29  | ASN  |
| 11  | K     | 35  | GLN  |
| 1   | N     | 80  | ASN  |
| 1   | N     | 98  | ASN  |
| 1   | N     | 170 | ASN  |
| 1   | N     | 178 | GLN  |
| 1   | N     | 180 | GLN  |
| 1   | N     | 422 | ASN  |
| 1   | N     | 503 | HIS  |
| 1   | N     | 512 | ASN  |
| 2   | O     | 10  | GLN  |
| 2   | O     | 91  | ASN  |
| 2   | O     | 203 | ASN  |
| 3   | P     | 50  | ASN  |
| 3   | P     | 68  | GLN  |
| 3   | P     | 161 | GLN  |
| 3   | P     | 230 | ASN  |
| 4   | Q     | 37  | GLN  |
| 4   | Q     | 101 | HIS  |
| 4   | Q     | 119 | GLN  |
| 5   | R     | 94  | ASN  |
| 6   | S     | 54  | ASN  |
| 6   | S     | 80  | GLN  |
| 6   | S     | 94  | HIS  |
| 7   | T     | 71  | HIS  |
| 8   | U     | 31  | GLN  |
| 8   | U     | 32  | ASN  |
| 10  | W     | 57  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | TPO  | T     | 11  | 7    | 8,10,11      | 1.46 | 2 (25%)  | 10,14,16    | 1.09 | 1 (10%)  |
| 9   | SAC  | V     | 1   | 9    | 7,8,9        | 2.71 | 2 (28%)  | 7,9,11      | 1.97 | 3 (42%)  |
| 2   | FME  | B     | 1   | 2    | 8,9,10       | 0.78 | 0        | 8,9,11      | 1.60 | 2 (25%)  |
| 1   | FME  | N     | 1   | 1    | 8,9,10       | 0.79 | 0        | 8,9,11      | 1.79 | 2 (25%)  |
| 7   | TPO  | G     | 11  | 7    | 8,10,11      | 1.36 | 1 (12%)  | 10,14,16    | 1.10 | 1 (10%)  |
| 1   | FME  | A     | 1   | 1    | 8,9,10       | 0.70 | 0        | 8,9,11      | 1.17 | 1 (12%)  |
| 9   | SAC  | I     | 1   | 9    | 7,8,9        | 2.41 | 2 (28%)  | 7,9,11      | 1.77 | 3 (42%)  |
| 2   | FME  | O     | 1   | 2    | 8,9,10       | 0.73 | 0        | 8,9,11      | 2.08 | 2 (25%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 7   | TPO  | T     | 11  | 7    | -       | 4/9/11/13 | -     |
| 9   | SAC  | V     | 1   | 9    | -       | 3/7/8/10  | -     |
| 2   | FME  | B     | 1   | 2    | -       | 1/7/9/11  | -     |
| 1   | FME  | N     | 1   | 1    | -       | 3/7/9/11  | -     |
| 7   | TPO  | G     | 11  | 7    | -       | 4/9/11/13 | -     |
| 1   | FME  | A     | 1   | 1    | -       | 3/7/9/11  | -     |
| 9   | SAC  | I     | 1   | 9    | -       | 3/7/8/10  | -     |
| 2   | FME  | O     | 1   | 2    | -       | 1/7/9/11  | -     |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 9   | V     | 1   | SAC  | OAC-C1A | 5.23 | 1.34        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 9   | I     | 1   | SAC  | OAC-C1A | 5.02 | 1.34        | 1.23     |
| 9   | V     | 1   | SAC  | CA-N    | 4.50 | 1.53        | 1.46     |
| 9   | I     | 1   | SAC  | CA-N    | 3.66 | 1.51        | 1.46     |
| 7   | T     | 11  | TPO  | CB-CA   | 2.81 | 1.59        | 1.53     |
| 7   | G     | 11  | TPO  | CB-CA   | 2.30 | 1.58        | 1.53     |
| 7   | T     | 11  | TPO  | P-O1P   | 2.04 | 1.56        | 1.50     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | N     | 1   | FME  | CA-N-CN     | -4.22 | 116.33      | 122.82   |
| 2   | O     | 1   | FME  | C-CA-N      | 4.22  | 117.64      | 109.50   |
| 2   | O     | 1   | FME  | CA-N-CN     | -3.93 | 116.77      | 122.82   |
| 9   | I     | 1   | SAC  | C-CA-N      | -3.09 | 103.53      | 109.50   |
| 9   | V     | 1   | SAC  | C2A-C1A-N   | 2.98  | 121.05      | 116.12   |
| 9   | V     | 1   | SAC  | C-CA-N      | -2.94 | 103.82      | 109.50   |
| 2   | B     | 1   | FME  | C-CA-N      | 2.78  | 114.85      | 109.50   |
| 2   | B     | 1   | FME  | CA-N-CN     | -2.74 | 118.61      | 122.82   |
| 1   | A     | 1   | FME  | CA-N-CN     | -2.44 | 119.08      | 122.82   |
| 9   | V     | 1   | SAC  | OAC-C1A-C2A | -2.27 | 118.01      | 122.05   |
| 9   | I     | 1   | SAC  | OAC-C1A-C2A | -2.22 | 118.10      | 122.05   |
| 9   | I     | 1   | SAC  | C2A-C1A-N   | 2.21  | 119.78      | 116.12   |
| 7   | T     | 11  | TPO  | O3P-P-OG1   | 2.17  | 114.30      | 105.85   |
| 1   | N     | 1   | FME  | O-C-CA      | -2.13 | 119.30      | 124.77   |
| 7   | G     | 11  | TPO  | O3P-P-OG1   | 2.07  | 113.91      | 105.85   |

There are no chirality outliers.

All (22) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | A     | 1   | FME  | O1-CN-N-CA   |
| 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  |
| 7   | G     | 11  | TPO  | O-C-CA-CB    |
| 9   | I     | 1   | SAC  | OAC-C1A-N-CA |
| 9   | I     | 1   | SAC  | CB-CA-N-C1A  |
| 1   | N     | 1   | FME  | O1-CN-N-CA   |
| 1   | N     | 1   | FME  | N-CA-CB-CG   |
| 1   | N     | 1   | FME  | C-CA-CB-CG   |

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

There are no ring outliers.

5 monomers are involved in 10 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | T     | 11  | TPO  | 1       | 0            |
| 2   | B     | 1   | FME  | 1       | 0            |
| 1   | N     | 1   | FME  | 1       | 0            |
| 1   | A     | 1   | FME  | 6       | 0            |
| 2   | O     | 1   | FME  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 42 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 | $\# Z  > 2$ |
| 19  | PGV  | A     | 3266 | -    | 50,50,50     | 0.87 | 1 (2%)      | 53,56,56    | 0.73 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | PEK  | C     | 3264 | -    | 52,52,52     | 1.46 | 5 (9%)   | 55,57,57    | 1.19 | 8 (14%)  |
| 27  | DMU  | M     | 3526 | -    | 34,34,34     | 3.28 | 8 (23%)  | 45,45,45    | 4.10 | 20 (44%) |
| 22  | CDL  | G     | 3269 | -    | 99,99,99     | 0.99 | 7 (7%)   | 105,111,111 | 0.89 | 6 (5%)   |
| 19  | PGV  | N     | 4524 | -    | 50,50,50     | 1.14 | 4 (8%)   | 53,56,56    | 1.04 | 4 (7%)   |
| 20  | CUA  | B     | 228  | 2    | 0,1,1        | -    | -        | -           | -    | -        |
| 22  | CDL  | T     | 4269 | -    | 99,99,99     | 0.98 | 5 (5%)   | 105,111,111 | 0.91 | 6 (5%)   |
| 18  | TGL  | A     | 3523 | -    | 62,62,62     | 1.09 | 3 (4%)   | 65,65,65    | 1.07 | 4 (6%)   |
| 25  | PSC  | E     | 3230 | -    | 51,51,51     | 1.22 | 3 (5%)   | 57,59,59    | 1.05 | 4 (7%)   |
| 22  | CDL  | P     | 4270 | -    | 99,99,99     | 0.77 | 1 (1%)   | 105,111,111 | 0.87 | 5 (4%)   |
| 18  | TGL  | Q     | 4523 | -    | 62,62,62     | 1.11 | 3 (4%)   | 65,65,65    | 1.05 | 6 (9%)   |
| 17  | HEA  | N     | 515  | 1    | 67,67,67     | 1.06 | 4 (5%)   | 81,103,103  | 1.13 | 5 (6%)   |
| 21  | CHD  | C     | 3525 | -    | 32,32,32     | 0.91 | 1 (3%)   | 51,51,51    | 1.66 | 11 (21%) |
| 23  | PEK  | C     | 3265 | -    | 52,52,52     | 1.64 | 8 (15%)  | 55,57,57    | 0.97 | 4 (7%)   |
| 23  | PEK  | G     | 4263 | -    | 52,52,52     | 1.62 | 9 (17%)  | 55,57,57    | 1.01 | 3 (5%)   |
| 27  | DMU  | Z     | 4526 | -    | 34,34,34     | 3.25 | 9 (26%)  | 45,45,45    | 4.08 | 20 (44%) |
| 25  | PSC  | O     | 4230 | -    | 51,51,51     | 1.23 | 3 (5%)   | 57,59,59    | 1.04 | 4 (7%)   |
| 18  | TGL  | N     | 4522 | -    | 62,62,62     | 1.47 | 8 (12%)  | 65,65,65    | 1.19 | 4 (6%)   |
| 19  | PGV  | C     | 3268 | -    | 50,50,50     | 1.09 | 4 (8%)   | 53,56,56    | 0.71 | 1 (1%)   |
| 21  | CHD  | C     | 3271 | -    | 32,32,32     | 0.89 | 1 (3%)   | 51,51,51    | 3.59 | 24 (47%) |
| 21  | CHD  | O     | 3085 | -    | 32,32,32     | 0.86 | 1 (3%)   | 51,51,51    | 1.88 | 16 (31%) |
| 19  | PGV  | A     | 3524 | -    | 50,50,50     | 1.10 | 3 (6%)   | 53,56,56    | 1.08 | 6 (11%)  |
| 18  | TGL  | A     | 3522 | -    | 62,62,62     | 1.41 | 6 (9%)   | 65,65,65    | 1.21 | 5 (7%)   |
| 18  | TGL  | A     | 3521 | -    | 62,62,62     | 1.11 | 4 (6%)   | 65,65,65    | 1.13 | 6 (9%)   |
| 17  | HEA  | A     | 515  | 1    | 67,67,67     | 1.04 | 5 (7%)   | 81,103,103  | 1.11 | 7 (8%)   |
| 19  | PGV  | C     | 3267 | -    | 50,50,50     | 0.82 | 1 (2%)   | 53,56,56    | 0.87 | 2 (3%)   |
| 17  | HEA  | A     | 516  | 1    | 67,67,67     | 1.30 | 4 (5%)   | 81,103,103  | 1.16 | 8 (9%)   |
| 17  | HEA  | N     | 516  | 1    | 67,67,67     | 1.19 | 3 (4%)   | 81,103,103  | 1.21 | 7 (8%)   |
| 23  | PEK  | P     | 4264 | -    | 52,52,52     | 1.46 | 6 (11%)  | 55,57,57    | 1.22 | 6 (10%)  |
| 19  | PGV  | N     | 4266 | -    | 50,50,50     | 0.91 | 2 (4%)   | 53,56,56    | 0.80 | 3 (5%)   |
| 19  | PGV  | P     | 4267 | -    | 50,50,50     | 0.85 | 1 (2%)   | 53,56,56    | 0.87 | 1 (1%)   |
| 20  | CUA  | O     | 228  | 2    | 0,1,1        | -    | -        | -           | -    | -        |
| 21  | CHD  | P     | 4525 | -    | 32,32,32     | 0.83 | 1 (3%)   | 51,51,51    | 1.62 | 8 (15%)  |
| 23  | PEK  | P     | 4265 | -    | 52,52,52     | 1.68 | 11 (21%) | 55,57,57    | 0.97 | 4 (7%)   |
| 19  | PGV  | P     | 4268 | -    | 50,50,50     | 1.10 | 3 (6%)   | 53,56,56    | 0.71 | 0        |
| 22  | CDL  | C     | 3270 | -    | 99,99,99     | 0.76 | 1 (1%)   | 105,111,111 | 0.88 | 5 (4%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | PEK  | T     | 3263 | -    | 52,52,52     | 1.66 | 10 (19%) | 55,57,57    | 0.99 | 3 (5%)   |
| 21  | CHD  | P     | 4271 | -    | 32,32,32     | 0.84 | 0        | 51,51,51    | 3.57 | 24 (47%) |
| 21  | CHD  | B     | 4085 | -    | 32,32,32     | 0.81 | 1 (3%)   | 51,51,51    | 1.83 | 15 (29%) |
| 21  | CHD  | J     | 3060 | -    | 32,32,32     | 1.13 | 1 (3%)   | 51,51,51    | 3.25 | 27 (52%) |
| 18  | TGL  | N     | 4521 | -    | 62,62,62     | 1.14 | 4 (6%)   | 65,65,65    | 1.10 | 5 (7%)   |
| 21  | CHD  | W     | 4060 | -    | 32,32,32     | 1.17 | 3 (9%)   | 51,51,51    | 3.29 | 26 (50%) |

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   |
|-----|------|-------|------|------|-----------|----------------|---------|
| 19  | PGV  | A     | 3266 | -    | -         | 13/55/55/55    | -       |
| 23  | PEK  | C     | 3264 | -    | -         | 21/56/56/56    | -       |
| 27  | DMU  | M     | 3526 | -    | 5/5/10/10 | 10/19/59/59    | 0/2/2/2 |
| 22  | CDL  | G     | 3269 | -    | -         | 65/110/110/110 | -       |
| 19  | PGV  | N     | 4524 | -    | -         | 31/55/55/55    | -       |
| 22  | CDL  | T     | 4269 | -    | -         | 66/110/110/110 | -       |
| 18  | TGL  | A     | 3523 | -    | -         | 25/65/65/65    | -       |
| 25  | PSC  | E     | 3230 | -    | -         | 35/55/55/55    | -       |
| 22  | CDL  | P     | 4270 | -    | -         | 76/110/110/110 | -       |
| 18  | TGL  | Q     | 4523 | -    | -         | 25/65/65/65    | -       |
| 17  | HEA  | N     | 515  | 1    | -         | 2/36/76/76     | -       |
| 21  | CHD  | C     | 3525 | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 23  | PEK  | C     | 3265 | -    | -         | 19/56/56/56    | -       |
| 23  | PEK  | G     | 4263 | -    | -         | 24/56/56/56    | -       |
| 27  | DMU  | Z     | 4526 | -    | 5/5/10/10 | 10/19/59/59    | 0/2/2/2 |
| 25  | PSC  | O     | 4230 | -    | -         | 34/55/55/55    | -       |
| 18  | TGL  | N     | 4522 | -    | -         | 32/65/65/65    | -       |
| 19  | PGV  | C     | 3268 | -    | -         | 29/55/55/55    | -       |
| 21  | CHD  | C     | 3271 | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |
| 21  | CHD  | O     | 3085 | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 19  | PGV  | A     | 3524 | -    | -         | 30/55/55/55    | -       |
| 18  | TGL  | A     | 3522 | -    | -         | 32/65/65/65    | -       |
| 18  | TGL  | A     | 3521 | -    | -         | 30/65/65/65    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions       | Rings   |
|-----|------|-------|------|------|-----------|----------------|---------|
| 17  | HEA  | A     | 515  | 1    | -         | 2/36/76/76     | -       |
| 19  | PGV  | C     | 3267 | -    | -         | 16/55/55/55    | -       |
| 17  | HEA  | A     | 516  | 1    | -         | 7/36/76/76     | -       |
| 17  | HEA  | N     | 516  | 1    | -         | 7/36/76/76     | -       |
| 23  | PEK  | P     | 4264 | -    | -         | 21/56/56/56    | -       |
| 19  | PGV  | N     | 4266 | -    | -         | 13/55/55/55    | -       |
| 19  | PGV  | P     | 4267 | -    | -         | 16/55/55/55    | -       |
| 21  | CHD  | P     | 4525 | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 23  | PEK  | P     | 4265 | -    | -         | 19/56/56/56    | -       |
| 19  | PGV  | P     | 4268 | -    | -         | 29/55/55/55    | -       |
| 22  | CDL  | C     | 3270 | -    | -         | 76/110/110/110 | -       |
| 23  | PEK  | T     | 3263 | -    | -         | 24/56/56/56    | -       |
| 21  | CHD  | P     | 4271 | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |
| 21  | CHD  | B     | 4085 | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 21  | CHD  | J     | 3060 | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |
| 18  | TGL  | N     | 4521 | -    | -         | 30/65/65/65    | -       |
| 21  | CHD  | W     | 4060 | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |

All (158) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 27  | M     | 3526 | DMU  | O7-C3   | -8.30 | 1.22        | 1.43     |
| 27  | Z     | 4526 | DMU  | O16-C6  | -8.17 | 1.26        | 1.40     |
| 27  | M     | 3526 | DMU  | O16-C6  | -8.00 | 1.26        | 1.40     |
| 27  | Z     | 4526 | DMU  | O7-C3   | -7.78 | 1.24        | 1.43     |
| 27  | M     | 3526 | DMU  | O5-C4   | -7.08 | 1.27        | 1.44     |
| 27  | Z     | 4526 | DMU  | O16-C18 | -6.97 | 1.24        | 1.43     |
| 27  | M     | 3526 | DMU  | O16-C18 | -6.92 | 1.24        | 1.43     |
| 27  | Z     | 4526 | DMU  | O5-C4   | -6.44 | 1.28        | 1.44     |
| 27  | M     | 3526 | DMU  | O1-C9   | -6.23 | 1.29        | 1.44     |
| 27  | Z     | 4526 | DMU  | O7-C10  | -6.11 | 1.24        | 1.41     |
| 27  | Z     | 4526 | DMU  | O1-C9   | -6.10 | 1.29        | 1.44     |
| 27  | M     | 3526 | DMU  | O7-C10  | -5.95 | 1.25        | 1.41     |
| 18  | A     | 3522 | TGL  | OG2-CB1 | 5.84  | 1.50        | 1.34     |
| 17  | A     | 516  | HEA  | FE-NC   | 5.60  | 2.13        | 1.95     |
| 18  | N     | 4522 | TGL  | OG2-CB1 | 5.56  | 1.50        | 1.34     |
| 27  | Z     | 4526 | DMU  | O1-C10  | -5.40 | 1.27        | 1.41     |
| 27  | M     | 3526 | DMU  | O1-C10  | -5.31 | 1.28        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 27  | M     | 3526 | DMU  | O5-C6   | -4.99 | 1.29        | 1.41     |
| 18  | N     | 4522 | TGL  | OG1-CA1 | 4.93  | 1.47        | 1.33     |
| 27  | Z     | 4526 | DMU  | O5-C6   | -4.88 | 1.29        | 1.41     |
| 18  | N     | 4521 | TGL  | OG2-CB1 | 4.84  | 1.48        | 1.34     |
| 23  | C     | 3264 | PEK  | C15-C14 | 4.79  | 1.58        | 1.31     |
| 23  | G     | 4263 | PEK  | C12-C11 | 4.76  | 1.58        | 1.31     |
| 23  | P     | 4264 | PEK  | C15-C14 | 4.75  | 1.58        | 1.31     |
| 23  | P     | 4264 | PEK  | C12-C11 | 4.73  | 1.58        | 1.31     |
| 23  | C     | 3264 | PEK  | C12-C11 | 4.62  | 1.57        | 1.31     |
| 23  | T     | 3263 | PEK  | C12-C11 | 4.61  | 1.57        | 1.31     |
| 18  | A     | 3522 | TGL  | OG1-CA1 | 4.57  | 1.46        | 1.33     |
| 18  | N     | 4522 | TGL  | OG3-CC1 | 4.54  | 1.46        | 1.33     |
| 18  | A     | 3523 | TGL  | OG1-CA1 | 4.41  | 1.46        | 1.33     |
| 23  | T     | 3263 | PEK  | C9-C8   | 4.36  | 1.56        | 1.31     |
| 23  | C     | 3265 | PEK  | C15-C14 | 4.36  | 1.56        | 1.31     |
| 23  | C     | 3265 | PEK  | C12-C11 | 4.35  | 1.56        | 1.31     |
| 23  | P     | 4265 | PEK  | C12-C11 | 4.35  | 1.56        | 1.31     |
| 25  | O     | 4230 | PSC  | C10-C9  | 4.34  | 1.56        | 1.31     |
| 18  | Q     | 4523 | TGL  | OG1-CA1 | 4.31  | 1.45        | 1.33     |
| 23  | P     | 4265 | PEK  | C6-C5   | 4.31  | 1.56        | 1.31     |
| 23  | P     | 4265 | PEK  | C15-C14 | 4.28  | 1.56        | 1.31     |
| 23  | T     | 3263 | PEK  | C6-C5   | 4.26  | 1.55        | 1.31     |
| 23  | C     | 3265 | PEK  | C6-C5   | 4.26  | 1.55        | 1.31     |
| 19  | N     | 4524 | PGV  | C12-C11 | 4.25  | 1.55        | 1.31     |
| 19  | A     | 3524 | PGV  | C12-C11 | 4.24  | 1.55        | 1.31     |
| 23  | G     | 4263 | PEK  | C9-C8   | 4.24  | 1.55        | 1.31     |
| 19  | P     | 4268 | PGV  | C12-C11 | 4.23  | 1.55        | 1.31     |
| 25  | O     | 4230 | PSC  | C13-C12 | 4.23  | 1.55        | 1.31     |
| 23  | P     | 4265 | PEK  | C9-C8   | 4.23  | 1.55        | 1.31     |
| 23  | C     | 3265 | PEK  | C9-C8   | 4.23  | 1.55        | 1.31     |
| 18  | A     | 3521 | TGL  | OG2-CB1 | 4.21  | 1.46        | 1.34     |
| 25  | E     | 3230 | PSC  | C10-C9  | 4.19  | 1.55        | 1.31     |
| 25  | E     | 3230 | PSC  | C13-C12 | 4.18  | 1.55        | 1.31     |
| 23  | G     | 4263 | PEK  | C15-C14 | 4.18  | 1.55        | 1.31     |
| 23  | G     | 4263 | PEK  | C6-C5   | 4.18  | 1.55        | 1.31     |
| 18  | A     | 3522 | TGL  | OG3-CC1 | 4.15  | 1.45        | 1.33     |
| 19  | C     | 3268 | PGV  | C12-C11 | 4.14  | 1.55        | 1.31     |
| 23  | T     | 3263 | PEK  | C15-C14 | 4.13  | 1.55        | 1.31     |
| 23  | C     | 3264 | PEK  | C9-C8   | 4.10  | 1.55        | 1.31     |
| 18  | Q     | 4523 | TGL  | OG2-CB1 | 4.10  | 1.45        | 1.34     |
| 17  | N     | 516  | HEA  | FE-NC   | 4.07  | 2.08        | 1.95     |
| 19  | N     | 4266 | PGV  | C12-C11 | 4.04  | 1.54        | 1.31     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | P     | 4264 | PEK  | C9-C8   | 4.03  | 1.54        | 1.31     |
| 23  | P     | 4264 | PEK  | C6-C5   | 4.03  | 1.54        | 1.31     |
| 18  | A     | 3523 | TGL  | OG3-CC1 | 4.00  | 1.45        | 1.33     |
| 23  | C     | 3264 | PEK  | C6-C5   | 3.97  | 1.54        | 1.31     |
| 19  | A     | 3266 | PGV  | C12-C11 | 3.96  | 1.54        | 1.31     |
| 18  | A     | 3521 | TGL  | OG1-CA1 | 3.81  | 1.44        | 1.33     |
| 18  | N     | 4521 | TGL  | OG1-CA1 | 3.80  | 1.44        | 1.33     |
| 17  | N     | 516  | HEA  | FE-NA   | 3.80  | 2.07        | 1.95     |
| 18  | Q     | 4523 | TGL  | OG3-CC1 | 3.78  | 1.44        | 1.33     |
| 21  | W     | 4060 | CHD  | C13-C17 | 3.76  | 1.61        | 1.55     |
| 18  | A     | 3523 | TGL  | OG2-CB1 | 3.74  | 1.44        | 1.34     |
| 21  | J     | 3060 | CHD  | C13-C17 | 3.54  | 1.61        | 1.55     |
| 23  | G     | 4263 | PEK  | C03-C02 | 3.52  | 1.61        | 1.50     |
| 17  | A     | 516  | HEA  | FE-NA   | 3.46  | 2.06        | 1.95     |
| 18  | A     | 3521 | TGL  | OG3-CC1 | 3.46  | 1.43        | 1.33     |
| 22  | T     | 4269 | CDL  | CB6-CB4 | 3.44  | 1.61        | 1.50     |
| 23  | T     | 3263 | PEK  | C03-C02 | 3.43  | 1.61        | 1.50     |
| 18  | N     | 4521 | TGL  | OG3-CC1 | 3.34  | 1.43        | 1.33     |
| 19  | P     | 4267 | PGV  | C12-C11 | 3.13  | 1.49        | 1.31     |
| 18  | N     | 4522 | TGL  | OG3-CG3 | 3.13  | 1.52        | 1.45     |
| 19  | C     | 3267 | PGV  | C12-C11 | 3.08  | 1.49        | 1.31     |
| 22  | G     | 3269 | CDL  | CB6-CB4 | 3.06  | 1.60        | 1.50     |
| 23  | P     | 4265 | PEK  | O03-C21 | 3.05  | 1.42        | 1.33     |
| 25  | O     | 4230 | PSC  | C2-C1   | 2.97  | 1.59        | 1.50     |
| 22  | G     | 3269 | CDL  | OA6-CA5 | 2.94  | 1.42        | 1.34     |
| 23  | C     | 3265 | PEK  | O03-C21 | 2.91  | 1.41        | 1.33     |
| 23  | G     | 4263 | PEK  | C01-C02 | 2.84  | 1.59        | 1.50     |
| 23  | T     | 3263 | PEK  | O03-C21 | 2.84  | 1.41        | 1.33     |
| 23  | T     | 3263 | PEK  | C01-C02 | 2.80  | 1.59        | 1.50     |
| 18  | A     | 3522 | TGL  | OG2-CG2 | 2.75  | 1.53        | 1.46     |
| 22  | T     | 4269 | CDL  | CB3-CB4 | 2.75  | 1.59        | 1.50     |
| 23  | T     | 3263 | PEK  | C22-C21 | 2.74  | 1.58        | 1.50     |
| 19  | P     | 4268 | PGV  | O01-C1  | 2.72  | 1.42        | 1.34     |
| 19  | C     | 3268 | PGV  | O01-C1  | 2.70  | 1.41        | 1.34     |
| 17  | A     | 515  | HEA  | CMA-C3A | -2.68 | 1.39        | 1.45     |
| 19  | N     | 4524 | PGV  | C20-C19 | 2.67  | 1.58        | 1.50     |
| 23  | C     | 3265 | PEK  | C03-C02 | 2.66  | 1.59        | 1.50     |
| 17  | N     | 516  | HEA  | CMA-C3A | -2.66 | 1.39        | 1.45     |
| 22  | G     | 3269 | CDL  | CB3-CB4 | 2.65  | 1.59        | 1.50     |
| 25  | E     | 3230 | PSC  | C2-C1   | 2.62  | 1.58        | 1.50     |
| 23  | P     | 4265 | PEK  | C03-C02 | 2.59  | 1.58        | 1.50     |
| 23  | G     | 4263 | PEK  | O03-C21 | 2.56  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | C     | 3270 | CDL  | C71-CB7 | 2.55  | 1.58        | 1.50     |
| 19  | A     | 3524 | PGV  | C20-C19 | 2.53  | 1.58        | 1.50     |
| 22  | T     | 4269 | CDL  | OA6-CA5 | 2.50  | 1.41        | 1.34     |
| 17  | N     | 515  | HEA  | C1C-C2C | 2.49  | 1.49        | 1.43     |
| 17  | N     | 515  | HEA  | C3C-C4C | 2.48  | 1.50        | 1.42     |
| 18  | A     | 3522 | TGL  | OG3-CG3 | 2.48  | 1.50        | 1.45     |
| 19  | P     | 4268 | PGV  | C2-C1   | 2.47  | 1.57        | 1.50     |
| 19  | N     | 4524 | PGV  | P-O11   | 2.47  | 1.69        | 1.59     |
| 17  | A     | 516  | HEA  | C4D-ND  | 2.47  | 1.43        | 1.38     |
| 23  | G     | 4263 | PEK  | C22-C21 | 2.45  | 1.57        | 1.50     |
| 23  | P     | 4265 | PEK  | C01-C02 | 2.44  | 1.58        | 1.50     |
| 22  | T     | 4269 | CDL  | CB2-C1  | 2.42  | 1.59        | 1.51     |
| 19  | N     | 4266 | PGV  | C01-C02 | 2.41  | 1.58        | 1.50     |
| 22  | G     | 3269 | CDL  | OB6-CB5 | 2.38  | 1.41        | 1.34     |
| 22  | P     | 4270 | CDL  | C71-CB7 | 2.34  | 1.57        | 1.50     |
| 19  | A     | 3524 | PGV  | P-O11   | 2.34  | 1.68        | 1.59     |
| 17  | N     | 515  | HEA  | C11-C3B | -2.33 | 1.48        | 1.51     |
| 19  | C     | 3268 | PGV  | C2-C1   | 2.33  | 1.57        | 1.50     |
| 18  | N     | 4522 | TGL  | CC2-CC1 | 2.31  | 1.57        | 1.50     |
| 18  | N     | 4522 | TGL  | OG2-CG2 | 2.31  | 1.52        | 1.46     |
| 23  | P     | 4264 | PEK  | O03-C01 | -2.26 | 1.40        | 1.45     |
| 17  | A     | 515  | HEA  | C3C-C4C | 2.26  | 1.49        | 1.42     |
| 22  | G     | 3269 | CDL  | CB2-C1  | 2.25  | 1.58        | 1.51     |
| 23  | C     | 3265 | PEK  | C01-C02 | 2.25  | 1.57        | 1.50     |
| 18  | A     | 3521 | TGL  | OG1-CG1 | -2.24 | 1.40        | 1.45     |
| 18  | N     | 4522 | TGL  | CG3-CG2 | 2.23  | 1.57        | 1.50     |
| 21  | B     | 4085 | CHD  | C13-C12 | -2.23 | 1.51        | 1.54     |
| 23  | P     | 4265 | PEK  | P-O11   | 2.23  | 1.68        | 1.59     |
| 27  | Z     | 4526 | DMU  | C8-C9   | 2.20  | 1.57        | 1.53     |
| 23  | P     | 4265 | PEK  | P-O12   | 2.19  | 1.68        | 1.59     |
| 22  | G     | 3269 | CDL  | C11-CA5 | 2.19  | 1.57        | 1.50     |
| 22  | T     | 4269 | CDL  | C11-CA5 | 2.19  | 1.57        | 1.50     |
| 23  | G     | 4263 | PEK  | P-O11   | 2.19  | 1.68        | 1.59     |
| 17  | N     | 515  | HEA  | CMA-C3A | -2.19 | 1.40        | 1.45     |
| 23  | P     | 4265 | PEK  | C22-C21 | 2.18  | 1.57        | 1.50     |
| 18  | N     | 4521 | TGL  | OG1-CG1 | -2.17 | 1.40        | 1.45     |
| 17  | A     | 516  | HEA  | CMA-C3A | -2.17 | 1.40        | 1.45     |
| 23  | T     | 3263 | PEK  | P-O11   | 2.17  | 1.67        | 1.59     |
| 17  | A     | 515  | HEA  | FE-NA   | 2.16  | 2.02        | 1.95     |
| 22  | G     | 3269 | CDL  | C71-CB7 | 2.15  | 1.56        | 1.50     |
| 23  | C     | 3265 | PEK  | P-O11   | 2.15  | 1.67        | 1.59     |
| 23  | P     | 4265 | PEK  | O01-C1  | 2.14  | 1.40        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | A     | 515  | HEA  | C13-C14 | 2.12  | 1.56        | 1.50     |
| 18  | N     | 4522 | TGL  | CB2-CB1 | 2.11  | 1.56        | 1.50     |
| 21  | P     | 4525 | CHD  | C8-C9   | 2.10  | 1.57        | 1.53     |
| 17  | A     | 515  | HEA  | CHC-C4B | 2.09  | 1.42        | 1.38     |
| 21  | W     | 4060 | CHD  | C8-C7   | 2.09  | 1.57        | 1.53     |
| 21  | O     | 3085 | CHD  | C8-C9   | 2.08  | 1.57        | 1.53     |
| 23  | C     | 3264 | PEK  | O03-C01 | -2.06 | 1.40        | 1.45     |
| 21  | W     | 4060 | CHD  | C20-C17 | 2.06  | 1.57        | 1.54     |
| 23  | T     | 3263 | PEK  | C2-C1   | 2.06  | 1.56        | 1.50     |
| 19  | C     | 3268 | PGV  | C04-C05 | 2.05  | 1.58        | 1.51     |
| 23  | P     | 4264 | PEK  | C2-C1   | 2.04  | 1.56        | 1.50     |
| 19  | N     | 4524 | PGV  | C03-C02 | 2.02  | 1.57        | 1.50     |
| 21  | C     | 3525 | CHD  | C13-C12 | -2.02 | 1.51        | 1.54     |
| 21  | C     | 3271 | CHD  | C19-C10 | -2.01 | 1.51        | 1.54     |
| 18  | A     | 3522 | TGL  | CB2-CB1 | 2.00  | 1.56        | 1.50     |

All (323) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | M     | 3526 | DMU  | C10-C5-C7   | 10.14 | 131.34      | 110.01   |
| 27  | Z     | 4526 | DMU  | C10-C5-C7   | 10.09 | 131.24      | 110.01   |
| 21  | P     | 4271 | CHD  | C17-C13-C14 | 9.93  | 110.08      | 100.11   |
| 21  | C     | 3271 | CHD  | C17-C13-C14 | 9.74  | 109.88      | 100.11   |
| 21  | J     | 3060 | CHD  | C17-C13-C14 | 8.89  | 109.03      | 100.11   |
| 21  | W     | 4060 | CHD  | C17-C13-C14 | 8.81  | 108.95      | 100.11   |
| 21  | P     | 4271 | CHD  | C17-C13-C12 | -8.76 | 109.78      | 117.67   |
| 21  | P     | 4271 | CHD  | C10-C9-C8   | 8.56  | 121.38      | 111.84   |
| 21  | C     | 3271 | CHD  | C10-C9-C8   | 8.54  | 121.36      | 111.84   |
| 21  | C     | 3271 | CHD  | C17-C13-C12 | -8.43 | 110.08      | 117.67   |
| 21  | C     | 3271 | CHD  | C19-C10-C9  | -8.20 | 100.16      | 111.18   |
| 27  | Z     | 4526 | DMU  | C8-C7-C5    | -7.99 | 96.81       | 110.83   |
| 21  | P     | 4271 | CHD  | C19-C10-C9  | -7.97 | 100.46      | 111.18   |
| 27  | M     | 3526 | DMU  | O1-C9-C11   | 7.84  | 125.87      | 106.44   |
| 27  | M     | 3526 | DMU  | C8-C7-C5    | -7.79 | 97.16       | 110.83   |
| 27  | Z     | 4526 | DMU  | C7-C8-C9    | 7.78  | 124.34      | 110.23   |
| 27  | Z     | 4526 | DMU  | O1-C9-C11   | 7.77  | 125.70      | 106.44   |
| 27  | M     | 3526 | DMU  | O5-C4-C3    | 7.67  | 125.58      | 109.72   |
| 27  | Z     | 4526 | DMU  | O5-C4-C3    | 7.57  | 125.36      | 109.72   |
| 27  | M     | 3526 | DMU  | C7-C8-C9    | 7.56  | 123.94      | 110.23   |
| 27  | Z     | 4526 | DMU  | O5-C6-O16   | 7.48  | 127.72      | 110.04   |
| 27  | M     | 3526 | DMU  | O1-C9-C8    | 7.22  | 122.71      | 109.70   |
| 27  | M     | 3526 | DMU  | O5-C6-O16   | 7.01  | 126.60      | 110.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | Z     | 4526 | DMU  | O1-C9-C8    | 6.99  | 122.29      | 109.70   |
| 27  | M     | 3526 | DMU  | C6-O5-C4    | 6.94  | 127.27      | 113.72   |
| 27  | Z     | 4526 | DMU  | C6-O5-C4    | 6.91  | 127.22      | 113.72   |
| 21  | W     | 4060 | CHD  | C13-C17-C20 | 6.84  | 127.77      | 119.48   |
| 27  | Z     | 4526 | DMU  | O5-C4-C57   | 6.77  | 123.23      | 106.44   |
| 27  | M     | 3526 | DMU  | O7-C3-C2    | 6.73  | 124.34      | 107.23   |
| 27  | M     | 3526 | DMU  | O5-C4-C57   | 6.58  | 122.74      | 106.44   |
| 21  | J     | 3060 | CHD  | C13-C17-C20 | 6.57  | 127.44      | 119.48   |
| 27  | Z     | 4526 | DMU  | O7-C3-C2    | 6.47  | 123.67      | 107.23   |
| 21  | C     | 3271 | CHD  | C14-C13-C12 | 6.46  | 113.32      | 107.42   |
| 21  | P     | 4271 | CHD  | C14-C13-C12 | 6.14  | 113.02      | 107.42   |
| 21  | C     | 3271 | CHD  | C19-C10-C1  | -6.05 | 98.69       | 108.31   |
| 21  | C     | 3271 | CHD  | C1-C10-C5   | 6.04  | 116.41      | 107.75   |
| 21  | P     | 4271 | CHD  | C1-C10-C5   | 5.99  | 116.35      | 107.75   |
| 21  | J     | 3060 | CHD  | C4-C3-C2    | 5.85  | 117.75      | 110.62   |
| 21  | P     | 4271 | CHD  | C19-C10-C1  | -5.79 | 99.10       | 108.31   |
| 27  | M     | 3526 | DMU  | C18-O16-C6  | 5.72  | 123.44      | 113.68   |
| 21  | P     | 4271 | CHD  | C9-C8-C7    | 5.71  | 119.04      | 111.86   |
| 21  | J     | 3060 | CHD  | C11-C12-C13 | 5.68  | 117.04      | 111.26   |
| 21  | J     | 3060 | CHD  | C11-C9-C10  | 5.66  | 119.45      | 113.70   |
| 21  | W     | 4060 | CHD  | C18-C13-C14 | -5.65 | 102.36      | 111.20   |
| 21  | C     | 3271 | CHD  | C9-C8-C7    | 5.64  | 118.95      | 111.86   |
| 21  | J     | 3060 | CHD  | C15-C14-C8  | -5.54 | 110.76      | 118.36   |
| 21  | W     | 4060 | CHD  | C15-C14-C8  | -5.52 | 110.79      | 118.36   |
| 21  | W     | 4060 | CHD  | C4-C3-C2    | 5.49  | 117.31      | 110.62   |
| 21  | W     | 4060 | CHD  | C11-C12-C13 | 5.43  | 116.79      | 111.26   |
| 21  | W     | 4060 | CHD  | C11-C9-C10  | 5.30  | 119.08      | 113.70   |
| 21  | W     | 4060 | CHD  | C6-C5-C10   | 5.29  | 118.29      | 112.66   |
| 21  | J     | 3060 | CHD  | C18-C13-C14 | -5.22 | 103.02      | 111.20   |
| 21  | W     | 4060 | CHD  | C5-C6-C7    | 5.20  | 120.58      | 114.40   |
| 27  | Z     | 4526 | DMU  | C18-O16-C6  | 5.15  | 122.48      | 113.68   |
| 21  | P     | 4271 | CHD  | C15-C14-C8  | -5.14 | 111.30      | 118.36   |
| 21  | J     | 3060 | CHD  | C5-C6-C7    | 5.14  | 120.51      | 114.40   |
| 21  | P     | 4271 | CHD  | C4-C3-C2    | 5.13  | 116.87      | 110.62   |
| 21  | C     | 3271 | CHD  | C15-C14-C8  | -5.11 | 111.35      | 118.36   |
| 21  | C     | 3271 | CHD  | C4-C3-C2    | 5.06  | 116.80      | 110.62   |
| 21  | J     | 3060 | CHD  | C6-C5-C10   | 4.98  | 117.95      | 112.66   |
| 21  | W     | 4060 | CHD  | C10-C9-C8   | 4.83  | 117.22      | 111.84   |
| 18  | A     | 3521 | TGL  | OG2-CB1-CB2 | 4.77  | 121.79      | 111.48   |
| 18  | N     | 4521 | TGL  | OG2-CB1-CB2 | 4.69  | 121.64      | 111.48   |
| 21  | W     | 4060 | CHD  | C2-C1-C10   | 4.69  | 120.66      | 112.74   |
| 21  | P     | 4525 | CHD  | C13-C17-C20 | 4.63  | 125.09      | 119.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | M     | 3526 | DMU  | O16-C6-C1   | 4.58  | 115.23      | 108.27   |
| 18  | N     | 4522 | TGL  | OG3-CG3-CG2 | 4.57  | 121.58      | 108.40   |
| 21  | J     | 3060 | CHD  | C10-C9-C8   | 4.54  | 116.90      | 111.84   |
| 18  | A     | 3522 | TGL  | OG3-CG3-CG2 | 4.50  | 121.37      | 108.40   |
| 18  | A     | 3523 | TGL  | OG2-CB1-CB2 | 4.45  | 121.10      | 111.48   |
| 27  | M     | 3526 | DMU  | C10-O7-C3   | 4.43  | 128.47      | 117.98   |
| 21  | C     | 3271 | CHD  | C4-C5-C10   | 4.43  | 117.37      | 112.66   |
| 21  | J     | 3060 | CHD  | C1-C10-C5   | 4.41  | 114.07      | 107.75   |
| 21  | J     | 3060 | CHD  | C2-C1-C10   | 4.39  | 120.16      | 112.74   |
| 21  | C     | 3525 | CHD  | C13-C17-C20 | 4.38  | 124.79      | 119.48   |
| 21  | W     | 4060 | CHD  | C1-C10-C5   | 4.21  | 113.79      | 107.75   |
| 21  | P     | 4271 | CHD  | C4-C5-C10   | 4.20  | 117.13      | 112.66   |
| 27  | Z     | 4526 | DMU  | C10-O7-C3   | 4.19  | 127.91      | 117.98   |
| 21  | J     | 3060 | CHD  | C9-C8-C7    | 4.15  | 117.08      | 111.86   |
| 18  | Q     | 4523 | TGL  | OG2-CB1-CB2 | 4.08  | 120.30      | 111.48   |
| 21  | O     | 3085 | CHD  | C10-C9-C8   | 4.07  | 116.38      | 111.84   |
| 27  | Z     | 4526 | DMU  | C6-C1-C2    | 4.03  | 118.50      | 110.01   |
| 21  | J     | 3060 | CHD  | C13-C14-C8  | 4.01  | 119.80      | 114.72   |
| 27  | M     | 3526 | DMU  | C6-C1-C2    | 4.00  | 118.44      | 110.01   |
| 21  | W     | 4060 | CHD  | C13-C14-C8  | 4.00  | 119.78      | 114.72   |
| 21  | B     | 4085 | CHD  | C15-C14-C8  | -3.99 | 112.88      | 118.36   |
| 21  | W     | 4060 | CHD  | C9-C8-C7    | 3.98  | 116.87      | 111.86   |
| 27  | Z     | 4526 | DMU  | O7-C10-O1   | 3.96  | 121.12      | 110.69   |
| 27  | Z     | 4526 | DMU  | O16-C6-C1   | 3.94  | 114.26      | 108.27   |
| 18  | N     | 4522 | TGL  | OG2-CB1-CB2 | 3.89  | 119.89      | 111.48   |
| 18  | A     | 3522 | TGL  | OG2-CB1-CB2 | 3.87  | 119.86      | 111.48   |
| 21  | O     | 3085 | CHD  | C16-C17-C13 | -3.87 | 99.79       | 103.54   |
| 21  | O     | 3085 | CHD  | C15-C14-C13 | -3.83 | 99.83       | 103.54   |
| 21  | B     | 4085 | CHD  | C15-C14-C13 | -3.83 | 99.83       | 103.54   |
| 27  | M     | 3526 | DMU  | O7-C10-O1   | 3.80  | 120.69      | 110.69   |
| 21  | C     | 3525 | CHD  | C15-C14-C8  | -3.78 | 113.17      | 118.36   |
| 27  | M     | 3526 | DMU  | O5-C6-C1    | 3.77  | 118.11      | 110.37   |
| 27  | Z     | 4526 | DMU  | O7-C3-C4    | 3.76  | 119.34      | 109.48   |
| 27  | Z     | 4526 | DMU  | O5-C6-C1    | 3.72  | 118.02      | 110.37   |
| 21  | C     | 3271 | CHD  | C18-C13-C12 | -3.71 | 105.35      | 109.06   |
| 21  | O     | 3085 | CHD  | C15-C14-C8  | -3.69 | 113.30      | 118.36   |
| 21  | P     | 4525 | CHD  | C15-C14-C8  | -3.65 | 113.35      | 118.36   |
| 19  | A     | 3524 | PGV  | P-O11-C03   | 3.65  | 142.25      | 121.35   |
| 21  | W     | 4060 | CHD  | C5-C4-C3    | 3.64  | 118.19      | 112.71   |
| 21  | P     | 4271 | CHD  | C1-C10-C9   | 3.62  | 116.96      | 111.34   |
| 21  | W     | 4060 | CHD  | C9-C11-C12  | 3.61  | 119.01      | 114.29   |
| 23  | T     | 3263 | PEK  | C03-C02-C01 | 3.60  | 120.19      | 111.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | C     | 3271 | CHD  | C1-C10-C9   | 3.59  | 116.91      | 111.34   |
| 27  | M     | 3526 | DMU  | C10-O1-C9   | 3.55  | 120.65      | 113.72   |
| 23  | C     | 3264 | PEK  | O03-C21-C22 | -3.51 | 101.14      | 111.83   |
| 21  | O     | 3085 | CHD  | C19-C10-C9  | -3.45 | 106.54      | 111.18   |
| 21  | P     | 4525 | CHD  | C5-C6-C7    | 3.45  | 118.50      | 114.40   |
| 23  | P     | 4264 | PEK  | O03-C21-C22 | -3.43 | 101.37      | 111.83   |
| 23  | G     | 4263 | PEK  | C03-C02-C01 | 3.42  | 119.77      | 111.78   |
| 21  | B     | 4085 | CHD  | C16-C17-C13 | -3.42 | 100.23      | 103.54   |
| 19  | N     | 4524 | PGV  | P-O11-C03   | 3.42  | 140.93      | 121.35   |
| 21  | P     | 4271 | CHD  | C6-C5-C10   | 3.39  | 116.27      | 112.66   |
| 27  | M     | 3526 | DMU  | O7-C3-C4    | 3.37  | 118.32      | 109.48   |
| 21  | J     | 3060 | CHD  | C1-C2-C3    | 3.37  | 114.94      | 110.48   |
| 21  | J     | 3060 | CHD  | C9-C11-C12  | 3.35  | 118.68      | 114.29   |
| 27  | M     | 3526 | DMU  | O7-C10-C5   | 3.34  | 116.31      | 108.09   |
| 21  | W     | 4060 | CHD  | C1-C2-C3    | 3.33  | 114.89      | 110.48   |
| 23  | T     | 3263 | PEK  | P-O11-C03   | 3.32  | 140.38      | 121.35   |
| 21  | B     | 4085 | CHD  | C1-C10-C5   | 3.32  | 112.51      | 107.75   |
| 23  | G     | 4263 | PEK  | P-O11-C03   | 3.30  | 140.24      | 121.35   |
| 21  | P     | 4271 | CHD  | C18-C13-C12 | -3.29 | 105.76      | 109.06   |
| 21  | P     | 4271 | CHD  | C14-C8-C7   | 3.29  | 116.21      | 111.85   |
| 21  | P     | 4525 | CHD  | C1-C10-C5   | 3.26  | 112.43      | 107.75   |
| 21  | P     | 4271 | CHD  | C5-C4-C3    | 3.24  | 117.59      | 112.71   |
| 21  | C     | 3271 | CHD  | C5-C6-C7    | 3.24  | 118.25      | 114.40   |
| 21  | B     | 4085 | CHD  | C18-C13-C12 | -3.23 | 105.82      | 109.06   |
| 21  | B     | 4085 | CHD  | C10-C9-C8   | 3.22  | 115.42      | 111.84   |
| 27  | Z     | 4526 | DMU  | C10-O1-C9   | 3.21  | 119.99      | 113.72   |
| 21  | W     | 4060 | CHD  | C17-C13-C12 | -3.20 | 114.79      | 117.67   |
| 21  | W     | 4060 | CHD  | C18-C13-C12 | -3.20 | 105.86      | 109.06   |
| 21  | W     | 4060 | CHD  | C14-C13-C12 | 3.18  | 110.32      | 107.42   |
| 21  | B     | 4085 | CHD  | C14-C8-C9   | -3.18 | 105.31      | 109.75   |
| 21  | J     | 3060 | CHD  | C5-C4-C3    | 3.18  | 117.50      | 112.71   |
| 21  | C     | 3271 | CHD  | C6-C5-C10   | 3.16  | 116.02      | 112.66   |
| 21  | C     | 3271 | CHD  | C5-C4-C3    | 3.14  | 117.45      | 112.71   |
| 21  | C     | 3271 | CHD  | C14-C8-C7   | 3.13  | 116.00      | 111.85   |
| 21  | O     | 3085 | CHD  | C5-C6-C7    | 3.12  | 118.11      | 114.40   |
| 27  | Z     | 4526 | DMU  | O7-C10-C5   | 3.11  | 115.74      | 108.09   |
| 21  | C     | 3525 | CHD  | C5-C6-C7    | 3.07  | 118.05      | 114.40   |
| 27  | Z     | 4526 | DMU  | C1-C2-C3    | 3.05  | 116.60      | 109.68   |
| 25  | O     | 4230 | PSC  | C01-O03-C19 | -3.04 | 106.01      | 117.12   |
| 23  | C     | 3265 | PEK  | P-O11-C03   | 3.02  | 138.65      | 121.35   |
| 25  | E     | 3230 | PSC  | C01-O03-C19 | -3.01 | 106.11      | 117.12   |
| 21  | W     | 4060 | CHD  | C16-C15-C14 | 3.00  | 111.02      | 105.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | P     | 4265 | PEK  | P-O11-C03   | 2.99  | 138.46      | 121.35   |
| 17  | A     | 515  | HEA  | C2D-C1D-ND  | 2.96  | 113.25      | 109.84   |
| 21  | B     | 4085 | CHD  | C1-C2-C3    | 2.96  | 114.40      | 110.48   |
| 27  | M     | 3526 | DMU  | C1-C2-C3    | 2.93  | 116.33      | 109.68   |
| 21  | P     | 4271 | CHD  | C5-C6-C7    | 2.93  | 117.88      | 114.40   |
| 21  | B     | 4085 | CHD  | C9-C11-C12  | 2.92  | 118.11      | 114.29   |
| 21  | J     | 3060 | CHD  | C16-C15-C14 | 2.89  | 110.81      | 105.14   |
| 17  | N     | 515  | HEA  | C12-C11-C3B | 2.89  | 116.64      | 112.12   |
| 21  | J     | 3060 | CHD  | C18-C13-C12 | -2.88 | 106.17      | 109.06   |
| 21  | P     | 4525 | CHD  | C14-C8-C9   | -2.85 | 105.77      | 109.75   |
| 21  | J     | 3060 | CHD  | C17-C13-C12 | -2.85 | 115.10      | 117.67   |
| 21  | C     | 3525 | CHD  | C16-C17-C13 | -2.85 | 100.78      | 103.54   |
| 21  | C     | 3525 | CHD  | C14-C13-C12 | -2.85 | 104.81      | 107.42   |
| 19  | N     | 4524 | PGV  | C03-C02-C01 | 2.84  | 118.42      | 111.78   |
| 19  | A     | 3524 | PGV  | C3-C2-C1    | -2.83 | 103.31      | 113.69   |
| 21  | O     | 3085 | CHD  | C9-C11-C12  | 2.82  | 117.99      | 114.29   |
| 25  | E     | 3230 | PSC  | C16-C15-C14 | 2.82  | 127.41      | 113.86   |
| 17  | A     | 516  | HEA  | CMB-C2B-C3B | -2.81 | 124.85      | 130.28   |
| 21  | C     | 3525 | CHD  | C10-C9-C8   | 2.78  | 114.94      | 111.84   |
| 22  | P     | 4270 | CDL  | CB6-OB8-CB7 | -2.78 | 106.97      | 117.12   |
| 23  | P     | 4264 | PEK  | O03-C21-O04 | 2.77  | 130.57      | 123.63   |
| 23  | G     | 4263 | PEK  | O03-C01-C02 | 2.77  | 116.38      | 108.40   |
| 18  | A     | 3521 | TGL  | OG3-CC1-OC1 | -2.76 | 116.72      | 123.63   |
| 21  | J     | 3060 | CHD  | C15-C16-C17 | 2.76  | 110.55      | 105.14   |
| 21  | P     | 4271 | CHD  | C15-C16-C17 | 2.76  | 110.55      | 105.14   |
| 21  | B     | 4085 | CHD  | C17-C13-C14 | 2.76  | 102.88      | 100.11   |
| 21  | B     | 4085 | CHD  | O3-C3-C4    | -2.75 | 104.36      | 109.84   |
| 21  | P     | 4525 | CHD  | C1-C2-C3    | 2.75  | 114.13      | 110.48   |
| 21  | P     | 4525 | CHD  | C9-C11-C12  | 2.74  | 117.88      | 114.29   |
| 21  | C     | 3525 | CHD  | C14-C8-C9   | -2.74 | 105.92      | 109.75   |
| 25  | O     | 4230 | PSC  | C16-C15-C14 | 2.74  | 127.01      | 113.86   |
| 21  | C     | 3271 | CHD  | C18-C13-C14 | -2.73 | 106.92      | 111.20   |
| 21  | C     | 3271 | CHD  | C15-C16-C17 | 2.73  | 110.49      | 105.14   |
| 21  | O     | 3085 | CHD  | C14-C13-C12 | -2.72 | 104.93      | 107.42   |
| 21  | C     | 3271 | CHD  | C1-C2-C3    | 2.72  | 114.08      | 110.48   |
| 25  | O     | 4230 | PSC  | C15-C14-C13 | 2.71  | 127.75      | 112.60   |
| 23  | P     | 4264 | PEK  | C3-C2-C1    | -2.70 | 103.81      | 113.69   |
| 17  | N     | 516  | HEA  | C27-C19-C20 | 2.70  | 119.91      | 115.23   |
| 21  | C     | 3525 | CHD  | C1-C10-C5   | 2.69  | 111.61      | 107.75   |
| 21  | P     | 4271 | CHD  | C18-C13-C14 | -2.68 | 107.01      | 111.20   |
| 22  | C     | 3270 | CDL  | OB6-CB5-C51 | -2.67 | 105.71      | 111.48   |
| 22  | C     | 3270 | CDL  | CB6-OB8-CB7 | -2.66 | 107.38      | 117.12   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21  | W     | 4060 | CHD  | C15-C16-C17 | 2.66  | 110.34      | 105.14   |
| 23  | P     | 4265 | PEK  | P-O12-C04   | 2.64  | 133.83      | 121.26   |
| 21  | J     | 3060 | CHD  | C19-C10-C9  | -2.64 | 107.63      | 111.18   |
| 21  | O     | 3085 | CHD  | C5-C4-C3    | 2.64  | 116.69      | 112.71   |
| 23  | C     | 3264 | PEK  | O03-C21-O04 | 2.63  | 130.22      | 123.63   |
| 25  | E     | 3230 | PSC  | C15-C14-C13 | 2.63  | 127.35      | 112.60   |
| 21  | O     | 3085 | CHD  | C17-C13-C14 | 2.62  | 102.74      | 100.11   |
| 21  | C     | 3271 | CHD  | C13-C17-C20 | -2.62 | 116.31      | 119.48   |
| 17  | N     | 516  | HEA  | C1D-ND-C4D  | -2.61 | 102.11      | 105.21   |
| 23  | T     | 3263 | PEK  | O03-C01-C02 | 2.60  | 115.90      | 108.40   |
| 18  | N     | 4521 | TGL  | OG3-CC1-OC1 | -2.59 | 117.14      | 123.63   |
| 21  | C     | 3271 | CHD  | C16-C15-C14 | 2.57  | 110.18      | 105.14   |
| 23  | C     | 3264 | PEK  | C3-C2-C1    | -2.57 | 104.29      | 113.69   |
| 21  | P     | 4271 | CHD  | C1-C2-C3    | 2.57  | 113.88      | 110.48   |
| 17  | A     | 516  | HEA  | C2B-C1B-NB  | 2.57  | 112.87      | 109.90   |
| 19  | C     | 3267 | PGV  | C9-C10-C11  | -2.56 | 98.25       | 112.60   |
| 17  | A     | 516  | HEA  | C4B-NB-C1B  | -2.55 | 102.19      | 105.21   |
| 21  | O     | 3085 | CHD  | C1-C2-C3    | 2.54  | 113.84      | 110.48   |
| 18  | A     | 3522 | TGL  | OG1-CA1-CA2 | 2.53  | 119.56      | 111.83   |
| 21  | P     | 4271 | CHD  | C16-C15-C14 | 2.52  | 110.08      | 105.14   |
| 21  | P     | 4271 | CHD  | C9-C11-C12  | 2.52  | 117.59      | 114.29   |
| 21  | O     | 3085 | CHD  | C18-C13-C12 | -2.51 | 106.55      | 109.06   |
| 21  | J     | 3060 | CHD  | C14-C13-C12 | 2.50  | 109.70      | 107.42   |
| 21  | O     | 3085 | CHD  | C14-C8-C9   | -2.50 | 106.26      | 109.75   |
| 19  | P     | 4267 | PGV  | C9-C10-C11  | -2.50 | 98.62       | 112.60   |
| 19  | N     | 4524 | PGV  | C3-C2-C1    | -2.50 | 104.55      | 113.69   |
| 17  | N     | 515  | HEA  | C3C-C4C-NC  | 2.49  | 111.90      | 109.80   |
| 21  | J     | 3060 | CHD  | C14-C8-C9   | 2.49  | 113.23      | 109.75   |
| 21  | P     | 4271 | CHD  | C13-C17-C20 | -2.48 | 116.48      | 119.48   |
| 17  | A     | 515  | HEA  | C12-C11-C3B | 2.47  | 115.99      | 112.12   |
| 18  | Q     | 4523 | TGL  | CB6-CB5-CB4 | 2.47  | 126.84      | 114.37   |
| 17  | A     | 516  | HEA  | C1D-ND-C4D  | -2.46 | 102.29      | 105.21   |
| 18  | N     | 4522 | TGL  | OG1-CA1-CA2 | 2.46  | 119.32      | 111.83   |
| 17  | N     | 516  | HEA  | CHA-C4D-C3D | -2.45 | 121.20      | 124.77   |
| 21  | J     | 3060 | CHD  | C4-C5-C10   | 2.45  | 115.27      | 112.66   |
| 23  | C     | 3265 | PEK  | P-O12-C04   | 2.44  | 132.87      | 121.26   |
| 18  | A     | 3522 | TGL  | OG3-CC1-OC1 | -2.43 | 117.54      | 123.63   |
| 17  | A     | 516  | HEA  | C4A-C3A-C2A | -2.43 | 104.71      | 106.81   |
| 21  | O     | 3085 | CHD  | C1-C10-C5   | 2.43  | 111.23      | 107.75   |
| 21  | J     | 3060 | CHD  | O7-C7-C6    | 2.42  | 115.88      | 109.86   |
| 21  | W     | 4060 | CHD  | C14-C8-C9   | 2.42  | 113.13      | 109.75   |
| 23  | C     | 3265 | PEK  | O03-C01-C02 | 2.41  | 115.36      | 108.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 515  | HEA  | C26-C15-C16 | 2.41  | 119.41      | 115.23   |
| 17  | N     | 515  | HEA  | C2D-C1D-ND  | 2.40  | 112.60      | 109.84   |
| 18  | A     | 3523 | TGL  | CB6-CB5-CB4 | 2.39  | 126.47      | 114.37   |
| 21  | C     | 3271 | CHD  | C9-C10-C5   | 2.38  | 111.82      | 108.51   |
| 21  | O     | 3085 | CHD  | O3-C3-C4    | -2.38 | 105.11      | 109.84   |
| 19  | A     | 3524 | PGV  | C03-C02-C01 | 2.38  | 117.32      | 111.78   |
| 23  | C     | 3264 | PEK  | C30-C29-C28 | -2.37 | 102.37      | 114.37   |
| 22  | T     | 4269 | CDL  | OB8-CB6-CB4 | 2.37  | 115.24      | 108.40   |
| 17  | N     | 516  | HEA  | C17-C18-C19 | 2.37  | 133.04      | 127.62   |
| 23  | P     | 4264 | PEK  | C30-C29-C28 | -2.36 | 102.45      | 114.37   |
| 18  | N     | 4522 | TGL  | OG3-CC1-OC1 | -2.35 | 117.75      | 123.63   |
| 21  | C     | 3271 | CHD  | C9-C11-C12  | 2.35  | 117.36      | 114.29   |
| 19  | N     | 4266 | PGV  | O03-C01-C02 | 2.34  | 115.15      | 108.40   |
| 17  | N     | 516  | HEA  | CMB-C2B-C3B | -2.31 | 125.80      | 130.28   |
| 22  | T     | 4269 | CDL  | C22-C21-C20 | 2.31  | 126.06      | 114.37   |
| 22  | G     | 3269 | CDL  | C22-C21-C20 | 2.30  | 126.01      | 114.37   |
| 17  | A     | 515  | HEA  | C1D-ND-C4D  | -2.30 | 102.48      | 105.21   |
| 22  | T     | 4269 | CDL  | C23-C22-C21 | 2.30  | 125.98      | 114.37   |
| 21  | B     | 4085 | CHD  | C5-C6-C7    | 2.29  | 117.12      | 114.40   |
| 21  | W     | 4060 | CHD  | O7-C7-C6    | 2.28  | 115.53      | 109.86   |
| 23  | P     | 4265 | PEK  | O03-C01-C02 | 2.28  | 114.96      | 108.40   |
| 21  | P     | 4525 | CHD  | C19-C10-C9  | -2.27 | 108.13      | 111.18   |
| 22  | G     | 3269 | CDL  | C23-C22-C21 | 2.27  | 125.82      | 114.37   |
| 21  | B     | 4085 | CHD  | C18-C13-C14 | 2.26  | 114.74      | 111.20   |
| 21  | C     | 3525 | CHD  | C19-C10-C9  | -2.26 | 108.15      | 111.18   |
| 17  | N     | 515  | HEA  | C2C-C1C-NC  | 2.25  | 113.75      | 110.14   |
| 22  | G     | 3269 | CDL  | OB8-CB6-CB4 | 2.25  | 114.88      | 108.40   |
| 22  | G     | 3269 | CDL  | C19-C18-C17 | 2.25  | 125.72      | 114.37   |
| 22  | T     | 4269 | CDL  | C19-C18-C17 | 2.24  | 125.70      | 114.37   |
| 18  | A     | 3521 | TGL  | CB6-CB5-CB4 | 2.24  | 125.69      | 114.37   |
| 17  | A     | 515  | HEA  | C26-C15-C14 | -2.24 | 117.89      | 123.63   |
| 23  | P     | 4264 | PEK  | C32-C31-C30 | -2.24 | 103.07      | 114.37   |
| 21  | W     | 4060 | CHD  | C19-C10-C9  | -2.23 | 108.17      | 111.18   |
| 25  | E     | 3230 | PSC  | C14-C13-C12 | -2.23 | 108.11      | 124.83   |
| 21  | W     | 4060 | CHD  | C4-C5-C10   | 2.23  | 115.03      | 112.66   |
| 22  | P     | 4270 | CDL  | OB6-CB5-C51 | -2.22 | 106.69      | 111.48   |
| 21  | P     | 4271 | CHD  | C9-C10-C5   | 2.20  | 111.58      | 108.51   |
| 23  | C     | 3264 | PEK  | C23-C22-C21 | -2.20 | 105.62      | 113.69   |
| 23  | C     | 3265 | PEK  | C11-C10-C9  | 2.20  | 122.87      | 112.02   |
| 21  | B     | 4085 | CHD  | C19-C10-C9  | -2.20 | 108.22      | 111.18   |
| 17  | N     | 516  | HEA  | C3C-C4C-NC  | 2.19  | 111.65      | 109.80   |
| 22  | P     | 4270 | CDL  | OB6-CB5-OB7 | 2.19  | 128.82      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18  | A     | 3523 | TGL  | OG1-CA1-CA2 | 2.19  | 118.50      | 111.83   |
| 23  | P     | 4264 | PEK  | C24-C23-C22 | -2.18 | 105.11      | 113.13   |
| 21  | C     | 3525 | CHD  | C15-C14-C13 | -2.18 | 101.43      | 103.54   |
| 21  | O     | 3085 | CHD  | C2-C1-C10   | 2.18  | 116.41      | 112.74   |
| 19  | N     | 4266 | PGV  | C01-O03-C19 | -2.17 | 109.18      | 117.12   |
| 21  | C     | 3525 | CHD  | C9-C11-C12  | 2.17  | 117.13      | 114.29   |
| 22  | T     | 4269 | CDL  | C83-C82-C81 | 2.16  | 125.29      | 114.37   |
| 18  | A     | 3521 | TGL  | CB5-CB4-CB3 | 2.16  | 125.29      | 114.37   |
| 17  | A     | 516  | HEA  | CHA-C4D-C3D | -2.15 | 121.63      | 124.77   |
| 19  | A     | 3524 | PGV  | P-O12-C04   | 2.15  | 133.66      | 121.35   |
| 17  | N     | 516  | HEA  | CHA-C4D-ND  | 2.15  | 126.73      | 124.42   |
| 22  | C     | 3270 | CDL  | C79-C78-C77 | 2.14  | 125.21      | 114.37   |
| 17  | A     | 515  | HEA  | CMC-C2C-C3C | 2.14  | 131.59      | 126.55   |
| 22  | P     | 4270 | CDL  | C82-C81-C80 | 2.14  | 125.20      | 114.37   |
| 21  | B     | 4085 | CHD  | C5-C4-C3    | 2.14  | 115.93      | 112.71   |
| 23  | P     | 4265 | PEK  | C11-C10-C9  | 2.14  | 122.55      | 112.02   |
| 17  | A     | 516  | HEA  | C27-C19-C20 | 2.14  | 118.94      | 115.23   |
| 17  | A     | 515  | HEA  | C4A-C3A-C2A | -2.13 | 104.96      | 106.81   |
| 18  | N     | 4521 | TGL  | CB6-CB5-CB4 | 2.13  | 125.14      | 114.37   |
| 23  | C     | 3264 | PEK  | C32-C31-C30 | -2.13 | 103.62      | 114.37   |
| 18  | A     | 3523 | TGL  | CB5-CB4-CB3 | 2.12  | 125.11      | 114.37   |
| 18  | A     | 3521 | TGL  | CC6-CC5-CC4 | 2.12  | 125.10      | 114.37   |
| 19  | N     | 4266 | PGV  | O01-C1-C2   | -2.12 | 106.90      | 111.48   |
| 25  | O     | 4230 | PSC  | C14-C13-C12 | -2.11 | 109.05      | 124.83   |
| 19  | C     | 3268 | PGV  | C21-C20-C19 | -2.10 | 105.99      | 113.69   |
| 18  | Q     | 4523 | TGL  | OG1-CA1-CA2 | 2.10  | 118.23      | 111.83   |
| 23  | C     | 3264 | PEK  | C24-C23-C22 | -2.10 | 105.43      | 113.13   |
| 22  | T     | 4269 | CDL  | C79-C78-C77 | 2.09  | 124.95      | 114.37   |
| 22  | C     | 3270 | CDL  | C82-C81-C80 | 2.09  | 124.95      | 114.37   |
| 22  | C     | 3270 | CDL  | OB6-CB5-OB7 | 2.09  | 128.60      | 123.70   |
| 18  | Q     | 4523 | TGL  | CB5-CB4-CB3 | 2.09  | 124.92      | 114.37   |
| 19  | A     | 3524 | PGV  | O01-C02-C03 | 2.08  | 115.82      | 108.34   |
| 19  | A     | 3524 | PGV  | C02-O01-C1  | 2.08  | 122.76      | 117.80   |
| 18  | N     | 4521 | TGL  | CB5-CB4-CB3 | 2.07  | 124.84      | 114.37   |
| 22  | P     | 4270 | CDL  | C79-C78-C77 | 2.07  | 124.83      | 114.37   |
| 18  | A     | 3521 | TGL  | OG2-CB1-OB1 | -2.07 | 118.87      | 123.70   |
| 22  | G     | 3269 | CDL  | C79-C78-C77 | 2.06  | 124.78      | 114.37   |
| 18  | N     | 4521 | TGL  | CC6-CC5-CC4 | 2.06  | 124.78      | 114.37   |
| 17  | N     | 515  | HEA  | C26-C15-C16 | 2.06  | 118.80      | 115.23   |
| 17  | A     | 516  | HEA  | C3D-C4D-ND  | 2.06  | 112.34      | 110.35   |
| 21  | J     | 3060 | CHD  | C19-C10-C1  | -2.04 | 105.06      | 108.31   |
| 23  | C     | 3264 | PEK  | C02-O01-C1  | -2.04 | 112.92      | 117.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19  | C     | 3267 | PGV  | O01-C1-C2   | -2.03 | 107.08      | 111.48   |
| 18  | Q     | 4523 | TGL  | CG3-OG3-CC1 | -2.03 | 109.71      | 117.12   |
| 18  | A     | 3522 | TGL  | CC6-CC5-CC4 | 2.02  | 124.58      | 114.37   |
| 22  | G     | 3269 | CDL  | C83-C82-C81 | 2.02  | 124.58      | 114.37   |
| 19  | N     | 4524 | PGV  | P-O12-C04   | 2.02  | 132.91      | 121.35   |
| 18  | Q     | 4523 | TGL  | OG3-CC1-OC1 | -2.00 | 118.62      | 123.63   |

All (30) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 21  | C     | 3271 | CHD  | C9   |
| 21  | C     | 3271 | CHD  | C12  |
| 21  | C     | 3271 | CHD  | C3   |
| 21  | C     | 3271 | CHD  | C8   |
| 21  | C     | 3271 | CHD  | C14  |
| 21  | J     | 3060 | CHD  | C9   |
| 21  | J     | 3060 | CHD  | C12  |
| 21  | J     | 3060 | CHD  | C17  |
| 21  | J     | 3060 | CHD  | C8   |
| 21  | J     | 3060 | CHD  | C14  |
| 21  | P     | 4271 | CHD  | C9   |
| 21  | P     | 4271 | CHD  | C12  |
| 21  | P     | 4271 | CHD  | C3   |
| 21  | P     | 4271 | CHD  | C8   |
| 21  | P     | 4271 | CHD  | C14  |
| 21  | W     | 4060 | CHD  | C9   |
| 21  | W     | 4060 | CHD  | C12  |
| 21  | W     | 4060 | CHD  | C17  |
| 21  | W     | 4060 | CHD  | C8   |
| 21  | W     | 4060 | CHD  | C14  |
| 27  | M     | 3526 | DMU  | C5   |
| 27  | M     | 3526 | DMU  | C6   |
| 27  | M     | 3526 | DMU  | C2   |
| 27  | M     | 3526 | DMU  | C4   |
| 27  | M     | 3526 | DMU  | C9   |
| 27  | Z     | 4526 | DMU  | C5   |
| 27  | Z     | 4526 | DMU  | C6   |
| 27  | Z     | 4526 | DMU  | C2   |
| 27  | Z     | 4526 | DMU  | C4   |
| 27  | Z     | 4526 | DMU  | C9   |

All (909) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | A     | 3521 | TGL  | CB2-CB1-OG2-CG2 |
| 18  | A     | 3521 | TGL  | OB1-CB1-OG2-CG2 |
| 18  | A     | 3523 | TGL  | OB1-CB1-OG2-CG2 |
| 18  | N     | 4521 | TGL  | CB2-CB1-OG2-CG2 |
| 18  | N     | 4521 | TGL  | OB1-CB1-OG2-CG2 |
| 18  | Q     | 4523 | TGL  | OB1-CB1-OG2-CG2 |
| 19  | A     | 3524 | PGV  | C03-O11-P-O12   |
| 19  | A     | 3524 | PGV  | C03-O11-P-O13   |
| 19  | A     | 3524 | PGV  | C02-C03-O11-P   |
| 19  | A     | 3524 | PGV  | C05-C04-O12-P   |
| 19  | A     | 3524 | PGV  | C2-C1-O01-C02   |
| 19  | C     | 3268 | PGV  | C04-O12-P-O11   |
| 19  | C     | 3268 | PGV  | C04-O12-P-O14   |
| 19  | C     | 3268 | PGV  | O12-C04-C05-C06 |
| 19  | C     | 3268 | PGV  | C04-C05-C06-O06 |
| 19  | N     | 4524 | PGV  | C03-O11-P-O12   |
| 19  | N     | 4524 | PGV  | C03-O11-P-O13   |
| 19  | N     | 4524 | PGV  | C02-C03-O11-P   |
| 19  | N     | 4524 | PGV  | C05-C04-O12-P   |
| 19  | N     | 4524 | PGV  | C2-C1-O01-C02   |
| 19  | P     | 4268 | PGV  | C04-O12-P-O11   |
| 19  | P     | 4268 | PGV  | C04-O12-P-O14   |
| 19  | P     | 4268 | PGV  | O12-C04-C05-C06 |
| 19  | P     | 4268 | PGV  | C04-C05-C06-O06 |
| 21  | J     | 3060 | CHD  | C16-C17-C20-C21 |
| 21  | J     | 3060 | CHD  | C16-C17-C20-C22 |
| 21  | W     | 4060 | CHD  | C16-C17-C20-C21 |
| 21  | W     | 4060 | CHD  | C16-C17-C20-C22 |
| 22  | C     | 3270 | CDL  | CA2-C1-CB2-OB2  |
| 22  | C     | 3270 | CDL  | CA2-OA2-PA1-OA3 |
| 22  | C     | 3270 | CDL  | CA2-OA2-PA1-OA4 |
| 22  | C     | 3270 | CDL  | CA2-OA2-PA1-OA5 |
| 22  | C     | 3270 | CDL  | CA3-OA5-PA1-OA2 |
| 22  | C     | 3270 | CDL  | C11-CA5-OA6-CA4 |
| 22  | C     | 3270 | CDL  | CB2-OB2-PB2-OB4 |
| 22  | G     | 3269 | CDL  | CB2-C1-CA2-OA2  |
| 22  | G     | 3269 | CDL  | CA2-OA2-PA1-OA3 |
| 22  | G     | 3269 | CDL  | C1-CB2-OB2-PB2  |
| 22  | G     | 3269 | CDL  | CB3-OB5-PB2-OB2 |
| 22  | G     | 3269 | CDL  | CB3-OB5-PB2-OB3 |
| 22  | G     | 3269 | CDL  | CB3-OB5-PB2-OB4 |
| 22  | G     | 3269 | CDL  | OB6-CB4-CB6-OB8 |
| 22  | P     | 4270 | CDL  | CA2-C1-CB2-OB2  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | P     | 4270 | CDL  | CA2-OA2-PA1-OA3 |
| 22  | P     | 4270 | CDL  | CA2-OA2-PA1-OA4 |
| 22  | P     | 4270 | CDL  | CA2-OA2-PA1-OA5 |
| 22  | P     | 4270 | CDL  | CA3-OA5-PA1-OA2 |
| 22  | P     | 4270 | CDL  | C11-CA5-OA6-CA4 |
| 22  | P     | 4270 | CDL  | CB2-OB2-PB2-OB4 |
| 22  | T     | 4269 | CDL  | CB2-C1-CA2-OA2  |
| 22  | T     | 4269 | CDL  | CA2-OA2-PA1-OA3 |
| 22  | T     | 4269 | CDL  | C1-CB2-OB2-PB2  |
| 22  | T     | 4269 | CDL  | CB3-OB5-PB2-OB2 |
| 22  | T     | 4269 | CDL  | CB3-OB5-PB2-OB3 |
| 22  | T     | 4269 | CDL  | CB3-OB5-PB2-OB4 |
| 22  | T     | 4269 | CDL  | OB6-CB4-CB6-OB8 |
| 23  | C     | 3264 | PEK  | O12-C04-C05-N   |
| 23  | C     | 3265 | PEK  | C04-O12-P-O11   |
| 23  | C     | 3265 | PEK  | C04-O12-P-O13   |
| 23  | G     | 4263 | PEK  | C04-O12-P-O13   |
| 23  | G     | 4263 | PEK  | O12-C04-C05-N   |
| 23  | P     | 4264 | PEK  | O12-C04-C05-N   |
| 23  | P     | 4265 | PEK  | C04-O12-P-O11   |
| 23  | P     | 4265 | PEK  | C04-O12-P-O13   |
| 23  | T     | 3263 | PEK  | C04-O12-P-O13   |
| 23  | T     | 3263 | PEK  | O12-C04-C05-N   |
| 25  | E     | 3230 | PSC  | C04-O12-P-O14   |
| 25  | E     | 3230 | PSC  | O02-C1-O01-C02  |
| 25  | E     | 3230 | PSC  | C13-C14-C15-C16 |
| 25  | O     | 4230 | PSC  | C04-O12-P-O14   |
| 25  | O     | 4230 | PSC  | O02-C1-O01-C02  |
| 25  | O     | 4230 | PSC  | C13-C14-C15-C16 |
| 27  | M     | 3526 | DMU  | O5-C6-O16-C18   |
| 27  | Z     | 4526 | DMU  | O5-C6-O16-C18   |
| 18  | A     | 3522 | TGL  | CG2-CG3-OG3-CC1 |
| 18  | N     | 4522 | TGL  | CG2-CG3-OG3-CC1 |
| 18  | A     | 3521 | TGL  | OC1-CC1-OG3-CG3 |
| 18  | A     | 3523 | TGL  | OC1-CC1-OG3-CG3 |
| 18  | N     | 4521 | TGL  | OC1-CC1-OG3-CG3 |
| 18  | Q     | 4523 | TGL  | OC1-CC1-OG3-CG3 |
| 19  | A     | 3524 | PGV  | O02-C1-O01-C02  |
| 19  | N     | 4524 | PGV  | O02-C1-O01-C02  |
| 22  | C     | 3270 | CDL  | OA7-CA5-OA6-CA4 |
| 22  | P     | 4270 | CDL  | OA7-CA5-OA6-CA4 |
| 18  | A     | 3523 | TGL  | CB2-CB1-OG2-CG2 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | Q     | 4523 | TGL  | CB2-CB1-OG2-CG2 |
| 27  | Z     | 4526 | DMU  | O6-C11-C9-O1    |
| 18  | A     | 3521 | TGL  | CC2-CC1-OG3-CG3 |
| 18  | A     | 3523 | TGL  | CC2-CC1-OG3-CG3 |
| 18  | N     | 4521 | TGL  | CC2-CC1-OG3-CG3 |
| 18  | N     | 4522 | TGL  | CA2-CA1-OG1-CG1 |
| 18  | Q     | 4523 | TGL  | CC2-CC1-OG3-CG3 |
| 18  | A     | 3521 | TGL  | CB3-CB4-CB5-CB6 |
| 18  | A     | 3522 | TGL  | CB3-CB4-CB5-CB6 |
| 18  | N     | 4521 | TGL  | CB3-CB4-CB5-CB6 |
| 22  | P     | 4270 | CDL  | C20-C21-C22-C23 |
| 18  | N     | 4522 | TGL  | CB3-CB4-CB5-CB6 |
| 22  | C     | 3270 | CDL  | C20-C21-C22-C23 |
| 18  | A     | 3523 | TGL  | CB3-CB4-CB5-CB6 |
| 22  | C     | 3270 | CDL  | C17-C18-C19-C20 |
| 22  | C     | 3270 | CDL  | C37-C38-C39-C40 |
| 22  | C     | 3270 | CDL  | C40-C41-C42-C43 |
| 22  | C     | 3270 | CDL  | C57-C58-C59-C60 |
| 22  | C     | 3270 | CDL  | C80-C81-C82-C83 |
| 22  | G     | 3269 | CDL  | C17-C18-C19-C20 |
| 22  | G     | 3269 | CDL  | C37-C38-C39-C40 |
| 22  | G     | 3269 | CDL  | C57-C58-C59-C60 |
| 22  | G     | 3269 | CDL  | C60-C61-C62-C63 |
| 22  | P     | 4270 | CDL  | C17-C18-C19-C20 |
| 22  | P     | 4270 | CDL  | C37-C38-C39-C40 |
| 22  | P     | 4270 | CDL  | C40-C41-C42-C43 |
| 22  | P     | 4270 | CDL  | C57-C58-C59-C60 |
| 22  | P     | 4270 | CDL  | C80-C81-C82-C83 |
| 22  | T     | 4269 | CDL  | C17-C18-C19-C20 |
| 22  | T     | 4269 | CDL  | C20-C21-C22-C23 |
| 22  | T     | 4269 | CDL  | C37-C38-C39-C40 |
| 22  | T     | 4269 | CDL  | C40-C41-C42-C43 |
| 22  | T     | 4269 | CDL  | C57-C58-C59-C60 |
| 22  | T     | 4269 | CDL  | C60-C61-C62-C63 |
| 22  | T     | 4269 | CDL  | C77-C78-C79-C80 |
| 18  | Q     | 4523 | TGL  | CB3-CB4-CB5-CB6 |
| 22  | C     | 3270 | CDL  | C77-C78-C79-C80 |
| 22  | G     | 3269 | CDL  | C20-C21-C22-C23 |
| 22  | G     | 3269 | CDL  | C40-C41-C42-C43 |
| 22  | G     | 3269 | CDL  | C77-C78-C79-C80 |
| 22  | G     | 3269 | CDL  | C80-C81-C82-C83 |
| 22  | P     | 4270 | CDL  | C77-C78-C79-C80 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | T     | 4269 | CDL  | C80-C81-C82-C83 |
| 19  | C     | 3268 | PGV  | O12-C04-C05-O05 |
| 19  | P     | 4268 | PGV  | O12-C04-C05-O05 |
| 22  | C     | 3270 | CDL  | O1-C1-CB2-OB2   |
| 22  | G     | 3269 | CDL  | O1-C1-CA2-OA2   |
| 22  | P     | 4270 | CDL  | O1-C1-CB2-OB2   |
| 22  | T     | 4269 | CDL  | O1-C1-CA2-OA2   |
| 18  | A     | 3522 | TGL  | CA2-CA1-OG1-CG1 |
| 22  | G     | 3269 | CDL  | C31-CA7-OA8-CA6 |
| 22  | T     | 4269 | CDL  | C31-CA7-OA8-CA6 |
| 27  | M     | 3526 | DMU  | O6-C11-C9-O1    |
| 22  | G     | 3269 | CDL  | OA9-CA7-OA8-CA6 |
| 22  | T     | 4269 | CDL  | OA9-CA7-OA8-CA6 |
| 22  | P     | 4270 | CDL  | C60-C61-C62-C63 |
| 22  | C     | 3270 | CDL  | C60-C61-C62-C63 |
| 18  | A     | 3523 | TGL  | CC2-CC3-CC4-CC5 |
| 18  | A     | 3522 | TGL  | OA1-CA1-OG1-CG1 |
| 18  | N     | 4522 | TGL  | OA1-CA1-OG1-CG1 |
| 18  | A     | 3522 | TGL  | OC1-CC1-OG3-CG3 |
| 18  | N     | 4522 | TGL  | OC1-CC1-OG3-CG3 |
| 18  | Q     | 4523 | TGL  | CC2-CC3-CC4-CC5 |
| 25  | E     | 3230 | PSC  | C20-C19-O03-C01 |
| 25  | O     | 4230 | PSC  | C20-C19-O03-C01 |
| 18  | A     | 3521 | TGL  | CA9-C20-C21-C22 |
| 18  | N     | 4521 | TGL  | CA9-C20-C21-C22 |
| 22  | P     | 4270 | CDL  | C62-C63-C64-C65 |
| 22  | C     | 3270 | CDL  | C62-C63-C64-C65 |
| 18  | N     | 4522 | TGL  | CC3-CC4-CC5-CC6 |
| 17  | A     | 516  | HEA  | C4D-C3D-CAD-CBD |
| 17  | N     | 516  | HEA  | C4D-C3D-CAD-CBD |
| 22  | C     | 3270 | CDL  | CB2-C1-CA2-OA2  |
| 22  | P     | 4270 | CDL  | CB2-C1-CA2-OA2  |
| 18  | A     | 3521 | TGL  | CA2-CA1-OG1-CG1 |
| 18  | N     | 4521 | TGL  | CA2-CA1-OG1-CG1 |
| 23  | C     | 3265 | PEK  | C22-C21-O03-C01 |
| 23  | P     | 4265 | PEK  | C22-C21-O03-C01 |
| 19  | A     | 3524 | PGV  | C20-C21-C22-C23 |
| 19  | N     | 4524 | PGV  | C20-C21-C22-C23 |
| 22  | T     | 4269 | CDL  | C52-C53-C54-C55 |
| 18  | A     | 3522 | TGL  | CC3-CC4-CC5-CC6 |
| 22  | G     | 3269 | CDL  | C52-C53-C54-C55 |
| 21  | C     | 3271 | CHD  | C13-C17-C20-C22 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 21  | P     | 4271 | CHD  | C13-C17-C20-C22 |
| 22  | C     | 3270 | CDL  | C23-C24-C25-C26 |
| 22  | P     | 4270 | CDL  | C23-C24-C25-C26 |
| 21  | C     | 3271 | CHD  | C17-C20-C22-C23 |
| 22  | G     | 3269 | CDL  | C15-C16-C17-C18 |
| 22  | G     | 3269 | CDL  | O1-C1-CB2-OB2   |
| 22  | T     | 4269 | CDL  | O1-C1-CB2-OB2   |
| 22  | T     | 4269 | CDL  | C15-C16-C17-C18 |
| 22  | G     | 3269 | CDL  | C73-C74-C75-C76 |
| 18  | A     | 3522 | TGL  | CB5-CB6-CB7-CB8 |
| 22  | T     | 4269 | CDL  | C73-C74-C75-C76 |
| 25  | E     | 3230 | PSC  | C20-C21-C22-C23 |
| 25  | O     | 4230 | PSC  | C20-C21-C22-C23 |
| 23  | C     | 3265 | PEK  | O04-C21-O03-C01 |
| 21  | P     | 4271 | CHD  | C17-C20-C22-C23 |
| 18  | N     | 4522 | TGL  | CB5-CB6-CB7-CB8 |
| 21  | C     | 3271 | CHD  | C21-C20-C22-C23 |
| 21  | P     | 4271 | CHD  | C21-C20-C22-C23 |
| 27  | M     | 3526 | DMU  | O5-C4-C57-O61   |
| 23  | P     | 4265 | PEK  | O04-C21-O03-C01 |
| 21  | J     | 3060 | CHD  | C13-C17-C20-C22 |
| 19  | A     | 3524 | PGV  | C1-C2-C3-C4     |
| 22  | G     | 3269 | CDL  | CA7-C31-C32-C33 |
| 22  | G     | 3269 | CDL  | CB7-C71-C72-C73 |
| 22  | T     | 4269 | CDL  | CA7-C31-C32-C33 |
| 23  | C     | 3264 | PEK  | C1-C2-C3-C4     |
| 23  | G     | 4263 | PEK  | C1-C2-C3-C4     |
| 19  | P     | 4268 | PGV  | C7-C8-C9-C10    |
| 27  | Z     | 4526 | DMU  | O5-C4-C57-O61   |
| 19  | C     | 3268 | PGV  | C7-C8-C9-C10    |
| 18  | A     | 3523 | TGL  | CA1-CA2-CA3-CA4 |
| 18  | Q     | 4523 | TGL  | CA1-CA2-CA3-CA4 |
| 19  | N     | 4524 | PGV  | C1-C2-C3-C4     |
| 22  | T     | 4269 | CDL  | CB7-C71-C72-C73 |
| 23  | T     | 3263 | PEK  | C1-C2-C3-C4     |
| 25  | E     | 3230 | PSC  | C1-C2-C3-C4     |
| 25  | O     | 4230 | PSC  | C1-C2-C3-C4     |
| 21  | W     | 4060 | CHD  | C13-C17-C20-C22 |
| 17  | A     | 516  | HEA  | C2D-C3D-CAD-CBD |
| 18  | A     | 3522 | TGL  | CB1-CB2-CB3-CB4 |
| 18  | N     | 4522 | TGL  | CB1-CB2-CB3-CB4 |
| 18  | A     | 3521 | TGL  | OA1-CA1-OG1-CG1 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | N     | 4521 | TGL  | OA1-CA1-OG1-CG1 |
| 22  | C     | 3270 | CDL  | O1-C1-CA2-OA2   |
| 19  | A     | 3524 | PGV  | C20-C19-O03-C01 |
| 25  | E     | 3230 | PSC  | O04-C19-O03-C01 |
| 25  | O     | 4230 | PSC  | O04-C19-O03-C01 |
| 23  | C     | 3265 | PEK  | C1-C2-C3-C4     |
| 23  | P     | 4265 | PEK  | C1-C2-C3-C4     |
| 25  | E     | 3230 | PSC  | C11-C12-C13-C14 |
| 25  | O     | 4230 | PSC  | C11-C12-C13-C14 |
| 23  | P     | 4264 | PEK  | C1-C2-C3-C4     |
| 25  | E     | 3230 | PSC  | C22-C23-C24-C25 |
| 19  | N     | 4524 | PGV  | C20-C19-O03-C01 |
| 22  | T     | 4269 | CDL  | C11-CA5-OA6-CA4 |
| 25  | E     | 3230 | PSC  | C2-C1-O01-C02   |
| 25  | O     | 4230 | PSC  | C2-C1-O01-C02   |
| 22  | G     | 3269 | CDL  | OA7-CA5-OA6-CA4 |
| 22  | T     | 4269 | CDL  | OA7-CA5-OA6-CA4 |
| 22  | G     | 3269 | CDL  | CA2-C1-CB2-OB2  |
| 22  | T     | 4269 | CDL  | CA2-C1-CB2-OB2  |
| 19  | C     | 3268 | PGV  | C20-C21-C22-C23 |
| 21  | P     | 4271 | CHD  | C13-C17-C20-C21 |
| 19  | P     | 4268 | PGV  | C20-C21-C22-C23 |
| 25  | O     | 4230 | PSC  | C22-C23-C24-C25 |
| 22  | G     | 3269 | CDL  | C11-CA5-OA6-CA4 |
| 27  | Z     | 4526 | DMU  | C3-C4-C57-O61   |
| 21  | C     | 3271 | CHD  | C13-C17-C20-C21 |
| 21  | J     | 3060 | CHD  | C13-C17-C20-C21 |
| 21  | W     | 4060 | CHD  | C13-C17-C20-C21 |
| 22  | P     | 4270 | CDL  | O1-C1-CA2-OA2   |
| 19  | C     | 3268 | PGV  | C02-C03-O11-P   |
| 19  | P     | 4268 | PGV  | C02-C03-O11-P   |
| 19  | A     | 3524 | PGV  | C04-C05-C06-O06 |
| 19  | N     | 4524 | PGV  | C04-C05-C06-O06 |
| 19  | N     | 4266 | PGV  | C15-C16-C17-C18 |
| 22  | G     | 3269 | CDL  | C22-C23-C24-C25 |
| 22  | T     | 4269 | CDL  | C63-C64-C65-C66 |
| 27  | M     | 3526 | DMU  | C25-C28-C31-C34 |
| 18  | A     | 3523 | TGL  | C12-C13-C14-C29 |
| 18  | Q     | 4523 | TGL  | C12-C13-C14-C29 |
| 19  | N     | 4266 | PGV  | C6-C7-C8-C9     |
| 22  | C     | 3270 | CDL  | C63-C64-C65-C66 |
| 22  | G     | 3269 | CDL  | C82-C83-C84-C85 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | P     | 4270 | CDL  | C63-C64-C65-C66 |
| 23  | P     | 4264 | PEK  | C23-C24-C25-C26 |
| 27  | Z     | 4526 | DMU  | C25-C28-C31-C34 |
| 19  | C     | 3268 | PGV  | C30-C31-C32-C33 |
| 19  | P     | 4268 | PGV  | C2-C3-C4-C5     |
| 22  | C     | 3270 | CDL  | C51-C52-C53-C54 |
| 22  | C     | 3270 | CDL  | C72-C73-C74-C75 |
| 22  | T     | 4269 | CDL  | C82-C83-C84-C85 |
| 23  | C     | 3264 | PEK  | C23-C24-C25-C26 |
| 19  | A     | 3524 | PGV  | O04-C19-O03-C01 |
| 19  | A     | 3266 | PGV  | C6-C7-C8-C9     |
| 19  | N     | 4524 | PGV  | C22-C23-C24-C25 |
| 19  | P     | 4268 | PGV  | C30-C31-C32-C33 |
| 22  | C     | 3270 | CDL  | C61-C62-C63-C64 |
| 22  | P     | 4270 | CDL  | C72-C73-C74-C75 |
| 23  | C     | 3265 | PEK  | C29-C30-C31-C32 |
| 19  | A     | 3524 | PGV  | O05-C05-C06-O06 |
| 19  | C     | 3268 | PGV  | O05-C05-C06-O06 |
| 19  | N     | 4524 | PGV  | O05-C05-C06-O06 |
| 19  | P     | 4268 | PGV  | O05-C05-C06-O06 |
| 18  | A     | 3522 | TGL  | C17-C18-C19-C33 |
| 18  | A     | 3523 | TGL  | C16-C15-CC9-CC8 |
| 18  | N     | 4521 | TGL  | C23-C24-C25-C26 |
| 18  | Q     | 4523 | TGL  | C16-C15-CC9-CC8 |
| 19  | A     | 3524 | PGV  | C22-C23-C24-C25 |
| 23  | P     | 4265 | PEK  | C29-C30-C31-C32 |
| 22  | C     | 3270 | CDL  | CB7-C71-C72-C73 |
| 19  | C     | 3268 | PGV  | C24-C25-C26-C27 |
| 22  | G     | 3269 | CDL  | C63-C64-C65-C66 |
| 22  | P     | 4270 | CDL  | C51-C52-C53-C54 |
| 22  | T     | 4269 | CDL  | C22-C23-C24-C25 |
| 19  | N     | 4524 | PGV  | O04-C19-O03-C01 |
| 22  | P     | 4270 | CDL  | C51-CB5-OB6-CB4 |
| 18  | N     | 4522 | TGL  | C17-C18-C19-C33 |
| 19  | C     | 3268 | PGV  | C14-C15-C16-C17 |
| 19  | P     | 4268 | PGV  | C14-C15-C16-C17 |
| 22  | C     | 3270 | CDL  | C73-C74-C75-C76 |
| 19  | A     | 3266 | PGV  | C15-C16-C17-C18 |
| 18  | A     | 3522 | TGL  | C24-C25-C26-C27 |
| 19  | C     | 3268 | PGV  | C2-C3-C4-C5     |
| 22  | G     | 3269 | CDL  | C79-C80-C81-C82 |
| 22  | P     | 4270 | CDL  | C61-C62-C63-C64 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | P     | 4270 | CDL  | CB7-C71-C72-C73 |
| 18  | A     | 3521 | TGL  | C23-C24-C25-C26 |
| 18  | N     | 4521 | TGL  | C22-C23-C24-C25 |
| 18  | N     | 4522 | TGL  | C24-C25-C26-C27 |
| 19  | A     | 3524 | PGV  | C14-C15-C16-C17 |
| 19  | P     | 4268 | PGV  | C24-C25-C26-C27 |
| 22  | T     | 4269 | CDL  | C79-C80-C81-C82 |
| 18  | A     | 3522 | TGL  | C21-C20-CA9-CA8 |
| 19  | N     | 4524 | PGV  | C14-C15-C16-C17 |
| 22  | P     | 4270 | CDL  | C73-C74-C75-C76 |
| 18  | A     | 3521 | TGL  | C22-C23-C24-C25 |
| 22  | T     | 4269 | CDL  | OB9-CB7-OB8-CB6 |
| 18  | A     | 3521 | TGL  | C12-C13-C14-C29 |
| 18  | N     | 4521 | TGL  | C12-C13-C14-C29 |
| 18  | N     | 4522 | TGL  | C21-C20-CA9-CA8 |
| 18  | A     | 3523 | TGL  | OG1-CG1-CG2-CG3 |
| 18  | Q     | 4523 | TGL  | OG1-CG1-CG2-CG3 |
| 23  | C     | 3264 | PEK  | O03-C01-C02-C03 |
| 27  | Z     | 4526 | DMU  | O16-C18-C19-C22 |
| 22  | T     | 4269 | CDL  | C13-C14-C15-C16 |
| 18  | N     | 4522 | TGL  | C16-C15-CC9-CC8 |
| 19  | A     | 3266 | PGV  | C29-C30-C31-C32 |
| 19  | N     | 4266 | PGV  | C29-C30-C31-C32 |
| 22  | C     | 3270 | CDL  | C74-C75-C76-C77 |
| 22  | G     | 3269 | CDL  | C13-C14-C15-C16 |
| 22  | G     | 3269 | CDL  | C33-C34-C35-C36 |
| 22  | G     | 3269 | CDL  | C41-C42-C43-C44 |
| 22  | P     | 4270 | CDL  | C74-C75-C76-C77 |
| 22  | T     | 4269 | CDL  | C41-C42-C43-C44 |
| 23  | G     | 4263 | PEK  | C22-C23-C24-C25 |
| 23  | T     | 3263 | PEK  | C22-C23-C24-C25 |
| 22  | G     | 3269 | CDL  | OB9-CB7-OB8-CB6 |
| 18  | A     | 3521 | TGL  | C14-C29-C30-C31 |
| 25  | E     | 3230 | PSC  | C29-C30-C31-C32 |
| 22  | T     | 4269 | CDL  | C33-C34-C35-C36 |
| 18  | A     | 3522 | TGL  | C16-C15-CC9-CC8 |
| 18  | N     | 4521 | TGL  | CB4-CB5-CB6-CB7 |
| 18  | N     | 4521 | TGL  | C14-C29-C30-C31 |
| 22  | C     | 3270 | CDL  | C55-C56-C57-C58 |
| 25  | O     | 4230 | PSC  | C29-C30-C31-C32 |
| 23  | P     | 4264 | PEK  | O04-C21-O03-C01 |
| 18  | A     | 3522 | TGL  | C21-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | N     | 4522 | TGL  | CC2-CC1-OG3-CG3 |
| 18  | A     | 3521 | TGL  | CB4-CB5-CB6-CB7 |
| 18  | N     | 4522 | TGL  | C21-C22-C23-C24 |
| 18  | A     | 3521 | TGL  | CC4-CC5-CC6-CC7 |
| 18  | A     | 3522 | TGL  | C22-C23-C24-C25 |
| 25  | E     | 3230 | PSC  | C2-C3-C4-C5     |
| 18  | N     | 4521 | TGL  | CC4-CC5-CC6-CC7 |
| 18  | N     | 4522 | TGL  | C22-C23-C24-C25 |
| 22  | P     | 4270 | CDL  | C55-C56-C57-C58 |
| 25  | O     | 4230 | PSC  | C2-C3-C4-C5     |
| 23  | C     | 3264 | PEK  | O04-C21-O03-C01 |
| 18  | A     | 3522 | TGL  | CC6-CC7-CC8-CC9 |
| 18  | N     | 4522 | TGL  | CC6-CC7-CC8-CC9 |
| 19  | C     | 3268 | PGV  | C23-C24-C25-C26 |
| 23  | T     | 3263 | PEK  | C31-C32-C33-C34 |
| 22  | C     | 3270 | CDL  | OB7-CB5-OB6-CB4 |
| 22  | P     | 4270 | CDL  | OB7-CB5-OB6-CB4 |
| 21  | W     | 4060 | CHD  | C21-C20-C22-C23 |
| 18  | A     | 3523 | TGL  | CB6-CB7-CB8-CB9 |
| 23  | T     | 3263 | PEK  | C25-C26-C27-C28 |
| 18  | A     | 3523 | TGL  | CB5-CB6-CB7-CB8 |
| 18  | Q     | 4523 | TGL  | CB6-CB7-CB8-CB9 |
| 19  | P     | 4268 | PGV  | C23-C24-C25-C26 |
| 22  | C     | 3270 | CDL  | C16-C17-C18-C19 |
| 23  | G     | 4263 | PEK  | C25-C26-C27-C28 |
| 23  | G     | 4263 | PEK  | C31-C32-C33-C34 |
| 23  | C     | 3264 | PEK  | C22-C21-O03-C01 |
| 22  | P     | 4270 | CDL  | C16-C17-C18-C19 |
| 18  | Q     | 4523 | TGL  | CB5-CB6-CB7-CB8 |
| 19  | P     | 4267 | PGV  | C22-C23-C24-C25 |
| 23  | P     | 4265 | PEK  | C25-C26-C27-C28 |
| 27  | M     | 3526 | DMU  | O16-C18-C19-C22 |
| 19  | N     | 4524 | PGV  | C24-C25-C26-C27 |
| 19  | A     | 3524 | PGV  | C24-C25-C26-C27 |
| 19  | C     | 3267 | PGV  | C22-C23-C24-C25 |
| 23  | C     | 3265 | PEK  | C25-C26-C27-C28 |
| 18  | A     | 3522 | TGL  | CC2-CC1-OG3-CG3 |
| 22  | C     | 3270 | CDL  | C51-CB5-OB6-CB4 |
| 23  | G     | 4263 | PEK  | C2-C1-O01-C02   |
| 23  | T     | 3263 | PEK  | C2-C1-O01-C02   |
| 19  | P     | 4268 | PGV  | C19-C20-C21-C22 |
| 22  | P     | 4270 | CDL  | C19-C20-C21-C22 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | P     | 4268 | PGV  | O02-C1-O01-C02  |
| 23  | T     | 3263 | PEK  | O02-C1-O01-C02  |
| 22  | C     | 3270 | CDL  | C19-C20-C21-C22 |
| 19  | C     | 3267 | PGV  | C11-C10-C9-C8   |
| 19  | P     | 4267 | PGV  | C11-C10-C9-C8   |
| 22  | G     | 3269 | CDL  | CA5-C11-C12-C13 |
| 22  | P     | 4270 | CDL  | CA5-C11-C12-C13 |
| 22  | T     | 4269 | CDL  | CA5-C11-C12-C13 |
| 19  | A     | 3266 | PGV  | C23-C24-C25-C26 |
| 22  | P     | 4270 | CDL  | C11-C12-C13-C14 |
| 22  | C     | 3270 | CDL  | C13-C14-C15-C16 |
| 19  | A     | 3266 | PGV  | C5-C6-C7-C8     |
| 19  | N     | 4266 | PGV  | C5-C6-C7-C8     |
| 22  | C     | 3270 | CDL  | C11-C12-C13-C14 |
| 22  | G     | 3269 | CDL  | C56-C57-C58-C59 |
| 22  | T     | 4269 | CDL  | C56-C57-C58-C59 |
| 18  | N     | 4521 | TGL  | C20-C21-C22-C23 |
| 19  | C     | 3268 | PGV  | C19-C20-C21-C22 |
| 22  | C     | 3270 | CDL  | CA5-C11-C12-C13 |
| 18  | A     | 3521 | TGL  | C20-C21-C22-C23 |
| 22  | G     | 3269 | CDL  | C39-C40-C41-C42 |
| 21  | J     | 3060 | CHD  | C21-C20-C22-C23 |
| 22  | T     | 4269 | CDL  | C39-C40-C41-C42 |
| 22  | P     | 4270 | CDL  | C13-C14-C15-C16 |
| 18  | A     | 3522 | TGL  | C18-C19-C33-C34 |
| 19  | C     | 3267 | PGV  | C25-C26-C27-C28 |
| 19  | N     | 4266 | PGV  | C23-C24-C25-C26 |
| 19  | P     | 4267 | PGV  | C25-C26-C27-C28 |
| 23  | T     | 3263 | PEK  | C27-C28-C29-C30 |
| 18  | A     | 3521 | TGL  | OG1-CG1-CG2-OG2 |
| 18  | A     | 3523 | TGL  | OG1-CG1-CG2-OG2 |
| 18  | N     | 4521 | TGL  | OG1-CG1-CG2-OG2 |
| 18  | Q     | 4523 | TGL  | OG1-CG1-CG2-OG2 |
| 18  | N     | 4522 | TGL  | C18-C19-C33-C34 |
| 22  | P     | 4270 | CDL  | C75-C76-C77-C78 |
| 22  | T     | 4269 | CDL  | C62-C63-C64-C65 |
| 23  | G     | 4263 | PEK  | C27-C28-C29-C30 |
| 22  | T     | 4269 | CDL  | C71-CB7-OB8-CB6 |
| 22  | G     | 3269 | CDL  | C23-C24-C25-C26 |
| 22  | T     | 4269 | CDL  | C23-C24-C25-C26 |
| 23  | C     | 3264 | PEK  | C16-C17-C18-C19 |
| 23  | P     | 4264 | PEK  | C16-C17-C18-C19 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | C     | 3270 | CDL  | C75-C76-C77-C78 |
| 19  | C     | 3268 | PGV  | O02-C1-O01-C02  |
| 23  | G     | 4263 | PEK  | O02-C1-O01-C02  |
| 18  | A     | 3522 | TGL  | CA7-CA8-CA9-C20 |
| 18  | A     | 3523 | TGL  | CB4-CB5-CB6-CB7 |
| 18  | N     | 4522 | TGL  | CA7-CA8-CA9-C20 |
| 22  | C     | 3270 | CDL  | C32-C33-C34-C35 |
| 22  | C     | 3270 | CDL  | C78-C79-C80-C81 |
| 22  | P     | 4270 | CDL  | C32-C33-C34-C35 |
| 22  | G     | 3269 | CDL  | C71-CB7-OB8-CB6 |
| 19  | N     | 4266 | PGV  | C7-C8-C9-C10    |
| 22  | P     | 4270 | CDL  | C78-C79-C80-C81 |
| 23  | C     | 3265 | PEK  | C16-C17-C18-C19 |
| 18  | Q     | 4523 | TGL  | CB4-CB5-CB6-CB7 |
| 22  | G     | 3269 | CDL  | C62-C63-C64-C65 |
| 18  | A     | 3521 | TGL  | C13-C14-C29-C30 |
| 23  | P     | 4265 | PEK  | C16-C17-C18-C19 |
| 23  | P     | 4264 | PEK  | C22-C21-O03-C01 |
| 18  | A     | 3521 | TGL  | C16-C15-CC9-CC8 |
| 19  | P     | 4267 | PGV  | C13-C14-C15-C16 |
| 22  | P     | 4270 | CDL  | C18-C19-C20-C21 |
| 18  | N     | 4521 | TGL  | C13-C14-C29-C30 |
| 22  | C     | 3270 | CDL  | C18-C19-C20-C21 |
| 19  | C     | 3267 | PGV  | C13-C14-C15-C16 |
| 19  | P     | 4267 | PGV  | C7-C8-C9-C10    |
| 19  | A     | 3524 | PGV  | C01-C02-C03-O11 |
| 19  | N     | 4524 | PGV  | C01-C02-C03-O11 |
| 22  | C     | 3270 | CDL  | OA5-CA3-CA4-CA6 |
| 22  | P     | 4270 | CDL  | OA5-CA3-CA4-CA6 |
| 22  | C     | 3270 | CDL  | C36-C37-C38-C39 |
| 18  | N     | 4521 | TGL  | C16-C15-CC9-CC8 |
| 19  | A     | 3266 | PGV  | C7-C8-C9-C10    |
| 21  | P     | 4271 | CHD  | C16-C17-C20-C21 |
| 27  | M     | 3526 | DMU  | C3-C4-C57-O61   |
| 17  | N     | 516  | HEA  | C2D-C3D-CAD-CBD |
| 22  | T     | 4269 | CDL  | C19-C20-C21-C22 |
| 18  | A     | 3522 | TGL  | C19-C33-C34-C35 |
| 18  | N     | 4522 | TGL  | C19-C33-C34-C35 |
| 19  | C     | 3268 | PGV  | C25-C26-C27-C28 |
| 22  | G     | 3269 | CDL  | C19-C20-C21-C22 |
| 22  | T     | 4269 | CDL  | C72-C73-C74-C75 |
| 21  | C     | 3271 | CHD  | C16-C17-C20-C21 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | N     | 4524 | PGV  | C5-C6-C7-C8     |
| 19  | C     | 3267 | PGV  | C7-C8-C9-C10    |
| 22  | P     | 4270 | CDL  | C14-C15-C16-C17 |
| 22  | C     | 3270 | CDL  | CA3-CA4-CA6-OA8 |
| 22  | C     | 3270 | CDL  | CB3-CB4-CB6-OB8 |
| 22  | P     | 4270 | CDL  | CA3-CA4-CA6-OA8 |
| 22  | P     | 4270 | CDL  | CB3-CB4-CB6-OB8 |
| 23  | C     | 3265 | PEK  | O03-C01-C02-C03 |
| 23  | P     | 4264 | PEK  | O03-C01-C02-C03 |
| 23  | P     | 4265 | PEK  | O03-C01-C02-C03 |
| 22  | G     | 3269 | CDL  | C72-C73-C74-C75 |
| 23  | C     | 3265 | PEK  | C2-C3-C4-C5     |
| 23  | P     | 4265 | PEK  | C2-C3-C4-C5     |
| 19  | N     | 4524 | PGV  | C2-C3-C4-C5     |
| 22  | P     | 4270 | CDL  | C36-C37-C38-C39 |
| 22  | C     | 3270 | CDL  | C14-C15-C16-C17 |
| 19  | A     | 3524 | PGV  | C5-C6-C7-C8     |
| 19  | C     | 3268 | PGV  | C29-C30-C31-C32 |
| 19  | P     | 4268 | PGV  | C25-C26-C27-C28 |
| 18  | N     | 4522 | TGL  | CC2-CC3-CC4-CC5 |
| 18  | A     | 3521 | TGL  | C17-C18-C19-C33 |
| 22  | G     | 3269 | CDL  | C14-C15-C16-C17 |
| 18  | N     | 4521 | TGL  | C17-C18-C19-C33 |
| 19  | A     | 3524 | PGV  | C03-C02-O01-C1  |
| 19  | N     | 4524 | PGV  | C03-C02-O01-C1  |
| 18  | A     | 3522 | TGL  | CB9-C10-C11-C12 |
| 18  | N     | 4521 | TGL  | CC2-CC3-CC4-CC5 |
| 18  | Q     | 4523 | TGL  | C23-C24-C25-C26 |
| 19  | P     | 4267 | PGV  | C24-C25-C26-C27 |
| 19  | P     | 4268 | PGV  | C29-C30-C31-C32 |
| 27  | Z     | 4526 | DMU  | C22-C25-C28-C31 |
| 18  | A     | 3521 | TGL  | CC2-CC3-CC4-CC5 |
| 18  | A     | 3522 | TGL  | CC4-CC5-CC6-CC7 |
| 18  | N     | 4522 | TGL  | CB9-C10-C11-C12 |
| 22  | T     | 4269 | CDL  | C14-C15-C16-C17 |
| 18  | N     | 4521 | TGL  | CA1-CA2-CA3-CA4 |
| 25  | E     | 3230 | PSC  | C21-C22-C23-C24 |
| 21  | W     | 4060 | CHD  | C17-C20-C22-C23 |
| 19  | A     | 3524 | PGV  | C2-C3-C4-C5     |
| 27  | M     | 3526 | DMU  | C34-C37-C40-C43 |
| 22  | C     | 3270 | CDL  | C71-C72-C73-C74 |
| 22  | G     | 3269 | CDL  | C38-C39-C40-C41 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | E     | 3230 | PSC  | C3-C4-C5-C6     |
| 25  | O     | 4230 | PSC  | C3-C4-C5-C6     |
| 21  | C     | 3271 | CHD  | C16-C17-C20-C22 |
| 21  | P     | 4271 | CHD  | C16-C17-C20-C22 |
| 19  | A     | 3524 | PGV  | C31-C32-C33-C34 |
| 18  | N     | 4522 | TGL  | CC4-CC5-CC6-CC7 |
| 22  | P     | 4270 | CDL  | C71-C72-C73-C74 |
| 25  | O     | 4230 | PSC  | C21-C22-C23-C24 |
| 18  | A     | 3523 | TGL  | CA9-C20-C21-C22 |
| 19  | C     | 3267 | PGV  | C24-C25-C26-C27 |
| 22  | C     | 3270 | CDL  | C59-C60-C61-C62 |
| 18  | A     | 3523 | TGL  | C23-C24-C25-C26 |
| 18  | Q     | 4523 | TGL  | CA9-C20-C21-C22 |
| 22  | T     | 4269 | CDL  | C38-C39-C40-C41 |
| 23  | P     | 4264 | PEK  | C22-C23-C24-C25 |
| 27  | M     | 3526 | DMU  | C22-C25-C28-C31 |
| 18  | A     | 3521 | TGL  | C25-C26-C27-C28 |
| 22  | P     | 4270 | CDL  | C12-C13-C14-C15 |
| 19  | N     | 4524 | PGV  | C31-C32-C33-C34 |
| 22  | T     | 4269 | CDL  | C44-C45-C46-C47 |
| 23  | C     | 3264 | PEK  | C22-C23-C24-C25 |
| 18  | N     | 4521 | TGL  | C25-C26-C27-C28 |
| 22  | C     | 3270 | CDL  | C84-C85-C86-C87 |
| 19  | N     | 4524 | PGV  | C13-C14-C15-C16 |
| 22  | C     | 3270 | CDL  | C12-C13-C14-C15 |
| 22  | P     | 4270 | CDL  | C84-C85-C86-C87 |
| 22  | G     | 3269 | CDL  | C44-C45-C46-C47 |
| 18  | A     | 3522 | TGL  | C29-C30-C31-C32 |
| 18  | N     | 4522 | TGL  | C29-C30-C31-C32 |
| 18  | A     | 3521 | TGL  | CA1-CA2-CA3-CA4 |
| 27  | Z     | 4526 | DMU  | C34-C37-C40-C43 |
| 22  | G     | 3269 | CDL  | C12-C13-C14-C15 |
| 22  | P     | 4270 | CDL  | C59-C60-C61-C62 |
| 19  | P     | 4268 | PGV  | C2-C1-O01-C02   |
| 19  | P     | 4267 | PGV  | C15-C16-C17-C18 |
| 23  | P     | 4265 | PEK  | C31-C32-C33-C34 |
| 19  | C     | 3267 | PGV  | C15-C16-C17-C18 |
| 22  | G     | 3269 | CDL  | CB5-C51-C52-C53 |
| 22  | T     | 4269 | CDL  | CB5-C51-C52-C53 |
| 23  | C     | 3265 | PEK  | C31-C32-C33-C34 |
| 18  | A     | 3522 | TGL  | CC2-CC3-CC4-CC5 |
| 19  | A     | 3524 | PGV  | C13-C14-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 27  | Z     | 4526 | DMU  | C19-C18-O16-C6  |
| 21  | J     | 3060 | CHD  | C17-C20-C22-C23 |
| 18  | A     | 3521 | TGL  | C16-C17-C18-C19 |
| 22  | P     | 4270 | CDL  | CA4-CA3-OA5-PA1 |
| 18  | A     | 3521 | TGL  | CC7-CC8-CC9-C15 |
| 18  | N     | 4521 | TGL  | C16-C17-C18-C19 |
| 22  | T     | 4269 | CDL  | C12-C13-C14-C15 |
| 18  | N     | 4522 | TGL  | C33-C34-C35-C36 |
| 18  | N     | 4521 | TGL  | CC7-CC8-CC9-C15 |
| 18  | A     | 3522 | TGL  | C33-C34-C35-C36 |
| 22  | G     | 3269 | CDL  | C24-C25-C26-C27 |
| 19  | C     | 3268 | PGV  | C2-C1-O01-C02   |
| 22  | T     | 4269 | CDL  | C24-C25-C26-C27 |
| 23  | P     | 4264 | PEK  | C24-C25-C26-C27 |
| 19  | A     | 3524 | PGV  | C12-C13-C14-C15 |
| 19  | N     | 4524 | PGV  | C12-C13-C14-C15 |
| 18  | A     | 3521 | TGL  | C21-C20-CA9-CA8 |
| 19  | N     | 4266 | PGV  | C31-C32-C33-C34 |
| 18  | A     | 3521 | TGL  | OG1-CG1-CG2-CG3 |
| 18  | N     | 4521 | TGL  | OG1-CG1-CG2-CG3 |
| 22  | G     | 3269 | CDL  | CA3-CA4-CA6-OA8 |
| 22  | T     | 4269 | CDL  | CA3-CA4-CA6-OA8 |
| 19  | A     | 3266 | PGV  | C31-C32-C33-C34 |
| 23  | C     | 3264 | PEK  | C24-C25-C26-C27 |
| 19  | A     | 3266 | PGV  | C4-C5-C6-C7     |
| 19  | C     | 3268 | PGV  | C13-C14-C15-C16 |
| 19  | P     | 4268 | PGV  | C13-C14-C15-C16 |
| 22  | G     | 3269 | CDL  | C35-C36-C37-C38 |
| 22  | T     | 4269 | CDL  | C58-C59-C60-C61 |
| 18  | N     | 4521 | TGL  | C21-C20-CA9-CA8 |
| 19  | A     | 3524 | PGV  | O01-C02-C03-O11 |
| 19  | C     | 3268 | PGV  | O01-C02-C03-O11 |
| 19  | P     | 4268 | PGV  | O01-C02-C03-O11 |
| 22  | C     | 3270 | CDL  | OA5-CA3-CA4-OA6 |
| 22  | P     | 4270 | CDL  | OA5-CA3-CA4-OA6 |
| 22  | G     | 3269 | CDL  | C58-C59-C60-C61 |
| 22  | C     | 3270 | CDL  | CA4-CA3-OA5-PA1 |
| 22  | G     | 3269 | CDL  | CB4-CB3-OB5-PB2 |
| 22  | T     | 4269 | CDL  | CB4-CB3-OB5-PB2 |
| 23  | C     | 3265 | PEK  | C30-C31-C32-C33 |
| 22  | T     | 4269 | CDL  | C35-C36-C37-C38 |
| 23  | P     | 4265 | PEK  | C30-C31-C32-C33 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | O     | 4230 | PSC  | C4-C5-C6-C7     |
| 22  | P     | 4270 | CDL  | C39-C40-C41-C42 |
| 22  | C     | 3270 | CDL  | OB6-CB4-CB6-OB8 |
| 22  | P     | 4270 | CDL  | OB6-CB4-CB6-OB8 |
| 23  | P     | 4265 | PEK  | C32-C33-C34-C35 |
| 23  | C     | 3264 | PEK  | C5-C6-C7-C8     |
| 23  | C     | 3264 | PEK  | C9-C10-C11-C12  |
| 23  | P     | 4264 | PEK  | C5-C6-C7-C8     |
| 23  | P     | 4264 | PEK  | C9-C10-C11-C12  |
| 25  | E     | 3230 | PSC  | C9-C10-C11-C12  |
| 25  | O     | 4230 | PSC  | C9-C10-C11-C12  |
| 27  | Z     | 4526 | DMU  | C28-C31-C34-C37 |
| 23  | G     | 4263 | PEK  | C21-C22-C23-C24 |
| 25  | E     | 3230 | PSC  | C4-C5-C6-C7     |
| 18  | A     | 3521 | TGL  | CC5-CC6-CC7-CC8 |
| 19  | N     | 4266 | PGV  | C4-C5-C6-C7     |
| 25  | E     | 3230 | PSC  | C14-C15-C16-C17 |
| 23  | T     | 3263 | PEK  | C21-C22-C23-C24 |
| 19  | N     | 4524 | PGV  | C26-C27-C28-C29 |
| 23  | C     | 3265 | PEK  | C32-C33-C34-C35 |
| 19  | P     | 4267 | PGV  | C30-C31-C32-C33 |
| 19  | A     | 3524 | PGV  | C26-C27-C28-C29 |
| 18  | A     | 3522 | TGL  | CC7-CC8-CC9-C15 |
| 22  | C     | 3270 | CDL  | C39-C40-C41-C42 |
| 22  | G     | 3269 | CDL  | C43-C44-C45-C46 |
| 25  | O     | 4230 | PSC  | C04-C05-N-C08   |
| 25  | O     | 4230 | PSC  | C15-C16-C17-C18 |
| 25  | O     | 4230 | PSC  | C14-C15-C16-C17 |
| 18  | N     | 4522 | TGL  | CC7-CC8-CC9-C15 |
| 19  | P     | 4268 | PGV  | C11-C10-C9-C8   |
| 23  | G     | 4263 | PEK  | C2-C3-C4-C5     |
| 25  | E     | 3230 | PSC  | C15-C16-C17-C18 |
| 22  | C     | 3270 | CDL  | OB5-CB3-CB4-CB6 |
| 22  | P     | 4270 | CDL  | OB5-CB3-CB4-CB6 |
| 22  | T     | 4269 | CDL  | C43-C44-C45-C46 |
| 22  | P     | 4270 | CDL  | C56-C57-C58-C59 |
| 23  | C     | 3265 | PEK  | C22-C23-C24-C25 |
| 23  | P     | 4264 | PEK  | C26-C27-C28-C29 |
| 23  | C     | 3264 | PEK  | C26-C27-C28-C29 |
| 22  | C     | 3270 | CDL  | C56-C57-C58-C59 |
| 22  | G     | 3269 | CDL  | C21-C22-C23-C24 |
| 19  | P     | 4267 | PGV  | C31-C32-C33-C34 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | O     | 4230 | PSC  | C03-C02-O01-C1  |
| 19  | C     | 3268 | PGV  | C11-C10-C9-C8   |
| 23  | G     | 4263 | PEK  | C28-C29-C30-C31 |
| 19  | C     | 3267 | PGV  | C31-C32-C33-C34 |
| 22  | T     | 4269 | CDL  | C21-C22-C23-C24 |
| 18  | N     | 4521 | TGL  | CC5-CC6-CC7-CC8 |
| 22  | G     | 3269 | CDL  | CB3-CB4-CB6-OB8 |
| 25  | E     | 3230 | PSC  | O03-C01-C02-C03 |
| 25  | O     | 4230 | PSC  | O03-C01-C02-C03 |
| 19  | C     | 3267 | PGV  | C30-C31-C32-C33 |
| 19  | N     | 4266 | PGV  | C30-C31-C32-C33 |
| 23  | T     | 3263 | PEK  | C28-C29-C30-C31 |
| 22  | C     | 3270 | CDL  | OA6-CA4-CA6-OA8 |
| 22  | G     | 3269 | CDL  | OA6-CA4-CA6-OA8 |
| 22  | P     | 4270 | CDL  | OA6-CA4-CA6-OA8 |
| 22  | T     | 4269 | CDL  | OA6-CA4-CA6-OA8 |
| 23  | G     | 4263 | PEK  | O03-C01-C02-O01 |
| 23  | T     | 3263 | PEK  | O03-C01-C02-O01 |
| 25  | E     | 3230 | PSC  | O03-C01-C02-O01 |
| 25  | O     | 4230 | PSC  | O03-C01-C02-O01 |
| 19  | C     | 3267 | PGV  | C23-C24-C25-C26 |
| 22  | C     | 3270 | CDL  | C38-C39-C40-C41 |
| 25  | O     | 4230 | PSC  | C04-C05-N-C07   |
| 19  | A     | 3266 | PGV  | C30-C31-C32-C33 |
| 23  | P     | 4265 | PEK  | C22-C23-C24-C25 |
| 18  | A     | 3523 | TGL  | C18-C19-C33-C34 |
| 25  | O     | 4230 | PSC  | C27-C28-C29-C30 |
| 22  | G     | 3269 | CDL  | C54-C55-C56-C57 |
| 25  | E     | 3230 | PSC  | C04-C05-N-C07   |
| 22  | P     | 4270 | CDL  | C38-C39-C40-C41 |
| 19  | C     | 3268 | PGV  | C01-C02-C03-O11 |
| 18  | N     | 4522 | TGL  | C25-C26-C27-C28 |
| 18  | A     | 3522 | TGL  | CB2-CB1-OG2-CG2 |
| 27  | M     | 3526 | DMU  | C28-C31-C34-C37 |
| 18  | Q     | 4523 | TGL  | C18-C19-C33-C34 |
| 18  | A     | 3522 | TGL  | C25-C26-C27-C28 |
| 25  | E     | 3230 | PSC  | C27-C28-C29-C30 |
| 22  | T     | 4269 | CDL  | C54-C55-C56-C57 |
| 18  | A     | 3522 | TGL  | OB1-CB1-OG2-CG2 |
| 19  | N     | 4524 | PGV  | O01-C02-C03-O11 |
| 22  | C     | 3270 | CDL  | OB5-CB3-CB4-OB6 |
| 22  | P     | 4270 | CDL  | OB5-CB3-CB4-OB6 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | T     | 3263 | PEK  | C2-C3-C4-C5     |
| 25  | E     | 3230 | PSC  | C04-C05-N-C08   |
| 19  | P     | 4267 | PGV  | C23-C24-C25-C26 |
| 23  | C     | 3264 | PEK  | O03-C01-C02-O01 |
| 23  | C     | 3265 | PEK  | O03-C01-C02-O01 |
| 23  | P     | 4264 | PEK  | O03-C01-C02-O01 |
| 23  | P     | 4265 | PEK  | O03-C01-C02-O01 |
| 22  | T     | 4269 | CDL  | CB3-CB4-CB6-OB8 |
| 23  | C     | 3265 | PEK  | C17-C18-C19-C20 |
| 23  | C     | 3264 | PEK  | C17-C18-C19-C20 |
| 22  | C     | 3270 | CDL  | C34-C35-C36-C37 |
| 18  | N     | 4522 | TGL  | OB1-CB1-OG2-CG2 |
| 23  | P     | 4265 | PEK  | C17-C18-C19-C20 |
| 19  | A     | 3524 | PGV  | C03-O11-P-O14   |
| 19  | N     | 4524 | PGV  | C03-O11-P-O14   |
| 22  | C     | 3270 | CDL  | CA3-OA5-PA1-OA3 |
| 22  | C     | 3270 | CDL  | CB2-OB2-PB2-OB3 |
| 22  | C     | 3270 | CDL  | CB2-OB2-PB2-OB5 |
| 22  | G     | 3269 | CDL  | CA2-OA2-PA1-OA4 |
| 22  | G     | 3269 | CDL  | CA2-OA2-PA1-OA5 |
| 22  | P     | 4270 | CDL  | CA3-OA5-PA1-OA3 |
| 22  | P     | 4270 | CDL  | CB2-OB2-PB2-OB3 |
| 22  | P     | 4270 | CDL  | CB2-OB2-PB2-OB5 |
| 22  | T     | 4269 | CDL  | CA2-OA2-PA1-OA4 |
| 22  | T     | 4269 | CDL  | CA2-OA2-PA1-OA5 |
| 23  | G     | 4263 | PEK  | C04-O12-P-O11   |
| 23  | G     | 4263 | PEK  | C04-O12-P-O14   |
| 23  | T     | 3263 | PEK  | C04-O12-P-O11   |
| 23  | T     | 3263 | PEK  | C04-O12-P-O14   |
| 25  | E     | 3230 | PSC  | C04-O12-P-O11   |
| 25  | E     | 3230 | PSC  | C04-O12-P-O13   |
| 25  | O     | 4230 | PSC  | C04-O12-P-O11   |
| 25  | O     | 4230 | PSC  | C04-O12-P-O13   |
| 25  | O     | 4230 | PSC  | C04-C05-N-C06   |
| 23  | G     | 4263 | PEK  | C14-C15-C16-C17 |
| 19  | C     | 3267 | PGV  | C02-C03-O11-P   |
| 19  | P     | 4267 | PGV  | C02-C03-O11-P   |
| 22  | C     | 3270 | CDL  | C1-CA2-OA2-PA1  |
| 22  | P     | 4270 | CDL  | C1-CA2-OA2-PA1  |
| 22  | P     | 4270 | CDL  | C31-C32-C33-C34 |
| 19  | N     | 4266 | PGV  | C25-C26-C27-C28 |
| 22  | P     | 4270 | CDL  | C34-C35-C36-C37 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | P     | 4264 | PEK  | C17-C18-C19-C20 |
| 23  | T     | 3263 | PEK  | C14-C15-C16-C17 |
| 25  | E     | 3230 | PSC  | C03-C02-O01-C1  |
| 19  | A     | 3266 | PGV  | C25-C26-C27-C28 |
| 25  | E     | 3230 | PSC  | C04-C05-N-C06   |
| 19  | P     | 4268 | PGV  | C01-C02-C03-O11 |
| 22  | C     | 3270 | CDL  | C31-C32-C33-C34 |
| 18  | N     | 4522 | TGL  | CB4-CB5-CB6-CB7 |
| 19  | C     | 3267 | PGV  | C20-C21-C22-C23 |
| 22  | G     | 3269 | CDL  | C84-C85-C86-C87 |
| 19  | P     | 4267 | PGV  | C20-C21-C22-C23 |
| 18  | N     | 4522 | TGL  | CB2-CB1-OG2-CG2 |
| 19  | P     | 4268 | PGV  | C3-C4-C5-C6     |
| 23  | G     | 4263 | PEK  | C33-C34-C35-C36 |
| 19  | P     | 4268 | PGV  | C4-C5-C6-C7     |
| 23  | T     | 3263 | PEK  | C33-C34-C35-C36 |
| 18  | A     | 3522 | TGL  | CB4-CB5-CB6-CB7 |
| 18  | N     | 4522 | TGL  | C13-C14-C29-C30 |
| 22  | P     | 4270 | CDL  | C42-C43-C44-C45 |
| 23  | T     | 3263 | PEK  | C24-C25-C26-C27 |
| 18  | N     | 4521 | TGL  | C21-C22-C23-C24 |
| 18  | A     | 3522 | TGL  | C13-C14-C29-C30 |
| 22  | P     | 4270 | CDL  | C44-C45-C46-C47 |
| 18  | Q     | 4523 | TGL  | CB9-C10-C11-C12 |
| 22  | C     | 3270 | CDL  | C44-C45-C46-C47 |
| 18  | A     | 3523 | TGL  | C15-C16-C17-C18 |
| 19  | A     | 3266 | PGV  | C9-C10-C11-C12  |
| 19  | N     | 4266 | PGV  | C9-C10-C11-C12  |
| 23  | P     | 4264 | PEK  | C3-C4-C5-C6     |
| 23  | P     | 4264 | PEK  | C25-C26-C27-C28 |
| 22  | T     | 4269 | CDL  | C84-C85-C86-C87 |
| 23  | T     | 3263 | PEK  | C35-C36-C37-C38 |
| 19  | C     | 3268 | PGV  | C3-C4-C5-C6     |
| 23  | C     | 3264 | PEK  | C25-C26-C27-C28 |
| 22  | C     | 3270 | CDL  | C42-C43-C44-C45 |
| 23  | P     | 4264 | PEK  | C31-C32-C33-C34 |
| 23  | C     | 3264 | PEK  | C3-C4-C5-C6     |
| 18  | A     | 3521 | TGL  | C21-C22-C23-C24 |
| 18  | Q     | 4523 | TGL  | C15-C16-C17-C18 |
| 23  | T     | 3263 | PEK  | C32-C33-C34-C35 |
| 18  | Q     | 4523 | TGL  | C33-C34-C35-C36 |
| 23  | G     | 4263 | PEK  | C24-C25-C26-C27 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | C     | 3264 | PEK  | C31-C32-C33-C34 |
| 19  | A     | 3524 | PGV  | C21-C22-C23-C24 |
| 23  | G     | 4263 | PEK  | C32-C33-C34-C35 |
| 21  | O     | 3085 | CHD  | C22-C23-C24-O25 |
| 18  | A     | 3523 | TGL  | C33-C34-C35-C36 |
| 21  | B     | 4085 | CHD  | C22-C23-C24-O25 |
| 21  | C     | 3271 | CHD  | C22-C23-C24-O26 |
| 21  | J     | 3060 | CHD  | C22-C23-C24-O25 |
| 18  | N     | 4521 | TGL  | CB1-CB2-CB3-CB4 |
| 21  | P     | 4271 | CHD  | C22-C23-C24-O26 |
| 21  | W     | 4060 | CHD  | C22-C23-C24-O25 |
| 22  | T     | 4269 | CDL  | C32-C33-C34-C35 |
| 17  | N     | 516  | HEA  | CAA-CBA-CGA-O1A |
| 21  | C     | 3271 | CHD  | C22-C23-C24-O25 |
| 23  | C     | 3265 | PEK  | C3-C4-C5-C6     |
| 19  | C     | 3268 | PGV  | C4-C5-C6-C7     |
| 19  | C     | 3267 | PGV  | C05-C04-O12-P   |
| 17  | A     | 515  | HEA  | CAD-CBD-CGD-O1D |
| 21  | P     | 4271 | CHD  | C22-C23-C24-O25 |
| 23  | G     | 4263 | PEK  | C35-C36-C37-C38 |
| 23  | P     | 4264 | PEK  | C28-C29-C30-C31 |
| 19  | N     | 4524 | PGV  | C21-C22-C23-C24 |
| 22  | P     | 4270 | CDL  | C54-C55-C56-C57 |
| 17  | N     | 515  | HEA  | CAD-CBD-CGD-O1D |
| 17  | A     | 516  | HEA  | CAA-CBA-CGA-O1A |
| 22  | G     | 3269 | CDL  | C32-C33-C34-C35 |
| 23  | G     | 4263 | PEK  | C6-C7-C8-C9     |
| 23  | T     | 3263 | PEK  | C6-C7-C8-C9     |
| 19  | C     | 3268 | PGV  | C28-C29-C30-C31 |
| 19  | P     | 4268 | PGV  | C28-C29-C30-C31 |
| 18  | A     | 3523 | TGL  | CB9-C10-C11-C12 |
| 23  | C     | 3265 | PEK  | C26-C27-C28-C29 |
| 18  | Q     | 4523 | TGL  | C11-C10-CB9-CB8 |
| 22  | P     | 4270 | CDL  | C43-C44-C45-C46 |
| 17  | N     | 516  | HEA  | CAA-CBA-CGA-O2A |
| 22  | P     | 4270 | CDL  | C33-C34-C35-C36 |
| 22  | C     | 3270 | CDL  | C54-C55-C56-C57 |
| 18  | A     | 3522 | TGL  | OG1-CA1-CA2-CA3 |
| 19  | A     | 3266 | PGV  | O03-C19-C20-C21 |
| 22  | C     | 3270 | CDL  | C33-C34-C35-C36 |
| 17  | A     | 516  | HEA  | CAA-CBA-CGA-O2A |
| 22  | C     | 3270 | CDL  | C43-C44-C45-C46 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | P     | 4265 | PEK  | C26-C27-C28-C29 |
| 18  | A     | 3523 | TGL  | OG1-CA1-CA2-CA3 |
| 19  | P     | 4268 | PGV  | C22-C23-C24-C25 |
| 21  | W     | 4060 | CHD  | C22-C23-C24-O26 |
| 19  | C     | 3267 | PGV  | C11-C12-C13-C14 |
| 23  | P     | 4265 | PEK  | C3-C4-C5-C6     |
| 18  | N     | 4522 | TGL  | OG1-CA1-CA2-CA3 |
| 21  | B     | 4085 | CHD  | C22-C23-C24-O26 |
| 21  | J     | 3060 | CHD  | C22-C23-C24-O26 |
| 25  | O     | 4230 | PSC  | C31-C32-C33-C34 |
| 18  | Q     | 4523 | TGL  | OG1-CA1-CA2-CA3 |
| 19  | N     | 4266 | PGV  | O03-C19-C20-C21 |
| 21  | O     | 3085 | CHD  | C22-C23-C24-O26 |
| 22  | C     | 3270 | CDL  | C76-C77-C78-C79 |
| 19  | C     | 3268 | PGV  | C22-C23-C24-C25 |
| 22  | P     | 4270 | CDL  | C76-C77-C78-C79 |
| 19  | P     | 4267 | PGV  | C11-C12-C13-C14 |
| 23  | T     | 3263 | PEK  | C3-C4-C5-C6     |
| 19  | P     | 4267 | PGV  | C05-C04-O12-P   |
| 19  | C     | 3267 | PGV  | C29-C30-C31-C32 |
| 19  | C     | 3268 | PGV  | C31-C32-C33-C34 |
| 17  | A     | 515  | HEA  | CAD-CBD-CGD-O2D |
| 17  | N     | 515  | HEA  | CAD-CBD-CGD-O2D |
| 23  | C     | 3264 | PEK  | C27-C28-C29-C30 |
| 23  | C     | 3264 | PEK  | C28-C29-C30-C31 |
| 22  | T     | 4269 | CDL  | C53-C54-C55-C56 |
| 22  | P     | 4270 | CDL  | C15-C16-C17-C18 |
| 17  | A     | 516  | HEA  | CAD-CBD-CGD-O2D |
| 19  | C     | 3267 | PGV  | C9-C10-C11-C12  |
| 19  | N     | 4266 | PGV  | C11-C12-C13-C14 |
| 25  | E     | 3230 | PSC  | C31-C32-C33-C34 |
| 19  | P     | 4268 | PGV  | C31-C32-C33-C34 |
| 18  | N     | 4522 | TGL  | OG2-CB1-CB2-CB3 |
| 23  | G     | 4263 | PEK  | C3-C4-C5-C6     |
| 17  | N     | 516  | HEA  | CAD-CBD-CGD-O2D |
| 21  | C     | 3525 | CHD  | C22-C23-C24-O26 |
| 21  | P     | 4525 | CHD  | C22-C23-C24-O26 |
| 17  | A     | 516  | HEA  | CAD-CBD-CGD-O1D |
| 19  | C     | 3268 | PGV  | C9-C10-C11-C12  |
| 17  | N     | 516  | HEA  | CAD-CBD-CGD-O1D |
| 19  | P     | 4267 | PGV  | C29-C30-C31-C32 |
| 18  | A     | 3522 | TGL  | OG2-CB1-CB2-CB3 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | C     | 3270 | CDL  | C15-C16-C17-C18 |
| 23  | P     | 4264 | PEK  | C27-C28-C29-C30 |
| 17  | N     | 516  | HEA  | C26-C15-C16-C17 |
| 21  | P     | 4525 | CHD  | C22-C23-C24-O25 |
| 21  | C     | 3525 | CHD  | C22-C23-C24-O25 |
| 19  | A     | 3266 | PGV  | C11-C12-C13-C14 |
| 19  | P     | 4267 | PGV  | C9-C10-C11-C12  |
| 19  | P     | 4268 | PGV  | C9-C10-C11-C12  |
| 25  | E     | 3230 | PSC  | C7-C8-C9-C10    |
| 25  | O     | 4230 | PSC  | C7-C8-C9-C10    |
| 19  | A     | 3524 | PGV  | O01-C1-C2-C3    |
| 25  | O     | 4230 | PSC  | O03-C19-C20-C21 |
| 22  | G     | 3269 | CDL  | C53-C54-C55-C56 |
| 18  | A     | 3523 | TGL  | OG3-CC1-CC2-CC3 |
| 19  | N     | 4524 | PGV  | O01-C1-C2-C3    |
| 18  | Q     | 4523 | TGL  | OG3-CC1-CC2-CC3 |
| 23  | C     | 3264 | PEK  | O01-C1-C2-C3    |
| 25  | E     | 3230 | PSC  | O03-C19-C20-C21 |
| 22  | G     | 3269 | CDL  | C78-C79-C80-C81 |
| 22  | G     | 3269 | CDL  | C11-C12-C13-C14 |
| 23  | P     | 4264 | PEK  | O01-C1-C2-C3    |
| 19  | A     | 3524 | PGV  | C3-C4-C5-C6     |
| 17  | A     | 516  | HEA  | C26-C15-C16-C17 |
| 19  | N     | 4524 | PGV  | C3-C4-C5-C6     |
| 23  | G     | 4263 | PEK  | C30-C31-C32-C33 |
| 22  | T     | 4269 | CDL  | C11-C12-C13-C14 |
| 18  | A     | 3521 | TGL  | CB1-CB2-CB3-CB4 |
| 27  | M     | 3526 | DMU  | C19-C18-O16-C6  |
| 22  | C     | 3270 | CDL  | C52-C51-CB5-OB6 |
| 23  | T     | 3263 | PEK  | C30-C31-C32-C33 |
| 18  | A     | 3523 | TGL  | OG2-CB1-CB2-CB3 |
| 18  | N     | 4521 | TGL  | OG3-CC1-CC2-CC3 |
| 18  | Q     | 4523 | TGL  | OG2-CB1-CB2-CB3 |
| 22  | P     | 4270 | CDL  | C52-C51-CB5-OB6 |
| 18  | A     | 3521 | TGL  | OG3-CC1-CC2-CC3 |
| 22  | C     | 3270 | CDL  | C12-C11-CA5-OA6 |
| 22  | P     | 4270 | CDL  | C12-C11-CA5-OA6 |
| 25  | O     | 4230 | PSC  | O01-C1-C2-C3    |
| 23  | C     | 3265 | PEK  | C24-C25-C26-C27 |
| 22  | T     | 4269 | CDL  | C78-C79-C80-C81 |
| 25  | E     | 3230 | PSC  | O01-C1-C2-C3    |
| 23  | T     | 3263 | PEK  | O01-C1-C2-C3    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | A     | 3523 | TGL  | C11-C10-CB9-CB8 |
| 23  | P     | 4265 | PEK  | C24-C25-C26-C27 |
| 19  | A     | 3524 | PGV  | O03-C19-C20-C21 |
| 23  | G     | 4263 | PEK  | O01-C1-C2-C3    |
| 25  | O     | 4230 | PSC  | O02-C1-C2-C3    |
| 25  | E     | 3230 | PSC  | O02-C1-C2-C3    |
| 22  | C     | 3270 | CDL  | C24-C25-C26-C27 |
| 22  | T     | 4269 | CDL  | C55-C56-C57-C58 |
| 19  | N     | 4524 | PGV  | O03-C19-C20-C21 |
| 23  | C     | 3264 | PEK  | O02-C1-C2-C3    |
| 25  | E     | 3230 | PSC  | O04-C19-C20-C21 |
| 19  | N     | 4524 | PGV  | C28-C29-C30-C31 |
| 19  | N     | 4524 | PGV  | O02-C1-C2-C3    |
| 22  | C     | 3270 | CDL  | C41-C42-C43-C44 |
| 18  | A     | 3523 | TGL  | OB1-CB1-CB2-CB3 |
| 25  | O     | 4230 | PSC  | O04-C19-C20-C21 |
| 22  | C     | 3270 | CDL  | C12-C11-CA5-OA7 |
| 25  | E     | 3230 | PSC  | C01-C02-C03-O11 |
| 25  | O     | 4230 | PSC  | C01-C02-C03-O11 |
| 23  | P     | 4264 | PEK  | O02-C1-C2-C3    |
| 22  | P     | 4270 | CDL  | C12-C11-CA5-OA7 |
| 22  | P     | 4270 | CDL  | C24-C25-C26-C27 |
| 25  | E     | 3230 | PSC  | C6-C7-C8-C9     |
| 18  | Q     | 4523 | TGL  | OB1-CB1-CB2-CB3 |
| 19  | A     | 3524 | PGV  | O02-C1-C2-C3    |
| 22  | P     | 4270 | CDL  | C52-C51-CB5-OB7 |

There are no ring outliers.

33 monomers are involved in 275 short contacts:

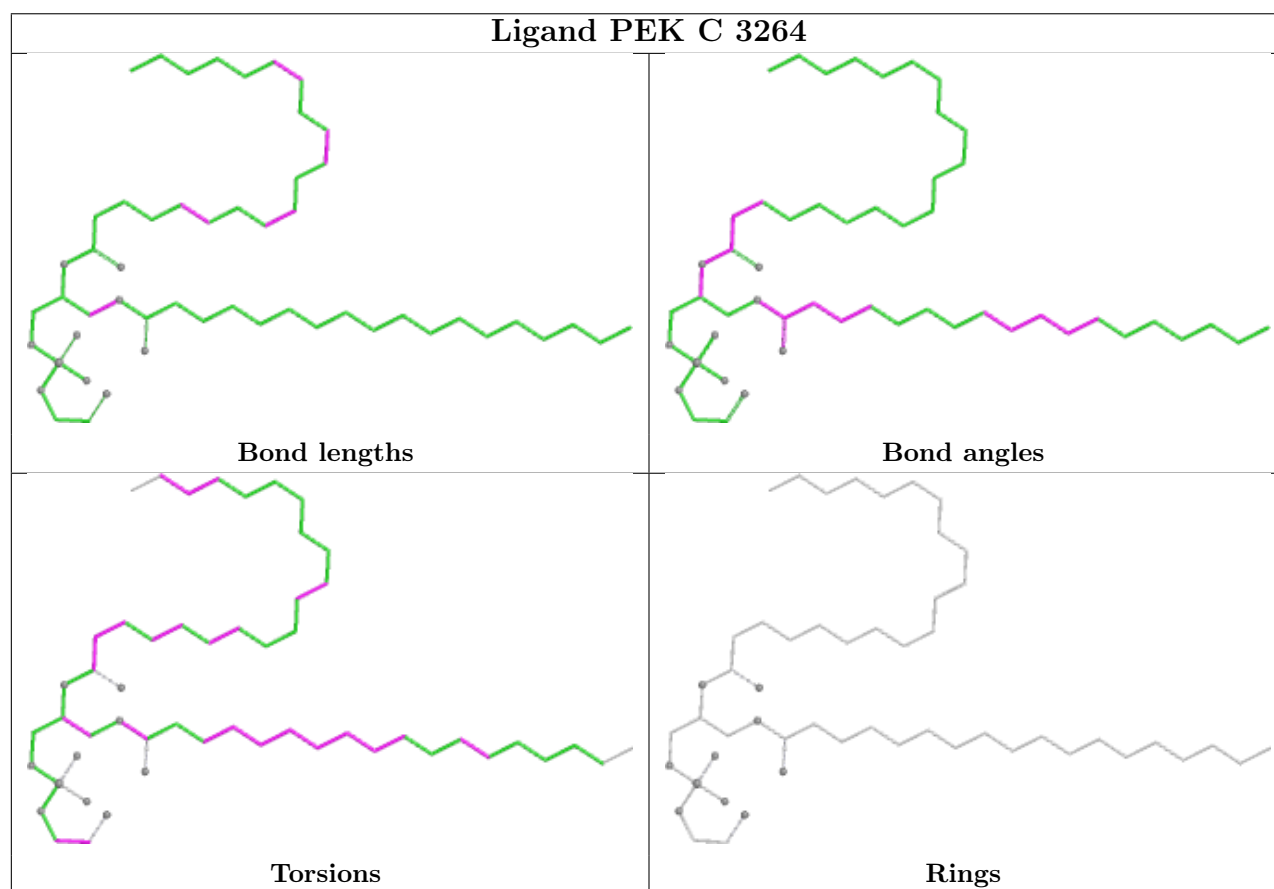
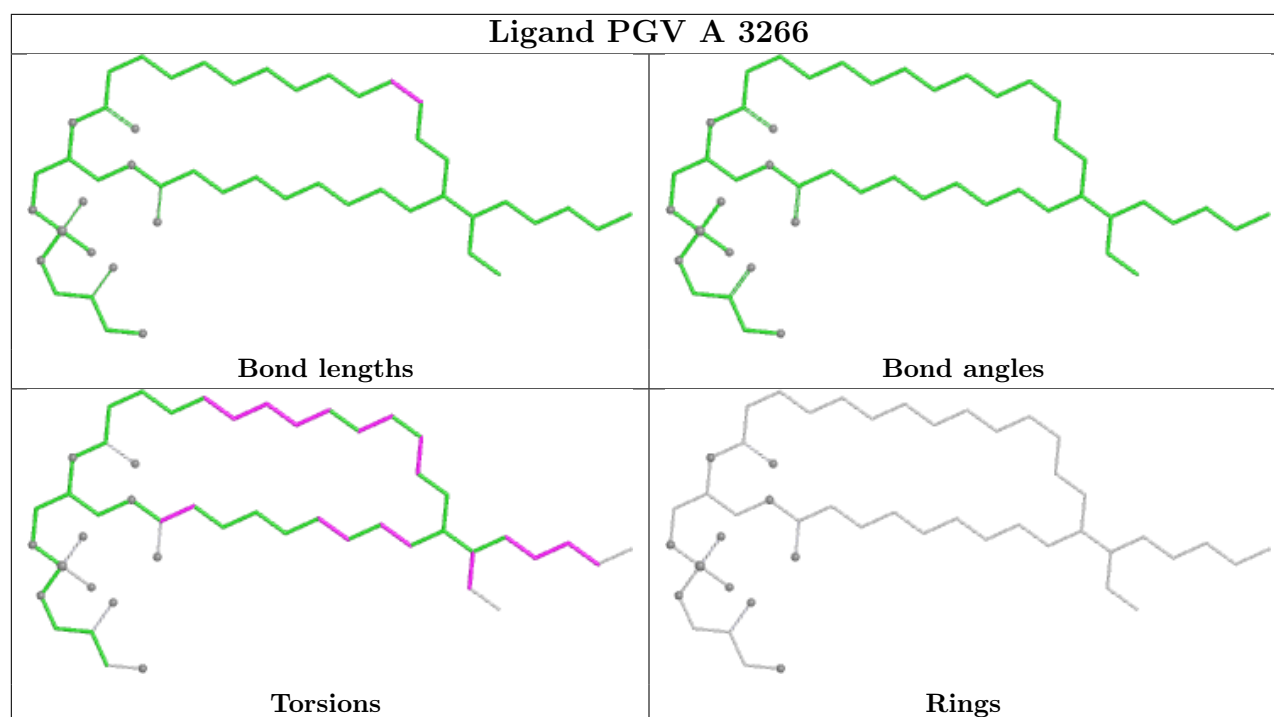
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 23  | C     | 3264 | PEK  | 4       | 0            |
| 22  | G     | 3269 | CDL  | 17      | 0            |
| 19  | N     | 4524 | PGV  | 6       | 0            |
| 22  | T     | 4269 | CDL  | 20      | 0            |
| 18  | A     | 3523 | TGL  | 6       | 0            |
| 25  | E     | 3230 | PSC  | 12      | 0            |
| 22  | P     | 4270 | CDL  | 20      | 0            |
| 18  | Q     | 4523 | TGL  | 6       | 0            |
| 17  | N     | 515  | HEA  | 2       | 0            |
| 23  | C     | 3265 | PEK  | 9       | 0            |
| 23  | G     | 4263 | PEK  | 6       | 0            |

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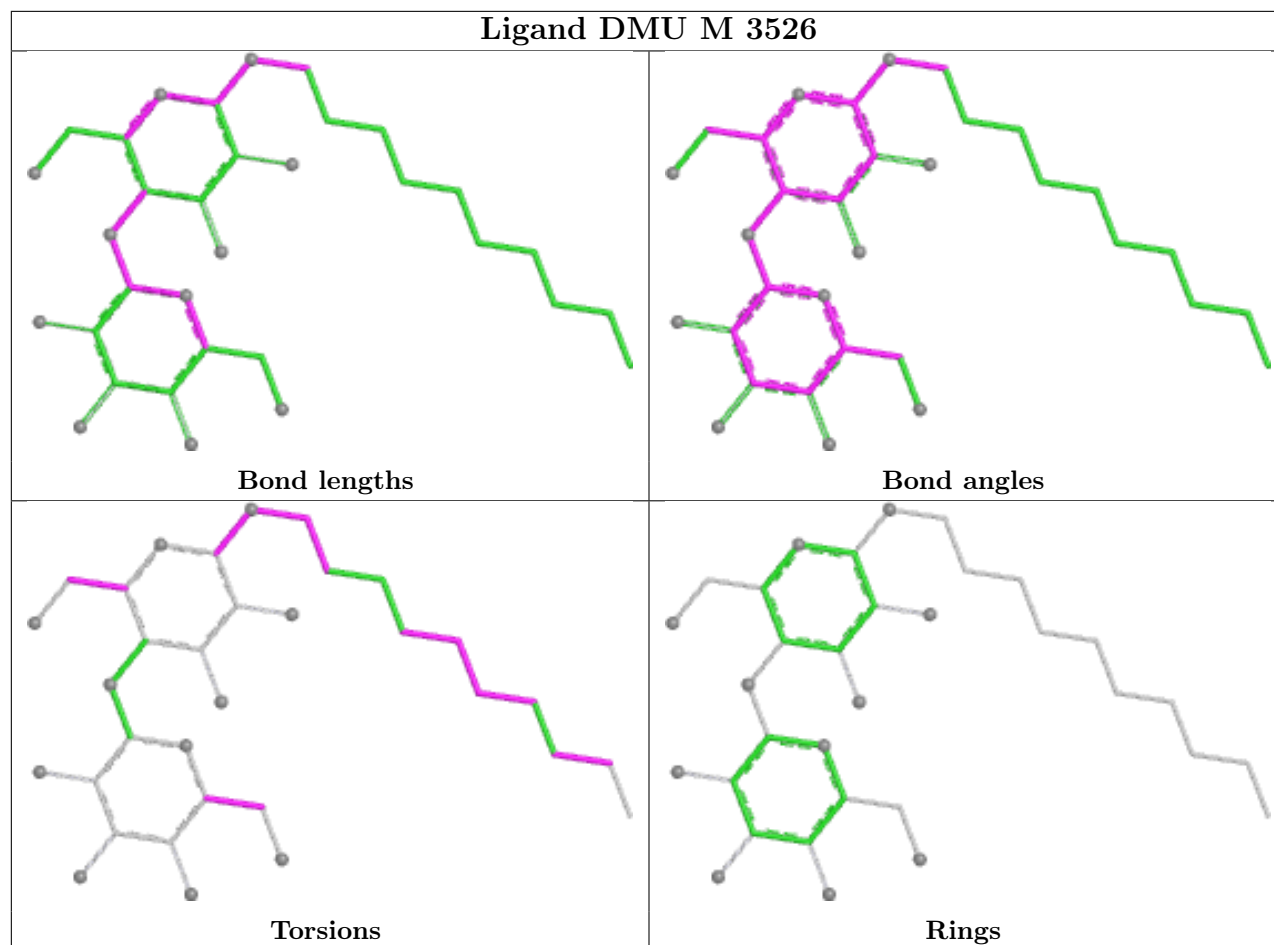
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 25  | O     | 4230 | PSC  | 11      | 0            |
| 18  | N     | 4522 | TGL  | 17      | 0            |
| 19  | C     | 3268 | PGV  | 3       | 0            |
| 21  | C     | 3271 | CHD  | 4       | 0            |
| 19  | A     | 3524 | PGV  | 7       | 0            |
| 18  | A     | 3522 | TGL  | 25      | 0            |
| 18  | A     | 3521 | TGL  | 16      | 0            |
| 17  | A     | 515  | HEA  | 2       | 0            |
| 19  | C     | 3267 | PGV  | 7       | 0            |
| 17  | A     | 516  | HEA  | 1       | 0            |
| 17  | N     | 516  | HEA  | 1       | 0            |
| 23  | P     | 4264 | PEK  | 4       | 0            |
| 19  | P     | 4267 | PGV  | 4       | 0            |
| 23  | P     | 4265 | PEK  | 4       | 0            |
| 19  | P     | 4268 | PGV  | 3       | 0            |
| 22  | C     | 3270 | CDL  | 23      | 0            |
| 23  | T     | 3263 | PEK  | 8       | 0            |
| 21  | P     | 4271 | CHD  | 2       | 0            |
| 21  | B     | 4085 | CHD  | 1       | 0            |
| 21  | J     | 3060 | CHD  | 3       | 0            |
| 18  | N     | 4521 | TGL  | 24      | 0            |
| 21  | W     | 4060 | CHD  | 3       | 0            |

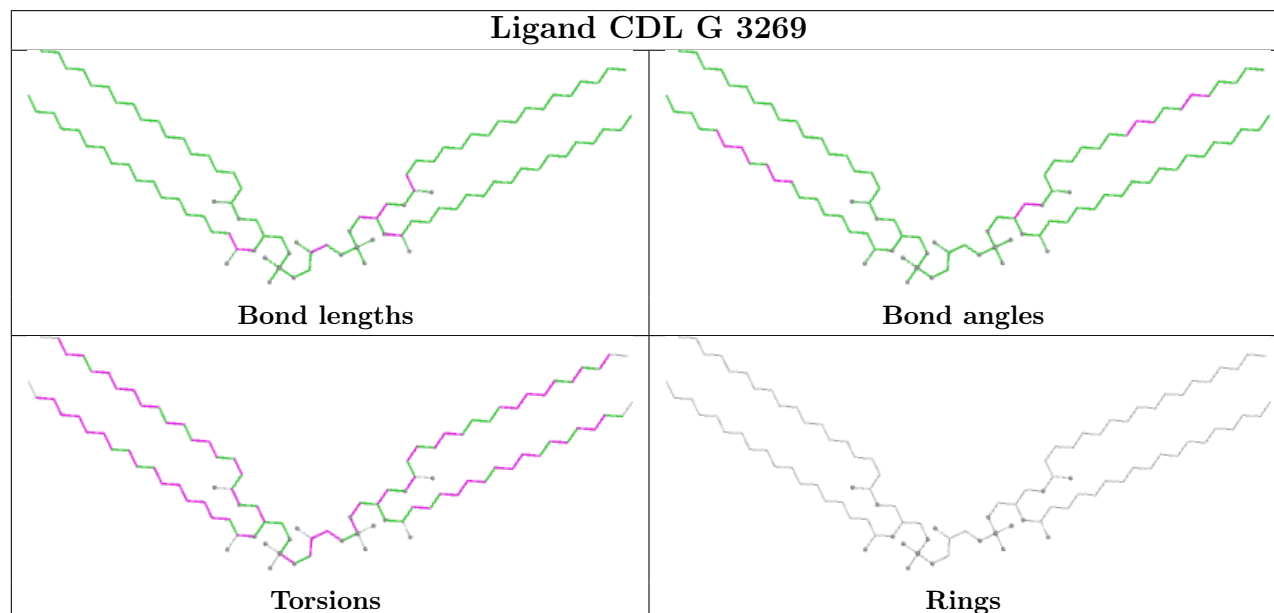
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

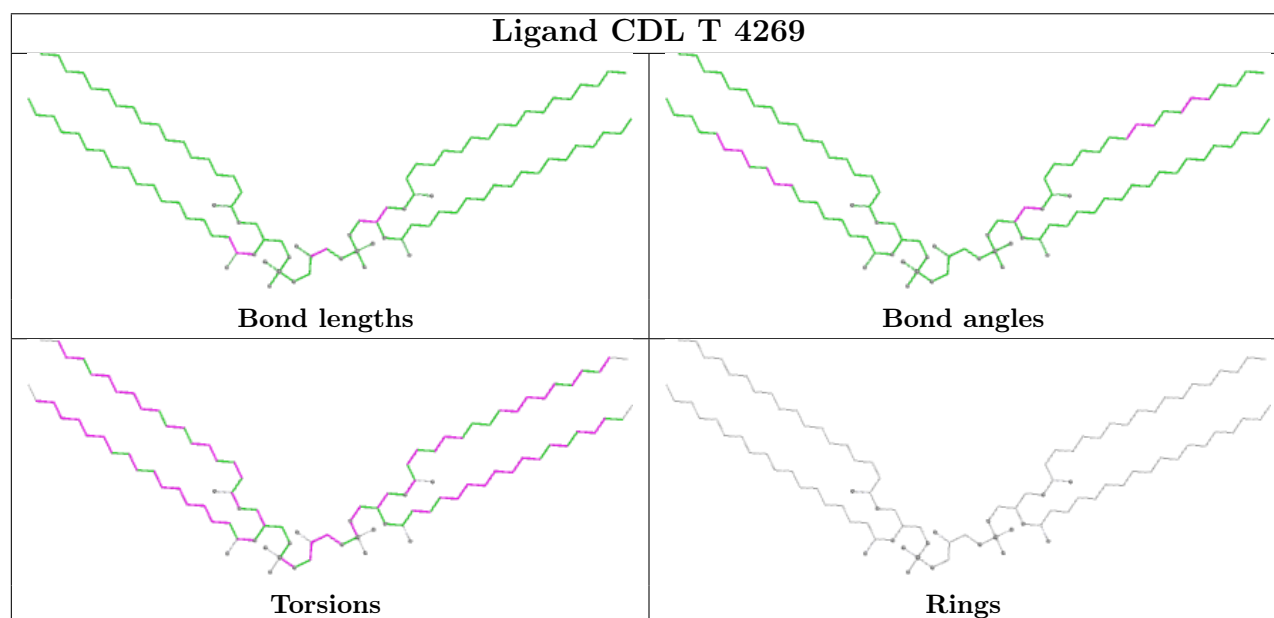
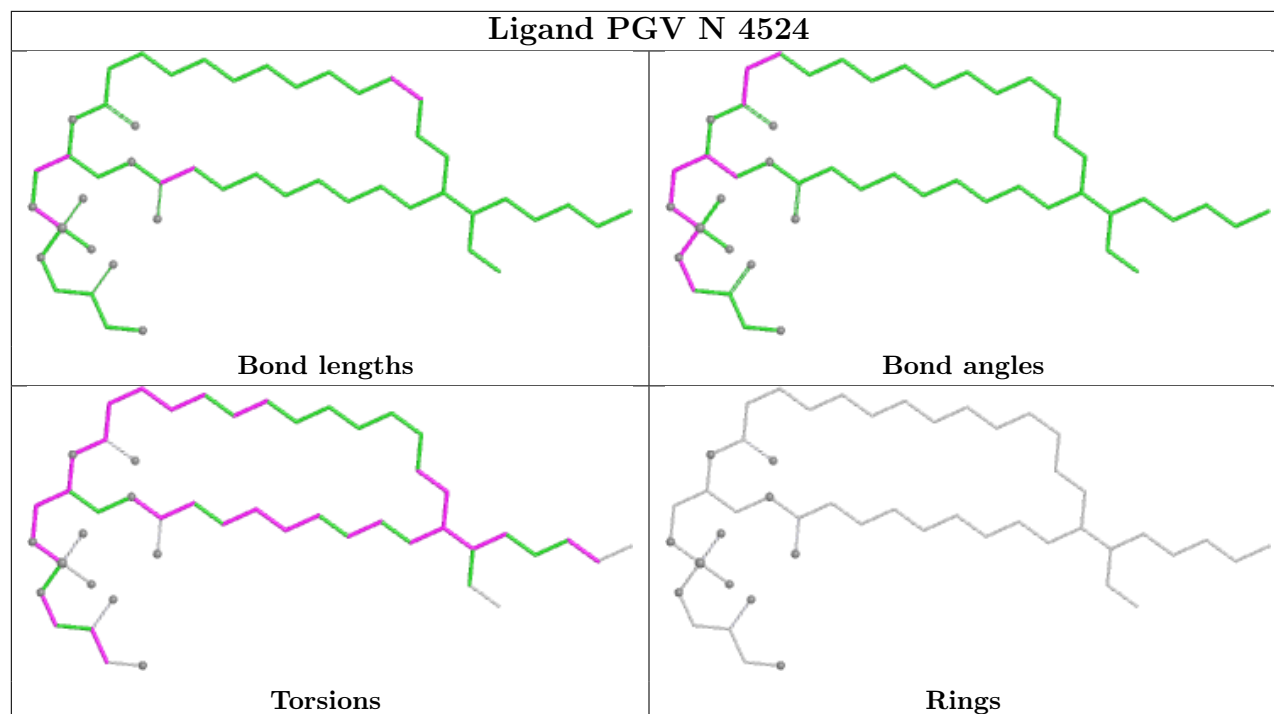


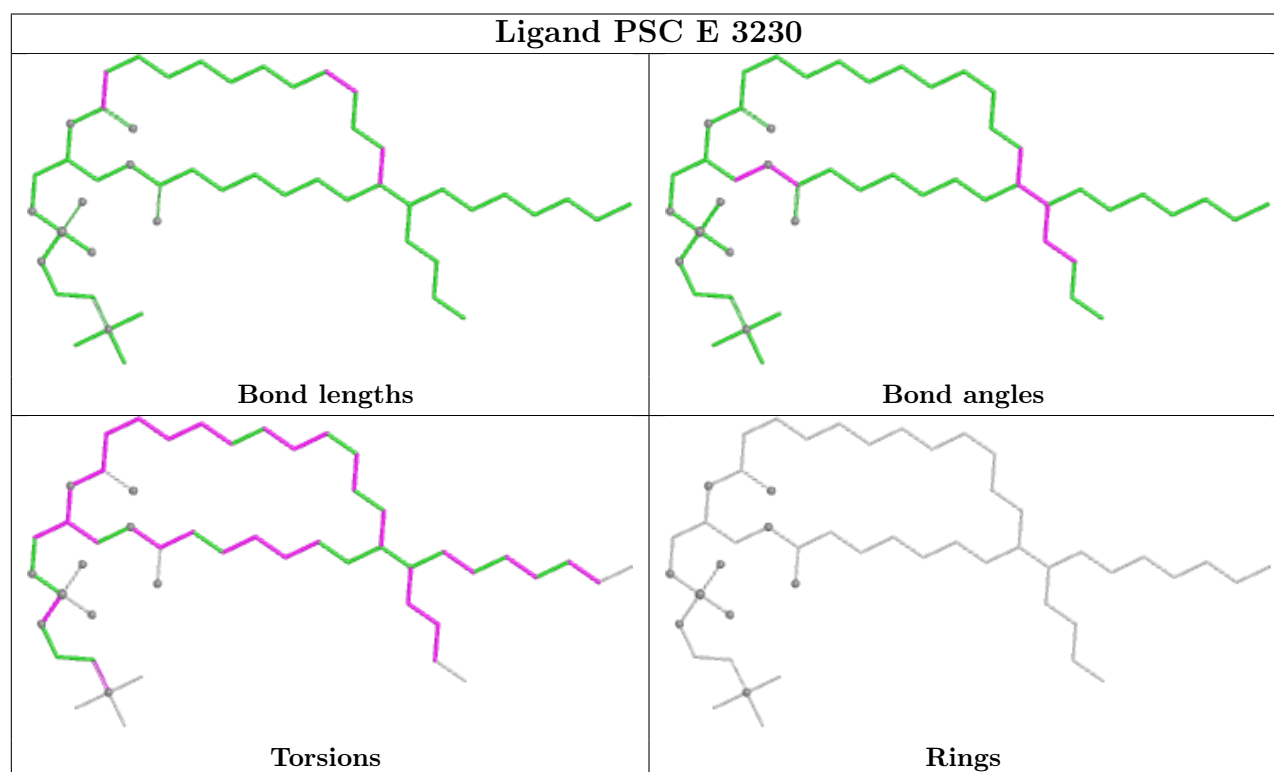
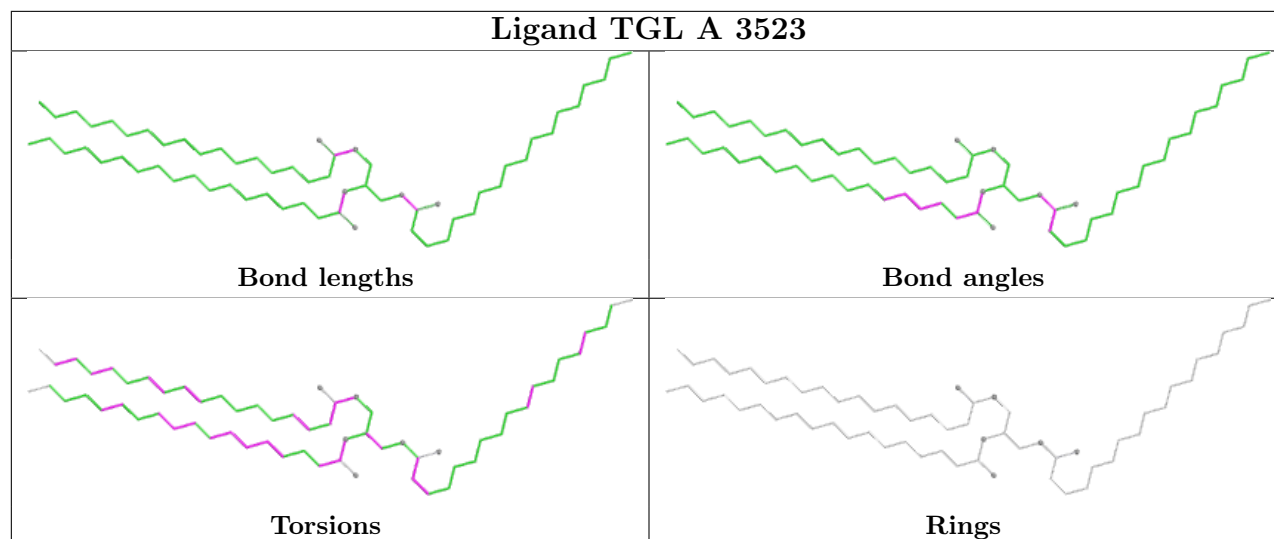
## Ligand DMU M 3526

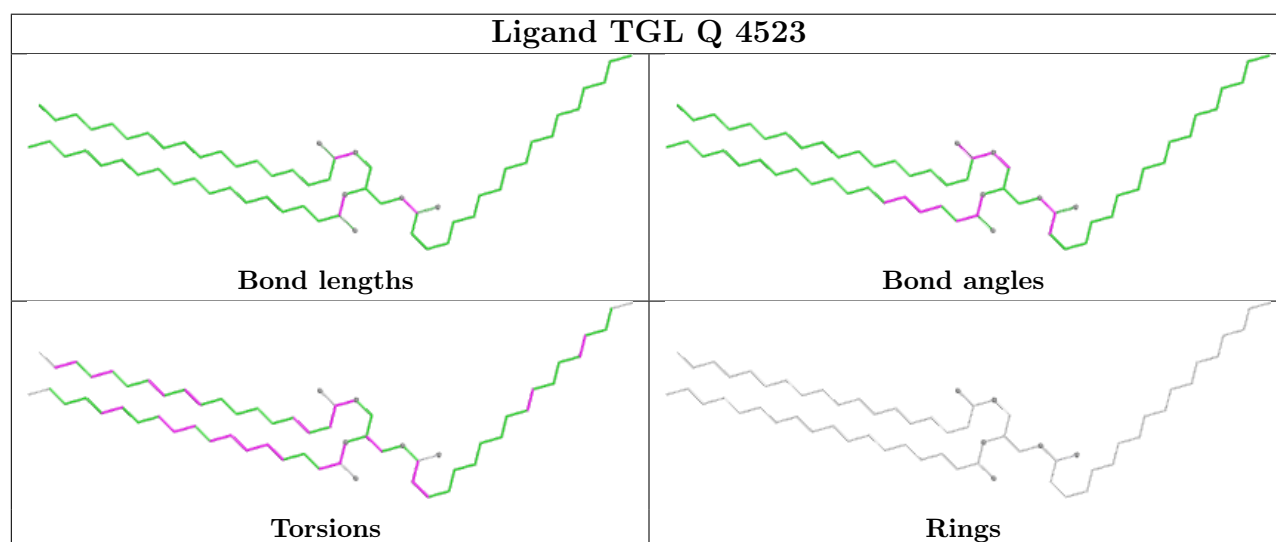
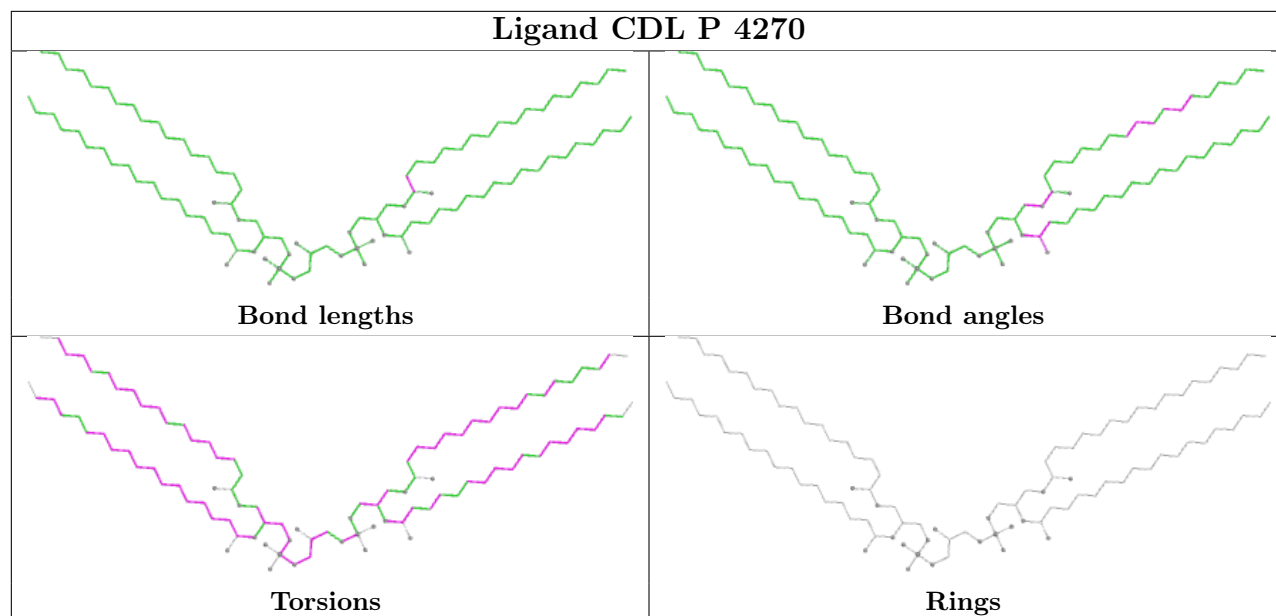


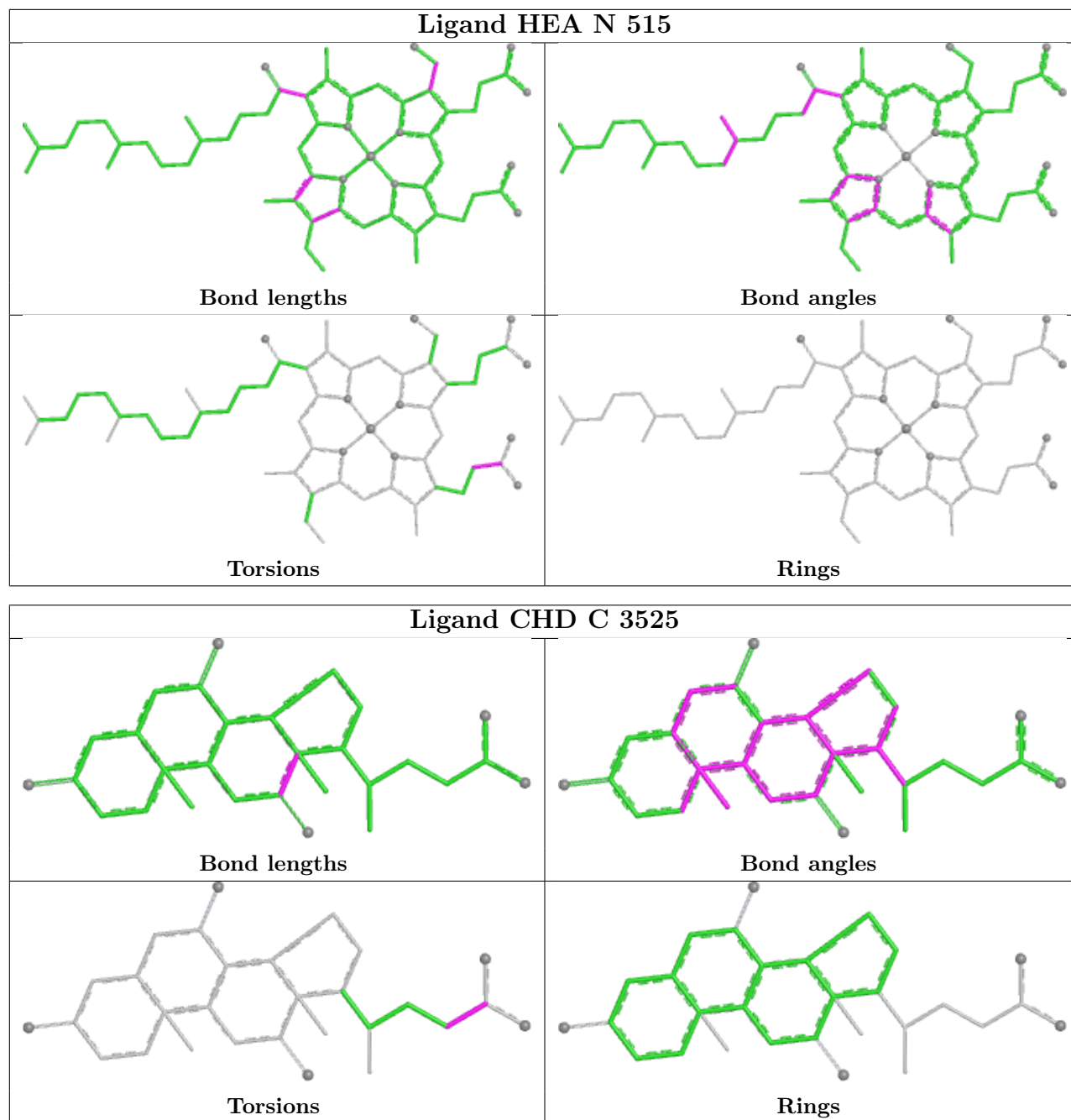
## Ligand CDL G 3269



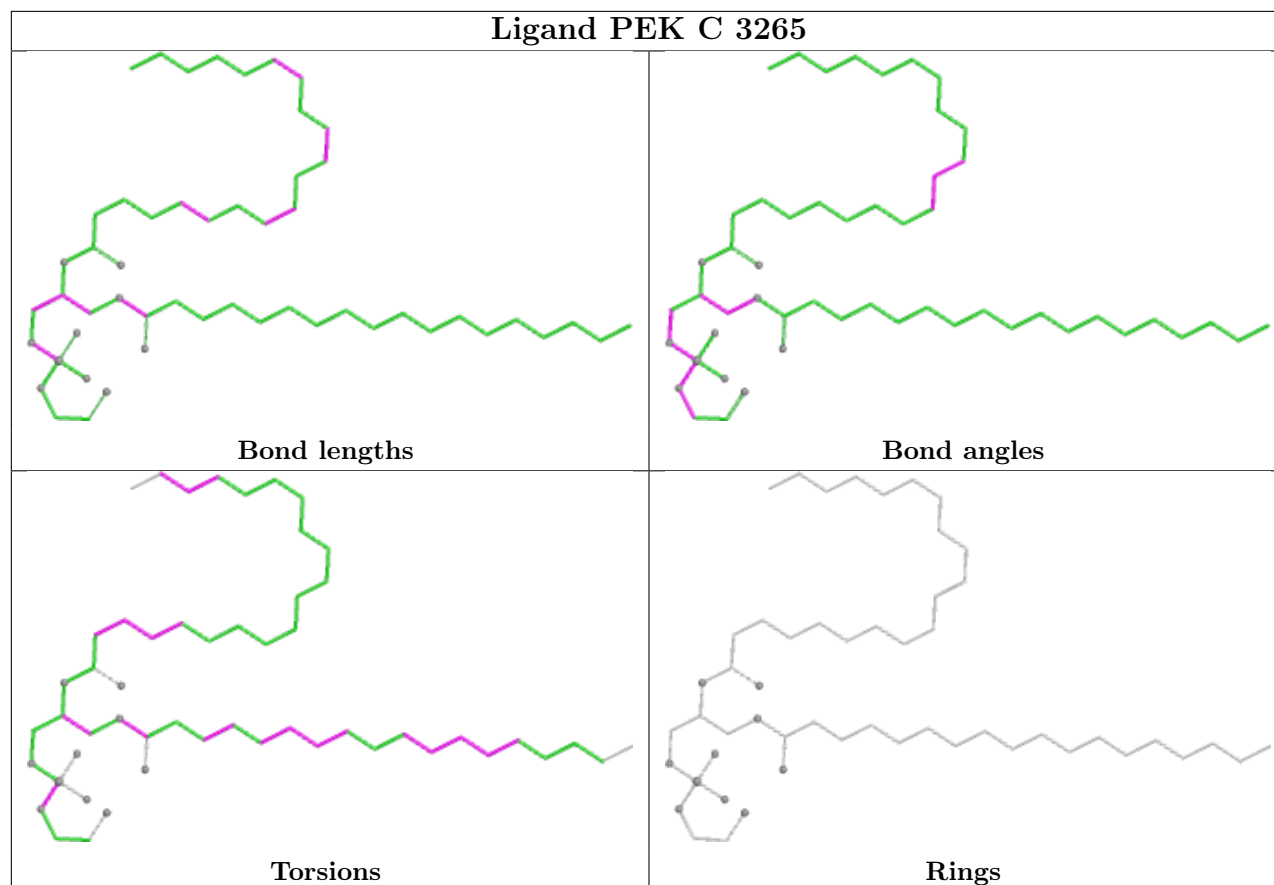




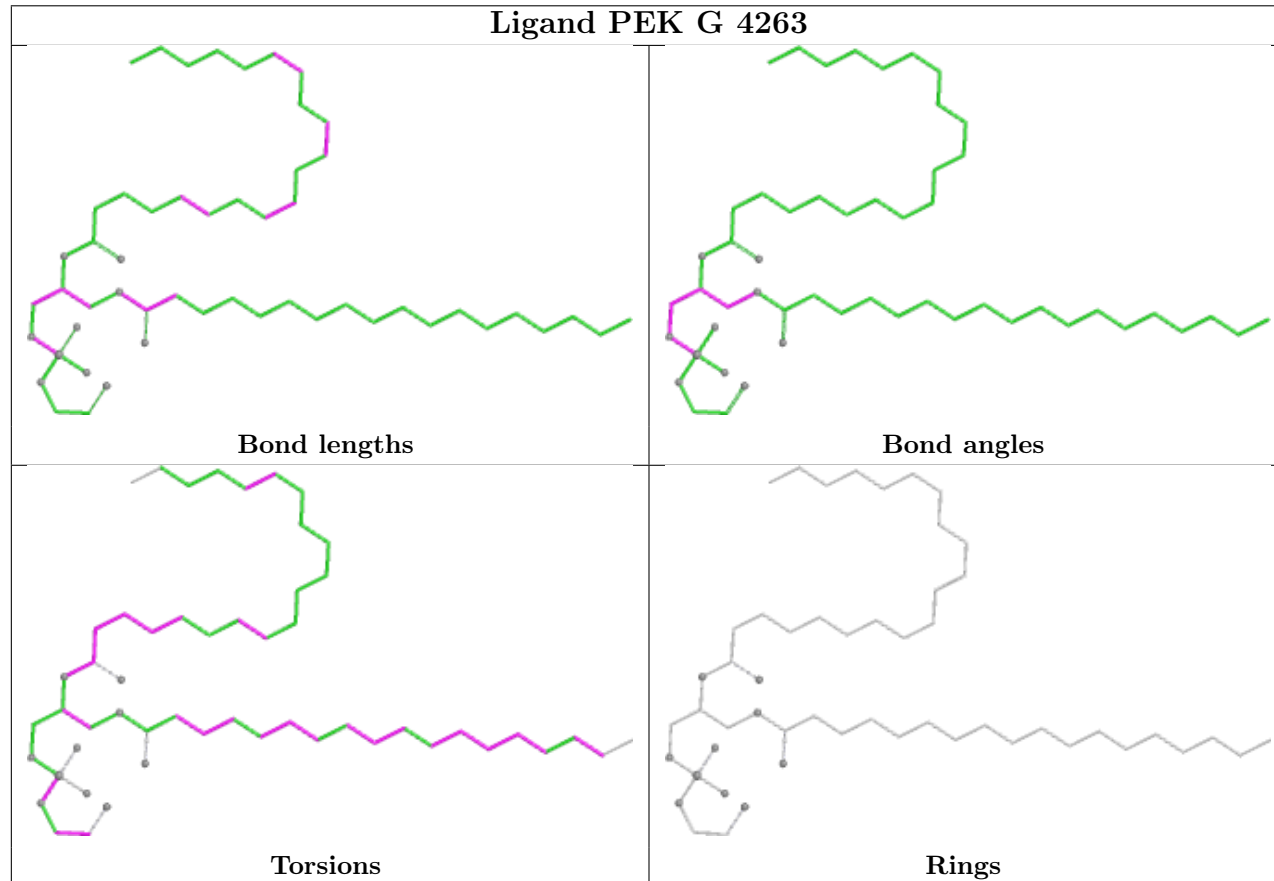




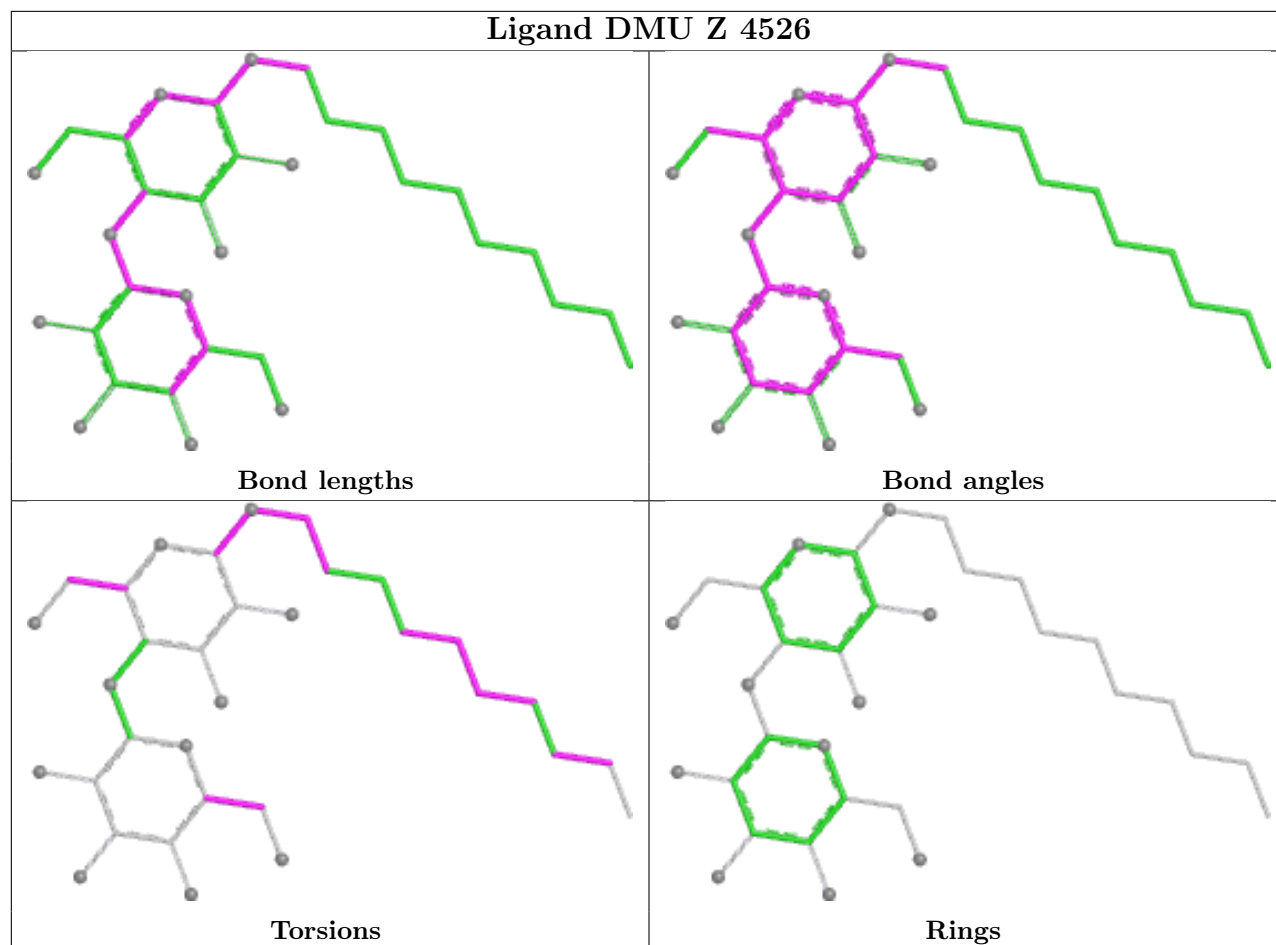
## Ligand PEK C 3265



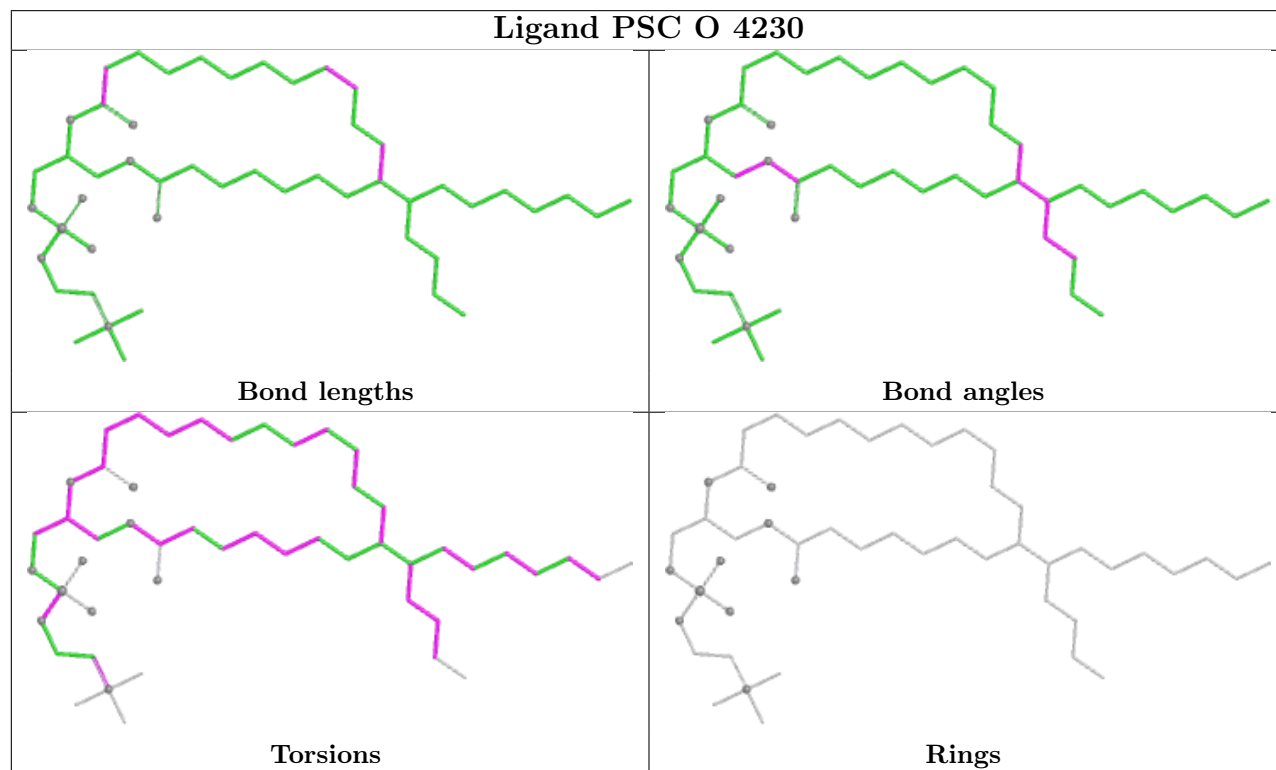
## Ligand PEK G 4263

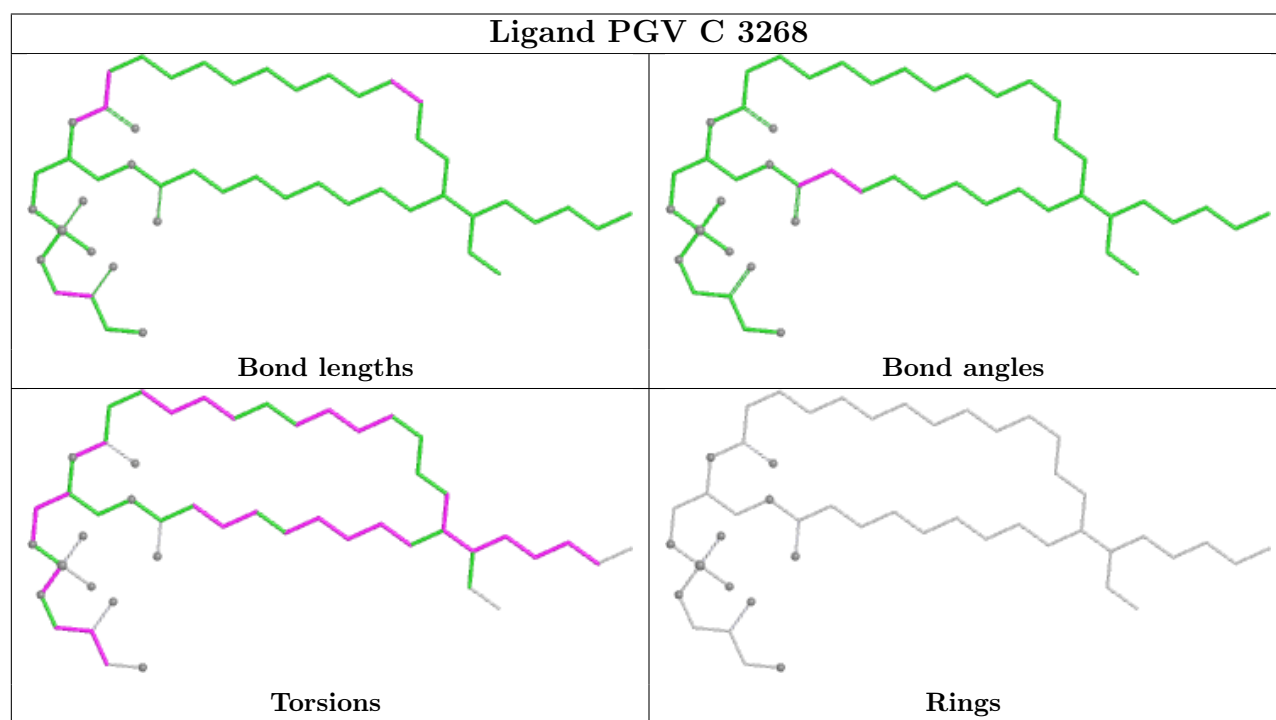
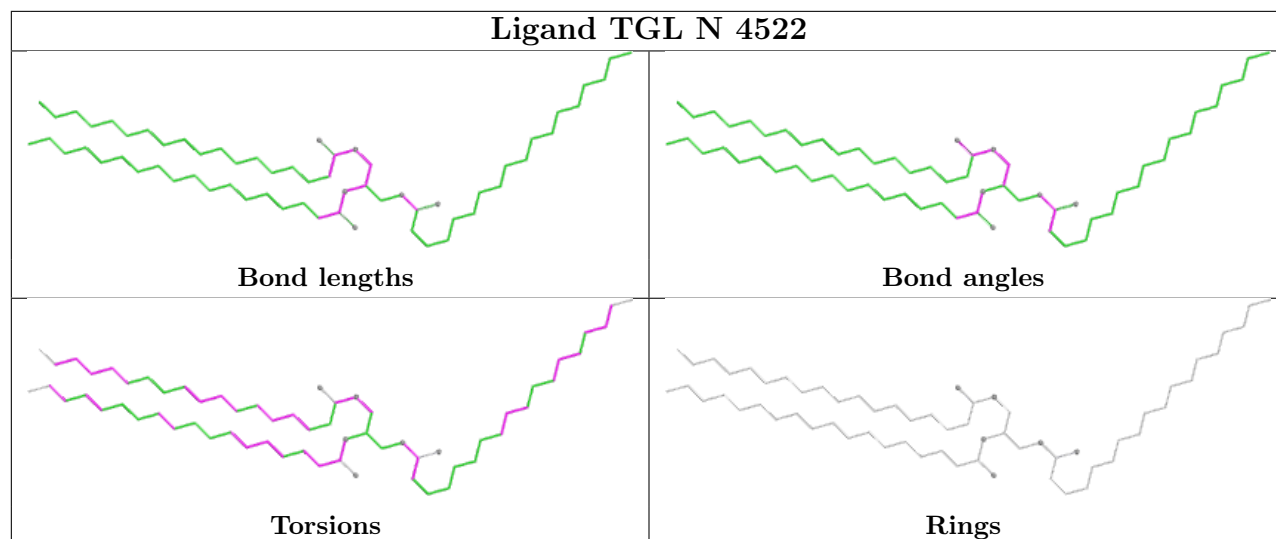


## Ligand DMU Z 4526

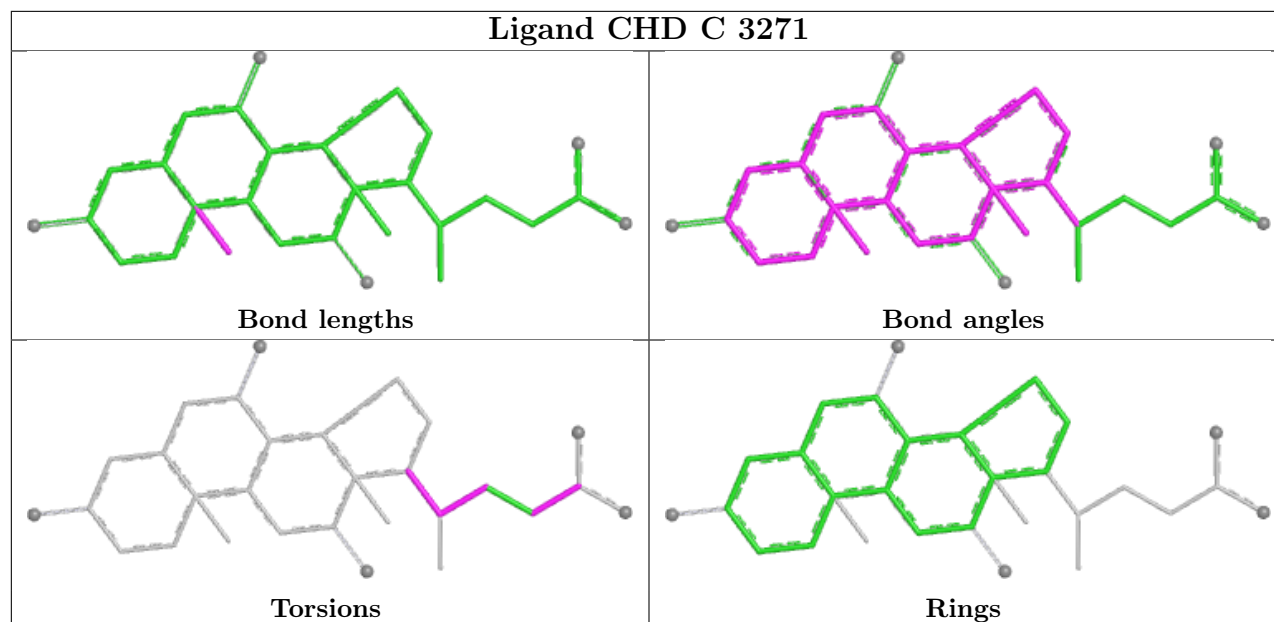


## Ligand PSC O 4230

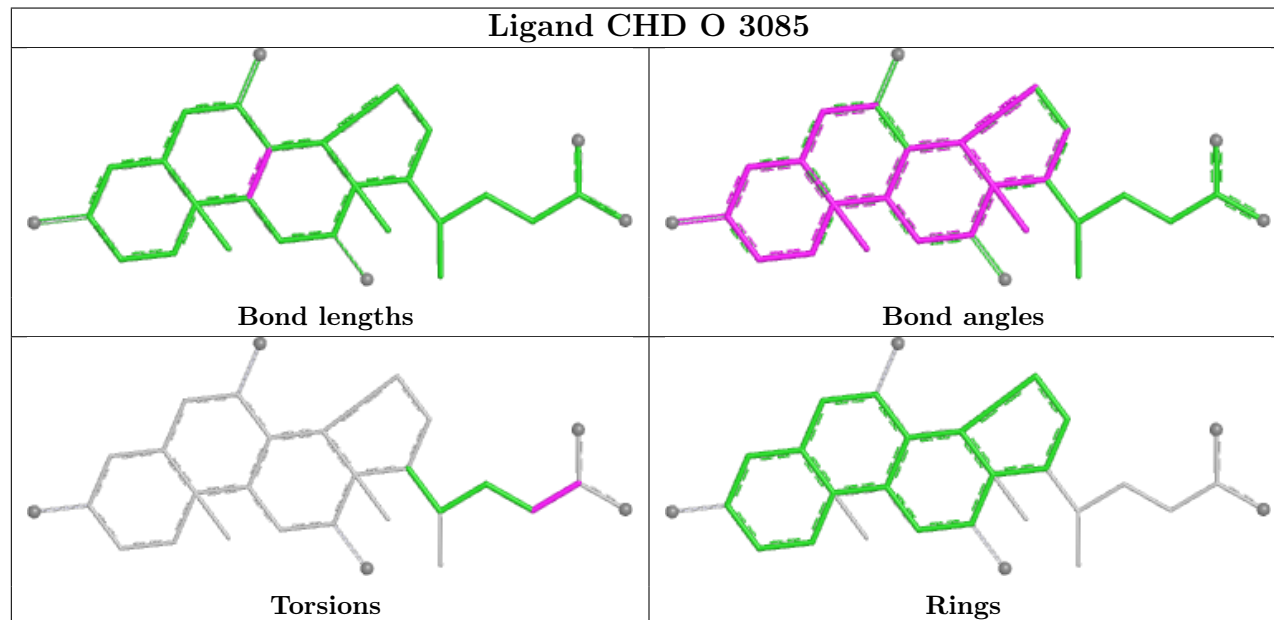


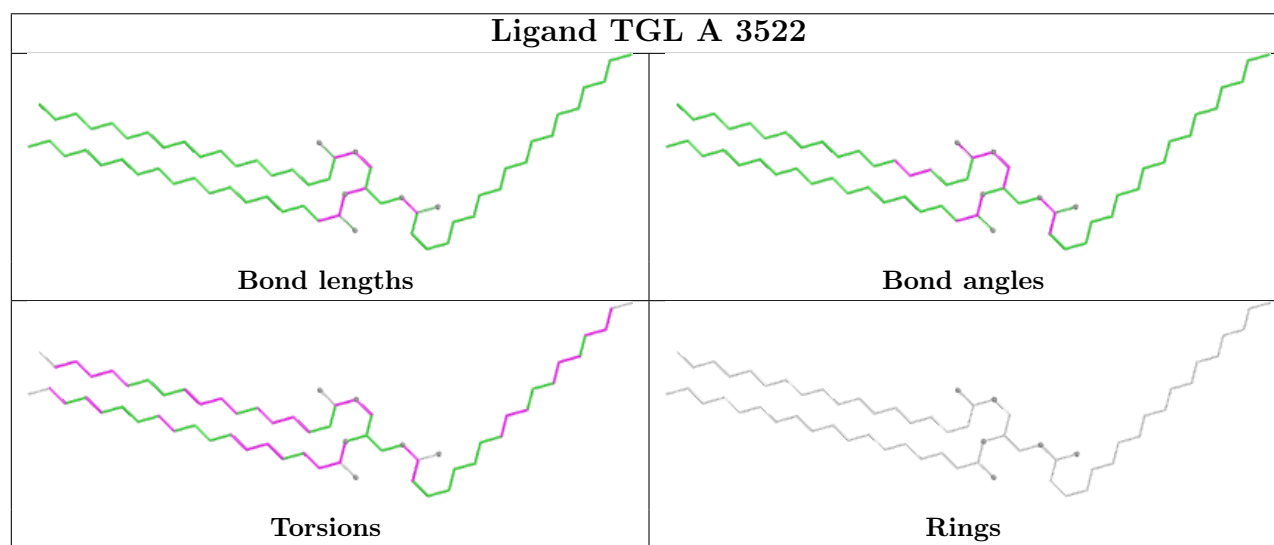
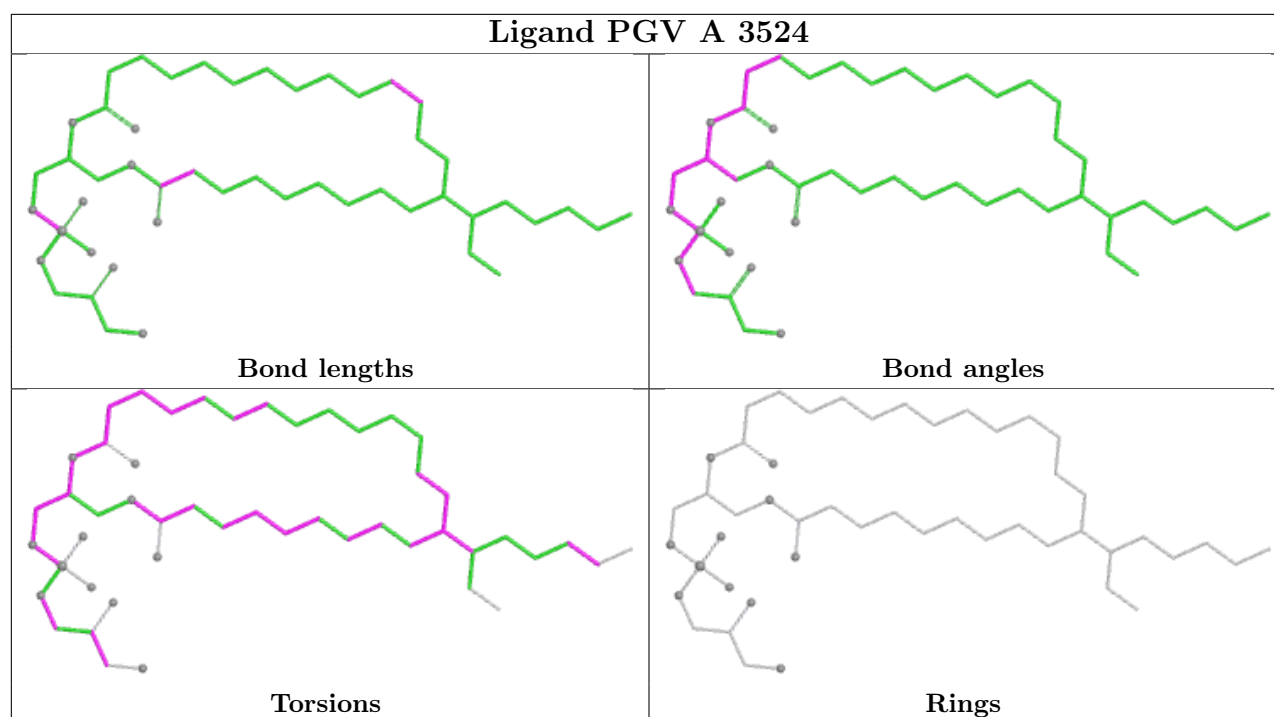


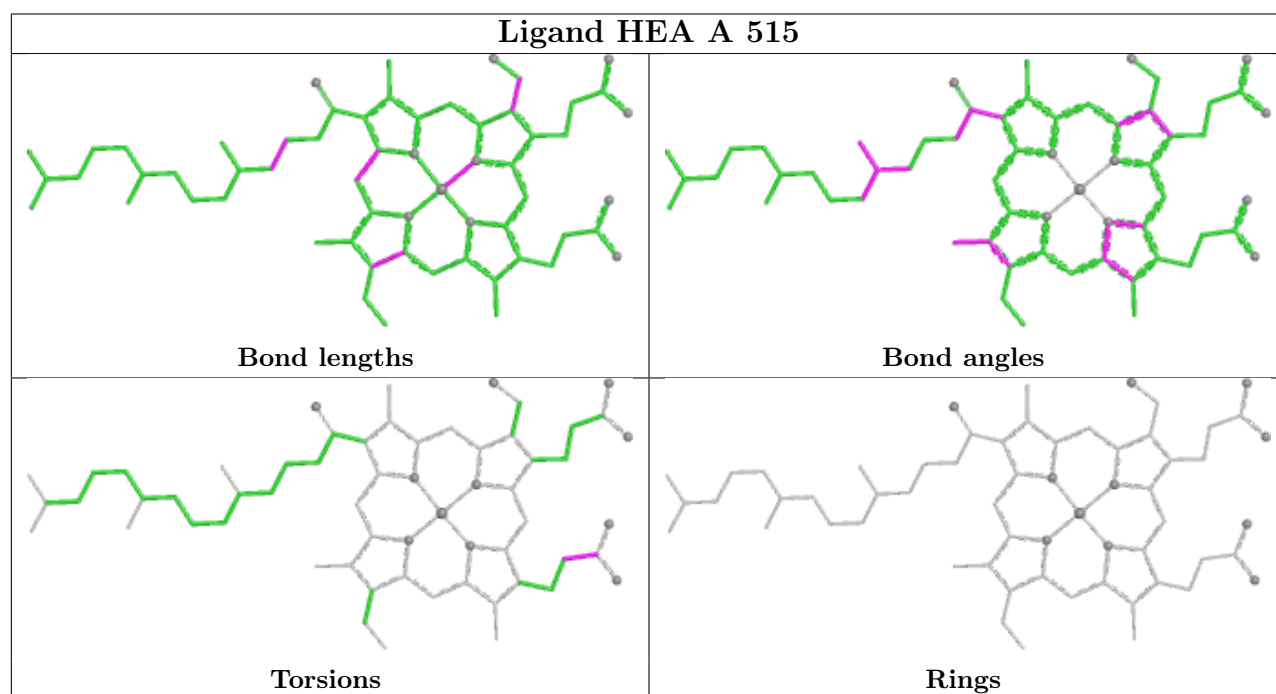
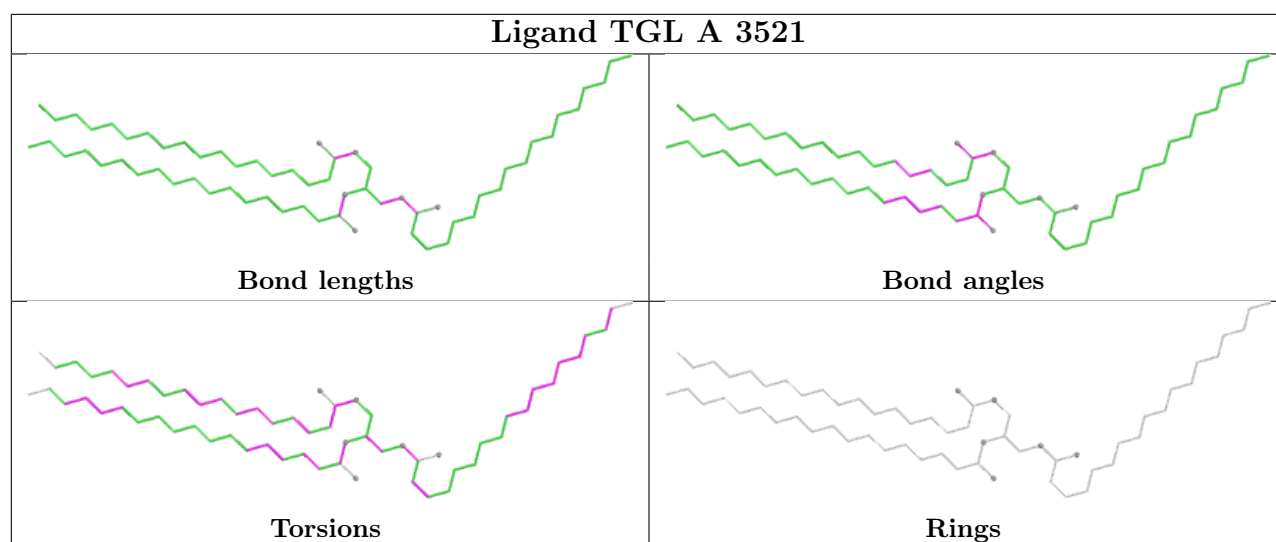
## Ligand CHD C 3271

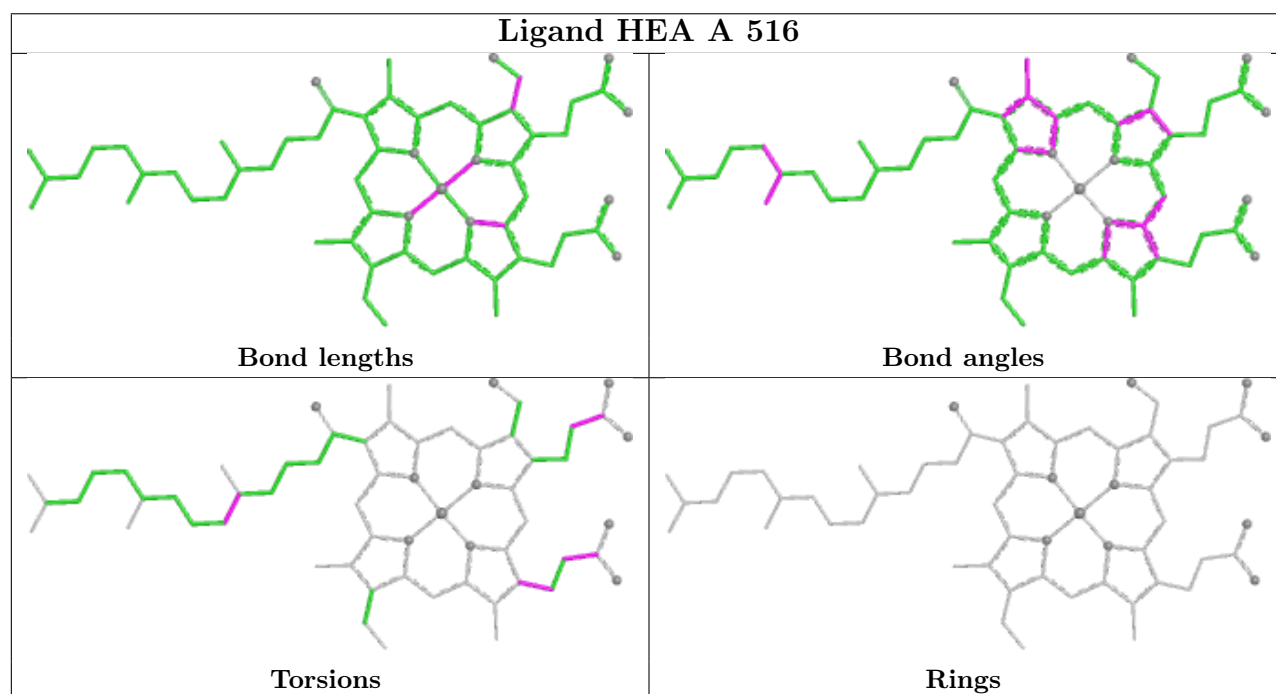
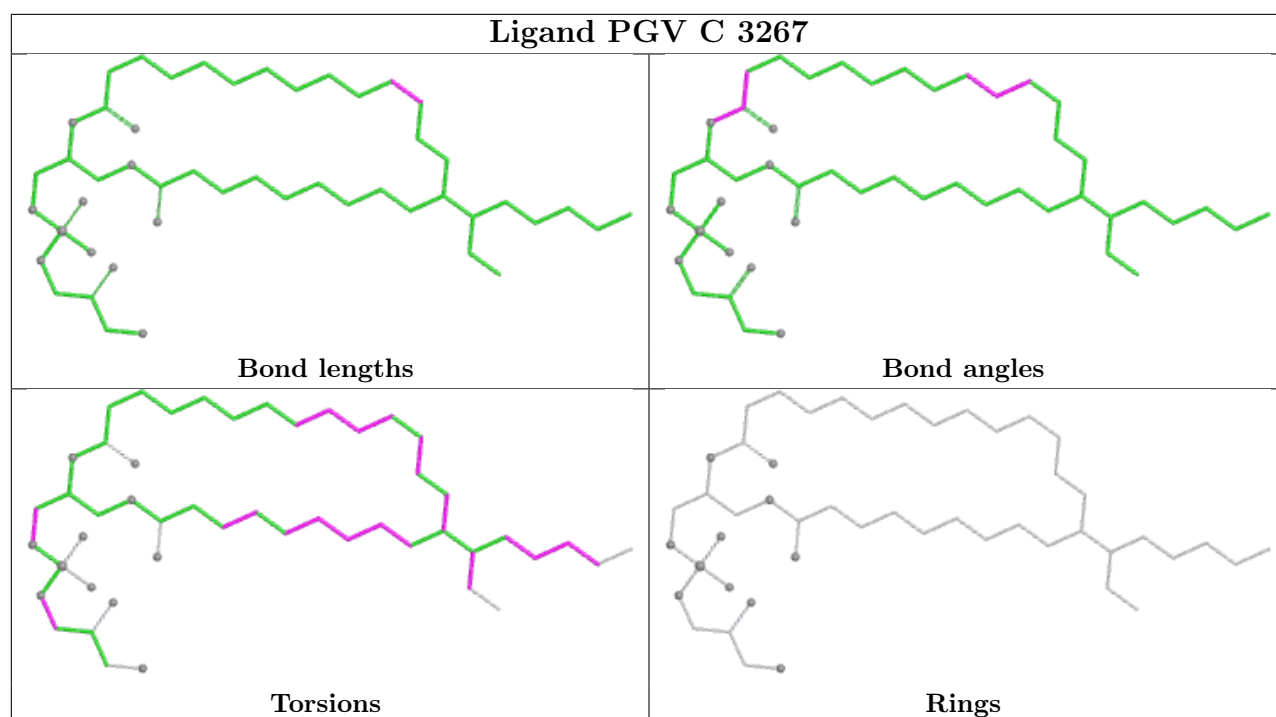


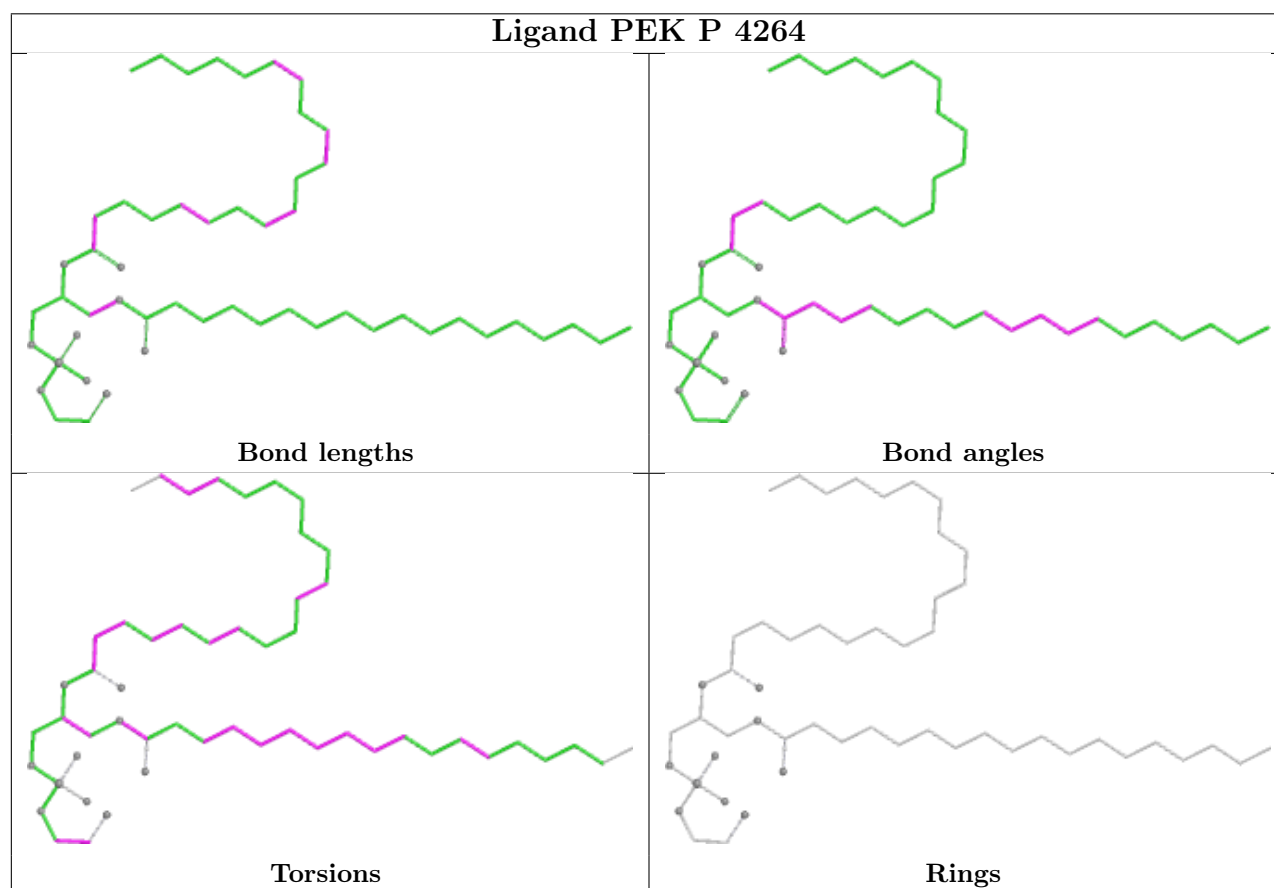
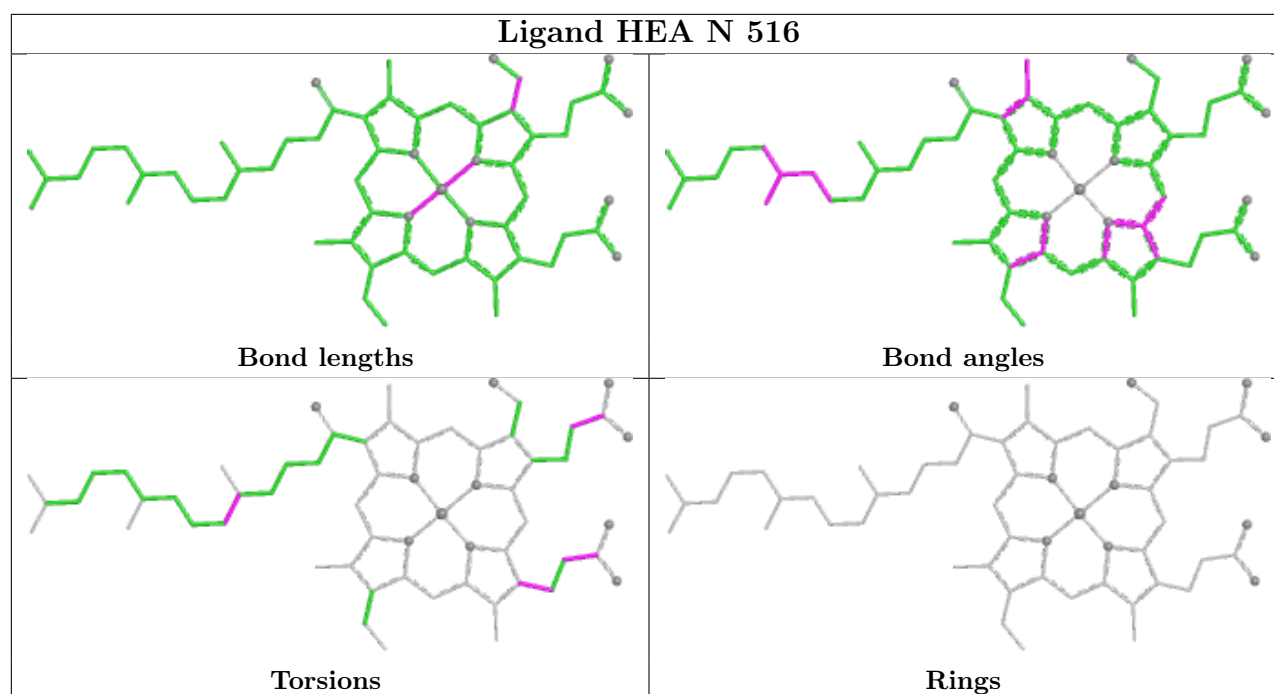
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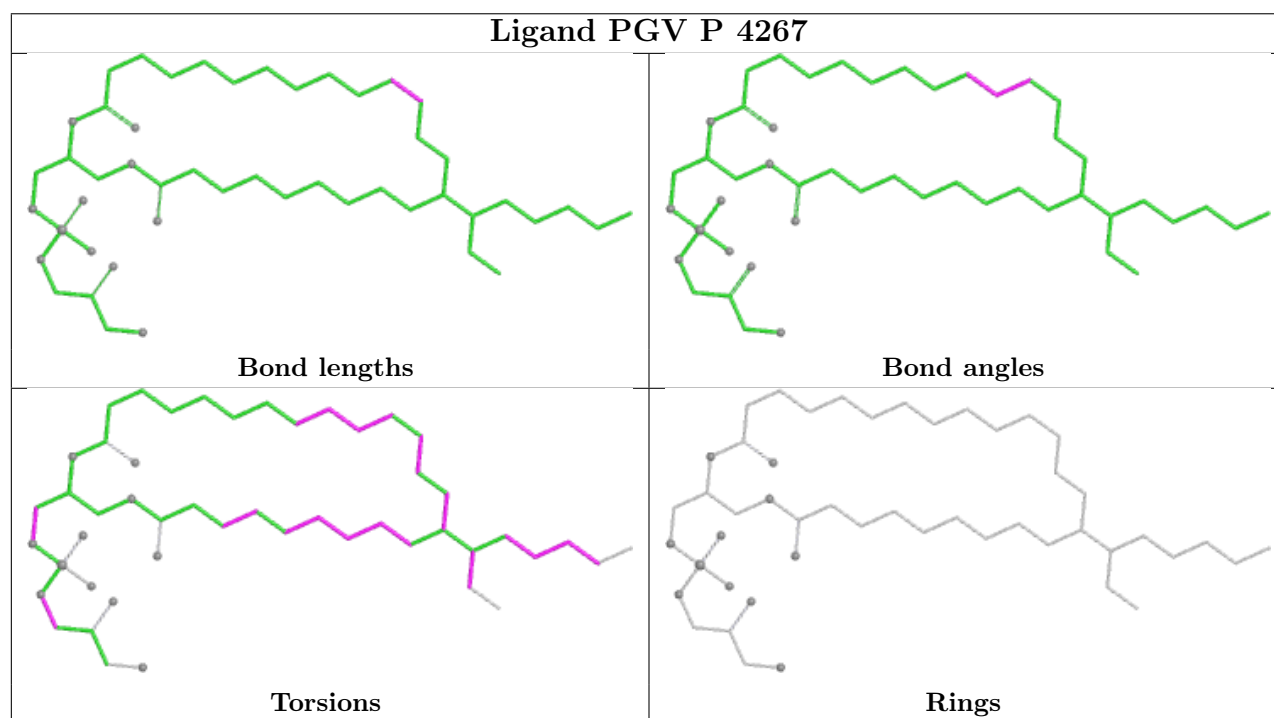
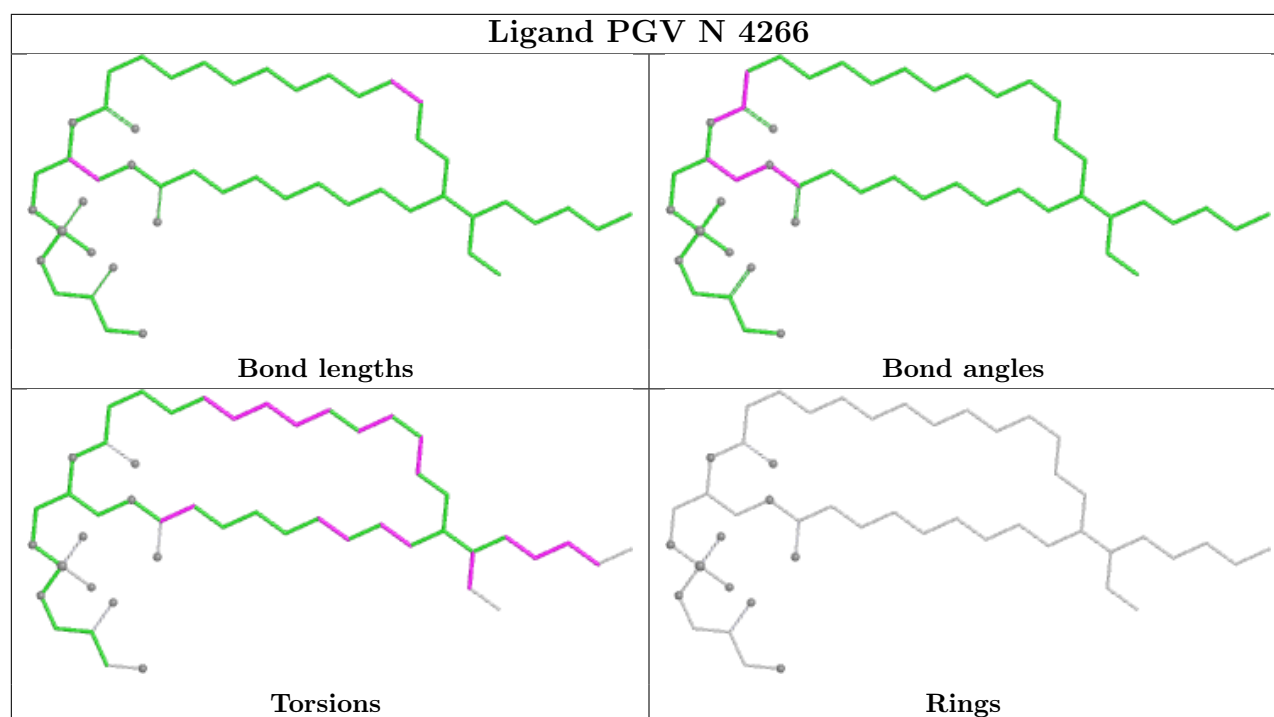




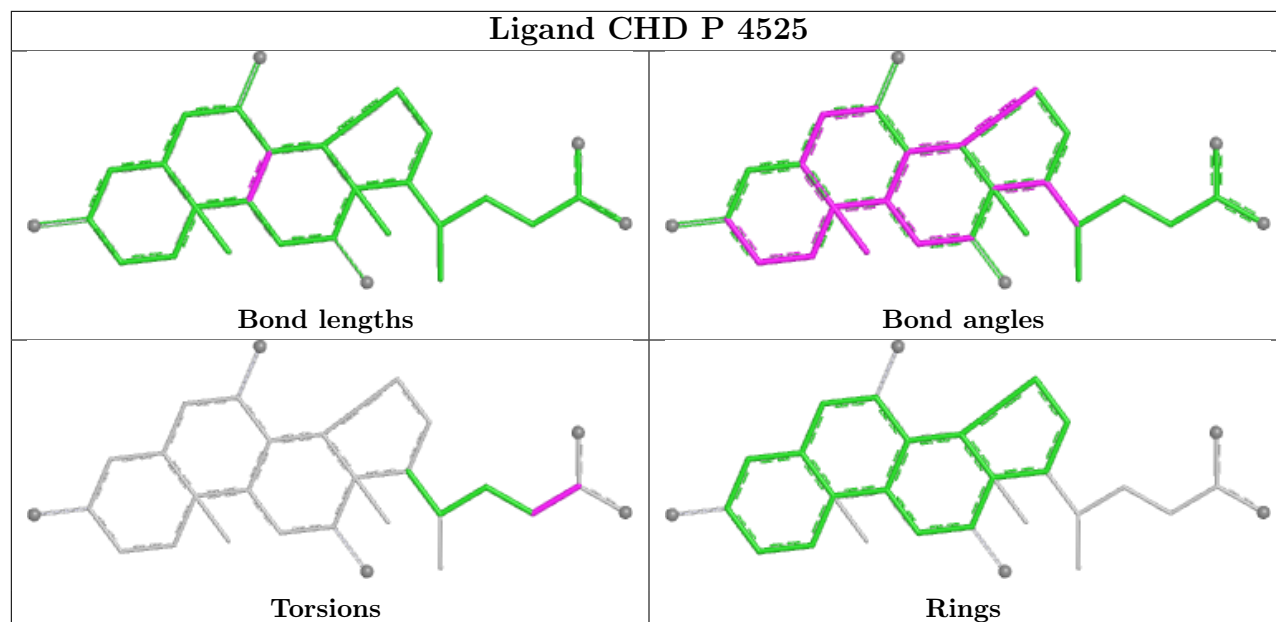




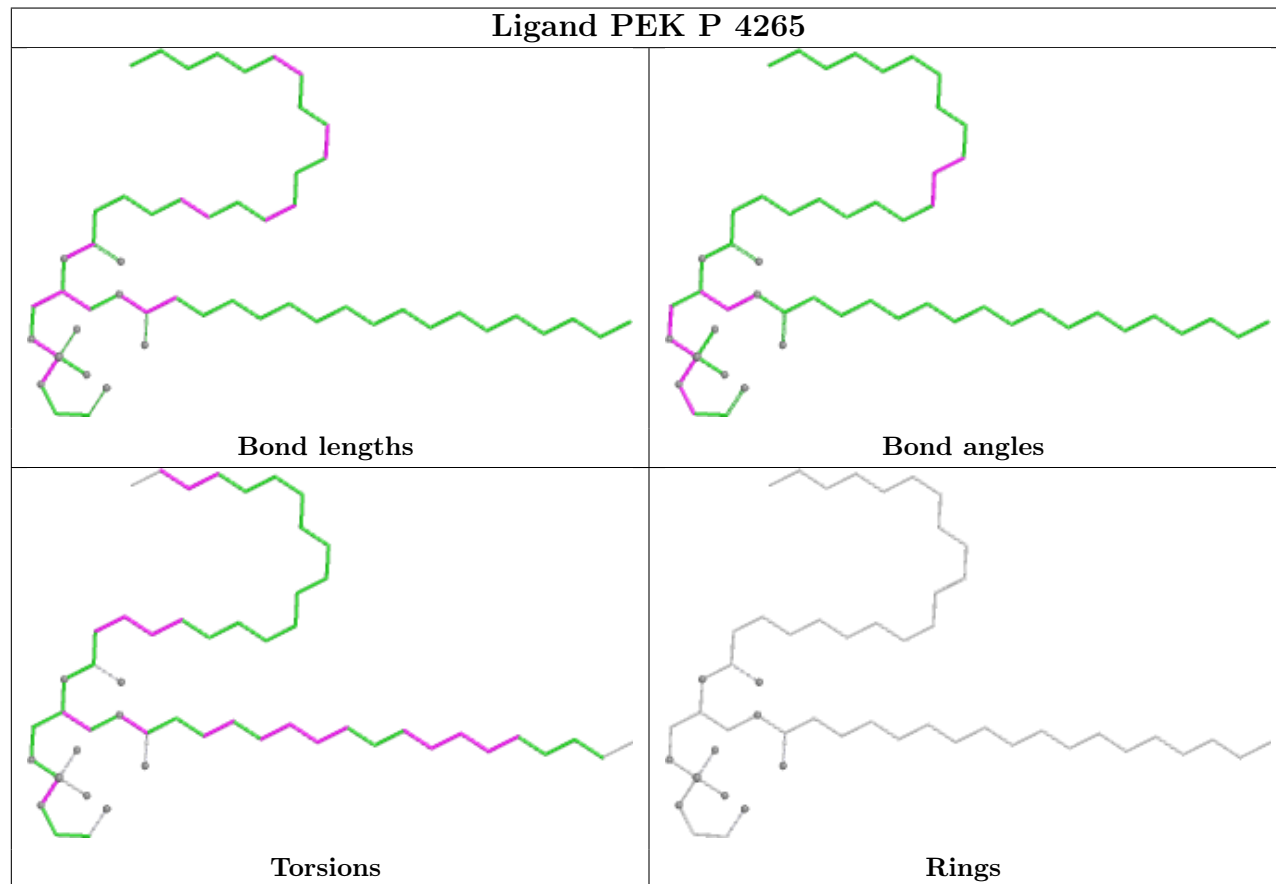


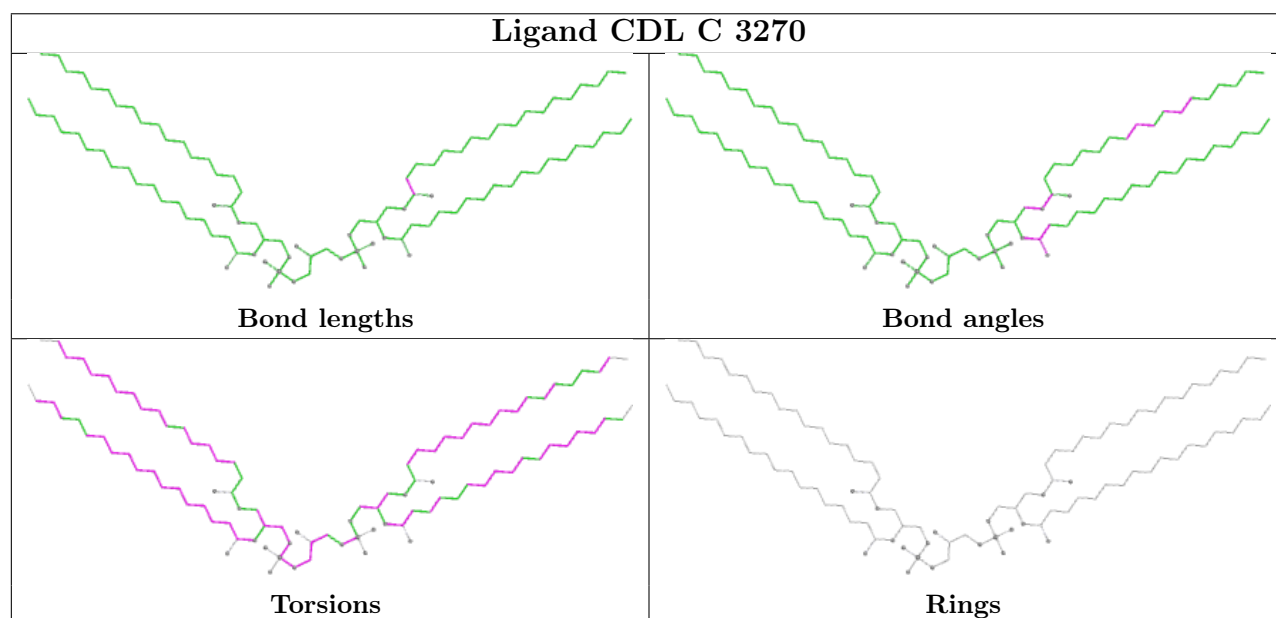
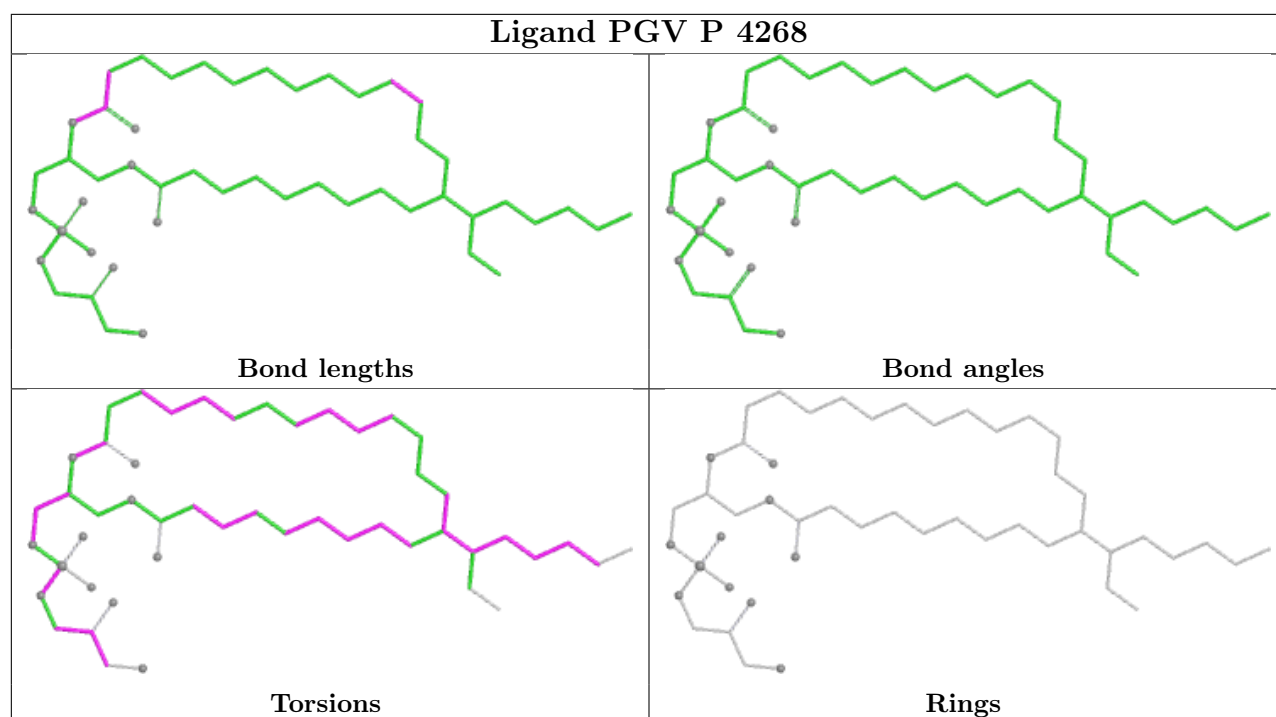


## Ligand CHD P 4525

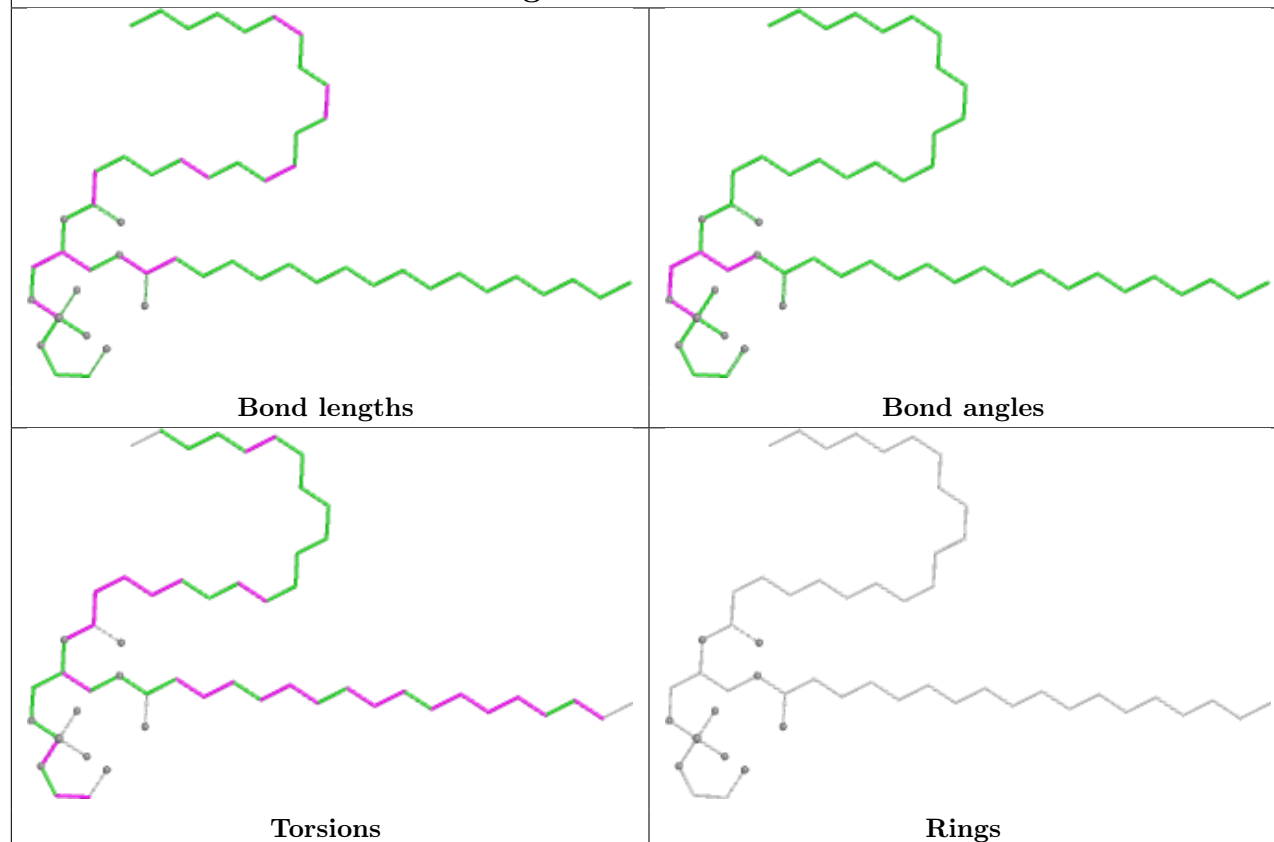


## Ligand PEK P 4265

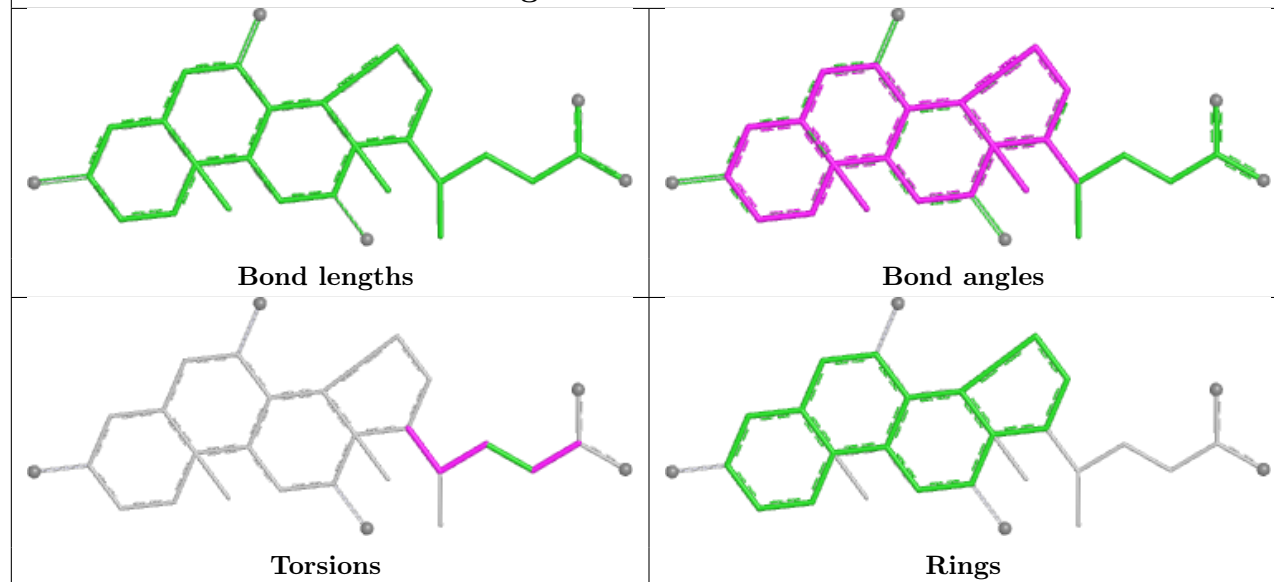




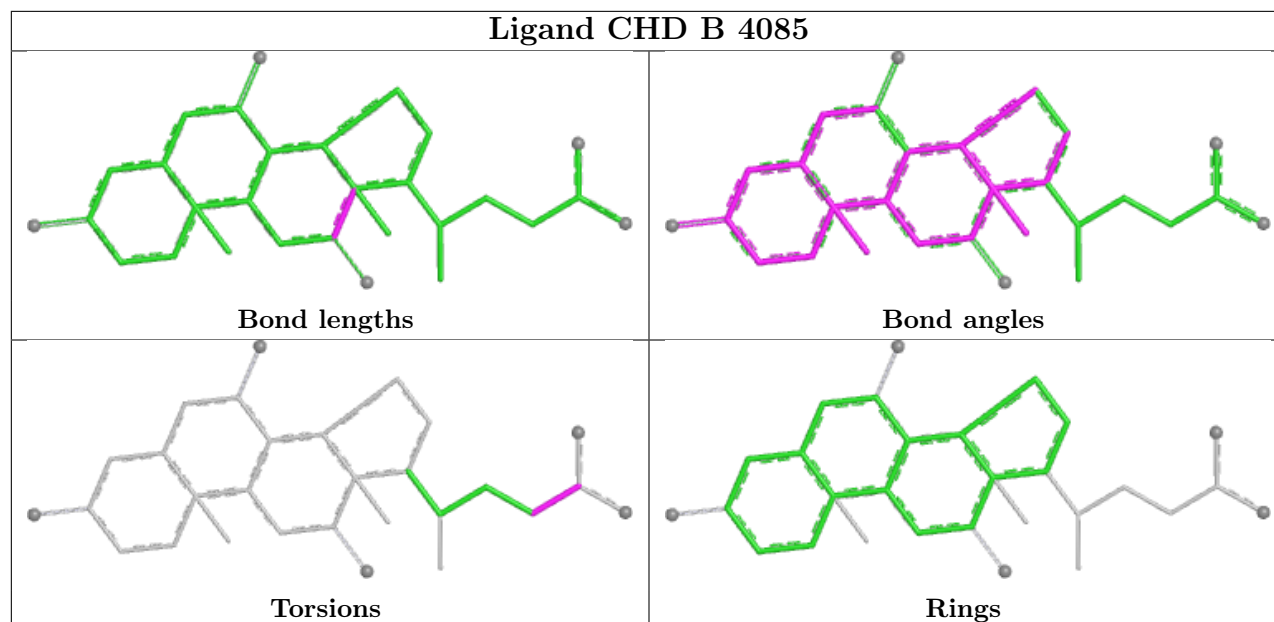
## Ligand PEK T 3263



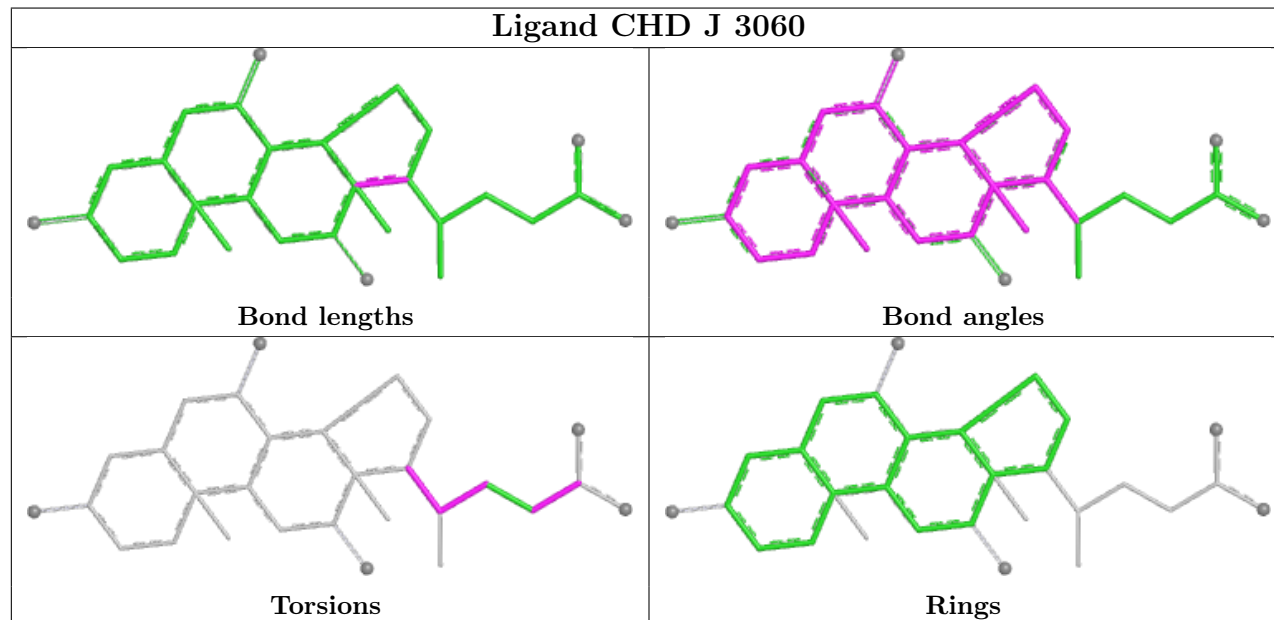
## Ligand CHD P 4271

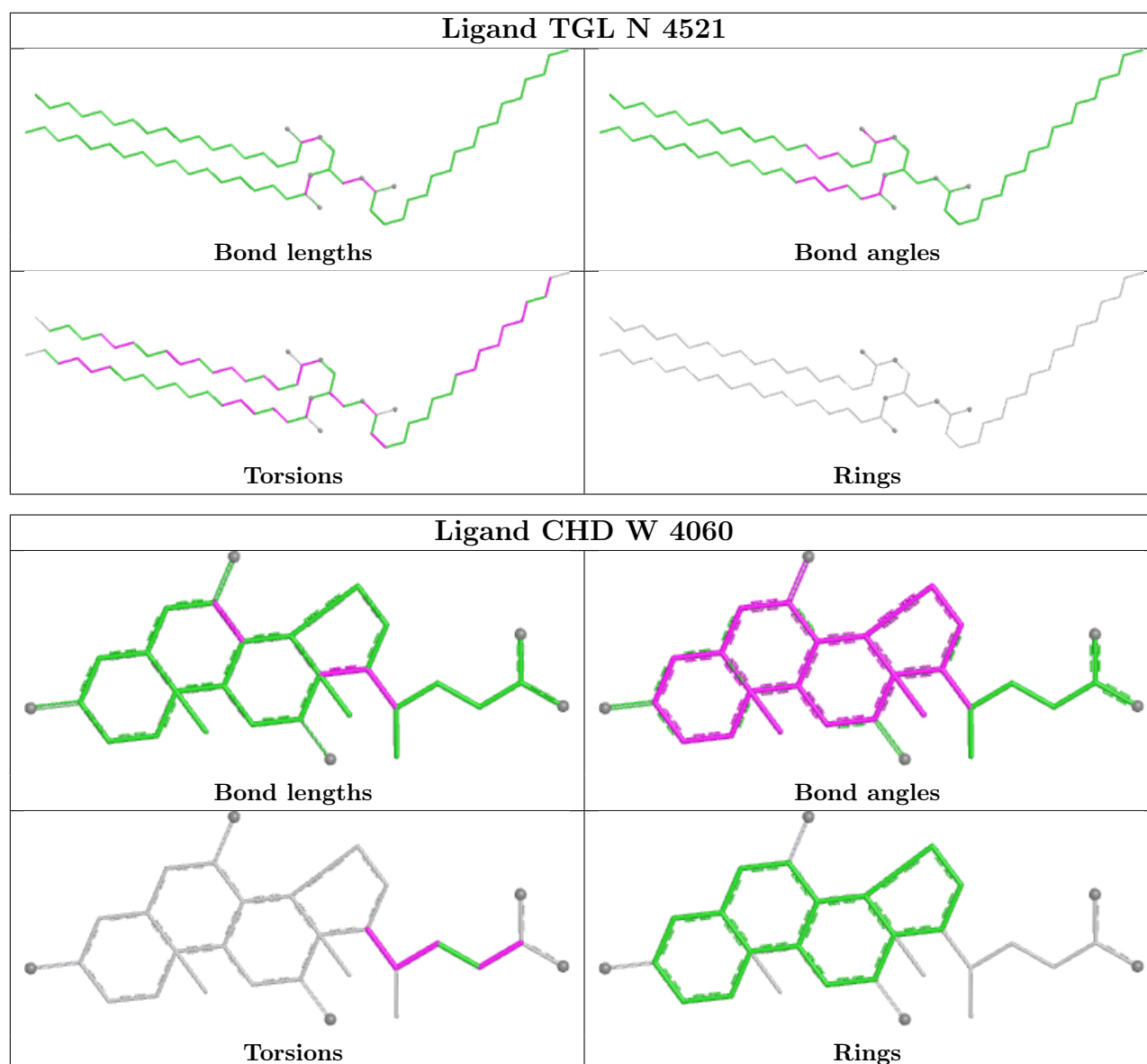


## Ligand CHD B 4085



## Ligand CHD J 3060





## 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%) | -0.58  | 6 (1%) 76 79   | 13, 19, 29, 66        | 0     |
| 1   | N     | 513/514 (99%) | -0.26  | 8 (1%) 70 74   | 17, 24, 34, 67        | 0     |
| 2   | B     | 226/227 (99%) | 0.28   | 21 (9%) 14 15  | 14, 27, 52, 83        | 0     |
| 2   | O     | 226/227 (99%) | 0.83   | 26 (11%) 9 10  | 21, 33, 60, 87        | 0     |
| 3   | C     | 259/261 (99%) | -0.27  | 6 (2%) 61 65   | 16, 23, 37, 65        | 0     |
| 3   | P     | 259/261 (99%) | -0.07  | 7 (2%) 56 60   | 18, 25, 39, 65        | 0     |
| 4   | D     | 144/147 (97%) | 0.63   | 14 (9%) 13 14  | 20, 30, 56, 81        | 0     |
| 4   | Q     | 144/147 (97%) | 1.76   | 41 (28%) 1 1   | 29, 41, 67, 98        | 0     |
| 5   | E     | 105/109 (96%) | 0.68   | 13 (12%) 8 8   | 23, 31, 57, 97        | 0     |
| 5   | R     | 105/109 (96%) | 1.42   | 28 (26%) 1 1   | 27, 37, 60, 97        | 0     |
| 6   | F     | 98/98 (100%)  | 0.82   | 10 (10%) 12 12 | 20, 29, 85, 100       | 0     |
| 6   | S     | 98/98 (100%)  | 1.10   | 13 (13%) 7 7   | 21, 31, 91, 100       | 0     |
| 7   | G     | 83/85 (97%)   | 1.36   | 24 (28%) 1 1   | 21, 31, 97, 99        | 0     |
| 7   | T     | 83/85 (97%)   | 1.65   | 25 (30%) 1 1   | 20, 35, 94, 98        | 0     |
| 8   | H     | 79/85 (92%)   | 1.22   | 16 (20%) 3 2   | 21, 34, 89, 100       | 0     |
| 8   | U     | 79/85 (92%)   | 1.46   | 19 (24%) 2 1   | 27, 38, 91, 100       | 0     |
| 9   | I     | 72/73 (98%)   | 1.28   | 18 (25%) 2 1   | 24, 41, 64, 81        | 0     |
| 9   | V     | 72/73 (98%)   | 1.81   | 21 (29%) 1 1   | 27, 47, 66, 91        | 0     |
| 10  | J     | 58/59 (98%)   | 0.82   | 8 (13%) 6 6    | 23, 32, 73, 94        | 0     |
| 10  | W     | 58/59 (98%)   | 1.32   | 9 (15%) 5 5    | 26, 38, 76, 100       | 0     |
| 11  | K     | 49/56 (87%)   | 0.85   | 4 (8%) 17 18   | 24, 34, 46, 67        | 0     |
| 11  | X     | 49/56 (87%)   | 1.51   | 12 (24%) 2 1   | 33, 41, 58, 75        | 0     |
| 12  | L     | 46/47 (97%)   | 0.14   | 3 (6%) 25 26   | 20, 25, 44, 92        | 0     |
| 12  | Y     | 46/47 (97%)   | 0.85   | 6 (13%) 7 7    | 26, 33, 58, 85        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------------|-----------------------|-------|
| 13  | M     | 43/46 (93%)     | 0.56   | 6 (13%) 6 6     | 21, 26, 77, 99        | 0     |
| 13  | Z     | 43/46 (93%)     | 1.18   | 8 (18%) 3 3     | 28, 35, 84, 100       | 0     |
| All | All   | 3550/3614 (98%) | 0.43   | 372 (10%) 11 12 | 13, 28, 62, 100       | 0     |

All (372) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 6   | S     | 1   | ALA  | 15.6 |
| 6   | F     | 1   | ALA  | 14.4 |
| 6   | S     | 97  | ALA  | 11.6 |
| 4   | Q     | 6   | VAL  | 10.7 |
| 6   | S     | 94  | HIS  | 10.5 |
| 4   | Q     | 5   | VAL  | 9.9  |
| 2   | O     | 227 | LEU  | 9.7  |
| 6   | F     | 97  | ALA  | 9.7  |
| 9   | V     | 3   | ALA  | 9.7  |
| 4   | Q     | 8   | SER  | 9.7  |
| 7   | G     | 4   | ALA  | 9.4  |
| 6   | F     | 96  | LEU  | 9.2  |
| 7   | T     | 3   | ALA  | 8.5  |
| 8   | U     | 8   | ILE  | 8.4  |
| 6   | S     | 96  | LEU  | 8.4  |
| 8   | H     | 8   | ILE  | 8.1  |
| 7   | T     | 36  | TRP  | 7.9  |
| 9   | V     | 5   | ALA  | 7.8  |
| 7   | T     | 5   | LYS  | 7.6  |
| 6   | S     | 93  | PRO  | 7.5  |
| 7   | G     | 5   | LYS  | 7.4  |
| 7   | G     | 3   | ALA  | 7.1  |
| 8   | H     | 47  | GLY  | 7.1  |
| 6   | S     | 98  | HIS  | 7.0  |
| 4   | D     | 5   | VAL  | 6.9  |
| 4   | D     | 4   | SER  | 6.9  |
| 4   | Q     | 4   | SER  | 6.8  |
| 7   | T     | 4   | ALA  | 6.7  |
| 1   | N     | 513 | LEU  | 6.7  |
| 2   | O     | 59  | GLN  | 6.7  |
| 2   | O     | 226 | MET  | 6.7  |
| 8   | H     | 50  | VAL  | 6.5  |
| 4   | Q     | 7   | LYS  | 6.4  |
| 7   | T     | 2   | SER  | 6.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | D     | 6   | VAL  | 6.4  |
| 6   | F     | 94  | HIS  | 6.3  |
| 7   | G     | 1   | ALA  | 6.3  |
| 10  | J     | 1   | PHE  | 6.2  |
| 6   | F     | 98  | HIS  | 6.1  |
| 9   | V     | 2   | THR  | 6.1  |
| 7   | G     | 42  | ARG  | 6.1  |
| 2   | O     | 113 | TYR  | 6.1  |
| 9   | I     | 3   | ALA  | 6.0  |
| 7   | G     | 36  | TRP  | 5.9  |
| 11  | K     | 6   | ALA  | 5.9  |
| 7   | G     | 7   | ASP  | 5.9  |
| 7   | G     | 2   | SER  | 5.9  |
| 7   | T     | 39  | SER  | 5.9  |
| 5   | R     | 109 | VAL  | 5.9  |
| 2   | O     | 224 | ALA  | 5.8  |
| 7   | T     | 42  | ARG  | 5.8  |
| 2   | B     | 59  | GLN  | 5.7  |
| 2   | B     | 90  | ILE  | 5.7  |
| 7   | T     | 37  | LEU  | 5.7  |
| 7   | T     | 10  | GLY  | 5.6  |
| 7   | T     | 8   | HIS  | 5.6  |
| 10  | W     | 58  | LYS  | 5.6  |
| 9   | V     | 37  | PHE  | 5.5  |
| 13  | M     | 40  | TYR  | 5.5  |
| 6   | F     | 3   | GLY  | 5.4  |
| 8   | U     | 46  | LYS  | 5.4  |
| 8   | U     | 47  | GLY  | 5.4  |
| 13  | M     | 43  | SER  | 5.4  |
| 2   | O     | 90  | ILE  | 5.3  |
| 7   | G     | 10  | GLY  | 5.3  |
| 7   | G     | 37  | LEU  | 5.3  |
| 8   | H     | 9   | LYS  | 5.3  |
| 4   | Q     | 51  | LEU  | 5.3  |
| 6   | F     | 95  | GLN  | 5.3  |
| 12  | L     | 2   | HIS  | 5.2  |
| 6   | S     | 3   | GLY  | 5.2  |
| 7   | T     | 7   | ASP  | 5.2  |
| 6   | S     | 95  | GLN  | 5.1  |
| 8   | U     | 7   | LYS  | 5.1  |
| 9   | V     | 4   | LEU  | 5.0  |
| 7   | T     | 1   | ALA  | 5.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | R     | 79  | LYS  | 5.0  |
| 10  | W     | 57  | HIS  | 5.0  |
| 9   | I     | 37  | PHE  | 5.0  |
| 7   | G     | 39  | SER  | 4.9  |
| 13  | Z     | 40  | TYR  | 4.9  |
| 2   | B     | 87  | MET  | 4.9  |
| 4   | Q     | 58  | GLU  | 4.9  |
| 4   | Q     | 33  | LEU  | 4.9  |
| 3   | P     | 3   | HIS  | 4.9  |
| 12  | Y     | 2   | HIS  | 4.9  |
| 10  | W     | 1   | PHE  | 4.8  |
| 8   | H     | 7   | LYS  | 4.8  |
| 7   | T     | 84  | LYS  | 4.8  |
| 13  | Z     | 41  | LYS  | 4.8  |
| 4   | Q     | 35  | ALA  | 4.8  |
| 6   | F     | 2   | SER  | 4.8  |
| 13  | Z     | 43  | SER  | 4.8  |
| 8   | U     | 48  | GLY  | 4.8  |
| 3   | C     | 38  | ASN  | 4.8  |
| 7   | T     | 38  | HIS  | 4.8  |
| 11  | X     | 6   | ALA  | 4.8  |
| 10  | J     | 56  | PRO  | 4.7  |
| 8   | H     | 46  | LYS  | 4.7  |
| 5   | R     | 105 | GLY  | 4.7  |
| 8   | H     | 10  | ASN  | 4.6  |
| 8   | U     | 45  | ALA  | 4.6  |
| 7   | T     | 9   | GLY  | 4.6  |
| 1   | A     | 514 | LYS  | 4.6  |
| 9   | I     | 2   | THR  | 4.6  |
| 7   | G     | 6   | GLY  | 4.6  |
| 2   | O     | 223 | SER  | 4.5  |
| 4   | Q     | 11  | TYR  | 4.5  |
| 4   | D     | 8   | SER  | 4.5  |
| 2   | B     | 113 | TYR  | 4.5  |
| 8   | H     | 44  | THR  | 4.5  |
| 7   | T     | 40  | GLY  | 4.4  |
| 3   | P     | 37  | PHE  | 4.3  |
| 13  | Z     | 42  | LYS  | 4.3  |
| 13  | M     | 39  | ASN  | 4.3  |
| 1   | N     | 514 | LYS  | 4.3  |
| 7   | G     | 38  | HIS  | 4.3  |
| 8   | U     | 50  | VAL  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7   | G     | 12  | GLY  | 4.2  |
| 10  | W     | 52  | TRP  | 4.2  |
| 4   | Q     | 39  | ALA  | 4.2  |
| 2   | O     | 65  | TRP  | 4.1  |
| 8   | U     | 9   | LYS  | 4.1  |
| 7   | G     | 40  | GLY  | 4.1  |
| 11  | X     | 47  | ARG  | 4.0  |
| 5   | R     | 83  | PRO  | 4.0  |
| 12  | Y     | 47  | LYS  | 4.0  |
| 11  | X     | 13  | TYR  | 4.0  |
| 7   | T     | 6   | GLY  | 4.0  |
| 1   | A     | 513 | LEU  | 4.0  |
| 2   | B     | 60  | GLU  | 4.0  |
| 5   | E     | 109 | VAL  | 4.0  |
| 9   | V     | 7   | PRO  | 4.0  |
| 8   | U     | 44  | THR  | 3.9  |
| 7   | G     | 9   | GLY  | 3.9  |
| 9   | I     | 29  | LEU  | 3.9  |
| 2   | O     | 217 | LYS  | 3.9  |
| 8   | U     | 10  | ASN  | 3.9  |
| 5   | R     | 5   | HIS  | 3.9  |
| 7   | G     | 8   | HIS  | 3.9  |
| 2   | O     | 225 | SER  | 3.9  |
| 6   | S     | 2   | SER  | 3.8  |
| 10  | W     | 56  | PRO  | 3.8  |
| 4   | D     | 11  | TYR  | 3.8  |
| 4   | Q     | 53  | ILE  | 3.7  |
| 2   | B     | 91  | ASN  | 3.7  |
| 4   | D     | 7   | LYS  | 3.7  |
| 7   | G     | 84  | LYS  | 3.6  |
| 5   | E     | 83  | PRO  | 3.6  |
| 4   | Q     | 9   | GLU  | 3.6  |
| 2   | B     | 65  | TRP  | 3.6  |
| 5   | R     | 108 | LYS  | 3.6  |
| 9   | V     | 8   | GLN  | 3.6  |
| 7   | G     | 41  | HIS  | 3.6  |
| 12  | Y     | 20  | ARG  | 3.6  |
| 3   | C     | 3   | HIS  | 3.6  |
| 7   | T     | 12  | GLY  | 3.5  |
| 9   | I     | 4   | LEU  | 3.5  |
| 8   | H     | 45  | ALA  | 3.5  |
| 7   | T     | 35  | SER  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8   | H     | 48  | GLY  | 3.4  |
| 8   | H     | 43  | MET  | 3.4  |
| 5   | R     | 89  | LEU  | 3.4  |
| 11  | K     | 47  | ARG  | 3.4  |
| 10  | J     | 58  | LYS  | 3.3  |
| 2   | O     | 60  | GLU  | 3.3  |
| 11  | X     | 52  | GLU  | 3.3  |
| 2   | O     | 87  | MET  | 3.3  |
| 4   | D     | 9   | GLU  | 3.3  |
| 5   | E     | 7   | THR  | 3.3  |
| 11  | X     | 7   | PRO  | 3.3  |
| 2   | O     | 91  | ASN  | 3.3  |
| 3   | P     | 38  | ASN  | 3.3  |
| 7   | T     | 33  | LEU  | 3.3  |
| 4   | Q     | 10  | ASP  | 3.3  |
| 13  | M     | 41  | LYS  | 3.2  |
| 5   | R     | 90  | ARG  | 3.2  |
| 2   | O     | 58  | ALA  | 3.2  |
| 1   | N     | 484 | THR  | 3.2  |
| 2   | O     | 32  | PHE  | 3.2  |
| 2   | B     | 16  | ILE  | 3.1  |
| 5   | R     | 76  | GLY  | 3.1  |
| 10  | W     | 55  | PHE  | 3.1  |
| 9   | V     | 36  | LYS  | 3.1  |
| 9   | V     | 73  | LYS  | 3.1  |
| 5   | R     | 7   | THR  | 3.1  |
| 4   | Q     | 62  | LEU  | 3.1  |
| 8   | U     | 49  | ASP  | 3.1  |
| 3   | P     | 44  | MET  | 3.1  |
| 10  | W     | 15  | ASP  | 3.0  |
| 4   | D     | 51  | LEU  | 3.0  |
| 5   | R     | 104 | LEU  | 3.0  |
| 2   | B     | 32  | PHE  | 3.0  |
| 2   | O     | 115 | ASP  | 3.0  |
| 8   | U     | 61  | LYS  | 3.0  |
| 12  | L     | 47  | LYS  | 3.0  |
| 5   | R     | 106 | LEU  | 3.0  |
| 5   | E     | 5   | HIS  | 3.0  |
| 4   | Q     | 32  | ASN  | 3.0  |
| 2   | B     | 61  | VAL  | 3.0  |
| 6   | S     | 92  | VAL  | 3.0  |
| 5   | R     | 99  | SER  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 49  | GLY  | 3.0  |
| 9   | I     | 5   | ALA  | 3.0  |
| 2   | O     | 126 | SER  | 2.9  |
| 9   | I     | 36  | LYS  | 2.9  |
| 2   | B     | 92  | ASN  | 2.9  |
| 13  | Z     | 39  | ASN  | 2.9  |
| 7   | T     | 41  | HIS  | 2.9  |
| 1   | N     | 113 | LEU  | 2.9  |
| 5   | R     | 84  | TYR  | 2.9  |
| 1   | N     | 297 | MET  | 2.9  |
| 7   | T     | 70  | PHE  | 2.9  |
| 8   | H     | 42  | ALA  | 2.9  |
| 5   | R     | 85  | VAL  | 2.9  |
| 4   | Q     | 38  | LYS  | 2.8  |
| 4   | Q     | 48  | TRP  | 2.8  |
| 4   | Q     | 34  | SER  | 2.8  |
| 2   | B     | 37  | LEU  | 2.8  |
| 5   | E     | 81  | ILE  | 2.8  |
| 9   | V     | 33  | THR  | 2.8  |
| 5   | R     | 80  | GLU  | 2.8  |
| 1   | A     | 298 | ASP  | 2.8  |
| 1   | A     | 382 | SER  | 2.8  |
| 9   | I     | 8   | GLN  | 2.7  |
| 10  | J     | 26  | ALA  | 2.7  |
| 2   | O     | 216 | LEU  | 2.7  |
| 10  | J     | 57  | HIS  | 2.7  |
| 13  | Z     | 32  | TRP  | 2.7  |
| 9   | I     | 34  | PHE  | 2.7  |
| 9   | V     | 68  | ILE  | 2.7  |
| 9   | I     | 26  | MET  | 2.6  |
| 3   | C     | 37  | PHE  | 2.6  |
| 5   | R     | 102 | GLU  | 2.6  |
| 7   | G     | 35  | SER  | 2.6  |
| 8   | U     | 52  | VAL  | 2.6  |
| 12  | Y     | 16  | GLU  | 2.6  |
| 13  | M     | 42  | LYS  | 2.6  |
| 7   | G     | 45  | PRO  | 2.6  |
| 1   | A     | 113 | LEU  | 2.6  |
| 10  | J     | 17  | GLY  | 2.6  |
| 10  | W     | 48  | TYR  | 2.6  |
| 12  | L     | 3   | TYR  | 2.6  |
| 9   | I     | 25  | PHE  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | Q     | 73  | ARG  | 2.6  |
| 5   | R     | 6   | GLU  | 2.6  |
| 4   | Q     | 30  | VAL  | 2.6  |
| 8   | U     | 42  | ALA  | 2.6  |
| 11  | X     | 20  | SER  | 2.6  |
| 5   | R     | 91  | PRO  | 2.5  |
| 5   | R     | 101 | PRO  | 2.5  |
| 3   | C     | 40  | MET  | 2.5  |
| 4   | Q     | 55  | GLU  | 2.5  |
| 4   | Q     | 59  | LEU  | 2.5  |
| 8   | H     | 49  | ASP  | 2.5  |
| 2   | O     | 221 | LYS  | 2.5  |
| 9   | V     | 65  | LYS  | 2.5  |
| 5   | E     | 85  | VAL  | 2.5  |
| 3   | P     | 40  | MET  | 2.5  |
| 2   | O     | 220 | GLU  | 2.5  |
| 9   | V     | 25  | PHE  | 2.5  |
| 2   | O     | 222 | TRP  | 2.5  |
| 11  | X     | 48  | VAL  | 2.5  |
| 8   | U     | 11  | TYR  | 2.5  |
| 10  | J     | 55  | PHE  | 2.5  |
| 4   | Q     | 143 | ASN  | 2.5  |
| 11  | X     | 54  | ARG  | 2.5  |
| 4   | Q     | 28  | ALA  | 2.5  |
| 5   | E     | 13  | ALA  | 2.5  |
| 9   | V     | 27  | VAL  | 2.5  |
| 2   | O     | 129 | LYS  | 2.5  |
| 6   | S     | 4   | GLY  | 2.4  |
| 2   | O     | 116 | LEU  | 2.4  |
| 13  | Z     | 37  | LEU  | 2.4  |
| 2   | B     | 58  | ALA  | 2.4  |
| 13  | M     | 38  | ASP  | 2.4  |
| 10  | J     | 52  | TRP  | 2.4  |
| 4   | Q     | 57  | VAL  | 2.4  |
| 4   | Q     | 133 | GLY  | 2.4  |
| 12  | Y     | 4   | GLU  | 2.4  |
| 7   | G     | 70  | PHE  | 2.4  |
| 5   | E     | 108 | LYS  | 2.4  |
| 11  | X     | 23  | THR  | 2.4  |
| 4   | Q     | 46  | ALA  | 2.4  |
| 9   | I     | 32  | ALA  | 2.4  |
| 6   | S     | 78  | GLU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9   | I     | 27  | VAL  | 2.4  |
| 4   | Q     | 72  | ASN  | 2.4  |
| 9   | I     | 30  | GLY  | 2.4  |
| 3   | P     | 33  | MET  | 2.4  |
| 8   | H     | 51  | SER  | 2.4  |
| 4   | Q     | 87  | PHE  | 2.4  |
| 9   | V     | 19  | PHE  | 2.4  |
| 4   | Q     | 107 | ILE  | 2.4  |
| 9   | V     | 15  | ARG  | 2.4  |
| 4   | Q     | 69  | ALA  | 2.4  |
| 2   | B     | 89  | GLU  | 2.4  |
| 4   | Q     | 138 | TRP  | 2.4  |
| 4   | D     | 31  | LYS  | 2.4  |
| 5   | R     | 93  | LEU  | 2.3  |
| 9   | I     | 15  | ARG  | 2.3  |
| 12  | Y     | 45  | LEU  | 2.3  |
| 5   | E     | 84  | TYR  | 2.3  |
| 6   | F     | 93  | PRO  | 2.3  |
| 7   | G     | 43  | GLU  | 2.3  |
| 8   | H     | 84  | LYS  | 2.3  |
| 8   | U     | 41  | LYS  | 2.3  |
| 4   | Q     | 52  | SER  | 2.3  |
| 2   | B     | 88  | ASP  | 2.3  |
| 2   | B     | 115 | ASP  | 2.3  |
| 7   | T     | 43  | GLU  | 2.3  |
| 8   | U     | 53  | CYS  | 2.3  |
| 9   | V     | 29  | LEU  | 2.3  |
| 2   | B     | 86  | MET  | 2.3  |
| 2   | O     | 93  | PRO  | 2.3  |
| 4   | Q     | 64  | PHE  | 2.2  |
| 11  | K     | 7   | PRO  | 2.2  |
| 5   | R     | 77  | PRO  | 2.2  |
| 4   | D     | 147 | LYS  | 2.2  |
| 4   | Q     | 31  | LYS  | 2.2  |
| 7   | G     | 33  | LEU  | 2.2  |
| 9   | I     | 7   | PRO  | 2.2  |
| 4   | Q     | 128 | VAL  | 2.2  |
| 10  | W     | 34  | VAL  | 2.2  |
| 9   | I     | 33  | THR  | 2.2  |
| 1   | N     | 298 | ASP  | 2.2  |
| 4   | D     | 52  | SER  | 2.2  |
| 9   | V     | 46  | ALA  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8   | U     | 43  | MET  | 2.1  |
| 5   | E     | 6   | GLU  | 2.1  |
| 8   | H     | 85  | ILE  | 2.1  |
| 13  | Z     | 38  | ASP  | 2.1  |
| 1   | N     | 483 | LEU  | 2.1  |
| 1   | A     | 297 | MET  | 2.1  |
| 5   | R     | 9   | GLU  | 2.1  |
| 5   | R     | 87  | GLN  | 2.1  |
| 9   | V     | 34  | PHE  | 2.1  |
| 2   | B     | 57  | ASP  | 2.1  |
| 6   | F     | 65  | ASP  | 2.1  |
| 4   | Q     | 115 | TRP  | 2.1  |
| 6   | S     | 53  | THR  | 2.1  |
| 11  | X     | 49  | THR  | 2.1  |
| 2   | B     | 82  | ARG  | 2.1  |
| 9   | I     | 73  | LYS  | 2.1  |
| 5   | E     | 9   | GLU  | 2.1  |
| 5   | E     | 80  | GLU  | 2.1  |
| 3   | C     | 44  | MET  | 2.1  |
| 11  | X     | 16  | ALA  | 2.1  |
| 4   | Q     | 68  | PHE  | 2.1  |
| 5   | E     | 39  | TYR  | 2.1  |
| 5   | R     | 81  | ILE  | 2.1  |
| 5   | R     | 86  | ILE  | 2.1  |
| 8   | U     | 85  | ILE  | 2.1  |
| 3   | C     | 39  | SER  | 2.1  |
| 3   | P     | 39  | SER  | 2.1  |
| 2   | B     | 217 | LYS  | 2.1  |
| 2   | O     | 47  | THR  | 2.1  |
| 7   | T     | 45  | PRO  | 2.1  |
| 2   | B     | 33  | LEU  | 2.1  |
| 2   | O     | 37  | LEU  | 2.1  |
| 4   | D     | 69  | ALA  | 2.1  |
| 9   | V     | 38  | ALA  | 2.1  |
| 5   | R     | 107 | ASP  | 2.1  |
| 4   | Q     | 19  | ARG  | 2.1  |
| 11  | X     | 45  | VAL  | 2.0  |
| 4   | D     | 19  | ARG  | 2.0  |
| 4   | D     | 39  | ALA  | 2.0  |
| 4   | Q     | 74  | SER  | 2.0  |
| 5   | R     | 78  | HIS  | 2.0  |
| 9   | V     | 21  | ILE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 11  | K     | 37  | GLY  | 2.0  |
| 7   | T     | 44  | ARG  | 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  | 0.27 | 0.21 | 98,99,100,100              | 0     |
| 7   | TPO  | G     | 11  | 11/12 | 0.51 | 0.30 | 71,79,100,100              | 0     |
| 7   | TPO  | T     | 11  | 11/12 | 0.52 | 0.30 | 71,81,100,100              | 0     |
| 9   | SAC  | I     | 1   | 9/10  | 0.69 | 0.24 | 91,93,94,96                | 0     |
| 1   | FME  | N     | 1   | 10/11 | 0.78 | 0.22 | 44,49,68,69                | 0     |
| 1   | FME  | A     | 1   | 10/11 | 0.80 | 0.18 | 41,45,67,71                | 0     |
| 2   | FME  | B     | 1   | 10/11 | 0.93 | 0.11 | 20,27,36,41                | 0     |
| 2   | FME  | O     | 1   | 10/11 | 0.93 | 0.11 | 32,33,40,42                | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 21  | CHD  | W     | 4060 | 29/29 | 0.63 | 0.27 | 84,98,100,100              | 0     |
| 23  | PEK  | T     | 3263 | 53/53 | 0.67 | 0.31 | 44,91,100,100              | 0     |
| 21  | CHD  | J     | 3060 | 29/29 | 0.68 | 0.25 | 83,96,100,100              | 0     |
| 23  | PEK  | C     | 3265 | 53/53 | 0.70 | 0.27 | 43,72,100,100              | 0     |
| 18  | TGL  | N     | 4522 | 63/63 | 0.71 | 0.28 | 38,63,76,84                | 0     |
| 18  | TGL  | N     | 4521 | 63/63 | 0.72 | 0.26 | 42,72,80,83                | 0     |
| 18  | TGL  | A     | 3521 | 63/63 | 0.73 | 0.27 | 45,70,80,84                | 0     |
| 19  | PGV  | A     | 3524 | 51/51 | 0.73 | 0.26 | 29,69,99,100               | 0     |

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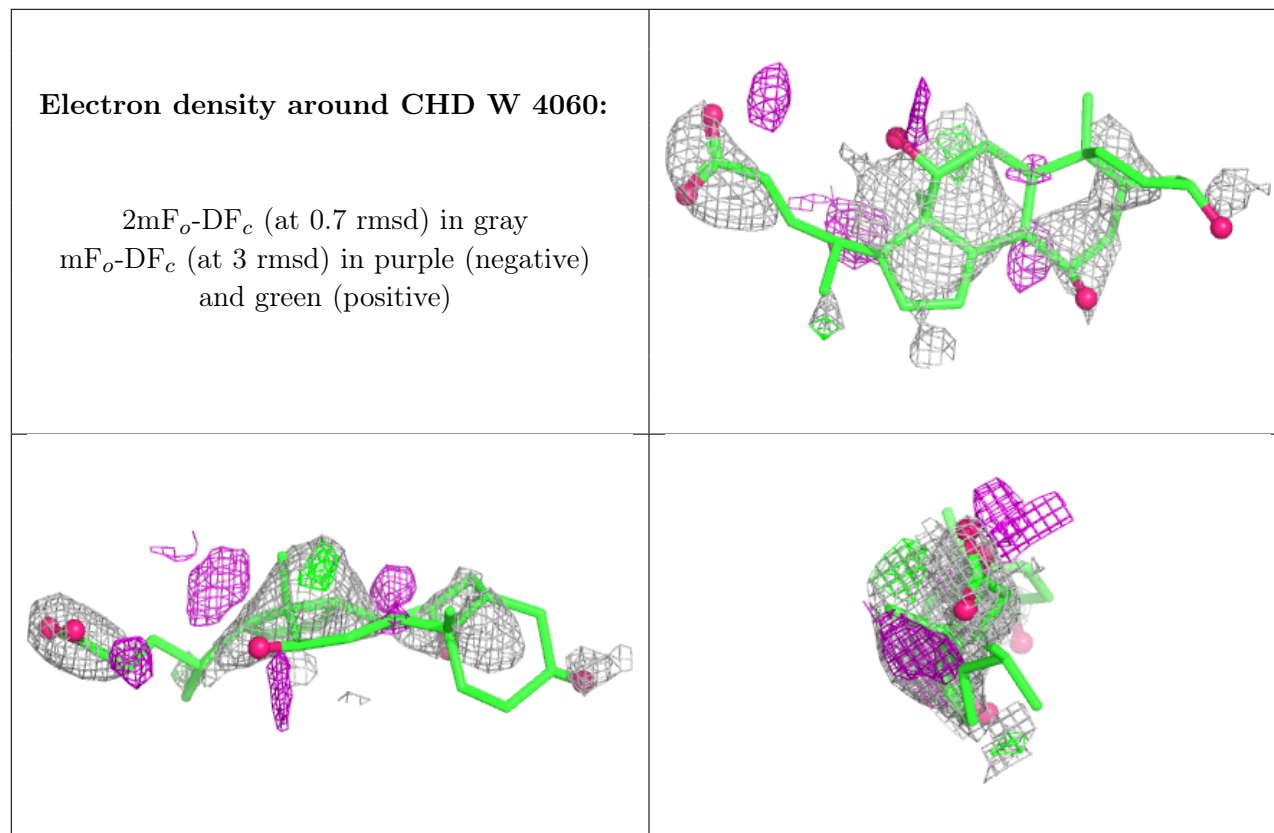
| Mol | Type | Chain | Res  | Atoms   | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|---------|------|------|----------------------------|-------|
| 19  | PGV  | C     | 3268 | 51/51   | 0.73 | 0.28 | 56,84,99,100               | 0     |
| 23  | PEK  | P     | 4265 | 53/53   | 0.73 | 0.28 | 44,70,100,100              | 0     |
| 19  | PGV  | N     | 4524 | 51/51   | 0.73 | 0.25 | 35,68,100,100              | 0     |
| 25  | PSC  | O     | 4230 | 52/52   | 0.73 | 0.29 | 46,79,100,100              | 0     |
| 23  | PEK  | G     | 4263 | 53/53   | 0.74 | 0.27 | 44,87,100,100              | 0     |
| 19  | PGV  | P     | 4268 | 51/51   | 0.74 | 0.27 | 62,83,98,100               | 0     |
| 21  | CHD  | C     | 3271 | 29/29   | 0.75 | 0.23 | 80,93,96,98                | 0     |
| 22  | CDL  | G     | 3269 | 100/100 | 0.75 | 0.27 | 48,87,100,100              | 0     |
| 22  | CDL  | T     | 4269 | 100/100 | 0.75 | 0.27 | 45,85,100,100              | 0     |
| 18  | TGL  | Q     | 4523 | 63/63   | 0.75 | 0.26 | 50,69,84,87                | 0     |
| 18  | TGL  | A     | 3523 | 63/63   | 0.76 | 0.26 | 49,66,83,87                | 0     |
| 25  | PSC  | E     | 3230 | 52/52   | 0.76 | 0.26 | 49,83,100,100              | 0     |
| 18  | TGL  | A     | 3522 | 63/63   | 0.76 | 0.28 | 31,61,76,79                | 0     |
| 22  | CDL  | P     | 4270 | 100/100 | 0.77 | 0.26 | 36,88,99,100               | 0     |
| 21  | CHD  | P     | 4271 | 29/29   | 0.77 | 0.23 | 79,91,95,97                | 0     |
| 22  | CDL  | C     | 3270 | 100/100 | 0.78 | 0.26 | 37,87,99,100               | 0     |
| 27  | DMU  | Z     | 4526 | 33/33   | 0.84 | 0.13 | 36,54,68,70                | 0     |
| 24  | UNX  | C     | 3262 | 1/1     | 0.88 | 0.34 | 33,33,33,33                | 0     |
| 24  | UNX  | P     | 4262 | 1/1     | 0.89 | 0.36 | 28,28,28,28                | 0     |
| 27  | DMU  | M     | 3526 | 33/33   | 0.91 | 0.12 | 28,45,64,67                | 0     |
| 16  | NA   | N     | 4519 | 1/1     | 0.94 | 0.08 | 30,30,30,30                | 0     |
| 23  | PEK  | P     | 4264 | 53/53   | 0.94 | 0.13 | 25,42,70,71                | 0     |
| 23  | PEK  | C     | 3264 | 53/53   | 0.95 | 0.13 | 21,41,70,72                | 0     |
| 16  | NA   | A     | 3519 | 1/1     | 0.95 | 0.06 | 25,25,25,25                | 0     |
| 21  | CHD  | P     | 4525 | 29/29   | 0.95 | 0.07 | 21,27,30,31                | 0     |
| 19  | PGV  | P     | 4267 | 51/51   | 0.96 | 0.10 | 20,29,57,59                | 0     |
| 19  | PGV  | C     | 3267 | 51/51   | 0.96 | 0.11 | 20,30,54,59                | 0     |
| 21  | CHD  | C     | 3525 | 29/29   | 0.96 | 0.06 | 18,25,28,32                | 0     |
| 19  | PGV  | A     | 3266 | 51/51   | 0.96 | 0.09 | 17,27,49,51                | 0     |
| 19  | PGV  | N     | 4266 | 51/51   | 0.96 | 0.09 | 19,30,48,53                | 0     |
| 15  | MG   | N     | 4518 | 1/1     | 0.96 | 0.05 | 27,27,27,27                | 0     |
| 20  | CUA  | O     | 228  | 2/2     | 0.97 | 0.04 | 24,24,24,27                | 0     |
| 21  | CHD  | O     | 3085 | 29/29   | 0.97 | 0.05 | 18,22,26,30                | 0     |
| 21  | CHD  | B     | 4085 | 29/29   | 0.97 | 0.05 | 18,22,29,33                | 0     |
| 15  | MG   | A     | 3518 | 1/1     | 0.99 | 0.03 | 17,17,17,17                | 0     |
| 17  | HEA  | A     | 515  | 60/60   | 0.99 | 0.05 | 13,19,30,33                | 0     |
| 17  | HEA  | A     | 516  | 60/60   | 0.99 | 0.05 | 12,17,25,27                | 0     |
| 17  | HEA  | N     | 515  | 60/60   | 0.99 | 0.06 | 17,23,33,35                | 0     |
| 26  | ZN   | F     | 99   | 1/1     | 0.99 | 0.02 | 25,25,25,25                | 0     |
| 26  | ZN   | S     | 99   | 1/1     | 0.99 | 0.02 | 28,28,28,28                | 0     |
| 20  | CUA  | B     | 228  | 2/2     | 0.99 | 0.02 | 16,16,16,18                | 0     |
| 17  | HEA  | N     | 516  | 60/60   | 0.99 | 0.05 | 15,19,29,30                | 0     |

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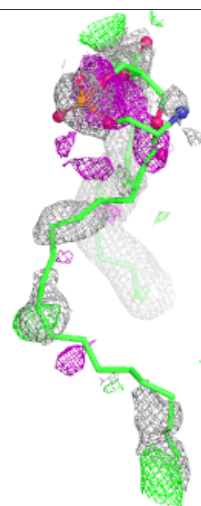
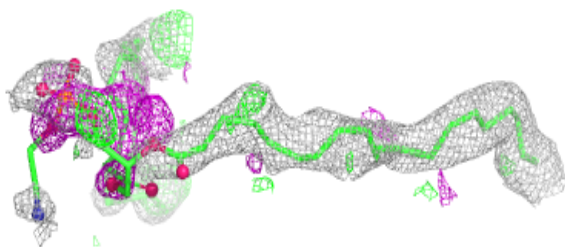
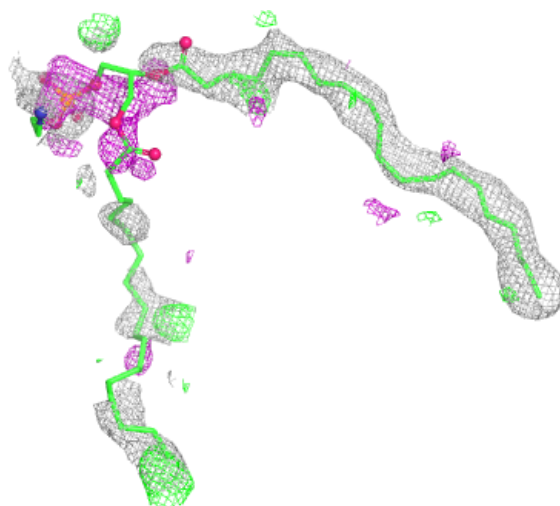
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 14  | CU   | A     | 517 | 1/1   | 1.00 | 0.02 | 16,16,16,16                 | 0     |
| 14  | CU   | N     | 517 | 1/1   | 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.



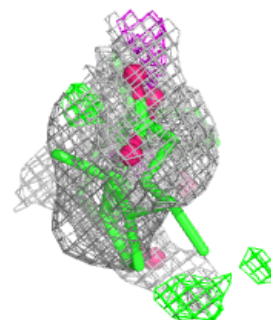
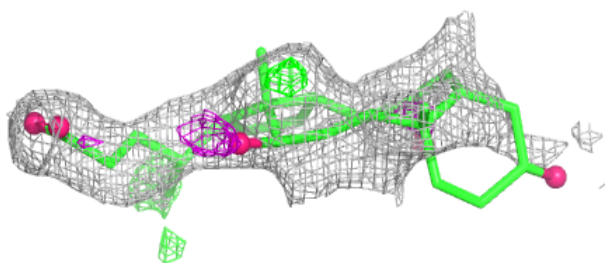
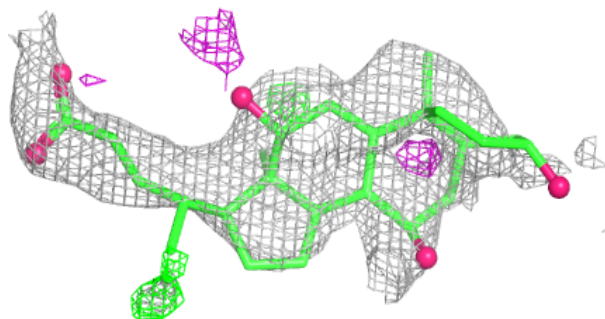
**Electron density around PEK T 3263:**

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



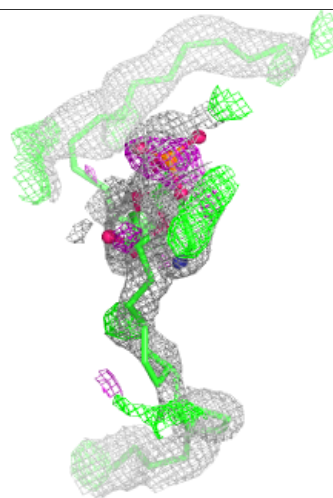
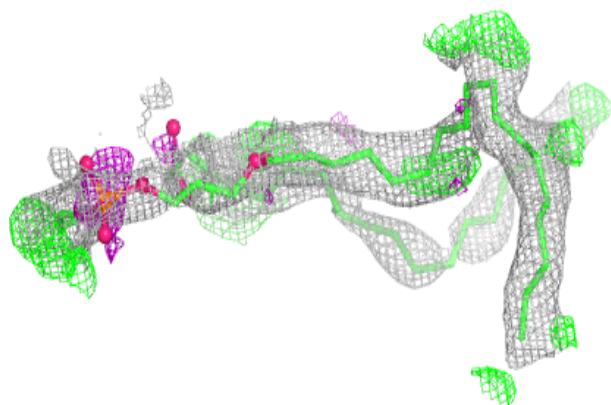
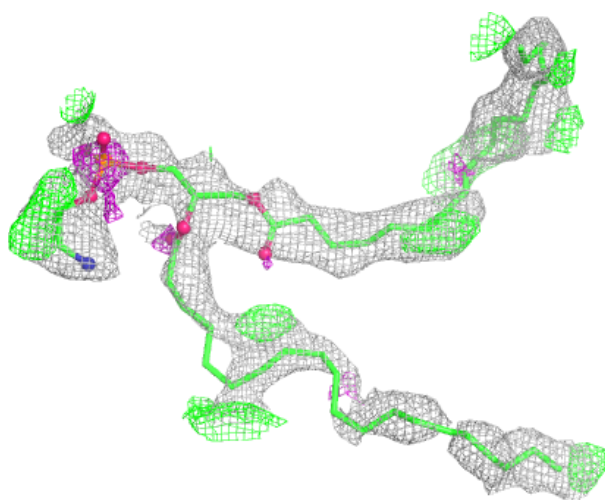
**Electron density around CHD J 3060:**

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



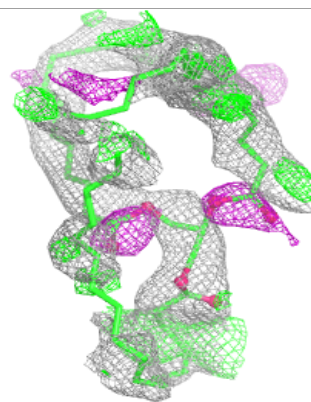
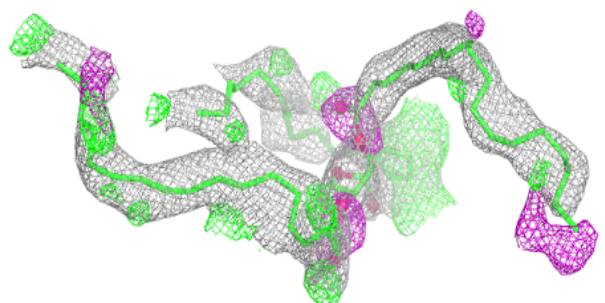
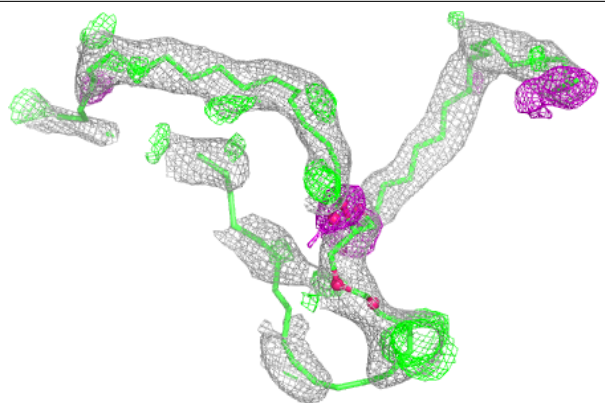
**Electron density around PEK C 3265:**

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

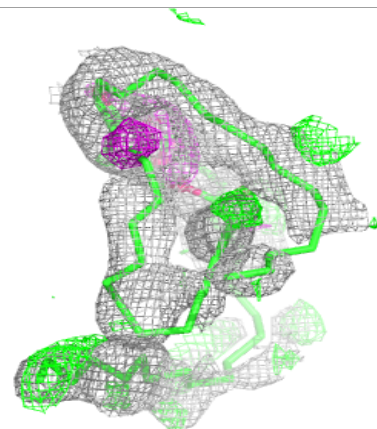
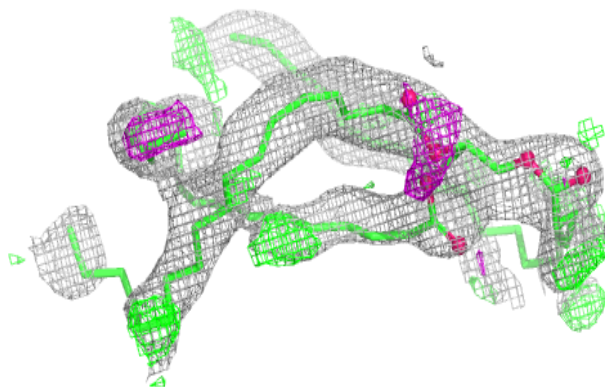
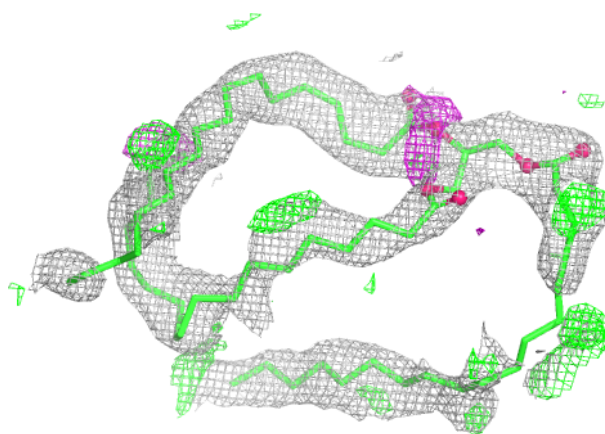


**Electron density around TGL N 4522:**

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

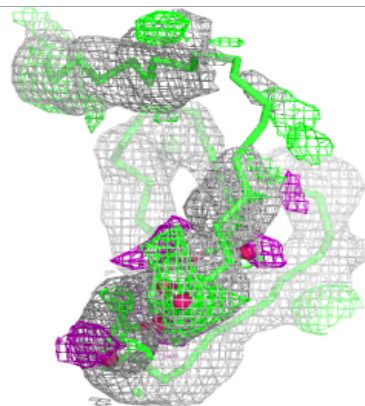
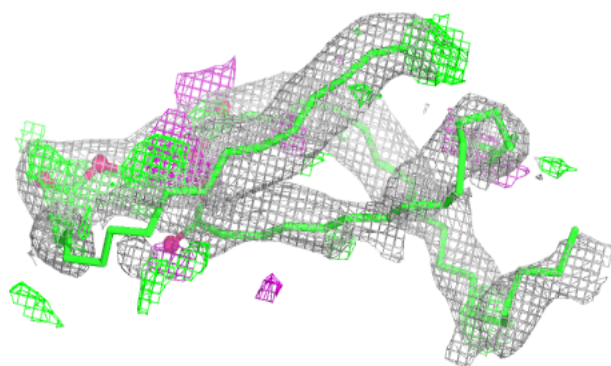
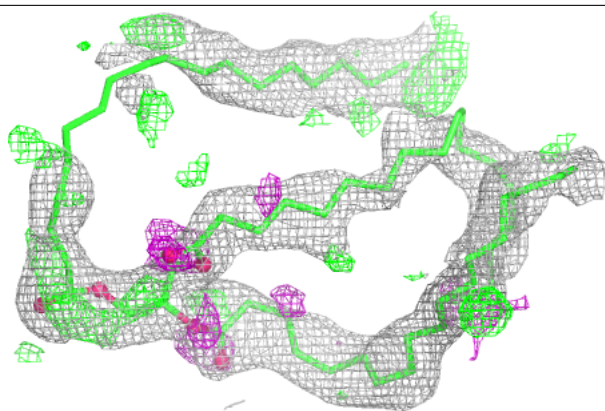
**Electron density around TGL N 4521:**

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

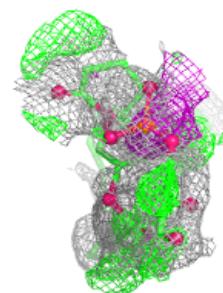
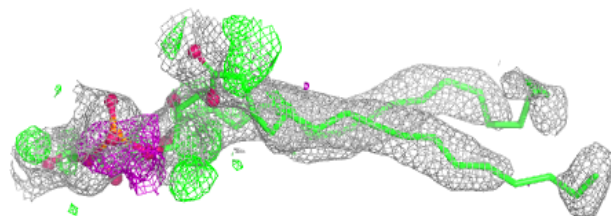
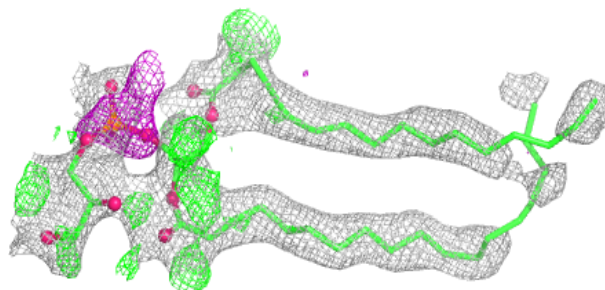


**Electron density around TGL A 3521:**

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and green (positive)

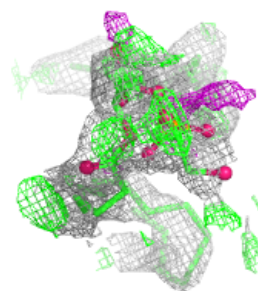
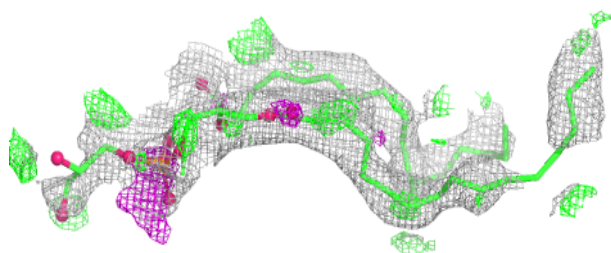
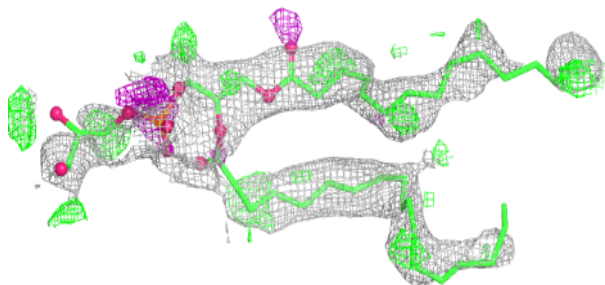
**Electron density around PGV A 3524:**

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and green (positive)



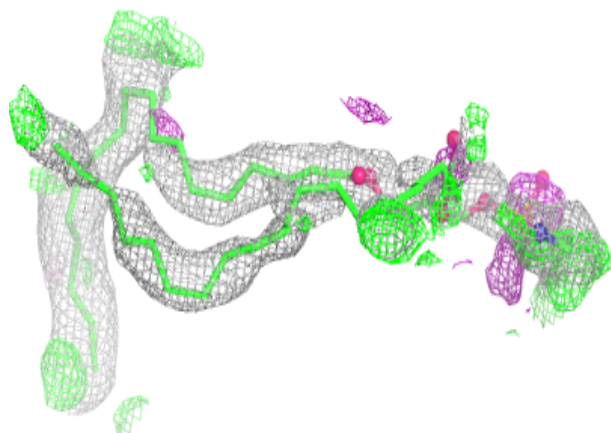
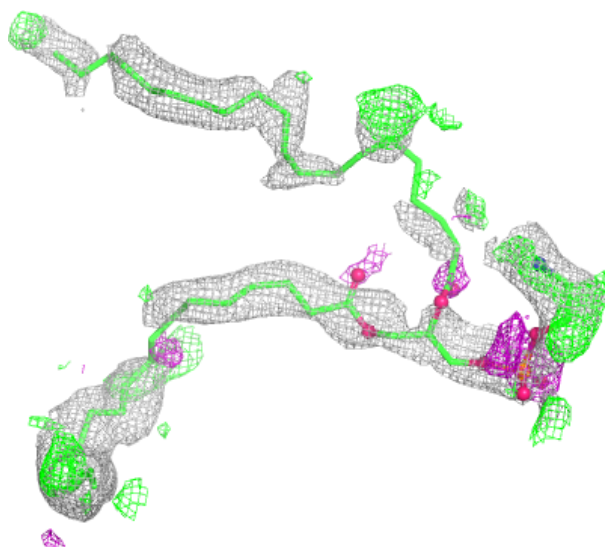
**Electron density around PGV C 3268:**

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



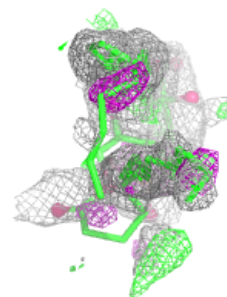
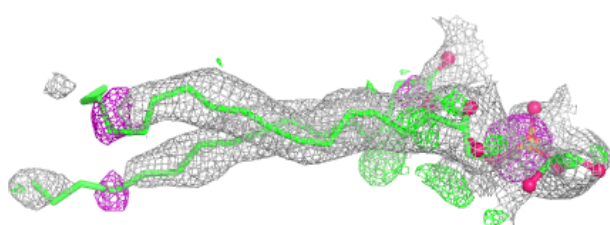
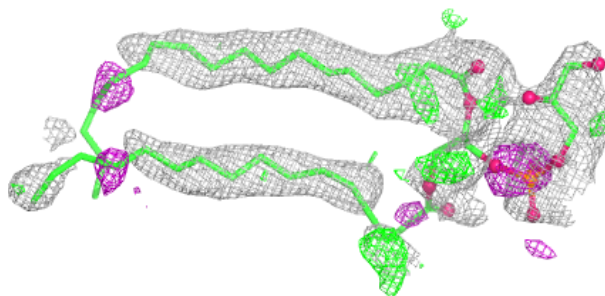
**Electron density around PEK P 4265:**

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and green (positive)

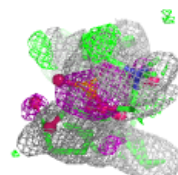
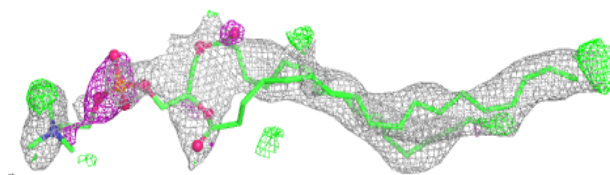
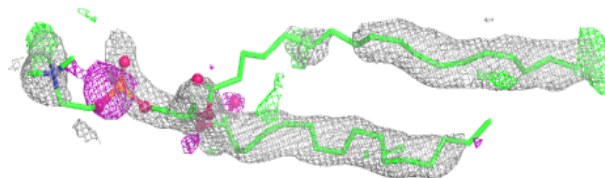


**Electron density around PGV N 4524:**

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and green (positive)

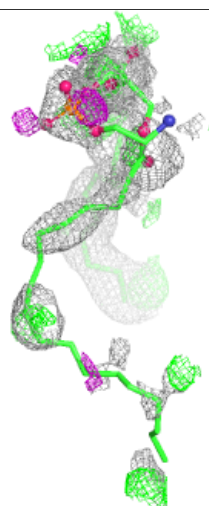
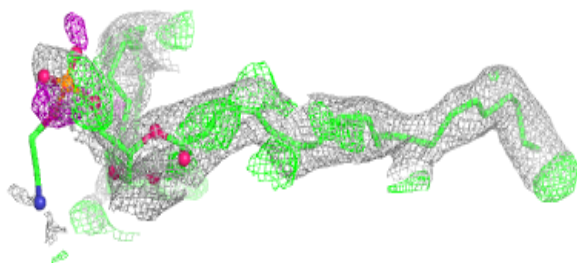
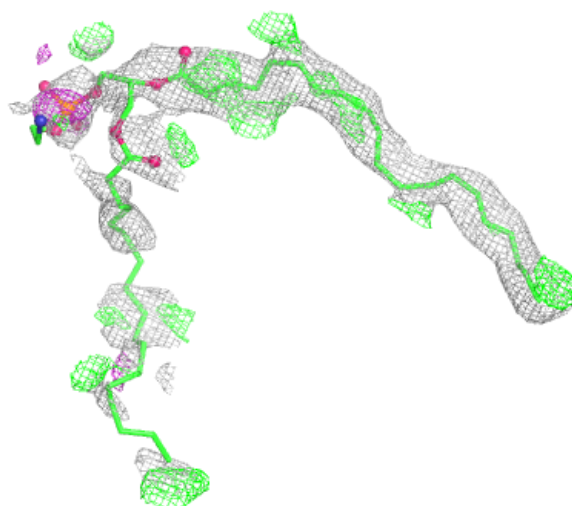
**Electron density around PSC O 4230:**

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and green (positive)



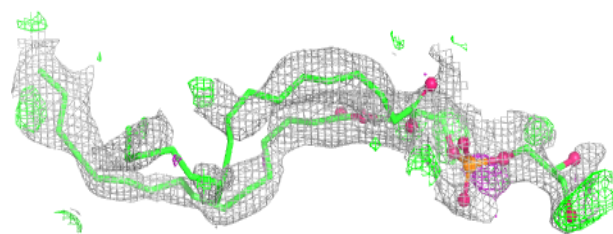
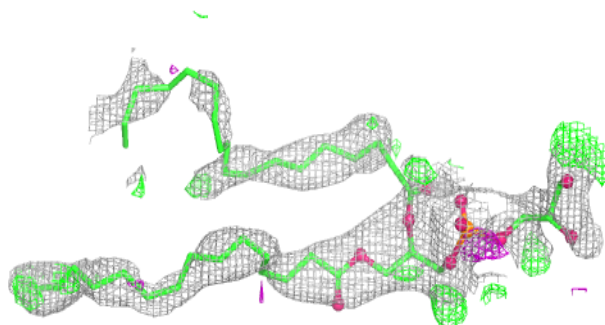
**Electron density around PEK G 4263:**

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and green (positive)

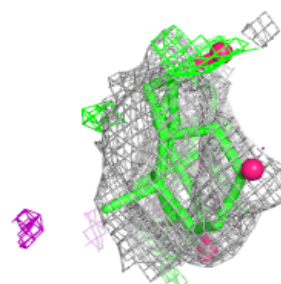
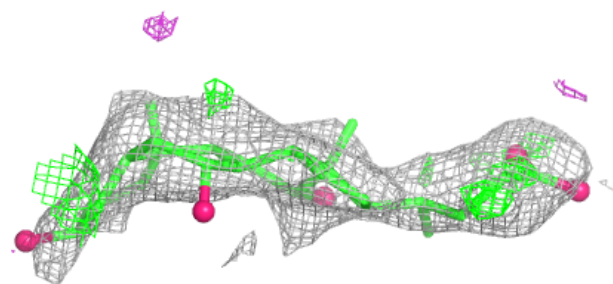
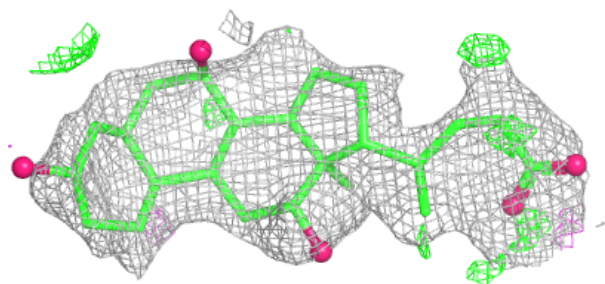


**Electron density around PGV P 4268:**

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

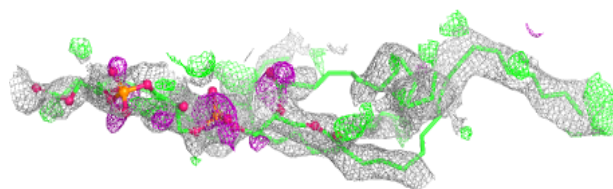
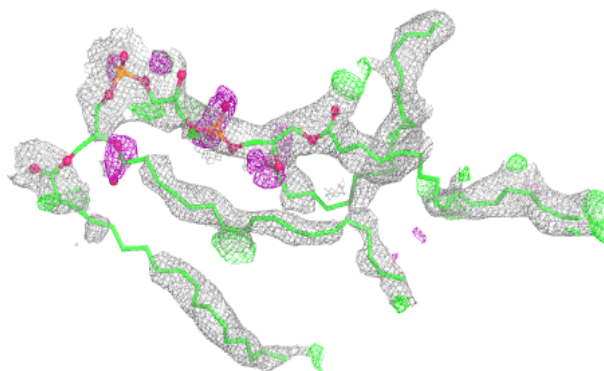
**Electron density around CHD C 3271:**

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

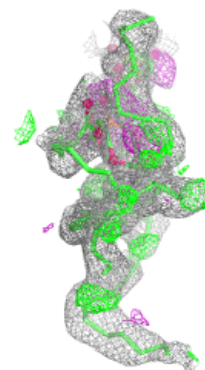
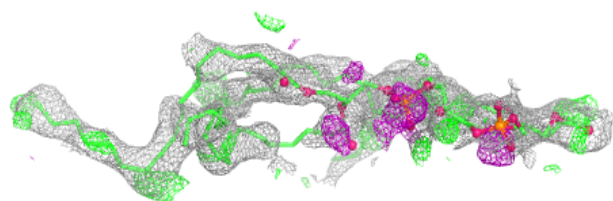
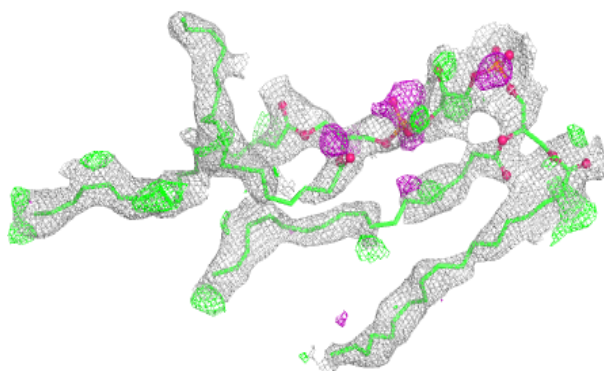


**Electron density around CDL G 3269:**

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

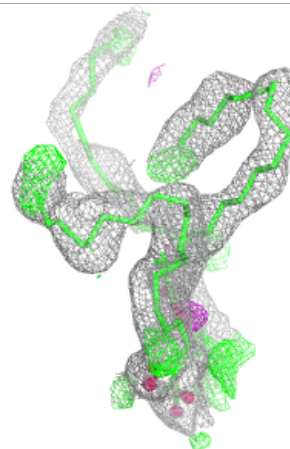
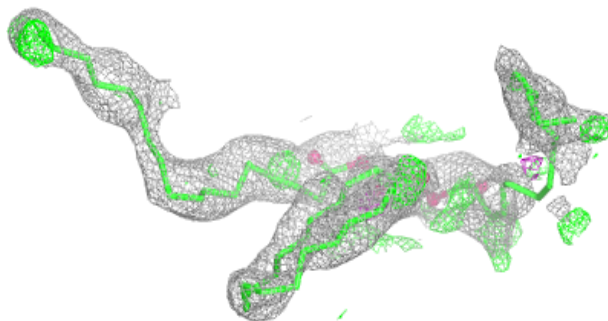
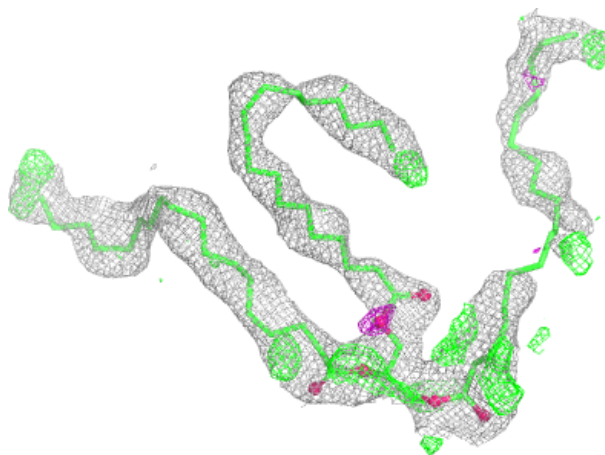
**Electron density around CDL T 4269:**

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



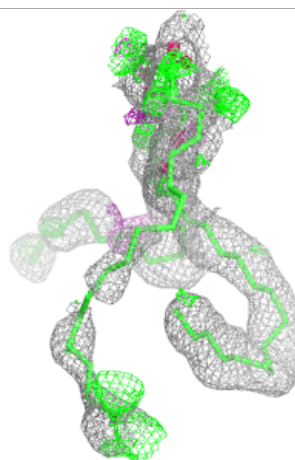
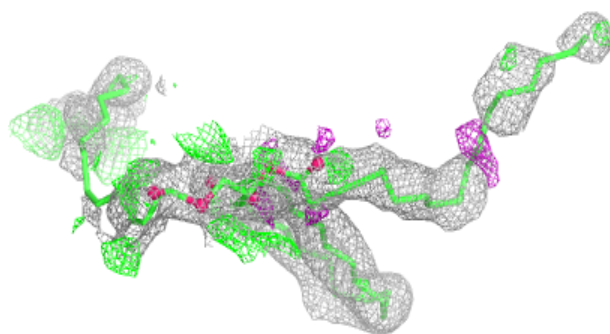
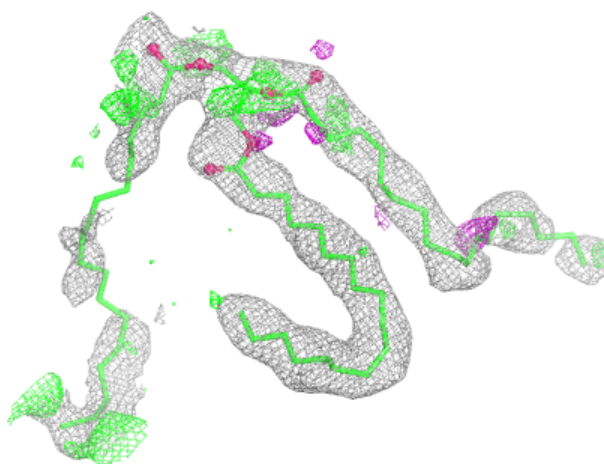
**Electron density around TGL Q 4523:**

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



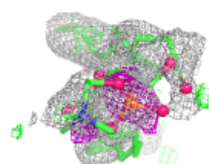
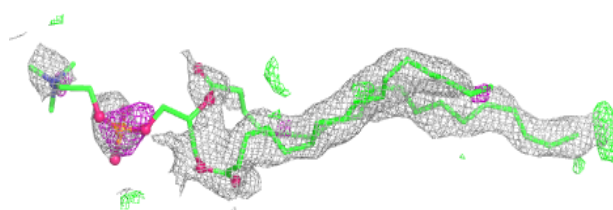
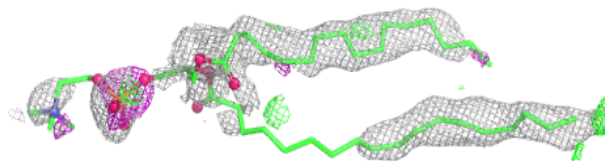
**Electron density around TGL A 3523:**

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

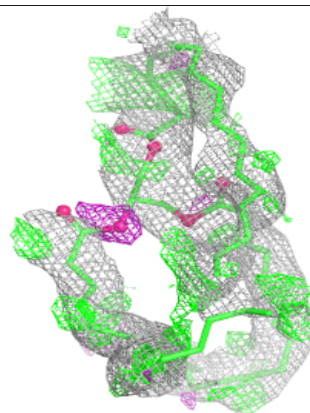
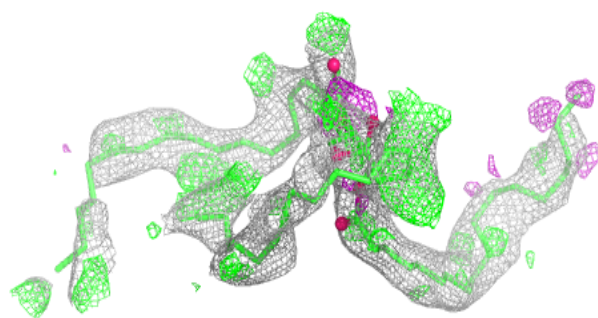
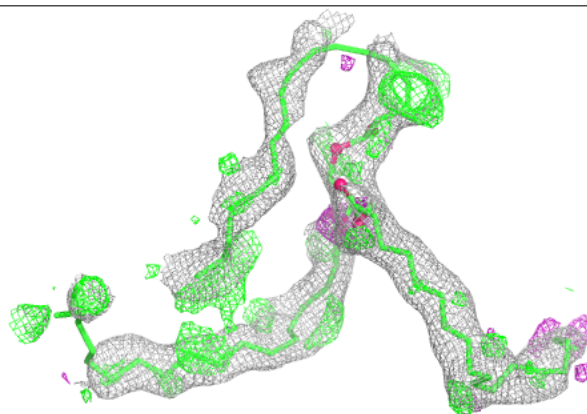


**Electron density around PSC E 3230:**

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

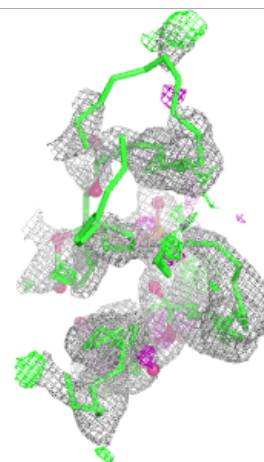
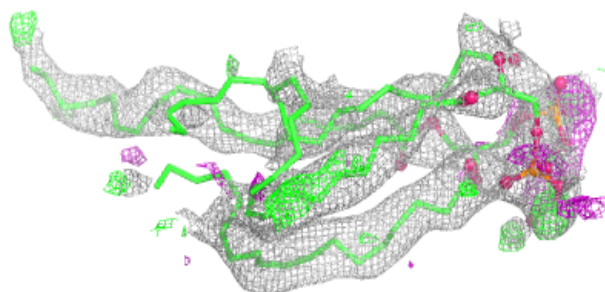
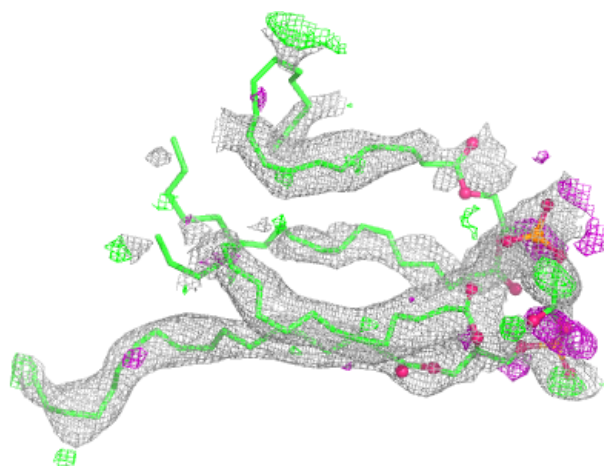
**Electron density around TGL A 3522:**

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



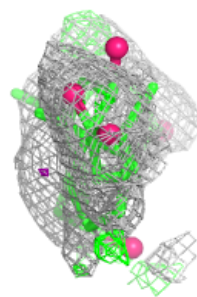
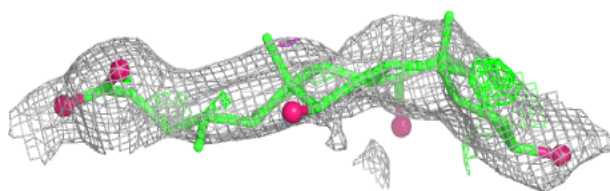
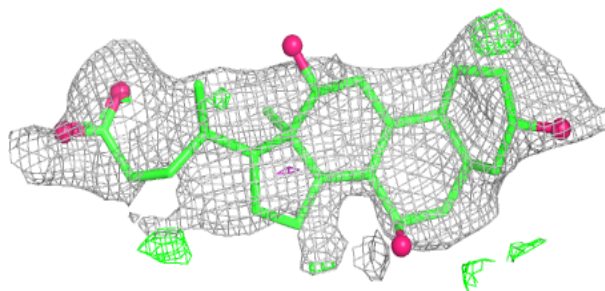
**Electron density around CDL P 4270:**

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

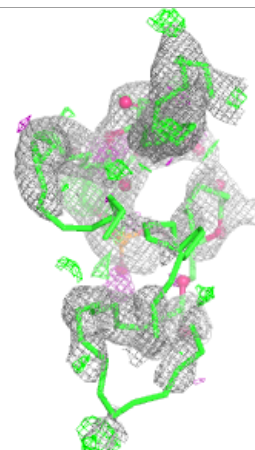
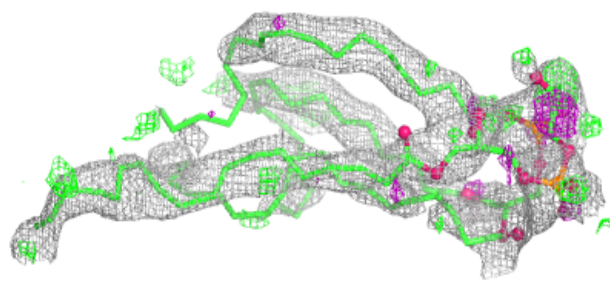
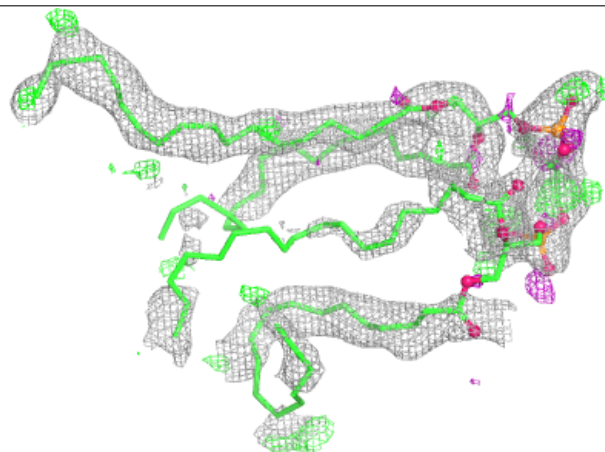


**Electron density around CHD P 4271:**

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

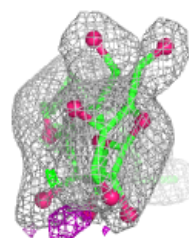
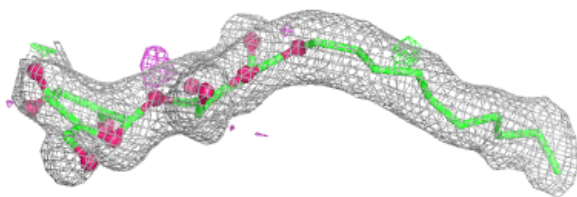
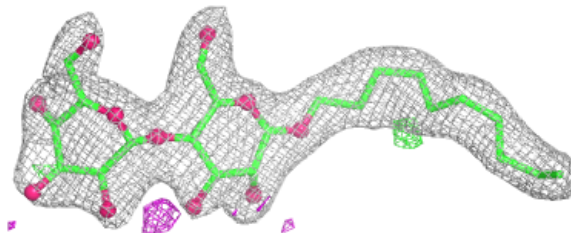
**Electron density around CDL C 3270:**

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

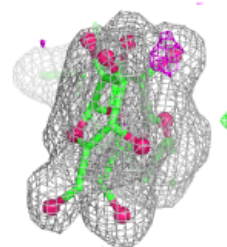
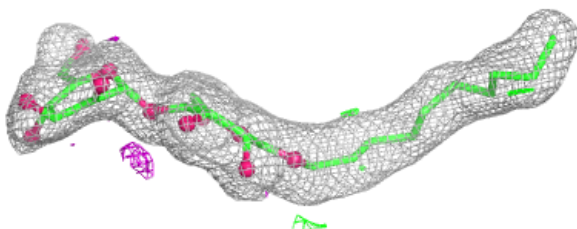
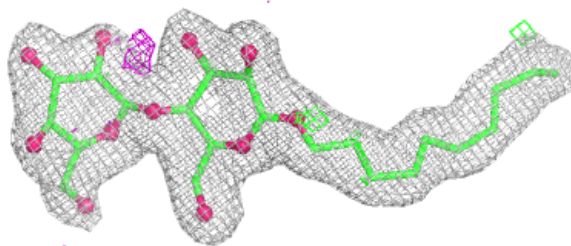


**Electron density around DMU Z 4526:**

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

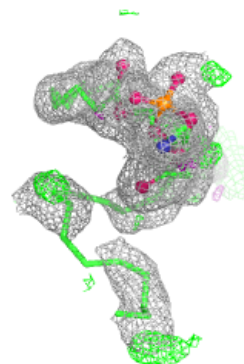
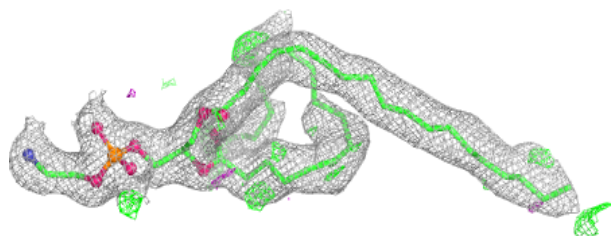
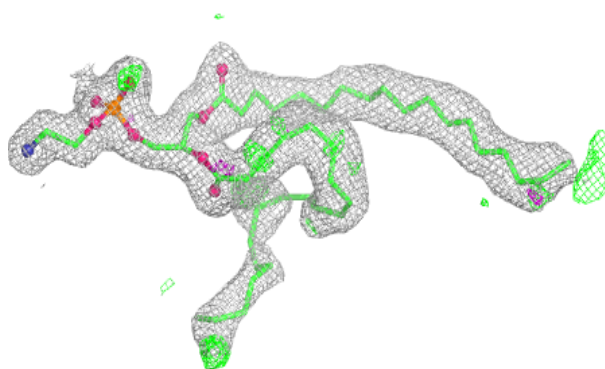
**Electron density around DMU M 3526:**

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

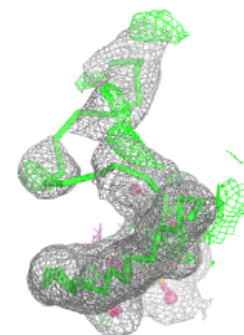
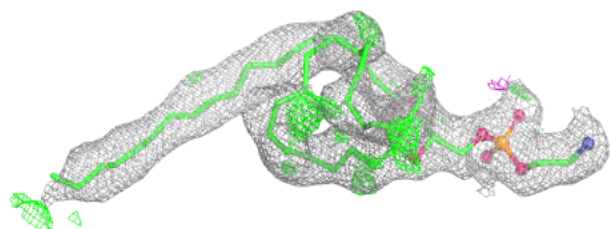
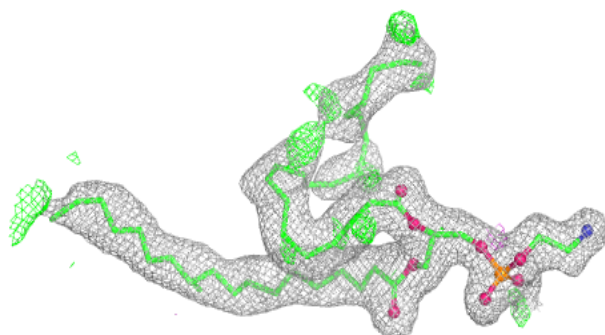


**Electron density around PEK P 4264:**

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

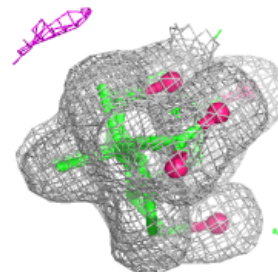
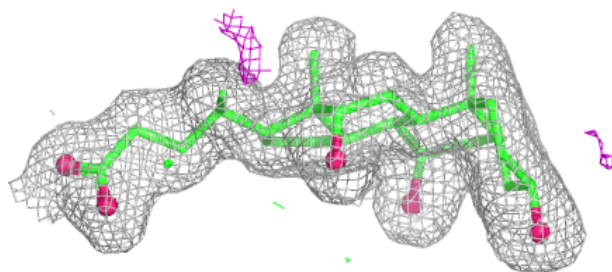
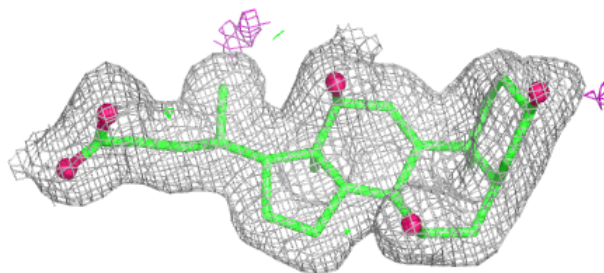
**Electron density around PEK C 3264:**

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

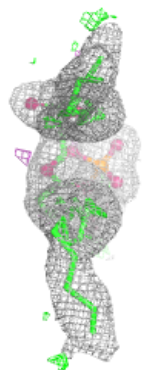
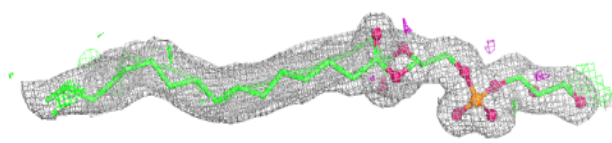
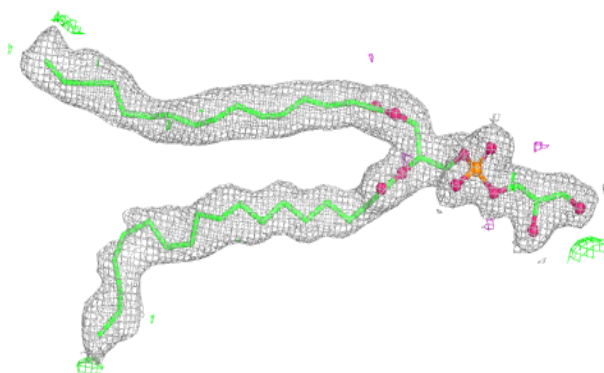


**Electron density around CHD P 4525:**

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

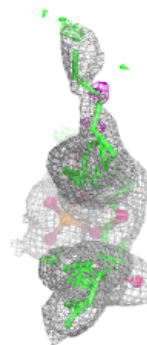
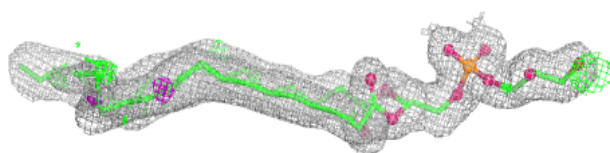
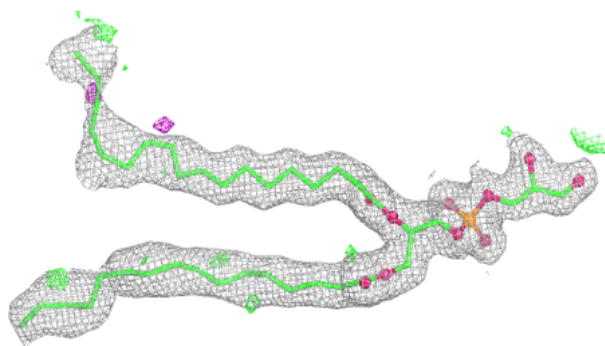
**Electron density around PGV P 4267:**

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

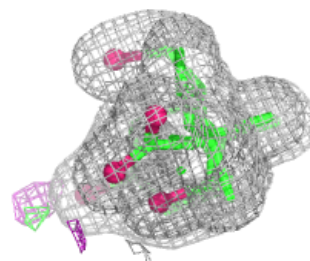
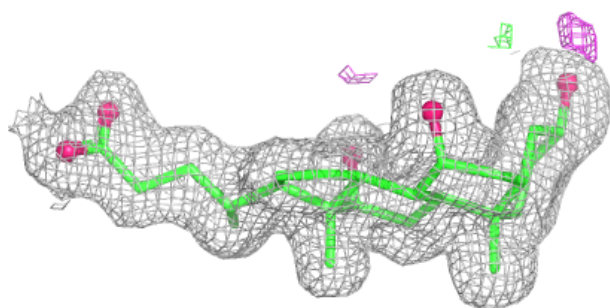
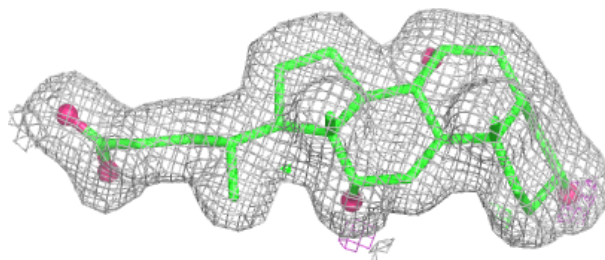


**Electron density around PGV C 3267:**

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

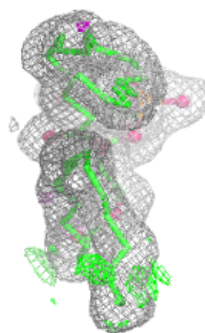
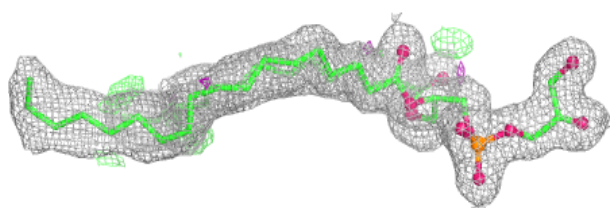
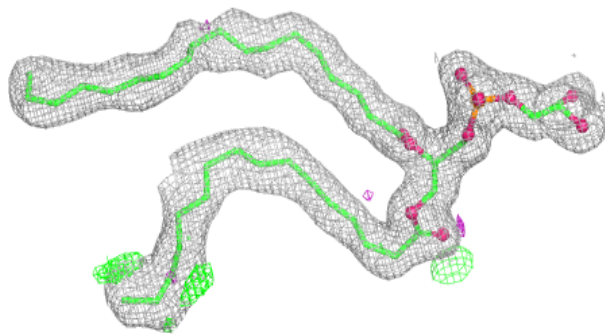
**Electron density around CHD C 3525:**

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

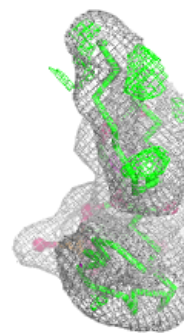
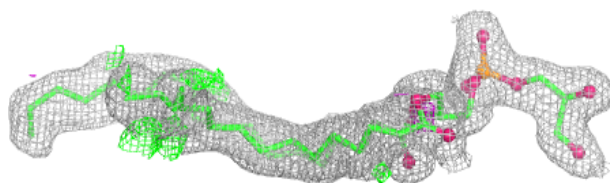
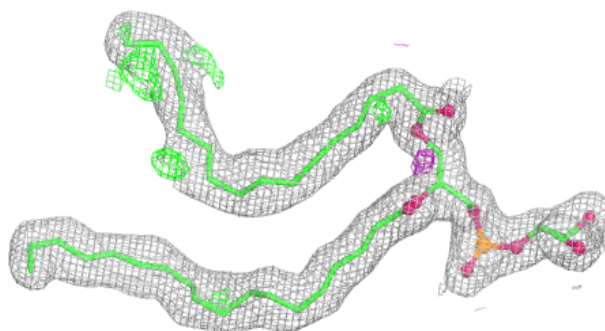


**Electron density around PGV A 3266:**

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

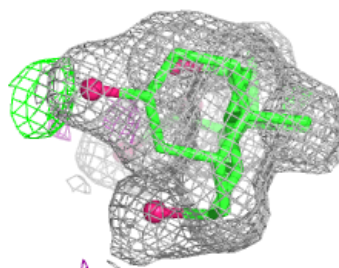
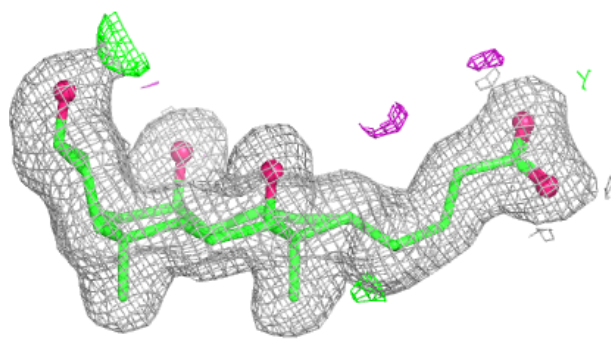
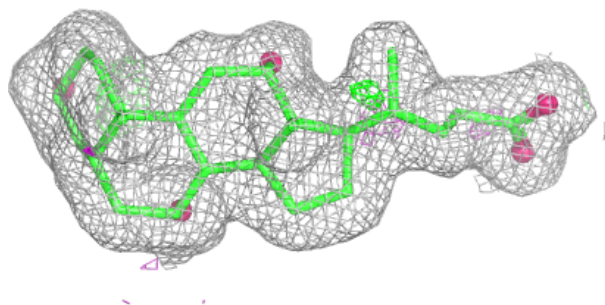
**Electron density around PGV N 4266:**

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

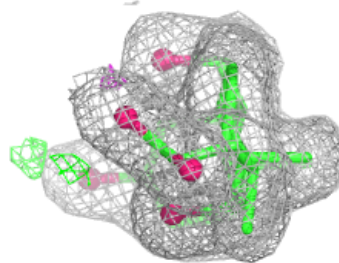
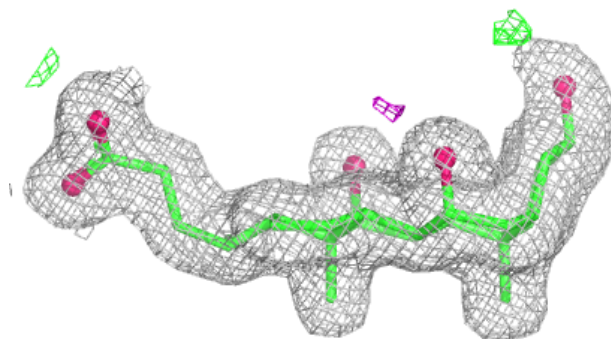
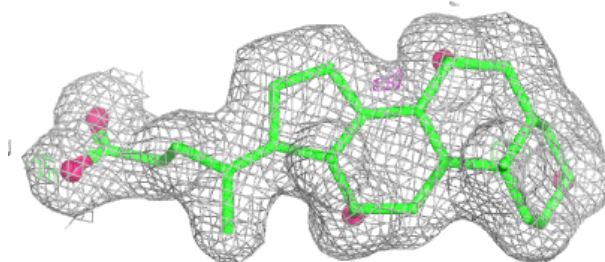


**Electron density around CHD O 3085:**

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

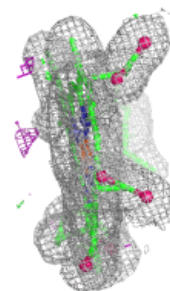
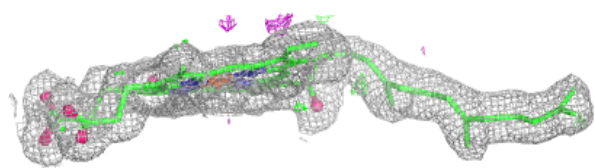
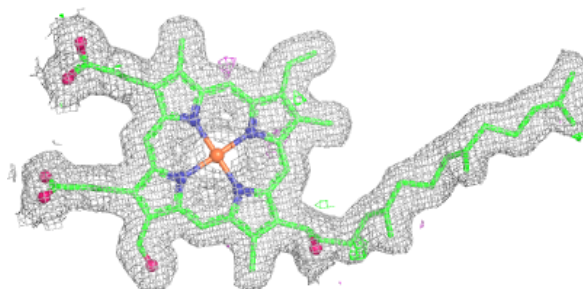
**Electron density around CHD B 4085:**

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

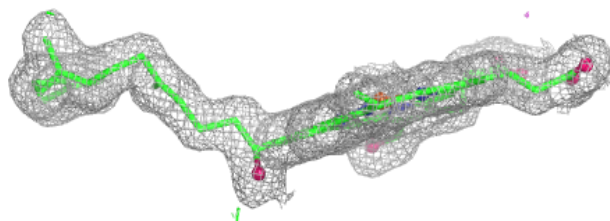
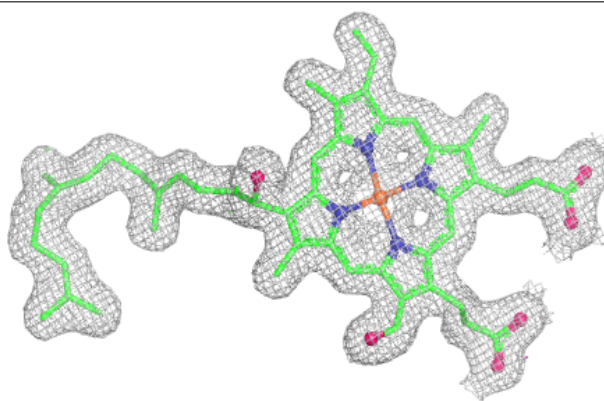


**Electron density around HEA A 515:**

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

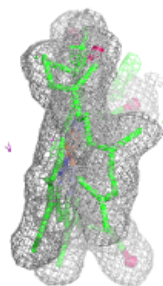
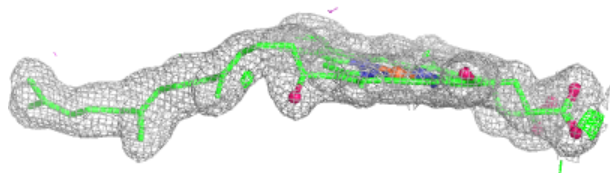
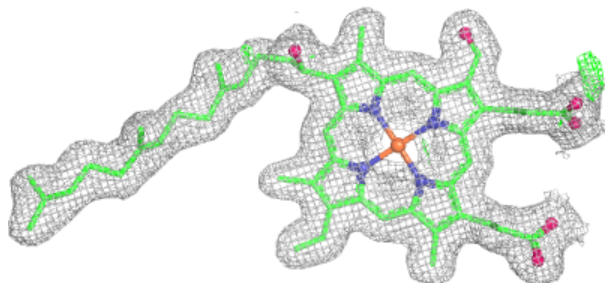
**Electron density around HEA A 516:**

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

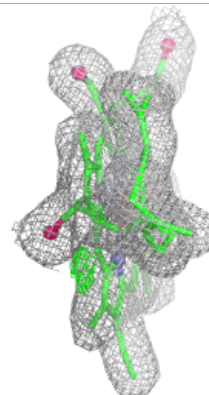
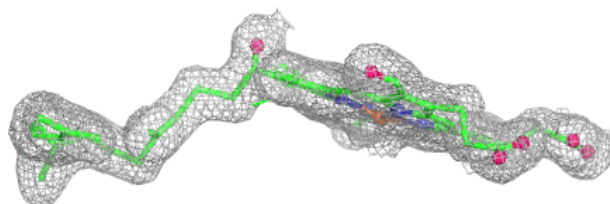
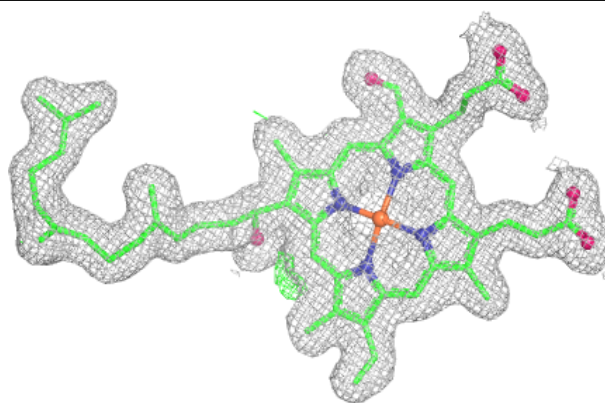


**Electron density around HEA N 515:**

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

**Electron density around HEA N 516:**

$2mF_o-DF_c$  (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.