



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:19 PM EDT

PDB ID : 3WG7 / pdb\_00003wg7  
Title : A 1.9 angstrom radiation damage free X-ray structure of large (420KDa) protein by femtosecond crystallography  
Authors : Hirata, K.; Shinzawa-Itoh, K.; Yano, N.; Takemura, S.; Kato, K.; Hatanaka, M.; Muramoto, K.; Kawahara, T.; Tsukihara, T.; Yamashita, E.; Tono, K.; Ueno, G.; Hikima, T.; Murakami, H.; Inubushi, Y.; Yabashi, M.; Ishikawa, T.; Yamamoto, M.; Ogura, T.; Sugimoto, H.; Shen, J.R.; Yoshikawa, S.; Ago, H.  
Deposited on : 2013-07-29  
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                      | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness           | : | 1.0.12                                                           |
| Ideal geometry (proteins) | : | Engh & Huber (2001)                                              |

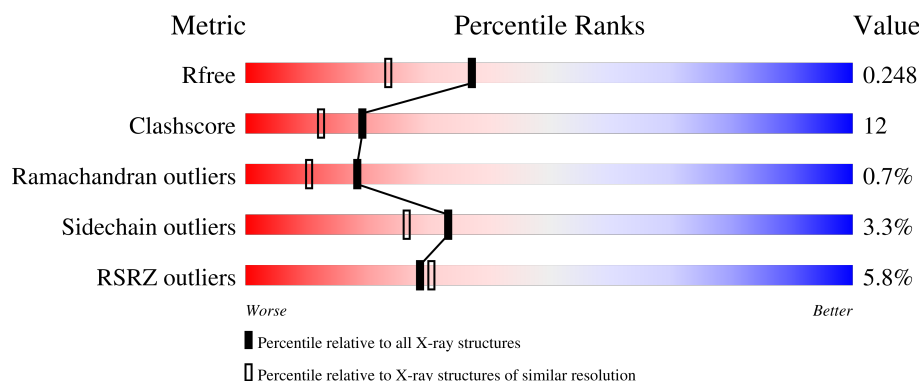
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 7789 (1.90-1.90)                                      |
| Clashscore            | 190562                      | 8410 (1.90-1.90)                                      |
| Ramachandran outliers | 187476                      | 8333 (1.90-1.90)                                      |
| Sidechain outliers    | 187428                      | 8333 (1.90-1.90)                                      |
| RSRZ outliers         | 180081                      | 7790 (1.90-1.90)                                      |

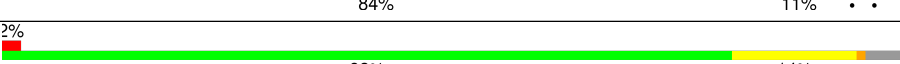
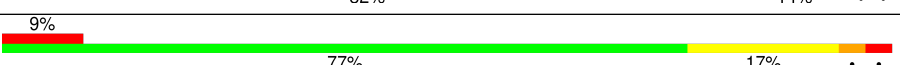
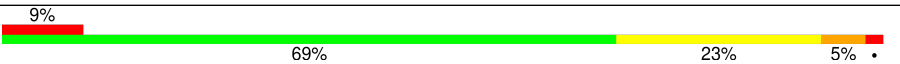
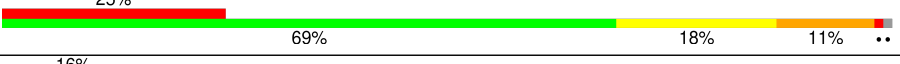
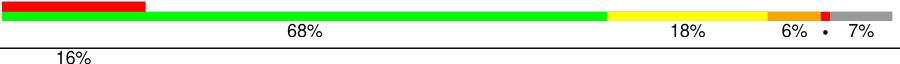
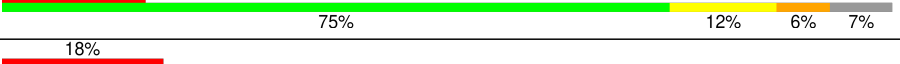
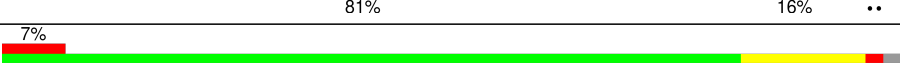
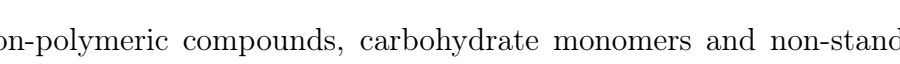
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 514    |  |
| 1   | N     | 514    |  |
| 2   | B     | 227    |  |

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | O     | 227    |    |
| 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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | FME  | O     | 1   | -         | -        | X       | -                |
| 23  | PSC  | N     | 610 | -         | -        | X       | -                |
| 25  | CDL  | C     | 304 | -         | -        | X       | -                |
| 25  | CDL  | G     | 101 | -         | -        | X       | -                |
| 25  | CDL  | T     | 102 | -         | -        | X       | -                |
| 27  | DMU  | M     | 101 | X         | -        | -       | -                |
| 27  | DMU  | Z     | 101 | X         | -        | -       | -                |

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 514      | Total | C    | N   | O   | S  | 0       | 6       | 0     |
|     |       |          | 4074  | 2725 | 629 | 684 | 36 |         |         |       |
| 1   | N     | 514      | Total | C    | N   | O   | S  | 0       | 6       | 0     |
|     |       |          | 4074  | 2725 | 629 | 684 | 36 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 227      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 1832  | 1189 | 282 | 343 | 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 subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 259      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2134  | 1427 | 339 | 353 | 15 |         |         |       |
| 3   | P     | 259      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2134  | 1427 | 339 | 353 | 15 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 144      | Total | C   | N   | O   | S | 0       | 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 subunit 5A, mitochondrial.

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

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

| 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 subunit 6A2, mitochondrial.

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

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

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

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

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

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

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

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

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

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

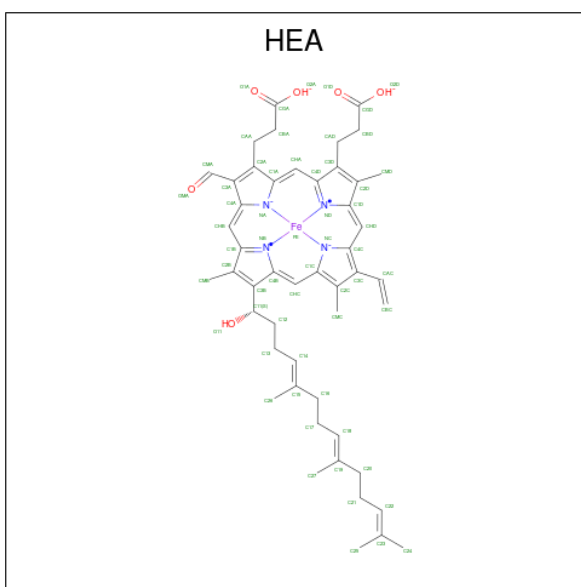
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 13  | M     | 43       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 335   | 223 | 53 | 59 |         |         |       |
| 13  | Z     | 43       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 335   | 223 | 53 | 59 |         |         |       |

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



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

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

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

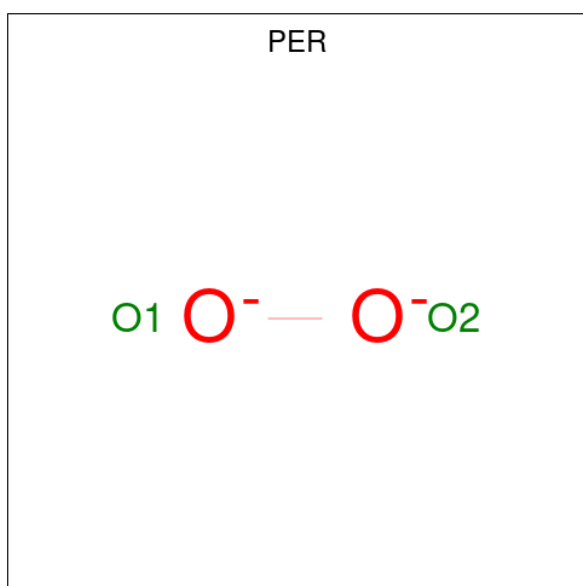
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

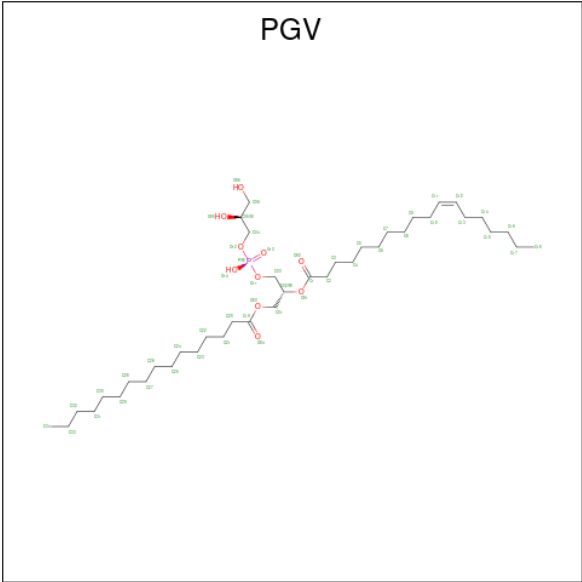
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 17  | A     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 17  | C     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 17  | N     | 1   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

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



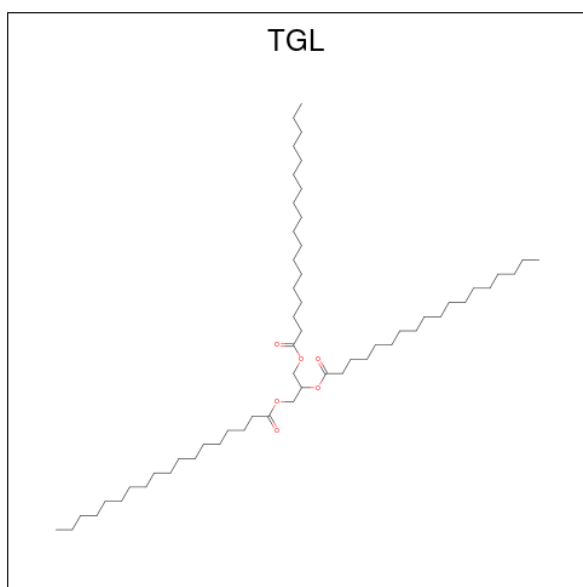
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 18  | A     | 1        | Total<br>4 | O<br>4 | 0       | 1       |
| 18  | N     | 1        | Total<br>4 | O<br>4 | 0       | 1       |

- 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).



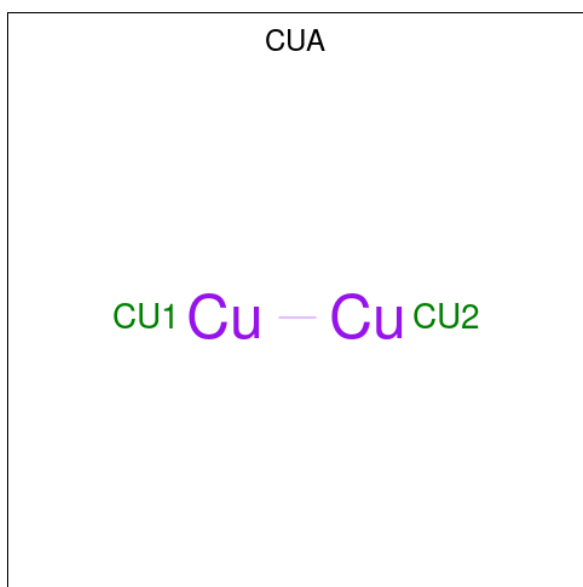
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | A     | 1        | 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 TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



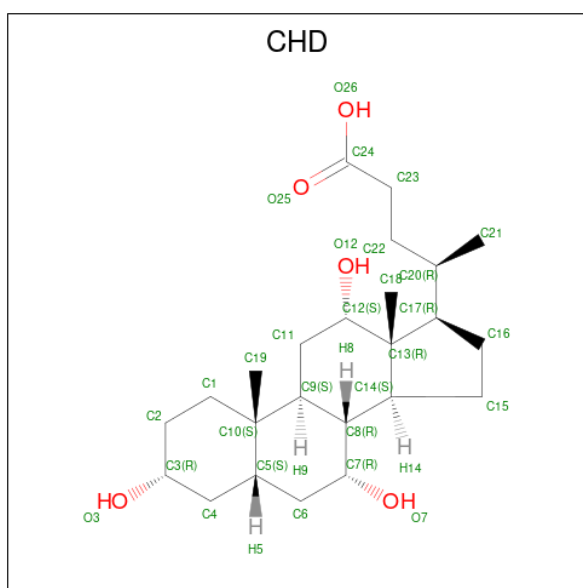
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 20  | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 20  | D     | 1        | Total | C  | O | 0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

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



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

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula:  $C_{24}H_{40}O_5$ ).



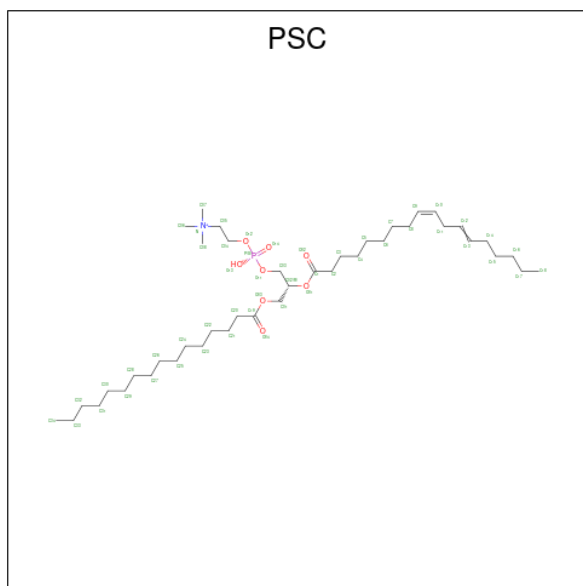
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 22  | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 22  | C     | 1        | Total | C  | O | 0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

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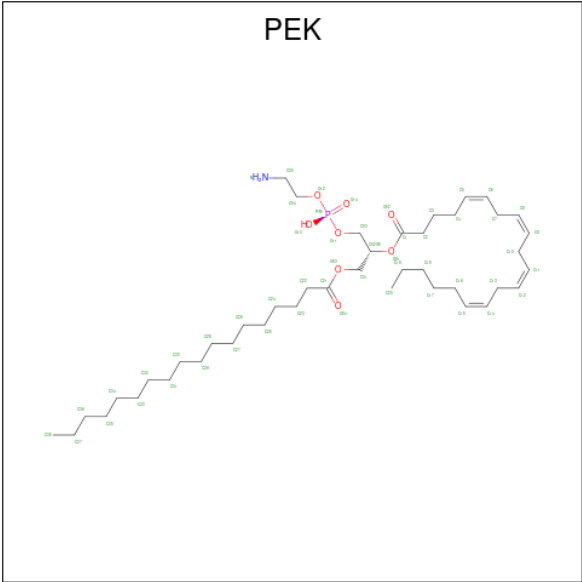
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 22  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 22  | G     | 1        | Total | C  | O | 0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

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula:  $C_{42}H_{81}NO_8P$ ).



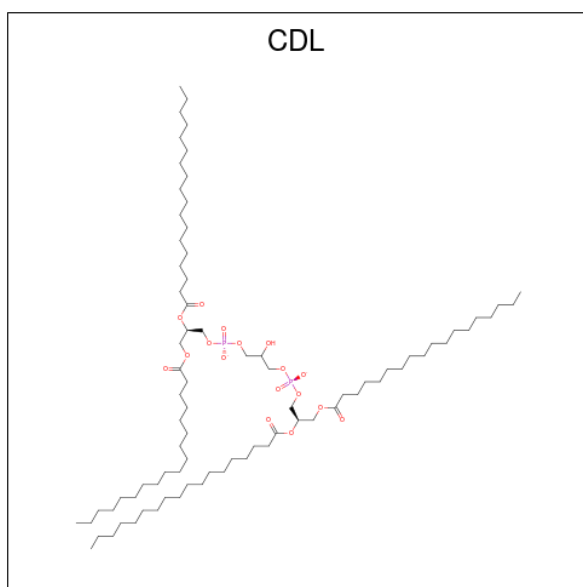
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 23  | B     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |
| 23  | N   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

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula:  $C_{43}H_{78}NO_8P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 24  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 24  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 24  | G     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 24  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 24  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 24  | T     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).

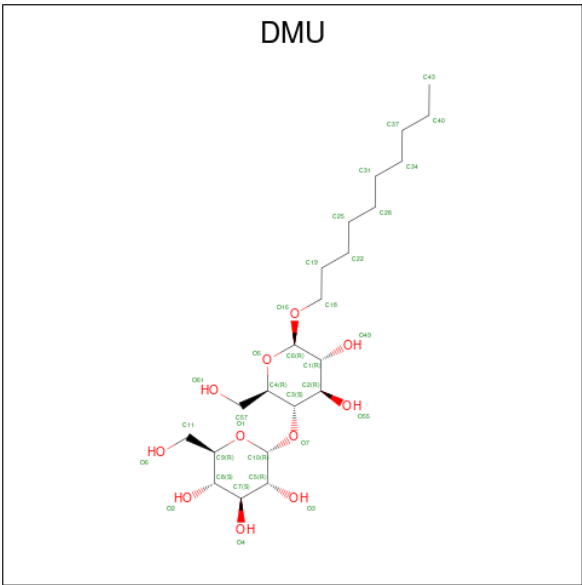


| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 25  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 25  | G     | 1       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

- Molecule 26 is 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     | 265      | Total | O   | 0       | 0       |
|     |       |          | 265   | 265 |         |         |
| 28  | B     | 194      | Total | O   | 0       | 0       |
|     |       |          | 194   | 194 |         |         |
| 28  | C     | 141      | Total | O   | 0       | 0       |
|     |       |          | 141   | 141 |         |         |
| 28  | D     | 160      | Total | O   | 0       | 0       |
|     |       |          | 160   | 160 |         |         |
| 28  | E     | 125      | Total | O   | 0       | 0       |
|     |       |          | 125   | 125 |         |         |
| 28  | F     | 112      | Total | O   | 0       | 0       |
|     |       |          | 112   | 112 |         |         |
| 28  | G     | 70       | Total | O   | 0       | 0       |
|     |       |          | 70    | 70  |         |         |
| 28  | H     | 70       | Total | O   | 0       | 0       |
|     |       |          | 70    | 70  |         |         |
| 28  | I     | 52       | Total | O   | 0       | 0       |
|     |       |          | 52    | 52  |         |         |
| 28  | J     | 31       | Total | O   | 0       | 0       |
|     |       |          | 31    | 31  |         |         |

Continued on next page...

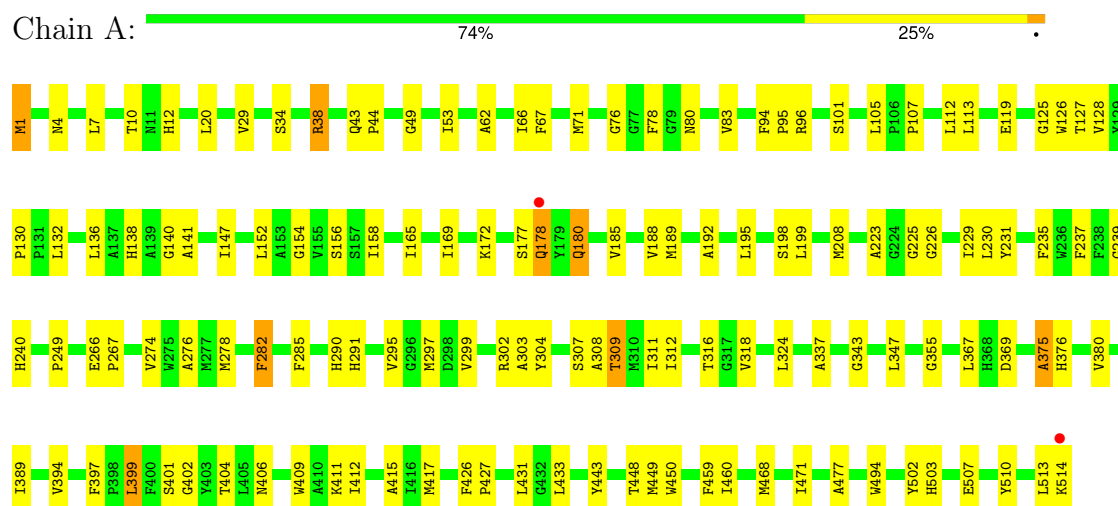
*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 28  | K     | 40       | Total<br>40  | O<br>40  | 0       | 0       |
| 28  | L     | 31       | Total<br>31  | O<br>31  | 0       | 0       |
| 28  | M     | 31       | Total<br>31  | O<br>31  | 0       | 0       |
| 28  | N     | 259      | Total<br>259 | O<br>259 | 0       | 0       |
| 28  | O     | 157      | Total<br>157 | O<br>157 | 0       | 0       |
| 28  | P     | 143      | Total<br>143 | O<br>143 | 0       | 0       |
| 28  | Q     | 90       | Total<br>90  | O<br>90  | 0       | 0       |
| 28  | R     | 103      | Total<br>103 | O<br>103 | 0       | 0       |
| 28  | S     | 122      | Total<br>122 | O<br>122 | 0       | 0       |
| 28  | T     | 56       | Total<br>56  | O<br>56  | 0       | 0       |
| 28  | U     | 51       | Total<br>51  | O<br>51  | 0       | 0       |
| 28  | V     | 42       | Total<br>42  | O<br>42  | 0       | 0       |
| 28  | W     | 38       | Total<br>38  | O<br>38  | 0       | 0       |
| 28  | X     | 34       | Total<br>34  | O<br>34  | 0       | 0       |
| 28  | Y     | 37       | Total<br>37  | O<br>37  | 0       | 0       |
| 28  | Z     | 24       | Total<br>24  | O<br>24  | 0       | 0       |

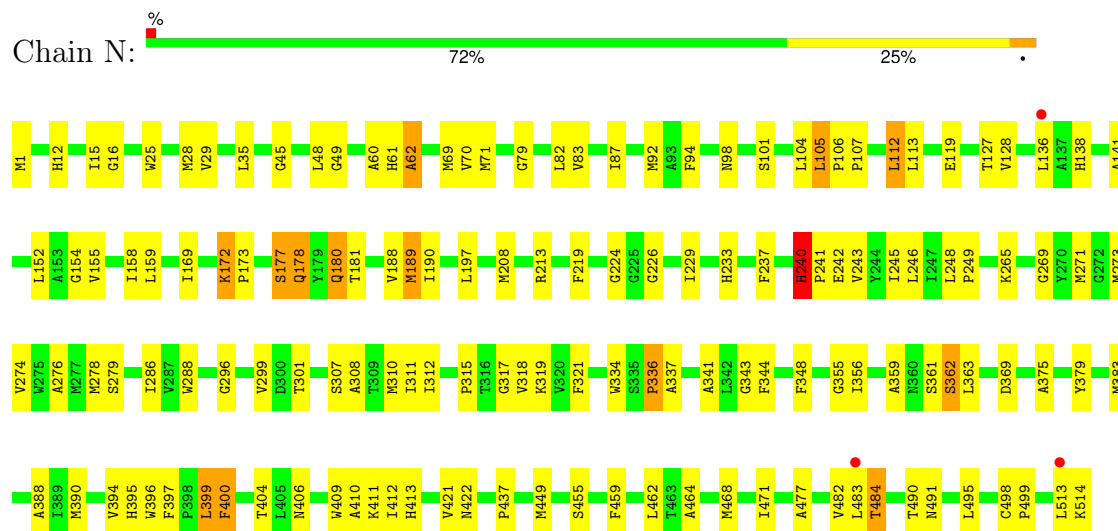
### 3 Residue-property plots

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

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

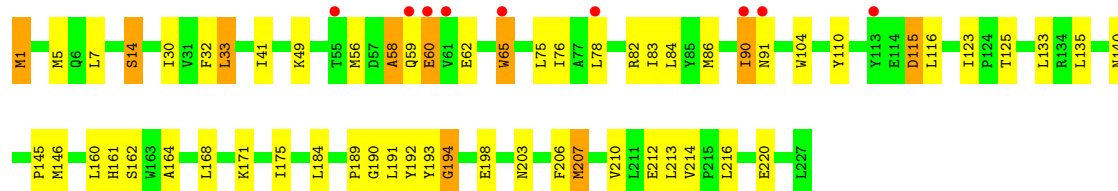


#### • Molecule 1: Cytochrome c oxidase subunit 1

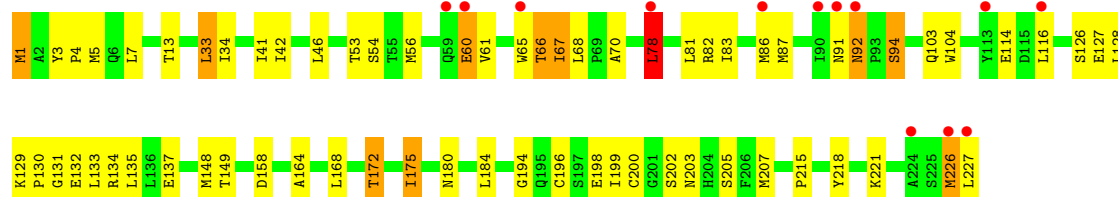


#### • Molecule 2: Cytochrome c oxidase subunit 2

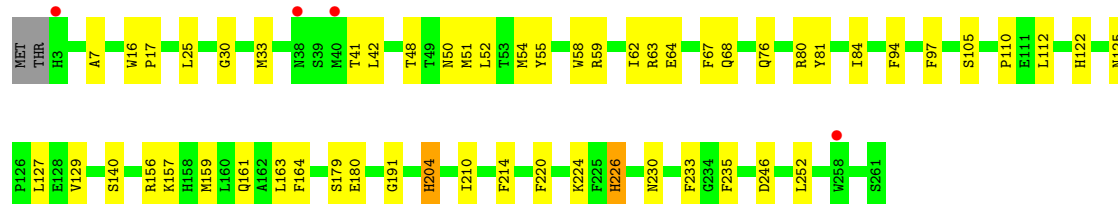
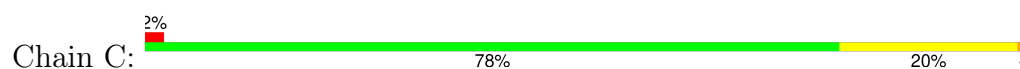




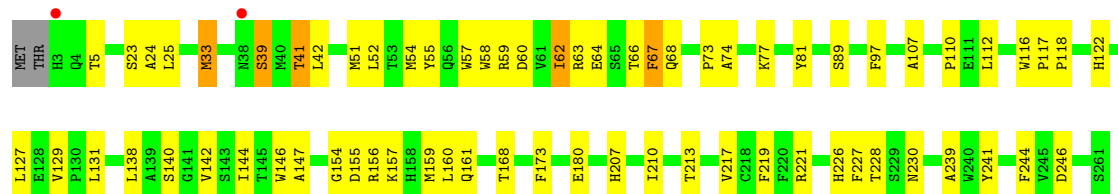
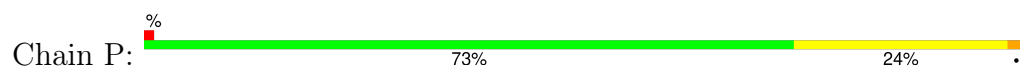
• Molecule 2: Cytochrome c oxidase subunit 2



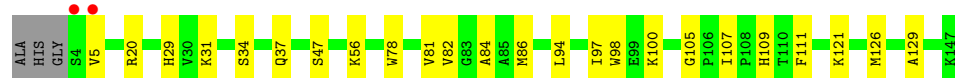
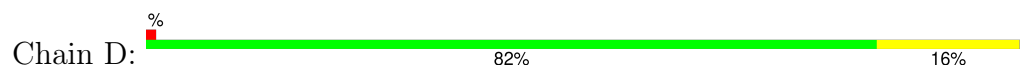
• Molecule 3: Cytochrome c oxidase subunit 3



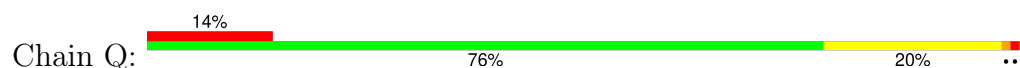
• Molecule 3: Cytochrome c oxidase subunit 3

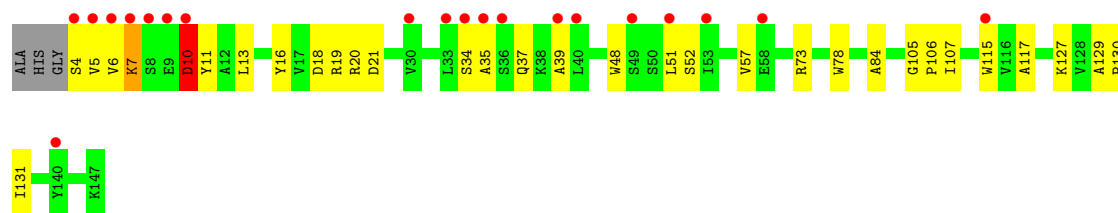


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

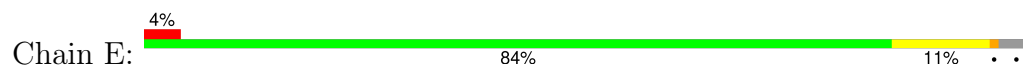


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

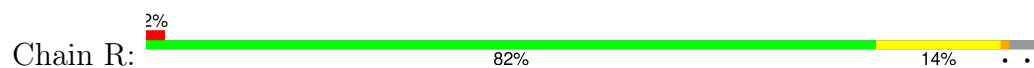




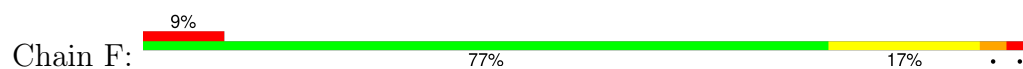
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



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



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



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

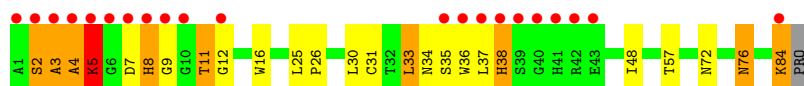


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

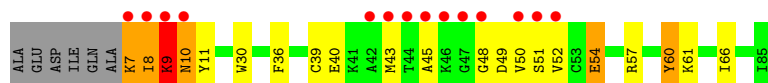


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

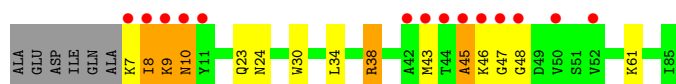
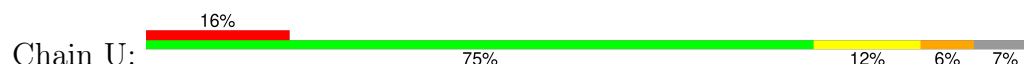




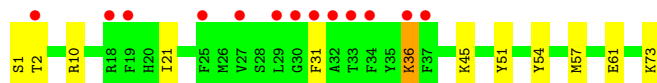
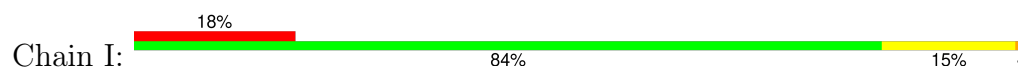
- Molecule 8: Cytochrome c oxidase subunit 6B1



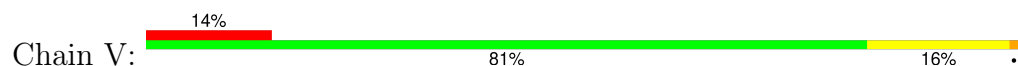
- Molecule 8: Cytochrome c oxidase subunit 6B1



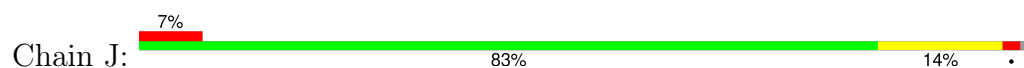
- Molecule 9: Cytochrome c oxidase subunit 6C



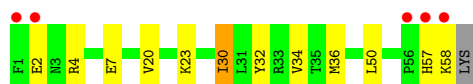
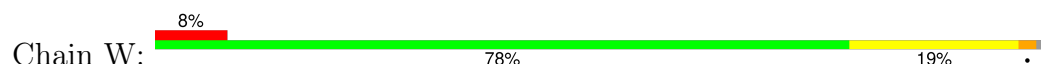
- Molecule 9: Cytochrome c oxidase subunit 6C



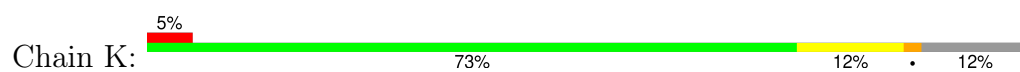
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



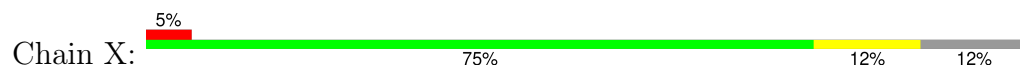
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



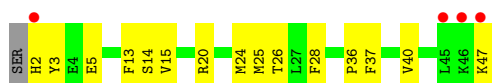
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



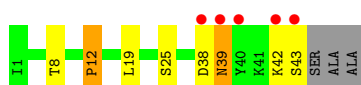
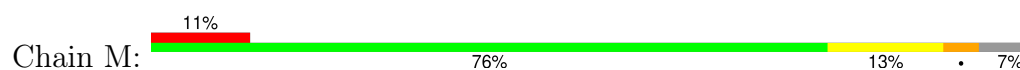
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



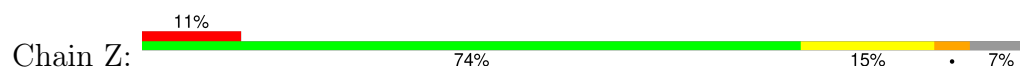
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 182.60Å 204.51Å 178.29Å<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)                            | 96.0 (40.00-1.90)<br>96.0 (40.00-1.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.24                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.49 (at 1.89Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0048                                             | Depositor        |
| R, $R_{free}$                                                           | 0.195 , 0.230<br>0.218 , 0.248                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 25229 reflections (1.99%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 24.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.252                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.42 , 66.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | 0.011 for l,k,h                                             | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 33302                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 24.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: PSC, CUA, TGL, HEA, CDL, PER, DMU, ZN, CHD, CU, NA, TPO, PEK, SAC, FME, PGV, MG

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$      | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.84         | 57/4203 (1.4%)   | 1.44        | 35/5742 (0.6%)   |
| 1   | N     | 1.76         | 62/4203 (1.5%)   | 1.43        | 38/5742 (0.7%)   |
| 2   | B     | 1.56         | 10/1868 (0.5%)   | 1.37        | 6/2545 (0.2%)    |
| 2   | O     | 1.45         | 16/1860 (0.9%)   | 1.28        | 9/2534 (0.4%)    |
| 3   | C     | 1.63         | 15/2221 (0.7%)   | 1.28        | 10/3035 (0.3%)   |
| 3   | P     | 1.62         | 21/2221 (0.9%)   | 1.28        | 7/3035 (0.2%)    |
| 4   | D     | 1.50         | 6/1229 (0.5%)    | 1.32        | 10/1658 (0.6%)   |
| 4   | Q     | 1.21         | 2/1229 (0.2%)    | 1.21        | 8/1658 (0.5%)    |
| 5   | E     | 1.53         | 2/871 (0.2%)     | 1.23        | 2/1182 (0.2%)    |
| 5   | R     | 1.25         | 1/871 (0.1%)     | 1.19        | 0/1182           |
| 6   | F     | 1.47         | 2/765 (0.3%)     | 1.33        | 2/1038 (0.2%)    |
| 6   | S     | 1.57         | 3/765 (0.4%)     | 1.34        | 3/1038 (0.3%)    |
| 7   | G     | 1.46         | 4/690 (0.6%)     | 1.32        | 6/937 (0.6%)     |
| 7   | T     | 1.44         | 3/690 (0.4%)     | 1.32        | 5/937 (0.5%)     |
| 8   | H     | 1.40         | 0/682            | 1.27        | 3/921 (0.3%)     |
| 8   | U     | 1.26         | 1/682 (0.1%)     | 1.21        | 1/921 (0.1%)     |
| 9   | I     | 1.20         | 0/605            | 1.26        | 1/802 (0.1%)     |
| 9   | V     | 1.12         | 1/605 (0.2%)     | 1.31        | 2/802 (0.2%)     |
| 10  | J     | 1.31         | 0/471            | 1.26        | 1/636 (0.2%)     |
| 10  | W     | 1.30         | 1/471 (0.2%)     | 1.29        | 1/636 (0.2%)     |
| 11  | K     | 1.43         | 0/398            | 1.30        | 2/546 (0.4%)     |
| 11  | X     | 1.27         | 3/398 (0.8%)     | 1.23        | 1/546 (0.2%)     |
| 12  | L     | 1.56         | 5/393 (1.3%)     | 1.43        | 3/526 (0.6%)     |
| 12  | Y     | 1.45         | 3/393 (0.8%)     | 1.27        | 4/526 (0.8%)     |
| 13  | M     | 1.50         | 1/345 (0.3%)     | 1.26        | 0/470            |
| 13  | Z     | 1.36         | 0/345            | 1.16        | 0/470            |
| All | All   | 1.57         | 219/29474 (0.7%) | 1.33        | 160/40065 (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   | N     | 0                   | 1                   |
| 6   | F     | 0                   | 1                   |
| 6   | S     | 0                   | 1                   |
| 8   | H     | 0                   | 1                   |
| 10  | J     | 0                   | 1                   |
| 10  | W     | 0                   | 1                   |
| All | All   | 0                   | 6                   |

All (219) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | N     | 83  | VAL  | CA-CB | 9.91  | 1.59        | 1.54     |
| 1   | N     | 337 | ALA  | N-CA  | 9.89  | 1.58        | 1.46     |
| 1   | A     | 404 | THR  | C-O   | 9.76  | 1.35        | 1.23     |
| 1   | A     | 154 | GLY  | N-CA  | 9.64  | 1.57        | 1.45     |
| 1   | N     | 288 | TRP  | N-CA  | 9.30  | 1.58        | 1.46     |
| 1   | N     | 359 | ALA  | N-CA  | 9.23  | 1.57        | 1.46     |
| 1   | N     | 69  | MET  | CA-C  | 8.99  | 1.60        | 1.52     |
| 2   | B     | 198 | GLU  | C-O   | 8.83  | 1.33        | 1.23     |
| 1   | N     | 79  | GLY  | N-CA  | 8.77  | 1.56        | 1.45     |
| 3   | C     | 129 | VAL  | CA-CB | 8.60  | 1.59        | 1.53     |
| 3   | P     | 226 | HIS  | N-CA  | 8.43  | 1.56        | 1.46     |
| 1   | A     | 443 | TYR  | C-O   | 8.36  | 1.33        | 1.24     |
| 1   | A     | 355 | GLY  | N-CA  | 8.28  | 1.56        | 1.45     |
| 1   | N     | 106 | PRO  | CA-C  | 8.21  | 1.59        | 1.52     |
| 1   | A     | 147 | ILE  | N-CA  | 8.04  | 1.56        | 1.46     |
| 1   | A     | 83  | VAL  | N-CA  | 7.78  | 1.55        | 1.46     |
| 7   | T     | 57  | THR  | C-O   | -7.66 | 1.14        | 1.24     |
| 3   | P     | 129 | VAL  | CA-CB | 7.57  | 1.59        | 1.53     |
| 6   | S     | 59  | GLY  | C-O   | 7.57  | 1.33        | 1.23     |
| 3   | P     | 147 | ALA  | N-CA  | 7.51  | 1.55        | 1.46     |
| 1   | A     | 295 | VAL  | CA-CB | 7.32  | 1.63        | 1.54     |
| 1   | N     | 404 | THR  | C-O   | 7.31  | 1.32        | 1.23     |
| 2   | O     | 198 | GLU  | C-O   | 7.26  | 1.31        | 1.23     |
| 1   | N     | 491 | ASN  | CA-CB | 7.25  | 1.61        | 1.53     |
| 1   | N     | 246 | LEU  | N-CA  | 7.15  | 1.55        | 1.46     |
| 1   | A     | 132 | LEU  | N-CA  | 7.11  | 1.55        | 1.46     |
| 2   | O     | 199 | ILE  | C-O   | 7.03  | 1.32        | 1.24     |
| 1   | N     | 128 | VAL  | N-CA  | 6.97  | 1.55        | 1.46     |
| 2   | O     | 66  | THR  | CA-C  | 6.97  | 1.59        | 1.52     |
| 1   | A     | 158 | ILE  | N-CA  | 6.96  | 1.54        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | N     | 219 | PHE  | N-CA  | 6.92  | 1.55        | 1.46     |
| 1   | N     | 158 | ILE  | N-CA  | 6.91  | 1.54        | 1.46     |
| 2   | O     | 78  | LEU  | CA-C  | 6.91  | 1.60        | 1.52     |
| 1   | A     | 12  | HIS  | CA-C  | 6.87  | 1.62        | 1.52     |
| 2   | B     | 190 | GLY  | C-O   | -6.83 | 1.17        | 1.24     |
| 1   | N     | 92  | MET  | CA-C  | 6.83  | 1.61        | 1.52     |
| 4   | D     | 56  | LYS  | C-O   | -6.78 | 1.16        | 1.24     |
| 1   | N     | 243 | VAL  | N-CA  | 6.75  | 1.55        | 1.46     |
| 1   | N     | 12  | HIS  | CA-C  | 6.73  | 1.61        | 1.52     |
| 3   | C     | 42  | LEU  | N-CA  | -6.69 | 1.38        | 1.46     |
| 2   | O     | 172 | THR  | N-CA  | 6.66  | 1.54        | 1.46     |
| 1   | A     | 239 | GLY  | N-CA  | 6.57  | 1.54        | 1.45     |
| 2   | O     | 175 | ILE  | N-CA  | 6.55  | 1.52        | 1.46     |
| 1   | N     | 459 | PHE  | N-CA  | 6.54  | 1.54        | 1.46     |
| 1   | A     | 324 | LEU  | N-CA  | 6.54  | 1.54        | 1.46     |
| 2   | B     | 162 | SER  | CA-C  | -6.50 | 1.44        | 1.52     |
| 3   | C     | 204 | HIS  | N-CA  | 6.48  | 1.54        | 1.46     |
| 1   | A     | 401 | SER  | N-CA  | 6.47  | 1.54        | 1.46     |
| 12  | Y     | 35  | ALA  | CA-CB | 6.42  | 1.59        | 1.54     |
| 2   | O     | 175 | ILE  | CA-C  | 6.38  | 1.57        | 1.52     |
| 2   | O     | 200 | CYS  | N-CA  | 6.35  | 1.52        | 1.46     |
| 3   | P     | 142 | VAL  | C-O   | 6.33  | 1.31        | 1.24     |
| 2   | B     | 194 | GLY  | C-O   | 6.32  | 1.30        | 1.23     |
| 3   | C     | 58  | TRP  | N-CA  | 6.30  | 1.54        | 1.46     |
| 1   | A     | 156 | SER  | N-CA  | 6.29  | 1.53        | 1.46     |
| 1   | A     | 49  | GLY  | C-O   | 6.28  | 1.31        | 1.23     |
| 2   | O     | 135 | LEU  | N-CA  | 6.28  | 1.54        | 1.46     |
| 3   | P     | 66  | THR  | N-CA  | 6.27  | 1.53        | 1.46     |
| 1   | A     | 397 | PHE  | CA-CB | 6.25  | 1.59        | 1.54     |
| 1   | N     | 245 | ILE  | N-CA  | 6.24  | 1.53        | 1.46     |
| 4   | D     | 97  | ILE  | N-CA  | 6.23  | 1.53        | 1.46     |
| 1   | A     | 502 | TYR  | C-O   | 6.22  | 1.31        | 1.24     |
| 4   | D     | 94  | LEU  | N-CA  | 6.22  | 1.54        | 1.46     |
| 3   | P     | 129 | VAL  | CA-C  | 6.22  | 1.57        | 1.52     |
| 1   | N     | 61  | HIS  | CA-CB | 6.19  | 1.62        | 1.53     |
| 1   | N     | 355 | GLY  | N-CA  | 6.13  | 1.53        | 1.45     |
| 13  | M     | 8   | THR  | C-N   | 6.13  | 1.41        | 1.33     |
| 1   | N     | 16  | GLY  | CA-C  | 6.11  | 1.58        | 1.52     |
| 11  | X     | 41  | ASN  | C-O   | 6.10  | 1.26        | 1.23     |
| 1   | A     | 105 | LEU  | CA-C  | 6.09  | 1.60        | 1.52     |
| 3   | P     | 73  | PRO  | CA-CB | 6.08  | 1.62        | 1.53     |
| 3   | C     | 30  | GLY  | N-CA  | 6.07  | 1.53        | 1.45     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | N     | 188 | VAL  | N-CA   | 6.07  | 1.53        | 1.46     |
| 1   | A     | 477 | ALA  | C-O    | -6.05 | 1.17        | 1.24     |
| 2   | B     | 207 | MET  | CA-CB  | 6.03  | 1.60        | 1.53     |
| 3   | P     | 23  | SER  | CA-C   | 6.02  | 1.60        | 1.52     |
| 1   | A     | 460 | ILE  | C-O    | 6.02  | 1.31        | 1.24     |
| 3   | P     | 146 | TRP  | C-O    | 6.02  | 1.31        | 1.24     |
| 7   | G     | 46  | ALA  | CA-C   | 6.00  | 1.60        | 1.52     |
| 6   | S     | 92  | VAL  | C-O    | -6.00 | 1.16        | 1.24     |
| 1   | N     | 242 | GLU  | CA-C   | 5.96  | 1.60        | 1.52     |
| 1   | N     | 224 | GLY  | C-O    | -5.96 | 1.20        | 1.24     |
| 3   | C     | 140 | SER  | CA-C   | 5.94  | 1.60        | 1.52     |
| 3   | P     | 89  | SER  | CA-C   | 5.92  | 1.60        | 1.52     |
| 2   | B     | 135 | LEU  | N-CA   | 5.90  | 1.53        | 1.46     |
| 3   | C     | 7   | ALA  | N-CA   | 5.90  | 1.53        | 1.46     |
| 1   | N     | 274 | VAL  | N-CA   | 5.89  | 1.53        | 1.46     |
| 6   | S     | 66  | ASN  | N-CA   | 5.89  | 1.53        | 1.46     |
| 1   | A     | 198 | SER  | CA-CB  | 5.86  | 1.62        | 1.53     |
| 1   | N     | 315 | PRO  | CA-C   | 5.86  | 1.61        | 1.52     |
| 1   | A     | 231 | TYR  | CA-CB  | 5.86  | 1.62        | 1.53     |
| 12  | Y     | 31  | SER  | CA-C   | 5.85  | 1.60        | 1.52     |
| 1   | A     | 199 | LEU  | N-CA   | 5.84  | 1.52        | 1.46     |
| 1   | A     | 282 | PHE  | CA-C   | 5.84  | 1.60        | 1.52     |
| 1   | N     | 276 | ALA  | CA-CB  | 5.83  | 1.62        | 1.53     |
| 1   | A     | 128 | VAL  | CA-C   | 5.82  | 1.60        | 1.52     |
| 2   | O     | 198 | GLU  | CA-C   | 5.79  | 1.59        | 1.52     |
| 1   | A     | 503 | HIS  | N-CA   | 5.78  | 1.53        | 1.46     |
| 1   | N     | 271 | MET  | N-CA   | 5.77  | 1.53        | 1.46     |
| 2   | B     | 192 | TYR  | CA-CB  | 5.76  | 1.64        | 1.53     |
| 4   | Q     | 106 | PRO  | C-O    | 5.76  | 1.30        | 1.23     |
| 1   | N     | 341 | ALA  | C-O    | -5.76 | 1.17        | 1.24     |
| 5   | E     | 95  | GLU  | CA-C   | 5.74  | 1.60        | 1.52     |
| 1   | N     | 94  | PHE  | CA-C   | 5.72  | 1.58        | 1.52     |
| 1   | N     | 348 | PHE  | N-CA   | 5.70  | 1.53        | 1.46     |
| 1   | A     | 66  | ILE  | N-CA   | 5.68  | 1.53        | 1.46     |
| 1   | N     | 319 | LYS  | C-O    | -5.67 | 1.17        | 1.24     |
| 4   | D     | 29  | HIS  | CA-C   | 5.67  | 1.60        | 1.52     |
| 1   | A     | 126 | TRP  | CA-C   | 5.67  | 1.62        | 1.52     |
| 1   | N     | 224 | GLY  | CA-C   | 5.65  | 1.57        | 1.51     |
| 1   | A     | 38  | ARG  | CZ-NH1 | 5.64  | 1.40        | 1.32     |
| 6   | F     | 72  | PHE  | C-O    | 5.64  | 1.31        | 1.23     |
| 7   | G     | 58  | LYS  | C-O    | 5.64  | 1.30        | 1.24     |
| 11  | X     | 41  | ASN  | N-CA   | 5.64  | 1.50        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 12  | HIS  | CA-CB  | 5.64  | 1.62        | 1.53     |
| 12  | L     | 15  | VAL  | CA-CB  | 5.64  | 1.60        | 1.54     |
| 1   | A     | 226 | GLY  | N-CA   | 5.63  | 1.51        | 1.45     |
| 1   | A     | 188 | VAL  | CA-C   | 5.62  | 1.60        | 1.52     |
| 3   | P     | 62  | ILE  | CA-CB  | 5.62  | 1.60        | 1.54     |
| 1   | N     | 395 | HIS  | CA-C   | 5.60  | 1.59        | 1.52     |
| 1   | A     | 152 | LEU  | CA-C   | 5.57  | 1.59        | 1.52     |
| 1   | N     | 399 | LEU  | C-O    | 5.57  | 1.30        | 1.24     |
| 1   | A     | 477 | ALA  | N-CA   | 5.56  | 1.53        | 1.46     |
| 7   | T     | 48  | ILE  | CA-C   | 5.54  | 1.58        | 1.52     |
| 1   | N     | 45  | GLY  | C-O    | 5.54  | 1.30        | 1.23     |
| 10  | W     | 20  | VAL  | CA-CB  | 5.53  | 1.61        | 1.54     |
| 2   | O     | 34  | ILE  | CA-CB  | 5.52  | 1.61        | 1.54     |
| 2   | O     | 205 | SER  | C-O    | 5.51  | 1.31        | 1.24     |
| 1   | A     | 230 | LEU  | CA-CB  | 5.51  | 1.62        | 1.53     |
| 1   | N     | 301 | THR  | CA-C   | 5.50  | 1.59        | 1.52     |
| 1   | N     | 237 | PHE  | CA-CB  | 5.50  | 1.61        | 1.53     |
| 1   | N     | 477 | ALA  | N-CA   | 5.50  | 1.52        | 1.46     |
| 4   | D     | 5   | VAL  | N-CA   | 5.50  | 1.52        | 1.46     |
| 1   | N     | 344 | PHE  | N-CA   | 5.49  | 1.52        | 1.46     |
| 3   | C     | 179 | SER  | CA-C   | 5.48  | 1.59        | 1.52     |
| 1   | A     | 240 | HIS  | CA-CB  | 5.45  | 1.60        | 1.53     |
| 12  | L     | 36  | PRO  | CA-C   | 5.43  | 1.60        | 1.52     |
| 12  | L     | 5   | GLU  | N-CA   | -5.41 | 1.39        | 1.45     |
| 1   | A     | 185 | VAL  | N-CA   | 5.40  | 1.52        | 1.46     |
| 1   | N     | 178 | GLN  | CA-C   | 5.40  | 1.60        | 1.52     |
| 3   | C     | 163 | LEU  | N-CA   | 5.39  | 1.52        | 1.46     |
| 5   | E     | 30  | ARG  | CZ-NH2 | 5.38  | 1.40        | 1.33     |
| 3   | C     | 235 | PHE  | N-CA   | 5.38  | 1.52        | 1.46     |
| 3   | P     | 219 | PHE  | N-CA   | 5.37  | 1.52        | 1.46     |
| 1   | A     | 309 | THR  | N-CA   | 5.36  | 1.52        | 1.46     |
| 1   | A     | 460 | ILE  | CA-C   | 5.36  | 1.59        | 1.52     |
| 6   | F     | 82  | CYS  | CA-CB  | 5.35  | 1.61        | 1.53     |
| 3   | C     | 129 | VAL  | CA-C   | 5.35  | 1.57        | 1.52     |
| 3   | P     | 67  | PHE  | N-CA   | 5.35  | 1.53        | 1.46     |
| 1   | A     | 402 | GLY  | CA-C   | 5.34  | 1.59        | 1.51     |
| 1   | N     | 48  | LEU  | C-O    | -5.34 | 1.17        | 1.23     |
| 9   | V     | 8   | GLN  | N-CA   | -5.33 | 1.39        | 1.46     |
| 12  | L     | 37  | PHE  | N-CA   | 5.33  | 1.52        | 1.46     |
| 3   | P     | 138 | LEU  | N-CA   | 5.33  | 1.52        | 1.46     |
| 1   | A     | 347 | LEU  | CA-C   | 5.31  | 1.60        | 1.52     |
| 3   | P     | 58  | TRP  | N-CA   | 5.31  | 1.53        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | P     | 122 | HIS  | N-CA   | 5.31  | 1.52        | 1.46     |
| 4   | D     | 81  | VAL  | CA-CB  | 5.31  | 1.60        | 1.54     |
| 1   | N     | 413 | HIS  | C-O    | 5.31  | 1.30        | 1.24     |
| 1   | A     | 29  | VAL  | CA-C   | 5.30  | 1.59        | 1.52     |
| 1   | N     | 60  | ALA  | CA-CB  | 5.30  | 1.61        | 1.53     |
| 1   | N     | 172 | LYS  | CA-CB  | 5.29  | 1.60        | 1.53     |
| 1   | N     | 400 | PHE  | N-CA   | 5.29  | 1.53        | 1.46     |
| 2   | O     | 135 | LEU  | CB-CG  | 5.29  | 1.64        | 1.53     |
| 7   | G     | 59  | PRO  | CA-CB  | 5.29  | 1.60        | 1.53     |
| 12  | L     | 28  | PHE  | N-CA   | 5.29  | 1.52        | 1.46     |
| 1   | A     | 127 | THR  | N-CA   | 5.28  | 1.53        | 1.46     |
| 3   | C     | 81  | TYR  | N-CA   | 5.28  | 1.52        | 1.46     |
| 1   | A     | 130 | PRO  | CA-CB  | 5.28  | 1.61        | 1.54     |
| 3   | P     | 244 | PHE  | CA-CB  | 5.26  | 1.61        | 1.53     |
| 1   | N     | 318 | VAL  | CA-CB  | 5.25  | 1.61        | 1.54     |
| 12  | Y     | 28  | PHE  | N-CA   | 5.25  | 1.52        | 1.46     |
| 2   | B     | 14  | SER  | N-CA   | 5.24  | 1.51        | 1.45     |
| 4   | Q     | 117 | ALA  | CA-C   | 5.22  | 1.59        | 1.52     |
| 1   | N     | 226 | GLY  | N-CA   | 5.21  | 1.50        | 1.45     |
| 2   | O     | 158 | ASP  | C-O    | -5.21 | 1.17        | 1.24     |
| 1   | N     | 177 | SER  | C-O    | 5.21  | 1.30        | 1.23     |
| 1   | N     | 233 | HIS  | CA-CB  | 5.20  | 1.61        | 1.53     |
| 3   | P     | 228 | THR  | CB-CG2 | 5.19  | 1.69        | 1.52     |
| 3   | C     | 214 | PHE  | CA-C   | 5.19  | 1.59        | 1.52     |
| 1   | A     | 389 | ILE  | CA-C   | 5.18  | 1.59        | 1.52     |
| 1   | A     | 309 | THR  | CA-C   | 5.17  | 1.59        | 1.52     |
| 3   | C     | 226 | HIS  | N-CA   | 5.17  | 1.52        | 1.46     |
| 1   | N     | 498 | CYS  | C-O    | -5.16 | 1.18        | 1.25     |
| 1   | A     | 399 | LEU  | CA-CB  | 5.16  | 1.61        | 1.53     |
| 5   | R     | 53  | ARG  | N-CA   | -5.16 | 1.39        | 1.46     |
| 8   | U     | 24  | ASN  | C-O    | 5.15  | 1.30        | 1.24     |
| 1   | A     | 235 | PHE  | N-CA   | 5.15  | 1.52        | 1.46     |
| 1   | N     | 62  | ALA  | C-O    | -5.14 | 1.18        | 1.24     |
| 2   | B     | 160 | LEU  | CA-C   | 5.13  | 1.59        | 1.52     |
| 1   | N     | 127 | THR  | N-CA   | 5.13  | 1.52        | 1.46     |
| 3   | P     | 227 | PHE  | CG-CD1 | 5.12  | 1.49        | 1.38     |
| 1   | A     | 20  | LEU  | N-CA   | 5.12  | 1.52        | 1.46     |
| 2   | B     | 125 | THR  | CA-C   | 5.12  | 1.59        | 1.52     |
| 3   | P     | 217 | VAL  | CA-CB  | 5.11  | 1.60        | 1.54     |
| 1   | N     | 437 | PRO  | C-O    | 5.10  | 1.29        | 1.23     |
| 1   | A     | 375 | ALA  | CA-C   | 5.09  | 1.59        | 1.52     |
| 3   | C     | 105 | SER  | N-CA   | 5.09  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | N     | 70  | VAL  | N-CA   | 5.08  | 1.52        | 1.46     |
| 1   | N     | 278 | MET  | N-CA   | 5.07  | 1.52        | 1.46     |
| 1   | N     | 98  | ASN  | N-CA   | 5.06  | 1.52        | 1.46     |
| 1   | A     | 276 | ALA  | CA-CB  | 5.06  | 1.61        | 1.53     |
| 1   | N     | 248 | LEU  | N-CA   | 5.06  | 1.51        | 1.46     |
| 1   | N     | 249 | PRO  | CA-C   | 5.05  | 1.60        | 1.52     |
| 1   | N     | 49  | GLY  | CA-C   | 5.05  | 1.58        | 1.52     |
| 1   | N     | 154 | GLY  | N-CA   | 5.05  | 1.52        | 1.45     |
| 1   | A     | 140 | GLY  | C-O    | 5.04  | 1.29        | 1.24     |
| 1   | A     | 318 | VAL  | CA-CB  | 5.04  | 1.60        | 1.54     |
| 2   | O     | 3   | TYR  | N-CA   | 5.04  | 1.51        | 1.45     |
| 2   | O     | 131 | GLY  | C-O    | -5.04 | 1.16        | 1.24     |
| 1   | A     | 316 | THR  | N-CA   | 5.04  | 1.52        | 1.46     |
| 11  | X     | 17  | VAL  | N-CA   | 5.03  | 1.52        | 1.46     |
| 1   | A     | 140 | GLY  | N-CA   | 5.03  | 1.51        | 1.45     |
| 1   | N     | 242 | GLU  | CD-OE1 | 5.03  | 1.34        | 1.25     |
| 7   | G     | 53  | LEU  | N-CA   | 5.01  | 1.52        | 1.45     |
| 7   | T     | 36  | TRP  | CB-CG  | 5.01  | 1.65        | 1.50     |
| 3   | P     | 146 | TRP  | CA-CB  | 5.01  | 1.61        | 1.53     |
| 1   | A     | 94  | PHE  | CA-C   | 5.00  | 1.58        | 1.52     |
| 1   | A     | 192 | ALA  | N-CA   | 5.00  | 1.52        | 1.46     |

All (160) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | N     | 240 | HIS  | N-CA-CB  | 8.84  | 120.85      | 110.42   |
| 1   | N     | 319 | LYS  | N-CA-C   | -8.36 | 102.11      | 111.14   |
| 1   | N     | 105 | LEU  | CA-C-N   | -8.19 | 111.95      | 120.38   |
| 1   | N     | 105 | LEU  | C-N-CA   | -8.19 | 111.95      | 120.38   |
| 1   | N     | 141 | ALA  | N-CA-C   | 8.14  | 122.47      | 112.54   |
| 1   | A     | 240 | HIS  | N-CA-CB  | 7.84  | 121.40      | 110.11   |
| 9   | V     | 8   | GLN  | CB-CG-CD | -7.76 | 99.41       | 112.60   |
| 12  | Y     | 20  | ARG  | N-CA-C   | -7.59 | 103.08      | 111.36   |
| 3   | C     | 125 | ASN  | CA-C-N   | -7.58 | 111.71      | 120.12   |
| 3   | C     | 125 | ASN  | C-N-CA   | -7.58 | 111.71      | 120.12   |
| 4   | Q     | 10  | ASP  | N-CA-C   | 7.54  | 121.97      | 111.56   |
| 1   | N     | 240 | HIS  | CA-C-N   | -7.43 | 110.85      | 119.32   |
| 1   | N     | 240 | HIS  | C-N-CA   | -7.43 | 110.85      | 119.32   |
| 11  | X     | 36  | ILE  | N-CA-C   | 7.34  | 119.66      | 111.88   |
| 1   | A     | 141 | ALA  | N-CA-C   | 7.29  | 121.44      | 112.54   |
| 2   | O     | 78  | LEU  | CA-C-N   | -7.18 | 111.58      | 119.19   |
| 2   | O     | 78  | LEU  | C-N-CA   | -7.18 | 111.58      | 119.19   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 8   | U     | 38  | ARG  | N-CA-C    | -7.17 | 103.54      | 111.36   |
| 5   | E     | 81  | ILE  | N-CA-C    | 7.07  | 117.18      | 110.53   |
| 1   | N     | 375 | ALA  | N-CA-C    | -7.07 | 103.50      | 111.14   |
| 3   | P     | 74  | ALA  | N-CA-C    | -7.04 | 103.69      | 111.36   |
| 3   | C     | 157 | LYS  | N-CA-C    | 7.00  | 118.56      | 111.07   |
| 1   | A     | 355 | GLY  | N-CA-C    | -7.00 | 103.81      | 112.77   |
| 1   | N     | 355 | GLY  | N-CA-C    | -6.93 | 103.90      | 112.77   |
| 1   | N     | 464 | ALA  | N-CA-C    | 6.81  | 118.70      | 111.28   |
| 3   | P     | 41  | THR  | N-CA-C    | 6.78  | 118.32      | 111.07   |
| 5   | E     | 67  | ILE  | N-CA-C    | -6.73 | 103.92      | 110.72   |
| 1   | N     | 101 | SER  | CA-CB-OG  | -6.73 | 97.64       | 111.10   |
| 1   | A     | 105 | LEU  | CA-C-N    | -6.66 | 113.52      | 120.38   |
| 1   | A     | 105 | LEU  | C-N-CA    | -6.66 | 113.52      | 120.38   |
| 4   | Q     | 105 | GLY  | CA-C-N    | -6.63 | 113.81      | 120.31   |
| 4   | Q     | 105 | GLY  | C-N-CA    | -6.63 | 113.81      | 120.31   |
| 1   | A     | 199 | LEU  | CA-C-N    | -6.56 | 112.24      | 119.19   |
| 1   | A     | 199 | LEU  | C-N-CA    | -6.56 | 112.24      | 119.19   |
| 4   | D     | 20  | ARG  | NE-CZ-NH2 | 6.51  | 125.06      | 119.20   |
| 1   | A     | 96  | ARG  | NE-CZ-NH2 | -6.49 | 113.36      | 119.20   |
| 7   | G     | 8   | HIS  | N-CA-C    | 6.48  | 124.59      | 110.80   |
| 1   | A     | 49  | GLY  | N-CA-C    | -6.44 | 101.92      | 110.74   |
| 1   | A     | 237 | PHE  | N-CA-C    | -6.38 | 104.32      | 111.28   |
| 6   | F     | 87  | THR  | N-CA-CB   | 6.37  | 119.34      | 110.17   |
| 7   | G     | 25  | LEU  | CA-C-N    | -6.36 | 112.28      | 119.28   |
| 7   | G     | 25  | LEU  | C-N-CA    | -6.36 | 112.28      | 119.28   |
| 1   | N     | 71  | MET  | CG-SD-CE  | -6.34 | 86.95       | 100.90   |
| 4   | Q     | 11  | TYR  | N-CA-C    | -6.33 | 105.42      | 113.01   |
| 8   | H     | 9   | LYS  | N-CA-C    | 6.33  | 119.06      | 109.63   |
| 1   | N     | 224 | GLY  | N-CA-C    | -6.32 | 104.80      | 115.80   |
| 1   | A     | 147 | ILE  | N-CA-C    | -6.32 | 104.33      | 110.72   |
| 1   | A     | 125 | GLY  | N-CA-C    | -6.32 | 104.83      | 112.48   |
| 1   | A     | 266 | GLU  | CA-C-N    | 6.32  | 126.23      | 119.85   |
| 1   | A     | 266 | GLU  | C-N-CA    | 6.32  | 126.23      | 119.85   |
| 1   | N     | 299 | VAL  | N-CA-C    | 6.20  | 116.87      | 110.36   |
| 1   | A     | 316 | THR  | N-CA-C    | -6.17 | 104.64      | 111.36   |
| 1   | A     | 71  | MET  | CG-SD-CE  | -6.08 | 87.53       | 100.90   |
| 1   | A     | 34  | SER  | N-CA-C    | -6.03 | 104.82      | 111.82   |
| 1   | A     | 380 | VAL  | N-CA-C    | 6.02  | 120.86      | 112.50   |
| 3   | P     | 140 | SER  | N-CA-C    | -6.02 | 105.43      | 112.89   |
| 4   | D     | 129 | ALA  | CA-C-N    | 6.02  | 126.54      | 120.04   |
| 4   | D     | 129 | ALA  | C-N-CA    | 6.02  | 126.54      | 120.04   |
| 1   | N     | 410 | ALA  | N-CA-C    | -5.99 | 104.68      | 112.23   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | D     | 5   | VAL  | N-CA-C   | 5.96  | 117.03      | 107.73   |
| 3   | C     | 16  | TRP  | CA-C-N   | -5.94 | 112.45      | 119.05   |
| 3   | C     | 16  | TRP  | C-N-CA   | -5.94 | 112.45      | 119.05   |
| 1   | A     | 240 | HIS  | CA-CB-CG | -5.93 | 107.87      | 113.80   |
| 2   | B     | 65  | TRP  | CB-CA-C  | 5.93  | 121.38      | 110.11   |
| 6   | S     | 45  | ASP  | CA-C-N   | -5.93 | 114.50      | 120.31   |
| 6   | S     | 45  | ASP  | C-N-CA   | -5.93 | 114.50      | 120.31   |
| 4   | D     | 100 | LYS  | N-CA-C   | -5.89 | 104.99      | 111.82   |
| 1   | A     | 119 | GLU  | CB-CA-C  | -5.88 | 109.81      | 116.63   |
| 2   | B     | 123 | ILE  | CB-CA-C  | -5.88 | 105.47      | 110.94   |
| 3   | P     | 23  | SER  | CA-CB-OG | -5.86 | 99.38       | 111.10   |
| 12  | L     | 15  | VAL  | N-CA-C   | -5.85 | 105.68      | 111.88   |
| 9   | V     | 38  | ALA  | N-CA-C   | 5.85  | 119.60      | 112.23   |
| 1   | A     | 127 | THR  | N-CA-C   | -5.83 | 106.00      | 113.23   |
| 4   | D     | 105 | GLY  | CA-C-N   | 5.82  | 125.75      | 119.76   |
| 4   | D     | 105 | GLY  | C-N-CA   | 5.82  | 125.75      | 119.76   |
| 1   | N     | 388 | ALA  | N-CA-C   | -5.80 | 105.04      | 111.36   |
| 7   | G     | 5   | LYS  | CB-CA-C  | 5.74  | 121.84      | 110.42   |
| 2   | O     | 92  | ASN  | N-CA-C   | 5.74  | 122.50      | 109.81   |
| 12  | Y     | 19  | TRP  | CA-CB-CG | -5.73 | 102.72      | 113.60   |
| 1   | A     | 101 | SER  | CA-CB-OG | -5.73 | 99.64       | 111.10   |
| 11  | K     | 13  | TYR  | CA-C-N   | 5.72  | 126.46      | 119.99   |
| 11  | K     | 13  | TYR  | C-N-CA   | 5.72  | 126.46      | 119.99   |
| 2   | O     | 65  | TRP  | N-CA-C   | 5.72  | 119.96      | 113.15   |
| 1   | N     | 82  | LEU  | CA-C-N   | -5.71 | 115.76      | 120.33   |
| 1   | N     | 82  | LEU  | C-N-CA   | -5.71 | 115.76      | 120.33   |
| 1   | A     | 78  | PHE  | N-CA-C   | 5.70  | 117.50      | 111.28   |
| 1   | A     | 223 | ALA  | N-CA-C   | -5.70 | 105.21      | 111.82   |
| 1   | N     | 455 | SER  | N-CA-C   | 5.70  | 117.49      | 111.28   |
| 3   | P     | 131 | LEU  | N-CA-C   | -5.68 | 105.00      | 111.14   |
| 7   | T     | 5   | LYS  | CB-CA-C  | 5.66  | 121.68      | 110.42   |
| 2   | B     | 83  | ILE  | N-CA-C   | 5.64  | 115.84      | 110.42   |
| 1   | N     | 15  | ILE  | N-CA-C   | -5.63 | 105.03      | 110.72   |
| 10  | J     | 57  | HIS  | CB-CA-C  | 5.62  | 119.96      | 110.79   |
| 1   | A     | 302 | ARG  | CA-CB-CG | -5.60 | 102.89      | 114.10   |
| 2   | O     | 67  | ILE  | N-CA-C   | 5.56  | 115.76      | 110.42   |
| 3   | C     | 80  | ARG  | CG-CD-NE | -5.52 | 99.86       | 112.00   |
| 1   | A     | 95  | PRO  | N-CA-C   | -5.50 | 106.54      | 114.18   |
| 8   | H     | 54  | GLU  | N-CA-C   | 5.45  | 117.65      | 111.11   |
| 3   | C     | 48  | THR  | N-CA-C   | 5.44  | 116.89      | 111.07   |
| 1   | A     | 249 | PRO  | CA-C-N   | 5.43  | 125.96      | 119.94   |
| 1   | A     | 249 | PRO  | C-N-CA   | 5.43  | 125.96      | 119.94   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | D     | 47  | SER  | N-CA-C   | 5.40  | 118.18      | 110.24   |
| 1   | A     | 10  | THR  | N-CA-C   | -5.40 | 104.11      | 111.56   |
| 2   | B     | 189 | PRO  | N-CA-C   | -5.39 | 103.68      | 111.22   |
| 1   | N     | 92  | MET  | CG-SD-CE | 5.39  | 112.75      | 100.90   |
| 3   | C     | 41  | THR  | N-CA-C   | 5.38  | 116.83      | 111.07   |
| 9   | I     | 21  | ILE  | N-CA-C   | -5.36 | 105.15      | 111.00   |
| 6   | S     | 49  | VAL  | N-CA-C   | -5.36 | 101.87      | 107.60   |
| 6   | F     | 94  | HIS  | N-CA-C   | 5.33  | 122.14      | 110.80   |
| 1   | N     | 189 | MET  | CB-CG-SD | -5.30 | 96.80       | 112.70   |
| 7   | G     | 58  | LYS  | CA-C-N   | -5.27 | 114.53      | 119.85   |
| 7   | G     | 58  | LYS  | C-N-CA   | -5.27 | 114.53      | 119.85   |
| 1   | A     | 67  | PHE  | N-CA-C   | 5.27  | 118.86      | 112.23   |
| 1   | N     | 362 | SER  | CA-CB-OG | -5.26 | 100.57      | 111.10   |
| 2   | B     | 58  | ALA  | N-CA-C   | 5.25  | 119.82      | 113.41   |
| 1   | A     | 38  | ARG  | CG-CD-NE | 5.25  | 123.55      | 112.00   |
| 4   | Q     | 129 | ALA  | CA-C-N   | 5.25  | 124.94      | 119.64   |
| 4   | Q     | 129 | ALA  | C-N-CA   | 5.25  | 124.94      | 119.64   |
| 3   | P     | 161 | GLN  | N-CA-C   | 5.23  | 117.39      | 111.11   |
| 1   | N     | 119 | GLU  | CB-CA-C  | -5.23 | 110.53      | 116.54   |
| 1   | N     | 343 | GLY  | N-CA-C   | -5.23 | 106.46      | 112.73   |
| 1   | N     | 482 | VAL  | CB-CA-C  | -5.22 | 103.32      | 111.26   |
| 2   | O     | 226 | MET  | N-CA-C   | -5.19 | 104.55      | 111.87   |
| 2   | B     | 161 | HIS  | N-CA-C   | -5.18 | 101.83      | 109.18   |
| 1   | N     | 29  | VAL  | CB-CA-C  | -5.17 | 105.15      | 112.14   |
| 4   | Q     | 107 | ILE  | CA-C-N   | -5.17 | 114.91      | 120.03   |
| 4   | Q     | 107 | ILE  | C-N-CA   | -5.17 | 114.91      | 120.03   |
| 12  | L     | 25  | MET  | CA-C-N   | 5.17  | 127.16      | 120.44   |
| 12  | L     | 25  | MET  | C-N-CA   | 5.17  | 127.16      | 120.44   |
| 3   | C     | 233 | PHE  | CA-C-N   | -5.14 | 114.27      | 119.98   |
| 3   | C     | 233 | PHE  | C-N-CA   | -5.14 | 114.27      | 119.98   |
| 1   | A     | 195 | LEU  | N-CA-C   | -5.12 | 105.61      | 111.14   |
| 1   | N     | 172 | LYS  | CA-C-N   | -5.12 | 115.92      | 119.66   |
| 1   | N     | 172 | LYS  | C-N-CA   | -5.12 | 115.92      | 119.66   |
| 1   | N     | 49  | GLY  | N-CA-C   | -5.11 | 103.74      | 110.74   |
| 1   | N     | 213 | ARG  | CA-C-N   | -5.11 | 114.26      | 122.08   |
| 1   | N     | 213 | ARG  | C-N-CA   | -5.11 | 114.26      | 122.08   |
| 4   | D     | 5   | VAL  | CA-C-N   | -5.11 | 115.78      | 122.37   |
| 4   | D     | 5   | VAL  | C-N-CA   | -5.11 | 115.78      | 122.37   |
| 3   | P     | 39  | SER  | N-CA-C   | 5.10  | 117.47      | 108.75   |
| 1   | N     | 477 | ALA  | N-CA-C   | 5.10  | 116.52      | 111.07   |
| 7   | T     | 76  | ASN  | CA-C-N   | -5.08 | 115.33      | 120.31   |
| 7   | T     | 76  | ASN  | C-N-CA   | -5.08 | 115.33      | 120.31   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 113 | LEU  | N-CA-C     | -5.08 | 105.82      | 111.36   |
| 12  | Y     | 16  | GLU  | CA-C-N     | -5.08 | 115.83      | 122.99   |
| 12  | Y     | 16  | GLU  | C-N-CA     | -5.08 | 115.83      | 122.99   |
| 1   | A     | 448 | THR  | N-CA-C     | 5.08  | 116.50      | 110.97   |
| 1   | N     | 271 | MET  | N-CA-C     | -5.08 | 105.93      | 111.82   |
| 2   | O     | 54  | SER  | N-CA-C     | -5.08 | 103.98      | 110.53   |
| 8   | H     | 66  | ILE  | N-CA-C     | 5.07  | 115.69      | 110.36   |
| 1   | N     | 112 | LEU  | CD1-CG-CD2 | -5.05 | 99.68       | 110.80   |
| 1   | N     | 286 | ILE  | N-CA-C     | 5.05  | 117.24      | 111.88   |
| 1   | A     | 267 | PRO  | N-CA-C     | -5.04 | 103.36      | 111.38   |
| 7   | T     | 25  | LEU  | CA-C-N     | -5.04 | 113.85      | 119.19   |
| 7   | T     | 25  | LEU  | C-N-CA     | -5.04 | 113.85      | 119.19   |
| 2   | O     | 202 | SER  | N-CA-C     | 5.03  | 118.19      | 111.75   |
| 10  | W     | 30  | ILE  | N-CA-C     | 5.03  | 115.25      | 110.42   |
| 2   | O     | 221 | LYS  | N-CA-C     | -5.02 | 105.70      | 111.07   |
| 1   | N     | 336 | PRO  | CB-CA-C    | -5.02 | 104.34      | 112.62   |
| 1   | N     | 361 | SER  | N-CA-C     | 5.00  | 117.38      | 111.33   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 6   | F     | 93  | PRO  | Peptide   |
| 8   | H     | 9   | LYS  | Peptide   |
| 10  | J     | 57  | HIS  | Peptide   |
| 1   | N     | 240 | HIS  | Sidechain |
| 6   | S     | 93  | PRO  | Peptide   |
| 10  | W     | 57  | HIS  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4074  | 0        | 4058     | 60      | 0            |
| 1   | N     | 4074  | 0        | 4058     | 80      | 0            |
| 2   | B     | 1832  | 0        | 1836     | 38      | 0            |
| 2   | O     | 1824  | 0        | 1833     | 53      | 2            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | C     | 2134  | 0        | 2051     | 41      | 0            |
| 3   | P     | 2134  | 0        | 2051     | 52      | 0            |
| 4   | D     | 1195  | 0        | 1183     | 16      | 0            |
| 4   | Q     | 1195  | 0        | 1183     | 31      | 0            |
| 5   | E     | 852   | 0        | 845      | 7       | 0            |
| 5   | R     | 852   | 0        | 845      | 11      | 2            |
| 6   | F     | 748   | 0        | 728      | 16      | 1            |
| 6   | S     | 748   | 0        | 728      | 37      | 7            |
| 7   | G     | 675   | 0        | 643      | 30      | 0            |
| 7   | T     | 675   | 0        | 643      | 34      | 0            |
| 8   | H     | 662   | 0        | 623      | 22      | 0            |
| 8   | U     | 662   | 0        | 623      | 11      | 0            |
| 9   | I     | 601   | 0        | 613      | 8       | 2            |
| 9   | V     | 601   | 0        | 613      | 9       | 0            |
| 10  | J     | 460   | 0        | 459      | 9       | 0            |
| 10  | W     | 460   | 0        | 459      | 8       | 0            |
| 11  | K     | 384   | 0        | 366      | 7       | 0            |
| 11  | X     | 384   | 0        | 366      | 4       | 0            |
| 12  | L     | 380   | 0        | 380      | 14      | 0            |
| 12  | Y     | 380   | 0        | 380      | 17      | 0            |
| 13  | M     | 335   | 0        | 352      | 10      | 0            |
| 13  | Z     | 335   | 0        | 352      | 11      | 0            |
| 14  | A     | 120   | 0        | 108      | 10      | 0            |
| 14  | N     | 120   | 0        | 108      | 8       | 0            |
| 15  | A     | 1     | 0        | 0        | 0       | 0            |
| 15  | N     | 1     | 0        | 0        | 0       | 0            |
| 16  | A     | 1     | 0        | 0        | 0       | 0            |
| 16  | N     | 1     | 0        | 0        | 0       | 0            |
| 17  | A     | 1     | 0        | 0        | 0       | 0            |
| 17  | C     | 1     | 0        | 0        | 1       | 0            |
| 17  | N     | 1     | 0        | 0        | 0       | 0            |
| 17  | P     | 1     | 0        | 0        | 0       | 0            |
| 18  | A     | 4     | 0        | 0        | 1       | 0            |
| 18  | N     | 4     | 0        | 0        | 1       | 0            |
| 19  | A     | 102   | 0        | 152      | 10      | 0            |
| 19  | C     | 102   | 0        | 152      | 6       | 0            |
| 19  | N     | 102   | 0        | 152      | 16      | 0            |
| 19  | P     | 102   | 0        | 152      | 11      | 0            |
| 20  | B     | 63    | 0        | 110      | 3       | 0            |
| 20  | D     | 63    | 0        | 110      | 13      | 0            |
| 20  | L     | 63    | 0        | 110      | 12      | 0            |
| 20  | N     | 63    | 0        | 110      | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20  | Q     | 63    | 0        | 110      | 11      | 0            |
| 20  | Y     | 63    | 0        | 110      | 17      | 0            |
| 21  | B     | 2     | 0        | 0        | 0       | 0            |
| 21  | O     | 2     | 0        | 0        | 0       | 0            |
| 22  | B     | 29    | 0        | 39       | 1       | 0            |
| 22  | C     | 58    | 0        | 78       | 4       | 0            |
| 22  | G     | 29    | 0        | 39       | 0       | 0            |
| 22  | J     | 29    | 0        | 39       | 5       | 0            |
| 22  | P     | 58    | 0        | 78       | 5       | 0            |
| 22  | W     | 29    | 0        | 38       | 5       | 0            |
| 23  | B     | 52    | 0        | 80       | 13      | 0            |
| 23  | N     | 52    | 0        | 80       | 21      | 0            |
| 24  | C     | 106   | 0        | 154      | 23      | 0            |
| 24  | G     | 53    | 0        | 77       | 6       | 0            |
| 24  | P     | 106   | 0        | 154      | 22      | 0            |
| 24  | T     | 53    | 0        | 77       | 12      | 0            |
| 25  | C     | 100   | 0        | 156      | 23      | 0            |
| 25  | G     | 100   | 0        | 156      | 37      | 0            |
| 25  | P     | 100   | 0        | 156      | 18      | 0            |
| 25  | T     | 100   | 0        | 156      | 29      | 0            |
| 26  | F     | 1     | 0        | 0        | 0       | 0            |
| 26  | S     | 1     | 0        | 0        | 0       | 0            |
| 27  | M     | 33    | 0        | 42       | 1       | 0            |
| 27  | Z     | 33    | 0        | 42       | 0       | 0            |
| 28  | A     | 265   | 0        | 0        | 10      | 0            |
| 28  | B     | 194   | 0        | 0        | 10      | 2            |
| 28  | C     | 141   | 0        | 0        | 8       | 0            |
| 28  | D     | 160   | 0        | 0        | 1       | 1            |
| 28  | E     | 125   | 0        | 0        | 3       | 0            |
| 28  | F     | 112   | 0        | 0        | 2       | 1            |
| 28  | G     | 70    | 0        | 0        | 7       | 0            |
| 28  | H     | 70    | 0        | 0        | 5       | 0            |
| 28  | I     | 52    | 0        | 0        | 1       | 0            |
| 28  | J     | 31    | 0        | 0        | 2       | 0            |
| 28  | K     | 40    | 0        | 0        | 3       | 1            |
| 28  | L     | 31    | 0        | 0        | 1       | 0            |
| 28  | M     | 31    | 0        | 0        | 1       | 2            |
| 28  | N     | 259   | 0        | 0        | 12      | 0            |
| 28  | O     | 157   | 0        | 0        | 11      | 6            |
| 28  | P     | 143   | 0        | 0        | 8       | 0            |
| 28  | Q     | 90    | 0        | 0        | 5       | 0            |
| 28  | R     | 103   | 0        | 0        | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | S     | 122   | 0        | 0        | 7       | 1            |
| 28  | T     | 56    | 0        | 0        | 2       | 0            |
| 28  | U     | 51    | 0        | 0        | 2       | 0            |
| 28  | V     | 42    | 0        | 0        | 5       | 0            |
| 28  | W     | 38    | 0        | 0        | 2       | 0            |
| 28  | X     | 34    | 0        | 0        | 3       | 0            |
| 28  | Y     | 37    | 0        | 0        | 4       | 0            |
| 28  | Z     | 24    | 0        | 0        | 1       | 0            |
| All | All   | 33302 | 0        | 31396    | 727     | 14           |

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 12.

All (727) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:S:76:LYS:CE      | 6:S:93:PRO:HG2     | 1.47                     | 1.41              |
| 6:S:43:LYS:H       | 6:S:43:LYS:CD      | 1.28                     | 1.39              |
| 6:S:43:LYS:HD3     | 6:S:43:LYS:N       | 1.33                     | 1.29              |
| 6:S:76:LYS:HD3     | 28:S:271:HOH:O     | 1.36                     | 1.25              |
| 18:A:606[A]:PER:O2 | 18:A:606[A]:PER:O1 | 1.55                     | 1.22              |
| 18:N:606[A]:PER:O2 | 18:N:606[A]:PER:O1 | 1.55                     | 1.19              |
| 20:L:101:TGL:OC1   | 20:L:101:TGL:HC41  | 1.41                     | 1.18              |
| 7:G:5:LYS:HB2      | 24:G:102:PEK:H362  | 1.21                     | 1.17              |
| 6:S:76:LYS:HE3     | 6:S:93:PRO:CG      | 1.80                     | 1.11              |
| 1:N:513:LEU:O      | 1:N:514:LYS:HB2    | 1.49                     | 1.07              |
| 19:P:304:PGV:H172  | 25:P:305:CDL:H651  | 1.35                     | 1.07              |
| 20:Q:201:TGL:HA91  | 20:Q:201:TGL:H231  | 1.29                     | 1.06              |
| 23:N:610:PSC:H342  | 2:O:41:ILE:HD13    | 1.36                     | 1.04              |
| 7:T:5:LYS:HB2      | 24:T:101:PEK:H351  | 1.39                     | 1.03              |
| 6:S:76:LYS:HE3     | 6:S:93:PRO:HG2     | 1.04                     | 1.02              |
| 6:S:76:LYS:HE2     | 6:S:93:PRO:HG2     | 1.38                     | 1.01              |
| 12:L:20:ARG:HH22   | 20:L:101:TGL:HC32  | 1.22                     | 1.01              |
| 3:C:67:PHE:HE1     | 25:C:304:CDL:H1    | 1.25                     | 1.01              |
| 6:S:95:GLN:HB2     | 28:S:240:HOH:O     | 1.64                     | 0.97              |
| 1:N:321:PHE:CD2    | 23:N:610:PSC:H341  | 2.00                     | 0.96              |
| 10:W:23:LYS:HE3    | 28:W:221:HOH:O     | 1.64                     | 0.95              |
| 11:X:47:ARG:HD3    | 28:X:116:HOH:O     | 1.67                     | 0.95              |
| 7:G:5:LYS:HG3      | 24:G:102:PEK:H383  | 1.48                     | 0.94              |
| 2:O:1:FME:HE1      | 2:O:133:LEU:CD1    | 1.98                     | 0.94              |
| 7:G:72:ASN:H       | 7:G:76:ASN:HD22    | 1.16                     | 0.93              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 19:A:608:PGV:H02    | 19:A:608:PGV:O14  | 1.67                     | 0.93              |
| 6:F:85:CYS:SG       | 6:F:87:THR:HG23   | 2.08                     | 0.93              |
| 23:N:610:PSC:H22    | 28:V:101:HOH:O    | 1.68                     | 0.92              |
| 3:C:224:LYS:CD      | 25:C:304:CDL:HB31 | 1.98                     | 0.92              |
| 24:C:307:PEK:H383   | 25:G:101:CDL:C27  | 2.01                     | 0.90              |
| 17:C:301:NA:NA      | 28:C:404:HOH:O    | 1.45                     | 0.89              |
| 7:G:5:LYS:HB2       | 24:G:102:PEK:C36  | 2.01                     | 0.89              |
| 7:T:5:LYS:CB        | 24:T:101:PEK:H351 | 2.02                     | 0.89              |
| 3:C:67:PHE:CE1      | 25:C:304:CDL:H1   | 2.08                     | 0.88              |
| 3:P:67:PHE:HE1      | 25:P:305:CDL:H1   | 1.36                     | 0.88              |
| 6:S:76:LYS:CE       | 6:S:93:PRO:CG     | 2.42                     | 0.88              |
| 19:N:608:PGV:H343   | 24:P:303:PEK:H382 | 1.56                     | 0.87              |
| 25:G:101:CDL:H202   | 25:G:101:CDL:H522 | 1.58                     | 0.86              |
| 1:N:514:LYS:HA      | 6:S:38:ALA:HB3    | 1.57                     | 0.86              |
| 19:P:301:PGV:H11    | 22:P:307:CHD:H152 | 1.58                     | 0.86              |
| 6:S:98:HIS:HB3      | 28:S:268:HOH:O    | 1.76                     | 0.85              |
| 12:L:20:ARG:NH2     | 20:L:101:TGL:HC32 | 1.91                     | 0.85              |
| 25:T:102:CDL:H511   | 25:T:102:CDL:H202 | 1.57                     | 0.85              |
| 8:U:7:LYS:O         | 8:U:8:ILE:HG22    | 1.77                     | 0.84              |
| 1:A:513:LEU:O       | 1:A:514:LYS:HB2   | 1.74                     | 0.84              |
| 4:D:78:TRP:HB3      | 20:D:201:TGL:HB22 | 1.56                     | 0.84              |
| 1:N:169[B]:ILE:HD11 | 1:N:189:MET:HE1   | 1.60                     | 0.84              |
| 25:G:101:CDL:H352   | 2:O:78:LEU:HD12   | 1.59                     | 0.83              |
| 20:L:101:TGL:OC1    | 20:L:101:TGL:CC4  | 2.23                     | 0.83              |
| 6:S:85:CYS:SG       | 6:S:87:THR:HG23   | 2.19                     | 0.83              |
| 7:T:72:ASN:H        | 7:T:76:ASN:HD22   | 1.23                     | 0.83              |
| 3:C:224:LYS:HD2     | 25:C:304:CDL:HB31 | 1.59                     | 0.82              |
| 6:S:75:HIS:H        | 6:S:80:GLN:HE22   | 1.23                     | 0.82              |
| 2:O:1:FME:CE        | 2:O:133:LEU:HD13  | 2.10                     | 0.81              |
| 3:P:63:ARG:HE       | 25:P:305:CDL:HA22 | 1.46                     | 0.81              |
| 8:H:40:GLU:OE2      | 28:H:130:HOH:O    | 1.98                     | 0.80              |
| 14:N:602:HEA:HBC1   | 14:N:602:HEA:HMC3 | 1.64                     | 0.80              |
| 19:A:608:PGV:H311   | 13:M:19:LEU:HD23  | 1.64                     | 0.80              |
| 25:C:304:CDL:H522   | 25:C:304:CDL:OB9  | 1.81                     | 0.80              |
| 12:L:2:HIS:CG       | 12:L:3:TYR:H      | 1.99                     | 0.80              |
| 7:G:84:LYS:H        | 7:G:84:LYS:HD2    | 1.47                     | 0.79              |
| 28:A:955:HOH:O      | 2:B:206:PHE:HE1   | 1.63                     | 0.79              |
| 24:C:302:PEK:HN2    | 7:G:76:ASN:HD21   | 1.27                     | 0.79              |
| 28:C:528:HOH:O      | 25:G:101:CDL:H673 | 1.81                     | 0.79              |
| 1:N:483:LEU:HD13    | 4:Q:6:VAL:HB      | 1.63                     | 0.79              |
| 3:P:33[A]:MET:HG2   | 28:P:455:HOH:O    | 1.83                     | 0.78              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 6:F:10:GLU:OE2      | 6:F:25:ARG:NH2    | 2.16                     | 0.78              |
| 1:N:321:PHE:HD2     | 23:N:610:PSC:H341 | 1.48                     | 0.78              |
| 24:P:303:PEK:H203   | 24:P:303:PEK:H15  | 1.65                     | 0.78              |
| 3:C:50:ASN:HD22     | 3:C:51[A]:MET:HE2 | 1.49                     | 0.77              |
| 6:S:43:LYS:CD       | 6:S:43:LYS:N      | 2.08                     | 0.77              |
| 24:C:307:PEK:H361   | 25:G:101:CDL:H273 | 1.66                     | 0.77              |
| 25:P:305:CDL:OB6    | 25:P:305:CDL:HB21 | 1.82                     | 0.77              |
| 7:G:11:TPO:HA       | 7:G:11:TPO:O2P    | 1.81                     | 0.77              |
| 5:E:90:ARG:HD2      | 28:E:279:HOH:O    | 1.83                     | 0.77              |
| 7:T:5:LYS:HG3       | 24:T:101:PEK:H371 | 1.67                     | 0.77              |
| 6:S:52:ILE:O        | 6:S:94:HIS:CE1    | 2.37                     | 0.77              |
| 28:N:953:HOH:O      | 24:P:303:PEK:H372 | 1.83                     | 0.77              |
| 24:C:307:PEK:C38    | 25:G:101:CDL:C27  | 2.62                     | 0.77              |
| 5:R:80:GLU:H        | 5:R:80:GLU:CD     | 1.93                     | 0.77              |
| 3:P:33[A]:MET:HE2   | 3:P:42:LEU:H      | 1.49                     | 0.76              |
| 2:O:1:FME:HE1       | 2:O:133:LEU:CD2   | 2.16                     | 0.76              |
| 23:B:304:PSC:C12    | 23:B:304:PSC:H342 | 2.14                     | 0.75              |
| 14:N:601:HEA:HBC1   | 14:N:601:HEA:HMC1 | 1.67                     | 0.75              |
| 28:P:530:HOH:O      | 6:S:1:ALA:HB2     | 1.87                     | 0.75              |
| 25:T:102:CDL:H311   | 25:T:102:CDL:CA5  | 2.17                     | 0.75              |
| 25:P:305:CDL:OB9    | 25:P:305:CDL:H532 | 1.87                     | 0.74              |
| 1:A:311[A]:ILE:HD13 | 25:T:102:CDL:H221 | 1.69                     | 0.74              |
| 7:G:84:LYS:HD2      | 7:G:84:LYS:N      | 2.02                     | 0.74              |
| 4:Q:34:SER:H        | 4:Q:37:GLN:NE2    | 1.86                     | 0.73              |
| 3:C:161:GLN:HE22    | 24:C:307:PEK:H21  | 1.52                     | 0.73              |
| 8:H:30:TRP:HB2      | 28:H:158:HOH:O    | 1.89                     | 0.73              |
| 12:L:26:THR:HG23    | 13:M:25:SER:CB    | 2.19                     | 0.73              |
| 19:N:607:PGV:H302   | 13:Z:19:LEU:CD2   | 2.19                     | 0.73              |
| 2:B:1:FME:HE1       | 2:B:133:LEU:HD22  | 1.70                     | 0.73              |
| 4:Q:6:VAL:HG13      | 4:Q:10:ASP:OD2    | 1.89                     | 0.72              |
| 12:Y:12:PRO:HB2     | 20:Y:101:TGL:HG11 | 1.68                     | 0.72              |
| 2:O:1:FME:CE        | 2:O:133:LEU:CD1   | 2.67                     | 0.72              |
| 4:Q:6:VAL:CG1       | 4:Q:10:ASP:OD2    | 2.37                     | 0.72              |
| 25:G:101:CDL:H111   | 25:G:101:CDL:HA21 | 1.71                     | 0.72              |
| 28:O:536:HOH:O      | 4:Q:21:ASP:HB2    | 1.89                     | 0.72              |
| 24:C:307:PEK:C38    | 25:G:101:CDL:H272 | 2.20                     | 0.72              |
| 1:A:417:MET:HE1     | 14:A:601:HEA:H263 | 1.72                     | 0.72              |
| 1:N:169[B]:ILE:CD1  | 1:N:189:MET:HE1   | 2.18                     | 0.72              |
| 25:P:305:CDL:H251   | 25:P:305:CDL:H391 | 1.72                     | 0.72              |
| 3:C:161:GLN:NE2     | 24:C:307:PEK:H21  | 2.05                     | 0.72              |
| 25:G:101:CDL:H751   | 25:G:101:CDL:H561 | 1.70                     | 0.72              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 3:P:107:ALA:HB2     | 19:P:301:PGV:H031 | 1.72                     | 0.72              |
| 19:N:607:PGV:H31    | 19:N:607:PGV:H202 | 1.72                     | 0.72              |
| 3:P:54:MET:HE1      | 19:P:304:PGV:H131 | 1.72                     | 0.71              |
| 12:Y:20:ARG:HH21    | 20:Y:101:TGL:HC32 | 1.55                     | 0.71              |
| 5:R:6:GLU:OE1       | 5:R:14:ARG:NH2    | 2.20                     | 0.71              |
| 4:Q:78:TRP:CA       | 20:Q:201:TGL:HB22 | 2.21                     | 0.71              |
| 24:P:303:PEK:HN2    | 7:T:76:ASN:HD21   | 1.34                     | 0.71              |
| 2:B:33:LEU:HD13     | 9:I:31:PHE:CD1    | 2.26                     | 0.71              |
| 2:B:56:MET:HG2      | 23:B:304:PSC:H221 | 1.73                     | 0.70              |
| 1:A:311[B]:ILE:HD11 | 24:P:308:PEK:H342 | 1.72                     | 0.70              |
| 14:A:602:HEA:HBC1   | 14:A:602:HEA:HMC1 | 1.73                     | 0.70              |
| 7:T:84:LYS:HZ3      | 7:T:84:LYS:H      | 1.39                     | 0.70              |
| 12:L:14:SER:H       | 20:L:101:TGL:HC31 | 1.55                     | 0.70              |
| 20:Q:201:TGL:HG32   | 20:Q:201:TGL:OB1  | 1.92                     | 0.70              |
| 1:N:28:MET:HE2      | 14:N:601:HEA:H271 | 1.74                     | 0.69              |
| 7:T:30:LEU:HD21     | 25:T:102:CDL:H471 | 1.74                     | 0.69              |
| 4:Q:19:ARG:HD2      | 4:Q:21:ASP:OD1    | 1.91                     | 0.69              |
| 4:D:78:TRP:N        | 20:D:201:TGL:HB21 | 2.06                     | 0.69              |
| 24:C:307:PEK:H382   | 25:G:101:CDL:H272 | 1.74                     | 0.69              |
| 3:C:63:ARG:HE       | 25:C:304:CDL:HA22 | 1.56                     | 0.69              |
| 1:N:321:PHE:CD2     | 23:N:610:PSC:C34  | 2.75                     | 0.69              |
| 7:T:3:ALA:O         | 7:T:4:ALA:CB      | 2.40                     | 0.69              |
| 4:Q:6:VAL:HG12      | 4:Q:7:LYS:H       | 1.57                     | 0.69              |
| 3:P:63:ARG:HE       | 25:P:305:CDL:CA2  | 2.06                     | 0.69              |
| 3:C:63:ARG:HE       | 25:C:304:CDL:CA2  | 2.06                     | 0.68              |
| 1:N:113:LEU:HD12    | 20:Y:101:TGL:H141 | 1.75                     | 0.68              |
| 4:D:78:TRP:CB       | 20:D:201:TGL:HB22 | 2.23                     | 0.68              |
| 6:F:1:ALA:HB3       | 6:S:65:ASP:OD1    | 1.93                     | 0.68              |
| 7:G:2:SER:OG        | 24:G:102:PEK:H301 | 1.93                     | 0.68              |
| 7:G:5:LYS:NZ        | 28:G:224:HOH:O    | 2.26                     | 0.68              |
| 25:G:101:CDL:H182   | 25:G:101:CDL:CB5  | 2.24                     | 0.68              |
| 2:B:32:PHE:CE2      | 20:B:301:TGL:HA52 | 2.29                     | 0.68              |
| 2:O:1:FME:HE2       | 2:O:133:LEU:HD13  | 1.76                     | 0.67              |
| 3:P:67:PHE:CE1      | 25:P:305:CDL:H1   | 2.25                     | 0.67              |
| 1:N:321:PHE:CE2     | 23:N:610:PSC:H341 | 2.30                     | 0.67              |
| 24:P:308:PEK:H382   | 25:T:102:CDL:H271 | 1.76                     | 0.67              |
| 6:S:64:GLU:O        | 6:S:65:ASP:HB2    | 1.94                     | 0.67              |
| 23:B:304:PSC:H342   | 23:B:304:PSC:H12  | 1.77                     | 0.67              |
| 1:N:107:PRO:HB3     | 3:P:25:LEU:HB2    | 1.77                     | 0.67              |
| 4:D:34:SER:H        | 4:D:37:GLN:HE21   | 1.43                     | 0.66              |
| 5:R:43:PRO:HB2      | 5:R:48:ILE:HD11   | 1.77                     | 0.66              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 11:K:39:GLU:HB3     | 28:K:137:HOH:O    | 1.95                     | 0.66              |
| 8:H:9:LYS:O         | 8:H:10:ASN:HB2    | 1.94                     | 0.66              |
| 1:N:406:ASN:HD21    | 19:N:607:PGV:H22  | 1.60                     | 0.66              |
| 2:B:115[B]:ASP:OD1  | 28:B:501:HOH:O    | 2.13                     | 0.66              |
| 1:N:334:TRP:CH2     | 2:O:46:LEU:HD13   | 2.31                     | 0.66              |
| 19:A:608:PGV:H152   | 19:A:608:PGV:H322 | 1.77                     | 0.66              |
| 7:G:1:ALA:HB2       | 19:P:301:PGV:H321 | 1.76                     | 0.66              |
| 4:Q:34:SER:H        | 4:Q:37:GLN:HE21   | 1.42                     | 0.66              |
| 8:H:7:LYS:O         | 8:H:8:ILE:HB      | 1.96                     | 0.66              |
| 2:O:218:TYR:HB3     | 28:O:513:HOH:O    | 1.94                     | 0.66              |
| 20:Q:201:TGL:HA91   | 20:Q:201:TGL:C23  | 2.15                     | 0.66              |
| 1:A:417:MET:CE      | 14:A:601:HEA:H263 | 2.25                     | 0.66              |
| 7:T:31:CYS:SG       | 25:T:102:CDL:H551 | 2.36                     | 0.66              |
| 1:N:159:LEU:HD21    | 28:P:499:HOH:O    | 1.96                     | 0.65              |
| 2:O:1:FME:HE1       | 2:O:133:LEU:HD11  | 1.78                     | 0.65              |
| 4:Q:78:TRP:CB       | 20:Q:201:TGL:HB22 | 2.27                     | 0.65              |
| 1:A:406:ASN:HD21    | 19:A:608:PGV:H22  | 1.62                     | 0.65              |
| 1:N:310:MET:HE3     | 1:N:356:ILE:HG23  | 1.77                     | 0.64              |
| 25:C:304:CDL:HB21   | 25:C:304:CDL:OB6  | 1.98                     | 0.64              |
| 4:Q:20:ARG:HG2      | 28:Q:317:HOH:O    | 1.96                     | 0.64              |
| 6:S:52:ILE:O        | 6:S:94:HIS:ND1    | 2.31                     | 0.64              |
| 1:N:273:MET:HE2     | 28:N:921:HOH:O    | 1.97                     | 0.63              |
| 3:C:224:LYS:HD3     | 25:C:304:CDL:HB31 | 1.80                     | 0.63              |
| 4:Q:78:TRP:HB3      | 20:Q:201:TGL:HB22 | 1.79                     | 0.63              |
| 2:O:132:GLU:HB3     | 2:O:137:GLU:HG3   | 1.80                     | 0.63              |
| 3:P:33[A]:MET:HE3   | 3:P:39:SER:OG     | 1.98                     | 0.63              |
| 23:N:610:PSC:H342   | 2:O:41:ILE:CD1    | 2.23                     | 0.62              |
| 3:P:5:THR:HG22      | 6:S:96:LEU:CD1    | 2.29                     | 0.62              |
| 23:N:610:PSC:C32    | 23:N:610:PSC:H12  | 2.29                     | 0.62              |
| 4:D:109:HIS:HD2     | 28:D:306:HOH:O    | 1.83                     | 0.62              |
| 6:F:95:GLN:C        | 6:F:97:ALA:H      | 2.06                     | 0.62              |
| 2:O:227:LEU:HD21    | 28:O:546:HOH:O    | 2.00                     | 0.61              |
| 25:G:101:CDL:H462   | 2:O:70:ALA:HB1    | 1.82                     | 0.61              |
| 10:J:7:GLU:HG3      | 28:J:209:HOH:O    | 2.01                     | 0.61              |
| 12:L:26:THR:HG23    | 13:M:25:SER:HB3   | 1.81                     | 0.61              |
| 5:E:12:ASP:OD1      | 5:E:44:GLU:HG3    | 1.98                     | 0.61              |
| 1:N:136[B]:LEU:HD21 | 28:N:892:HOH:O    | 2.00                     | 0.61              |
| 2:B:140:ASN:HB3     | 28:B:502:HOH:O    | 2.00                     | 0.61              |
| 7:T:3:ALA:O         | 7:T:4:ALA:HB3     | 1.99                     | 0.61              |
| 12:Y:12:PRO:CB      | 20:Y:101:TGL:HG11 | 2.31                     | 0.61              |
| 2:B:7:LEU:HD12      | 20:B:301:TGL:HC52 | 1.83                     | 0.61              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 2:B:82:ARG:HH11     | 2:B:86:MET:HE1    | 1.66                     | 0.61              |
| 1:N:136[B]:LEU:CD2  | 28:N:893:HOH:O    | 2.48                     | 0.61              |
| 4:Q:78:TRP:HA       | 20:Q:201:TGL:HB22 | 1.83                     | 0.60              |
| 12:Y:24:MET:SD      | 20:Y:101:TGL:H152 | 2.41                     | 0.60              |
| 7:T:2:SER:OG        | 24:T:101:PEK:H292 | 2.00                     | 0.60              |
| 1:A:311[A]:ILE:HG13 | 25:T:102:CDL:H432 | 1.83                     | 0.60              |
| 10:J:33:ARG:HG2     | 22:J:101:CHD:H152 | 1.82                     | 0.60              |
| 3:P:59:ARG:HA       | 25:P:305:CDL:H512 | 1.82                     | 0.60              |
| 13:M:42:LYS:HB3     | 28:M:2326:HOH:O   | 2.01                     | 0.60              |
| 3:P:246:ASP:HB2     | 28:P:473:HOH:O    | 2.02                     | 0.60              |
| 7:T:31:CYS:SG       | 25:T:102:CDL:C55  | 2.90                     | 0.60              |
| 14:N:602:HEA:HBC1   | 14:N:602:HEA:CMC  | 2.32                     | 0.60              |
| 6:S:43:LYS:H        | 6:S:43:LYS:HD3    | 0.48                     | 0.60              |
| 4:D:121:LYS:HD3     | 11:K:52:GLU:HA    | 1.83                     | 0.60              |
| 3:C:246:ASP:HB2     | 28:C:459:HOH:O    | 2.02                     | 0.59              |
| 1:N:177:SER:H       | 1:N:180:GLN:HE21  | 1.50                     | 0.59              |
| 5:R:72:LYS:HB2      | 5:R:82:TYR:CD2    | 2.37                     | 0.59              |
| 9:I:45:LYS:HG3      | 28:I:144:HOH:O    | 2.02                     | 0.59              |
| 3:C:54:MET:HE1      | 19:C:303:PGV:H142 | 1.84                     | 0.59              |
| 1:N:484:THR:HG22    | 13:Z:2:THR:HG23   | 1.84                     | 0.59              |
| 3:P:33[A]:MET:HE1   | 3:P:41:THR:HB     | 1.84                     | 0.59              |
| 3:P:54:MET:HE3      | 25:P:305:CDL:H612 | 1.83                     | 0.59              |
| 20:D:201:TGL:H242   | 20:D:201:TGL:H202 | 1.84                     | 0.59              |
| 5:R:80:GLU:HG3      | 28:R:279:HOH:O    | 2.02                     | 0.59              |
| 2:O:83:ILE:O        | 2:O:87:MET:HG3    | 2.02                     | 0.59              |
| 3:P:60:ASP:O        | 3:P:64:GLU:HG3    | 2.03                     | 0.59              |
| 5:R:79:LYS:HD2      | 5:R:79:LYS:N      | 2.16                     | 0.59              |
| 7:T:31:CYS:SG       | 25:T:102:CDL:H532 | 2.42                     | 0.59              |
| 1:A:1:FME:HE2       | 1:A:4:ASN:HD22    | 1.67                     | 0.59              |
| 23:B:304:PSC:H22    | 23:B:304:PSC:H231 | 1.83                     | 0.59              |
| 3:C:161:GLN:HE22    | 24:C:307:PEK:C2   | 2.15                     | 0.59              |
| 6:S:43:LYS:HD2      | 6:S:88:HIS:CE1    | 2.38                     | 0.59              |
| 7:G:3:ALA:O         | 7:G:4:ALA:CB      | 2.51                     | 0.58              |
| 12:Y:12:PRO:CG      | 20:Y:101:TGL:HG11 | 2.32                     | 0.58              |
| 3:C:210:ILE:HG12    | 19:C:303:PGV:H132 | 1.84                     | 0.58              |
| 1:N:449:MET:SD      | 2:O:5:MET:HG2     | 2.43                     | 0.58              |
| 12:Y:20:ARG:NH2     | 20:Y:101:TGL:HC32 | 2.18                     | 0.58              |
| 4:Q:73:ARG:HH11     | 4:Q:73:ARG:HG2    | 1.67                     | 0.58              |
| 6:F:75:HIS:H        | 6:F:80:GLN:HE22   | 1.51                     | 0.58              |
| 20:L:101:TGL:HC61   | 20:L:101:TGL:HC22 | 1.86                     | 0.58              |
| 1:N:177:SER:H       | 1:N:180:GLN:NE2   | 2.02                     | 0.58              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 23:N:610:PSC:H21    | 23:N:610:PSC:H222 | 1.84                     | 0.58              |
| 4:Q:127:LYS:HD2     | 28:V:109:HOH:O    | 2.04                     | 0.58              |
| 1:A:136[B]:LEU:HD11 | 28:A:927:HOH:O    | 2.04                     | 0.58              |
| 2:O:127:GLU:HG2     | 28:O:543:HOH:O    | 2.04                     | 0.58              |
| 6:S:94:HIS:CD2      | 6:S:95:GLN:H      | 2.21                     | 0.58              |
| 10:J:37:THR:OG1     | 22:J:101:CHD:H5   | 2.04                     | 0.57              |
| 6:F:92:VAL:HG23     | 6:F:92:VAL:O      | 2.02                     | 0.57              |
| 25:G:101:CDL:H242   | 25:G:101:CDL:H542 | 1.86                     | 0.57              |
| 25:G:101:CDL:H171   | 1:N:307:SER:HB3   | 1.85                     | 0.57              |
| 19:N:607:PGV:H322   | 13:Z:19:LEU:HD23  | 1.86                     | 0.57              |
| 3:C:161:GLN:NE2     | 24:C:307:PEK:C2   | 2.67                     | 0.57              |
| 1:N:422:ASN:OD1     | 20:N:609:TGL:H262 | 2.03                     | 0.57              |
| 3:C:33[A]:MET:HE1   | 10:J:45:TYR:OH    | 2.04                     | 0.57              |
| 2:O:128:LEU:HD11    | 2:O:134:ARG:HA    | 1.87                     | 0.57              |
| 1:A:431:LEU:HD21    | 1:A:450:TRP:HB2   | 1.85                     | 0.57              |
| 7:G:72:ASN:H        | 7:G:76:ASN:ND2    | 1.96                     | 0.57              |
| 28:N:945:HOH:O      | 2:O:56:MET:SD     | 2.58                     | 0.57              |
| 3:P:33[A]:MET:CE    | 3:P:42:LEU:H      | 2.18                     | 0.57              |
| 24:P:308:PEK:H311   | 7:T:26:PRO:HB3    | 1.86                     | 0.57              |
| 1:A:177:SER:H       | 1:A:180:GLN:HE21  | 1.53                     | 0.57              |
| 1:N:229:ILE:HD11    | 2:O:175:ILE:HD13  | 1.87                     | 0.57              |
| 7:T:5:LYS:CG        | 24:T:101:PEK:H371 | 2.34                     | 0.57              |
| 1:N:400:PHE:O       | 20:Y:101:TGL:H281 | 2.04                     | 0.57              |
| 10:W:4:ARG:HD2      | 10:W:7:GLU:OE2    | 2.05                     | 0.57              |
| 22:C:305:CHD:C23    | 22:C:305:CHD:H162 | 2.35                     | 0.57              |
| 12:L:13:PHE:HB3     | 20:L:101:TGL:HG12 | 1.85                     | 0.57              |
| 6:F:95:GLN:HB3      | 28:F:280:HOH:O    | 2.03                     | 0.56              |
| 7:G:45:PRO:HD2      | 28:G:203:HOH:O    | 2.06                     | 0.56              |
| 4:Q:19:ARG:HG2      | 4:Q:21:ASP:OD1    | 2.04                     | 0.56              |
| 1:A:274:VAL:HG12    | 1:A:278:MET:HE2   | 1.87                     | 0.56              |
| 25:G:101:CDL:H561   | 25:G:101:CDL:H771 | 1.87                     | 0.56              |
| 12:L:26:THR:HG22    | 28:L:226:HOH:O    | 2.05                     | 0.56              |
| 25:G:101:CDL:H771   | 25:G:101:CDL:C56  | 2.35                     | 0.56              |
| 6:S:78:GLU:HB2      | 28:S:317:HOH:O    | 2.05                     | 0.56              |
| 2:B:32:PHE:HE2      | 20:B:301:TGL:HA52 | 1.67                     | 0.56              |
| 23:B:304:PSC:H241   | 23:B:304:PSC:H42  | 1.86                     | 0.56              |
| 7:G:8:HIS:O         | 7:G:9:GLY:C       | 2.47                     | 0.56              |
| 7:T:11:TPO:HG22     | 7:T:16:TRP:HE1    | 1.71                     | 0.56              |
| 24:C:307:PEK:H361   | 25:G:101:CDL:C27  | 2.34                     | 0.56              |
| 24:C:307:PEK:H041   | 7:G:17:ARG:HH22   | 1.71                     | 0.56              |
| 25:G:101:CDL:C35    | 2:O:78:LEU:HD12   | 2.35                     | 0.56              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 12:L:26:THR:HG23  | 13:M:25:SER:HB2     | 1.88                     | 0.56              |
| 1:N:113:LEU:HD12  | 20:Y:101:TGL:C14    | 2.36                     | 0.56              |
| 24:P:308:PEK:H383 | 25:T:102:CDL:H273   | 1.88                     | 0.56              |
| 20:L:101:TGL:HC61 | 20:L:101:TGL:CC1    | 2.36                     | 0.56              |
| 4:Q:6:VAL:HG12    | 4:Q:7:LYS:N         | 2.20                     | 0.56              |
| 1:A:297:MET:HG2   | 28:C:531:HOH:O      | 2.05                     | 0.56              |
| 24:G:102:PEK:H241 | 28:G:266:HOH:O      | 2.06                     | 0.56              |
| 3:P:210:ILE:HD13  | 19:P:304:PGV:H301   | 1.87                     | 0.55              |
| 7:T:72:ASN:N      | 7:T:76:ASN:HD22     | 1.99                     | 0.55              |
| 20:Y:101:TGL:OG3  | 20:Y:101:TGL:OA1    | 2.24                     | 0.55              |
| 1:N:172:LYS:HD2   | 1:N:181:THR:CG2     | 2.36                     | 0.55              |
| 1:N:409:TRP:HB3   | 1:N:471:ILE:HG12    | 1.88                     | 0.55              |
| 3:P:77:LYS:NZ     | 28:P:482:HOH:O      | 2.36                     | 0.55              |
| 1:N:483:LEU:HD21  | 13:Z:4:LYS:HE3      | 1.87                     | 0.55              |
| 20:N:609:TGL:HC31 | 28:V:102:HOH:O      | 2.07                     | 0.55              |
| 3:P:5:THR:HG22    | 6:S:96:LEU:HD13     | 1.88                     | 0.55              |
| 6:S:43:LYS:HE3    | 28:S:282:HOH:O      | 2.06                     | 0.55              |
| 1:A:225:GLY:HA3   | 3:C:112:LEU:HD21    | 1.88                     | 0.55              |
| 1:N:28:MET:HE2    | 14:N:601:HEA:C27    | 2.37                     | 0.55              |
| 8:U:48:GLY:HA2    | 28:U:133:HOH:O      | 2.06                     | 0.55              |
| 1:A:1:FME:HE1     | 28:A:963:HOH:O      | 2.06                     | 0.54              |
| 12:Y:12:PRO:HG2   | 20:Y:101:TGL:HG11   | 1.89                     | 0.54              |
| 2:B:33:LEU:HD13   | 9:I:31:PHE:HD1      | 1.70                     | 0.54              |
| 6:F:64:GLU:O      | 6:F:65:ASP:HB2      | 2.07                     | 0.54              |
| 3:P:168:THR:HG22  | 24:P:308:PEK:H14    | 1.88                     | 0.54              |
| 3:C:94:PHE:HD2    | 28:C:509:HOH:O      | 1.90                     | 0.54              |
| 11:X:52:GLU:HG2   | 28:X:120:HOH:O      | 2.06                     | 0.54              |
| 1:N:308:ALA:O     | 1:N:311[B]:ILE:HG22 | 2.08                     | 0.54              |
| 14:N:601:HEA:HBC1 | 14:N:601:HEA:CMC    | 2.37                     | 0.54              |
| 8:H:50:VAL:HG23   | 28:H:156:HOH:O      | 2.07                     | 0.54              |
| 1:N:321:PHE:HD2   | 23:N:610:PSC:C34    | 2.15                     | 0.54              |
| 4:Q:10:ASP:HB3    | 4:Q:13:LEU:HD12     | 1.88                     | 0.54              |
| 1:A:513:LEU:O     | 1:A:514:LYS:CB      | 2.46                     | 0.54              |
| 3:C:54:MET:HE1    | 19:C:303:PGV:C14    | 2.38                     | 0.54              |
| 1:N:513:LEU:O     | 1:N:514:LYS:CB      | 2.31                     | 0.54              |
| 7:G:41:HIS:HB3    | 7:G:74:ARG:CZ       | 2.37                     | 0.54              |
| 2:O:91:ASN:HD22   | 2:O:149:THR:HG21    | 1.73                     | 0.54              |
| 28:P:529:HOH:O    | 25:T:102:CDL:H673   | 2.06                     | 0.54              |
| 7:T:5:LYS:HD2     | 24:T:101:PEK:H371   | 1.89                     | 0.54              |
| 25:G:101:CDL:H171 | 1:N:307:SER:CB      | 2.38                     | 0.53              |
| 8:H:43:MET:HE1    | 8:U:43:MET:HE1      | 1.89                     | 0.53              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:N:265:LYS:HB2    | 1:N:490:THR:HG21    | 1.90                     | 0.53              |
| 2:O:53:THR:HG21    | 28:Q:344:HOH:O      | 2.07                     | 0.53              |
| 12:Y:12:PRO:HB2    | 20:Y:101:TGL:CG1    | 2.37                     | 0.53              |
| 28:B:452:HOH:O     | 20:D:201:TGL:HC61   | 2.08                     | 0.53              |
| 1:N:113:LEU:HD12   | 20:Y:101:TGL:C13    | 2.38                     | 0.53              |
| 3:P:77:LYS:NZ      | 3:P:81:TYR:OH       | 2.40                     | 0.53              |
| 4:Q:19:ARG:CD      | 4:Q:21:ASP:OD1      | 2.57                     | 0.53              |
| 25:T:102:CDL:H571  | 25:T:102:CDL:H781   | 1.91                     | 0.53              |
| 25:T:102:CDL:H172  | 28:T:222:HOH:O      | 2.07                     | 0.53              |
| 1:A:309:THR:O      | 1:A:312[B]:ILE:HG22 | 2.08                     | 0.53              |
| 7:G:84:LYS:HG2     | 28:G:253:HOH:O      | 2.08                     | 0.53              |
| 1:N:411:LYS:NZ     | 28:N:890:HOH:O      | 2.41                     | 0.53              |
| 1:A:311[B]:ILE:CD1 | 24:P:308:PEK:H342   | 2.39                     | 0.53              |
| 8:H:43:MET:CE      | 8:H:49:ASP:H        | 2.22                     | 0.53              |
| 8:U:45:ALA:O       | 8:U:47:GLY:N        | 2.42                     | 0.53              |
| 2:B:49:LYS:HD3     | 20:D:201:TGL:HC72   | 1.91                     | 0.53              |
| 3:C:191:GLY:HA3    | 28:G:204:HOH:O      | 2.09                     | 0.53              |
| 25:G:101:CDL:H542  | 25:G:101:CDL:C24    | 2.38                     | 0.53              |
| 8:H:36:PHE:CD1     | 8:H:57:ARG:HB2      | 2.44                     | 0.53              |
| 1:A:165:ILE:HG22   | 1:A:169[B]:ILE:HD12 | 1.91                     | 0.53              |
| 23:N:610:PSC:H12   | 23:N:610:PSC:H321   | 1.90                     | 0.53              |
| 4:Q:6:VAL:HG12     | 4:Q:10:ASP:OD2      | 2.07                     | 0.53              |
| 7:T:5:LYS:HG3      | 24:T:101:PEK:C37    | 2.37                     | 0.53              |
| 1:N:152:LEU:HD22   | 3:P:24:ALA:HB1      | 1.91                     | 0.53              |
| 28:O:479:HOH:O     | 20:Q:201:TGL:HC72   | 2.09                     | 0.53              |
| 12:Y:20:ARG:NH2    | 12:Y:24:MET:HG3     | 2.23                     | 0.53              |
| 3:C:156:ARG:HE     | 22:C:305:CHD:C24    | 2.22                     | 0.53              |
| 1:A:112:LEU:HG     | 28:A:749:HOH:O      | 2.10                     | 0.52              |
| 10:J:55:PHE:HB2    | 28:J:230:HOH:O      | 2.09                     | 0.52              |
| 8:H:8:ILE:HG23     | 8:H:8:ILE:O         | 2.09                     | 0.52              |
| 1:N:321:PHE:CZ     | 23:N:610:PSC:H162   | 2.45                     | 0.52              |
| 2:O:1:FME:HE1      | 2:O:133:LEU:HD22    | 1.92                     | 0.52              |
| 3:P:207:HIS:HD2    | 3:P:241:TYR:OH      | 1.92                     | 0.52              |
| 28:B:582:HOH:O     | 24:P:308:PEK:H301   | 2.08                     | 0.52              |
| 2:O:116:LEU:HD13   | 2:O:226:MET:HG3     | 1.91                     | 0.52              |
| 2:O:196:CYS:HB2    | 2:O:207:MET:HG3     | 1.92                     | 0.52              |
| 10:W:2:GLU:HA      | 28:W:218:HOH:O      | 2.09                     | 0.52              |
| 20:L:101:TGL:HC61  | 20:L:101:TGL:CC2    | 2.39                     | 0.52              |
| 23:N:610:PSC:H12   | 23:N:610:PSC:H322   | 1.92                     | 0.52              |
| 1:A:43:GLN:HB2     | 1:A:44:PRO:HD2      | 1.91                     | 0.52              |
| 3:C:84:ILE:HD11    | 24:T:101:PEK:H031   | 1.92                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 23:B:304:PSC:H342   | 23:B:304:PSC:C13    | 2.39                     | 0.52              |
| 3:C:59:ARG:HG3      | 25:C:304:CDL:H512   | 1.90                     | 0.52              |
| 1:N:390:MET:O       | 1:N:394[A]:VAL:HG22 | 2.10                     | 0.52              |
| 3:P:168:THR:CG2     | 24:P:308:PEK:H14    | 2.40                     | 0.52              |
| 19:P:301:PGV:H21    | 28:P:512:HOH:O      | 2.09                     | 0.52              |
| 1:N:208:MET:HE2     | 3:P:97:PHE:CD1      | 2.44                     | 0.51              |
| 25:T:102:CDL:HA21   | 25:T:102:CDL:H122   | 1.93                     | 0.51              |
| 9:V:8:GLN:HG3       | 28:V:116:HOH:O      | 2.08                     | 0.51              |
| 1:A:177:SER:H       | 1:A:180:GLN:NE2     | 2.08                     | 0.51              |
| 20:N:609:TGL:H191   | 28:N:933:HOH:O      | 2.09                     | 0.51              |
| 1:A:76:GLY:O        | 1:A:80:ASN:HB2      | 2.11                     | 0.51              |
| 1:A:297:MET:HB2     | 28:A:924:HOH:O      | 2.11                     | 0.51              |
| 6:S:76:LYS:CD       | 28:S:271:HOH:O      | 2.19                     | 0.51              |
| 19:P:301:PGV:H42    | 22:P:307:CHD:H151   | 1.93                     | 0.51              |
| 2:O:82:ARG:HG2      | 2:O:86:MET:HE3      | 1.91                     | 0.51              |
| 19:A:608:PGV:P      | 19:A:608:PGV:H061   | 2.50                     | 0.51              |
| 1:N:336:PRO:HB2     | 1:N:394[B]:VAL:HG11 | 1.93                     | 0.51              |
| 5:E:16:VAL:HG21     | 5:E:46:LYS:HG3      | 1.92                     | 0.51              |
| 1:N:112:LEU:HD23    | 1:N:113:LEU:HD23    | 1.93                     | 0.51              |
| 23:B:304:PSC:H042   | 28:E:217:HOH:O      | 2.10                     | 0.50              |
| 3:P:110:PRO:HB3     | 8:U:30:TRP:CE3      | 2.46                     | 0.50              |
| 23:N:610:PSC:H21    | 23:N:610:PSC:C22    | 2.40                     | 0.50              |
| 1:A:308:ALA:HA      | 25:T:102:CDL:H212   | 1.94                     | 0.50              |
| 14:A:601:HEA:HMC3   | 14:A:601:HEA:HBC1   | 1.93                     | 0.50              |
| 24:C:307:PEK:C04    | 7:G:17:ARG:HH22     | 2.25                     | 0.50              |
| 1:N:136[B]:LEU:HD22 | 28:N:893:HOH:O      | 2.09                     | 0.50              |
| 1:N:406:ASN:HD21    | 19:N:607:PGV:C2     | 2.25                     | 0.50              |
| 12:Y:35:ALA:HB3     | 12:Y:36:PRO:HD3     | 1.94                     | 0.50              |
| 1:A:299:VAL:HG23    | 2:B:84:LEU:HG       | 1.94                     | 0.50              |
| 28:O:458:HOH:O      | 8:U:61:LYS:HE3      | 2.10                     | 0.50              |
| 3:P:51[A]:MET:SD    | 25:P:305:CDL:H621   | 2.51                     | 0.50              |
| 2:B:104:TRP:CG      | 2:B:203:ASN:HB2     | 2.46                     | 0.50              |
| 3:C:55:TYR:CE1      | 25:C:304:CDL:H521   | 2.47                     | 0.50              |
| 6:F:87:THR:HG21     | 28:F:222:HOH:O      | 2.12                     | 0.50              |
| 7:T:2:SER:OG        | 24:T:101:PEK:C29    | 2.59                     | 0.50              |
| 1:A:285:PHE:CD2     | 7:T:4:ALA:HB2       | 2.47                     | 0.50              |
| 19:C:303:PGV:H12    | 25:C:304:CDL:H651   | 1.93                     | 0.50              |
| 23:N:610:PSC:H072   | 9:V:10:ARG:HH21     | 1.77                     | 0.50              |
| 1:A:343:GLY:HA2     | 20:D:201:TGL:H211   | 1.92                     | 0.50              |
| 7:G:9:GLY:HA3       | 28:N:812:HOH:O      | 2.12                     | 0.50              |
| 23:B:304:PSC:H212   | 23:B:304:PSC:O01    | 2.12                     | 0.50              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 8:H:9:LYS:HG3       | 8:H:11:TYR:H      | 1.77                     | 0.50              |
| 3:P:210:ILE:HG21    | 19:P:304:PGV:H282 | 1.93                     | 0.50              |
| 19:A:608:PGV:H251   | 13:M:12:PRO:HG3   | 1.93                     | 0.49              |
| 3:P:107:ALA:HB2     | 19:P:301:PGV:C03  | 2.41                     | 0.49              |
| 3:P:207:HIS:CD2     | 3:P:241:TYR:OH    | 2.65                     | 0.49              |
| 3:C:127:LEU:HD13    | 25:G:101:CDL:OB3  | 2.11                     | 0.49              |
| 25:C:304:CDL:HB22   | 25:C:304:CDL:CB5  | 2.42                     | 0.49              |
| 6:F:55:LYS:HG3      | 6:F:73:TRP:CZ3    | 2.48                     | 0.49              |
| 24:P:303:PEK:H15    | 24:P:303:PEK:C20  | 2.36                     | 0.49              |
| 3:C:164:PHE:CD1     | 22:C:305:CHD:H192 | 2.48                     | 0.49              |
| 5:E:86:ILE:O        | 5:E:90:ARG:HG2    | 2.12                     | 0.49              |
| 1:N:155:VAL:HG21    | 19:N:608:PGV:H142 | 1.95                     | 0.49              |
| 1:N:169[B]:ILE:HD11 | 1:N:189:MET:CE    | 2.36                     | 0.49              |
| 4:Q:130:PRO:HD2     | 4:Q:131:ILE:HD12  | 1.94                     | 0.49              |
| 1:A:415:ALA:HB1     | 20:D:201:TGL:H132 | 1.94                     | 0.49              |
| 19:N:608:PGV:H61    | 3:P:54:MET:HG2    | 1.94                     | 0.49              |
| 19:N:608:PGV:H21    | 3:P:57:TRP:CZ2    | 2.47                     | 0.49              |
| 4:Q:7:LYS:HA        | 28:Q:373:HOH:O    | 2.13                     | 0.49              |
| 2:B:58:ALA:O        | 2:B:62:GLU:HG3    | 2.12                     | 0.49              |
| 4:D:34:SER:H        | 4:D:37:GLN:NE2    | 2.10                     | 0.49              |
| 25:P:305:CDL:H431   | 10:W:34:VAL:HG11  | 1.93                     | 0.49              |
| 1:A:514:LYS:HA      | 6:F:38:ALA:HB3    | 1.93                     | 0.49              |
| 25:G:101:CDL:HA21   | 25:G:101:CDL:C11  | 2.39                     | 0.49              |
| 2:O:13:THR:HB       | 2:O:168:LEU:HD23  | 1.95                     | 0.49              |
| 13:Z:40:TYR:O       | 13:Z:42:LYS:N     | 2.45                     | 0.49              |
| 3:C:224:LYS:HD3     | 25:C:304:CDL:CB3  | 2.42                     | 0.49              |
| 24:C:307:PEK:H292   | 28:O:486:HOH:O    | 2.13                     | 0.49              |
| 4:D:82:VAL:HG12     | 4:D:86:MET:HE2    | 1.94                     | 0.49              |
| 7:G:3:ALA:O         | 7:G:4:ALA:HB2     | 2.11                     | 0.49              |
| 1:N:317:GLY:O       | 1:N:321:PHE:CD1   | 2.66                     | 0.49              |
| 7:T:2:SER:O         | 7:T:3:ALA:HB3     | 2.11                     | 0.49              |
| 19:N:608:PGV:C34    | 24:P:303:PEK:H382 | 2.35                     | 0.48              |
| 28:R:294:HOH:O      | 9:V:11:GLY:HA2    | 2.12                     | 0.48              |
| 1:A:459:PHE:HE2     | 28:A:949:HOH:O    | 1.96                     | 0.48              |
| 2:B:30:ILE:HD13     | 28:B:571:HOH:O    | 2.13                     | 0.48              |
| 7:G:2:SER:HB2       | 1:N:197:LEU:HD21  | 1.95                     | 0.48              |
| 25:G:101:CDL:H522   | 25:G:101:CDL:C20  | 2.37                     | 0.48              |
| 3:P:62:ILE:HD12     | 25:P:305:CDL:H511 | 1.94                     | 0.48              |
| 1:A:1:FME:CE        | 1:A:4:ASN:HD22    | 2.27                     | 0.48              |
| 1:A:303:ALA:HB1     | 25:T:102:CDL:H132 | 1.95                     | 0.48              |
| 7:G:2:SER:HB2       | 1:N:197:LEU:HD11  | 1.96                     | 0.48              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 25:T:102:CDL:H571   | 25:T:102:CDL:C78  | 2.43                     | 0.48              |
| 12:Y:25:MET:HE3     | 20:Y:101:TGL:HA81 | 1.96                     | 0.48              |
| 2:O:1:FME:CE        | 2:O:133:LEU:HD22  | 2.43                     | 0.48              |
| 1:A:409:TRP:HB3     | 1:A:471:ILE:HG12  | 1.95                     | 0.48              |
| 4:D:78:TRP:CA       | 20:D:201:TGL:CB2  | 2.92                     | 0.48              |
| 9:I:57:MET:O        | 9:I:61:GLU:HG2    | 2.13                     | 0.48              |
| 11:K:44:PRO:CA      | 11:K:47:ARG:HH21  | 2.27                     | 0.48              |
| 24:P:303:PEK:H11    | 24:P:303:PEK:H161 | 1.96                     | 0.48              |
| 2:B:41:ILE:HD13     | 23:B:304:PSC:H341 | 1.96                     | 0.48              |
| 2:B:86:MET:HE3      | 2:B:86:MET:HB2    | 1.76                     | 0.48              |
| 6:S:54:ASN:HD22     | 6:S:54:ASN:C      | 2.22                     | 0.48              |
| 1:A:172:LYS:NZ      | 1:A:178:GLN:HE22  | 2.12                     | 0.47              |
| 2:B:56:MET:CG       | 23:B:304:PSC:H221 | 2.43                     | 0.47              |
| 3:C:204:HIS:HB2     | 3:C:252:LEU:HD11  | 1.97                     | 0.47              |
| 7:G:37:LEU:HD21     | 25:G:101:CDL:H361 | 1.96                     | 0.47              |
| 23:N:610:PSC:C13    | 23:N:610:PSC:H343 | 2.44                     | 0.47              |
| 12:Y:46:LYS:HG2     | 28:Y:229:HOH:O    | 2.15                     | 0.47              |
| 12:L:20:ARG:HH22    | 20:L:101:TGL:HC52 | 1.79                     | 0.47              |
| 10:W:36:MET:HB3     | 22:W:101:CHD:H181 | 1.97                     | 0.47              |
| 12:Y:41:ARG:HG3     | 13:Z:40:TYR:CE1   | 2.50                     | 0.47              |
| 8:H:43:MET:CE       | 8:U:43:MET:HE1    | 2.44                     | 0.47              |
| 1:N:87:ILE:O        | 1:N:173:PRO:HD3   | 2.14                     | 0.47              |
| 1:N:172:LYS:NZ      | 1:N:178:GLN:HE22  | 2.13                     | 0.47              |
| 9:V:61:GLU:OE1      | 9:V:64:ARG:NE     | 2.45                     | 0.47              |
| 3:C:226:HIS:CE1     | 25:C:304:CDL:HB32 | 2.50                     | 0.47              |
| 8:U:7:LYS:HB2       | 28:U:139:HOH:O    | 2.14                     | 0.47              |
| 1:A:229:ILE:HD11    | 2:B:175:ILE:HD13  | 1.96                     | 0.47              |
| 8:H:9:LYS:O         | 8:H:10:ASN:CB     | 2.62                     | 0.47              |
| 2:O:94:SER:OG       | 2:O:148:MET:HE2   | 2.15                     | 0.47              |
| 24:P:308:PEK:C38    | 25:T:102:CDL:C27  | 2.93                     | 0.47              |
| 22:J:101:CHD:H192   | 22:J:101:CHD:H3   | 1.96                     | 0.47              |
| 23:N:610:PSC:H42    | 23:N:610:PSC:H241 | 1.97                     | 0.47              |
| 24:P:308:PEK:H362   | 24:P:308:PEK:H332 | 1.78                     | 0.47              |
| 1:A:311[A]:ILE:HD13 | 25:T:102:CDL:C22  | 2.41                     | 0.47              |
| 1:N:104:LEU:C       | 1:N:107:PRO:HD2   | 2.40                     | 0.47              |
| 19:N:607:PGV:H302   | 13:Z:19:LEU:HD22  | 1.96                     | 0.47              |
| 6:S:76:LYS:CE       | 28:S:271:HOH:O    | 2.57                     | 0.47              |
| 7:T:2:SER:O         | 24:T:101:PEK:H322 | 2.15                     | 0.47              |
| 3:C:52:LEU:HD23     | 25:C:304:CDL:H362 | 1.97                     | 0.47              |
| 2:O:42:ILE:HG21     | 20:Q:201:TGL:H232 | 1.96                     | 0.47              |
| 3:P:127:LEU:HD22    | 25:T:102:CDL:HB62 | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:T:102:CDL:H712 | 25:T:102:CDL:H521 | 1.97                     | 0.47              |
| 2:B:56:MET:HG2    | 23:B:304:PSC:H201 | 1.95                     | 0.46              |
| 25:G:101:CDL:H732 | 25:G:101:CDL:H541 | 1.97                     | 0.46              |
| 12:L:24:MET:SD    | 20:L:101:TGL:HC82 | 2.55                     | 0.46              |
| 28:C:536:HOH:O    | 24:T:101:PEK:H262 | 2.14                     | 0.46              |
| 7:G:23:LEU:HD12   | 25:G:101:CDL:H271 | 1.97                     | 0.46              |
| 9:I:36:LYS:HB2    | 9:I:36:LYS:HE3    | 1.64                     | 0.46              |
| 2:O:4:PRO:HB2     | 11:X:43:SER:HA    | 1.96                     | 0.46              |
| 7:T:7:ASP:O       | 7:T:9:GLY:N       | 2.49                     | 0.46              |
| 24:C:302:PEK:H102 | 24:C:302:PEK:H72  | 1.73                     | 0.46              |
| 4:D:78:TRP:N      | 20:D:201:TGL:CB2  | 2.77                     | 0.46              |
| 19:N:607:PGV:H21  | 19:N:607:PGV:H52  | 1.64                     | 0.46              |
| 2:B:14:SER:HB3    | 2:B:168:LEU:CD2   | 2.46                     | 0.46              |
| 24:C:302:PEK:H161 | 24:C:302:PEK:C12  | 2.45                     | 0.46              |
| 4:D:78:TRP:CA     | 20:D:201:TGL:HB22 | 2.45                     | 0.46              |
| 25:G:101:CDL:H152 | 1:N:307:SER:OG    | 2.15                     | 0.46              |
| 1:N:62:ALA:HB2    | 14:N:601:HEA:HBD1 | 1.96                     | 0.46              |
| 2:O:215:PRO:HD3   | 9:V:60:PHE:CD2    | 2.50                     | 0.46              |
| 1:A:468:MET:HG3   | 28:A:937:HOH:O    | 2.15                     | 0.46              |
| 24:C:307:PEK:H383 | 25:G:101:CDL:H271 | 1.89                     | 0.46              |
| 1:N:240:HIS:O     | 1:N:241:PRO:C     | 2.56                     | 0.46              |
| 19:N:608:PGV:H343 | 24:P:303:PEK:C38  | 2.36                     | 0.46              |
| 2:O:67:ILE:CD1    | 28:O:486:HOH:O    | 2.62                     | 0.46              |
| 7:T:33:LEU:O      | 7:T:34:ASN:C      | 2.59                     | 0.46              |
| 25:T:102:CDL:H342 | 25:T:102:CDL:OA7  | 2.16                     | 0.46              |
| 19:A:607:PGV:H343 | 24:C:302:PEK:H382 | 1.97                     | 0.46              |
| 8:H:60:TYR:CD1    | 8:H:60:TYR:C      | 2.93                     | 0.46              |
| 2:B:164:ALA:O     | 2:B:194:GLY:HA3   | 2.15                     | 0.46              |
| 1:N:310:MET:HE3   | 1:N:356:ILE:CG2   | 2.45                     | 0.46              |
| 10:W:32:TYR:OH    | 22:W:101:CHD:H213 | 2.15                     | 0.46              |
| 8:H:54:GLU:OE1    | 8:H:54:GLU:HA     | 2.16                     | 0.46              |
| 5:R:76:GLY:O      | 5:R:79:LYS:HE3    | 2.16                     | 0.46              |
| 1:A:507:GLU:CD    | 28:A:945:HOH:O    | 2.59                     | 0.45              |
| 6:F:95:GLN:O      | 6:F:97:ALA:N      | 2.40                     | 0.45              |
| 7:T:2:SER:O       | 7:T:3:ALA:CB      | 2.64                     | 0.45              |
| 2:B:30:ILE:CD1    | 28:B:571:HOH:O    | 2.63                     | 0.45              |
| 3:C:62:ILE:HD12   | 25:C:304:CDL:H511 | 1.99                     | 0.45              |
| 11:K:44:PRO:HA    | 11:K:47:ARG:HH21  | 1.80                     | 0.45              |
| 13:M:39:ASN:OD1   | 13:M:39:ASN:N     | 2.49                     | 0.45              |
| 2:O:129:LYS:O     | 2:O:132:GLU:HG3   | 2.17                     | 0.45              |
| 22:W:101:CHD:O12  | 22:W:101:CHD:H222 | 2.15                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:A:337:ALA:HB2     | 1:A:394[A]:VAL:HG23 | 1.99                     | 0.45              |
| 2:O:114:GLU:HG3     | 28:O:505:HOH:O      | 2.15                     | 0.45              |
| 2:O:128:LEU:HD22    | 2:O:132:GLU:HB2     | 1.97                     | 0.45              |
| 2:O:130:PRO:HA      | 4:Q:115:TRP:CZ3     | 2.52                     | 0.45              |
| 25:P:305:CDL:H561   | 25:P:305:CDL:H531   | 1.50                     | 0.45              |
| 19:A:608:PGV:H311   | 13:M:19:LEU:CD2     | 2.41                     | 0.45              |
| 1:N:25:TRP:CH2      | 20:Y:101:TGL:H292   | 2.52                     | 0.45              |
| 4:D:98:TRP:CE2      | 27:M:101:DMU:H11    | 2.52                     | 0.45              |
| 20:Q:201:TGL:HG31   | 20:Q:201:TGL:HC21   | 1.77                     | 0.45              |
| 5:R:77:PRO:O        | 5:R:79:LYS:HD2      | 2.16                     | 0.45              |
| 7:T:11:TPO:CG2      | 7:T:11:TPO:O        | 2.65                     | 0.45              |
| 1:A:307:SER:HB2     | 25:T:102:CDL:H192   | 1.99                     | 0.45              |
| 1:A:311[B]:ILE:HG12 | 1:A:311[B]:ILE:O    | 2.15                     | 0.45              |
| 3:C:110:PRO:HB3     | 8:H:30:TRP:CE3      | 2.52                     | 0.45              |
| 8:H:43:MET:HE3      | 8:H:48:GLY:HA3      | 1.98                     | 0.45              |
| 13:M:39:ASN:O       | 13:M:43:SER:HB2     | 2.16                     | 0.45              |
| 1:N:383:MET:HG2     | 1:N:421:VAL:HG21    | 1.97                     | 0.45              |
| 3:P:154:GLY:HA2     | 6:S:6:VAL:HB        | 1.97                     | 0.45              |
| 20:Y:101:TGL:H172   | 28:Y:235:HOH:O      | 2.17                     | 0.45              |
| 23:B:304:PSC:H073   | 5:E:11:PHE:CG       | 2.52                     | 0.45              |
| 7:G:43:GLU:HA       | 28:G:269:HOH:O      | 2.16                     | 0.45              |
| 1:A:208:MET:HE2     | 3:C:97:PHE:CD1      | 2.52                     | 0.45              |
| 1:A:290:HIS:CD2     | 1:A:291:HIS:CD2     | 3.04                     | 0.45              |
| 2:B:168:LEU:HD13    | 2:B:184:LEU:HG      | 1.97                     | 0.45              |
| 1:N:296:GLY:HA2     | 8:U:23:GLN:OE1      | 2.17                     | 0.45              |
| 1:A:399:LEU:HB2     | 1:A:494:TRP:CZ3     | 2.52                     | 0.45              |
| 5:E:90:ARG:HG3      | 28:E:239:HOH:O      | 2.16                     | 0.45              |
| 11:K:8:ASP:HB2      | 28:K:111:HOH:O      | 2.16                     | 0.45              |
| 11:K:24:PHE:CE1     | 11:K:28:VAL:HG21    | 2.52                     | 0.45              |
| 1:N:468:MET:HG3     | 28:N:923:HOH:O      | 2.17                     | 0.45              |
| 7:G:2:SER:CB        | 1:N:197:LEU:HD11    | 2.47                     | 0.44              |
| 28:B:452:HOH:O      | 20:D:201:TGL:CC6    | 2.64                     | 0.44              |
| 1:N:321:PHE:HD2     | 23:N:610:PSC:C33    | 2.30                     | 0.44              |
| 2:O:164:ALA:O       | 2:O:194:GLY:HA3     | 2.16                     | 0.44              |
| 4:Q:73:ARG:HG2      | 4:Q:73:ARG:NH1      | 2.32                     | 0.44              |
| 22:W:101:CHD:H232   | 22:W:101:CHD:H211   | 1.60                     | 0.44              |
| 1:A:304:TYR:CD2     | 1:A:304:TYR:C       | 2.94                     | 0.44              |
| 1:A:411:LYS:NZ      | 28:A:908:HOH:O      | 2.50                     | 0.44              |
| 3:C:220:PHE:HB2     | 25:C:304:CDL:H712   | 1.99                     | 0.44              |
| 2:O:116:LEU:CD2     | 2:O:226:MET:HG2     | 2.48                     | 0.44              |
| 1:A:53:ILE:HD11     | 12:L:40:VAL:HG13    | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:64:GLU:O      | 6:F:65:ASP:CB     | 2.62                     | 0.44              |
| 1:N:334:TRP:HH2   | 2:O:46:LEU:HD13   | 1.81                     | 0.44              |
| 4:Q:19:ARG:CG     | 4:Q:21:ASP:OD1    | 2.65                     | 0.44              |
| 3:C:64:GLU:HA     | 3:C:68:GLN:HE21   | 1.83                     | 0.44              |
| 2:O:33:LEU:HD13   | 9:V:31:PHE:CD1    | 2.53                     | 0.44              |
| 24:P:308:PEK:C38  | 25:T:102:CDL:H271 | 2.46                     | 0.44              |
| 22:W:101:CHD:H111 | 22:W:101:CHD:H12A | 1.85                     | 0.44              |
| 13:Z:40:TYR:C     | 13:Z:42:LYS:H     | 2.26                     | 0.44              |
| 2:B:76:ILE:HG13   | 28:B:571:HOH:O    | 2.18                     | 0.44              |
| 19:N:607:PGV:H251 | 13:Z:12:PRO:HB3   | 2.00                     | 0.44              |
| 3:P:52:LEU:HD23   | 25:P:305:CDL:H362 | 2.00                     | 0.44              |
| 6:S:10:GLU:OE2    | 6:S:25:ARG:NH1    | 2.49                     | 0.44              |
| 14:A:601:HEA:HHC  | 14:A:601:HEA:H122 | 2.00                     | 0.44              |
| 2:B:207:MET:HE3   | 2:B:207:MET:HB2   | 1.79                     | 0.44              |
| 28:N:951:HOH:O    | 6:S:37:LYS:HE2    | 2.18                     | 0.44              |
| 22:C:306:CHD:H212 | 22:C:306:CHD:H12  | 1.99                     | 0.44              |
| 24:C:307:PEK:H372 | 1:N:279:SER:OG    | 2.18                     | 0.44              |
| 1:N:321:PHE:HB3   | 23:N:610:PSC:H331 | 2.00                     | 0.44              |
| 1:N:379:TYR:CZ    | 1:N:383:MET:HE1   | 2.53                     | 0.44              |
| 14:A:601:HEA:H212 | 14:A:601:HEA:H271 | 1.44                     | 0.43              |
| 3:C:55:TYR:CD1    | 25:C:304:CDL:H181 | 2.53                     | 0.43              |
| 3:C:122:HIS:HD2   | 28:C:467:HOH:O    | 2.00                     | 0.43              |
| 6:S:52:ILE:C      | 6:S:94:HIS:HD1    | 2.25                     | 0.43              |
| 8:U:34:LEU:O      | 8:U:38:ARG:HG3    | 2.19                     | 0.43              |
| 12:Y:42:HIS:O     | 12:Y:46:LYS:HG3   | 2.18                     | 0.43              |
| 25:G:101:CDL:H352 | 2:O:78:LEU:CD1    | 2.38                     | 0.43              |
| 1:N:105:LEU:HD23  | 1:N:105:LEU:HA    | 1.86                     | 0.43              |
| 19:N:607:PGV:H211 | 28:Z:222:HOH:O    | 2.18                     | 0.43              |
| 23:N:610:PSC:H21  | 23:N:610:PSC:C21  | 2.48                     | 0.43              |
| 24:P:308:PEK:H382 | 25:T:102:CDL:C27  | 2.47                     | 0.43              |
| 7:T:12:GLY:CA     | 28:T:207:HOH:O    | 2.65                     | 0.43              |
| 20:Y:101:TGL:H202 | 20:Y:101:TGL:H231 | 1.67                     | 0.43              |
| 10:J:29:ASN:HD22  | 10:J:29:ASN:H     | 1.66                     | 0.43              |
| 2:B:146:MET:HA    | 2:B:213:LEU:HD12  | 2.01                     | 0.43              |
| 8:H:7:LYS:HA      | 28:H:145:HOH:O    | 2.18                     | 0.43              |
| 3:P:112:LEU:HD13  | 3:P:118:PRO:HG3   | 1.99                     | 0.43              |
| 5:R:44:GLU:OE1    | 9:V:6:LYS:NZ      | 2.40                     | 0.43              |
| 9:V:51:TYR:O      | 9:V:52:ARG:C      | 2.61                     | 0.43              |
| 1:A:62:ALA:HB2    | 14:A:601:HEA:HBD1 | 2.00                     | 0.43              |
| 8:H:43:MET:HE3    | 8:H:49:ASP:N      | 2.33                     | 0.43              |
| 12:L:2:HIS:CG     | 12:L:3:TYR:N      | 2.70                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:144:ILE:CD1   | 3:P:239:ALA:HA    | 2.48                     | 0.43              |
| 6:S:62:CYS:HB3    | 6:S:85:CYS:HB3    | 2.01                     | 0.43              |
| 2:B:193:TYR:CD1   | 2:B:210:VAL:HG22  | 2.54                     | 0.43              |
| 1:N:399:LEU:O     | 1:N:499:PRO:HA    | 2.18                     | 0.43              |
| 6:F:54:ASN:H      | 6:F:54:ASN:HD22   | 1.65                     | 0.43              |
| 10:J:37:THR:OG1   | 22:J:101:CHD:H191 | 2.18                     | 0.43              |
| 13:Z:36:HIS:HD2   | 13:Z:39:ASN:HD22  | 1.67                     | 0.43              |
| 1:A:449:MET:SD    | 2:B:5:MET:HG2     | 2.59                     | 0.43              |
| 22:B:303:CHD:H12  | 22:B:303:CHD:H212 | 2.00                     | 0.43              |
| 24:C:302:PEK:H171 | 24:C:302:PEK:H203 | 1.81                     | 0.43              |
| 8:H:54:GLU:OE2    | 8:H:57:ARG:NH2    | 2.44                     | 0.43              |
| 12:L:20:ARG:HH22  | 20:L:101:TGL:CC3  | 2.11                     | 0.43              |
| 1:N:172:LYS:HZ2   | 1:N:178:GLN:HE22  | 1.67                     | 0.43              |
| 5:R:80:GLU:CD     | 5:R:80:GLU:N      | 2.69                     | 0.43              |
| 19:A:607:PGV:H183 | 24:C:302:PEK:H322 | 2.01                     | 0.43              |
| 24:P:308:PEK:H6   | 24:P:308:PEK:H221 | 2.01                     | 0.43              |
| 14:A:602:HEA:HAD2 | 14:A:602:HEA:HH4  | 1.76                     | 0.43              |
| 3:P:62:ILE:CD1    | 3:P:221:ARG:HD2   | 2.49                     | 0.43              |
| 4:Q:48:TRP:HB2    | 5:R:96:LEU:O      | 2.18                     | 0.43              |
| 4:Q:52:SER:HB2    | 28:Q:340:HOH:O    | 2.18                     | 0.43              |
| 4:D:78:TRP:CA     | 20:D:201:TGL:HB21 | 2.49                     | 0.42              |
| 7:G:3:ALA:HA      | 28:G:261:HOH:O    | 2.19                     | 0.42              |
| 25:C:304:CDL:H182 | 25:C:304:CDL:H352 | 2.00                     | 0.42              |
| 24:C:307:PEK:H383 | 25:G:101:CDL:H273 | 1.93                     | 0.42              |
| 19:P:301:PGV:H202 | 19:P:301:PGV:H231 | 1.74                     | 0.42              |
| 25:T:102:CDL:CB5  | 25:T:102:CDL:H181 | 2.50                     | 0.42              |
| 12:Y:39:ILE:O     | 12:Y:42:HIS:HB3   | 2.19                     | 0.42              |
| 25:C:304:CDL:OB6  | 25:C:304:CDL:CB2  | 2.67                     | 0.42              |
| 25:C:304:CDL:CB5  | 25:C:304:CDL:CB2  | 2.98                     | 0.42              |
| 25:G:101:CDL:H202 | 25:G:101:CDL:C52  | 2.39                     | 0.42              |
| 2:O:103:GLN:HB3   | 2:O:104:TRP:CE2   | 2.55                     | 0.42              |
| 3:P:213:THR:HG23  | 25:P:305:CDL:H771 | 2.01                     | 0.42              |
| 1:A:367:LEU:HD21  | 1:A:433:LEU:HD23  | 2.02                     | 0.42              |
| 19:C:308:PGV:H51  | 19:C:308:PGV:H21  | 1.88                     | 0.42              |
| 1:N:396:TRP:O     | 1:N:397:PHE:C     | 2.62                     | 0.42              |
| 25:P:305:CDL:H222 | 25:P:305:CDL:H192 | 1.80                     | 0.42              |
| 20:Q:201:TGL:HA32 | 20:Q:201:TGL:HB51 | 2.00                     | 0.42              |
| 12:Y:46:LYS:CD    | 28:Y:229:HOH:O    | 2.67                     | 0.42              |
| 25:G:101:CDL:H591 | 25:G:101:CDL:C77  | 2.49                     | 0.42              |
| 2:O:60:GLU:CD     | 2:O:60:GLU:H      | 2.26                     | 0.42              |
| 10:W:30:ILE:O     | 10:W:34:VAL:HG23  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:282:PHE:HA    | 7:T:4:ALA:CB      | 2.49                     | 0.42              |
| 2:B:216:LEU:O     | 2:B:220:GLU:HG3   | 2.20                     | 0.42              |
| 23:N:610:PSC:H062 | 23:N:610:PSC:H042 | 1.85                     | 0.42              |
| 28:A:955:HOH:O    | 2:B:206:PHE:CE1   | 2.51                     | 0.42              |
| 1:N:269:GLY:HA2   | 28:O:500:HOH:O    | 2.19                     | 0.42              |
| 2:O:168:LEU:HD13  | 2:O:184:LEU:HG    | 2.01                     | 0.42              |
| 3:P:155:ASP:OD2   | 6:S:2:SER:HA      | 2.20                     | 0.42              |
| 28:B:580:HOH:O    | 4:D:126:MET:SD    | 2.62                     | 0.42              |
| 11:K:52:GLU:HG3   | 28:K:131:HOH:O    | 2.18                     | 0.42              |
| 3:P:5:THR:HG22    | 6:S:96:LEU:HD11   | 1.99                     | 0.42              |
| 3:P:173:PHE:CD2   | 3:P:173:PHE:C     | 2.98                     | 0.42              |
| 6:S:43:LYS:N      | 6:S:43:LYS:HD2    | 2.24                     | 0.42              |
| 10:W:58:LYS:HD3   | 10:W:58:LYS:HA    | 1.70                     | 0.42              |
| 13:Z:40:TYR:C     | 13:Z:42:LYS:N     | 2.77                     | 0.42              |
| 25:G:101:CDL:H132 | 2:O:81:LEU:HD13   | 2.01                     | 0.42              |
| 9:I:51:TYR:HA     | 9:I:54:TYR:HB2    | 2.02                     | 0.42              |
| 2:O:1:FME:HE1     | 2:O:133:LEU:HD21  | 1.99                     | 0.42              |
| 4:D:107:ILE:HD12  | 4:D:111:PHE:CD1   | 2.54                     | 0.42              |
| 1:N:229:ILE:HD11  | 2:O:175:ILE:CD1   | 2.50                     | 0.42              |
| 3:P:157:LYS:HD3   | 28:P:520:HOH:O    | 2.20                     | 0.42              |
| 2:B:191:LEU:HD23  | 2:B:212:GLU:HA    | 2.01                     | 0.41              |
| 25:G:101:CDL:H771 | 25:G:101:CDL:H591 | 2.02                     | 0.41              |
| 19:A:608:PGV:C31  | 13:M:19:LEU:HD23  | 2.42                     | 0.41              |
| 7:G:50:TYR:HB3    | 7:G:52:HIS:CE1    | 2.55                     | 0.41              |
| 8:H:52:VAL:HG12   | 28:H:166:HOH:O    | 2.19                     | 0.41              |
| 19:N:607:PGV:H131 | 19:N:607:PGV:H301 | 2.02                     | 0.41              |
| 20:N:609:TGL:H152 | 2:O:7:LEU:HD11    | 2.01                     | 0.41              |
| 22:P:307:CHD:H212 | 22:P:307:CHD:H12  | 2.01                     | 0.41              |
| 7:T:38:HIS:HE1    | 25:T:102:CDL:H121 | 1.83                     | 0.41              |
| 7:G:5:LYS:CG      | 24:G:102:PEK:H383 | 2.35                     | 0.41              |
| 1:A:426:PHE:HB3   | 1:A:427:PRO:HD3   | 2.03                     | 0.41              |
| 1:A:468:MET:HE1   | 14:A:601:HEA:H271 | 2.02                     | 0.41              |
| 3:C:63:ARG:HE     | 25:C:304:CDL:HA21 | 1.83                     | 0.41              |
| 3:C:76:GLN:NE2    | 28:C:435:HOH:O    | 2.46                     | 0.41              |
| 3:C:210:ILE:HG21  | 19:C:303:PGV:H281 | 2.01                     | 0.41              |
| 24:C:307:PEK:C36  | 25:G:101:CDL:H273 | 2.45                     | 0.41              |
| 5:E:12:ASP:HB3    | 5:E:46:LYS:HE2    | 2.03                     | 0.41              |
| 4:Q:57:VAL:HG21   | 28:R:258:HOH:O    | 2.20                     | 0.41              |
| 9:V:49:ASP:HB3    | 28:V:132:HOH:O    | 2.20                     | 0.41              |
| 1:A:513:LEU:HD23  | 1:A:513:LEU:HA    | 1.55                     | 0.41              |
| 2:O:172:THR:CG2   | 2:O:180:ASN:HB3   | 2.50                     | 0.41              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 24:P:303:PEK:H161   | 24:P:303:PEK:C11  | 2.49                     | 0.41              |
| 7:T:30:LEU:CD2      | 25:T:102:CDL:H471 | 2.44                     | 0.41              |
| 1:A:375:ALA:O       | 1:A:376:HIS:C     | 2.64                     | 0.41              |
| 2:B:60:GLU:H        | 2:B:60:GLU:HG3    | 1.56                     | 0.41              |
| 2:B:90:ILE:H        | 2:B:90:ILE:HG13   | 1.73                     | 0.41              |
| 6:F:55:LYS:HA       | 6:F:74:LEU:O      | 2.20                     | 0.41              |
| 4:Q:39:ALA:HB1      | 28:Q:354:HOH:O    | 2.21                     | 0.41              |
| 7:T:11:TPO:HG22     | 7:T:11:TPO:O      | 2.20                     | 0.41              |
| 12:Y:20:ARG:HD3     | 28:Y:211:HOH:O    | 2.20                     | 0.41              |
| 25:G:101:CDL:H602   | 25:G:101:CDL:H631 | 1.87                     | 0.41              |
| 4:Q:16:TYR:OH       | 4:Q:18:ASP:OD2    | 2.37                     | 0.41              |
| 8:U:9:LYS:HB3       | 8:U:10:ASN:H      | 1.66                     | 0.41              |
| 1:A:417:MET:HE1     | 14:A:601:HEA:C26  | 2.47                     | 0.41              |
| 2:B:145:PRO:HA      | 2:B:214:VAL:O     | 2.20                     | 0.41              |
| 8:H:43:MET:HE2      | 8:H:49:ASP:H      | 1.86                     | 0.41              |
| 1:N:136[B]:LEU:HD11 | 28:N:935:HOH:O    | 2.20                     | 0.41              |
| 1:N:468:MET:HE2     | 1:N:468:MET:HB3   | 1.81                     | 0.41              |
| 3:P:144:ILE:HD13    | 3:P:239:ALA:HA    | 2.03                     | 0.41              |
| 1:A:412:ILE:HG12    | 4:D:84:ALA:HB3    | 2.03                     | 0.41              |
| 6:F:92:VAL:O        | 6:F:92:VAL:CG2    | 2.66                     | 0.41              |
| 25:G:101:CDL:H541   | 25:G:101:CDL:H712 | 2.03                     | 0.41              |
| 14:N:601:HEA:HHC    | 14:N:601:HEA:H122 | 2.03                     | 0.41              |
| 1:A:107:PRO:HB3     | 3:C:25:LEU:HB2    | 2.03                     | 0.40              |
| 2:B:1:FME:HE3       | 28:B:418:HOH:O    | 2.21                     | 0.40              |
| 1:N:35:LEU:HD11     | 1:N:462:LEU:HB2   | 2.03                     | 0.40              |
| 2:O:67:ILE:HD13     | 28:O:486:HOH:O    | 2.20                     | 0.40              |
| 3:P:64:GLU:HA       | 3:P:68:GLN:HE21   | 1.86                     | 0.40              |
| 3:P:156:ARG:HE      | 22:P:306:CHD:C23  | 2.33                     | 0.40              |
| 7:T:5:LYS:CD        | 24:T:101:PEK:H371 | 2.49                     | 0.40              |
| 25:T:102:CDL:H712   | 25:T:102:CDL:C52  | 2.51                     | 0.40              |
| 2:B:168:LEU:HD23    | 2:B:168:LEU:HA    | 1.94                     | 0.40              |
| 1:A:510:TYR:CD1     | 1:A:510:TYR:C     | 3.00                     | 0.40              |
| 9:I:73:LYS:HA       | 9:I:73:LYS:HD2    | 1.60                     | 0.40              |
| 1:N:189:MET:HG3     | 1:N:190:ILE:N     | 2.29                     | 0.40              |
| 2:O:104:TRP:CG      | 2:O:203:ASN:HB2   | 2.56                     | 0.40              |
| 3:P:160:LEU:HD13    | 22:P:306:CHD:H181 | 2.03                     | 0.40              |
| 23:B:304:PSC:C07    | 9:I:10:ARG:HH21   | 2.34                     | 0.40              |
| 10:J:52:TRP:O       | 10:J:57:HIS:HE1   | 2.02                     | 0.40              |
| 8:H:39:CYS:O        | 8:H:43:MET:HG2    | 2.21                     | 0.40              |
| 10:J:32:TYR:OH      | 22:J:101:CHD:H213 | 2.22                     | 0.40              |
| 1:N:412:ILE:HD13    | 4:Q:84:ALA:HB3    | 2.04                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:P:33[A]:MET:CE | 3:P:41:THR:HB     | 2.50                     | 0.40              |
| 3:P:55:TYR:CE1   | 25:P:305:CDL:H171 | 2.57                     | 0.40              |
| 3:P:116:TRP:HA   | 3:P:117:PRO:C     | 2.46                     | 0.40              |
| 7:T:72:ASN:H     | 7:T:76:ASN:ND2    | 2.03                     | 0.40              |
| 11:X:54:ARG:NH2  | 28:X:130:HOH:O    | 2.53                     | 0.40              |

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 28:F:294:HOH:O | 28:K:114:HOH:O[2_585]  | 1.63                     | 0.57              |
| 9:I:2:THR:CG2  | 5:R:80:GLU:OE1[3_647]  | 1.83                     | 0.37              |
| 28:B:586:HOH:O | 28:M:2318:HOH:O[2_584] | 1.90                     | 0.30              |
| 2:O:126:SER:O  | 6:S:94:HIS:CB[2_684]   | 1.93                     | 0.27              |
| 6:S:95:GLN:N   | 28:O:535:HOH:O[2_685]  | 1.95                     | 0.25              |
| 6:F:94:HIS:CE1 | 28:D:393:HOH:O[2_585]  | 1.98                     | 0.22              |
| 6:S:94:HIS:CD2 | 28:O:535:HOH:O[2_685]  | 2.00                     | 0.20              |
| 9:I:2:THR:CB   | 5:R:80:GLU:OE1[3_647]  | 2.06                     | 0.14              |
| 6:S:94:HIS:CA  | 28:O:547:HOH:O[2_685]  | 2.07                     | 0.13              |
| 28:B:592:HOH:O | 28:M:2318:HOH:O[2_584] | 2.09                     | 0.11              |
| 28:O:533:HOH:O | 28:S:307:HOH:O[2_684]  | 2.10                     | 0.10              |
| 6:S:95:GLN:CA  | 28:O:535:HOH:O[2_685]  | 2.10                     | 0.10              |
| 2:O:126:SER:O  | 6:S:94:HIS:CG[2_684]   | 2.12                     | 0.08              |
| 6:S:95:GLN:N   | 28:O:547:HOH:O[2_685]  | 2.18                     | 0.02              |

## 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     | 518/514 (101%) | 500 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | N     | 518/514 (101%) | 501 (97%) | 17 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | B     | 226/227 (100%)  | 213 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 2   | O     | 225/227 (99%)   | 214 (95%)  | 10 (4%)  | 1 (0%)   | 30          | 22  |
| 3   | C     | 260/261 (100%)  | 254 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 3   | P     | 260/261 (100%)  | 255 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 4   | D     | 142/147 (97%)   | 138 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 4   | Q     | 142/147 (97%)   | 136 (96%)  | 5 (4%)   | 1 (1%)   | 18          | 10  |
| 5   | E     | 103/109 (94%)   | 102 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 5   | R     | 103/109 (94%)   | 103 (100%) | 0        | 0        | 100         | 100 |
| 6   | F     | 96/98 (98%)     | 91 (95%)   | 2 (2%)   | 3 (3%)   | 3           | 0   |
| 6   | S     | 96/98 (98%)     | 90 (94%)   | 3 (3%)   | 3 (3%)   | 3           | 0   |
| 7   | G     | 81/85 (95%)     | 69 (85%)   | 7 (9%)   | 5 (6%)   | 1           | 0   |
| 7   | T     | 81/85 (95%)     | 68 (84%)   | 8 (10%)  | 5 (6%)   | 1           | 0   |
| 8   | H     | 77/85 (91%)     | 71 (92%)   | 3 (4%)   | 3 (4%)   | 2           | 0   |
| 8   | U     | 77/85 (91%)     | 70 (91%)   | 4 (5%)   | 3 (4%)   | 2           | 0   |
| 9   | I     | 71/73 (97%)     | 69 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 9   | V     | 71/73 (97%)     | 70 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 10  | J     | 56/59 (95%)     | 55 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 10  | W     | 56/59 (95%)     | 55 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 11  | K     | 47/56 (84%)     | 46 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 11  | X     | 47/56 (84%)     | 46 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 12  | L     | 44/47 (94%)     | 42 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 12  | Y     | 44/47 (94%)     | 41 (93%)   | 3 (7%)   | 0        | 100         | 100 |
| 13  | M     | 41/46 (89%)     | 38 (93%)   | 3 (7%)   | 0        | 100         | 100 |
| 13  | Z     | 41/46 (89%)     | 39 (95%)   | 2 (5%)   | 0        | 100         | 100 |
| All | All   | 3523/3614 (98%) | 3376 (96%) | 123 (4%) | 24 (1%)  | 18          | 10  |

All (24) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 94  | HIS  |
| 6   | F     | 96  | LEU  |
| 7   | G     | 4   | ALA  |
| 7   | G     | 8   | HIS  |
| 8   | H     | 8   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | S     | 94  | HIS  |
| 6   | S     | 95  | GLN  |
| 7   | T     | 3   | ALA  |
| 7   | T     | 5   | LYS  |
| 7   | T     | 8   | HIS  |
| 8   | U     | 8   | ILE  |
| 8   | U     | 46  | LYS  |
| 6   | F     | 95  | GLN  |
| 7   | G     | 37  | LEU  |
| 7   | T     | 38  | HIS  |
| 7   | G     | 7   | ASP  |
| 2   | O     | 92  | ASN  |
| 7   | T     | 4   | ALA  |
| 8   | U     | 45  | ALA  |
| 4   | Q     | 35  | ALA  |
| 6   | S     | 96  | LEU  |
| 7   | G     | 5   | LYS  |
| 8   | H     | 10  | ASN  |
| 8   | H     | 45  | ALA  |

### 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     | 432/426 (101%) | 425 (98%) | 7 (2%)   | 55          | 54 |
| 1   | N     | 432/426 (101%) | 423 (98%) | 9 (2%)   | 47          | 44 |
| 2   | B     | 211/210 (100%) | 198 (94%) | 13 (6%)  | 16          | 9  |
| 2   | O     | 210/210 (100%) | 203 (97%) | 7 (3%)   | 33          | 26 |
| 3   | C     | 227/226 (100%) | 223 (98%) | 4 (2%)   | 51          | 50 |
| 3   | P     | 227/226 (100%) | 222 (98%) | 5 (2%)   | 45          | 42 |
| 4   | D     | 128/129 (99%)  | 127 (99%) | 1 (1%)   | 73          | 75 |
| 4   | Q     | 128/129 (99%)  | 123 (96%) | 5 (4%)   | 28          | 21 |
| 5   | E     | 92/95 (97%)    | 89 (97%)  | 3 (3%)   | 33          | 26 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 5   | R     | 92/95 (97%)     | 88 (96%)   | 4 (4%)   | 26          | 18  |
| 6   | F     | 81/81 (100%)    | 75 (93%)   | 6 (7%)   | 13          | 6   |
| 6   | S     | 81/81 (100%)    | 76 (94%)   | 5 (6%)   | 16          | 9   |
| 7   | G     | 67/68 (98%)     | 63 (94%)   | 4 (6%)   | 17          | 9   |
| 7   | T     | 67/68 (98%)     | 60 (90%)   | 7 (10%)  | 7           | 2   |
| 8   | H     | 71/75 (95%)     | 66 (93%)   | 5 (7%)   | 14          | 7   |
| 8   | U     | 71/75 (95%)     | 69 (97%)   | 2 (3%)   | 38          | 32  |
| 9   | I     | 57/57 (100%)    | 56 (98%)   | 1 (2%)   | 51          | 50  |
| 9   | V     | 57/57 (100%)    | 54 (95%)   | 3 (5%)   | 20          | 12  |
| 10  | J     | 49/50 (98%)     | 49 (100%)  | 0        | 100         | 100 |
| 10  | W     | 49/50 (98%)     | 48 (98%)   | 1 (2%)   | 48          | 46  |
| 11  | K     | 39/46 (85%)     | 38 (97%)   | 1 (3%)   | 40          | 35  |
| 11  | X     | 39/46 (85%)     | 39 (100%)  | 0        | 100         | 100 |
| 12  | L     | 39/40 (98%)     | 38 (97%)   | 1 (3%)   | 40          | 35  |
| 12  | Y     | 39/40 (98%)     | 36 (92%)   | 3 (8%)   | 12          | 5   |
| 13  | M     | 37/38 (97%)     | 34 (92%)   | 3 (8%)   | 11          | 5   |
| 13  | Z     | 37/38 (97%)     | 34 (92%)   | 3 (8%)   | 11          | 5   |
| All | All   | 3059/3082 (99%) | 2956 (97%) | 103 (3%) | 33          | 25  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | LEU  |
| 1   | A     | 38  | ARG  |
| 1   | A     | 138 | HIS  |
| 1   | A     | 178 | GLN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 189 | MET  |
| 1   | A     | 369 | ASP  |
| 2   | B     | 33  | LEU  |
| 2   | B     | 59  | GLN  |
| 2   | B     | 60  | GLU  |
| 2   | B     | 65  | TRP  |
| 2   | B     | 75  | LEU  |
| 2   | B     | 78  | LEU  |
| 2   | B     | 90  | ILE  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | B     | 91     | ASN  |
| 2   | B     | 110    | TYR  |
| 2   | B     | 115[A] | ASP  |
| 2   | B     | 115[B] | ASP  |
| 2   | B     | 116    | LEU  |
| 2   | B     | 171    | LYS  |
| 3   | C     | 17     | PRO  |
| 3   | C     | 159    | MET  |
| 3   | C     | 180    | GLU  |
| 3   | C     | 230    | ASN  |
| 4   | D     | 31     | LYS  |
| 5   | E     | 5      | HIS  |
| 5   | E     | 70     | VAL  |
| 5   | E     | 90     | ARG  |
| 6   | F     | 54     | ASN  |
| 6   | F     | 78     | GLU  |
| 6   | F     | 80     | GLN  |
| 6   | F     | 87     | THR  |
| 6   | F     | 95     | GLN  |
| 6   | F     | 96     | LEU  |
| 7   | G     | 2      | SER  |
| 7   | G     | 33     | LEU  |
| 7   | G     | 37     | LEU  |
| 7   | G     | 79     | PRO  |
| 8   | H     | 7      | LYS  |
| 8   | H     | 9      | LYS  |
| 8   | H     | 51     | SER  |
| 8   | H     | 60     | TYR  |
| 8   | H     | 61     | LYS  |
| 9   | I     | 36     | LYS  |
| 11  | K     | 47     | ARG  |
| 12  | L     | 47     | LYS  |
| 13  | M     | 12     | PRO  |
| 13  | M     | 38     | ASP  |
| 13  | M     | 39     | ASN  |
| 1   | N     | 138    | HIS  |
| 1   | N     | 180    | GLN  |
| 1   | N     | 312[A] | ILE  |
| 1   | N     | 312[B] | ILE  |
| 1   | N     | 362    | SER  |
| 1   | N     | 363    | LEU  |
| 1   | N     | 369    | ASP  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | N     | 484   | THR  |
| 1   | N     | 495   | LEU  |
| 2   | O     | 33    | LEU  |
| 2   | O     | 60    | GLU  |
| 2   | O     | 61    | VAL  |
| 2   | O     | 66    | THR  |
| 2   | O     | 68    | LEU  |
| 2   | O     | 78    | LEU  |
| 2   | O     | 94    | SER  |
| 3   | P     | 33[A] | MET  |
| 3   | P     | 33[B] | MET  |
| 3   | P     | 159   | MET  |
| 3   | P     | 180   | GLU  |
| 3   | P     | 230   | ASN  |
| 4   | Q     | 4     | SER  |
| 4   | Q     | 5     | VAL  |
| 4   | Q     | 7     | LYS  |
| 4   | Q     | 10    | ASP  |
| 4   | Q     | 51    | LEU  |
| 5   | R     | 5     | HIS  |
| 5   | R     | 46    | LYS  |
| 5   | R     | 79    | LYS  |
| 5   | R     | 109   | VAL  |
| 6   | S     | 43    | LYS  |
| 6   | S     | 54    | ASN  |
| 6   | S     | 80    | GLN  |
| 6   | S     | 94    | HIS  |
| 6   | S     | 95    | GLN  |
| 7   | T     | 2     | SER  |
| 7   | T     | 5     | LYS  |
| 7   | T     | 8     | HIS  |
| 7   | T     | 33    | LEU  |
| 7   | T     | 35    | SER  |
| 7   | T     | 37    | LEU  |
| 7   | T     | 84    | LYS  |
| 8   | U     | 9     | LYS  |
| 8   | U     | 10    | ASN  |
| 9   | V     | 8     | GLN  |
| 9   | V     | 36    | LYS  |
| 9   | V     | 52    | ARG  |
| 10  | W     | 50    | LEU  |
| 12  | Y     | 2     | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | Y     | 20  | ARG  |
| 12  | Y     | 26  | THR  |
| 13  | Z     | 2   | THR  |
| 13  | Z     | 38  | ASP  |
| 13  | Z     | 42  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ASN  |
| 1   | A     | 55  | ASN  |
| 1   | A     | 178 | GLN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 422 | ASN  |
| 1   | A     | 503 | HIS  |
| 2   | B     | 59  | GLN  |
| 2   | B     | 92  | ASN  |
| 3   | C     | 50  | ASN  |
| 3   | C     | 56  | GLN  |
| 3   | C     | 68  | GLN  |
| 3   | C     | 76  | GLN  |
| 3   | C     | 149 | HIS  |
| 3   | C     | 161 | GLN  |
| 3   | C     | 230 | ASN  |
| 4   | D     | 29  | HIS  |
| 4   | D     | 37  | GLN  |
| 4   | D     | 109 | HIS  |
| 4   | D     | 119 | GLN  |
| 4   | D     | 143 | ASN  |
| 5   | E     | 94  | ASN  |
| 6   | F     | 54  | ASN  |
| 6   | F     | 80  | GLN  |
| 7   | G     | 34  | ASN  |
| 7   | G     | 38  | HIS  |
| 7   | G     | 76  | ASN  |
| 8   | H     | 31  | GLN  |
| 8   | H     | 37  | HIS  |
| 10  | J     | 29  | ASN  |
| 10  | J     | 57  | HIS  |
| 11  | K     | 35  | GLN  |
| 1   | N     | 178 | GLN  |
| 1   | N     | 180 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 422 | ASN  |
| 2   | O     | 10  | GLN  |
| 2   | O     | 91  | ASN  |
| 3   | P     | 50  | ASN  |
| 3   | P     | 56  | GLN  |
| 3   | P     | 68  | GLN  |
| 4   | Q     | 32  | ASN  |
| 4   | Q     | 37  | GLN  |
| 4   | Q     | 109 | HIS  |
| 5   | R     | 94  | ASN  |
| 6   | S     | 54  | ASN  |
| 6   | S     | 80  | GLN  |
| 6   | S     | 95  | GLN  |
| 6   | S     | 98  | HIS  |
| 7   | T     | 76  | ASN  |
| 8   | U     | 12  | GLN  |
| 8   | U     | 37  | HIS  |
| 10  | W     | 29  | ASN  |
| 10  | W     | 57  | HIS  |
| 13  | Z     | 36  | 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      | 1.77 | 1 (12%)     | 10,14,16    | 1.33 | 1 (10%)     |
| 2   | FME  | B     | 1   | 2    | 8,9,10       | 1.39 | 1 (12%)     | 8,9,11      | 7.58 | 4 (50%)     |
| 7   | TPO  | G     | 11  | 7    | 8,10,11      | 1.67 | 2 (25%)     | 10,14,16    | 1.56 | 2 (20%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | FME  | O     | 1   | 2    | 8,9,10       | 0.97 | 0        | 8,9,11      | 1.92 | 3 (37%)  |
| 9   | SAC  | V     | 1   | 9    | 7,8,9        | 2.22 | 2 (28%)  | 7,9,11      | 1.40 | 1 (14%)  |
| 1   | FME  | A     | 1   | 1    | 8,9,10       | 0.50 | 0        | 8,9,11      | 1.39 | 1 (12%)  |
| 9   | SAC  | I     | 1   | 9    | 7,8,9        | 2.29 | 2 (28%)  | 7,9,11      | 1.31 | 1 (14%)  |
| 1   | FME  | N     | 1   | 1    | 8,9,10       | 0.88 | 0        | 8,9,11      | 1.48 | 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    | -       | 3/9/11/13 | -     |
| 2   | FME  | B     | 1   | 2    | -       | 2/7/9/11  | -     |
| 7   | TPO  | G     | 11  | 7    | -       | 7/9/11/13 | -     |
| 2   | FME  | O     | 1   | 2    | -       | 2/7/9/11  | -     |
| 9   | SAC  | V     | 1   | 9    | -       | 5/7/8/10  | -     |
| 1   | FME  | A     | 1   | 1    | -       | 2/7/9/11  | -     |
| 9   | SAC  | I     | 1   | 9    | -       | 1/7/8/10  | -     |
| 1   | FME  | N     | 1   | 1    | -       | 2/7/9/11  | -     |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | I     | 1   | SAC  | OAC-C1A | 5.14  | 1.34        | 1.23     |
| 9   | V     | 1   | SAC  | OAC-C1A | 4.87  | 1.34        | 1.23     |
| 7   | T     | 11  | TPO  | P-O1P   | 3.48  | 1.61        | 1.50     |
| 9   | V     | 1   | SAC  | CA-N    | 3.04  | 1.51        | 1.46     |
| 7   | G     | 11  | TPO  | P-O1P   | 2.82  | 1.59        | 1.50     |
| 9   | I     | 1   | SAC  | CA-N    | 2.65  | 1.50        | 1.46     |
| 2   | B     | 1   | FME  | O1-CN   | -2.59 | 1.12        | 1.22     |
| 7   | G     | 11  | TPO  | P-OG1   | 2.51  | 1.63        | 1.59     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2   | B     | 1   | FME  | CA-N-CN   | -20.41 | 91.43       | 122.82   |
| 2   | B     | 1   | FME  | O1-CN-N   | 4.73   | 137.52      | 125.32   |
| 7   | T     | 11  | TPO  | CG2-CB-CA | 3.19   | 119.47      | 113.26   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | O     | 1   | FME  | O1-CN-N   | -3.02 | 117.51      | 125.32   |
| 2   | B     | 1   | FME  | O-C-CA    | -2.95 | 117.18      | 124.77   |
| 7   | G     | 11  | TPO  | CG2-CB-CA | 2.94  | 119.00      | 113.26   |
| 1   | N     | 1   | FME  | C-CA-N    | 2.89  | 115.08      | 109.50   |
| 2   | O     | 1   | FME  | CG-CB-CA  | -2.68 | 104.68      | 112.87   |
| 2   | B     | 1   | FME  | CB-CA-N   | -2.53 | 105.91      | 110.52   |
| 1   | A     | 1   | FME  | C-CA-N    | 2.50  | 114.32      | 109.50   |
| 9   | I     | 1   | SAC  | C-CA-N    | 2.48  | 114.28      | 109.50   |
| 2   | O     | 1   | FME  | CB-CA-N   | -2.38 | 106.18      | 110.52   |
| 9   | V     | 1   | SAC  | C2A-C1A-N | 2.34  | 120.00      | 116.12   |
| 1   | N     | 1   | FME  | O-C-CA    | -2.09 | 119.39      | 124.77   |
| 7   | G     | 11  | TPO  | O2P-P-OG1 | 2.04  | 113.79      | 105.85   |

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | A     | 1   | FME  | N-CA-CB-CG   |
| 2   | B     | 1   | FME  | O1-CN-N-CA   |
| 7   | G     | 11  | TPO  | N-CA-CB-CG2  |
| 7   | G     | 11  | TPO  | N-CA-CB-OG1  |
| 7   | G     | 11  | TPO  | C-CA-CB-CG2  |
| 7   | G     | 11  | TPO  | O-C-CA-CB    |
| 7   | G     | 11  | TPO  | CA-CB-OG1-P  |
| 9   | I     | 1   | SAC  | O-C-CA-CB    |
| 1   | N     | 1   | FME  | N-CA-CB-CG   |
| 7   | T     | 11  | TPO  | N-CA-CB-CG2  |
| 7   | T     | 11  | TPO  | N-CA-CB-OG1  |
| 7   | T     | 11  | TPO  | C-CA-CB-CG2  |
| 9   | V     | 1   | SAC  | O-C-CA-CB    |
| 9   | V     | 1   | SAC  | C-CA-CB-OG   |
| 9   | V     | 1   | SAC  | C2A-C1A-N-CA |
| 9   | V     | 1   | SAC  | OAC-C1A-N-CA |
| 9   | V     | 1   | SAC  | N-CA-CB-OG   |
| 2   | B     | 1   | FME  | CB-CG-SD-CE  |
| 1   | A     | 1   | FME  | C-CA-CB-CG   |
| 2   | O     | 1   | FME  | C-CA-CB-CG   |
| 1   | N     | 1   | FME  | C-CA-CB-CG   |
| 2   | O     | 1   | FME  | CA-CB-CG-SD  |
| 7   | G     | 11  | TPO  | CB-OG1-P-O1P |
| 7   | G     | 11  | TPO  | CG2-CB-OG1-P |

There are no ring outliers.

5 monomers are involved in 18 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | T     | 11  | TPO  | 3       | 0            |
| 2   | B     | 1   | FME  | 2       | 0            |
| 7   | G     | 11  | TPO  | 1       | 0            |
| 2   | O     | 1   | FME  | 9       | 0            |
| 1   | A     | 1   | FME  | 3       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 10 are monoatomic - leaving 46 for Mogul analysis.

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

| Mol | Type | Chain | Res    | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|--------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |        |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 23  | PSC  | N     | 610    | -    | 51,51,51     | 1.25 | 3 (5%)      | 57,59,59    | 1.27 | 4 (7%)      |
| 19  | PGV  | N     | 607    | -    | 50,50,50     | 1.03 | 2 (4%)      | 53,56,56    | 1.32 | 8 (15%)     |
| 22  | CHD  | B     | 303    | -    | 32,32,32     | 1.45 | 4 (12%)     | 51,51,51    | 1.92 | 13 (25%)    |
| 19  | PGV  | N     | 608    | -    | 50,50,50     | 1.06 | 2 (4%)      | 53,56,56    | 1.51 | 6 (11%)     |
| 20  | TGL  | Q     | 201    | -    | 62,62,62     | 1.60 | 7 (11%)     | 65,65,65    | 1.33 | 11 (16%)    |
| 22  | CHD  | P     | 306    | -    | 32,32,32     | 0.90 | 1 (3%)      | 51,51,51    | 2.45 | 19 (37%)    |
| 20  | TGL  | Y     | 101    | -    | 62,62,62     | 1.44 | 6 (9%)      | 65,65,65    | 1.56 | 11 (16%)    |
| 19  | PGV  | C     | 308    | -    | 50,50,50     | 1.19 | 2 (4%)      | 53,56,56    | 1.22 | 4 (7%)      |
| 18  | PER  | N     | 606[B] | 15   | 1,1,1        | 0.90 | 0           | -           |      |             |
| 27  | DMU  | M     | 101    | -    | 34,34,34     | 0.67 | 0           | 45,45,45    | 2.38 | 14 (31%)    |
| 25  | CDL  | C     | 304    | -    | 99,99,99     | 1.53 | 16 (16%)    | 105,111,111 | 1.51 | 13 (12%)    |
| 25  | CDL  | T     | 102    | -    | 99,99,99     | 1.45 | 12 (12%)    | 105,111,111 | 1.35 | 12 (11%)    |
| 14  | HEA  | N     | 602    | 1,18 | 67,67,67     | 2.12 | 22 (32%)    | 81,103,103  | 1.76 | 28 (34%)    |

| Mol | Type | Chain | Res    | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 20  | TGL  | N     | 609    | -     | 62,62,62     | 1.39 | 6 (9%)   | 65,65,65    | 1.62 | 9 (13%)  |
| 21  | CUA  | O     | 301    | 2     | 0,1,1        | -    | -        | -           |      |          |
| 22  | CHD  | C     | 306    | -     | 32,32,32     | 1.20 | 3 (9%)   | 51,51,51    | 1.77 | 12 (23%) |
| 18  | PER  | A     | 606[A] | 15,14 | 1,1,1        | 0.90 | 0        | -           |      |          |
| 24  | PEK  | T     | 101    | -     | 52,52,52     | 1.05 | 2 (3%)   | 55,57,57    | 1.24 | 4 (7%)   |
| 14  | HEA  | N     | 601    | 1     | 67,67,67     | 2.11 | 19 (28%) | 81,103,103  | 1.81 | 22 (27%) |
| 24  | PEK  | P     | 303    | -     | 52,52,52     | 1.09 | 3 (5%)   | 55,57,57    | 1.39 | 6 (10%)  |
| 25  | CDL  | G     | 101    | -     | 99,99,99     | 1.45 | 12 (12%) | 105,111,111 | 1.30 | 9 (8%)   |
| 27  | DMU  | Z     | 101    | -     | 34,34,34     | 0.74 | 1 (2%)   | 45,45,45    | 1.83 | 12 (26%) |
| 14  | HEA  | A     | 601    | 1     | 67,67,67     | 2.54 | 25 (37%) | 81,103,103  | 2.32 | 30 (37%) |
| 19  | PGV  | A     | 608    | -     | 50,50,50     | 1.23 | 2 (4%)   | 53,56,56    | 1.44 | 6 (11%)  |
| 24  | PEK  | P     | 308    | -     | 52,52,52     | 1.15 | 2 (3%)   | 55,57,57    | 1.10 | 4 (7%)   |
| 20  | TGL  | B     | 301    | -     | 62,62,62     | 1.36 | 6 (9%)   | 65,65,65    | 1.68 | 11 (16%) |
| 20  | TGL  | L     | 101    | -     | 62,62,62     | 1.47 | 6 (9%)   | 65,65,65    | 1.48 | 10 (15%) |
| 21  | CUA  | B     | 302    | 2     | 0,1,1        | -    | -        | -           |      |          |
| 22  | CHD  | J     | 101    | -     | 32,32,32     | 0.71 | 0        | 51,51,51    | 2.59 | 25 (49%) |
| 24  | PEK  | G     | 102    | -     | 52,52,52     | 1.13 | 2 (3%)   | 55,57,57    | 1.25 | 6 (10%)  |
| 22  | CHD  | C     | 305    | -     | 32,32,32     | 0.81 | 0        | 51,51,51    | 1.99 | 18 (35%) |
| 19  | PGV  | A     | 607    | -     | 50,50,50     | 1.16 | 5 (10%)  | 53,56,56    | 1.31 | 5 (9%)   |
| 24  | PEK  | C     | 302    | -     | 52,52,52     | 1.00 | 2 (3%)   | 55,57,57    | 1.10 | 6 (10%)  |
| 23  | PSC  | B     | 304    | -     | 51,51,51     | 1.21 | 3 (5%)   | 57,59,59    | 1.17 | 4 (7%)   |
| 25  | CDL  | P     | 305    | -     | 99,99,99     | 1.49 | 15 (15%) | 105,111,111 | 1.40 | 13 (12%) |
| 19  | PGV  | P     | 301    | -     | 50,50,50     | 1.07 | 2 (4%)   | 53,56,56    | 1.21 | 5 (9%)   |
| 20  | TGL  | D     | 201    | -     | 62,62,62     | 1.60 | 7 (11%)  | 65,65,65    | 1.64 | 13 (20%) |
| 19  | PGV  | C     | 303    | -     | 50,50,50     | 0.96 | 2 (4%)   | 53,56,56    | 1.40 | 7 (13%)  |
| 18  | PER  | A     | 606[B] | 15    | 1,1,1        | 0.88 | 0        | -           |      |          |
| 22  | CHD  | P     | 307    | -     | 32,32,32     | 1.33 | 4 (12%)  | 51,51,51    | 1.40 | 8 (15%)  |
| 14  | HEA  | A     | 602    | 1,18  | 67,67,67     | 2.44 | 26 (38%) | 81,103,103  | 2.23 | 25 (30%) |
| 22  | CHD  | W     | 101    | -     | 32,32,32     | 0.83 | 0        | 51,51,51    | 3.06 | 17 (33%) |
| 18  | PER  | N     | 606[A] | 15,14 | 1,1,1        | 0.91 | 0        | -           |      |          |
| 19  | PGV  | P     | 304    | -     | 50,50,50     | 0.98 | 2 (4%)   | 53,56,56    | 1.05 | 2 (3%)   |
| 22  | CHD  | G     | 103    | -     | 32,32,32     | 1.56 | 7 (21%)  | 51,51,51    | 2.47 | 18 (35%) |
| 24  | PEK  | C     | 307    | -     | 52,52,52     | 1.10 | 2 (3%)   | 55,57,57    | 1.20 | 4 (7%)   |

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   |
|-----|------|-------|-----|------|-----------|----------------|---------|
| 23  | PSC  | N     | 610 | -    | -         | 25/55/55/55    | -       |
| 19  | PGV  | N     | 607 | -    | -         | 28/55/55/55    | -       |
| 22  | CHD  | B     | 303 | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 19  | PGV  | N     | 608 | -    | -         | 12/55/55/55    | -       |
| 20  | TGL  | Q     | 201 | -    | -         | 41/65/65/65    | -       |
| 22  | CHD  | P     | 306 | -    | -         | 8/9/74/74      | 0/4/4/4 |
| 20  | TGL  | Y     | 101 | -    | -         | 39/65/65/65    | -       |
| 19  | PGV  | C     | 308 | -    | -         | 32/55/55/55    | -       |
| 27  | DMU  | M     | 101 | -    | 2/2/10/10 | 7/19/59/59     | 0/2/2/2 |
| 25  | CDL  | C     | 304 | -    | -         | 62/110/110/110 | -       |
| 25  | CDL  | T     | 102 | -    | -         | 65/110/110/110 | -       |
| 14  | HEA  | N     | 602 | 1,18 | -         | 5/36/76/76     | -       |
| 20  | TGL  | N     | 609 | -    | -         | 37/65/65/65    | -       |
| 22  | CHD  | C     | 306 | -    | -         | 1/9/74/74      | 0/4/4/4 |
| 24  | PEK  | T     | 101 | -    | -         | 25/56/56/56    | -       |
| 14  | HEA  | N     | 601 | 1    | -         | 7/36/76/76     | -       |
| 24  | PEK  | P     | 303 | -    | -         | 25/56/56/56    | -       |
| 25  | CDL  | G     | 101 | -    | -         | 77/110/110/110 | -       |
| 27  | DMU  | Z     | 101 | -    | 2/2/10/10 | 7/19/59/59     | 0/2/2/2 |
| 14  | HEA  | A     | 601 | 1    | -         | 8/36/76/76     | -       |
| 19  | PGV  | A     | 608 | -    | -         | 32/55/55/55    | -       |
| 24  | PEK  | P     | 308 | -    | -         | 36/56/56/56    | -       |
| 20  | TGL  | B     | 301 | -    | -         | 32/65/65/65    | -       |
| 20  | TGL  | L     | 101 | -    | -         | 33/65/65/65    | -       |
| 22  | CHD  | J     | 101 | -    | -         | 7/9/74/74      | 0/4/4/4 |
| 24  | PEK  | G     | 102 | -    | -         | 29/56/56/56    | -       |
| 22  | CHD  | C     | 305 | -    | -         | 6/9/74/74      | 0/4/4/4 |
| 19  | PGV  | A     | 607 | -    | -         | 9/55/55/55     | -       |
| 24  | PEK  | C     | 302 | -    | -         | 17/56/56/56    | -       |
| 23  | PSC  | B     | 304 | -    | -         | 34/55/55/55    | -       |
| 25  | CDL  | P     | 305 | -    | -         | 58/110/110/110 | -       |
| 19  | PGV  | P     | 301 | -    | -         | 30/55/55/55    | -       |
| 20  | TGL  | D     | 201 | -    | -         | 38/65/65/65    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 19  | PGV  | C     | 303 | -    | -       | 19/55/55/55 | -       |
| 22  | CHD  | P     | 307 | -    | -       | 2/9/74/74   | 0/4/4/4 |
| 14  | HEA  | A     | 602 | 1,18 | -       | 7/36/76/76  | -       |
| 22  | CHD  | W     | 101 | -    | -       | 7/9/74/74   | 0/4/4/4 |
| 19  | PGV  | P     | 304 | -    | -       | 12/55/55/55 | -       |
| 22  | CHD  | G     | 103 | -    | -       | 2/9/74/74   | 0/4/4/4 |
| 24  | PEK  | C     | 307 | -    | -       | 36/56/56/56 | -       |

All (243) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | A     | 601 | HEA  | FE-NA   | 9.36  | 2.26        | 1.95     |
| 14  | A     | 602 | HEA  | FE-NA   | 6.84  | 2.17        | 1.95     |
| 14  | N     | 601 | HEA  | FE-NC   | 6.57  | 2.16        | 1.95     |
| 14  | A     | 601 | HEA  | CHA-C1A | 6.29  | 1.50        | 1.38     |
| 14  | A     | 601 | HEA  | FE-NC   | 6.22  | 2.15        | 1.95     |
| 14  | N     | 601 | HEA  | FE-NA   | 6.02  | 2.15        | 1.95     |
| 20  | L     | 101 | TGL  | OG2-CB1 | 5.99  | 1.51        | 1.34     |
| 14  | A     | 602 | HEA  | FE-NC   | 5.82  | 2.14        | 1.95     |
| 20  | Y     | 101 | TGL  | OG2-CB1 | 5.45  | 1.49        | 1.34     |
| 19  | A     | 608 | PGV  | O03-C19 | 5.44  | 1.49        | 1.33     |
| 20  | D     | 201 | TGL  | OB1-CB1 | 5.44  | 1.38        | 1.22     |
| 20  | Q     | 201 | TGL  | OG2-CB1 | 5.42  | 1.49        | 1.34     |
| 20  | D     | 201 | TGL  | OG2-CB1 | 5.39  | 1.49        | 1.34     |
| 20  | B     | 301 | TGL  | OG1-CA1 | 5.32  | 1.48        | 1.33     |
| 24  | P     | 308 | PEK  | O01-C1  | 5.19  | 1.48        | 1.34     |
| 20  | Q     | 201 | TGL  | OG1-CA1 | 5.17  | 1.48        | 1.33     |
| 20  | Y     | 101 | TGL  | OG3-CC1 | 5.16  | 1.48        | 1.33     |
| 14  | A     | 602 | HEA  | CMD-C2D | 5.10  | 1.61        | 1.50     |
| 20  | Q     | 201 | TGL  | OB1-CB1 | 5.08  | 1.37        | 1.22     |
| 23  | N     | 610 | PSC  | O01-C1  | 5.06  | 1.48        | 1.34     |
| 25  | G     | 101 | CDL  | OB8-CB7 | 5.06  | 1.48        | 1.33     |
| 20  | D     | 201 | TGL  | OG1-CA1 | 5.06  | 1.48        | 1.33     |
| 25  | C     | 304 | CDL  | OA8-CA7 | 5.05  | 1.48        | 1.33     |
| 20  | N     | 609 | TGL  | OG3-CC1 | 5.04  | 1.48        | 1.33     |
| 24  | C     | 307 | PEK  | O03-C21 | 5.01  | 1.48        | 1.33     |
| 14  | N     | 602 | HEA  | FE-NC   | 5.01  | 2.11        | 1.95     |
| 14  | A     | 602 | HEA  | C1C-NC  | -5.00 | 1.30        | 1.39     |
| 24  | C     | 307 | PEK  | O01-C1  | 4.98  | 1.48        | 1.34     |
| 24  | G     | 102 | PEK  | O03-C21 | 4.97  | 1.47        | 1.33     |
| 25  | P     | 305 | CDL  | OA8-CA7 | 4.94  | 1.47        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 20  | N     | 609 | TGL  | OG1-CA1 | 4.89  | 1.47        | 1.33     |
| 24  | G     | 102 | PEK  | O01-C1  | 4.85  | 1.48        | 1.34     |
| 19  | C     | 308 | PGV  | O01-C1  | 4.85  | 1.48        | 1.34     |
| 20  | B     | 301 | TGL  | OG3-CC1 | 4.83  | 1.47        | 1.33     |
| 19  | N     | 607 | PGV  | O03-C19 | 4.83  | 1.47        | 1.33     |
| 24  | T     | 101 | PEK  | O03-C21 | 4.83  | 1.47        | 1.33     |
| 25  | G     | 101 | CDL  | OA6-CA5 | 4.83  | 1.47        | 1.34     |
| 25  | T     | 102 | CDL  | OA8-CA7 | 4.81  | 1.47        | 1.33     |
| 23  | B     | 304 | PSC  | O01-C1  | 4.81  | 1.47        | 1.34     |
| 25  | T     | 102 | CDL  | OA6-CA5 | 4.80  | 1.47        | 1.34     |
| 25  | C     | 304 | CDL  | OA6-CA5 | 4.74  | 1.47        | 1.34     |
| 19  | P     | 301 | PGV  | O03-C19 | 4.70  | 1.47        | 1.33     |
| 24  | P     | 308 | PEK  | O03-C21 | 4.69  | 1.47        | 1.33     |
| 19  | A     | 608 | PGV  | O01-C1  | 4.69  | 1.47        | 1.34     |
| 20  | L     | 101 | TGL  | OG1-CA1 | 4.64  | 1.46        | 1.33     |
| 14  | A     | 601 | HEA  | C1A-NA  | -4.63 | 1.30        | 1.39     |
| 20  | L     | 101 | TGL  | OG3-CC1 | 4.61  | 1.46        | 1.33     |
| 19  | C     | 308 | PGV  | O03-C19 | 4.58  | 1.46        | 1.33     |
| 23  | N     | 610 | PSC  | O03-C19 | 4.53  | 1.46        | 1.33     |
| 24  | C     | 302 | PEK  | O03-C21 | 4.50  | 1.46        | 1.33     |
| 25  | P     | 305 | CDL  | OB8-CB7 | 4.49  | 1.46        | 1.33     |
| 19  | N     | 608 | PGV  | O03-C19 | 4.48  | 1.46        | 1.33     |
| 25  | P     | 305 | CDL  | OA6-CA5 | 4.47  | 1.46        | 1.34     |
| 25  | G     | 101 | CDL  | OB6-CB5 | 4.47  | 1.46        | 1.34     |
| 14  | N     | 602 | HEA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 25  | T     | 102 | CDL  | OB6-CB5 | 4.41  | 1.46        | 1.34     |
| 24  | T     | 101 | PEK  | O01-C1  | 4.39  | 1.46        | 1.34     |
| 25  | C     | 304 | CDL  | OB8-CB7 | 4.38  | 1.46        | 1.33     |
| 20  | Q     | 201 | TGL  | OG3-CC1 | 4.38  | 1.46        | 1.33     |
| 14  | N     | 602 | HEA  | C1A-NA  | -4.37 | 1.31        | 1.39     |
| 14  | A     | 602 | HEA  | C12-C11 | 4.36  | 1.60        | 1.53     |
| 24  | P     | 303 | PEK  | O03-C21 | 4.32  | 1.45        | 1.33     |
| 14  | A     | 602 | HEA  | CHB-C4A | 4.32  | 1.46        | 1.38     |
| 25  | T     | 102 | CDL  | C42-C41 | -4.30 | 1.30        | 1.51     |
| 20  | N     | 609 | TGL  | OG2-CB1 | 4.30  | 1.46        | 1.34     |
| 14  | N     | 601 | HEA  | C1D-ND  | -4.26 | 1.32        | 1.40     |
| 14  | N     | 602 | HEA  | CMD-C2D | 4.25  | 1.59        | 1.50     |
| 14  | N     | 601 | HEA  | FE-ND   | 4.25  | 2.08        | 1.94     |
| 25  | G     | 101 | CDL  | OA8-CA7 | 4.23  | 1.45        | 1.33     |
| 23  | N     | 610 | PSC  | C13-C12 | 4.22  | 1.55        | 1.31     |
| 23  | B     | 304 | PSC  | O03-C19 | 4.21  | 1.45        | 1.33     |
| 19  | P     | 301 | PGV  | O01-C1  | 4.16  | 1.46        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | B     | 304 | PSC  | C13-C12 | 4.14  | 1.55        | 1.31     |
| 19  | A     | 607 | PGV  | O03-C19 | 4.13  | 1.45        | 1.33     |
| 14  | A     | 602 | HEA  | CHA-C1A | 4.11  | 1.46        | 1.38     |
| 14  | N     | 602 | HEA  | FE-NA   | 4.10  | 2.08        | 1.95     |
| 25  | T     | 102 | CDL  | OB8-CB7 | 4.09  | 1.45        | 1.33     |
| 19  | P     | 304 | PGV  | O03-C19 | 4.09  | 1.45        | 1.33     |
| 14  | A     | 601 | HEA  | CHC-C1C | 4.08  | 1.48        | 1.39     |
| 19  | N     | 607 | PGV  | O01-C1  | 4.08  | 1.45        | 1.34     |
| 14  | A     | 601 | HEA  | C1C-NC  | -4.05 | 1.32        | 1.39     |
| 20  | D     | 201 | TGL  | OG3-CC1 | 4.04  | 1.45        | 1.33     |
| 24  | C     | 302 | PEK  | O01-C1  | 3.99  | 1.45        | 1.34     |
| 25  | C     | 304 | CDL  | C59-C58 | -3.96 | 1.32        | 1.51     |
| 20  | Y     | 101 | TGL  | C20-CA9 | -3.96 | 1.32        | 1.51     |
| 14  | A     | 601 | HEA  | C4C-NC  | -3.95 | 1.32        | 1.39     |
| 14  | A     | 601 | HEA  | FE-NB   | 3.95  | 2.07        | 1.94     |
| 25  | C     | 304 | CDL  | C79-C78 | -3.93 | 1.32        | 1.51     |
| 14  | N     | 601 | HEA  | CHA-C1A | 3.90  | 1.46        | 1.38     |
| 20  | Y     | 101 | TGL  | OG1-CA1 | 3.89  | 1.44        | 1.33     |
| 14  | A     | 602 | HEA  | CMB-C2B | 3.88  | 1.58        | 1.50     |
| 22  | G     | 103 | CHD  | C10-C5  | -3.86 | 1.49        | 1.55     |
| 14  | A     | 601 | HEA  | CHB-C4A | 3.84  | 1.45        | 1.38     |
| 20  | N     | 609 | TGL  | C10-CB9 | -3.81 | 1.32        | 1.51     |
| 25  | P     | 305 | CDL  | C59-C58 | -3.81 | 1.32        | 1.51     |
| 14  | A     | 601 | HEA  | CMB-C2B | 3.80  | 1.58        | 1.50     |
| 20  | L     | 101 | TGL  | C20-CA9 | -3.76 | 1.33        | 1.51     |
| 20  | D     | 201 | TGL  | C10-CB9 | -3.76 | 1.33        | 1.51     |
| 25  | P     | 305 | CDL  | OB6-CB5 | 3.76  | 1.44        | 1.34     |
| 25  | P     | 305 | CDL  | C62-C61 | -3.73 | 1.33        | 1.51     |
| 14  | N     | 602 | HEA  | C1B-C2B | -3.73 | 1.37        | 1.44     |
| 25  | T     | 102 | CDL  | C39-C38 | -3.70 | 1.33        | 1.51     |
| 14  | N     | 602 | HEA  | C4B-C3B | -3.70 | 1.38        | 1.44     |
| 19  | C     | 303 | PGV  | O03-C19 | 3.69  | 1.44        | 1.33     |
| 20  | Q     | 201 | TGL  | C10-CB9 | -3.68 | 1.33        | 1.51     |
| 25  | P     | 305 | CDL  | C79-C78 | -3.68 | 1.33        | 1.51     |
| 25  | G     | 101 | CDL  | C82-C81 | -3.68 | 1.33        | 1.51     |
| 20  | N     | 609 | TGL  | C20-CA9 | -3.67 | 1.33        | 1.51     |
| 22  | B     | 303 | CHD  | C4-C3   | 3.65  | 1.58        | 1.52     |
| 14  | N     | 602 | HEA  | CHA-C1A | 3.64  | 1.45        | 1.38     |
| 14  | N     | 601 | HEA  | C1B-C2B | -3.62 | 1.37        | 1.44     |
| 14  | N     | 602 | HEA  | C3A-C4A | -3.62 | 1.39        | 1.46     |
| 25  | G     | 101 | CDL  | C59-C58 | -3.61 | 1.33        | 1.51     |
| 25  | T     | 102 | CDL  | C59-C58 | -3.60 | 1.33        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | A     | 601 | HEA  | FE-ND   | 3.60  | 2.06        | 1.94     |
| 25  | T     | 102 | CDL  | C22-C21 | -3.60 | 1.33        | 1.51     |
| 25  | C     | 304 | CDL  | C82-C81 | -3.59 | 1.33        | 1.51     |
| 25  | G     | 101 | CDL  | C79-C78 | -3.59 | 1.33        | 1.51     |
| 25  | P     | 305 | CDL  | C39-C38 | -3.59 | 1.33        | 1.51     |
| 24  | P     | 303 | PEK  | C2-C1   | 3.59  | 1.61        | 1.50     |
| 25  | T     | 102 | CDL  | C82-C81 | -3.59 | 1.33        | 1.51     |
| 14  | N     | 601 | HEA  | C4A-NA  | -3.58 | 1.32        | 1.39     |
| 25  | C     | 304 | CDL  | C19-C18 | -3.57 | 1.34        | 1.51     |
| 20  | L     | 101 | TGL  | C10-CB9 | -3.55 | 1.34        | 1.51     |
| 25  | C     | 304 | CDL  | C22-C21 | -3.55 | 1.34        | 1.51     |
| 25  | C     | 304 | CDL  | C39-C38 | -3.55 | 1.34        | 1.51     |
| 25  | C     | 304 | CDL  | C62-C61 | -3.53 | 1.34        | 1.51     |
| 25  | C     | 304 | CDL  | C42-C41 | -3.51 | 1.34        | 1.51     |
| 25  | T     | 102 | CDL  | C19-C18 | -3.51 | 1.34        | 1.51     |
| 25  | G     | 101 | CDL  | C62-C61 | -3.51 | 1.34        | 1.51     |
| 20  | Y     | 101 | TGL  | C10-CB9 | -3.49 | 1.34        | 1.51     |
| 20  | B     | 301 | TGL  | C20-CA9 | -3.49 | 1.34        | 1.51     |
| 25  | P     | 305 | CDL  | C82-C81 | -3.48 | 1.34        | 1.51     |
| 14  | A     | 601 | HEA  | CMA-C3A | 3.48  | 1.53        | 1.45     |
| 25  | T     | 102 | CDL  | C79-C78 | -3.46 | 1.34        | 1.51     |
| 20  | B     | 301 | TGL  | C10-CB9 | -3.46 | 1.34        | 1.51     |
| 25  | P     | 305 | CDL  | C19-C18 | -3.45 | 1.34        | 1.51     |
| 25  | G     | 101 | CDL  | C42-C41 | -3.45 | 1.34        | 1.51     |
| 14  | A     | 602 | HEA  | C4D-ND  | -3.43 | 1.32        | 1.38     |
| 14  | A     | 601 | HEA  | C4B-NB  | -3.43 | 1.34        | 1.40     |
| 25  | P     | 305 | CDL  | C42-C41 | -3.42 | 1.34        | 1.51     |
| 25  | C     | 304 | CDL  | OB6-CB5 | 3.39  | 1.43        | 1.34     |
| 14  | N     | 601 | HEA  | CHC-C4B | 3.32  | 1.45        | 1.38     |
| 25  | P     | 305 | CDL  | C22-C21 | -3.31 | 1.35        | 1.51     |
| 20  | Q     | 201 | TGL  | C15-CC9 | -3.31 | 1.35        | 1.51     |
| 14  | A     | 602 | HEA  | FE-NB   | 3.30  | 2.05        | 1.94     |
| 25  | G     | 101 | CDL  | C39-C38 | -3.30 | 1.35        | 1.51     |
| 20  | Y     | 101 | TGL  | C15-CC9 | -3.29 | 1.35        | 1.51     |
| 20  | D     | 201 | TGL  | C15-CC9 | -3.28 | 1.35        | 1.51     |
| 20  | B     | 301 | TGL  | OG2-CB1 | 3.24  | 1.43        | 1.34     |
| 14  | N     | 601 | HEA  | C1A-C2A | -3.24 | 1.39        | 1.45     |
| 14  | A     | 602 | HEA  | FE-ND   | 3.23  | 2.04        | 1.94     |
| 14  | N     | 602 | HEA  | C4D-ND  | -3.22 | 1.32        | 1.38     |
| 20  | N     | 609 | TGL  | C15-CC9 | -3.21 | 1.35        | 1.51     |
| 20  | Q     | 201 | TGL  | C20-CA9 | -3.21 | 1.35        | 1.51     |
| 25  | T     | 102 | CDL  | C62-C61 | -3.20 | 1.35        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | N     | 601 | HEA  | CHD-C1D | 3.19  | 1.44        | 1.38     |
| 14  | A     | 601 | HEA  | C1A-C2A | -3.18 | 1.39        | 1.45     |
| 20  | D     | 201 | TGL  | C20-CA9 | -3.17 | 1.36        | 1.51     |
| 14  | N     | 602 | HEA  | C1A-C2A | -3.17 | 1.39        | 1.45     |
| 24  | P     | 303 | PEK  | O01-C1  | 3.16  | 1.43        | 1.34     |
| 25  | G     | 101 | CDL  | C19-C18 | -3.16 | 1.36        | 1.51     |
| 19  | C     | 303 | PGV  | O01-C1  | 3.15  | 1.43        | 1.34     |
| 14  | N     | 602 | HEA  | CHB-C4A | 3.15  | 1.44        | 1.38     |
| 22  | P     | 307 | CHD  | C8-C7   | 3.11  | 1.59        | 1.53     |
| 19  | P     | 304 | PGV  | O01-C1  | 3.10  | 1.43        | 1.34     |
| 20  | L     | 101 | TGL  | C15-CC9 | -3.09 | 1.36        | 1.51     |
| 20  | B     | 301 | TGL  | C15-CC9 | -3.04 | 1.36        | 1.51     |
| 14  | A     | 602 | HEA  | C11-C3B | 3.02  | 1.55        | 1.51     |
| 14  | A     | 602 | HEA  | C1A-C2A | -3.02 | 1.39        | 1.45     |
| 14  | A     | 601 | HEA  | C1D-ND  | -3.02 | 1.35        | 1.40     |
| 14  | A     | 602 | HEA  | C18-C19 | 3.02  | 1.40        | 1.33     |
| 14  | A     | 602 | HEA  | C1A-NA  | -3.01 | 1.33        | 1.39     |
| 22  | G     | 103 | CHD  | C6-C5   | 3.00  | 1.58        | 1.53     |
| 22  | C     | 306 | CHD  | C18-C13 | 2.99  | 1.59        | 1.54     |
| 25  | G     | 101 | CDL  | C22-C21 | -2.99 | 1.36        | 1.51     |
| 14  | N     | 601 | HEA  | C3A-C4A | -2.97 | 1.40        | 1.46     |
| 22  | G     | 103 | CHD  | C18-C13 | 2.97  | 1.59        | 1.54     |
| 14  | N     | 602 | HEA  | C1D-C2D | -2.93 | 1.38        | 1.44     |
| 14  | N     | 602 | HEA  | C1C-NC  | -2.92 | 1.34        | 1.39     |
| 22  | B     | 303 | CHD  | C4-C5   | 2.92  | 1.58        | 1.53     |
| 14  | N     | 601 | HEA  | C1A-NA  | -2.90 | 1.34        | 1.39     |
| 14  | A     | 602 | HEA  | CHC-C1C | 2.89  | 1.45        | 1.39     |
| 14  | A     | 602 | HEA  | CHD-C4C | 2.87  | 1.45        | 1.39     |
| 22  | P     | 307 | CHD  | C11-C12 | 2.84  | 1.57        | 1.53     |
| 14  | N     | 601 | HEA  | CHC-C1C | 2.83  | 1.45        | 1.39     |
| 14  | A     | 602 | HEA  | C3A-C2A | 2.80  | 1.43        | 1.37     |
| 14  | N     | 601 | HEA  | C1C-NC  | -2.80 | 1.34        | 1.39     |
| 14  | A     | 602 | HEA  | CAD-C3D | 2.73  | 1.58        | 1.51     |
| 14  | A     | 602 | HEA  | C4A-NA  | -2.67 | 1.34        | 1.39     |
| 14  | A     | 601 | HEA  | C3A-C4A | -2.64 | 1.41        | 1.46     |
| 14  | A     | 601 | HEA  | CBD-CGD | 2.64  | 1.56        | 1.50     |
| 14  | N     | 601 | HEA  | CHA-C4D | 2.62  | 1.45        | 1.39     |
| 14  | A     | 602 | HEA  | CMC-C2C | 2.61  | 1.56        | 1.50     |
| 14  | N     | 602 | HEA  | CHC-C4B | 2.59  | 1.43        | 1.38     |
| 19  | A     | 607 | PGV  | O01-C1  | 2.58  | 1.41        | 1.34     |
| 14  | N     | 601 | HEA  | CMB-C2B | 2.55  | 1.56        | 1.50     |
| 25  | C     | 304 | CDL  | OB6-CB4 | -2.55 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | A     | 602 | HEA  | CHB-C1B | 2.53  | 1.45        | 1.39     |
| 14  | A     | 601 | HEA  | C1C-C2C | -2.51 | 1.37        | 1.43     |
| 22  | G     | 103 | CHD  | C13-C12 | 2.50  | 1.58        | 1.54     |
| 14  | A     | 601 | HEA  | CHB-C1B | 2.46  | 1.44        | 1.39     |
| 22  | C     | 306 | CHD  | C21-C20 | 2.45  | 1.59        | 1.53     |
| 14  | A     | 601 | HEA  | O1D-CGD | 2.44  | 1.30        | 1.22     |
| 14  | A     | 602 | HEA  | C4B-NB  | -2.44 | 1.36        | 1.40     |
| 14  | N     | 602 | HEA  | C4C-NC  | -2.43 | 1.35        | 1.39     |
| 22  | G     | 103 | CHD  | C11-C9  | 2.41  | 1.57        | 1.53     |
| 14  | N     | 601 | HEA  | O11-C11 | 2.37  | 1.48        | 1.42     |
| 14  | N     | 601 | HEA  | C4D-ND  | -2.37 | 1.34        | 1.38     |
| 14  | A     | 602 | HEA  | CHC-C4B | 2.33  | 1.43        | 1.38     |
| 27  | Z     | 101 | DMU  | O16-C6  | 2.33  | 1.44        | 1.40     |
| 22  | C     | 306 | CHD  | C11-C9  | 2.33  | 1.57        | 1.53     |
| 14  | A     | 601 | HEA  | O11-C11 | 2.32  | 1.48        | 1.42     |
| 14  | A     | 602 | HEA  | C20-C19 | 2.30  | 1.56        | 1.51     |
| 25  | P     | 305 | CDL  | PB2-OB3 | 2.30  | 1.58        | 1.50     |
| 14  | N     | 602 | HEA  | OMA-CMA | 2.28  | 1.27        | 1.22     |
| 14  | N     | 602 | HEA  | CBD-CGD | 2.28  | 1.55        | 1.50     |
| 14  | N     | 602 | HEA  | FE-ND   | 2.26  | 2.01        | 1.94     |
| 19  | A     | 607 | PGV  | P-O14   | -2.24 | 1.45        | 1.55     |
| 14  | N     | 602 | HEA  | C16-C15 | 2.23  | 1.55        | 1.51     |
| 25  | C     | 304 | CDL  | CA2-C1  | 2.22  | 1.58        | 1.51     |
| 25  | P     | 305 | CDL  | O1-C1   | 2.21  | 1.49        | 1.43     |
| 14  | A     | 601 | HEA  | C4A-NA  | -2.20 | 1.35        | 1.39     |
| 22  | P     | 306 | CHD  | C8-C9   | 2.19  | 1.58        | 1.53     |
| 25  | P     | 305 | CDL  | CB2-C1  | 2.17  | 1.58        | 1.51     |
| 14  | N     | 602 | HEA  | C20-C19 | 2.15  | 1.55        | 1.51     |
| 22  | B     | 303 | CHD  | C11-C9  | 2.15  | 1.57        | 1.53     |
| 14  | A     | 601 | HEA  | C1D-C2D | -2.15 | 1.40        | 1.44     |
| 22  | B     | 303 | CHD  | C13-C12 | 2.11  | 1.57        | 1.54     |
| 14  | A     | 602 | HEA  | C1D-C2D | -2.08 | 1.40        | 1.44     |
| 19  | N     | 608 | PGV  | O06-C06 | 2.08  | 1.51        | 1.42     |
| 25  | C     | 304 | CDL  | PB2-OB3 | 2.07  | 1.58        | 1.50     |
| 14  | N     | 601 | HEA  | C4D-C3D | -2.06 | 1.41        | 1.45     |
| 25  | C     | 304 | CDL  | CB2-C1  | 2.05  | 1.58        | 1.51     |
| 22  | G     | 103 | CHD  | C20-C17 | 2.05  | 1.57        | 1.54     |
| 22  | P     | 307 | CHD  | C6-C5   | 2.04  | 1.57        | 1.53     |
| 14  | A     | 601 | HEA  | C3B-C2B | 2.03  | 1.39        | 1.34     |
| 22  | P     | 307 | CHD  | C21-C20 | 2.02  | 1.58        | 1.53     |
| 14  | N     | 602 | HEA  | CMA-C3A | 2.01  | 1.49        | 1.45     |
| 22  | G     | 103 | CHD  | O26-C24 | -2.01 | 1.24        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | A     | 607 | PGV  | C01-C02 | 2.00  | 1.57        | 1.50     |
| 14  | A     | 601 | HEA  | C4D-ND  | -2.00 | 1.34        | 1.38     |
| 19  | A     | 607 | PGV  | C8-C7   | 2.00  | 1.61        | 1.51     |

All (454) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | W     | 101 | CHD  | C17-C13-C12 | 9.82  | 126.50      | 117.67   |
| 22  | G     | 103 | CHD  | C1-C2-C3    | -9.55 | 97.84       | 110.48   |
| 22  | W     | 101 | CHD  | C13-C17-C20 | 8.62  | 129.93      | 119.48   |
| 22  | W     | 101 | CHD  | C18-C13-C12 | -7.92 | 101.13      | 109.06   |
| 22  | W     | 101 | CHD  | C17-C13-C14 | -7.30 | 92.79       | 100.11   |
| 14  | A     | 601 | HEA  | OMA-CMA-C3A | -6.91 | 110.01      | 125.62   |
| 20  | N     | 609 | TGL  | CG2-OG2-CB1 | 6.85  | 134.19      | 117.80   |
| 14  | A     | 602 | HEA  | CHB-C1B-NB  | -6.78 | 117.13      | 124.42   |
| 27  | M     | 101 | DMU  | O7-C10-C5   | -6.69 | 91.64       | 108.09   |
| 20  | Y     | 101 | TGL  | OG2-CB1-CB2 | 6.42  | 125.37      | 111.48   |
| 25  | T     | 102 | CDL  | OA6-CA5-C11 | 6.25  | 125.01      | 111.48   |
| 14  | A     | 601 | HEA  | CHB-C4A-NA  | -6.16 | 117.75      | 124.45   |
| 22  | G     | 103 | CHD  | C4-C5-C10   | -6.14 | 106.12      | 112.66   |
| 22  | C     | 305 | CHD  | C23-C22-C20 | -6.09 | 103.09      | 114.46   |
| 24  | T     | 101 | PEK  | O01-C1-C2   | 6.05  | 124.56      | 111.48   |
| 22  | J     | 101 | CHD  | C10-C9-C8   | 6.03  | 118.56      | 111.84   |
| 25  | C     | 304 | CDL  | OA6-CA5-C11 | 6.02  | 124.51      | 111.48   |
| 25  | G     | 101 | CDL  | OB6-CB5-C51 | 5.96  | 124.38      | 111.48   |
| 27  | M     | 101 | DMU  | O1-C9-C8    | 5.93  | 120.38      | 109.70   |
| 20  | D     | 201 | TGL  | OG2-CB1-CB2 | -5.90 | 98.72       | 111.48   |
| 22  | P     | 306 | CHD  | C18-C13-C12 | -5.87 | 103.18      | 109.06   |
| 22  | B     | 303 | CHD  | C4-C3-C2    | 5.69  | 117.56      | 110.62   |
| 20  | D     | 201 | TGL  | OG2-CB1-OB1 | 5.68  | 136.97      | 123.70   |
| 14  | A     | 601 | HEA  | C4A-C3A-C2A | -5.51 | 102.03      | 106.81   |
| 14  | A     | 601 | HEA  | C4A-CHB-C1B | 5.49  | 137.69      | 126.02   |
| 14  | N     | 602 | HEA  | OMA-CMA-C3A | -5.41 | 113.40      | 125.62   |
| 19  | N     | 608 | PGV  | O03-C19-O04 | -5.40 | 110.13      | 123.63   |
| 22  | J     | 101 | CHD  | C9-C8-C7    | 5.40  | 118.65      | 111.86   |
| 22  | J     | 101 | CHD  | C6-C5-C4    | -5.24 | 105.24      | 111.23   |
| 24  | P     | 303 | PEK  | C2-C3-C4    | 5.21  | 124.73      | 113.35   |
| 27  | Z     | 101 | DMU  | C10-O1-C9   | 5.21  | 123.89      | 113.72   |
| 14  | A     | 601 | HEA  | CHA-C4D-ND  | 5.19  | 130.00      | 124.42   |
| 14  | A     | 601 | HEA  | C17-C18-C19 | 5.16  | 139.42      | 127.62   |
| 25  | G     | 101 | CDL  | OA6-CA5-C11 | 5.15  | 122.62      | 111.48   |
| 24  | G     | 102 | PEK  | O01-C1-C2   | 5.14  | 122.61      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | B     | 301 | TGL  | CG2-OG2-CB1 | 5.12  | 130.04      | 117.80   |
| 27  | M     | 101 | DMU  | O1-C10-C5   | 5.06  | 120.76      | 110.37   |
| 23  | N     | 610 | PSC  | O01-C1-C2   | 5.05  | 122.40      | 111.48   |
| 22  | P     | 306 | CHD  | C6-C7-C8    | 5.04  | 117.01      | 111.50   |
| 14  | A     | 602 | HEA  | OMA-CMA-C3A | -4.96 | 114.42      | 125.62   |
| 22  | C     | 306 | CHD  | C18-C13-C12 | 4.95  | 114.01      | 109.06   |
| 19  | P     | 301 | PGV  | O03-C19-C20 | 4.93  | 126.88      | 111.83   |
| 25  | P     | 305 | CDL  | CB4-OB6-CB5 | -4.91 | 106.03      | 117.80   |
| 14  | A     | 602 | HEA  | CMB-C2B-C1B | 4.91  | 132.70      | 125.03   |
| 14  | A     | 602 | HEA  | CHA-C4D-ND  | 4.82  | 129.62      | 124.42   |
| 14  | A     | 601 | HEA  | CHB-C1B-NB  | -4.82 | 119.24      | 124.42   |
| 19  | C     | 308 | PGV  | O01-C1-C2   | 4.81  | 121.89      | 111.48   |
| 27  | Z     | 101 | DMU  | O1-C9-C8    | 4.81  | 118.36      | 109.70   |
| 19  | C     | 303 | PGV  | O03-C19-O04 | -4.74 | 111.76      | 123.63   |
| 23  | B     | 304 | PSC  | O01-C1-C2   | 4.70  | 121.64      | 111.48   |
| 22  | P     | 306 | CHD  | C15-C14-C13 | 4.60  | 108.00      | 103.54   |
| 22  | G     | 103 | CHD  | C15-C14-C13 | 4.59  | 108.00      | 103.54   |
| 24  | P     | 303 | PEK  | O01-C1-O02  | -4.57 | 113.02      | 123.70   |
| 14  | A     | 602 | HEA  | C4A-C3A-C2A | -4.57 | 102.85      | 106.81   |
| 22  | J     | 101 | CHD  | C4-C5-C10   | 4.54  | 117.49      | 112.66   |
| 22  | P     | 306 | CHD  | C19-C10-C9  | -4.51 | 105.11      | 111.18   |
| 22  | J     | 101 | CHD  | C14-C8-C7   | 4.49  | 117.80      | 111.85   |
| 25  | T     | 102 | CDL  | OB6-CB5-C51 | 4.46  | 121.14      | 111.48   |
| 14  | A     | 601 | HEA  | C2B-C1B-NB  | 4.44  | 115.04      | 109.90   |
| 14  | N     | 601 | HEA  | C3A-C2A-C1A | -4.44 | 102.84      | 107.05   |
| 22  | P     | 306 | CHD  | C4-C5-C10   | 4.42  | 117.37      | 112.66   |
| 24  | C     | 307 | PEK  | O01-C1-C2   | 4.40  | 121.01      | 111.48   |
| 22  | W     | 101 | CHD  | C14-C8-C7   | 4.39  | 117.68      | 111.85   |
| 27  | M     | 101 | DMU  | C8-C7-C5    | 4.35  | 118.47      | 110.83   |
| 25  | P     | 305 | CDL  | OA6-CA5-C11 | 4.34  | 120.88      | 111.48   |
| 22  | W     | 101 | CHD  | C11-C12-C13 | 4.31  | 115.65      | 111.26   |
| 20  | B     | 301 | TGL  | CG3-OG3-CC1 | 4.30  | 132.85      | 117.12   |
| 22  | G     | 103 | CHD  | C18-C13-C14 | 4.28  | 117.91      | 111.20   |
| 14  | N     | 601 | HEA  | O2D-CGD-CBD | 4.28  | 127.53      | 114.00   |
| 22  | J     | 101 | CHD  | C14-C8-C9   | -4.28 | 103.78      | 109.75   |
| 19  | A     | 608 | PGV  | O03-C19-C20 | 4.28  | 124.88      | 111.83   |
| 25  | P     | 305 | CDL  | OB8-CB7-C71 | 4.27  | 124.87      | 111.83   |
| 24  | C     | 307 | PEK  | O03-C21-C22 | 4.26  | 124.83      | 111.83   |
| 22  | J     | 101 | CHD  | C13-C17-C20 | 4.25  | 124.63      | 119.48   |
| 20  | N     | 609 | TGL  | OG2-CB1-CB2 | 4.24  | 120.66      | 111.48   |
| 22  | B     | 303 | CHD  | C19-C10-C5  | -4.21 | 103.40      | 110.44   |
| 20  | B     | 301 | TGL  | OG1-CA1-CA2 | 4.19  | 124.60      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | A     | 602 | HEA  | C13-C12-C11 | -4.18 | 107.72      | 114.39   |
| 20  | L     | 101 | TGL  | OG3-CC1-CC2 | 4.17  | 124.55      | 111.83   |
| 22  | P     | 306 | CHD  | O7-C7-C6    | -4.16 | 99.52       | 109.86   |
| 19  | A     | 608 | PGV  | C4-C3-C2    | -4.15 | 97.87       | 113.13   |
| 14  | N     | 602 | HEA  | CHA-C4D-ND  | 4.11  | 128.84      | 124.42   |
| 22  | J     | 101 | CHD  | C14-C13-C12 | 4.10  | 111.16      | 107.42   |
| 25  | C     | 304 | CDL  | CB4-OB6-CB5 | -4.08 | 108.03      | 117.80   |
| 19  | N     | 608 | PGV  | O03-C19-C20 | 4.07  | 124.24      | 111.83   |
| 20  | B     | 301 | TGL  | OG2-CB1-CB2 | 4.06  | 120.25      | 111.48   |
| 22  | J     | 101 | CHD  | C11-C12-C13 | 4.04  | 115.38      | 111.26   |
| 22  | W     | 101 | CHD  | C18-C13-C17 | 3.95  | 117.40      | 111.20   |
| 22  | W     | 101 | CHD  | C15-C14-C8  | 3.94  | 123.76      | 118.36   |
| 22  | P     | 306 | CHD  | C19-C10-C1  | -3.93 | 102.06      | 108.31   |
| 19  | C     | 308 | PGV  | O03-C19-C20 | 3.92  | 123.80      | 111.83   |
| 22  | B     | 303 | CHD  | C15-C14-C13 | 3.92  | 107.35      | 103.54   |
| 24  | P     | 303 | PEK  | O03-C21-C22 | 3.92  | 123.78      | 111.83   |
| 19  | P     | 301 | PGV  | O01-C1-C2   | 3.90  | 119.92      | 111.48   |
| 22  | G     | 103 | CHD  | C19-C10-C1  | -3.89 | 102.12      | 108.31   |
| 14  | A     | 602 | HEA  | CMD-C2D-C1D | 3.86  | 131.06      | 125.03   |
| 22  | J     | 101 | CHD  | C19-C10-C9  | -3.85 | 106.00      | 111.18   |
| 20  | N     | 609 | TGL  | CG3-OG3-CC1 | 3.82  | 131.09      | 117.12   |
| 27  | M     | 101 | DMU  | O7-C10-O1   | -3.82 | 100.64      | 110.69   |
| 27  | Z     | 101 | DMU  | O49-C1-C2   | -3.82 | 101.38      | 110.38   |
| 14  | A     | 602 | HEA  | C2B-C1B-NB  | 3.80  | 114.29      | 109.90   |
| 19  | C     | 303 | PGV  | O01-C1-C2   | 3.79  | 119.68      | 111.48   |
| 22  | P     | 306 | CHD  | C16-C17-C13 | 3.78  | 107.21      | 103.54   |
| 14  | A     | 602 | HEA  | C4A-CHB-C1B | 3.77  | 134.04      | 126.02   |
| 14  | A     | 602 | HEA  | CAD-C3D-C4D | -3.76 | 118.14      | 124.70   |
| 22  | W     | 101 | CHD  | C6-C5-C10   | 3.74  | 116.64      | 112.66   |
| 22  | C     | 305 | CHD  | C6-C7-C8    | 3.74  | 115.58      | 111.50   |
| 20  | B     | 301 | TGL  | OG2-CG2-CG1 | 3.72  | 121.68      | 108.34   |
| 19  | A     | 607 | PGV  | O03-C19-C20 | 3.72  | 123.17      | 111.83   |
| 22  | G     | 103 | CHD  | C13-C14-C8  | -3.71 | 110.02      | 114.72   |
| 14  | A     | 601 | HEA  | CMB-C2B-C1B | 3.71  | 130.82      | 125.03   |
| 14  | A     | 602 | HEA  | CMB-C2B-C3B | -3.70 | 123.12      | 130.28   |
| 22  | B     | 303 | CHD  | C18-C13-C12 | -3.70 | 105.36      | 109.06   |
| 27  | Z     | 101 | DMU  | C18-O16-C6  | -3.67 | 107.42      | 113.68   |
| 22  | P     | 306 | CHD  | O3-C3-C4    | -3.65 | 102.57      | 109.84   |
| 14  | A     | 602 | HEA  | C1D-C2D-C3D | -3.65 | 103.15      | 106.98   |
| 20  | Q     | 201 | TGL  | OG2-CB1-CB2 | -3.63 | 103.63      | 111.48   |
| 24  | P     | 308 | PEK  | O01-C1-C2   | 3.63  | 119.33      | 111.48   |
| 25  | P     | 305 | CDL  | OB6-CB5-C51 | 3.62  | 119.31      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | N     | 601 | HEA  | CHC-C4B-NB  | 3.62  | 128.84      | 124.37   |
| 14  | N     | 601 | HEA  | C2B-C1B-NB  | 3.59  | 114.05      | 109.90   |
| 24  | P     | 308 | PEK  | O03-C21-C22 | 3.58  | 122.75      | 111.83   |
| 22  | C     | 306 | CHD  | C1-C2-C3    | -3.58 | 105.74      | 110.48   |
| 22  | C     | 305 | CHD  | C18-C13-C12 | -3.56 | 105.49      | 109.06   |
| 19  | N     | 607 | PGV  | O01-C1-C2   | 3.55  | 119.17      | 111.48   |
| 14  | N     | 601 | HEA  | CHA-C1A-NA  | -3.55 | 120.58      | 124.45   |
| 22  | C     | 306 | CHD  | C16-C17-C13 | -3.54 | 100.11      | 103.54   |
| 22  | P     | 306 | CHD  | C11-C12-C13 | 3.53  | 114.86      | 111.26   |
| 27  | M     | 101 | DMU  | O3-C5-C7    | 3.53  | 118.70      | 110.38   |
| 24  | G     | 102 | PEK  | O03-C21-C22 | 3.52  | 122.57      | 111.83   |
| 22  | P     | 307 | CHD  | C19-C10-C1  | -3.51 | 102.72      | 108.31   |
| 22  | C     | 305 | CHD  | C1-C10-C5   | 3.51  | 112.79      | 107.75   |
| 19  | A     | 608 | PGV  | C02-O01-C1  | 3.50  | 126.17      | 117.80   |
| 22  | C     | 305 | CHD  | C17-C13-C12 | -3.50 | 114.52      | 117.67   |
| 20  | Y     | 101 | TGL  | OG3-CC1-CC2 | 3.50  | 122.50      | 111.83   |
| 14  | A     | 602 | HEA  | CHB-C4A-NA  | -3.49 | 120.65      | 124.45   |
| 23  | N     | 610 | PSC  | O03-C19-C20 | 3.49  | 122.47      | 111.83   |
| 20  | B     | 301 | TGL  | OG3-CC1-CC2 | 3.48  | 122.45      | 111.83   |
| 19  | N     | 608 | PGV  | O01-C1-O02  | -3.47 | 115.60      | 123.70   |
| 27  | Z     | 101 | DMU  | O2-C8-C9    | 3.45  | 117.83      | 109.32   |
| 14  | N     | 601 | HEA  | O2D-CGD-O1D | -3.44 | 114.48      | 123.33   |
| 25  | P     | 305 | CDL  | OB8-CB7-OB9 | -3.44 | 115.03      | 123.63   |
| 22  | W     | 101 | CHD  | C1-C10-C5   | 3.43  | 112.67      | 107.75   |
| 14  | A     | 601 | HEA  | CAA-CBA-CGA | -3.43 | 104.56      | 113.67   |
| 20  | L     | 101 | TGL  | OG1-CA1-CA2 | 3.43  | 122.29      | 111.83   |
| 27  | M     | 101 | DMU  | C10-C5-C7   | 3.43  | 117.22      | 110.01   |
| 14  | N     | 602 | HEA  | O11-C11-C3B | -3.42 | 104.98      | 111.26   |
| 24  | T     | 101 | PEK  | O01-C1-O02  | -3.41 | 115.74      | 123.70   |
| 20  | B     | 301 | TGL  | CB3-CB2-CB1 | -3.40 | 101.23      | 113.69   |
| 22  | B     | 303 | CHD  | C6-C5-C10   | 3.40  | 116.27      | 112.66   |
| 20  | N     | 609 | TGL  | OG1-CA1-CA2 | 3.39  | 122.19      | 111.83   |
| 22  | B     | 303 | CHD  | C13-C17-C20 | -3.39 | 115.37      | 119.48   |
| 14  | N     | 601 | HEA  | CMD-C2D-C1D | 3.39  | 130.33      | 125.03   |
| 19  | N     | 607 | PGV  | C4-C3-C2    | -3.38 | 100.70      | 113.13   |
| 19  | A     | 607 | PGV  | O03-C19-O04 | -3.38 | 115.18      | 123.63   |
| 20  | Q     | 201 | TGL  | OG1-CA1-CA2 | 3.37  | 122.12      | 111.83   |
| 14  | A     | 601 | HEA  | CHA-C4D-C3D | -3.37 | 119.86      | 124.77   |
| 14  | A     | 601 | HEA  | C1B-C2B-C3B | -3.36 | 102.91      | 106.80   |
| 22  | G     | 103 | CHD  | C17-C13-C12 | -3.35 | 114.65      | 117.67   |
| 14  | N     | 602 | HEA  | C1A-CHA-C4D | -3.34 | 118.93      | 126.02   |
| 22  | W     | 101 | CHD  | C22-C20-C17 | 3.34  | 117.25      | 110.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | N     | 609 | TGL  | OG2-CG2-CG1 | 3.32  | 120.26      | 108.34   |
| 22  | B     | 303 | CHD  | C1-C10-C5   | 3.32  | 112.51      | 107.75   |
| 22  | J     | 101 | CHD  | C1-C2-C3    | 3.31  | 114.87      | 110.48   |
| 27  | M     | 101 | DMU  | C7-C8-C9    | 3.30  | 116.21      | 110.23   |
| 22  | J     | 101 | CHD  | C19-C10-C1  | -3.29 | 103.08      | 108.31   |
| 20  | Y     | 101 | TGL  | OG1-CA1-OA1 | -3.29 | 115.40      | 123.63   |
| 14  | A     | 602 | HEA  | CHA-C4D-C3D | -3.27 | 120.01      | 124.77   |
| 24  | P     | 308 | PEK  | O03-C21-O04 | -3.26 | 115.47      | 123.63   |
| 22  | P     | 307 | CHD  | C4-C5-C10   | -3.26 | 109.19      | 112.66   |
| 22  | P     | 306 | CHD  | C15-C14-C8  | 3.25  | 122.81      | 118.36   |
| 20  | D     | 201 | TGL  | CB3-CB2-CB1 | 3.23  | 125.53      | 113.69   |
| 19  | N     | 607 | PGV  | C3-C2-C1    | -3.23 | 101.87      | 113.69   |
| 22  | W     | 101 | CHD  | C6-C5-C4    | -3.21 | 107.56      | 111.23   |
| 19  | C     | 303 | PGV  | O03-C19-C20 | 3.21  | 121.61      | 111.83   |
| 14  | N     | 601 | HEA  | OMA-CMA-C3A | -3.20 | 118.41      | 125.62   |
| 25  | G     | 101 | CDL  | OA8-CA7-C31 | 3.18  | 121.53      | 111.83   |
| 27  | M     | 101 | DMU  | C10-O1-C9   | 3.18  | 119.92      | 113.72   |
| 20  | Y     | 101 | TGL  | OG1-CA1-CA2 | 3.17  | 121.51      | 111.83   |
| 24  | T     | 101 | PEK  | O03-C21-C22 | 3.17  | 121.51      | 111.83   |
| 20  | Q     | 201 | TGL  | OG1-CG1-CG2 | 3.17  | 117.53      | 108.40   |
| 25  | C     | 304 | CDL  | C52-C51-CB5 | -3.13 | 102.22      | 113.69   |
| 22  | P     | 306 | CHD  | C6-C5-C10   | 3.13  | 115.99      | 112.66   |
| 25  | T     | 102 | CDL  | OA8-CA7-C31 | 3.13  | 121.36      | 111.83   |
| 20  | B     | 301 | TGL  | CG1-OG1-CA1 | 3.12  | 128.53      | 117.12   |
| 25  | C     | 304 | CDL  | OB6-CB5-C51 | 3.12  | 118.23      | 111.48   |
| 25  | P     | 305 | CDL  | OA8-CA7-C31 | 3.10  | 121.29      | 111.83   |
| 14  | N     | 601 | HEA  | C3C-C4C-NC  | 3.10  | 112.41      | 109.80   |
| 22  | C     | 306 | CHD  | C6-C5-C4    | -3.09 | 107.69      | 111.23   |
| 22  | G     | 103 | CHD  | C18-C13-C12 | -3.08 | 105.97      | 109.06   |
| 25  | C     | 304 | CDL  | OB8-CB7-C71 | 3.06  | 121.17      | 111.83   |
| 22  | J     | 101 | CHD  | C15-C14-C8  | 3.05  | 122.55      | 118.36   |
| 14  | A     | 601 | HEA  | C26-C15-C16 | -3.05 | 109.93      | 115.23   |
| 14  | N     | 602 | HEA  | C4C-C3C-C2C | -3.05 | 103.51      | 107.30   |
| 19  | N     | 608 | PGV  | C01-O03-C19 | -3.03 | 106.05      | 117.12   |
| 22  | C     | 306 | CHD  | C5-C6-C7    | 3.02  | 117.99      | 114.40   |
| 25  | C     | 304 | CDL  | OA8-CA7-C31 | 3.01  | 121.03      | 111.83   |
| 22  | P     | 306 | CHD  | C11-C9-C8   | 3.01  | 115.34      | 110.89   |
| 14  | A     | 602 | HEA  | CHD-C4C-NC  | 3.00  | 129.30      | 123.86   |
| 20  | L     | 101 | TGL  | OG2-CB1-CB2 | 3.00  | 117.97      | 111.48   |
| 24  | G     | 102 | PEK  | O03-C01-C02 | 2.99  | 117.02      | 108.40   |
| 22  | P     | 306 | CHD  | C22-C23-C24 | -2.96 | 104.61      | 112.49   |
| 14  | A     | 602 | HEA  | CAD-C3D-C2D | 2.95  | 133.40      | 127.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | P     | 306 | CHD  | C21-C20-C22 | -2.94 | 105.79      | 110.34   |
| 19  | A     | 608 | PGV  | C01-O03-C19 | 2.94  | 127.85      | 117.12   |
| 25  | G     | 101 | CDL  | OA6-CA5-OA7 | -2.93 | 116.85      | 123.70   |
| 14  | N     | 601 | HEA  | C17-C18-C19 | 2.93  | 134.32      | 127.62   |
| 14  | N     | 602 | HEA  | C12-C11-C3B | 2.93  | 116.69      | 112.12   |
| 14  | A     | 601 | HEA  | CHA-C1A-NA  | -2.92 | 121.27      | 124.45   |
| 20  | N     | 609 | TGL  | OG2-CG2-CG3 | 2.92  | 118.80      | 108.34   |
| 14  | A     | 602 | HEA  | C2D-C1D-ND  | 2.90  | 113.18      | 109.84   |
| 14  | A     | 602 | HEA  | C16-C15-C14 | -2.90 | 114.66      | 121.17   |
| 22  | C     | 305 | CHD  | C21-C20-C17 | 2.88  | 117.20      | 112.88   |
| 20  | Q     | 201 | TGL  | OG3-CC1-CC2 | 2.87  | 120.59      | 111.83   |
| 22  | C     | 306 | CHD  | C11-C12-C13 | 2.86  | 114.18      | 111.26   |
| 20  | D     | 201 | TGL  | OG3-CG3-CG2 | -2.86 | 100.14      | 108.40   |
| 25  | C     | 304 | CDL  | OA6-CA5-OA7 | -2.86 | 117.01      | 123.70   |
| 24  | C     | 302 | PEK  | O03-C21-O04 | -2.86 | 116.47      | 123.63   |
| 20  | D     | 201 | TGL  | OG1-CG1-CG2 | 2.85  | 116.62      | 108.40   |
| 19  | C     | 308 | PGV  | C01-O03-C19 | 2.84  | 127.52      | 117.12   |
| 14  | A     | 601 | HEA  | C20-C19-C18 | 2.84  | 127.55      | 121.17   |
| 20  | D     | 201 | TGL  | C21-C20-CA9 | 2.84  | 128.71      | 114.37   |
| 19  | A     | 607 | PGV  | C23-C22-C21 | -2.81 | 100.15      | 114.37   |
| 22  | G     | 103 | CHD  | C16-C15-C14 | -2.79 | 99.67       | 105.14   |
| 14  | N     | 602 | HEA  | O2A-CGA-CBA | 2.78  | 122.78      | 114.00   |
| 19  | A     | 608 | PGV  | O03-C19-O04 | -2.77 | 116.69      | 123.63   |
| 25  | T     | 102 | CDL  | OA6-CA5-OA7 | -2.77 | 117.23      | 123.70   |
| 23  | B     | 304 | PSC  | O03-C19-C20 | 2.77  | 120.27      | 111.83   |
| 25  | G     | 101 | CDL  | C19-C18-C17 | 2.76  | 128.34      | 114.37   |
| 14  | N     | 602 | HEA  | C13-C12-C11 | -2.76 | 109.98      | 114.39   |
| 22  | W     | 101 | CHD  | C11-C9-C10  | 2.76  | 116.50      | 113.70   |
| 19  | P     | 304 | PGV  | O01-C1-C2   | 2.76  | 117.45      | 111.48   |
| 22  | P     | 306 | CHD  | C14-C8-C9   | -2.76 | 105.90      | 109.75   |
| 20  | Q     | 201 | TGL  | OG2-CB1-OB1 | 2.75  | 130.14      | 123.70   |
| 25  | G     | 101 | CDL  | CB6-OB8-CB7 | 2.75  | 127.17      | 117.12   |
| 14  | N     | 601 | HEA  | C12-C11-C3B | 2.74  | 116.40      | 112.12   |
| 22  | P     | 306 | CHD  | C1-C10-C9   | 2.74  | 115.59      | 111.34   |
| 27  | M     | 101 | DMU  | O16-C6-C1   | 2.73  | 112.41      | 108.27   |
| 22  | J     | 101 | CHD  | C16-C17-C13 | 2.73  | 106.19      | 103.54   |
| 25  | P     | 305 | CDL  | C52-C51-CB5 | -2.72 | 103.72      | 113.69   |
| 27  | M     | 101 | DMU  | C28-C25-C22 | -2.72 | 100.61      | 114.37   |
| 20  | Y     | 101 | TGL  | OG1-CG1-CG2 | 2.71  | 116.20      | 108.40   |
| 27  | M     | 101 | DMU  | O7-C3-C4    | -2.70 | 102.39      | 109.48   |
| 22  | G     | 103 | CHD  | C5-C4-C3    | -2.70 | 108.64      | 112.71   |
| 14  | N     | 602 | HEA  | CHB-C1B-C2B | -2.68 | 120.80      | 125.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | D     | 201 | TGL  | CG2-OG2-CB1 | 2.68  | 124.20      | 117.80   |
| 22  | J     | 101 | CHD  | C11-C9-C8   | -2.68 | 106.94      | 110.89   |
| 25  | G     | 101 | CDL  | OA8-CA7-OA9 | -2.67 | 116.95      | 123.63   |
| 25  | T     | 102 | CDL  | OB8-CB7-OB9 | -2.66 | 116.97      | 123.63   |
| 22  | C     | 305 | CHD  | C19-C10-C1  | -2.66 | 104.08      | 108.31   |
| 24  | C     | 307 | PEK  | O03-C01-C02 | 2.65  | 116.04      | 108.40   |
| 14  | N     | 602 | HEA  | C4A-C3A-C2A | -2.65 | 104.52      | 106.81   |
| 22  | G     | 103 | CHD  | C14-C8-C9   | 2.65  | 113.45      | 109.75   |
| 22  | W     | 101 | CHD  | O12-C12-C11 | 2.65  | 114.51      | 109.12   |
| 22  | P     | 307 | CHD  | C22-C23-C24 | -2.65 | 105.43      | 112.49   |
| 22  | P     | 307 | CHD  | C11-C9-C10  | -2.65 | 111.02      | 113.70   |
| 19  | C     | 303 | PGV  | O01-C1-O02  | -2.64 | 117.53      | 123.70   |
| 25  | G     | 101 | CDL  | OB6-CB5-OB7 | -2.64 | 117.54      | 123.70   |
| 27  | Z     | 101 | DMU  | C7-C8-C9    | 2.63  | 115.00      | 110.23   |
| 20  | Y     | 101 | TGL  | OG2-CB1-OB1 | -2.63 | 117.56      | 123.70   |
| 20  | Y     | 101 | TGL  | OG3-CG3-CG2 | 2.63  | 115.97      | 108.40   |
| 22  | C     | 305 | CHD  | C22-C23-C24 | -2.63 | 105.49      | 112.49   |
| 25  | T     | 102 | CDL  | OB8-CB7-C71 | 2.62  | 119.82      | 111.83   |
| 20  | D     | 201 | TGL  | OG3-CC1-OC1 | -2.62 | 117.08      | 123.63   |
| 19  | N     | 607 | PGV  | C02-O01-C1  | 2.61  | 124.05      | 117.80   |
| 23  | N     | 610 | PSC  | O01-C1-O02  | -2.61 | 117.61      | 123.70   |
| 25  | C     | 304 | CDL  | OA8-CA6-CA4 | 2.61  | 115.91      | 108.40   |
| 24  | C     | 302 | PEK  | O01-C1-C2   | 2.60  | 117.10      | 111.48   |
| 20  | N     | 609 | TGL  | OG3-CC1-CC2 | 2.60  | 119.75      | 111.83   |
| 14  | N     | 601 | HEA  | O11-C11-C3B | -2.59 | 106.51      | 111.26   |
| 22  | C     | 305 | CHD  | C14-C13-C12 | 2.59  | 109.78      | 107.42   |
| 14  | N     | 601 | HEA  | C3D-C4D-ND  | 2.58  | 112.85      | 110.35   |
| 20  | Y     | 101 | TGL  | OG3-CC1-OC1 | -2.58 | 117.18      | 123.63   |
| 19  | A     | 608 | PGV  | O01-C02-C03 | 2.57  | 117.56      | 108.34   |
| 27  | M     | 101 | DMU  | O6-C11-C9   | -2.57 | 102.60      | 111.33   |
| 14  | N     | 601 | HEA  | C1A-CHA-C4D | 2.56  | 131.45      | 126.02   |
| 19  | P     | 301 | PGV  | O01-C1-O02  | -2.55 | 117.74      | 123.70   |
| 14  | N     | 601 | HEA  | O2A-CGA-CBA | 2.55  | 122.05      | 114.00   |
| 20  | B     | 301 | TGL  | C15-CC9-CC8 | 2.54  | 127.22      | 114.37   |
| 14  | N     | 602 | HEA  | CHA-C1A-NA  | 2.53  | 127.21      | 124.45   |
| 22  | C     | 306 | CHD  | C5-C4-C3    | -2.52 | 108.91      | 112.71   |
| 14  | N     | 601 | HEA  | O1A-CGA-CBA | -2.52 | 115.11      | 123.09   |
| 14  | A     | 602 | HEA  | C21-C20-C19 | 2.52  | 121.53      | 113.19   |
| 14  | A     | 602 | HEA  | CHC-C4B-NB  | 2.52  | 127.48      | 124.37   |
| 25  | P     | 305 | CDL  | OB2-PB2-OB3 | 2.51  | 118.90      | 108.94   |
| 14  | N     | 601 | HEA  | C4A-C3A-C2A | 2.51  | 108.99      | 106.81   |
| 25  | C     | 304 | CDL  | CA4-OA6-CA5 | 2.50  | 123.78      | 117.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | C     | 303 | PGV  | C02-O01-C1  | 2.50  | 123.78      | 117.80   |
| 19  | C     | 303 | PGV  | O01-C02-C03 | -2.49 | 99.40       | 108.34   |
| 19  | N     | 607 | PGV  | O03-C19-C20 | 2.49  | 119.42      | 111.83   |
| 22  | B     | 303 | CHD  | C4-C5-C10   | 2.49  | 115.31      | 112.66   |
| 14  | N     | 601 | HEA  | C13-C12-C11 | -2.47 | 110.45      | 114.39   |
| 22  | G     | 103 | CHD  | C1-C10-C9   | 2.47  | 115.17      | 111.34   |
| 22  | C     | 306 | CHD  | O25-C24-C23 | -2.47 | 115.27      | 123.09   |
| 14  | N     | 602 | HEA  | C3C-C4C-NC  | 2.46  | 111.87      | 109.80   |
| 22  | J     | 101 | CHD  | C6-C7-C8    | 2.46  | 114.19      | 111.50   |
| 19  | P     | 301 | PGV  | O04-C19-C20 | -2.45 | 114.18      | 123.78   |
| 14  | N     | 601 | HEA  | CHB-C1B-C2B | -2.45 | 121.16      | 125.03   |
| 24  | P     | 303 | PEK  | O02-C1-C2   | 2.44  | 133.34      | 123.78   |
| 20  | L     | 101 | TGL  | OG3-CC1-OC1 | -2.44 | 117.52      | 123.63   |
| 22  | C     | 305 | CHD  | C14-C8-C9   | -2.44 | 106.34      | 109.75   |
| 14  | A     | 602 | HEA  | C17-C18-C19 | 2.43  | 133.19      | 127.62   |
| 22  | G     | 103 | CHD  | C15-C16-C17 | 2.43  | 109.90      | 105.14   |
| 27  | Z     | 101 | DMU  | O4-C7-C8    | -2.42 | 104.66      | 110.38   |
| 24  | C     | 302 | PEK  | O01-C02-C01 | -2.42 | 99.65       | 108.34   |
| 14  | N     | 602 | HEA  | CHC-C4B-NB  | 2.42  | 127.36      | 124.37   |
| 14  | A     | 602 | HEA  | C1B-C2B-C3B | -2.42 | 103.99      | 106.80   |
| 22  | W     | 101 | CHD  | C19-C10-C1  | -2.42 | 104.46      | 108.31   |
| 20  | D     | 201 | TGL  | C16-C15-CC9 | 2.41  | 126.56      | 114.37   |
| 22  | P     | 306 | CHD  | C2-C1-C10   | 2.41  | 116.81      | 112.74   |
| 22  | J     | 101 | CHD  | O7-C7-C8    | 2.41  | 115.04      | 109.52   |
| 19  | C     | 303 | PGV  | O14-P-O13   | 2.40  | 123.62      | 112.44   |
| 22  | G     | 103 | CHD  | C14-C13-C12 | 2.40  | 109.61      | 107.42   |
| 23  | N     | 610 | PSC  | C21-C20-C19 | -2.39 | 104.94      | 113.69   |
| 20  | Y     | 101 | TGL  | CA4-CA3-CA2 | -2.39 | 104.36      | 113.13   |
| 22  | J     | 101 | CHD  | C22-C20-C17 | 2.37  | 115.25      | 110.33   |
| 14  | N     | 602 | HEA  | CAD-CBD-CGD | -2.37 | 107.38      | 113.67   |
| 22  | J     | 101 | CHD  | C23-C22-C20 | -2.37 | 110.04      | 114.46   |
| 22  | C     | 305 | CHD  | C18-C13-C17 | 2.37  | 114.91      | 111.20   |
| 22  | G     | 103 | CHD  | C19-C10-C5  | -2.37 | 106.48      | 110.44   |
| 25  | P     | 305 | CDL  | C57-C56-C55 | -2.36 | 102.41      | 114.37   |
| 14  | N     | 602 | HEA  | C1C-CHC-C4B | -2.36 | 120.69      | 126.25   |
| 24  | C     | 302 | PEK  | C2-C3-C4    | -2.35 | 108.22      | 113.35   |
| 22  | W     | 101 | CHD  | C16-C17-C20 | 2.34  | 115.73      | 112.18   |
| 14  | N     | 602 | HEA  | CHA-C4D-C3D | -2.34 | 121.36      | 124.77   |
| 14  | A     | 601 | HEA  | C4C-CHD-C1D | 2.34  | 131.75      | 126.25   |
| 22  | C     | 305 | CHD  | C16-C17-C13 | 2.33  | 105.80      | 103.54   |
| 14  | N     | 601 | HEA  | C4C-C3C-C2C | -2.33 | 104.41      | 107.30   |
| 25  | P     | 305 | CDL  | OA6-CA5-OA7 | -2.32 | 118.27      | 123.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | P     | 307 | CHD  | O25-C24-C23 | -2.32 | 115.72      | 123.09   |
| 22  | P     | 307 | CHD  | C1-C10-C5   | 2.32  | 111.07      | 107.75   |
| 14  | N     | 602 | HEA  | CHC-C1C-C2C | -2.32 | 120.70      | 127.43   |
| 22  | C     | 305 | CHD  | C5-C6-C7    | 2.32  | 117.16      | 114.40   |
| 20  | D     | 201 | TGL  | CG3-OG3-CC1 | 2.32  | 125.58      | 117.12   |
| 25  | G     | 101 | CDL  | OB8-CB6-CB4 | 2.31  | 115.05      | 108.40   |
| 20  | L     | 101 | TGL  | CC4-CC3-CC2 | -2.31 | 104.65      | 113.13   |
| 20  | Q     | 201 | TGL  | OG2-CG2-CG1 | 2.31  | 116.62      | 108.34   |
| 24  | C     | 302 | PEK  | C23-C22-C21 | 2.30  | 122.13      | 113.69   |
| 22  | B     | 303 | CHD  | C10-C9-C8   | -2.30 | 109.27      | 111.84   |
| 20  | Q     | 201 | TGL  | C15-CC9-CC8 | 2.30  | 125.99      | 114.37   |
| 22  | C     | 306 | CHD  | C17-C13-C14 | -2.30 | 97.81       | 100.11   |
| 22  | C     | 306 | CHD  | C22-C20-C17 | -2.29 | 105.59      | 110.33   |
| 22  | C     | 305 | CHD  | O12-C12-C11 | 2.29  | 113.77      | 109.12   |
| 20  | Q     | 201 | TGL  | C16-C15-CC9 | 2.29  | 125.92      | 114.37   |
| 27  | Z     | 101 | DMU  | O1-C10-C5   | 2.28  | 115.06      | 110.37   |
| 22  | B     | 303 | CHD  | C19-C10-C1  | -2.28 | 104.68      | 108.31   |
| 27  | Z     | 101 | DMU  | O4-C7-C5    | -2.28 | 105.01      | 110.38   |
| 20  | N     | 609 | TGL  | CG1-OG1-CA1 | 2.27  | 125.43      | 117.12   |
| 19  | N     | 607 | PGV  | O01-C02-C01 | 2.27  | 116.49      | 108.34   |
| 20  | Y     | 101 | TGL  | CG2-OG2-CB1 | 2.27  | 123.23      | 117.80   |
| 22  | J     | 101 | CHD  | C19-C10-C5  | 2.27  | 114.22      | 110.44   |
| 23  | B     | 304 | PSC  | O01-C1-O02  | -2.27 | 118.41      | 123.70   |
| 20  | Q     | 201 | TGL  | C21-C20-CA9 | 2.26  | 125.81      | 114.37   |
| 22  | J     | 101 | CHD  | C15-C14-C13 | 2.26  | 105.74      | 103.54   |
| 22  | B     | 303 | CHD  | O26-C24-C23 | 2.26  | 121.15      | 114.00   |
| 22  | B     | 303 | CHD  | C16-C17-C20 | -2.26 | 108.75      | 112.18   |
| 20  | Y     | 101 | TGL  | CG3-OG3-CC1 | 2.26  | 125.38      | 117.12   |
| 19  | N     | 607 | PGV  | C9-C8-C7    | -2.26 | 102.95      | 114.37   |
| 14  | A     | 601 | HEA  | CMD-C2D-C1D | 2.25  | 128.55      | 125.03   |
| 14  | N     | 601 | HEA  | C4D-C3D-C2D | -2.25 | 103.62      | 106.89   |
| 14  | A     | 601 | HEA  | CHC-C4B-NB  | -2.24 | 121.60      | 124.37   |
| 20  | D     | 201 | TGL  | OG1-CA1-CA2 | 2.24  | 118.66      | 111.83   |
| 25  | C     | 304 | CDL  | C56-C55-C54 | -2.23 | 103.07      | 114.37   |
| 14  | N     | 602 | HEA  | CHD-C1D-ND  | 2.23  | 127.12      | 124.37   |
| 14  | A     | 601 | HEA  | C16-C15-C14 | 2.22  | 126.16      | 121.17   |
| 22  | C     | 305 | CHD  | C6-C5-C10   | 2.22  | 115.03      | 112.66   |
| 22  | P     | 306 | CHD  | C1-C10-C5   | 2.22  | 110.94      | 107.75   |
| 22  | J     | 101 | CHD  | C18-C13-C12 | -2.22 | 106.83      | 109.06   |
| 25  | C     | 304 | CDL  | C39-C38-C37 | 2.22  | 125.59      | 114.37   |
| 14  | A     | 602 | HEA  | CHB-C1B-C2B | 2.22  | 128.53      | 125.03   |
| 20  | L     | 101 | TGL  | CG2-OG2-CB1 | 2.21  | 123.09      | 117.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 305 | CHD  | C16-C17-C20 | 2.21  | 115.52      | 112.18   |
| 25  | T     | 102 | CDL  | C83-C82-C81 | 2.21  | 125.53      | 114.37   |
| 25  | T     | 102 | CDL  | C12-C11-CA5 | -2.21 | 105.61      | 113.69   |
| 19  | A     | 607 | PGV  | O01-C1-C2   | 2.20  | 116.23      | 111.48   |
| 20  | Q     | 201 | TGL  | CG2-OG2-CB1 | 2.19  | 123.04      | 117.80   |
| 25  | T     | 102 | CDL  | CA4-OA6-CA5 | 2.19  | 123.04      | 117.80   |
| 20  | D     | 201 | TGL  | CG1-OG1-CA1 | 2.19  | 125.11      | 117.12   |
| 23  | B     | 304 | PSC  | O03-C19-O04 | -2.18 | 118.18      | 123.63   |
| 14  | A     | 601 | HEA  | CAA-C2A-C1A | -2.17 | 120.44      | 124.85   |
| 25  | T     | 102 | CDL  | C59-C58-C57 | 2.17  | 125.33      | 114.37   |
| 25  | T     | 102 | CDL  | C63-C62-C61 | 2.17  | 125.32      | 114.37   |
| 24  | G     | 102 | PEK  | O01-C02-C01 | 2.17  | 116.11      | 108.34   |
| 20  | B     | 301 | TGL  | OA1-CA1-CA2 | -2.17 | 115.31      | 123.78   |
| 22  | W     | 101 | CHD  | C19-C10-C5  | -2.16 | 106.82      | 110.44   |
| 22  | B     | 303 | CHD  | C11-C12-C13 | -2.16 | 109.06      | 111.26   |
| 22  | C     | 306 | CHD  | C14-C8-C9   | 2.16  | 112.77      | 109.75   |
| 14  | A     | 601 | HEA  | C1C-CHC-C4B | 2.16  | 131.33      | 126.25   |
| 14  | A     | 601 | HEA  | C21-C20-C19 | -2.16 | 106.03      | 113.19   |
| 22  | G     | 103 | CHD  | C6-C5-C10   | -2.16 | 110.36      | 112.66   |
| 22  | G     | 103 | CHD  | C9-C10-C5   | 2.16  | 111.51      | 108.51   |
| 24  | C     | 302 | PEK  | C03-C02-C01 | 2.15  | 116.80      | 111.78   |
| 14  | N     | 602 | HEA  | CHA-C1A-C2A | -2.15 | 121.47      | 124.86   |
| 24  | C     | 307 | PEK  | O03-C21-O04 | -2.14 | 118.27      | 123.63   |
| 22  | J     | 101 | CHD  | C2-C1-C10   | 2.14  | 116.35      | 112.74   |
| 19  | N     | 608 | PGV  | O01-C1-C2   | 2.14  | 116.10      | 111.48   |
| 22  | J     | 101 | CHD  | C5-C6-C7    | -2.14 | 111.86      | 114.40   |
| 24  | P     | 303 | PEK  | O03-C21-O04 | -2.13 | 118.30      | 123.63   |
| 14  | N     | 601 | HEA  | CBC-CAC-C3C | -2.13 | 116.88      | 127.53   |
| 24  | T     | 101 | PEK  | C01-O03-C21 | 2.13  | 124.90      | 117.12   |
| 14  | N     | 602 | HEA  | C2B-C1B-NB  | 2.13  | 112.36      | 109.90   |
| 22  | P     | 307 | CHD  | C23-C22-C20 | -2.13 | 110.49      | 114.46   |
| 14  | N     | 602 | HEA  | C12-C13-C14 | -2.12 | 106.58      | 112.16   |
| 19  | N     | 607 | PGV  | C26-C25-C24 | -2.12 | 103.63      | 114.37   |
| 24  | P     | 308 | PEK  | O03-C01-C02 | 2.12  | 114.51      | 108.40   |
| 27  | Z     | 101 | DMU  | C8-C7-C5    | 2.12  | 114.55      | 110.83   |
| 14  | N     | 602 | HEA  | O2D-CGD-CBD | 2.12  | 120.69      | 114.00   |
| 27  | Z     | 101 | DMU  | O5-C4-C57   | 2.11  | 111.68      | 106.44   |
| 14  | A     | 601 | HEA  | CHB-C4A-C3A | 2.11  | 128.77      | 125.21   |
| 14  | A     | 601 | HEA  | C25-C23-C22 | -2.11 | 116.31      | 122.66   |
| 22  | G     | 103 | CHD  | C15-C14-C8  | 2.11  | 121.25      | 118.36   |
| 19  | P     | 301 | PGV  | O03-C01-C02 | 2.11  | 114.47      | 108.40   |
| 20  | Q     | 201 | TGL  | OG3-CC1-OC1 | -2.11 | 118.36      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 306 | CHD  | C16-C15-C14 | -2.10 | 101.03      | 105.14   |
| 14  | A     | 601 | HEA  | C1D-ND-C4D  | 2.10  | 107.69      | 105.21   |
| 20  | N     | 609 | TGL  | C15-CC9-CC8 | 2.10  | 124.97      | 114.37   |
| 14  | N     | 602 | HEA  | CHB-C4A-NA  | -2.10 | 122.17      | 124.45   |
| 14  | A     | 601 | HEA  | O2A-CGA-CBA | 2.09  | 120.62      | 114.00   |
| 25  | P     | 305 | CDL  | OA4-PA1-OA3 | 2.09  | 122.17      | 112.44   |
| 14  | A     | 601 | HEA  | C12-C11-C3B | 2.09  | 115.38      | 112.12   |
| 20  | D     | 201 | TGL  | C11-C10-CB9 | 2.08  | 124.90      | 114.37   |
| 20  | B     | 301 | TGL  | C16-C15-CC9 | 2.08  | 124.89      | 114.37   |
| 14  | A     | 602 | HEA  | C21-C22-C23 | -2.08 | 120.70      | 127.64   |
| 14  | A     | 601 | HEA  | CMB-C2B-C3B | -2.08 | 126.25      | 130.28   |
| 22  | J     | 101 | CHD  | C17-C13-C14 | -2.08 | 98.03       | 100.11   |
| 14  | N     | 602 | HEA  | C21-C20-C19 | 2.08  | 120.06      | 113.19   |
| 24  | G     | 102 | PEK  | O03-C21-O04 | -2.07 | 118.44      | 123.63   |
| 22  | C     | 305 | CHD  | C11-C9-C8   | 2.07  | 113.96      | 110.89   |
| 14  | A     | 602 | HEA  | C27-C19-C20 | 2.07  | 118.82      | 115.23   |
| 22  | C     | 305 | CHD  | C4-C5-C10   | 2.07  | 114.86      | 112.66   |
| 25  | P     | 305 | CDL  | OB6-CB5-OB7 | -2.07 | 118.87      | 123.70   |
| 19  | P     | 304 | PGV  | C04-C05-C06 | -2.07 | 104.81      | 111.77   |
| 19  | A     | 607 | PGV  | C02-O01-C1  | 2.06  | 122.73      | 117.80   |
| 25  | T     | 102 | CDL  | C62-C61-C60 | 2.06  | 124.80      | 114.37   |
| 14  | A     | 601 | HEA  | C4C-NC-C1C  | 2.06  | 109.18      | 105.82   |
| 14  | N     | 602 | HEA  | CHD-C1D-C2D | -2.06 | 121.09      | 126.95   |
| 27  | Z     | 101 | DMU  | C10-O7-C3   | -2.06 | 113.10      | 117.98   |
| 22  | P     | 307 | CHD  | C1-C2-C3    | -2.06 | 107.76      | 110.48   |
| 20  | L     | 101 | TGL  | C29-C14-C13 | -2.06 | 103.98      | 114.37   |
| 20  | L     | 101 | TGL  | C16-C15-CC9 | 2.05  | 124.72      | 114.37   |
| 25  | P     | 305 | CDL  | OA8-CA7-OA9 | -2.05 | 118.51      | 123.63   |
| 20  | L     | 101 | TGL  | OG2-CG2-CG1 | 2.04  | 115.67      | 108.34   |
| 25  | C     | 304 | CDL  | OB6-CB5-OB7 | -2.04 | 118.95      | 123.70   |
| 14  | A     | 601 | HEA  | CHA-C1A-C2A | 2.03  | 128.07      | 124.86   |
| 27  | M     | 101 | DMU  | O5-C6-O16   | -2.03 | 105.25      | 110.04   |
| 24  | G     | 102 | PEK  | C01-O03-C21 | 2.03  | 124.54      | 117.12   |
| 19  | C     | 308 | PGV  | O04-C19-C20 | -2.03 | 115.84      | 123.78   |
| 25  | C     | 304 | CDL  | CA6-OA8-CA7 | 2.03  | 124.53      | 117.12   |
| 20  | L     | 101 | TGL  | CA9-CA8-CA7 | -2.03 | 104.12      | 114.37   |
| 24  | P     | 303 | PEK  | O12-P-O14   | 2.03  | 116.97      | 108.94   |
| 14  | N     | 602 | HEA  | O1A-CGA-CBA | -2.03 | 116.67      | 123.09   |
| 14  | N     | 602 | HEA  | CHB-C1B-NB  | 2.02  | 126.59      | 124.42   |
| 14  | N     | 602 | HEA  | C13-C14-C15 | -2.01 | 123.02      | 127.62   |
| 19  | N     | 608 | PGV  | O14-P-O11   | 2.00  | 116.63      | 107.57   |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 27  | M     | 101 | DMU  | C5   |
| 27  | M     | 101 | DMU  | C9   |
| 27  | Z     | 101 | DMU  | C5   |
| 27  | Z     | 101 | DMU  | C9   |

All (959) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 608 | PGV  | C04-O12-P-O11   |
| 19  | A     | 608 | PGV  | C04-O12-P-O13   |
| 19  | A     | 608 | PGV  | C04-O12-P-O14   |
| 19  | A     | 608 | PGV  | C02-C03-O11-P   |
| 19  | A     | 608 | PGV  | C05-C04-O12-P   |
| 19  | A     | 608 | PGV  | C2-C1-O01-C02   |
| 19  | A     | 608 | PGV  | O04-C19-O03-C01 |
| 19  | A     | 608 | PGV  | C20-C19-O03-C01 |
| 19  | C     | 308 | PGV  | C03-O11-P-O12   |
| 19  | C     | 308 | PGV  | C03-O11-P-O13   |
| 19  | N     | 607 | PGV  | O12-C04-C05-C06 |
| 19  | N     | 607 | PGV  | O02-C1-O01-C02  |
| 19  | N     | 607 | PGV  | C2-C1-O01-C02   |
| 19  | P     | 301 | PGV  | C03-O11-P-O12   |
| 19  | P     | 301 | PGV  | C03-O11-P-O13   |
| 19  | P     | 301 | PGV  | C03-O11-P-O14   |
| 19  | P     | 301 | PGV  | C04-O12-P-O11   |
| 19  | P     | 301 | PGV  | C04-O12-P-O14   |
| 19  | P     | 301 | PGV  | O01-C02-C03-O11 |
| 19  | P     | 301 | PGV  | C02-C03-O11-P   |
| 20  | D     | 201 | TGL  | OG1-CG1-CG2-OG2 |
| 20  | L     | 101 | TGL  | CB2-CB1-OG2-CG2 |
| 20  | Q     | 201 | TGL  | CC2-CC1-OG3-CG3 |
| 20  | Q     | 201 | TGL  | OC1-CC1-OG3-CG3 |
| 20  | Y     | 101 | TGL  | CB2-CB1-OG2-CG2 |
| 22  | J     | 101 | CHD  | C13-C17-C20-C21 |
| 22  | J     | 101 | CHD  | C13-C17-C20-C22 |
| 22  | J     | 101 | CHD  | C16-C17-C20-C21 |
| 22  | W     | 101 | CHD  | C13-C17-C20-C22 |
| 22  | W     | 101 | CHD  | C16-C17-C20-C21 |
| 22  | W     | 101 | CHD  | C16-C17-C20-C22 |
| 23  | B     | 304 | PSC  | C03-O11-P-O12   |
| 23  | B     | 304 | PSC  | C03-O11-P-O13   |
| 23  | B     | 304 | PSC  | C04-O12-P-O11   |
| 23  | B     | 304 | PSC  | C04-O12-P-O13   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | B     | 304 | PSC  | C04-O12-P-O14   |
| 23  | N     | 610 | PSC  | C03-O11-P-O12   |
| 23  | N     | 610 | PSC  | C03-O11-P-O13   |
| 23  | N     | 610 | PSC  | C2-C1-O01-C02   |
| 23  | N     | 610 | PSC  | O04-C19-O03-C01 |
| 23  | N     | 610 | PSC  | C20-C19-O03-C01 |
| 24  | C     | 302 | PEK  | C5-C6-C7-C8     |
| 24  | C     | 307 | PEK  | C04-O12-P-O11   |
| 24  | C     | 307 | PEK  | O03-C01-C02-O01 |
| 24  | C     | 307 | PEK  | O12-C04-C05-N   |
| 24  | G     | 102 | PEK  | O12-C04-C05-N   |
| 24  | G     | 102 | PEK  | C2-C1-O01-C02   |
| 24  | G     | 102 | PEK  | C9-C10-C11-C12  |
| 24  | P     | 308 | PEK  | C03-O11-P-O12   |
| 24  | P     | 308 | PEK  | C03-O11-P-O13   |
| 24  | P     | 308 | PEK  | C03-O11-P-O14   |
| 24  | P     | 308 | PEK  | C04-O12-P-O11   |
| 24  | P     | 308 | PEK  | O12-C04-C05-N   |
| 24  | T     | 101 | PEK  | C03-O11-P-O12   |
| 24  | T     | 101 | PEK  | C03-O11-P-O13   |
| 24  | T     | 101 | PEK  | O12-C04-C05-N   |
| 24  | T     | 101 | PEK  | C11-C12-C13-C14 |
| 25  | C     | 304 | CDL  | CA2-OA2-PA1-OA4 |
| 25  | C     | 304 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | C     | 304 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | C     | 304 | CDL  | CA3-OA5-PA1-OA3 |
| 25  | C     | 304 | CDL  | CA4-CA3-OA5-PA1 |
| 25  | C     | 304 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | C     | 304 | CDL  | C11-CA5-OA6-CA4 |
| 25  | C     | 304 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | G     | 101 | CDL  | O1-C1-CA2-OA2   |
| 25  | G     | 101 | CDL  | CB2-C1-CA2-OA2  |
| 25  | G     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 25  | G     | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | G     | 101 | CDL  | CA3-OA5-PA1-OA4 |
| 25  | G     | 101 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | G     | 101 | CDL  | C11-CA5-OA6-CA4 |
| 25  | G     | 101 | CDL  | C31-CA7-OA8-CA6 |
| 25  | G     | 101 | CDL  | C1-CB2-OB2-PB2  |
| 25  | G     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | G     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | G     | 101 | CDL  | CB3-OB5-PB2-OB2 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | G     | 101 | CDL  | CB3-OB5-PB2-OB3 |
| 25  | G     | 101 | CDL  | C51-CB5-OB6-CB4 |
| 25  | P     | 305 | CDL  | CA2-OA2-PA1-OA4 |
| 25  | P     | 305 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | P     | 305 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | P     | 305 | CDL  | CA3-OA5-PA1-OA3 |
| 25  | P     | 305 | CDL  | C11-CA5-OA6-CA4 |
| 25  | P     | 305 | CDL  | CB2-OB2-PB2-OB3 |
| 25  | P     | 305 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | P     | 305 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | P     | 305 | CDL  | CB3-OB5-PB2-OB3 |
| 25  | P     | 305 | CDL  | CB3-OB5-PB2-OB4 |
| 25  | P     | 305 | CDL  | OB7-CB5-OB6-CB4 |
| 25  | P     | 305 | CDL  | C51-CB5-OB6-CB4 |
| 25  | T     | 102 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | T     | 102 | CDL  | CA3-OA5-PA1-OA3 |
| 25  | T     | 102 | CDL  | CA3-OA5-PA1-OA4 |
| 25  | T     | 102 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | T     | 102 | CDL  | OA9-CA7-OA8-CA6 |
| 25  | T     | 102 | CDL  | C31-CA7-OA8-CA6 |
| 25  | T     | 102 | CDL  | C1-CB2-OB2-PB2  |
| 25  | T     | 102 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | T     | 102 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | T     | 102 | CDL  | CB3-OB5-PB2-OB3 |
| 25  | G     | 101 | CDL  | OA9-CA7-OA8-CA6 |
| 19  | N     | 607 | PGV  | O04-C19-O03-C01 |
| 20  | D     | 201 | TGL  | OC1-CC1-OG3-CG3 |
| 20  | L     | 101 | TGL  | OB1-CB1-OG2-CG2 |
| 20  | Y     | 101 | TGL  | OB1-CB1-OG2-CG2 |
| 24  | G     | 102 | PEK  | O02-C1-O01-C02  |
| 25  | G     | 101 | CDL  | OB7-CB5-OB6-CB4 |
| 25  | P     | 305 | CDL  | OA7-CA5-OA6-CA4 |
| 19  | N     | 607 | PGV  | C20-C19-O03-C01 |
| 20  | D     | 201 | TGL  | CC2-CC1-OG3-CG3 |
| 20  | L     | 101 | TGL  | CA2-CA1-OG1-CG1 |
| 23  | B     | 304 | PSC  | C20-C19-O03-C01 |
| 25  | T     | 102 | CDL  | C11-CA5-OA6-CA4 |
| 14  | A     | 601 | HEA  | C27-C19-C20-C21 |
| 14  | A     | 601 | HEA  | C18-C19-C20-C21 |
| 25  | C     | 304 | CDL  | C31-CA7-OA8-CA6 |
| 19  | C     | 303 | PGV  | C10-C11-C12-C13 |
| 19  | P     | 301 | PGV  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | N     | 610 | PSC  | C11-C12-C13-C14 |
| 24  | C     | 307 | PEK  | C4-C5-C6-C7     |
| 24  | P     | 308 | PEK  | C10-C11-C12-C13 |
| 20  | L     | 101 | TGL  | OA1-CA1-OG1-CG1 |
| 20  | N     | 609 | TGL  | OC1-CC1-OG3-CG3 |
| 25  | C     | 304 | CDL  | OA9-CA7-OA8-CA6 |
| 19  | A     | 608 | PGV  | O02-C1-O01-C02  |
| 23  | N     | 610 | PSC  | O02-C1-O01-C02  |
| 22  | J     | 101 | CHD  | C16-C17-C20-C22 |
| 19  | N     | 607 | PGV  | O12-C04-C05-O05 |
| 23  | B     | 304 | PSC  | O04-C19-O03-C01 |
| 27  | M     | 101 | DMU  | O6-C11-C9-C8    |
| 27  | Z     | 101 | DMU  | O6-C11-C9-O1    |
| 22  | C     | 305 | CHD  | C17-C20-C22-C23 |
| 20  | N     | 609 | TGL  | CC2-CC1-OG3-CG3 |
| 14  | N     | 601 | HEA  | C19-C20-C21-C22 |
| 25  | P     | 305 | CDL  | C19-C20-C21-C22 |
| 25  | G     | 101 | CDL  | C58-C59-C60-C61 |
| 24  | C     | 302 | PEK  | C10-C11-C12-C13 |
| 24  | C     | 307 | PEK  | C10-C11-C12-C13 |
| 24  | C     | 307 | PEK  | C13-C14-C15-C16 |
| 24  | P     | 303 | PEK  | C13-C14-C15-C16 |
| 24  | P     | 308 | PEK  | C13-C14-C15-C16 |
| 24  | T     | 101 | PEK  | C7-C8-C9-C10    |
| 25  | P     | 305 | CDL  | C53-C54-C55-C56 |
| 19  | C     | 308 | PGV  | O12-C04-C05-C06 |
| 25  | C     | 304 | CDL  | CB2-C1-CA2-OA2  |
| 25  | G     | 101 | CDL  | CA2-C1-CB2-OB2  |
| 25  | P     | 305 | CDL  | CB2-C1-CA2-OA2  |
| 25  | P     | 305 | CDL  | CA2-C1-CB2-OB2  |
| 25  | G     | 101 | CDL  | C71-CB7-OB8-CB6 |
| 25  | T     | 102 | CDL  | C71-CB7-OB8-CB6 |
| 19  | A     | 607 | PGV  | C26-C27-C28-C29 |
| 24  | P     | 308 | PEK  | C33-C34-C35-C36 |
| 25  | C     | 304 | CDL  | C80-C81-C82-C83 |
| 20  | D     | 201 | TGL  | C20-C21-C22-C23 |
| 20  | Y     | 101 | TGL  | C20-C21-C22-C23 |
| 19  | C     | 308 | PGV  | C20-C21-C22-C23 |
| 27  | Z     | 101 | DMU  | O6-C11-C9-C8    |
| 23  | N     | 610 | PSC  | C20-C21-C22-C23 |
| 19  | C     | 308 | PGV  | O12-C04-C05-O05 |
| 25  | C     | 304 | CDL  | O1-C1-CA2-OA2   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | B     | 304 | PSC  | C22-C23-C24-C25 |
| 25  | P     | 305 | CDL  | CB5-C51-C52-C53 |
| 22  | P     | 306 | CHD  | C17-C20-C22-C23 |
| 25  | G     | 101 | CDL  | CA5-C11-C12-C13 |
| 24  | P     | 303 | PEK  | C4-C5-C6-C7     |
| 19  | C     | 308 | PGV  | O05-C05-C06-O06 |
| 24  | G     | 102 | PEK  | C33-C34-C35-C36 |
| 20  | B     | 301 | TGL  | OB1-CB1-OG2-CG2 |
| 20  | Q     | 201 | TGL  | C16-C15-CC9-CC8 |
| 25  | G     | 101 | CDL  | C60-C61-C62-C63 |
| 19  | N     | 607 | PGV  | C19-C20-C21-C22 |
| 20  | D     | 201 | TGL  | CB1-CB2-CB3-CB4 |
| 20  | Y     | 101 | TGL  | CA1-CA2-CA3-CA4 |
| 20  | Y     | 101 | TGL  | CB1-CB2-CB3-CB4 |
| 24  | C     | 307 | PEK  | C1-C2-C3-C4     |
| 24  | G     | 102 | PEK  | C21-C22-C23-C24 |
| 24  | T     | 101 | PEK  | C1-C2-C3-C4     |
| 25  | T     | 102 | CDL  | CB5-C51-C52-C53 |
| 25  | T     | 102 | CDL  | CB7-C71-C72-C73 |
| 25  | T     | 102 | CDL  | OB9-CB7-OB8-CB6 |
| 20  | B     | 301 | TGL  | CC2-CC1-OG3-CG3 |
| 22  | C     | 305 | CHD  | C20-C22-C23-C24 |
| 25  | T     | 102 | CDL  | C79-C80-C81-C82 |
| 22  | C     | 305 | CHD  | C21-C20-C22-C23 |
| 19  | C     | 308 | PGV  | C1-C2-C3-C4     |
| 20  | B     | 301 | TGL  | CB1-CB2-CB3-CB4 |
| 24  | P     | 303 | PEK  | C1-C2-C3-C4     |
| 25  | T     | 102 | CDL  | CA7-C31-C32-C33 |
| 19  | N     | 607 | PGV  | C02-C01-O03-C19 |
| 23  | N     | 610 | PSC  | C22-C23-C24-C25 |
| 25  | G     | 101 | CDL  | O1-C1-CB2-OB2   |
| 25  | P     | 305 | CDL  | O1-C1-CA2-OA2   |
| 25  | P     | 305 | CDL  | O1-C1-CB2-OB2   |
| 25  | T     | 102 | CDL  | O1-C1-CB2-OB2   |
| 20  | B     | 301 | TGL  | OC1-CC1-OG3-CG3 |
| 22  | P     | 306 | CHD  | C21-C20-C22-C23 |
| 23  | B     | 304 | PSC  | C11-C12-C13-C14 |
| 24  | C     | 307 | PEK  | C7-C8-C9-C10    |
| 24  | G     | 102 | PEK  | C10-C11-C12-C13 |
| 25  | G     | 101 | CDL  | OB9-CB7-OB8-CB6 |
| 22  | W     | 101 | CHD  | C13-C17-C20-C21 |
| 25  | C     | 304 | CDL  | C61-C62-C63-C64 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | T     | 102 | CDL  | CA2-C1-CB2-OB2  |
| 19  | C     | 303 | PGV  | C24-C25-C26-C27 |
| 20  | Q     | 201 | TGL  | CB1-CB2-CB3-CB4 |
| 27  | Z     | 101 | DMU  | O16-C18-C19-C22 |
| 24  | C     | 307 | PEK  | C22-C21-O03-C01 |
| 20  | B     | 301 | TGL  | CB2-CB1-OG2-CG2 |
| 23  | B     | 304 | PSC  | C2-C1-O01-C02   |
| 25  | C     | 304 | CDL  | C51-CB5-OB6-CB4 |
| 23  | B     | 304 | PSC  | O02-C1-O01-C02  |
| 24  | G     | 102 | PEK  | C7-C8-C9-C10    |
| 24  | P     | 308 | PEK  | C7-C8-C9-C10    |
| 24  | C     | 307 | PEK  | C24-C25-C26-C27 |
| 25  | C     | 304 | CDL  | O1-C1-CB2-OB2   |
| 19  | C     | 308 | PGV  | C04-C05-C06-O06 |
| 24  | P     | 308 | PEK  | C1-C2-C3-C4     |
| 19  | A     | 608 | PGV  | C03-C02-O01-C1  |
| 20  | D     | 201 | TGL  | CG3-CG2-OG2-CB1 |
| 20  | Q     | 201 | TGL  | CG3-CG2-OG2-CB1 |
| 23  | N     | 610 | PSC  | C01-C02-O01-C1  |
| 24  | C     | 307 | PEK  | C2-C3-C4-C5     |
| 20  | N     | 609 | TGL  | OB1-CB1-OG2-CG2 |
| 19  | P     | 301 | PGV  | C2-C1-O01-C02   |
| 19  | P     | 301 | PGV  | C20-C19-O03-C01 |
| 20  | L     | 101 | TGL  | CB1-CB2-CB3-CB4 |
| 24  | C     | 307 | PEK  | O04-C21-O03-C01 |
| 19  | N     | 607 | PGV  | C4-C5-C6-C7     |
| 20  | B     | 301 | TGL  | C10-C11-C12-C13 |
| 20  | L     | 101 | TGL  | CB4-CB5-CB6-CB7 |
| 20  | N     | 609 | TGL  | CC2-CC3-CC4-CC5 |
| 20  | Q     | 201 | TGL  | CA6-CA7-CA8-CA9 |
| 20  | Q     | 201 | TGL  | CB5-CB6-CB7-CB8 |
| 23  | B     | 304 | PSC  | C29-C30-C31-C32 |
| 24  | P     | 303 | PEK  | C16-C17-C18-C19 |
| 19  | C     | 303 | PGV  | C13-C14-C15-C16 |
| 19  | P     | 301 | PGV  | C24-C25-C26-C27 |
| 20  | D     | 201 | TGL  | CC7-CC8-CC9-C15 |
| 20  | L     | 101 | TGL  | C11-C10-CB9-CB8 |
| 20  | L     | 101 | TGL  | C21-C22-C23-C24 |
| 20  | Y     | 101 | TGL  | CA7-CA8-CA9-C20 |
| 20  | Y     | 101 | TGL  | CB6-CB7-CB8-CB9 |
| 25  | C     | 304 | CDL  | C23-C24-C25-C26 |
| 25  | C     | 304 | CDL  | C59-C60-C61-C62 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | G     | 101 | CDL  | C23-C24-C25-C26 |
| 25  | G     | 101 | CDL  | C36-C37-C38-C39 |
| 25  | G     | 101 | CDL  | C37-C38-C39-C40 |
| 25  | P     | 305 | CDL  | C74-C75-C76-C77 |
| 19  | A     | 608 | PGV  | C10-C11-C12-C13 |
| 24  | T     | 101 | PEK  | C13-C14-C15-C16 |
| 20  | B     | 301 | TGL  | C16-C15-CC9-CC8 |
| 20  | Y     | 101 | TGL  | C18-C19-C33-C34 |
| 25  | G     | 101 | CDL  | C16-C17-C18-C19 |
| 25  | G     | 101 | CDL  | C63-C64-C65-C66 |
| 25  | P     | 305 | CDL  | C22-C23-C24-C25 |
| 25  | P     | 305 | CDL  | C72-C73-C74-C75 |
| 25  | T     | 102 | CDL  | C76-C77-C78-C79 |
| 20  | L     | 101 | TGL  | CB3-CB4-CB5-CB6 |
| 20  | L     | 101 | TGL  | CC5-CC6-CC7-CC8 |
| 20  | N     | 609 | TGL  | CB6-CB7-CB8-CB9 |
| 20  | N     | 609 | TGL  | C12-C13-C14-C29 |
| 20  | N     | 609 | TGL  | C15-C16-C17-C18 |
| 25  | C     | 304 | CDL  | C72-C73-C74-C75 |
| 25  | C     | 304 | CDL  | C79-C80-C81-C82 |
| 25  | G     | 101 | CDL  | C20-C21-C22-C23 |
| 27  | M     | 101 | DMU  | C19-C22-C25-C28 |
| 20  | D     | 201 | TGL  | CB9-C10-C11-C12 |
| 20  | N     | 609 | TGL  | CC5-CC6-CC7-CC8 |
| 24  | C     | 302 | PEK  | C32-C33-C34-C35 |
| 24  | G     | 102 | PEK  | C34-C35-C36-C37 |
| 25  | T     | 102 | CDL  | C75-C76-C77-C78 |
| 19  | C     | 303 | PGV  | C27-C28-C29-C30 |
| 25  | P     | 305 | CDL  | C16-C17-C18-C19 |
| 25  | T     | 102 | CDL  | C72-C73-C74-C75 |
| 24  | P     | 303 | PEK  | C31-C32-C33-C34 |
| 25  | G     | 101 | CDL  | C76-C77-C78-C79 |
| 24  | C     | 307 | PEK  | C2-C1-O01-C02   |
| 24  | T     | 101 | PEK  | C27-C28-C29-C30 |
| 19  | N     | 608 | PGV  | C23-C24-C25-C26 |
| 19  | P     | 301 | PGV  | C26-C27-C28-C29 |
| 20  | B     | 301 | TGL  | C11-C12-C13-C14 |
| 20  | N     | 609 | TGL  | CB5-CB6-CB7-CB8 |
| 20  | Q     | 201 | TGL  | CC5-CC6-CC7-CC8 |
| 24  | P     | 303 | PEK  | C28-C29-C30-C31 |
| 25  | C     | 304 | CDL  | C36-C37-C38-C39 |
| 25  | C     | 304 | CDL  | C78-C79-C80-C81 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | N     | 609 | TGL  | CC4-CC5-CC6-CC7 |
| 20  | N     | 609 | TGL  | C16-C15-CC9-CC8 |
| 27  | Z     | 101 | DMU  | C22-C25-C28-C31 |
| 20  | D     | 201 | TGL  | C11-C12-C13-C14 |
| 19  | A     | 608 | PGV  | C14-C15-C16-C17 |
| 19  | C     | 308 | PGV  | C30-C31-C32-C33 |
| 19  | N     | 607 | PGV  | C14-C15-C16-C17 |
| 25  | C     | 304 | CDL  | C60-C61-C62-C63 |
| 25  | C     | 304 | CDL  | C82-C83-C84-C85 |
| 24  | G     | 102 | PEK  | C22-C21-O03-C01 |
| 19  | A     | 608 | PGV  | C7-C8-C9-C10    |
| 19  | N     | 608 | PGV  | C13-C14-C15-C16 |
| 19  | P     | 301 | PGV  | C30-C31-C32-C33 |
| 20  | B     | 301 | TGL  | CA6-CA7-CA8-CA9 |
| 20  | B     | 301 | TGL  | C22-C23-C24-C25 |
| 20  | N     | 609 | TGL  | CA4-CA5-CA6-CA7 |
| 23  | B     | 304 | PSC  | C28-C29-C30-C31 |
| 24  | G     | 102 | PEK  | C23-C24-C25-C26 |
| 25  | G     | 101 | CDL  | C77-C78-C79-C80 |
| 25  | G     | 101 | CDL  | C80-C81-C82-C83 |
| 19  | A     | 608 | PGV  | C20-C21-C22-C23 |
| 19  | N     | 607 | PGV  | C25-C26-C27-C28 |
| 19  | P     | 304 | PGV  | C30-C31-C32-C33 |
| 20  | D     | 201 | TGL  | CA3-CA4-CA5-CA6 |
| 23  | B     | 304 | PSC  | C30-C31-C32-C33 |
| 25  | T     | 102 | CDL  | C11-C12-C13-C14 |
| 27  | M     | 101 | DMU  | C22-C25-C28-C31 |
| 19  | N     | 608 | PGV  | C27-C28-C29-C30 |
| 19  | P     | 301 | PGV  | C4-C5-C6-C7     |
| 20  | B     | 301 | TGL  | C16-C17-C18-C19 |
| 20  | N     | 609 | TGL  | C10-C11-C12-C13 |
| 20  | Q     | 201 | TGL  | C21-C20-CA9-CA8 |
| 24  | T     | 101 | PEK  | C32-C33-C34-C35 |
| 25  | C     | 304 | CDL  | C53-C54-C55-C56 |
| 25  | C     | 304 | CDL  | C63-C64-C65-C66 |
| 25  | G     | 101 | CDL  | C82-C83-C84-C85 |
| 25  | P     | 305 | CDL  | C37-C38-C39-C40 |
| 19  | N     | 607 | PGV  | C28-C29-C30-C31 |
| 20  | N     | 609 | TGL  | CA5-CA6-CA7-CA8 |
| 23  | N     | 610 | PSC  | C3-C4-C5-C6     |
| 19  | P     | 301 | PGV  | C20-C21-C22-C23 |
| 20  | D     | 201 | TGL  | C14-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | N     | 609 | TGL  | CB4-CB5-CB6-CB7 |
| 20  | Q     | 201 | TGL  | CC6-CC7-CC8-CC9 |
| 24  | P     | 308 | PEK  | C28-C29-C30-C31 |
| 25  | G     | 101 | CDL  | C73-C74-C75-C76 |
| 25  | T     | 102 | CDL  | C31-C32-C33-C34 |
| 19  | P     | 304 | PGV  | C1-C2-C3-C4     |
| 23  | B     | 304 | PSC  | C19-C20-C21-C22 |
| 20  | Q     | 201 | TGL  | C21-C22-C23-C24 |
| 19  | A     | 608 | PGV  | C11-C10-C9-C8   |
| 19  | C     | 303 | PGV  | C12-C13-C14-C15 |
| 19  | N     | 608 | PGV  | C11-C10-C9-C8   |
| 24  | P     | 303 | PEK  | C2-C3-C4-C5     |
| 24  | G     | 102 | PEK  | C4-C5-C6-C7     |
| 19  | N     | 607 | PGV  | C20-C21-C22-C23 |
| 20  | B     | 301 | TGL  | C12-C13-C14-C29 |
| 23  | B     | 304 | PSC  | C27-C28-C29-C30 |
| 25  | T     | 102 | CDL  | C73-C74-C75-C76 |
| 19  | C     | 308 | PGV  | C2-C3-C4-C5     |
| 25  | G     | 101 | CDL  | C79-C80-C81-C82 |
| 19  | C     | 308 | PGV  | C14-C15-C16-C17 |
| 20  | Q     | 201 | TGL  | CB9-C10-C11-C12 |
| 24  | G     | 102 | PEK  | C26-C27-C28-C29 |
| 19  | P     | 301 | PGV  | C22-C23-C24-C25 |
| 23  | N     | 610 | PSC  | C2-C3-C4-C5     |
| 24  | C     | 302 | PEK  | C23-C24-C25-C26 |
| 24  | C     | 307 | PEK  | C28-C29-C30-C31 |
| 19  | P     | 301 | PGV  | O02-C1-O01-C02  |
| 24  | C     | 307 | PEK  | O02-C1-O01-C02  |
| 25  | C     | 304 | CDL  | OB7-CB5-OB6-CB4 |
| 25  | C     | 304 | CDL  | C20-C21-C22-C23 |
| 25  | T     | 102 | CDL  | C20-C21-C22-C23 |
| 25  | T     | 102 | CDL  | C62-C63-C64-C65 |
| 20  | B     | 301 | TGL  | CB4-CB5-CB6-CB7 |
| 20  | D     | 201 | TGL  | CA7-CA8-CA9-C20 |
| 20  | Q     | 201 | TGL  | C23-C24-C25-C26 |
| 25  | T     | 102 | CDL  | C54-C55-C56-C57 |
| 25  | T     | 102 | CDL  | C55-C56-C57-C58 |
| 19  | C     | 308 | PGV  | C26-C27-C28-C29 |
| 20  | B     | 301 | TGL  | CA5-CA6-CA7-CA8 |
| 20  | D     | 201 | TGL  | C13-C14-C29-C30 |
| 20  | D     | 201 | TGL  | C18-C19-C33-C34 |
| 23  | B     | 304 | PSC  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | P     | 308 | PEK  | C32-C33-C34-C35 |
| 25  | G     | 101 | CDL  | C83-C84-C85-C86 |
| 20  | L     | 101 | TGL  | C10-C11-C12-C13 |
| 24  | C     | 302 | PEK  | C28-C29-C30-C31 |
| 25  | P     | 305 | CDL  | C59-C60-C61-C62 |
| 19  | A     | 608 | PGV  | C24-C25-C26-C27 |
| 20  | B     | 301 | TGL  | C17-C18-C19-C33 |
| 20  | Y     | 101 | TGL  | C19-C33-C34-C35 |
| 19  | C     | 303 | PGV  | C26-C27-C28-C29 |
| 20  | L     | 101 | TGL  | CA3-CA4-CA5-CA6 |
| 24  | C     | 302 | PEK  | C16-C17-C18-C19 |
| 24  | P     | 308 | PEK  | C26-C27-C28-C29 |
| 25  | T     | 102 | CDL  | C13-C14-C15-C16 |
| 20  | L     | 101 | TGL  | CB2-CB3-CB4-CB5 |
| 20  | N     | 609 | TGL  | C21-C20-CA9-CA8 |
| 20  | Y     | 101 | TGL  | CB3-CB4-CB5-CB6 |
| 24  | C     | 307 | PEK  | C22-C23-C24-C25 |
| 25  | C     | 304 | CDL  | C57-C58-C59-C60 |
| 25  | G     | 101 | CDL  | C33-C34-C35-C36 |
| 20  | L     | 101 | TGL  | C16-C15-CC9-CC8 |
| 20  | Y     | 101 | TGL  | C10-C11-C12-C13 |
| 20  | Y     | 101 | TGL  | C22-C23-C24-C25 |
| 23  | N     | 610 | PSC  | C29-C30-C31-C32 |
| 25  | G     | 101 | CDL  | C31-C32-C33-C34 |
| 20  | N     | 609 | TGL  | CB2-CB1-OG2-CG2 |
| 25  | C     | 304 | CDL  | C51-C52-C53-C54 |
| 25  | C     | 304 | CDL  | C38-C39-C40-C41 |
| 24  | G     | 102 | PEK  | O04-C21-O03-C01 |
| 20  | L     | 101 | TGL  | C21-C20-CA9-CA8 |
| 20  | N     | 609 | TGL  | CB7-CB8-CB9-C10 |
| 25  | C     | 304 | CDL  | C74-C75-C76-C77 |
| 20  | N     | 609 | TGL  | C14-C29-C30-C31 |
| 20  | Y     | 101 | TGL  | CA9-C20-C21-C22 |
| 19  | C     | 308 | PGV  | C5-C6-C7-C8     |
| 25  | T     | 102 | CDL  | C57-C58-C59-C60 |
| 24  | P     | 303 | PEK  | C26-C27-C28-C29 |
| 25  | T     | 102 | CDL  | C59-C60-C61-C62 |
| 19  | N     | 607 | PGV  | C7-C8-C9-C10    |
| 19  | P     | 301 | PGV  | O04-C19-O03-C01 |
| 25  | P     | 305 | CDL  | C14-C15-C16-C17 |
| 25  | G     | 101 | CDL  | C81-C82-C83-C84 |
| 20  | Y     | 101 | TGL  | CC3-CC4-CC5-CC6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | P     | 303 | PEK  | C2-C1-O01-C02   |
| 20  | Q     | 201 | TGL  | C19-C33-C34-C35 |
| 20  | B     | 301 | TGL  | CC4-CC5-CC6-CC7 |
| 20  | Q     | 201 | TGL  | C12-C13-C14-C29 |
| 24  | C     | 307 | PEK  | C16-C17-C18-C19 |
| 25  | T     | 102 | CDL  | C42-C43-C44-C45 |
| 20  | Q     | 201 | TGL  | OG1-CG1-CG2-OG2 |
| 24  | G     | 102 | PEK  | O03-C01-C02-O01 |
| 24  | G     | 102 | PEK  | C15-C16-C17-C18 |
| 24  | P     | 308 | PEK  | O03-C01-C02-O01 |
| 25  | C     | 304 | CDL  | OA6-CA4-CA6-OA8 |
| 25  | G     | 101 | CDL  | OA6-CA4-CA6-OA8 |
| 19  | P     | 301 | PGV  | C5-C6-C7-C8     |
| 20  | Q     | 201 | TGL  | C16-C17-C18-C19 |
| 20  | Y     | 101 | TGL  | CA4-CA5-CA6-CA7 |
| 25  | P     | 305 | CDL  | C36-C37-C38-C39 |
| 25  | P     | 305 | CDL  | C40-C41-C42-C43 |
| 24  | T     | 101 | PEK  | C22-C21-O03-C01 |
| 19  | P     | 304 | PGV  | C24-C25-C26-C27 |
| 25  | P     | 305 | CDL  | C35-C36-C37-C38 |
| 19  | N     | 607 | PGV  | C13-C14-C15-C16 |
| 24  | P     | 308 | PEK  | C29-C30-C31-C32 |
| 25  | T     | 102 | CDL  | C41-C42-C43-C44 |
| 19  | P     | 301 | PGV  | C29-C30-C31-C32 |
| 20  | B     | 301 | TGL  | C20-C21-C22-C23 |
| 20  | N     | 609 | TGL  | C23-C24-C25-C26 |
| 25  | C     | 304 | CDL  | C58-C59-C60-C61 |
| 25  | G     | 101 | CDL  | C14-C15-C16-C17 |
| 20  | Q     | 201 | TGL  | CC2-CC3-CC4-CC5 |
| 25  | C     | 304 | CDL  | C41-C42-C43-C44 |
| 25  | P     | 305 | CDL  | C79-C80-C81-C82 |
| 19  | C     | 308 | PGV  | C24-C25-C26-C27 |
| 23  | B     | 304 | PSC  | C26-C27-C28-C29 |
| 25  | P     | 305 | CDL  | C41-C42-C43-C44 |
| 20  | L     | 101 | TGL  | C18-C19-C33-C34 |
| 24  | C     | 307 | PEK  | C33-C34-C35-C36 |
| 20  | D     | 201 | TGL  | CC5-CC6-CC7-CC8 |
| 25  | G     | 101 | CDL  | C38-C39-C40-C41 |
| 19  | P     | 301 | PGV  | C1-C2-C3-C4     |
| 19  | N     | 607 | PGV  | C29-C30-C31-C32 |
| 20  | N     | 609 | TGL  | CA3-CA4-CA5-CA6 |
| 25  | P     | 305 | CDL  | C42-C43-C44-C45 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 608 | PGV  | C4-C5-C6-C7     |
| 20  | D     | 201 | TGL  | CC6-CC7-CC8-CC9 |
| 20  | L     | 101 | TGL  | C24-C25-C26-C27 |
| 19  | P     | 301 | PGV  | C13-C14-C15-C16 |
| 20  | D     | 201 | TGL  | C19-C33-C34-C35 |
| 24  | C     | 307 | PEK  | C32-C33-C34-C35 |
| 25  | C     | 304 | CDL  | C17-C18-C19-C20 |
| 19  | P     | 301 | PGV  | C11-C10-C9-C8   |
| 19  | P     | 304 | PGV  | C11-C10-C9-C8   |
| 24  | C     | 302 | PEK  | C15-C16-C17-C18 |
| 20  | B     | 301 | TGL  | CA4-CA5-CA6-CA7 |
| 20  | Y     | 101 | TGL  | C13-C14-C29-C30 |
| 24  | T     | 101 | PEK  | C26-C27-C28-C29 |
| 25  | C     | 304 | CDL  | C42-C43-C44-C45 |
| 19  | A     | 608 | PGV  | C01-C02-C03-O11 |
| 19  | N     | 607 | PGV  | C01-C02-C03-O11 |
| 19  | P     | 301 | PGV  | C01-C02-C03-O11 |
| 24  | P     | 308 | PEK  | C01-C02-C03-O11 |
| 25  | C     | 304 | CDL  | OA5-CA3-CA4-CA6 |
| 20  | Q     | 201 | TGL  | CB4-CB5-CB6-CB7 |
| 20  | Y     | 101 | TGL  | C11-C12-C13-C14 |
| 25  | P     | 305 | CDL  | C73-C74-C75-C76 |
| 25  | P     | 305 | CDL  | C81-C82-C83-C84 |
| 24  | P     | 308 | PEK  | C16-C17-C18-C19 |
| 19  | A     | 608 | PGV  | C19-C20-C21-C22 |
| 24  | C     | 302 | PEK  | C24-C25-C26-C27 |
| 25  | G     | 101 | CDL  | C43-C44-C45-C46 |
| 20  | D     | 201 | TGL  | C16-C15-CC9-CC8 |
| 19  | A     | 607 | PGV  | C29-C30-C31-C32 |
| 20  | Y     | 101 | TGL  | CB7-CB8-CB9-C10 |
| 25  | G     | 101 | CDL  | C52-C53-C54-C55 |
| 19  | C     | 303 | PGV  | C19-C20-C21-C22 |
| 20  | Q     | 201 | TGL  | OG1-CG1-CG2-CG3 |
| 20  | Q     | 201 | TGL  | CG1-CG2-CG3-OG3 |
| 23  | N     | 610 | PSC  | O03-C01-C02-C03 |
| 24  | C     | 307 | PEK  | O03-C01-C02-C03 |
| 24  | G     | 102 | PEK  | O03-C01-C02-C03 |
| 24  | P     | 308 | PEK  | O03-C01-C02-C03 |
| 25  | T     | 102 | CDL  | CA3-CA4-CA6-OA8 |
| 25  | G     | 101 | CDL  | C53-C54-C55-C56 |
| 27  | M     | 101 | DMU  | O6-C11-C9-O1    |
| 23  | B     | 304 | PSC  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | C     | 307 | PEK  | C25-C26-C27-C28 |
| 23  | B     | 304 | PSC  | C24-C25-C26-C27 |
| 25  | G     | 101 | CDL  | C59-C60-C61-C62 |
| 25  | C     | 304 | CDL  | C40-C41-C42-C43 |
| 19  | N     | 607 | PGV  | C26-C27-C28-C29 |
| 19  | C     | 303 | PGV  | C20-C21-C22-C23 |
| 20  | Q     | 201 | TGL  | CC7-CC8-CC9-C15 |
| 25  | G     | 101 | CDL  | C62-C63-C64-C65 |
| 22  | P     | 306 | CHD  | C16-C17-C20-C21 |
| 20  | L     | 101 | TGL  | CA6-CA7-CA8-CA9 |
| 25  | P     | 305 | CDL  | C21-C22-C23-C24 |
| 24  | P     | 308 | PEK  | C31-C32-C33-C34 |
| 24  | T     | 101 | PEK  | C25-C26-C27-C28 |
| 25  | P     | 305 | CDL  | C76-C77-C78-C79 |
| 20  | Q     | 201 | TGL  | CA9-C20-C21-C22 |
| 24  | T     | 101 | PEK  | C31-C32-C33-C34 |
| 19  | P     | 304 | PGV  | C19-C20-C21-C22 |
| 19  | N     | 607 | PGV  | C10-C11-C12-C13 |
| 14  | A     | 602 | HEA  | C4D-C3D-CAD-CBD |
| 19  | C     | 308 | PGV  | O01-C02-C03-O11 |
| 24  | T     | 101 | PEK  | O04-C21-O03-C01 |
| 19  | A     | 608 | PGV  | C29-C30-C31-C32 |
| 19  | C     | 303 | PGV  | C7-C8-C9-C10    |
| 20  | N     | 609 | TGL  | C16-C17-C18-C19 |
| 24  | P     | 308 | PEK  | C35-C36-C37-C38 |
| 25  | C     | 304 | CDL  | C84-C85-C86-C87 |
| 19  | P     | 301 | PGV  | C28-C29-C30-C31 |
| 20  | D     | 201 | TGL  | CA2-CA3-CA4-CA5 |
| 20  | D     | 201 | TGL  | C23-C24-C25-C26 |
| 20  | L     | 101 | TGL  | CC9-C15-C16-C17 |
| 20  | Y     | 101 | TGL  | C14-C29-C30-C31 |
| 24  | T     | 101 | PEK  | C33-C34-C35-C36 |
| 19  | C     | 303 | PGV  | C28-C29-C30-C31 |
| 19  | N     | 607 | PGV  | C5-C6-C7-C8     |
| 20  | D     | 201 | TGL  | CC3-CC4-CC5-CC6 |
| 20  | Q     | 201 | TGL  | CB6-CB7-CB8-CB9 |
| 20  | Y     | 101 | TGL  | CB9-C10-C11-C12 |
| 25  | T     | 102 | CDL  | C36-C37-C38-C39 |
| 19  | N     | 608 | PGV  | C31-C32-C33-C34 |
| 24  | C     | 302 | PEK  | C25-C26-C27-C28 |
| 20  | L     | 101 | TGL  | OG2-CG2-CG3-OG3 |
| 20  | N     | 609 | TGL  | OG1-CG1-CG2-OG2 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | C     | 304 | CDL  | OB6-CB4-CB6-OB8 |
| 20  | L     | 101 | TGL  | CC3-CC4-CC5-CC6 |
| 19  | C     | 303 | PGV  | C31-C32-C33-C34 |
| 24  | C     | 307 | PEK  | C26-C27-C28-C29 |
| 25  | T     | 102 | CDL  | C81-C82-C83-C84 |
| 19  | N     | 608 | PGV  | C15-C16-C17-C18 |
| 24  | C     | 307 | PEK  | C35-C36-C37-C38 |
| 25  | T     | 102 | CDL  | C84-C85-C86-C87 |
| 19  | C     | 308 | PGV  | O01-C1-C2-C3    |
| 20  | L     | 101 | TGL  | CB7-CB8-CB9-C10 |
| 20  | Q     | 201 | TGL  | CB7-CB8-CB9-C10 |
| 25  | T     | 102 | CDL  | C63-C64-C65-C66 |
| 25  | P     | 305 | CDL  | C77-C78-C79-C80 |
| 20  | B     | 301 | TGL  | C29-C30-C31-C32 |
| 20  | D     | 201 | TGL  | CC1-CC2-CC3-CC4 |
| 19  | A     | 607 | PGV  | C31-C32-C33-C34 |
| 20  | D     | 201 | TGL  | OG2-CB1-CB2-CB3 |
| 20  | L     | 101 | TGL  | CB6-CB7-CB8-CB9 |
| 19  | C     | 303 | PGV  | C23-C24-C25-C26 |
| 25  | G     | 101 | CDL  | C42-C43-C44-C45 |
| 27  | Z     | 101 | DMU  | C25-C28-C31-C34 |
| 19  | P     | 304 | PGV  | C10-C11-C12-C13 |
| 24  | P     | 303 | PEK  | C7-C8-C9-C10    |
| 24  | P     | 308 | PEK  | C4-C5-C6-C7     |
| 19  | P     | 304 | PGV  | C7-C8-C9-C10    |
| 20  | B     | 301 | TGL  | CA3-CA4-CA5-CA6 |
| 25  | C     | 304 | CDL  | C73-C74-C75-C76 |
| 20  | B     | 301 | TGL  | CA9-C20-C21-C22 |
| 25  | G     | 101 | CDL  | C55-C56-C57-C58 |
| 20  | B     | 301 | TGL  | C21-C22-C23-C24 |
| 20  | Q     | 201 | TGL  | C11-C12-C13-C14 |
| 20  | B     | 301 | TGL  | C18-C19-C33-C34 |
| 20  | Q     | 201 | TGL  | CC3-CC4-CC5-CC6 |
| 20  | Q     | 201 | TGL  | CC9-C15-C16-C17 |
| 19  | N     | 607 | PGV  | C02-C03-O11-P   |
| 19  | N     | 607 | PGV  | C15-C16-C17-C18 |
| 19  | P     | 301 | PGV  | C14-C15-C16-C17 |
| 20  | B     | 301 | TGL  | C21-C20-CA9-CA8 |
| 25  | G     | 101 | CDL  | C71-C72-C73-C74 |
| 25  | P     | 305 | CDL  | C58-C59-C60-C61 |
| 20  | N     | 609 | TGL  | C29-C30-C31-C32 |
| 25  | C     | 304 | CDL  | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 608 | PGV  | C22-C23-C24-C25 |
| 19  | P     | 304 | PGV  | C22-C23-C24-C25 |
| 19  | C     | 308 | PGV  | C01-C02-C03-O11 |
| 25  | G     | 101 | CDL  | OA5-CA3-CA4-CA6 |
| 25  | P     | 305 | CDL  | OA5-CA3-CA4-CA6 |
| 20  | Y     | 101 | TGL  | C29-C30-C31-C32 |
| 25  | C     | 304 | CDL  | C64-C65-C66-C67 |
| 25  | G     | 101 | CDL  | C51-C52-C53-C54 |
| 19  | C     | 308 | PGV  | C27-C28-C29-C30 |
| 25  | P     | 305 | CDL  | C63-C64-C65-C66 |
| 24  | G     | 102 | PEK  | C22-C23-C24-C25 |
| 19  | C     | 308 | PGV  | C20-C19-O03-C01 |
| 19  | A     | 607 | PGV  | C23-C24-C25-C26 |
| 20  | B     | 301 | TGL  | C15-C16-C17-C18 |
| 24  | P     | 303 | PEK  | C30-C31-C32-C33 |
| 24  | P     | 303 | PEK  | C33-C34-C35-C36 |
| 25  | C     | 304 | CDL  | C35-C36-C37-C38 |
| 14  | A     | 602 | HEA  | C2D-C3D-CAD-CBD |
| 27  | Z     | 101 | DMU  | C34-C37-C40-C43 |
| 20  | N     | 609 | TGL  | C22-C23-C24-C25 |
| 19  | A     | 608 | PGV  | O03-C01-C02-C03 |
| 19  | N     | 607 | PGV  | O03-C01-C02-C03 |
| 25  | C     | 304 | CDL  | CA3-CA4-CA6-OA8 |
| 25  | C     | 304 | CDL  | CB3-CB4-CB6-OB8 |
| 19  | N     | 608 | PGV  | C30-C31-C32-C33 |
| 24  | C     | 302 | PEK  | C27-C28-C29-C30 |
| 25  | T     | 102 | CDL  | C12-C13-C14-C15 |
| 25  | T     | 102 | CDL  | C22-C23-C24-C25 |
| 20  | Y     | 101 | TGL  | C24-C25-C26-C27 |
| 20  | L     | 101 | TGL  | CC1-CC2-CC3-CC4 |
| 24  | C     | 307 | PEK  | O01-C02-C03-O11 |
| 24  | P     | 308 | PEK  | O01-C02-C03-O11 |
| 25  | C     | 304 | CDL  | OA5-CA3-CA4-OA6 |
| 25  | P     | 305 | CDL  | OA5-CA3-CA4-OA6 |
| 25  | P     | 305 | CDL  | OB5-CB3-CB4-OB6 |
| 27  | M     | 101 | DMU  | C34-C37-C40-C43 |
| 20  | Y     | 101 | TGL  | CB2-CB3-CB4-CB5 |
| 23  | B     | 304 | PSC  | C21-C22-C23-C24 |
| 19  | C     | 303 | PGV  | C22-C23-C24-C25 |
| 19  | P     | 301 | PGV  | C2-C3-C4-C5     |
| 24  | G     | 102 | PEK  | C24-C25-C26-C27 |
| 19  | C     | 308 | PGV  | O03-C01-C02-O01 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | B     | 301 | TGL  | OG1-CG1-CG2-OG2 |
| 25  | G     | 101 | CDL  | OB6-CB4-CB6-OB8 |
| 23  | B     | 304 | PSC  | C9-C10-C11-C12  |
| 23  | B     | 304 | PSC  | C10-C11-C12-C13 |
| 23  | N     | 610 | PSC  | C9-C10-C11-C12  |
| 24  | C     | 307 | PEK  | C6-C7-C8-C9     |
| 24  | C     | 307 | PEK  | C9-C10-C11-C12  |
| 24  | G     | 102 | PEK  | C5-C6-C7-C8     |
| 24  | P     | 303 | PEK  | C11-C10-C9-C8   |
| 24  | P     | 303 | PEK  | C11-C12-C13-C14 |
| 24  | P     | 308 | PEK  | C9-C10-C11-C12  |
| 24  | P     | 308 | PEK  | C12-C13-C14-C15 |
| 24  | T     | 101 | PEK  | C12-C13-C14-C15 |
| 20  | L     | 101 | TGL  | C20-C21-C22-C23 |
| 24  | P     | 303 | PEK  | C27-C28-C29-C30 |
| 25  | G     | 101 | CDL  | C41-C42-C43-C44 |
| 24  | P     | 308 | PEK  | C30-C31-C32-C33 |
| 25  | G     | 101 | CDL  | C21-C22-C23-C24 |
| 25  | P     | 305 | CDL  | C52-C53-C54-C55 |
| 23  | N     | 610 | PSC  | C15-C16-C17-C18 |
| 20  | Y     | 101 | TGL  | CB4-CB5-CB6-CB7 |
| 19  | A     | 608 | PGV  | C2-C3-C4-C5     |
| 20  | D     | 201 | TGL  | CB4-CB5-CB6-CB7 |
| 25  | T     | 102 | CDL  | C77-C78-C79-C80 |
| 19  | A     | 608 | PGV  | O05-C05-C06-O06 |
| 19  | N     | 607 | PGV  | C30-C31-C32-C33 |
| 20  | B     | 301 | TGL  | CC9-C15-C16-C17 |
| 20  | Q     | 201 | TGL  | C25-C26-C27-C28 |
| 24  | T     | 101 | PEK  | C29-C30-C31-C32 |
| 25  | T     | 102 | CDL  | C78-C79-C80-C81 |
| 20  | Y     | 101 | TGL  | CA2-CA1-OG1-CG1 |
| 24  | T     | 101 | PEK  | C01-C02-C03-O11 |
| 19  | C     | 308 | PGV  | C4-C5-C6-C7     |
| 20  | D     | 201 | TGL  | C17-C18-C19-C33 |
| 20  | B     | 301 | TGL  | CA1-CA2-CA3-CA4 |
| 20  | D     | 201 | TGL  | CB5-CB6-CB7-CB8 |
| 20  | Y     | 101 | TGL  | C25-C26-C27-C28 |
| 23  | B     | 304 | PSC  | C15-C16-C17-C18 |
| 25  | C     | 304 | CDL  | C62-C63-C64-C65 |
| 25  | T     | 102 | CDL  | C21-C22-C23-C24 |
| 25  | G     | 101 | CDL  | C17-C18-C19-C20 |
| 19  | C     | 308 | PGV  | O04-C19-O03-C01 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | P     | 305 | CDL  | CA5-C11-C12-C13 |
| 22  | P     | 306 | CHD  | C20-C22-C23-C24 |
| 19  | A     | 608 | PGV  | C31-C32-C33-C34 |
| 20  | N     | 609 | TGL  | C18-C19-C33-C34 |
| 19  | N     | 607 | PGV  | C03-C02-O01-C1  |
| 23  | B     | 304 | PSC  | C01-C02-O01-C1  |
| 20  | Y     | 101 | TGL  | OA1-CA1-OG1-CG1 |
| 19  | N     | 607 | PGV  | O01-C02-C03-O11 |
| 24  | T     | 101 | PEK  | O01-C02-C03-O11 |
| 19  | C     | 308 | PGV  | C25-C26-C27-C28 |
| 25  | T     | 102 | CDL  | C56-C57-C58-C59 |
| 20  | D     | 201 | TGL  | OG1-CG1-CG2-CG3 |
| 20  | N     | 609 | TGL  | C21-C22-C23-C24 |
| 25  | C     | 304 | CDL  | C71-C72-C73-C74 |
| 25  | P     | 305 | CDL  | C80-C81-C82-C83 |
| 20  | D     | 201 | TGL  | CA9-C20-C21-C22 |
| 20  | Q     | 201 | TGL  | OG2-CG2-CG3-OG3 |
| 20  | Y     | 101 | TGL  | OG2-CG2-CG3-OG3 |
| 23  | B     | 304 | PSC  | O03-C01-C02-O01 |
| 23  | N     | 610 | PSC  | O03-C01-C02-O01 |
| 23  | N     | 610 | PSC  | C31-C32-C33-C34 |
| 19  | N     | 608 | PGV  | C24-C25-C26-C27 |
| 20  | L     | 101 | TGL  | C22-C23-C24-C25 |
| 25  | G     | 101 | CDL  | C12-C13-C14-C15 |
| 25  | P     | 305 | CDL  | C34-C35-C36-C37 |
| 19  | A     | 607 | PGV  | C27-C28-C29-C30 |
| 20  | D     | 201 | TGL  | C11-C10-CB9-CB8 |
| 20  | L     | 101 | TGL  | CA2-CA3-CA4-CA5 |
| 25  | C     | 304 | CDL  | C13-C14-C15-C16 |
| 20  | B     | 301 | TGL  | C23-C24-C25-C26 |
| 20  | L     | 101 | TGL  | OG1-CA1-CA2-CA3 |
| 25  | T     | 102 | CDL  | C52-C53-C54-C55 |
| 14  | A     | 601 | HEA  | C26-C15-C16-C17 |
| 24  | C     | 307 | PEK  | C31-C32-C33-C34 |
| 20  | N     | 609 | TGL  | C13-C14-C29-C30 |
| 19  | N     | 607 | PGV  | C31-C32-C33-C34 |
| 24  | C     | 302 | PEK  | C30-C31-C32-C33 |
| 25  | P     | 305 | CDL  | C11-C12-C13-C14 |
| 20  | D     | 201 | TGL  | CA4-CA5-CA6-CA7 |
| 25  | G     | 101 | CDL  | C15-C16-C17-C18 |
| 25  | T     | 102 | CDL  | C33-C34-C35-C36 |
| 25  | G     | 101 | CDL  | C57-C58-C59-C60 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | P     | 305 | CDL  | C20-C21-C22-C23 |
| 19  | P     | 304 | PGV  | C11-C12-C13-C14 |
| 19  | C     | 303 | PGV  | C02-C03-O11-P   |
| 19  | P     | 304 | PGV  | C02-C03-O11-P   |
| 25  | G     | 101 | CDL  | CB4-CB3-OB5-PB2 |
| 19  | C     | 308 | PGV  | C31-C32-C33-C34 |
| 20  | L     | 101 | TGL  | C17-C18-C19-C33 |
| 20  | N     | 609 | TGL  | C24-C25-C26-C27 |
| 23  | B     | 304 | PSC  | C23-C24-C25-C26 |
| 19  | A     | 608 | PGV  | O01-C02-C03-O11 |
| 25  | G     | 101 | CDL  | OA5-CA3-CA4-OA6 |
| 20  | Y     | 101 | TGL  | CA6-CA7-CA8-CA9 |
| 24  | P     | 303 | PEK  | C32-C33-C34-C35 |
| 14  | A     | 601 | HEA  | C4A-C3A-CMA-OMA |
| 14  | N     | 601 | HEA  | C4A-C3A-CMA-OMA |
| 25  | T     | 102 | CDL  | C37-C38-C39-C40 |
| 25  | T     | 102 | CDL  | OA6-CA4-CA6-OA8 |
| 19  | P     | 301 | PGV  | C23-C24-C25-C26 |
| 25  | C     | 304 | CDL  | C16-C17-C18-C19 |
| 20  | L     | 101 | TGL  | CG1-CG2-CG3-OG3 |
| 23  | B     | 304 | PSC  | O03-C01-C02-C03 |
| 25  | G     | 101 | CDL  | CA3-CA4-CA6-OA8 |
| 19  | P     | 301 | PGV  | C31-C32-C33-C34 |
| 23  | B     | 304 | PSC  | C4-C5-C6-C7     |
| 19  | A     | 608 | PGV  | C1-C2-C3-C4     |
| 24  | P     | 303 | PEK  | C15-C16-C17-C18 |
| 20  | Q     | 201 | TGL  | CA5-CA6-CA7-CA8 |
| 20  | Y     | 101 | TGL  | CC5-CC6-CC7-CC8 |
| 20  | L     | 101 | TGL  | C23-C24-C25-C26 |
| 19  | A     | 608 | PGV  | C11-C12-C13-C14 |
| 20  | D     | 201 | TGL  | CA6-CA7-CA8-CA9 |
| 19  | C     | 308 | PGV  | C03-O11-P-O14   |
| 24  | C     | 307 | PEK  | C04-O12-P-O14   |
| 24  | G     | 102 | PEK  | C03-O11-P-O12   |
| 24  | G     | 102 | PEK  | C04-O12-P-O14   |
| 24  | P     | 308 | PEK  | C04-O12-P-O13   |
| 25  | C     | 304 | CDL  | CB2-OB2-PB2-OB3 |
| 25  | C     | 304 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | G     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 25  | G     | 101 | CDL  | CB3-OB5-PB2-OB4 |
| 25  | P     | 305 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | T     | 102 | CDL  | CB3-OB5-PB2-OB2 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | T     | 102 | CDL  | CB3-OB5-PB2-OB4 |
| 19  | A     | 608 | PGV  | C9-C10-C11-C12  |
| 22  | P     | 306 | CHD  | C16-C17-C20-C22 |
| 25  | T     | 102 | CDL  | CB4-CB3-OB5-PB2 |
| 27  | M     | 101 | DMU  | C18-C19-C22-C25 |
| 25  | G     | 101 | CDL  | C34-C35-C36-C37 |
| 19  | C     | 308 | PGV  | C15-C16-C17-C18 |
| 19  | C     | 303 | PGV  | C1-C2-C3-C4     |
| 25  | T     | 102 | CDL  | C53-C54-C55-C56 |
| 24  | P     | 303 | PEK  | C23-C24-C25-C26 |
| 27  | M     | 101 | DMU  | C25-C28-C31-C34 |
| 25  | C     | 304 | CDL  | C12-C13-C14-C15 |
| 23  | N     | 610 | PSC  | C04-C05-N-C06   |
| 23  | N     | 610 | PSC  | C04-C05-N-C07   |
| 24  | G     | 102 | PEK  | C25-C26-C27-C28 |
| 24  | P     | 303 | PEK  | C29-C30-C31-C32 |
| 19  | A     | 608 | PGV  | C27-C28-C29-C30 |
| 24  | P     | 308 | PEK  | C17-C18-C19-C20 |
| 20  | D     | 201 | TGL  | CC9-C15-C16-C17 |
| 20  | B     | 301 | TGL  | C13-C14-C29-C30 |
| 20  | Y     | 101 | TGL  | C12-C13-C14-C29 |
| 24  | C     | 302 | PEK  | C34-C35-C36-C37 |
| 23  | N     | 610 | PSC  | C30-C31-C32-C33 |
| 24  | C     | 302 | PEK  | C13-C14-C15-C16 |
| 19  | C     | 303 | PGV  | C14-C15-C16-C17 |
| 14  | N     | 601 | HEA  | C15-C16-C17-C18 |
| 20  | Y     | 101 | TGL  | CG1-CG2-CG3-OG3 |
| 25  | T     | 102 | CDL  | C60-C61-C62-C63 |
| 25  | C     | 304 | CDL  | C76-C77-C78-C79 |
| 19  | A     | 608 | PGV  | O12-C04-C05-O05 |
| 24  | P     | 308 | PEK  | C15-C16-C17-C18 |
| 25  | C     | 304 | CDL  | C12-C11-CA5-OA6 |
| 20  | Q     | 201 | TGL  | CB2-CB3-CB4-CB5 |
| 25  | C     | 304 | CDL  | C34-C35-C36-C37 |
| 20  | D     | 201 | TGL  | OB1-CB1-CB2-CB3 |
| 19  | A     | 608 | PGV  | O12-C04-C05-C06 |
| 22  | C     | 305 | CHD  | C16-C17-C20-C22 |
| 25  | C     | 304 | CDL  | C1-CA2-OA2-PA1  |
| 24  | T     | 101 | PEK  | C28-C29-C30-C31 |
| 20  | Q     | 201 | TGL  | C10-C11-C12-C13 |
| 14  | A     | 601 | HEA  | C14-C15-C16-C17 |
| 19  | C     | 303 | PGV  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | T     | 101 | PEK  | C3-C4-C5-C6     |
| 19  | N     | 608 | PGV  | C25-C26-C27-C28 |
| 25  | T     | 102 | CDL  | C44-C45-C46-C47 |
| 20  | Q     | 201 | TGL  | OG2-CB1-CB2-CB3 |
| 25  | T     | 102 | CDL  | C80-C81-C82-C83 |
| 14  | A     | 602 | HEA  | CAD-CBD-CGD-O2D |
| 14  | N     | 602 | HEA  | CAD-CBD-CGD-O1D |
| 23  | N     | 610 | PSC  | C04-C05-N-C08   |
| 19  | C     | 308 | PGV  | O02-C1-C2-C3    |
| 19  | C     | 308 | PGV  | C23-C24-C25-C26 |
| 25  | P     | 305 | CDL  | C60-C61-C62-C63 |
| 22  | J     | 101 | CHD  | C22-C23-C24-O25 |
| 25  | T     | 102 | CDL  | C58-C59-C60-C61 |
| 24  | C     | 302 | PEK  | C7-C8-C9-C10    |
| 24  | P     | 308 | PEK  | C23-C24-C25-C26 |
| 25  | C     | 304 | CDL  | C14-C15-C16-C17 |
| 20  | B     | 301 | TGL  | CG1-CG2-OG2-CB1 |
| 20  | N     | 609 | TGL  | CG1-CG2-OG2-CB1 |
| 24  | G     | 102 | PEK  | C01-C02-O01-C1  |
| 25  | C     | 304 | CDL  | CA3-CA4-OA6-CA5 |
| 22  | J     | 101 | CHD  | C17-C20-C22-C23 |
| 25  | G     | 101 | CDL  | C61-C62-C63-C64 |
| 22  | B     | 303 | CHD  | C22-C23-C24-O25 |
| 22  | G     | 103 | CHD  | C22-C23-C24-O25 |
| 25  | P     | 305 | CDL  | C43-C44-C45-C46 |
| 24  | P     | 303 | PEK  | O02-C1-O01-C02  |
| 14  | A     | 602 | HEA  | CAD-CBD-CGD-O1D |
| 22  | C     | 306 | CHD  | C22-C23-C24-O25 |
| 20  | L     | 101 | TGL  | CA9-C20-C21-C22 |
| 25  | G     | 101 | CDL  | CA4-CA3-OA5-PA1 |
| 25  | P     | 305 | CDL  | CA4-CA3-OA5-PA1 |
| 22  | C     | 305 | CHD  | C22-C23-C24-O26 |
| 22  | P     | 306 | CHD  | C22-C23-C24-O25 |
| 20  | D     | 201 | TGL  | C12-C13-C14-C29 |
| 20  | N     | 609 | TGL  | C11-C10-CB9-CB8 |
| 24  | P     | 303 | PEK  | C35-C36-C37-C38 |
| 20  | N     | 609 | TGL  | C17-C18-C19-C33 |
| 25  | P     | 305 | CDL  | C51-C52-C53-C54 |
| 19  | A     | 607 | PGV  | C11-C12-C13-C14 |
| 25  | T     | 102 | CDL  | C43-C44-C45-C46 |
| 23  | N     | 610 | PSC  | C10-C11-C12-C13 |
| 24  | C     | 302 | PEK  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | C     | 307 | PEK  | C11-C10-C9-C8   |
| 24  | C     | 307 | PEK  | C12-C13-C14-C15 |
| 24  | G     | 102 | PEK  | C12-C13-C14-C15 |
| 24  | P     | 303 | PEK  | C5-C6-C7-C8     |
| 24  | P     | 308 | PEK  | C5-C6-C7-C8     |
| 24  | P     | 308 | PEK  | C6-C7-C8-C9     |
| 24  | P     | 308 | PEK  | C11-C10-C9-C8   |
| 24  | T     | 101 | PEK  | C5-C6-C7-C8     |
| 24  | T     | 101 | PEK  | C11-C10-C9-C8   |
| 14  | N     | 602 | HEA  | CAD-CBD-CGD-O2D |
| 23  | B     | 304 | PSC  | C04-C05-N-C08   |
| 14  | A     | 602 | HEA  | C26-C15-C16-C17 |
| 14  | N     | 602 | HEA  | C26-C15-C16-C17 |
| 24  | C     | 302 | PEK  | C17-C18-C19-C20 |
| 20  | Q     | 201 | TGL  | C20-C21-C22-C23 |
| 22  | G     | 103 | CHD  | C22-C23-C24-O26 |
| 20  | Y     | 101 | TGL  | C17-C18-C19-C33 |
| 22  | P     | 306 | CHD  | C13-C17-C20-C21 |
| 22  | J     | 101 | CHD  | C22-C23-C24-O26 |
| 24  | P     | 308 | PEK  | C24-C25-C26-C27 |
| 14  | A     | 601 | HEA  | CAD-CBD-CGD-O1D |
| 19  | C     | 308 | PGV  | C05-C04-O12-P   |
| 25  | P     | 305 | CDL  | C55-C56-C57-C58 |
| 14  | N     | 602 | HEA  | CAA-CBA-CGA-O2A |
| 14  | A     | 602 | HEA  | CAA-CBA-CGA-O2A |
| 14  | N     | 602 | HEA  | CAA-CBA-CGA-O1A |
| 20  | Y     | 101 | TGL  | C15-C16-C17-C18 |
| 19  | C     | 308 | PGV  | C29-C30-C31-C32 |
| 24  | P     | 308 | PEK  | C3-C4-C5-C6     |
| 19  | N     | 608 | PGV  | O03-C19-C20-C21 |
| 20  | D     | 201 | TGL  | C21-C22-C23-C24 |
| 20  | D     | 201 | TGL  | C29-C30-C31-C32 |
| 24  | P     | 303 | PEK  | O03-C21-C22-C23 |
| 22  | B     | 303 | CHD  | C22-C23-C24-O26 |
| 22  | C     | 305 | CHD  | C22-C23-C24-O25 |
| 24  | C     | 307 | PEK  | C01-C02-C03-O11 |
| 25  | P     | 305 | CDL  | OB5-CB3-CB4-CB6 |
| 20  | Y     | 101 | TGL  | C23-C24-C25-C26 |
| 24  | C     | 302 | PEK  | C21-C22-C23-C24 |
| 24  | T     | 101 | PEK  | O01-C1-C2-C3    |
| 19  | C     | 303 | PGV  | C9-C10-C11-C12  |
| 25  | T     | 102 | CDL  | C82-C83-C84-C85 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | D     | 201 | TGL  | C16-C17-C18-C19 |
| 22  | W     | 101 | CHD  | C22-C23-C24-O25 |
| 25  | T     | 102 | CDL  | O1-C1-CA2-OA2   |
| 19  | P     | 301 | PGV  | C11-C12-C13-C14 |
| 23  | B     | 304 | PSC  | C12-C13-C14-C15 |
| 23  | N     | 610 | PSC  | C12-C13-C14-C15 |
| 19  | N     | 607 | PGV  | C22-C23-C24-C25 |
| 22  | W     | 101 | CHD  | C22-C23-C24-O26 |
| 25  | P     | 305 | CDL  | C18-C19-C20-C21 |
| 25  | G     | 101 | CDL  | C22-C23-C24-C25 |
| 20  | Q     | 201 | TGL  | CA1-CA2-CA3-CA4 |
| 25  | C     | 304 | CDL  | CA6-CA4-OA6-CA5 |
| 19  | A     | 607 | PGV  | C11-C10-C9-C8   |
| 23  | N     | 610 | PSC  | C6-C7-C8-C9     |
| 20  | N     | 609 | TGL  | C19-C33-C34-C35 |
| 22  | P     | 306 | CHD  | C22-C23-C24-O26 |
| 24  | T     | 101 | PEK  | C21-C22-C23-C24 |
| 20  | Y     | 101 | TGL  | C16-C15-CC9-CC8 |
| 25  | G     | 101 | CDL  | C84-C85-C86-C87 |
| 25  | T     | 102 | CDL  | C83-C84-C85-C86 |
| 20  | B     | 301 | TGL  | C19-C33-C34-C35 |
| 20  | N     | 609 | TGL  | CC7-CC8-CC9-C15 |
| 19  | C     | 308 | PGV  | O03-C01-C02-C03 |
| 20  | Y     | 101 | TGL  | OG1-CG1-CG2-CG3 |
| 25  | G     | 101 | CDL  | CB3-CB4-CB6-OB8 |
| 20  | N     | 609 | TGL  | C25-C26-C27-C28 |
| 24  | C     | 307 | PEK  | C17-C18-C19-C20 |
| 25  | P     | 305 | CDL  | C84-C85-C86-C87 |
| 25  | G     | 101 | CDL  | C52-C51-CB5-OB6 |
| 20  | N     | 609 | TGL  | CA6-CA7-CA8-CA9 |
| 25  | G     | 101 | CDL  | C13-C14-C15-C16 |
| 24  | P     | 308 | PEK  | O01-C1-C2-C3    |
| 22  | P     | 307 | CHD  | C22-C23-C24-O25 |
| 25  | T     | 102 | CDL  | C32-C31-CA7-OA8 |
| 22  | W     | 101 | CHD  | C21-C20-C22-C23 |
| 19  | N     | 608 | PGV  | C11-C12-C13-C14 |
| 24  | G     | 102 | PEK  | C3-C4-C5-C6     |
| 24  | G     | 102 | PEK  | C31-C32-C33-C34 |
| 24  | P     | 303 | PEK  | O01-C1-C2-C3    |
| 14  | A     | 601 | HEA  | CAD-CBD-CGD-O2D |
| 25  | G     | 101 | CDL  | C12-C11-CA5-OA6 |
| 25  | G     | 101 | CDL  | C32-C31-CA7-OA8 |

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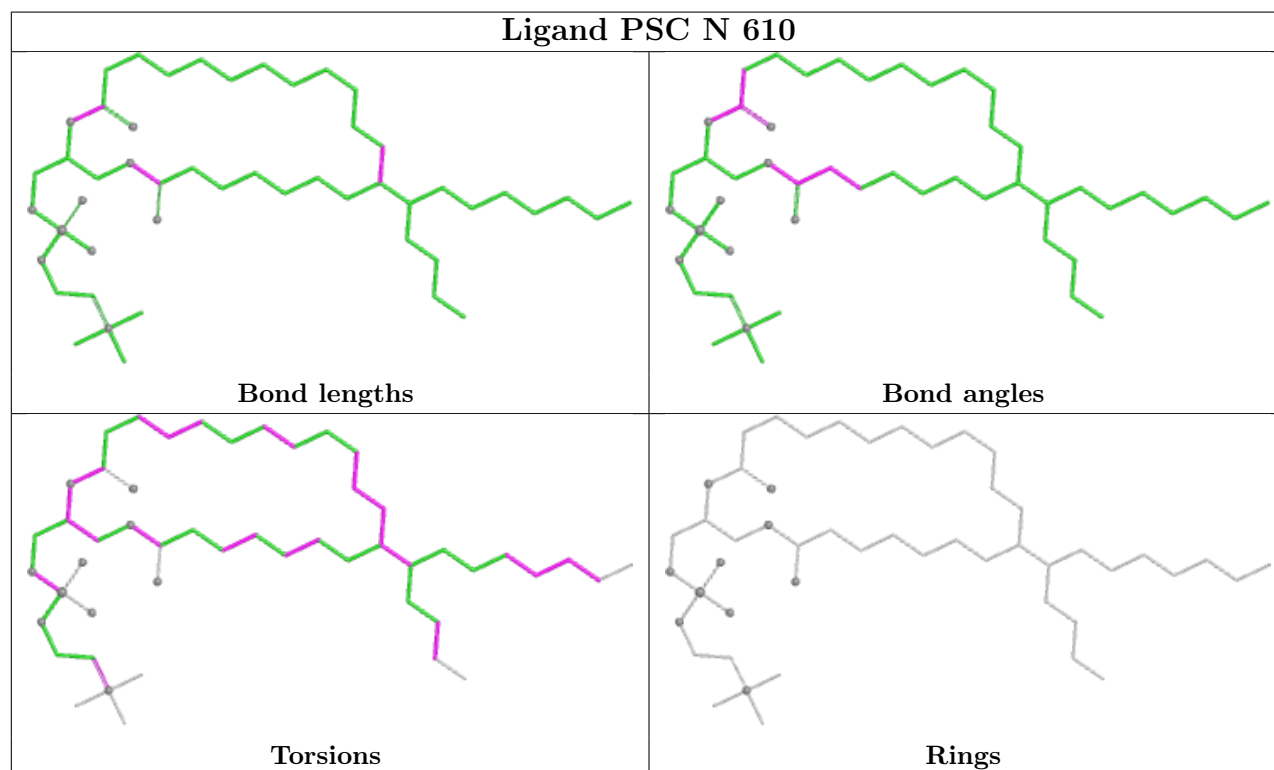
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | C     | 308 | PGV  | C12-C13-C14-C15 |
| 20  | Y     | 101 | TGL  | C33-C34-C35-C36 |
| 19  | N     | 608 | PGV  | C4-C5-C6-C7     |
| 20  | Q     | 201 | TGL  | CA3-CA4-CA5-CA6 |
| 24  | G     | 102 | PEK  | C35-C36-C37-C38 |
| 24  | C     | 307 | PEK  | C21-C22-C23-C24 |
| 23  | B     | 304 | PSC  | O03-C19-C20-C21 |
| 14  | A     | 602 | HEA  | CAA-CBA-CGA-O1A |
| 20  | Q     | 201 | TGL  | OG3-CC1-CC2-CC3 |
| 20  | Y     | 101 | TGL  | OG1-CG1-CG2-OG2 |
| 14  | N     | 601 | HEA  | CAD-CBD-CGD-O1D |
| 14  | N     | 601 | HEA  | CAD-CBD-CGD-O2D |
| 25  | T     | 102 | CDL  | CA4-CA6-OA8-CA7 |
| 20  | Q     | 201 | TGL  | C17-C18-C19-C33 |
| 20  | L     | 101 | TGL  | OA1-CA1-CA2-CA3 |
| 23  | B     | 304 | PSC  | C04-C05-N-C07   |
| 20  | N     | 609 | TGL  | CA7-CA8-CA9-C20 |
| 27  | Z     | 101 | DMU  | C19-C22-C25-C28 |
| 20  | D     | 201 | TGL  | CB2-CB3-CB4-CB5 |
| 24  | G     | 102 | PEK  | C28-C29-C30-C31 |
| 19  | P     | 304 | PGV  | C05-C04-O12-P   |
| 14  | N     | 601 | HEA  | CAA-CBA-CGA-O1A |
| 22  | P     | 307 | CHD  | C22-C23-C24-O26 |
| 24  | P     | 308 | PEK  | O02-C1-C2-C3    |
| 25  | T     | 102 | CDL  | C64-C65-C66-C67 |
| 23  | B     | 304 | PSC  | O04-C19-C20-C21 |
| 20  | Q     | 201 | TGL  | C13-C14-C29-C30 |
| 24  | C     | 307 | PEK  | O01-C1-C2-C3    |
| 20  | Q     | 201 | TGL  | OC1-CC1-CC2-CC3 |
| 25  | T     | 102 | CDL  | C32-C31-CA7-OA9 |
| 24  | P     | 303 | PEK  | O02-C1-C2-C3    |
| 25  | G     | 101 | CDL  | C12-C11-CA5-OA7 |
| 25  | G     | 101 | CDL  | C32-C31-CA7-OA9 |
| 24  | C     | 307 | PEK  | C14-C15-C16-C17 |
| 19  | C     | 303 | PGV  | C05-C04-O12-P   |
| 19  | A     | 607 | PGV  | C19-C20-C21-C22 |
| 24  | C     | 307 | PEK  | O02-C1-C2-C3    |
| 19  | P     | 304 | PGV  | C23-C24-C25-C26 |
| 25  | G     | 101 | CDL  | C78-C79-C80-C81 |
| 19  | A     | 607 | PGV  | O03-C19-C20-C21 |
| 14  | A     | 601 | HEA  | CAA-CBA-CGA-O1A |
| 14  | N     | 601 | HEA  | CAA-CBA-CGA-O2A |

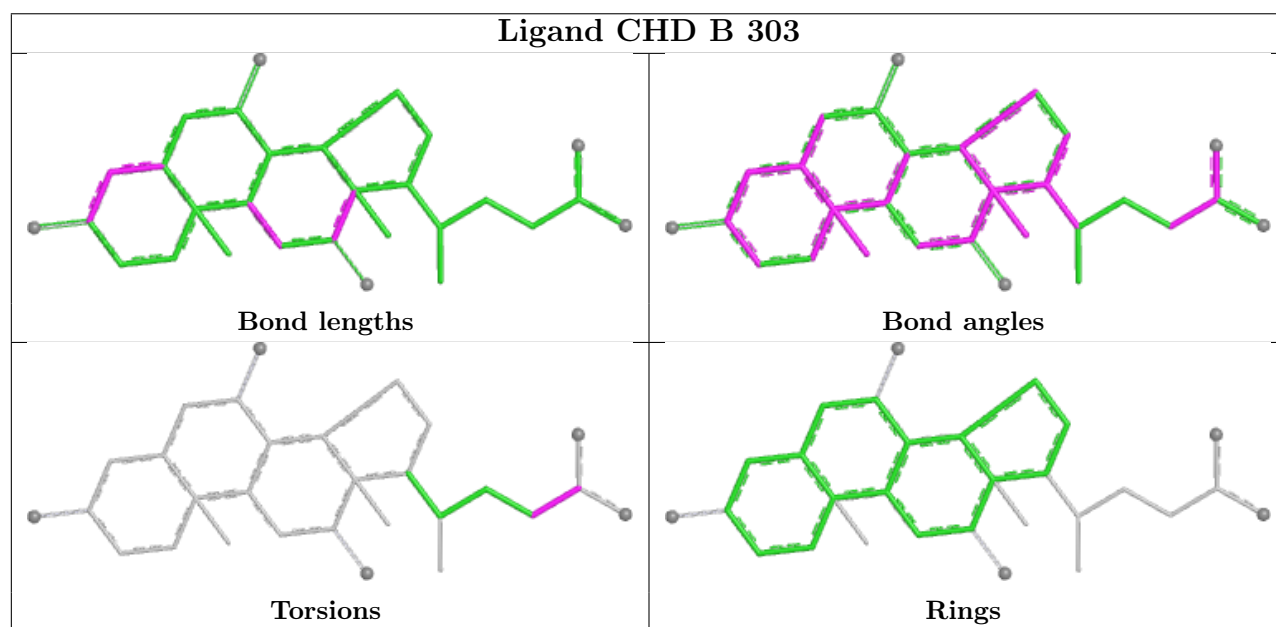
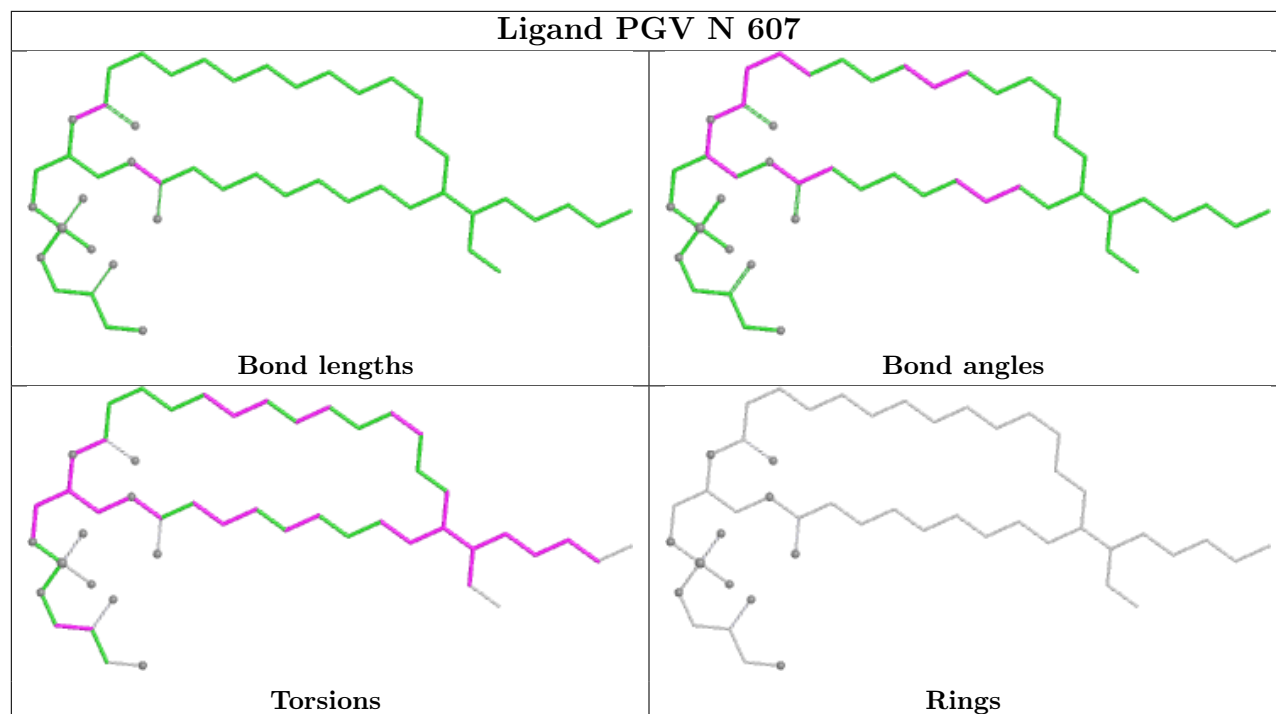
There are no ring outliers.

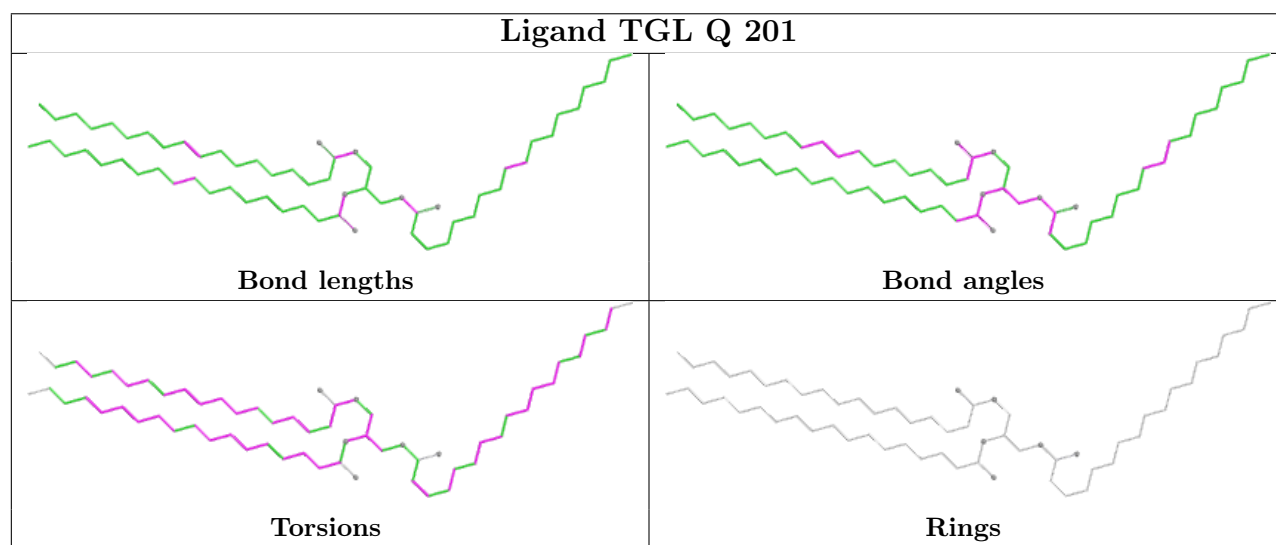
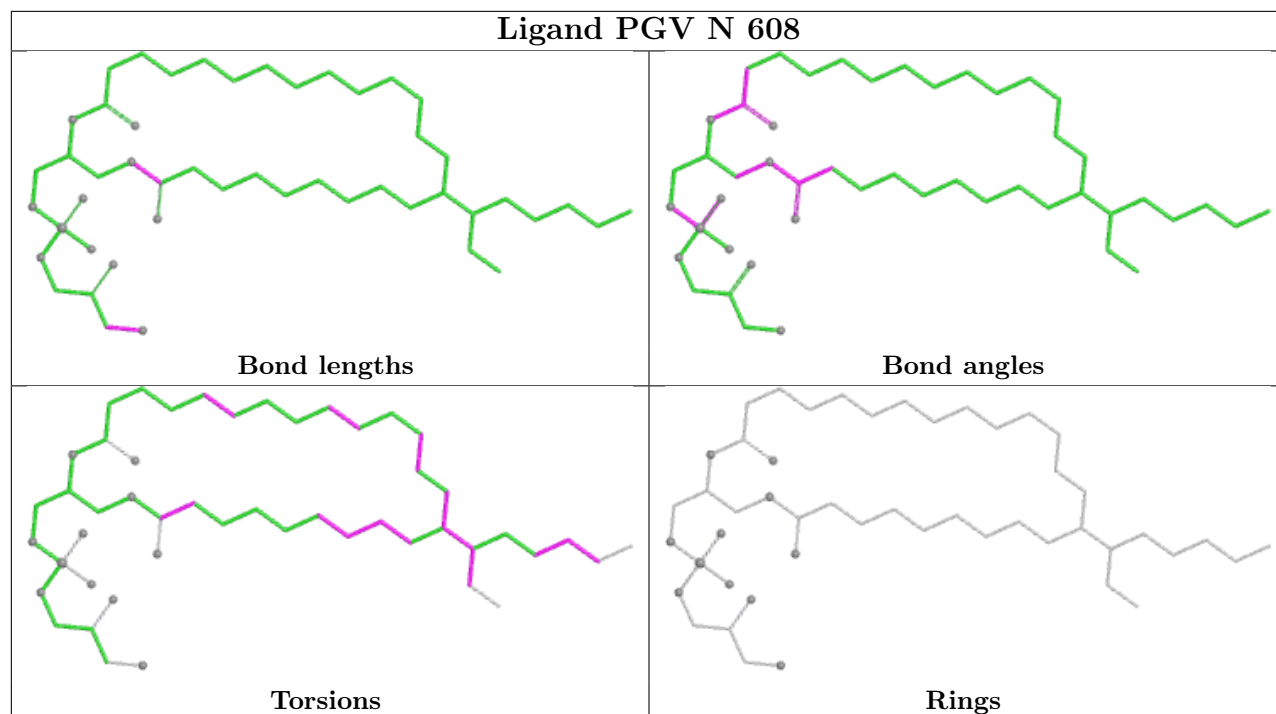
40 monomers are involved in 325 short contacts:

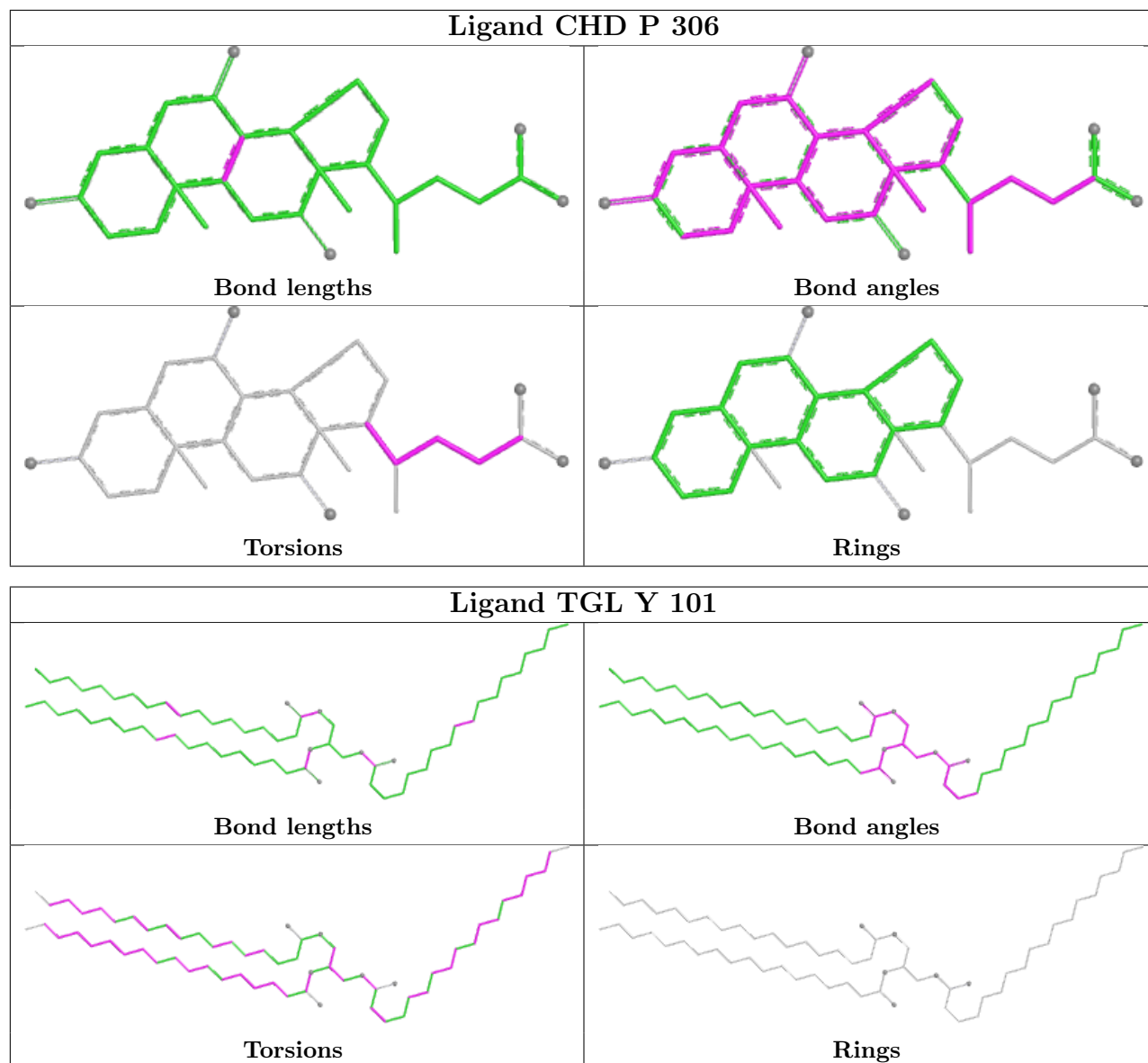
| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 23  | N     | 610    | PSC  | 21      | 0            |
| 19  | N     | 607    | PGV  | 10      | 0            |
| 22  | B     | 303    | CHD  | 1       | 0            |
| 19  | N     | 608    | PGV  | 6       | 0            |
| 20  | Q     | 201    | TGL  | 11      | 0            |
| 22  | P     | 306    | CHD  | 2       | 0            |
| 20  | Y     | 101    | TGL  | 17      | 0            |
| 19  | C     | 308    | PGV  | 1       | 0            |
| 27  | M     | 101    | DMU  | 1       | 0            |
| 25  | C     | 304    | CDL  | 23      | 0            |
| 25  | T     | 102    | CDL  | 29      | 0            |
| 14  | N     | 602    | HEA  | 2       | 0            |
| 20  | N     | 609    | TGL  | 4       | 0            |
| 22  | C     | 306    | CHD  | 1       | 0            |
| 18  | A     | 606[A] | PER  | 1       | 0            |
| 24  | T     | 101    | PEK  | 12      | 0            |
| 14  | N     | 601    | HEA  | 6       | 0            |
| 24  | P     | 303    | PEK  | 9       | 0            |
| 25  | G     | 101    | CDL  | 37      | 0            |
| 14  | A     | 601    | HEA  | 8       | 0            |
| 19  | A     | 608    | PGV  | 8       | 0            |
| 24  | P     | 308    | PEK  | 13      | 0            |
| 20  | B     | 301    | TGL  | 3       | 0            |
| 20  | L     | 101    | TGL  | 12      | 0            |
| 22  | J     | 101    | CHD  | 5       | 0            |
| 24  | G     | 102    | PEK  | 6       | 0            |
| 22  | C     | 305    | CHD  | 3       | 0            |
| 19  | A     | 607    | PGV  | 2       | 0            |
| 24  | C     | 302    | PEK  | 6       | 0            |
| 23  | B     | 304    | PSC  | 13      | 0            |
| 25  | P     | 305    | CDL  | 18      | 0            |
| 19  | P     | 301    | PGV  | 7       | 0            |
| 20  | D     | 201    | TGL  | 13      | 0            |
| 19  | C     | 303    | PGV  | 5       | 0            |
| 22  | P     | 307    | CHD  | 3       | 0            |
| 14  | A     | 602    | HEA  | 2       | 0            |
| 22  | W     | 101    | CHD  | 5       | 0            |
| 18  | N     | 606[A] | PER  | 1       | 0            |
| 19  | P     | 304    | PGV  | 4       | 0            |
| 24  | C     | 307    | PEK  | 17      | 0            |

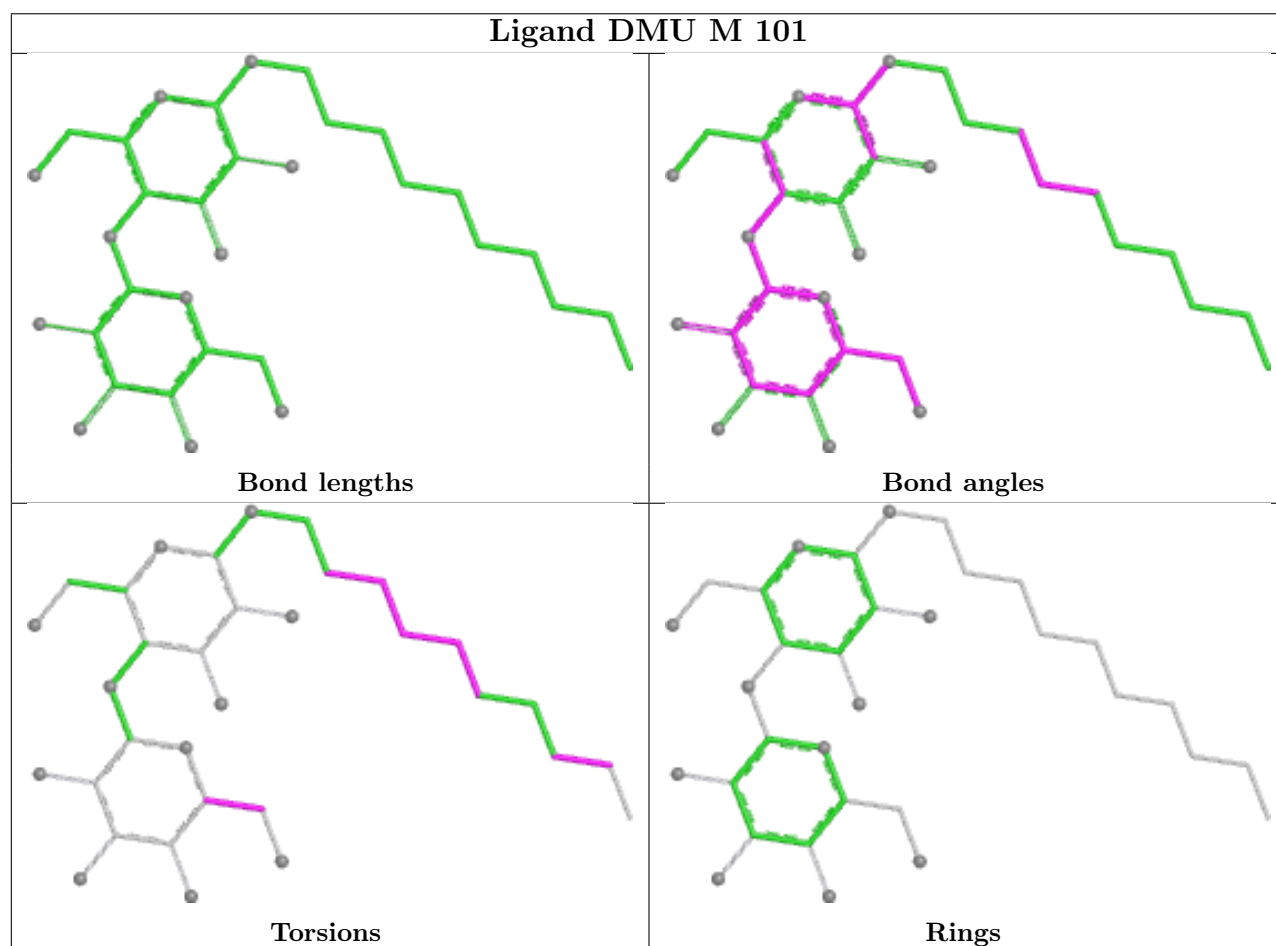
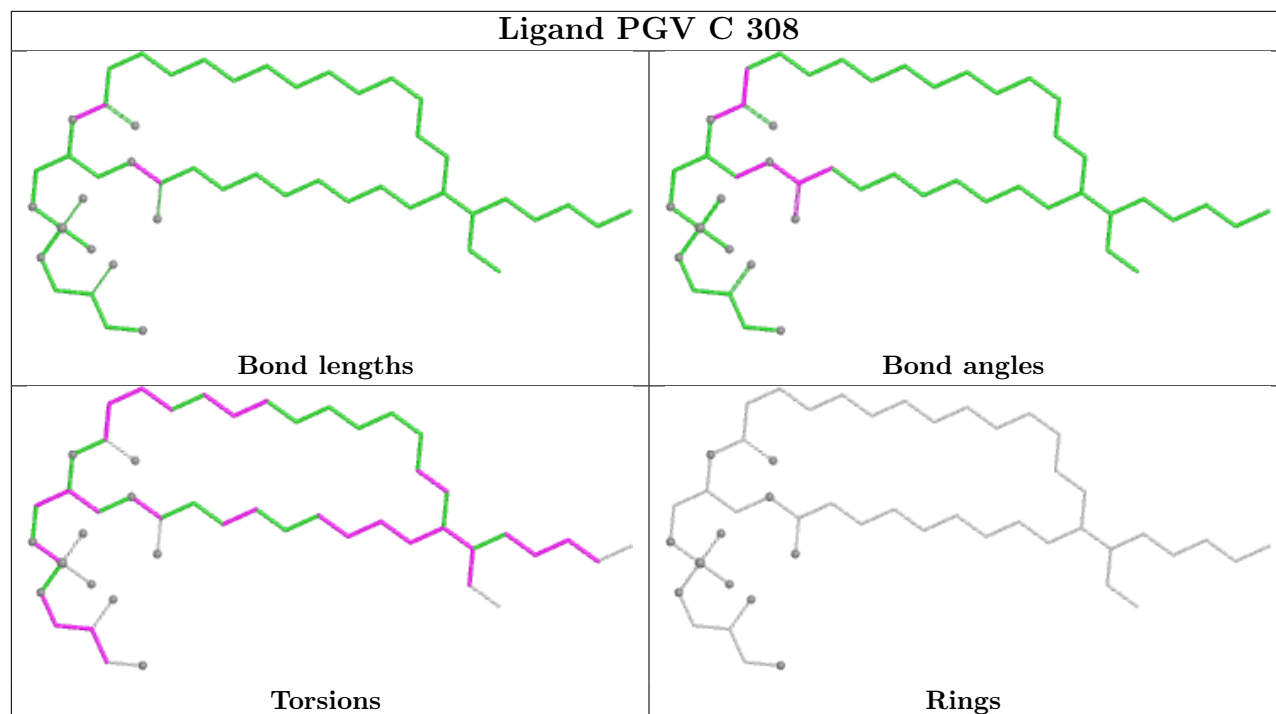
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

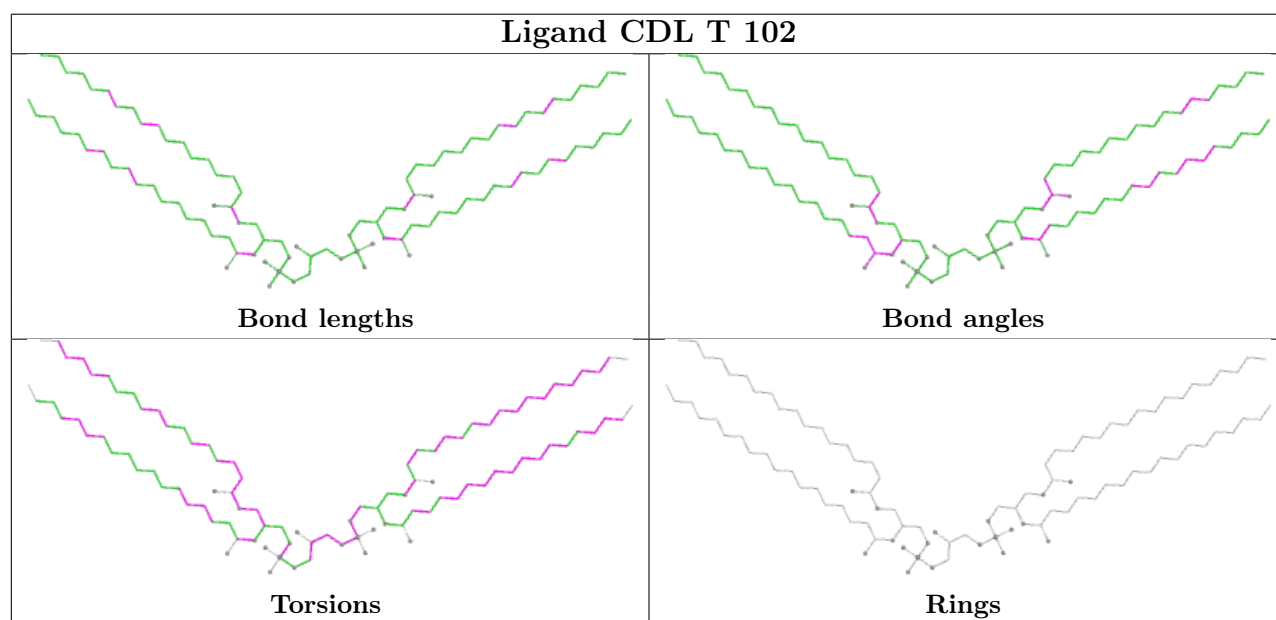
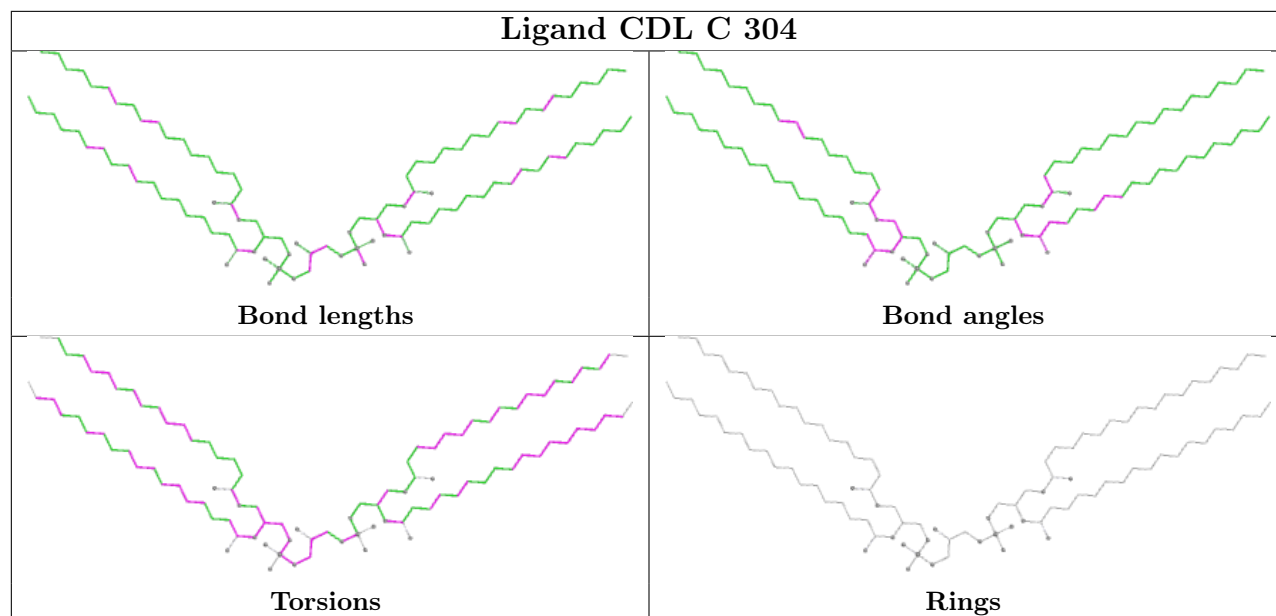


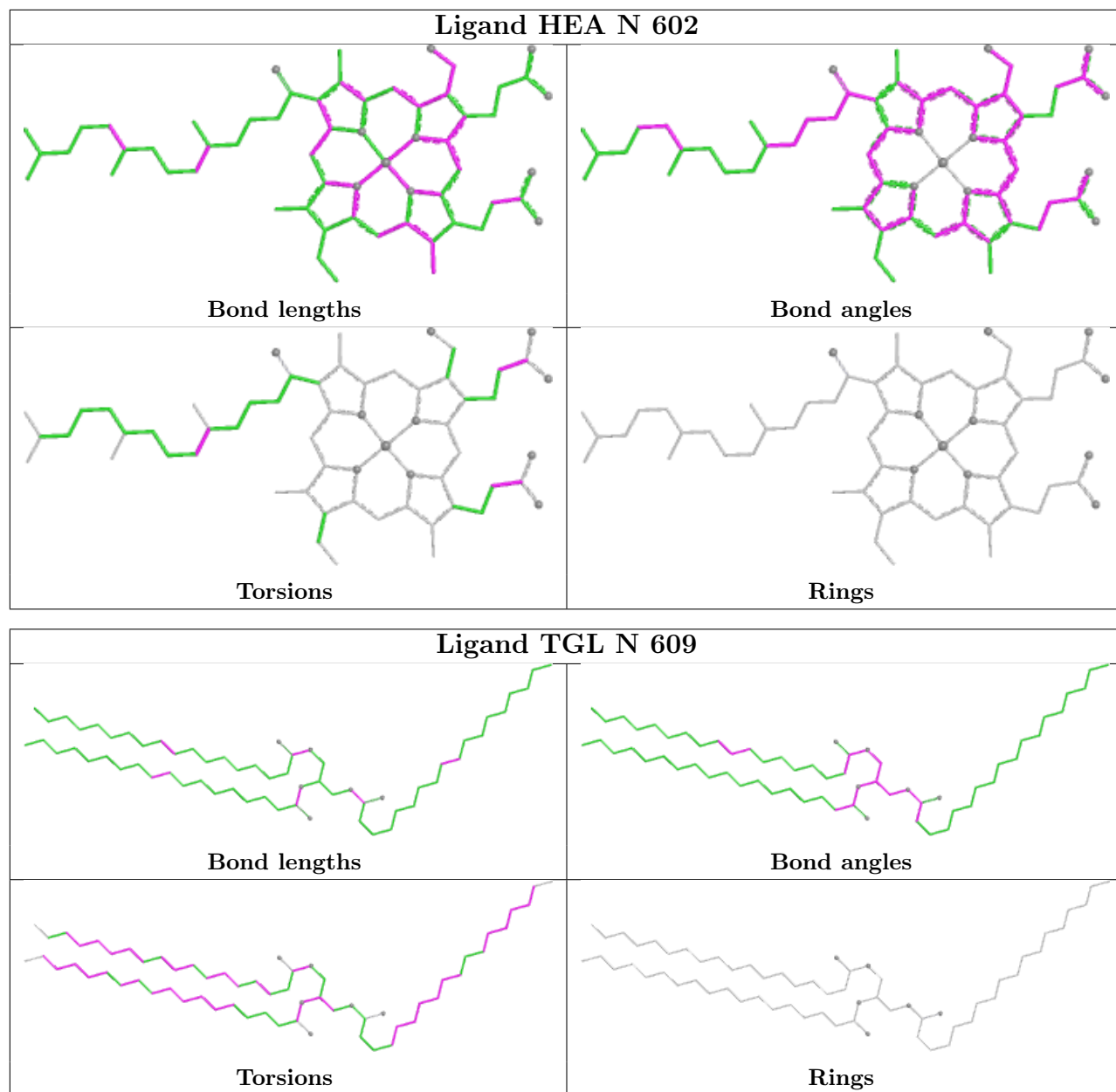


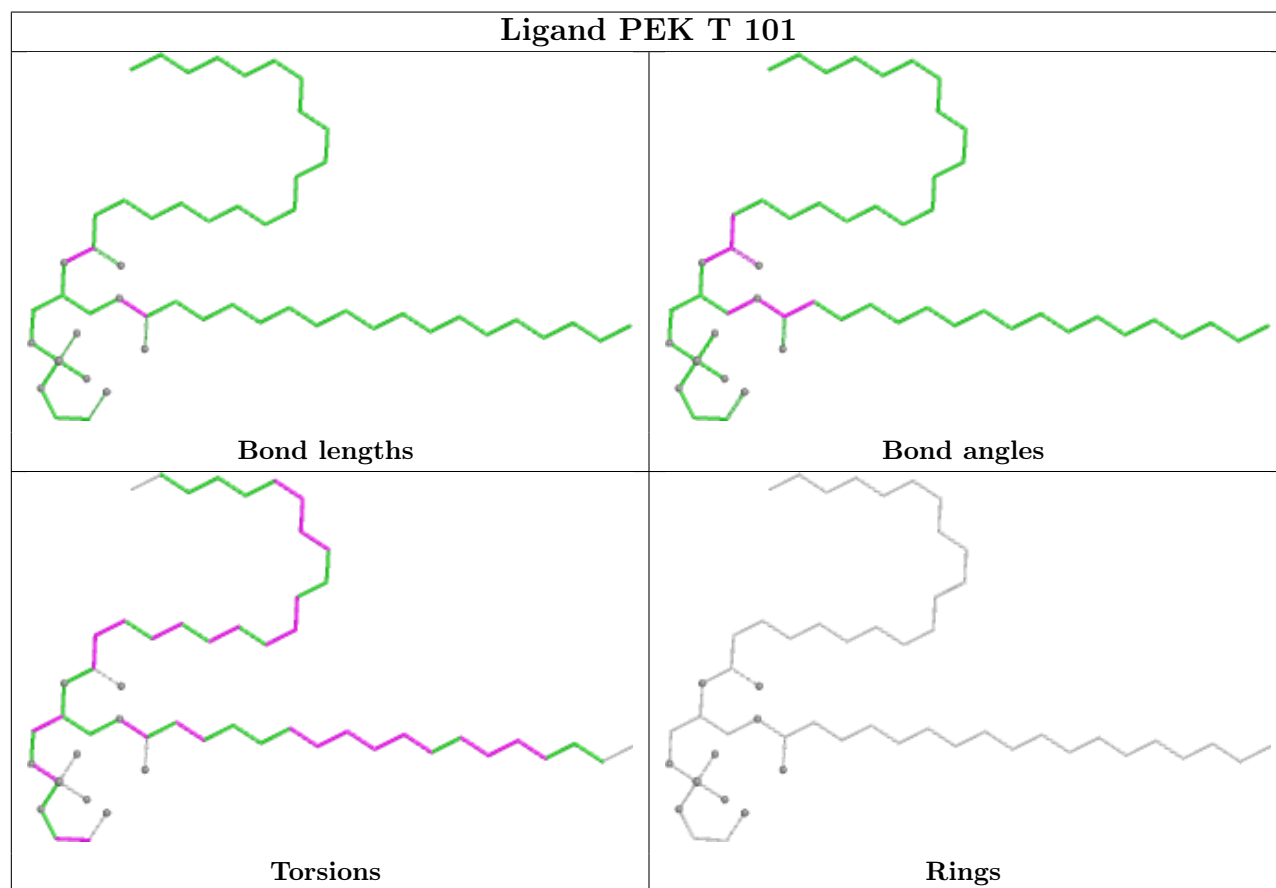
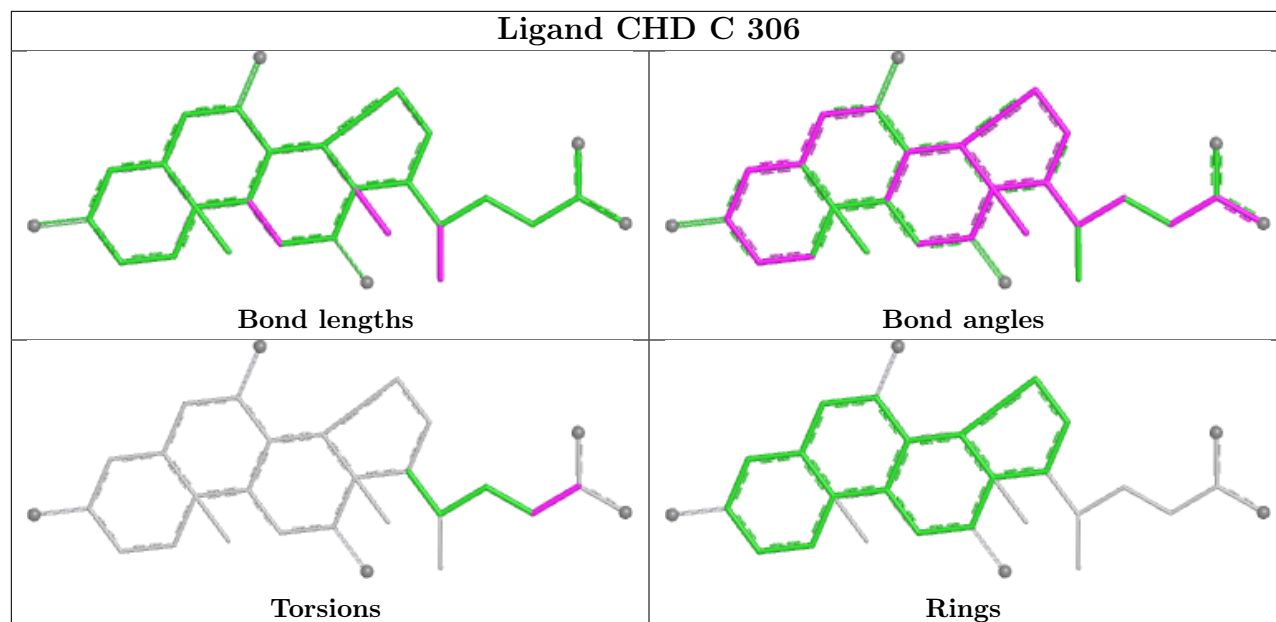


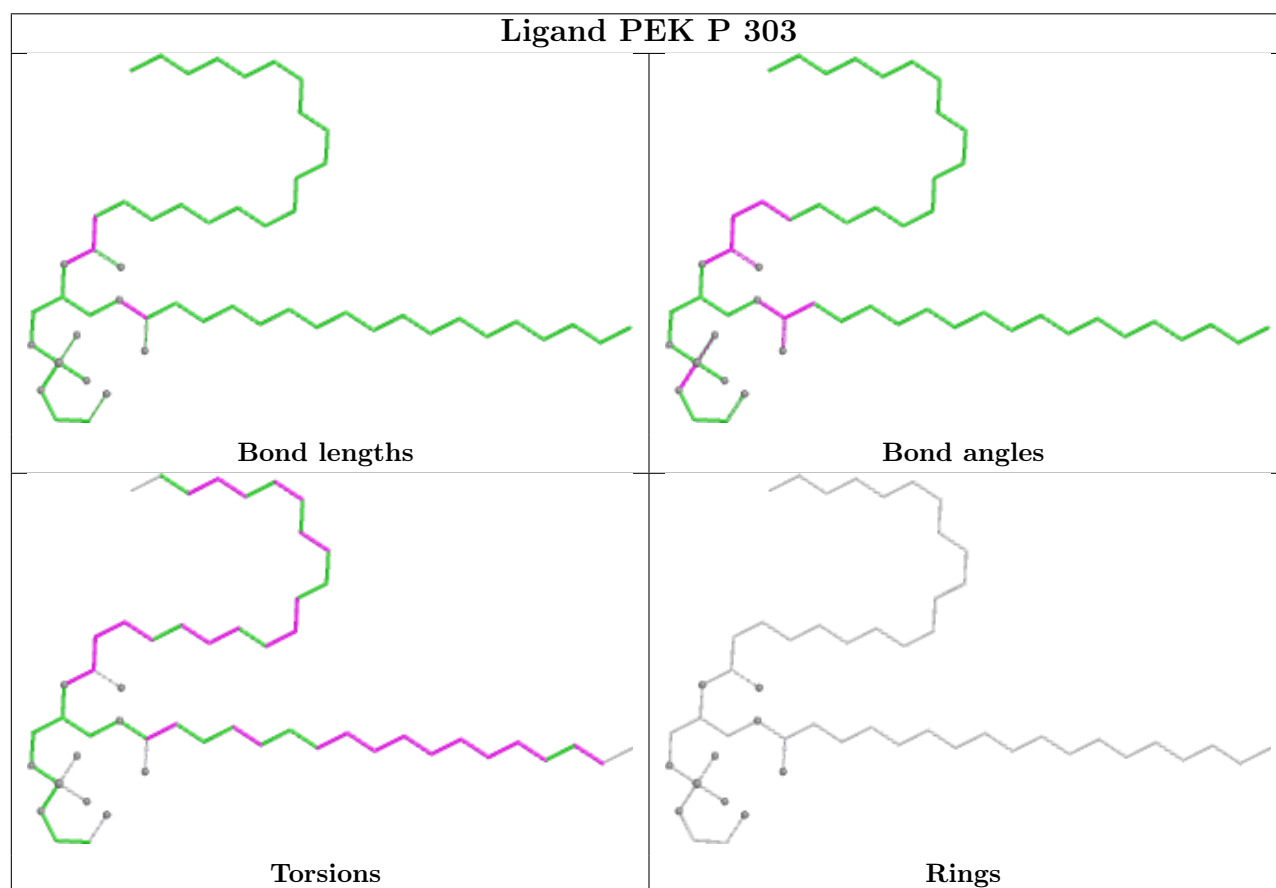
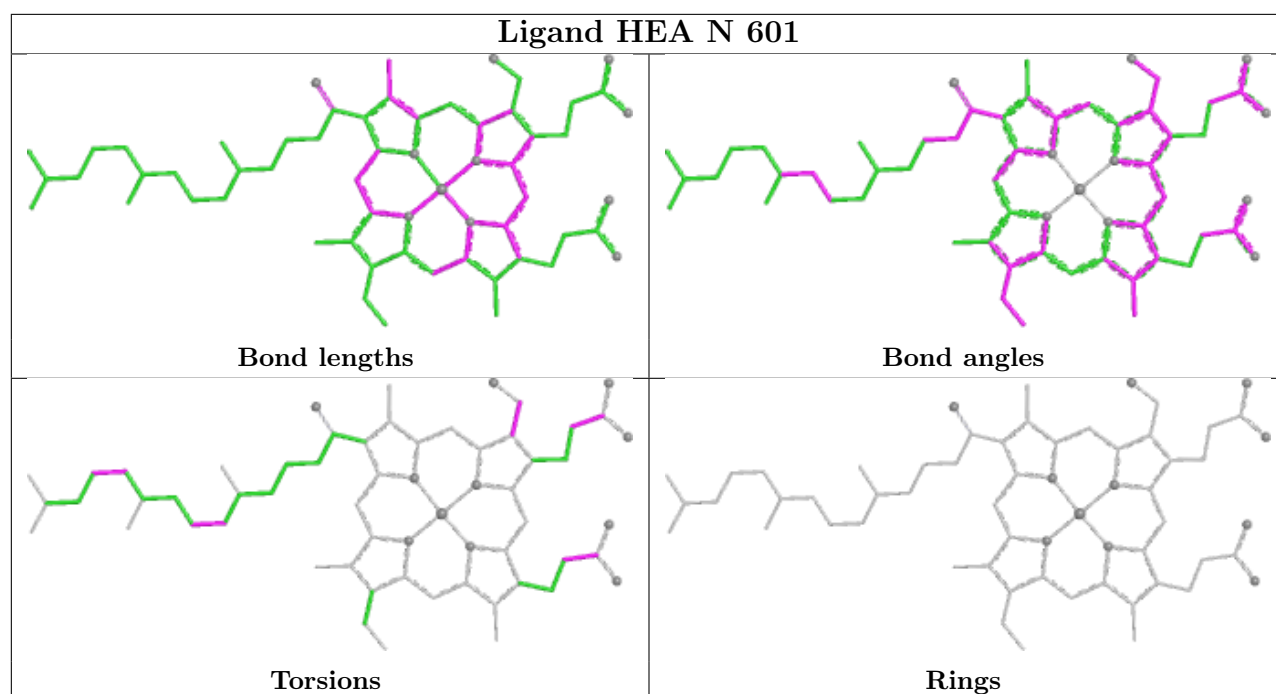


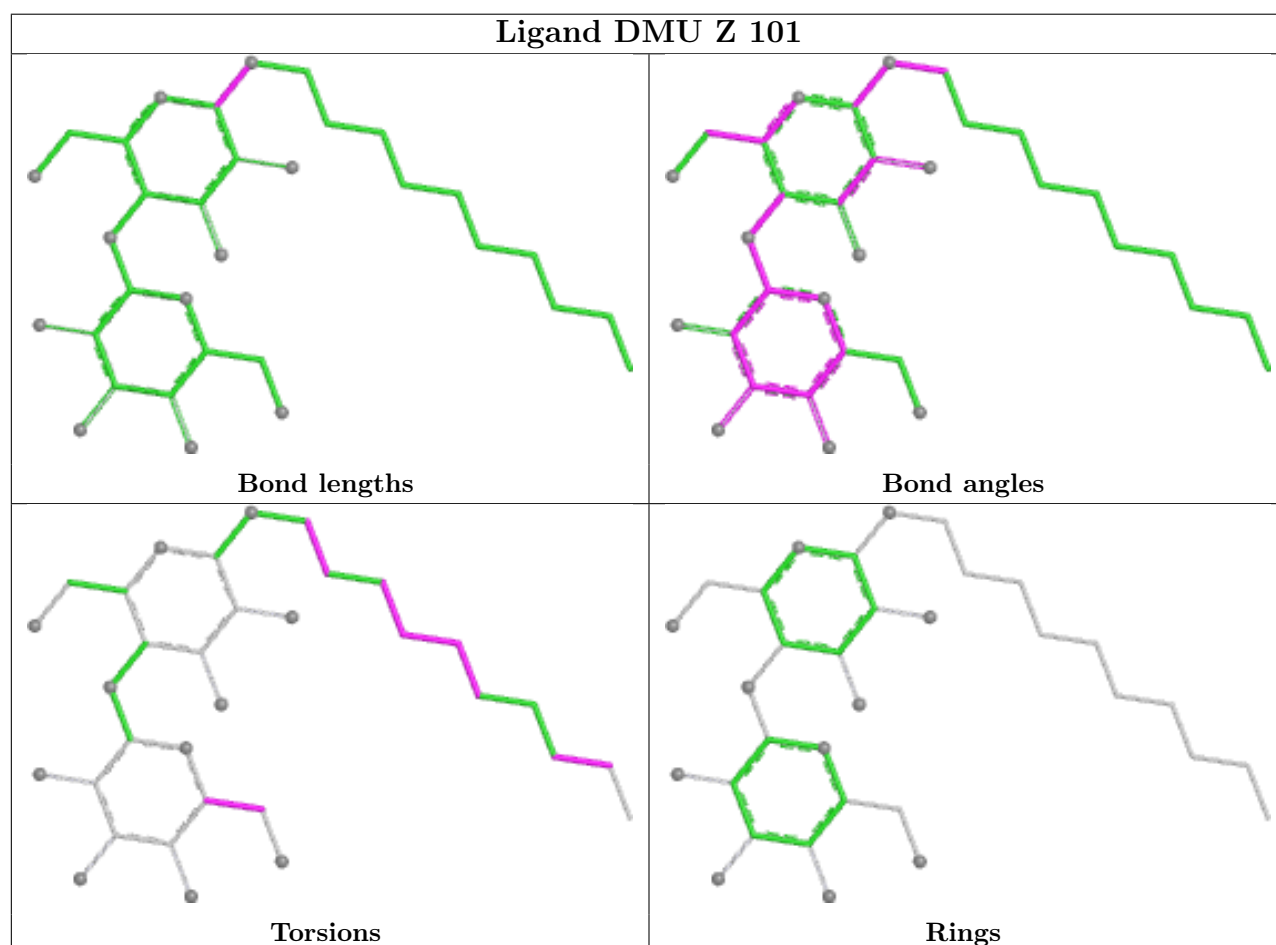
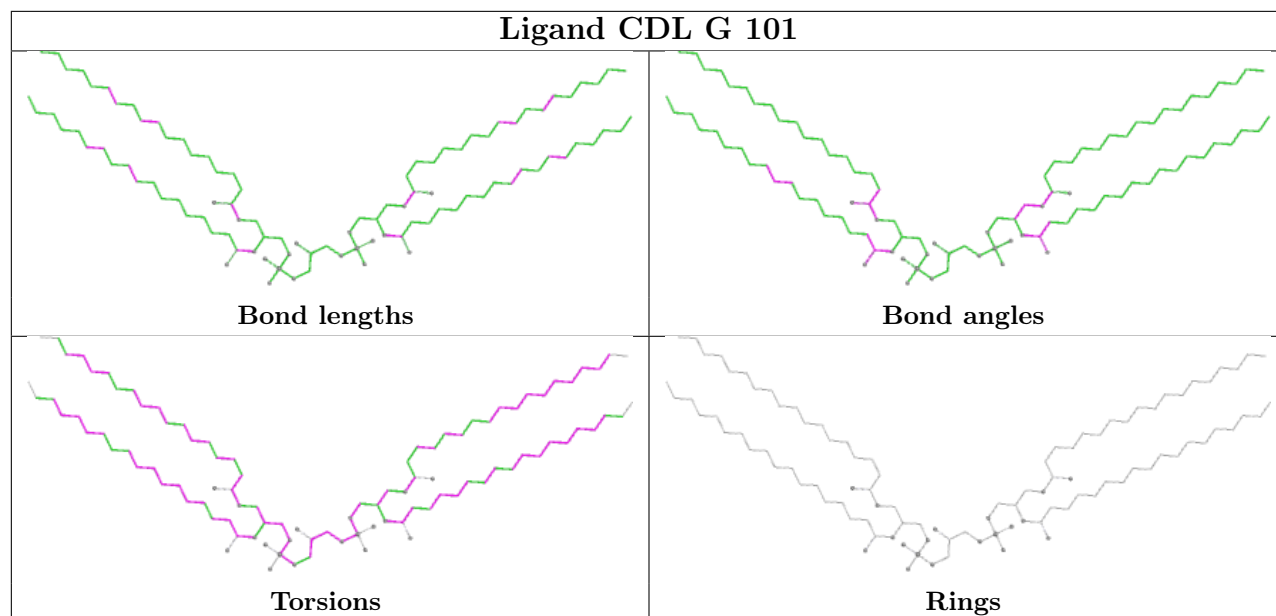


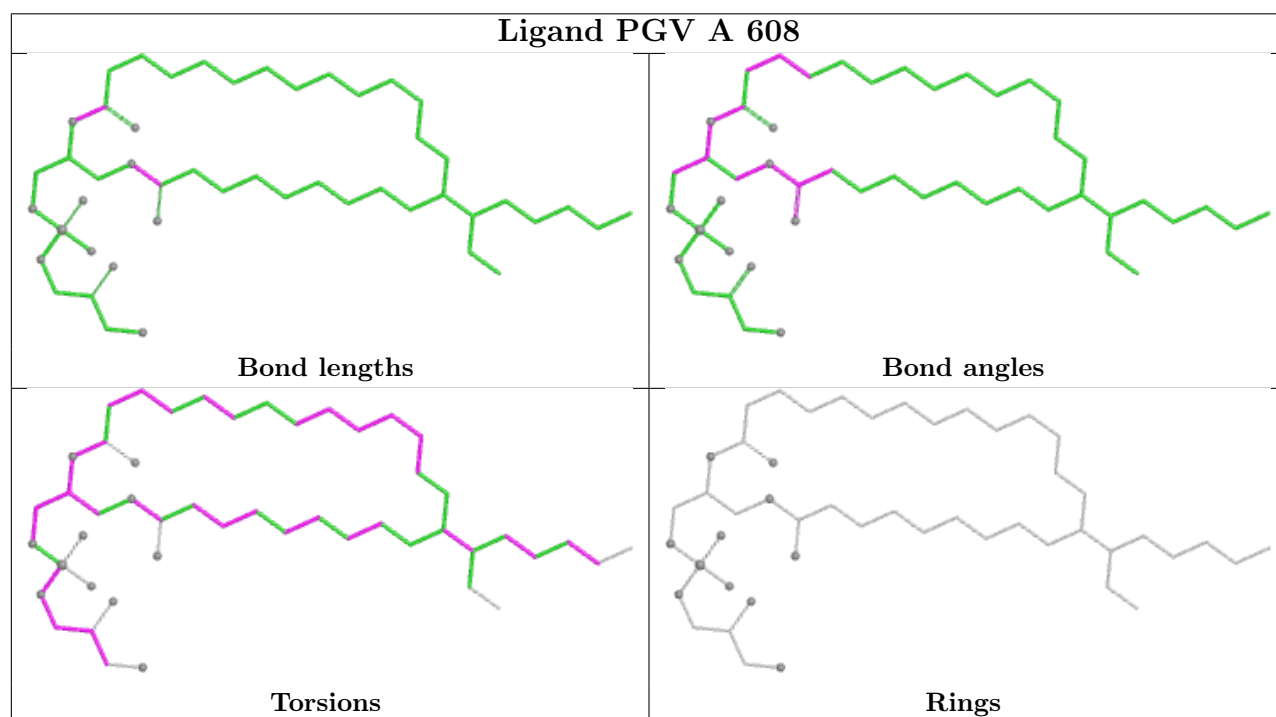
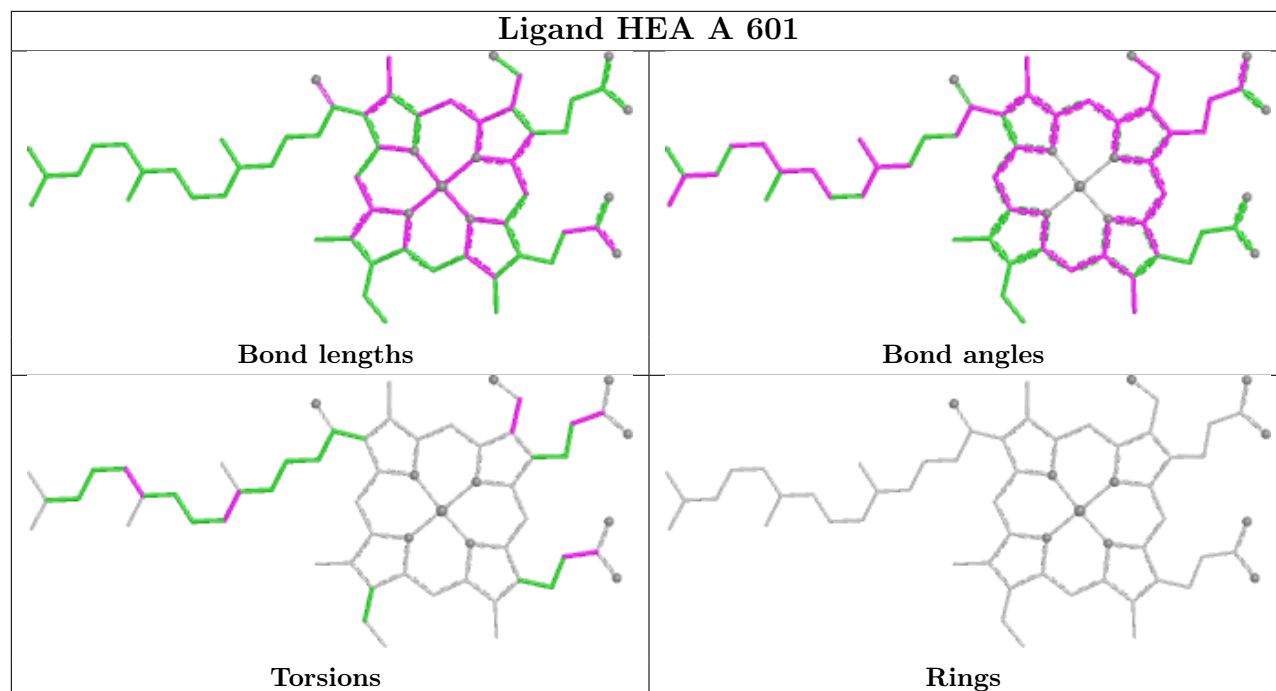




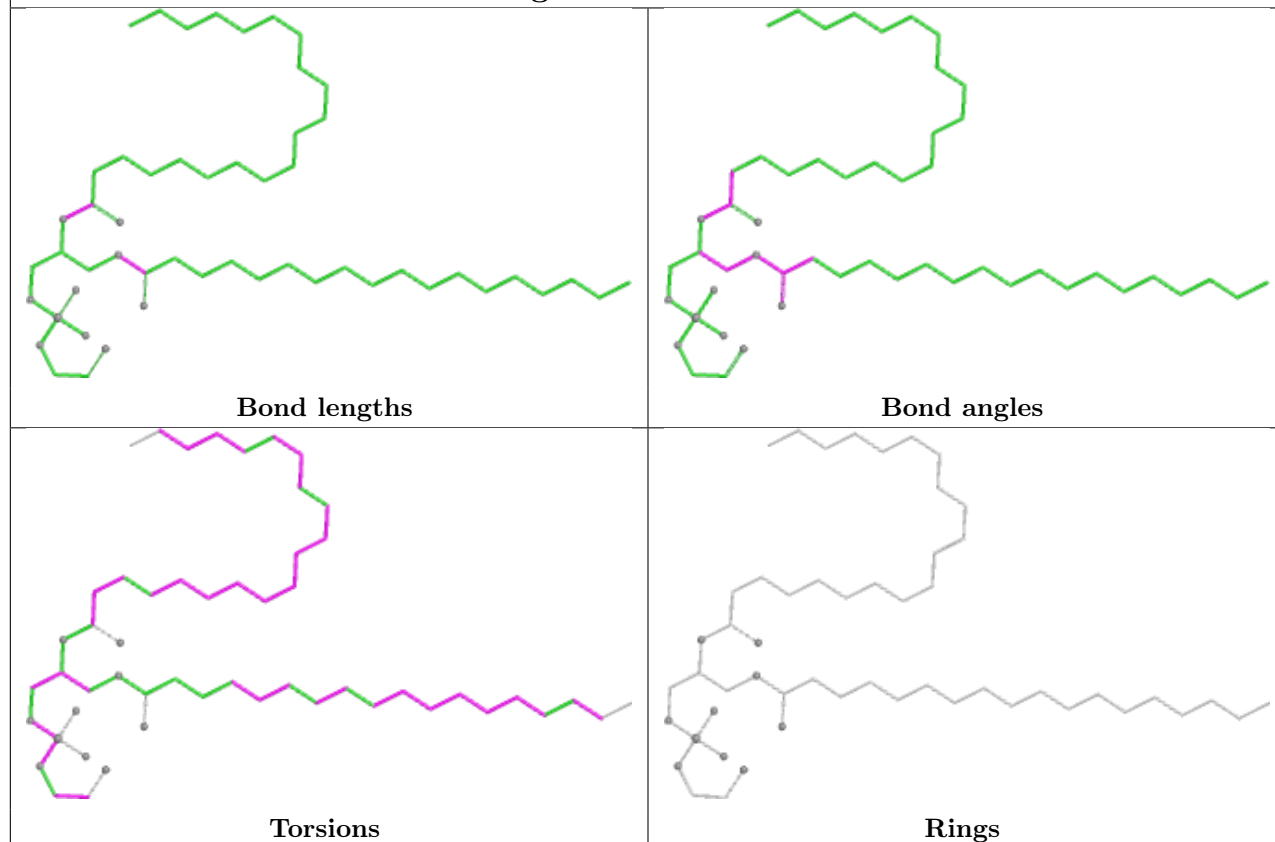




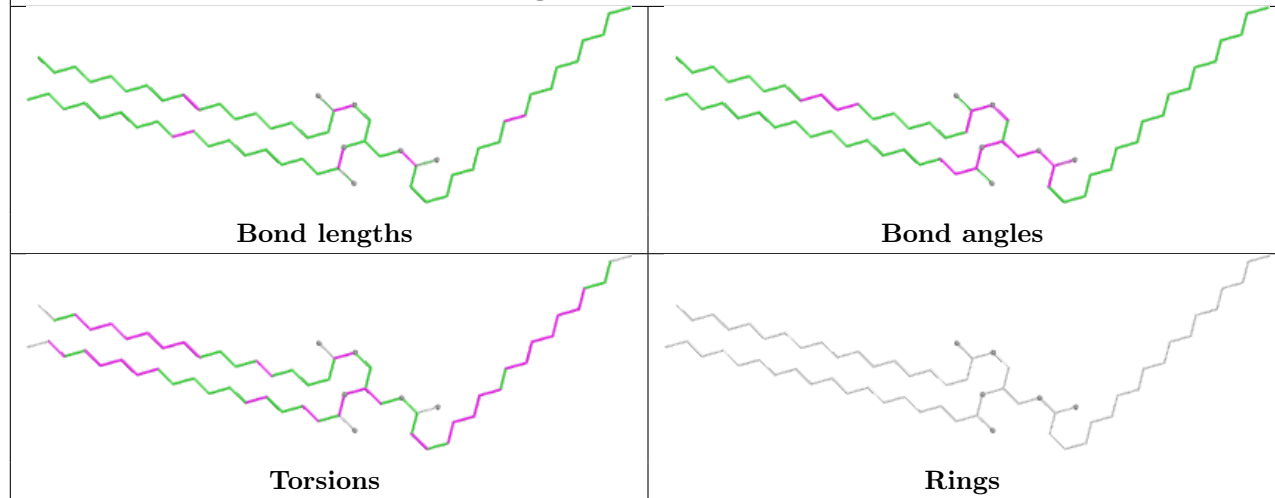


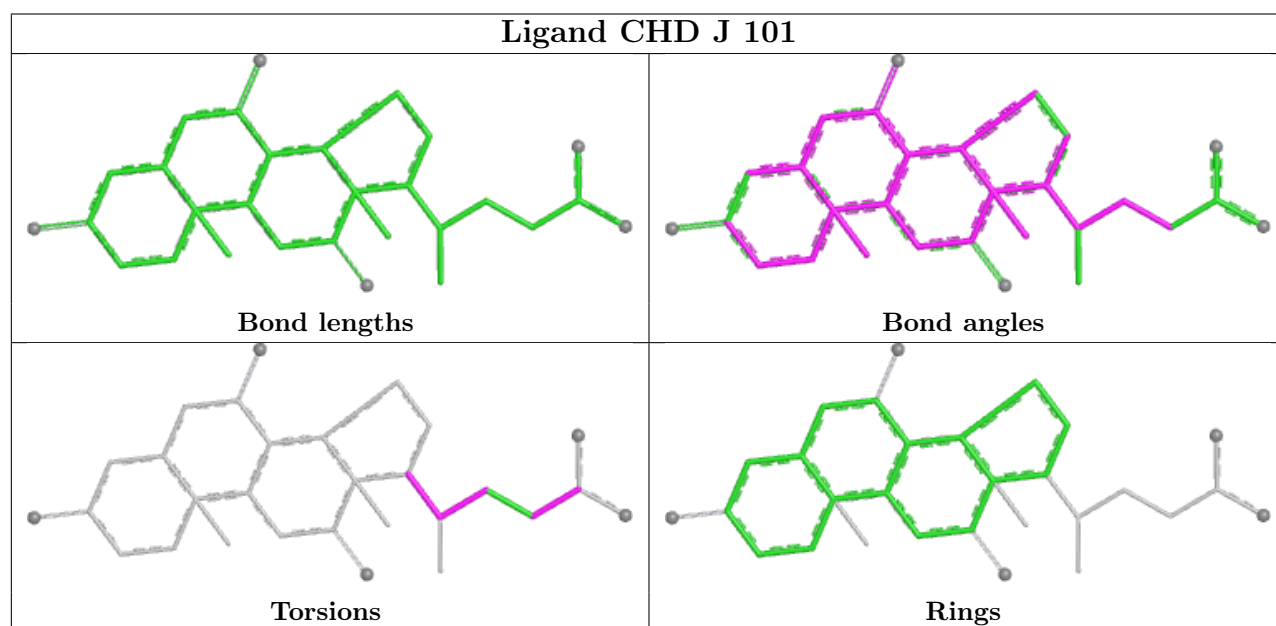
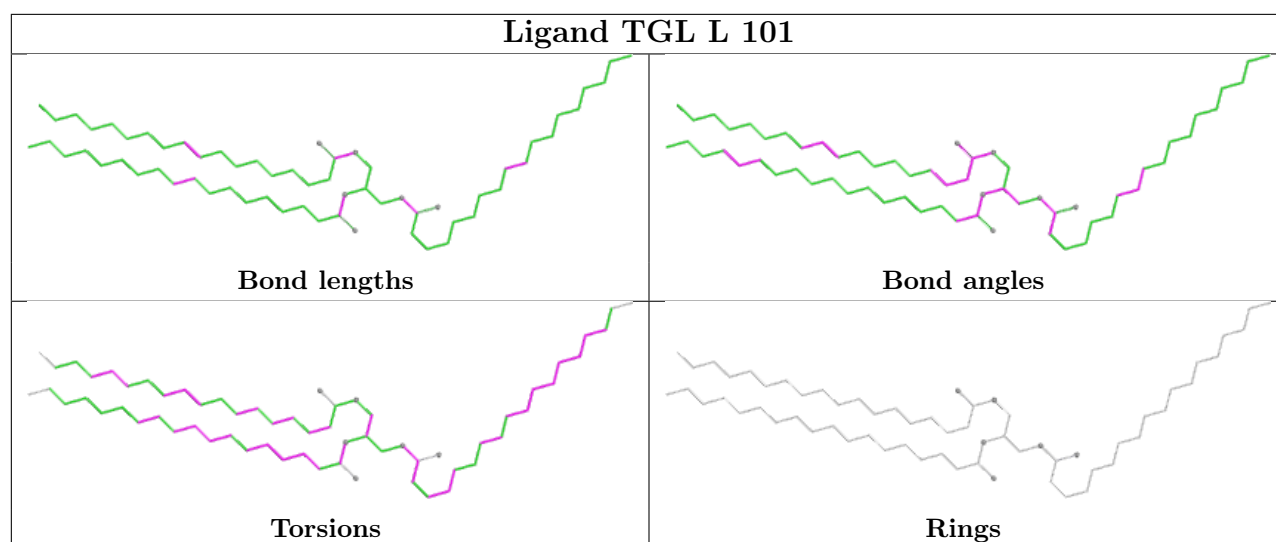


## Ligand PEK P 308

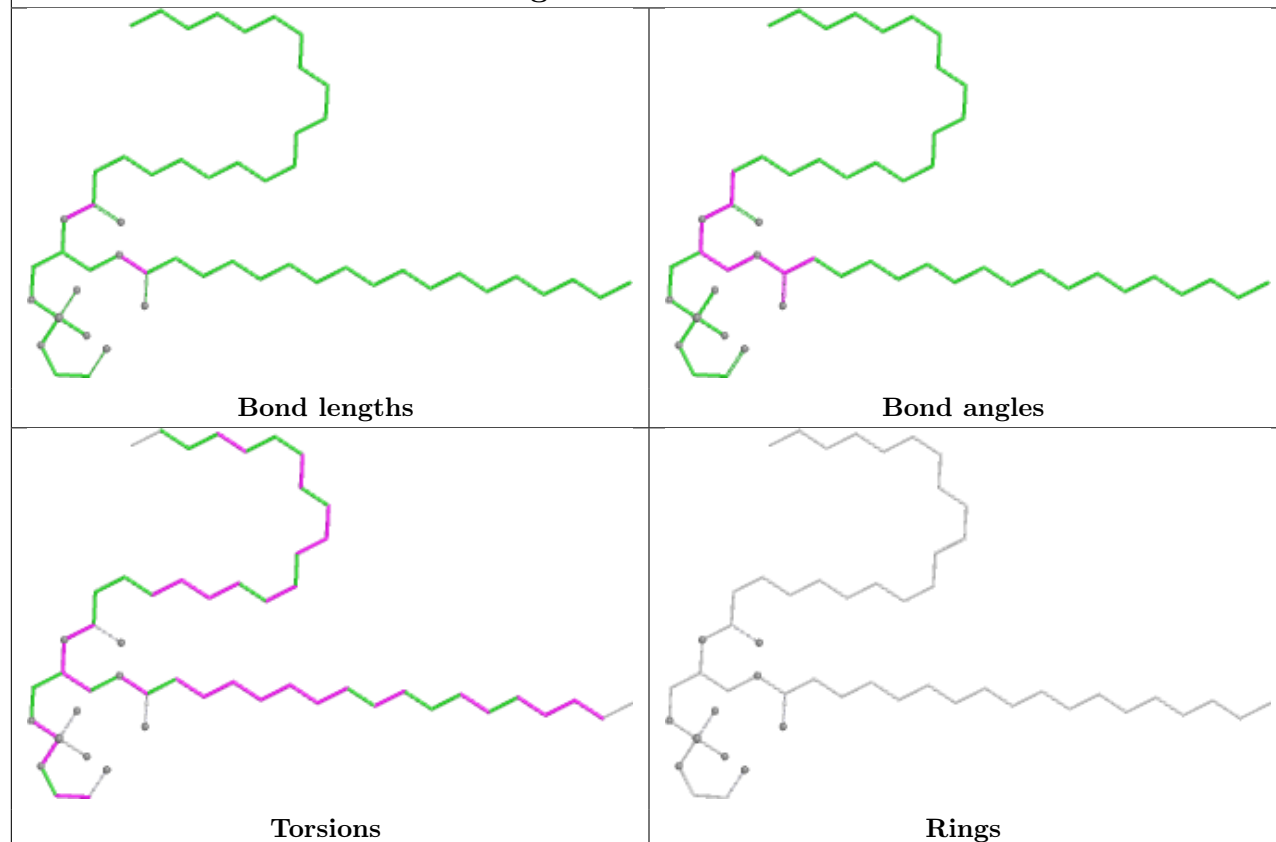


## Ligand TGL B 301

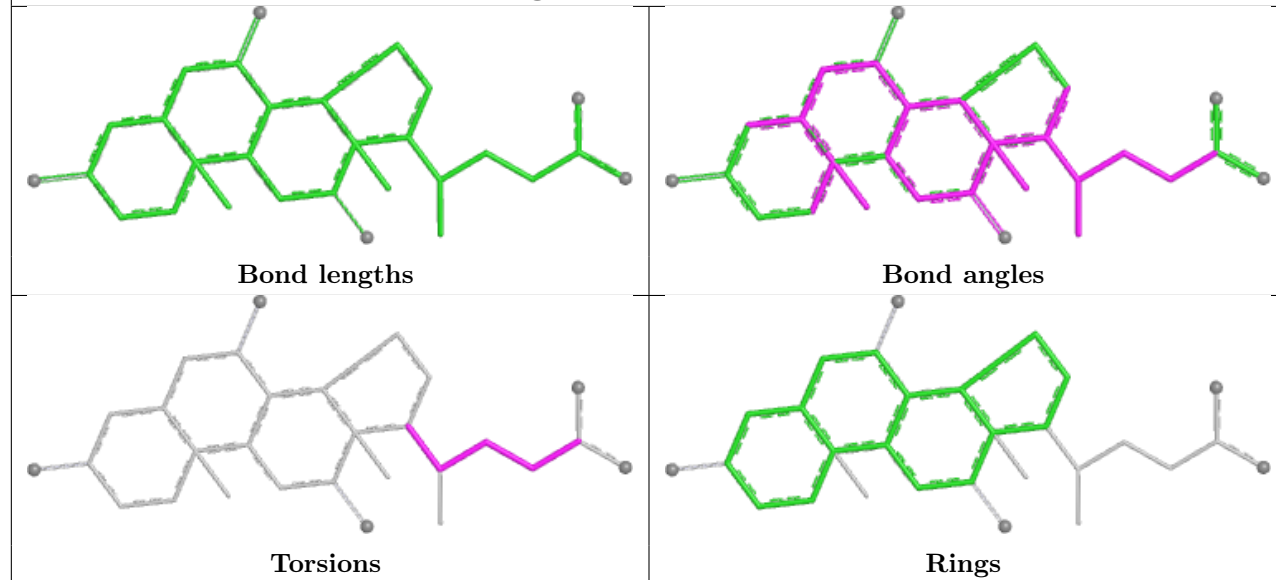


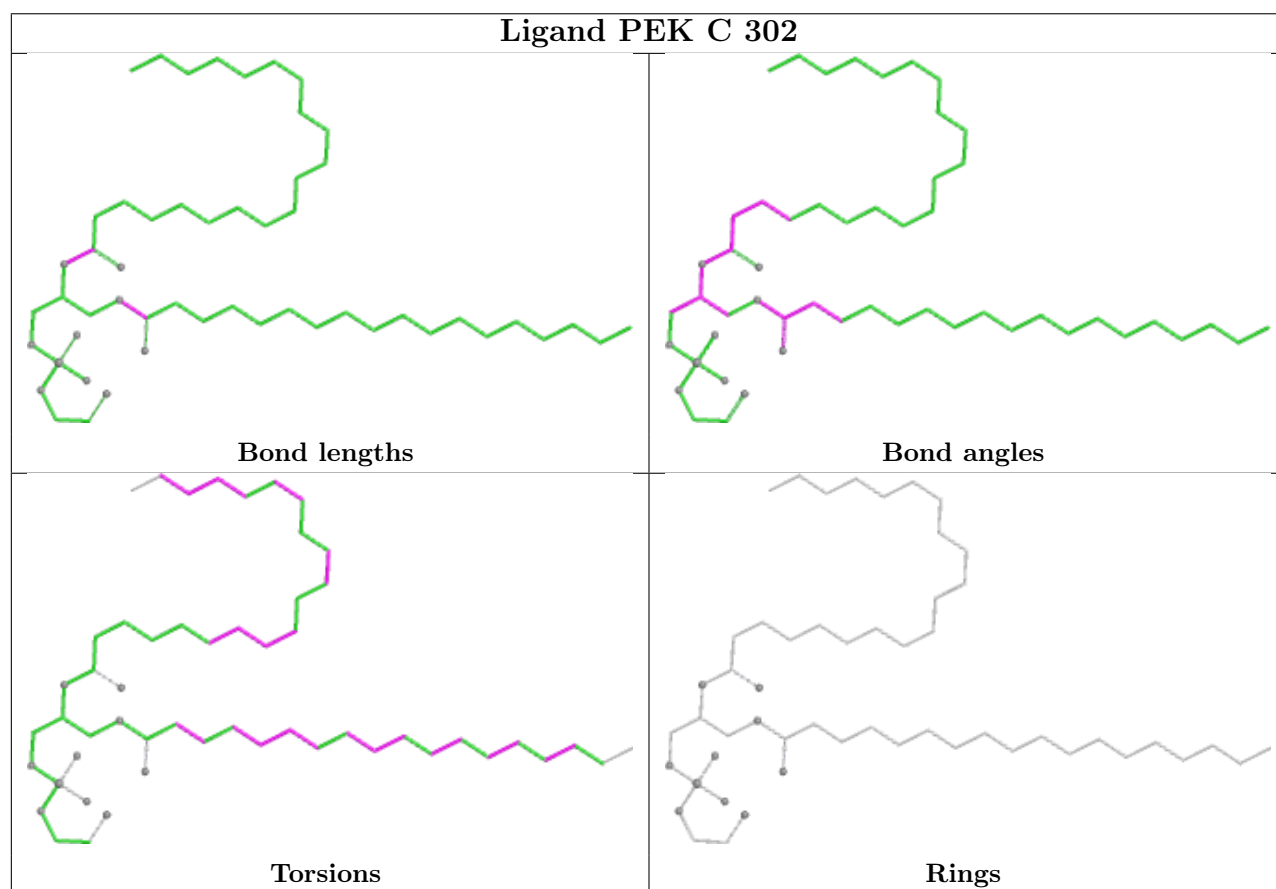
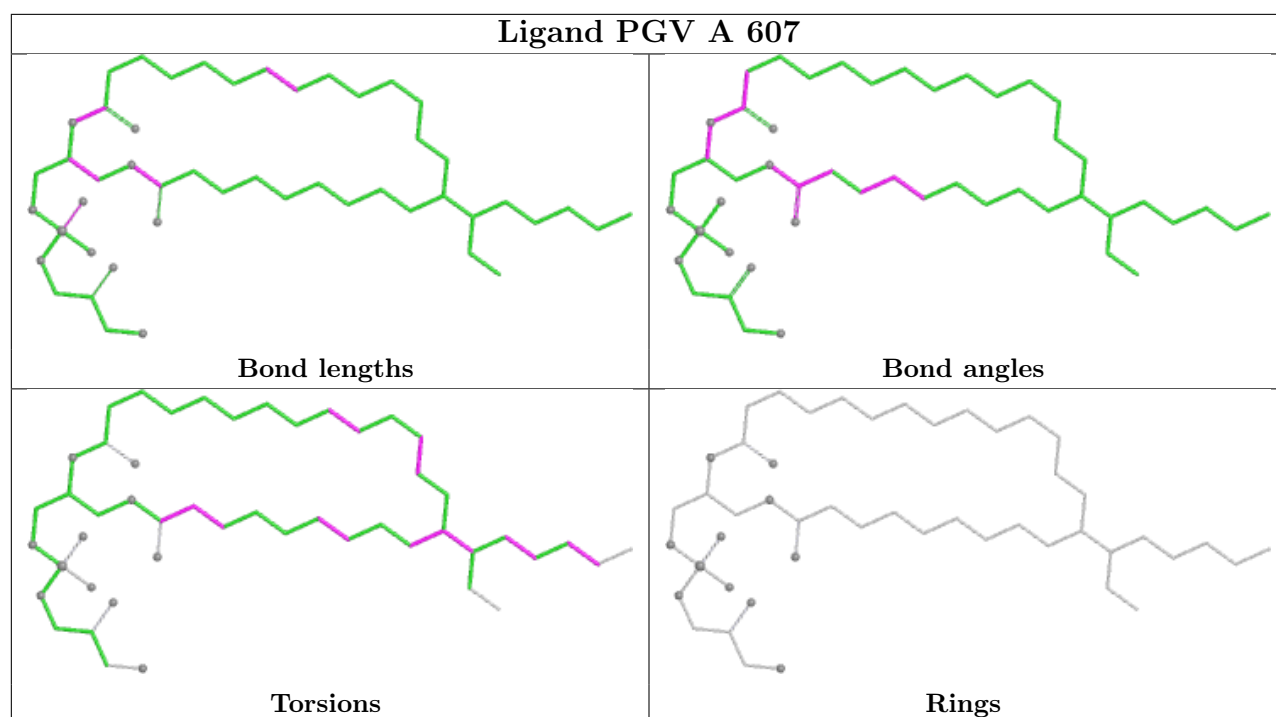


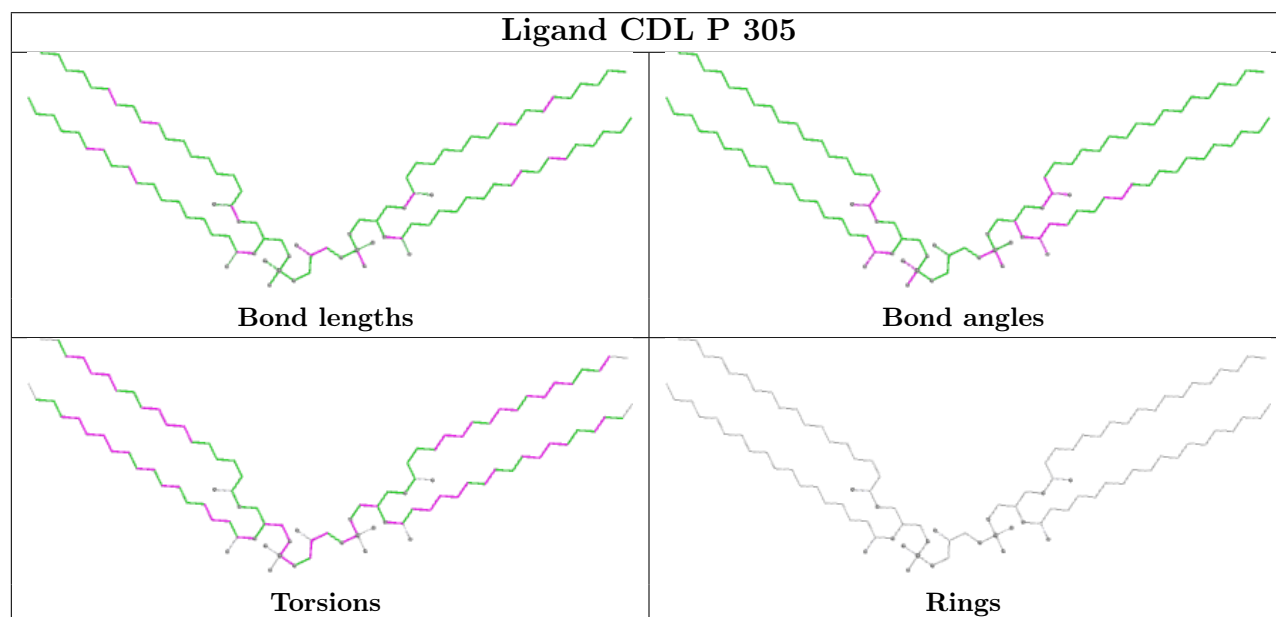
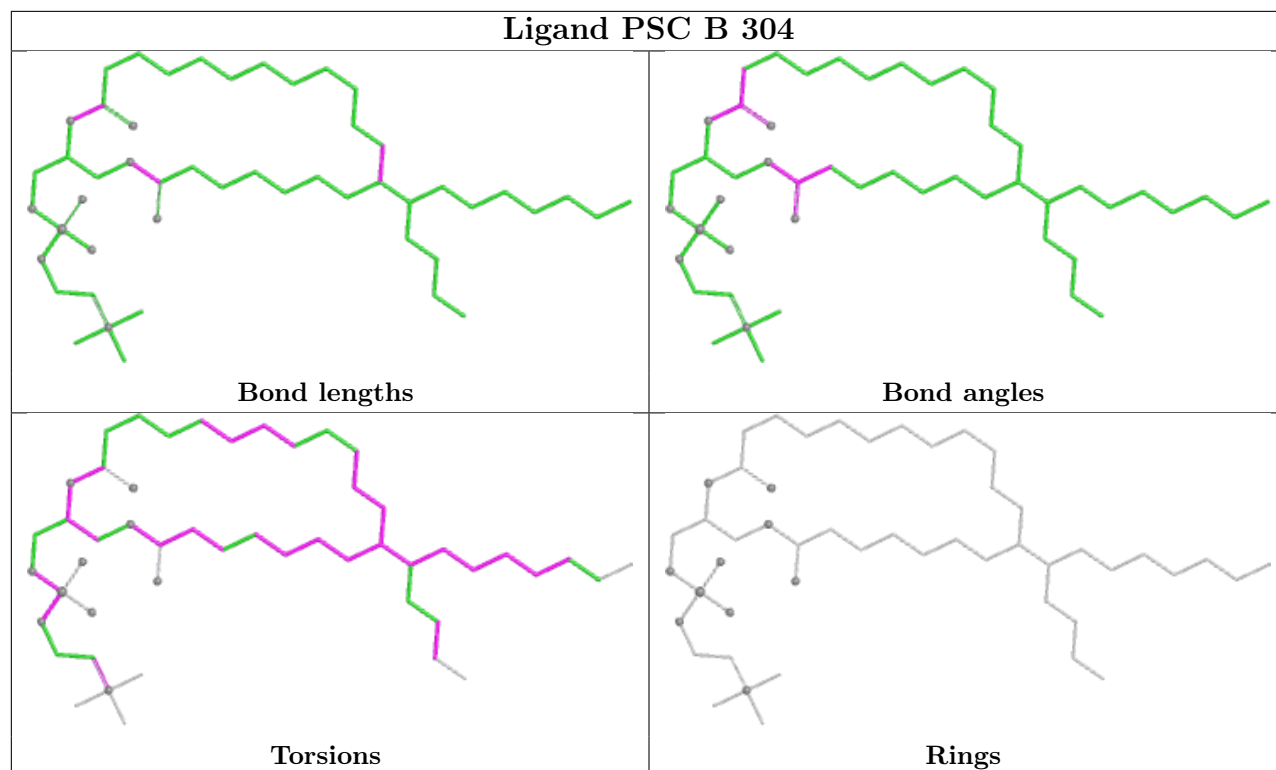
## Ligand PEK G 102

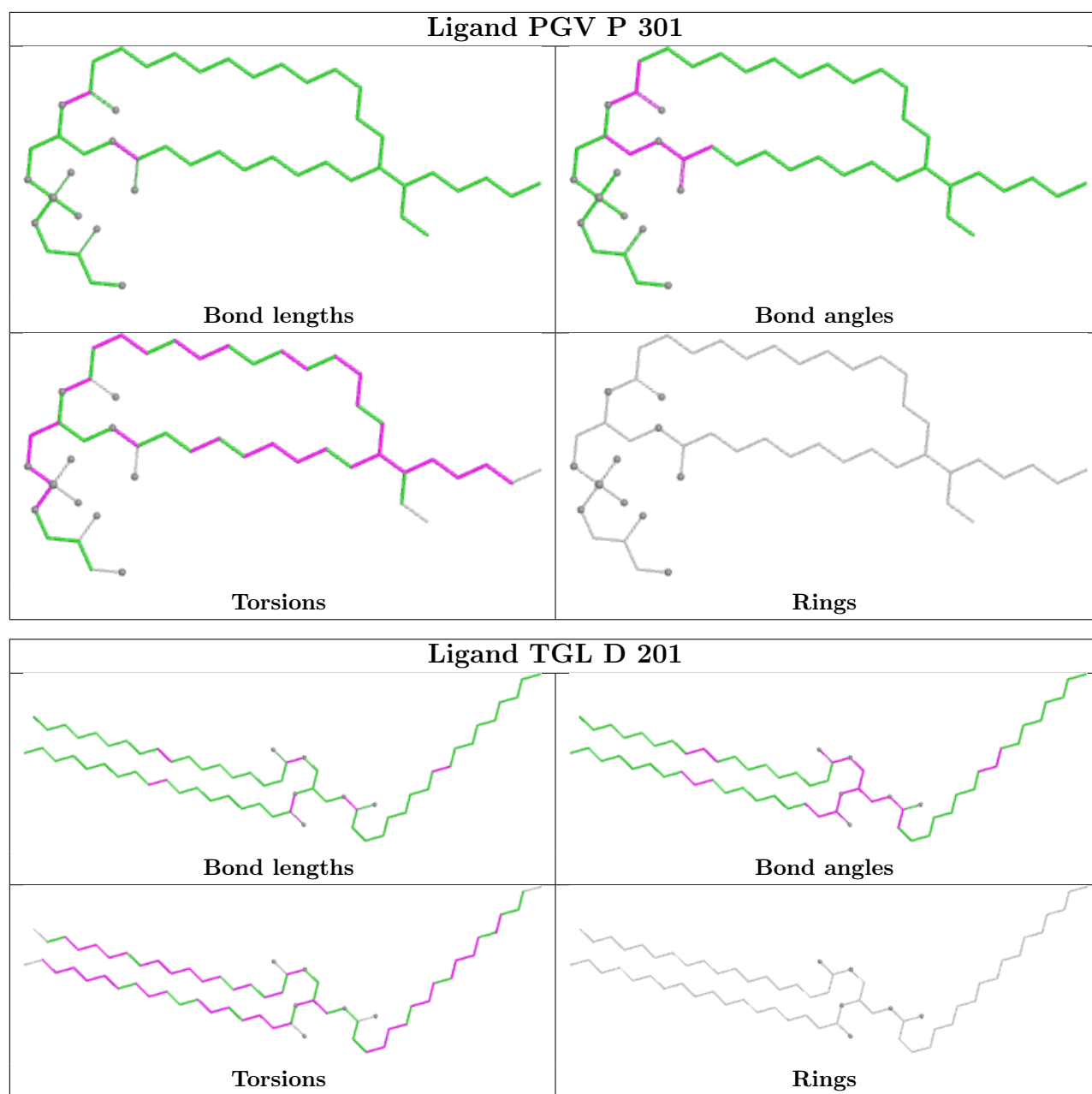


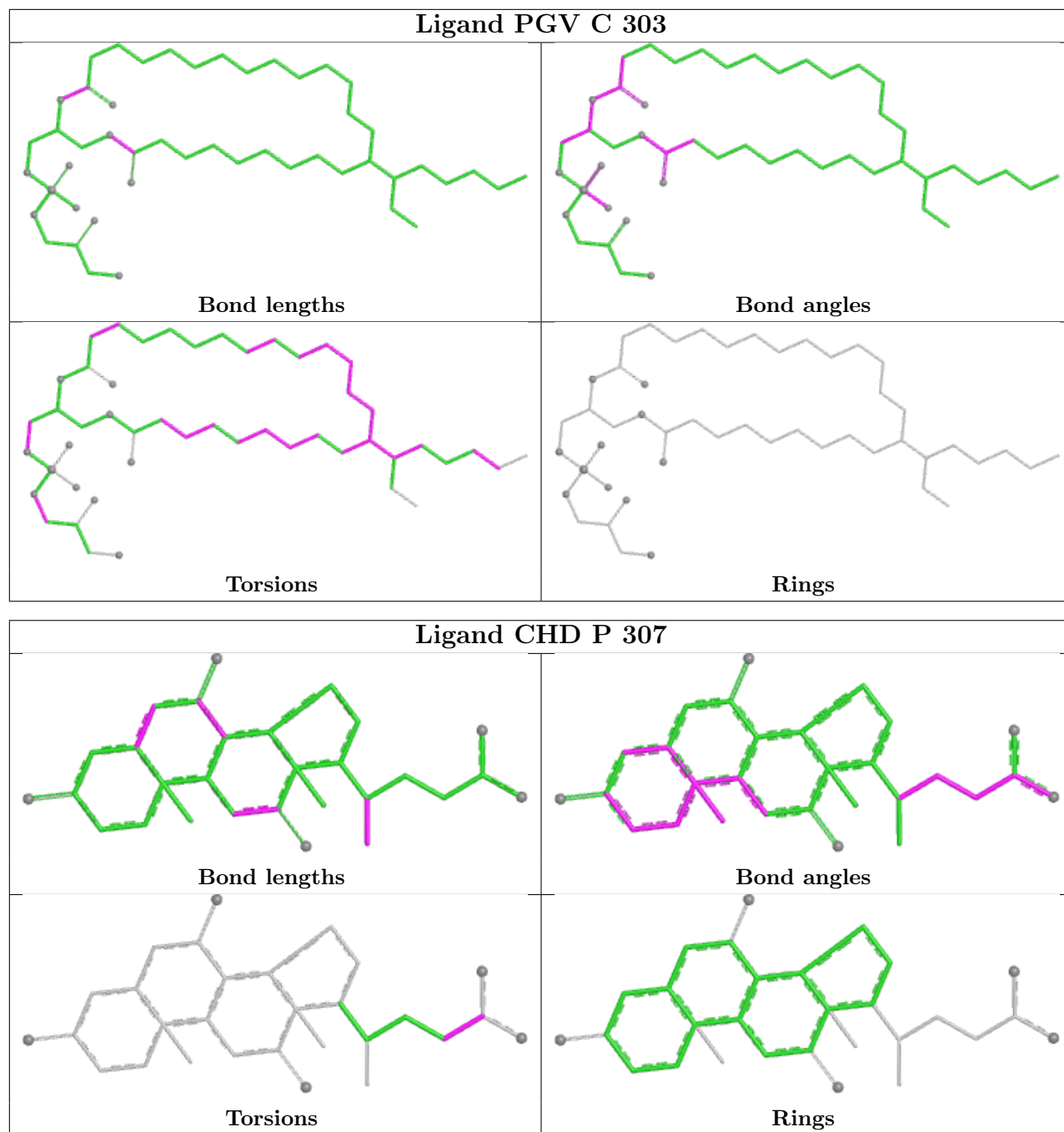
## Ligand CHD C 305

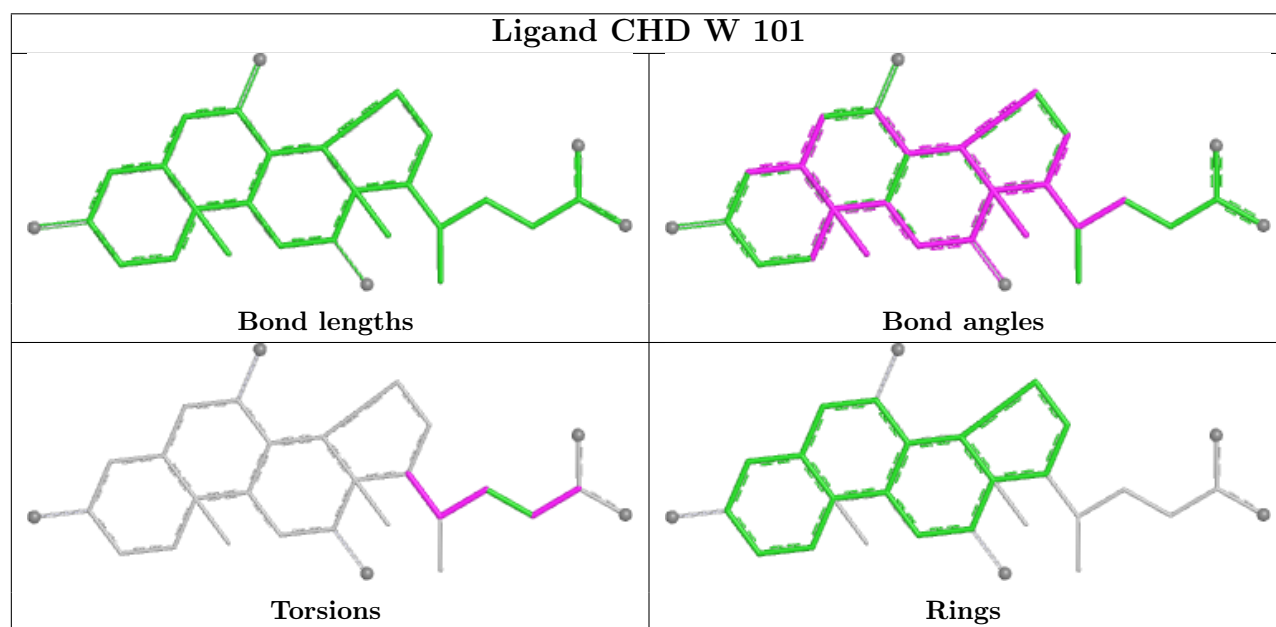
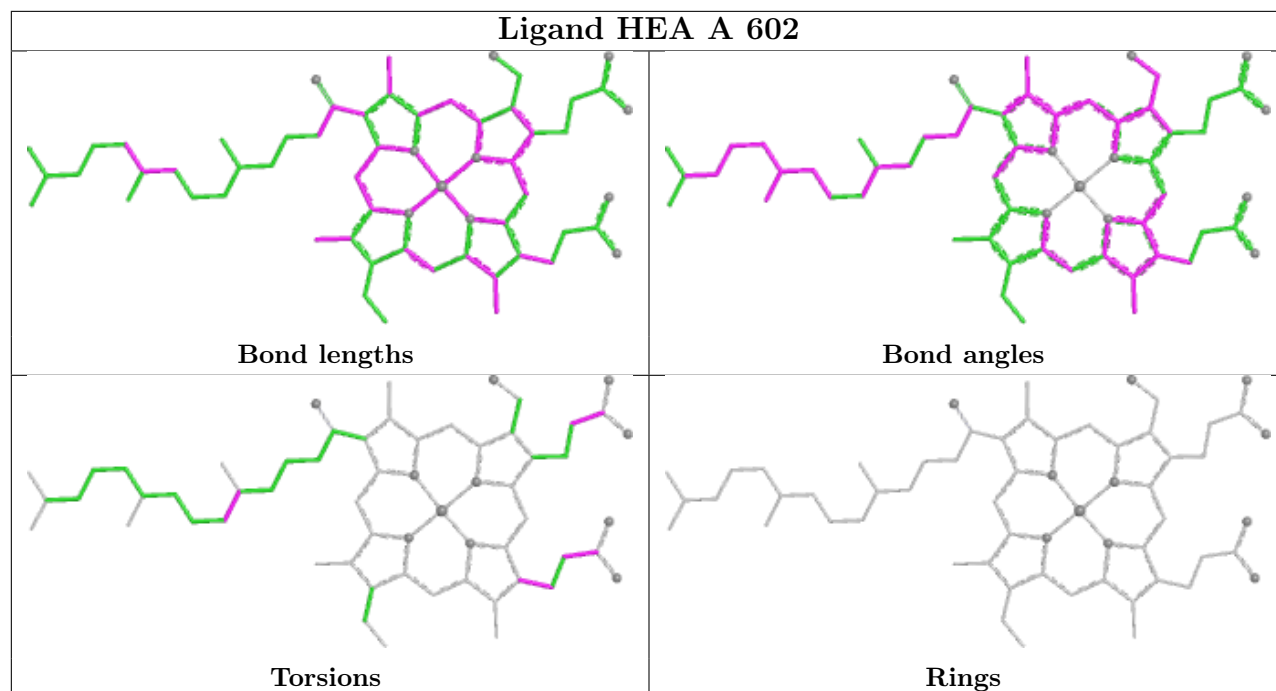




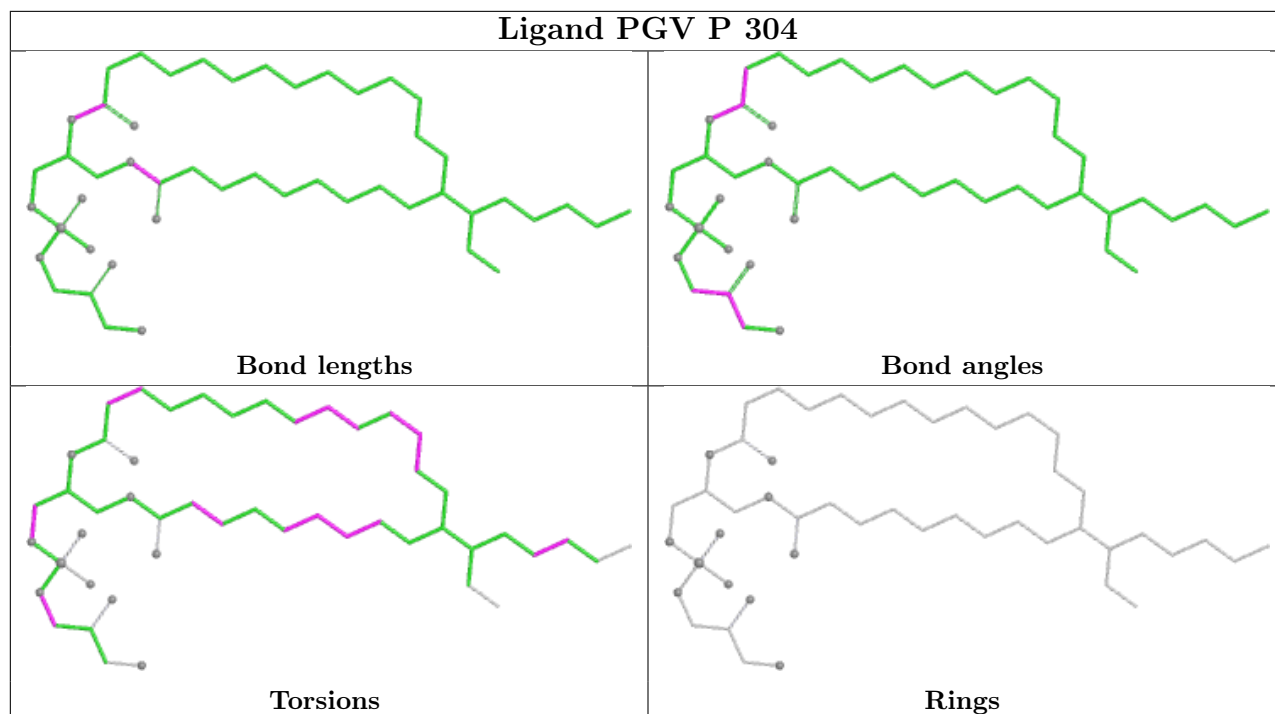




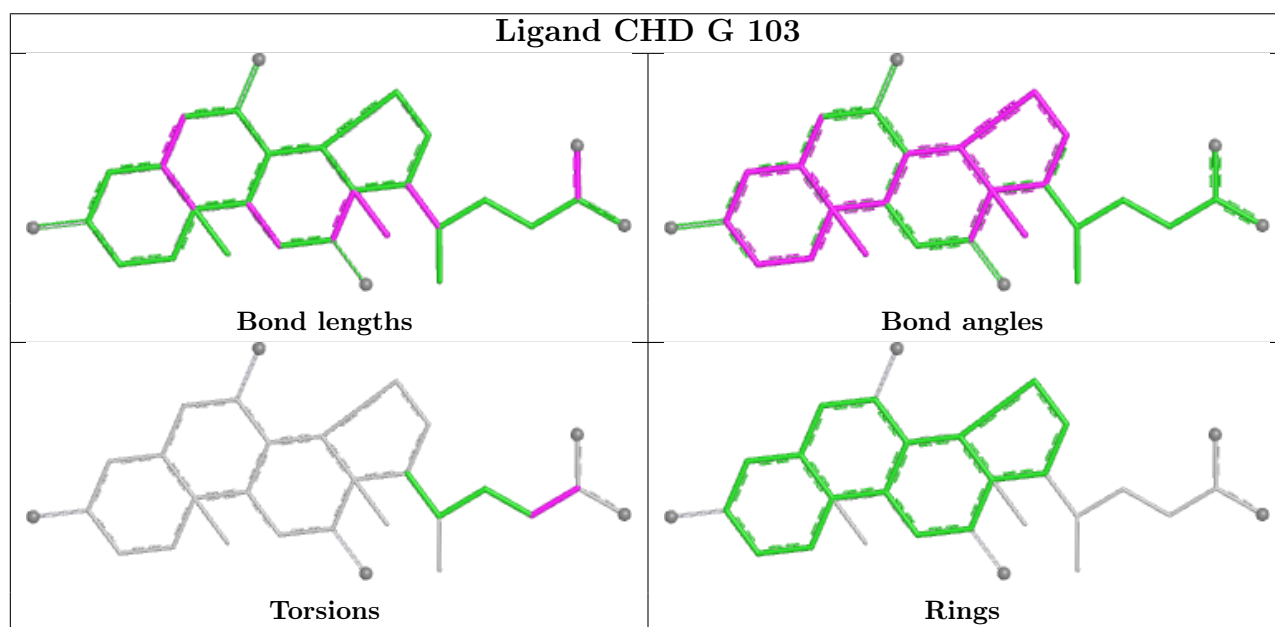


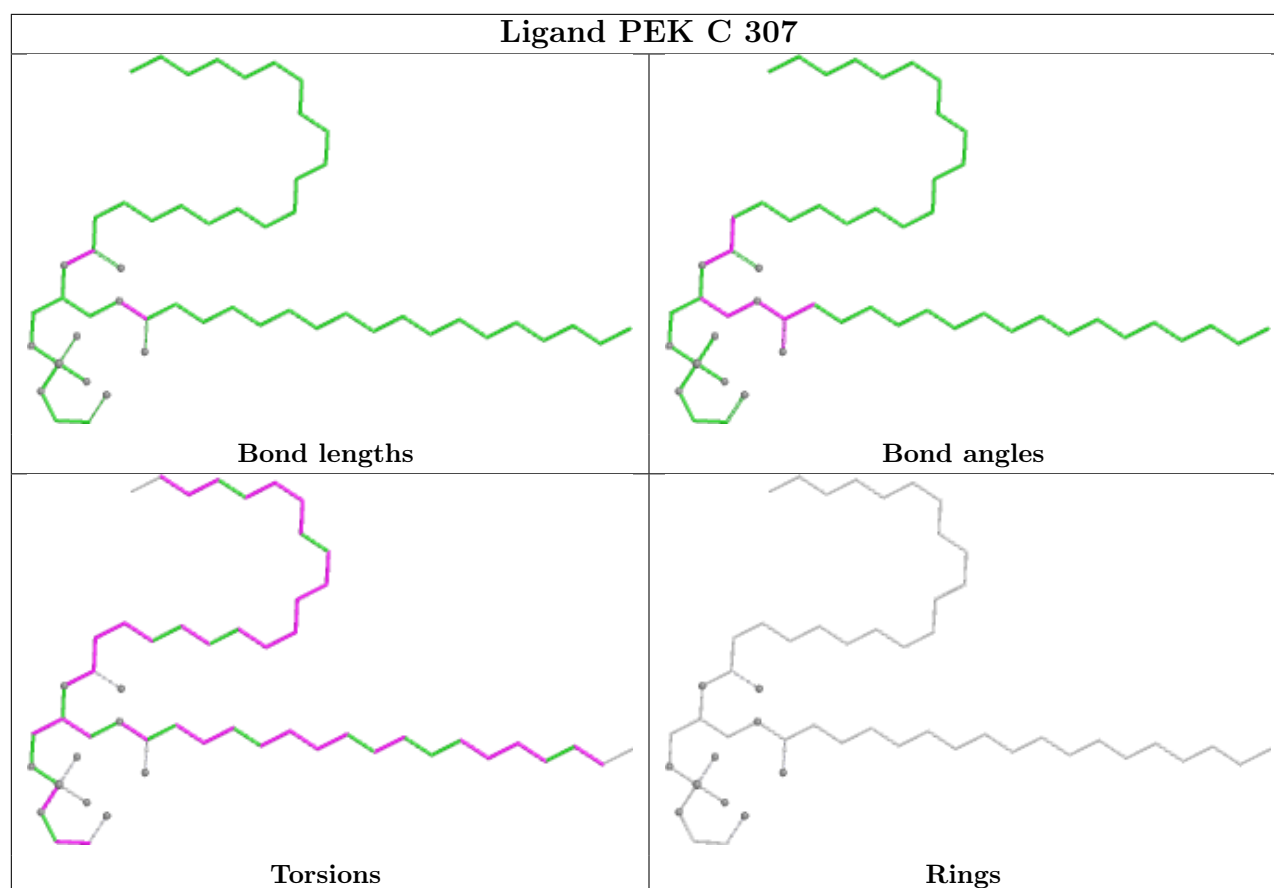


## Ligand PGV P 304



## Ligand CHD G 103





## 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%) | -0.21  | 2 (0%) 88 90  | 6, 15, 22, 51         | 6 (1%) |
| 1   | N     | 513/514 (99%) | -0.21  | 3 (0%) 85 87  | 6, 14, 20, 51         | 6 (1%) |
| 2   | B     | 226/227 (99%) | 0.16   | 9 (3%) 42 45  | 9, 18, 39, 65         | 1 (0%) |
| 2   | O     | 226/227 (99%) | 0.31   | 13 (5%) 29 30 | 11, 17, 41, 62        | 0      |
| 3   | C     | 259/261 (99%) | -0.10  | 4 (1%) 72 75  | 11, 17, 26, 59        | 3 (1%) |
| 3   | P     | 259/261 (99%) | -0.08  | 2 (0%) 82 85  | 9, 16, 26, 46         | 3 (1%) |
| 4   | D     | 144/147 (97%) | 0.14   | 2 (1%) 73 76  | 12, 18, 35, 57        | 0      |
| 4   | Q     | 144/147 (97%) | 0.96   | 20 (13%) 6 6  | 13, 23, 48, 106       | 0      |
| 5   | E     | 105/109 (96%) | 0.08   | 4 (3%) 44 47  | 11, 17, 41, 88        | 0      |
| 5   | R     | 105/109 (96%) | 0.41   | 2 (1%) 66 70  | 13, 18, 36, 89        | 0      |
| 6   | F     | 98/98 (100%)  | 0.79   | 9 (9%) 14 15  | 15, 23, 68, 118       | 0      |
| 6   | S     | 98/98 (100%)  | 0.67   | 9 (9%) 14 15  | 13, 20, 61, 97        | 0      |
| 7   | G     | 83/85 (97%)   | 0.98   | 21 (25%) 1 1  | 11, 20, 73, 90        | 0      |
| 7   | T     | 83/85 (97%)   | 1.15   | 21 (25%) 1 1  | 10, 20, 77, 101       | 0      |
| 8   | H     | 79/85 (92%)   | 0.83   | 14 (17%) 4 3  | 16, 24, 62, 76        | 0      |
| 8   | U     | 79/85 (92%)   | 0.78   | 14 (17%) 4 3  | 14, 21, 63, 76        | 0      |
| 9   | I     | 72/73 (98%)   | 0.90   | 13 (18%) 3 3  | 15, 26, 53, 63        | 0      |
| 9   | V     | 72/73 (98%)   | 1.02   | 10 (13%) 6 6  | 13, 26, 47, 58        | 0      |
| 10  | J     | 58/59 (98%)   | 0.67   | 4 (6%) 23 24  | 17, 25, 45, 86        | 0      |
| 10  | W     | 58/59 (98%)   | 0.72   | 5 (8%) 16 17  | 13, 22, 51, 91        | 0      |
| 11  | K     | 49/56 (87%)   | 0.54   | 3 (6%) 27 29  | 16, 22, 36, 42        | 0      |
| 11  | X     | 49/56 (87%)   | 0.93   | 3 (6%) 27 29  | 16, 21, 37, 43        | 0      |
| 12  | L     | 46/47 (97%)   | 0.28   | 4 (8%) 16 17  | 15, 19, 37, 64        | 0      |
| 12  | Y     | 46/47 (97%)   | 0.44   | 4 (8%) 16 17  | 12, 19, 38, 70        | 0      |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|----------------|-----------------------|---------|
| 13  | M     | 43/46 (93%)     | 0.31   | 5 (11%) 9 10   | 14, 18, 44, 77        | 0       |
| 13  | Z     | 43/46 (93%)     | 0.64   | 5 (11%) 9 10   | 12, 18, 48, 66        | 0       |
| All | All   | 3550/3614 (98%) | 0.24   | 205 (5%) 29 30 | 6, 17, 43, 118        | 19 (0%) |

All (205) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 6   | F     | 1   | ALA  | 12.6 |
| 6   | F     | 97  | ALA  | 10.6 |
| 6   | S     | 97  | ALA  | 10.6 |
| 6   | F     | 96  | LEU  | 8.8  |
| 6   | S     | 1   | ALA  | 8.7  |
| 7   | T     | 36  | TRP  | 8.1  |
| 4   | Q     | 6   | VAL  | 7.8  |
| 4   | Q     | 5   | VAL  | 7.3  |
| 6   | S     | 96  | LEU  | 7.1  |
| 7   | T     | 10  | GLY  | 7.0  |
| 4   | D     | 4   | SER  | 6.2  |
| 6   | S     | 98  | HIS  | 6.2  |
| 8   | H     | 44  | THR  | 6.2  |
| 8   | H     | 47  | GLY  | 6.0  |
| 7   | T     | 8   | HIS  | 5.9  |
| 7   | G     | 10  | GLY  | 5.8  |
| 6   | F     | 94  | HIS  | 5.8  |
| 8   | H     | 8   | ILE  | 5.7  |
| 10  | W     | 1   | PHE  | 5.5  |
| 9   | V     | 37  | PHE  | 5.5  |
| 6   | F     | 98  | HIS  | 5.4  |
| 8   | U     | 8   | ILE  | 5.4  |
| 6   | F     | 95  | GLN  | 5.4  |
| 6   | S     | 95  | GLN  | 5.4  |
| 7   | T     | 9   | GLY  | 5.4  |
| 4   | D     | 5   | VAL  | 5.3  |
| 7   | G     | 7   | ASP  | 5.3  |
| 4   | Q     | 8   | SER  | 5.3  |
| 7   | T     | 2   | SER  | 5.3  |
| 7   | T     | 37  | LEU  | 5.3  |
| 7   | G     | 9   | GLY  | 5.2  |
| 6   | S     | 94  | HIS  | 5.1  |
| 5   | E     | 109 | VAL  | 5.1  |
| 6   | S     | 2   | SER  | 5.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | Q     | 4   | SER  | 4.9  |
| 7   | G     | 36  | TRP  | 4.8  |
| 9   | I     | 37  | PHE  | 4.8  |
| 2   | B     | 60  | GLU  | 4.8  |
| 5   | R     | 109 | VAL  | 4.6  |
| 8   | H     | 10  | ASN  | 4.5  |
| 10  | W     | 58  | LYS  | 4.5  |
| 8   | H     | 45  | ALA  | 4.4  |
| 2   | O     | 227 | LEU  | 4.4  |
| 2   | O     | 113 | TYR  | 4.4  |
| 7   | G     | 2   | SER  | 4.4  |
| 7   | G     | 1   | ALA  | 4.4  |
| 7   | T     | 38  | HIS  | 4.3  |
| 7   | T     | 7   | ASP  | 4.3  |
| 13  | M     | 42  | LYS  | 4.3  |
| 4   | Q     | 7   | LYS  | 4.3  |
| 6   | S     | 93  | PRO  | 4.3  |
| 7   | T     | 84  | LYS  | 4.2  |
| 7   | G     | 84  | LYS  | 4.2  |
| 8   | U     | 44  | THR  | 4.1  |
| 7   | T     | 1   | ALA  | 4.1  |
| 12  | Y     | 20  | ARG  | 4.0  |
| 7   | G     | 37  | LEU  | 4.0  |
| 10  | J     | 58  | LYS  | 4.0  |
| 5   | R     | 5   | HIS  | 3.9  |
| 3   | C     | 38  | ASN  | 3.9  |
| 6   | F     | 2   | SER  | 3.9  |
| 7   | T     | 4   | ALA  | 3.9  |
| 8   | U     | 47  | GLY  | 3.9  |
| 13  | Z     | 43  | SER  | 3.9  |
| 5   | E     | 5   | HIS  | 3.8  |
| 8   | U     | 45  | ALA  | 3.8  |
| 2   | O     | 90  | ILE  | 3.8  |
| 6   | F     | 3   | GLY  | 3.8  |
| 6   | S     | 3   | GLY  | 3.8  |
| 12  | L     | 2   | HIS  | 3.7  |
| 9   | V     | 22  | VAL  | 3.7  |
| 10  | W     | 57  | HIS  | 3.7  |
| 4   | Q     | 35  | ALA  | 3.6  |
| 7   | G     | 5   | LYS  | 3.6  |
| 12  | L     | 47  | LYS  | 3.6  |
| 2   | B     | 65  | TRP  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 59  | GLN  | 3.5  |
| 7   | G     | 41  | HIS  | 3.5  |
| 7   | G     | 8   | HIS  | 3.4  |
| 7   | G     | 3   | ALA  | 3.4  |
| 8   | H     | 7   | LYS  | 3.4  |
| 13  | M     | 43  | SER  | 3.4  |
| 7   | T     | 39  | SER  | 3.4  |
| 9   | I     | 32  | ALA  | 3.4  |
| 9   | I     | 33  | THR  | 3.4  |
| 7   | T     | 42  | ARG  | 3.3  |
| 7   | T     | 5   | LYS  | 3.3  |
| 2   | O     | 59  | GLN  | 3.3  |
| 3   | P     | 38  | ASN  | 3.3  |
| 7   | T     | 3   | ALA  | 3.2  |
| 8   | U     | 42  | ALA  | 3.2  |
| 9   | I     | 34  | PHE  | 3.2  |
| 2   | O     | 116 | LEU  | 3.2  |
| 9   | V     | 34  | PHE  | 3.2  |
| 5   | E     | 7   | THR  | 3.1  |
| 8   | U     | 7   | LYS  | 3.1  |
| 7   | G     | 33  | LEU  | 3.1  |
| 13  | Z     | 39  | ASN  | 3.1  |
| 9   | I     | 25  | PHE  | 3.1  |
| 8   | H     | 9   | LYS  | 3.1  |
| 7   | G     | 38  | HIS  | 3.1  |
| 7   | G     | 6   | GLY  | 3.1  |
| 8   | H     | 52  | VAL  | 3.1  |
| 2   | O     | 226 | MET  | 3.0  |
| 2   | B     | 90  | ILE  | 3.0  |
| 2   | O     | 91  | ASN  | 3.0  |
| 4   | Q     | 10  | ASP  | 3.0  |
| 9   | V     | 2   | THR  | 3.0  |
| 4   | Q     | 39  | ALA  | 3.0  |
| 3   | P     | 3   | HIS  | 2.9  |
| 13  | M     | 38  | ASP  | 2.9  |
| 8   | U     | 43  | MET  | 2.9  |
| 10  | J     | 1   | PHE  | 2.9  |
| 7   | G     | 4   | ALA  | 2.9  |
| 4   | Q     | 140 | TYR  | 2.9  |
| 12  | Y     | 2   | HIS  | 2.9  |
| 2   | O     | 86  | MET  | 2.9  |
| 7   | T     | 6   | GLY  | 2.9  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 8   | U     | 9      | LYS  | 2.8  |
| 2   | O     | 224    | ALA  | 2.8  |
| 8   | U     | 52     | VAL  | 2.8  |
| 8   | U     | 10     | ASN  | 2.8  |
| 2   | B     | 61     | VAL  | 2.8  |
| 9   | V     | 25     | PHE  | 2.7  |
| 9   | I     | 27     | VAL  | 2.7  |
| 9   | I     | 36     | LYS  | 2.7  |
| 2   | B     | 91     | ASN  | 2.7  |
| 10  | J     | 52     | TRP  | 2.7  |
| 7   | G     | 42     | ARG  | 2.7  |
| 4   | Q     | 9      | GLU  | 2.7  |
| 8   | H     | 50     | VAL  | 2.7  |
| 8   | H     | 43     | MET  | 2.6  |
| 9   | I     | 19     | PHE  | 2.6  |
| 7   | T     | 41     | HIS  | 2.6  |
| 2   | B     | 78     | LEU  | 2.6  |
| 7   | G     | 40     | GLY  | 2.6  |
| 7   | T     | 43     | GLU  | 2.6  |
| 10  | J     | 57     | HIS  | 2.6  |
| 12  | L     | 45     | LEU  | 2.6  |
| 7   | T     | 40     | GLY  | 2.6  |
| 11  | X     | 6      | ALA  | 2.6  |
| 7   | G     | 39     | SER  | 2.6  |
| 9   | V     | 33     | THR  | 2.6  |
| 3   | C     | 3      | HIS  | 2.5  |
| 4   | Q     | 33     | LEU  | 2.5  |
| 2   | O     | 65     | TRP  | 2.5  |
| 13  | Z     | 40     | TYR  | 2.5  |
| 13  | Z     | 42     | LYS  | 2.5  |
| 1   | N     | 513    | LEU  | 2.5  |
| 8   | H     | 51     | SER  | 2.5  |
| 10  | W     | 2      | GLU  | 2.5  |
| 11  | X     | 13     | TYR  | 2.4  |
| 1   | N     | 136[A] | LEU  | 2.4  |
| 2   | O     | 60     | GLU  | 2.4  |
| 2   | O     | 92     | ASN  | 2.4  |
| 5   | E     | 6      | GLU  | 2.4  |
| 13  | M     | 39     | ASN  | 2.4  |
| 9   | I     | 29     | LEU  | 2.4  |
| 9   | V     | 36     | LYS  | 2.4  |
| 4   | Q     | 30     | VAL  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7   | G     | 12  | GLY  | 2.4  |
| 8   | U     | 50  | VAL  | 2.4  |
| 13  | Z     | 32  | TRP  | 2.4  |
| 13  | M     | 40  | TYR  | 2.3  |
| 9   | I     | 31  | PHE  | 2.3  |
| 3   | C     | 40  | MET  | 2.3  |
| 4   | Q     | 40  | LEU  | 2.3  |
| 12  | Y     | 47  | LYS  | 2.3  |
| 9   | V     | 27  | VAL  | 2.3  |
| 1   | N     | 483 | LEU  | 2.3  |
| 7   | T     | 12  | GLY  | 2.3  |
| 2   | B     | 55  | THR  | 2.3  |
| 7   | G     | 43  | GLU  | 2.2  |
| 9   | I     | 30  | GLY  | 2.2  |
| 10  | W     | 56  | PRO  | 2.2  |
| 2   | O     | 78  | LEU  | 2.2  |
| 8   | H     | 48  | GLY  | 2.2  |
| 8   | U     | 11  | TYR  | 2.2  |
| 9   | I     | 2   | THR  | 2.2  |
| 9   | V     | 32  | ALA  | 2.2  |
| 2   | B     | 113 | TYR  | 2.2  |
| 4   | Q     | 34  | SER  | 2.2  |
| 4   | Q     | 49  | SER  | 2.2  |
| 11  | X     | 7   | PRO  | 2.2  |
| 8   | U     | 46  | LYS  | 2.2  |
| 1   | A     | 178 | GLN  | 2.1  |
| 3   | C     | 258 | TRP  | 2.1  |
| 4   | Q     | 36  | SER  | 2.1  |
| 12  | L     | 46  | LYS  | 2.1  |
| 4   | Q     | 53  | ILE  | 2.1  |
| 9   | I     | 18  | ARG  | 2.1  |
| 8   | H     | 42  | ALA  | 2.1  |
| 11  | K     | 47  | ARG  | 2.1  |
| 1   | A     | 514 | LYS  | 2.1  |
| 8   | U     | 48  | GLY  | 2.1  |
| 12  | Y     | 24  | MET  | 2.1  |
| 8   | H     | 46  | LYS  | 2.0  |
| 9   | V     | 31  | PHE  | 2.0  |
| 11  | K     | 7   | PRO  | 2.0  |
| 4   | Q     | 51  | LEU  | 2.0  |
| 4   | Q     | 115 | TRP  | 2.0  |
| 11  | K     | 6   | ALA  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | Q     | 58  | GLU  | 2.0  |
| 7   | T     | 35  | SER  | 2.0  |
| 6   | F     | 54  | ASN  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 9   | SAC  | V     | 1   | 9/10  | 0.42 | 0.23 | 63,69,72,74                | 0     |
| 9   | SAC  | I     | 1   | 9/10  | 0.62 | 0.25 | 43,49,64,67                | 0     |
| 7   | TPO  | T     | 11  | 11/12 | 0.65 | 0.26 | 52,69,96,97                | 0     |
| 7   | TPO  | G     | 11  | 11/12 | 0.68 | 0.26 | 65,74,106,115              | 0     |
| 1   | FME  | A     | 1   | 10/11 | 0.89 | 0.12 | 25,33,52,71                | 0     |
| 1   | FME  | N     | 1   | 10/11 | 0.90 | 0.12 | 18,28,48,58                | 0     |
| 2   | FME  | B     | 1   | 10/11 | 0.94 | 0.09 | 15,16,24,33                | 0     |
| 2   | FME  | O     | 1   | 10/11 | 0.96 | 0.08 | 15,16,24,24                | 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 22  | CHD  | J     | 101 | 29/29 | 0.62 | 0.27 | 56,93,101,102              | 0     |
| 22  | CHD  | W     | 101 | 29/29 | 0.62 | 0.26 | 52,82,95,101               | 0     |
| 20  | TGL  | Q     | 201 | 63/63 | 0.71 | 0.20 | 30,47,66,71                | 0     |
| 19  | PGV  | P     | 301 | 51/51 | 0.73 | 0.22 | 45,70,102,114              | 0     |
| 24  | PEK  | C     | 307 | 53/53 | 0.74 | 0.22 | 34,59,94,103               | 0     |
| 19  | PGV  | C     | 308 | 51/51 | 0.75 | 0.21 | 34,64,99,101               | 0     |
| 24  | PEK  | G     | 102 | 53/53 | 0.75 | 0.23 | 37,71,111,121              | 0     |

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| Mol | Type | Chain | Res    | Atoms   | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|---------|------|------|-----------------------------|-------|
| 25  | CDL  | T     | 102    | 100/100 | 0.75 | 0.22 | 31,67,118,128               | 0     |
| 24  | PEK  | T     | 101    | 53/53   | 0.76 | 0.26 | 36,76,114,118               | 0     |
| 25  | CDL  | G     | 101    | 100/100 | 0.77 | 0.20 | 34,66,99,138                | 0     |
| 20  | TGL  | Y     | 101    | 63/63   | 0.78 | 0.20 | 33,49,76,81                 | 0     |
| 19  | PGV  | N     | 607    | 51/51   | 0.78 | 0.20 | 27,49,103,114               | 0     |
| 23  | PSC  | B     | 304    | 52/52   | 0.79 | 0.22 | 36,84,130,137               | 0     |
| 22  | CHD  | P     | 306    | 29/29   | 0.79 | 0.15 | 34,44,49,56                 | 0     |
| 24  | PEK  | P     | 308    | 53/53   | 0.80 | 0.20 | 25,55,100,118               | 0     |
| 20  | TGL  | L     | 101    | 63/63   | 0.80 | 0.19 | 28,44,70,80                 | 0     |
| 19  | PGV  | A     | 608    | 51/51   | 0.80 | 0.19 | 24,51,72,84                 | 0     |
| 25  | CDL  | P     | 305    | 100/100 | 0.80 | 0.20 | 28,60,102,116               | 0     |
| 20  | TGL  | D     | 201    | 63/63   | 0.80 | 0.18 | 23,45,66,74                 | 0     |
| 23  | PSC  | N     | 610    | 52/52   | 0.81 | 0.21 | 24,61,117,126               | 0     |
| 22  | CHD  | C     | 305    | 29/29   | 0.81 | 0.14 | 41,47,53,59                 | 0     |
| 25  | CDL  | C     | 304    | 100/100 | 0.82 | 0.19 | 26,59,88,108                | 0     |
| 20  | TGL  | N     | 609    | 63/63   | 0.83 | 0.17 | 31,54,73,76                 | 0     |
| 20  | TGL  | B     | 301    | 63/63   | 0.84 | 0.17 | 28,51,75,84                 | 0     |
| 17  | NA   | P     | 302    | 1/1     | 0.88 | 0.09 | 29,29,29,29                 | 0     |
| 27  | DMU  | M     | 101    | 33/33   | 0.88 | 0.11 | 25,29,39,40                 | 0     |
| 27  | DMU  | Z     | 101    | 33/33   | 0.88 | 0.10 | 18,31,34,39                 | 0     |
| 16  | MG   | N     | 604    | 1/1     | 0.91 | 0.07 | 17,17,17,17                 | 0     |
| 17  | NA   | C     | 301    | 1/1     | 0.93 | 0.22 | 37,37,37,37                 | 0     |
| 22  | CHD  | B     | 303    | 29/29   | 0.93 | 0.07 | 8,10,13,19                  | 0     |
| 24  | PEK  | P     | 303    | 53/53   | 0.94 | 0.11 | 13,29,70,77                 | 0     |
| 22  | CHD  | P     | 307    | 29/29   | 0.94 | 0.07 | 12,19,23,26                 | 0     |
| 24  | PEK  | C     | 302    | 53/53   | 0.94 | 0.12 | 13,33,60,65                 | 0     |
| 22  | CHD  | C     | 306    | 29/29   | 0.95 | 0.07 | 17,21,25,29                 | 0     |
| 22  | CHD  | G     | 103    | 29/29   | 0.95 | 0.06 | 8,10,12,16                  | 0     |
| 17  | NA   | N     | 605    | 1/1     | 0.95 | 0.06 | 12,12,12,12                 | 0     |
| 19  | PGV  | C     | 303    | 51/51   | 0.95 | 0.10 | 13,22,55,63                 | 0     |
| 19  | PGV  | N     | 608    | 51/51   | 0.95 | 0.10 | 12,30,49,58                 | 0     |
| 19  | PGV  | A     | 607    | 51/51   | 0.96 | 0.10 | 13,26,49,57                 | 0     |
| 19  | PGV  | P     | 304    | 51/51   | 0.96 | 0.09 | 12,27,51,54                 | 0     |
| 14  | HEA  | A     | 601    | 60/60   | 0.97 | 0.08 | 10,12,37,46                 | 0     |
| 14  | HEA  | A     | 602    | 60/60   | 0.97 | 0.06 | 9,12,18,19                  | 0     |
| 21  | CUA  | O     | 301    | 2/2     | 0.97 | 0.04 | 14,14,14,15                 | 0     |
| 14  | HEA  | N     | 601    | 60/60   | 0.97 | 0.07 | 10,13,32,39                 | 0     |
| 16  | MG   | A     | 604    | 1/1     | 0.97 | 0.06 | 14,14,14,14                 | 0     |
| 14  | HEA  | N     | 602    | 60/60   | 0.98 | 0.06 | 9,12,18,21                  | 0     |
| 18  | PER  | A     | 606[A] | 2/2     | 0.98 | 0.18 | 10,10,10,12                 | 0     |
| 18  | PER  | A     | 606[B] | 2/2     | 0.98 | 0.18 | 11,11,11,11                 | 2     |
| 18  | PER  | N     | 606[A] | 2/2     | 0.98 | 0.08 | 10,10,10,12                 | 0     |

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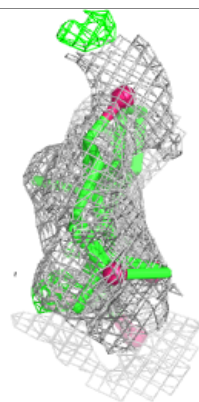
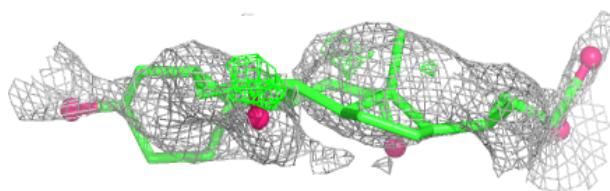
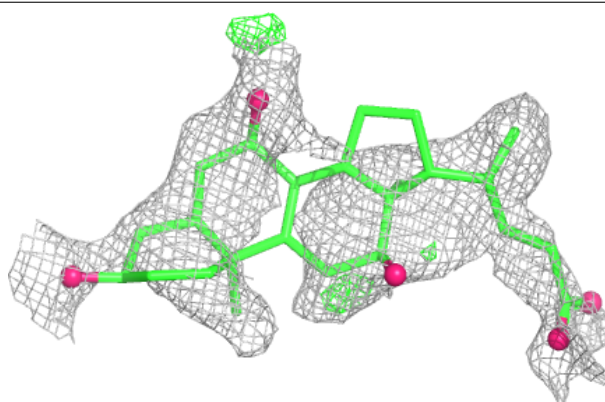
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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 18  | PER  | N     | 606[B] | 2/2   | 0.98 | 0.08 | 11,11,11,11                 | 2     |
| 17  | NA   | A     | 605    | 1/1   | 0.98 | 0.04 | 14,14,14,14                 | 0     |
| 26  | ZN   | F     | 101    | 1/1   | 0.99 | 0.02 | 19,19,19,19                 | 0     |
| 26  | ZN   | S     | 101    | 1/1   | 0.99 | 0.02 | 18,18,18,18                 | 0     |
| 21  | CUA  | B     | 302    | 2/2   | 0.99 | 0.03 | 14,14,14,15                 | 0     |
| 15  | CU   | N     | 603    | 1/1   | 0.99 | 0.04 | 14,14,14,14                 | 0     |
| 15  | CU   | A     | 603    | 1/1   | 1.00 | 0.07 | 15,15,15,15                 | 0     |

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

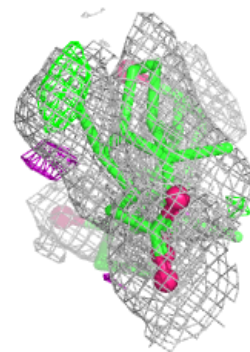
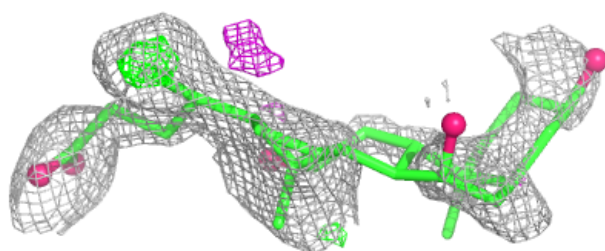
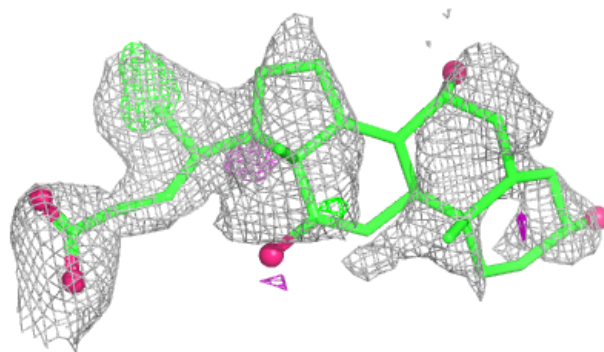
**Electron density around CHD J 101:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

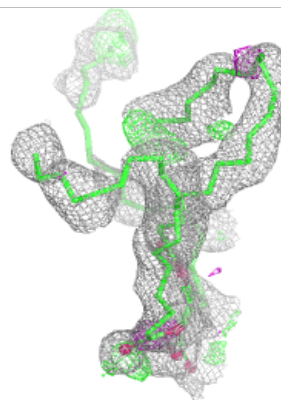
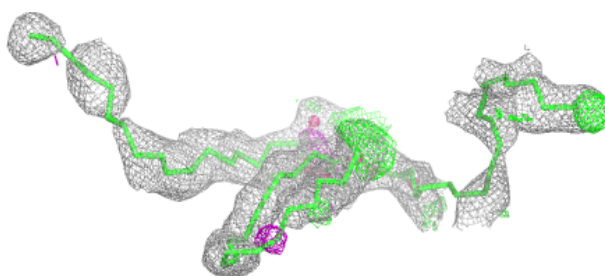
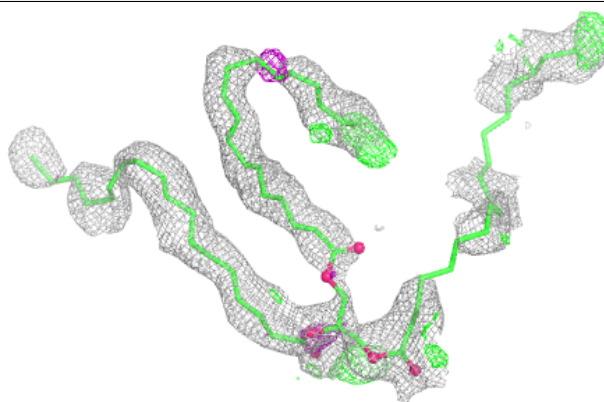


**Electron density around CHD W 101:**

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

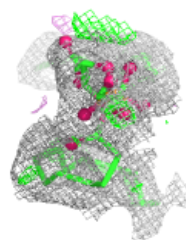
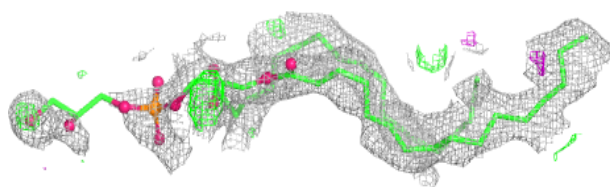
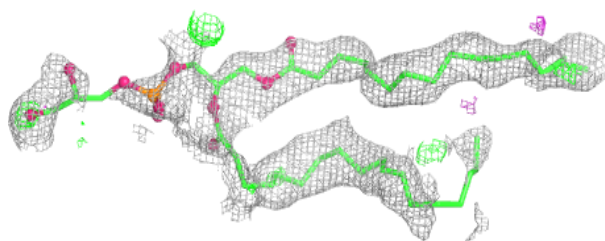
**Electron density around TGL Q 201:**

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



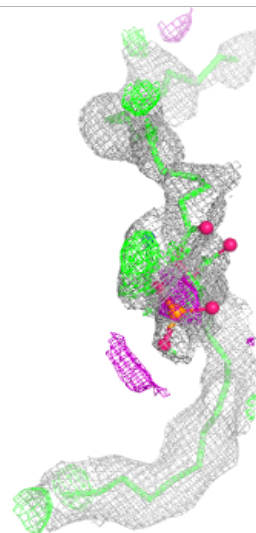
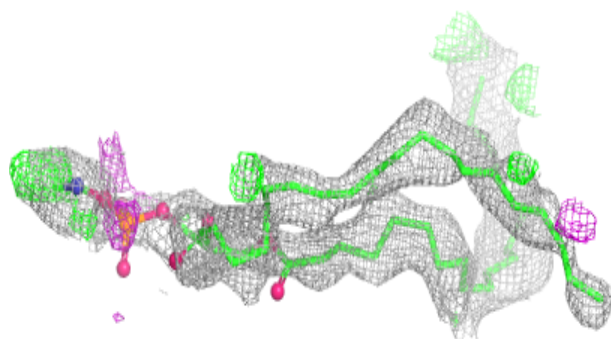
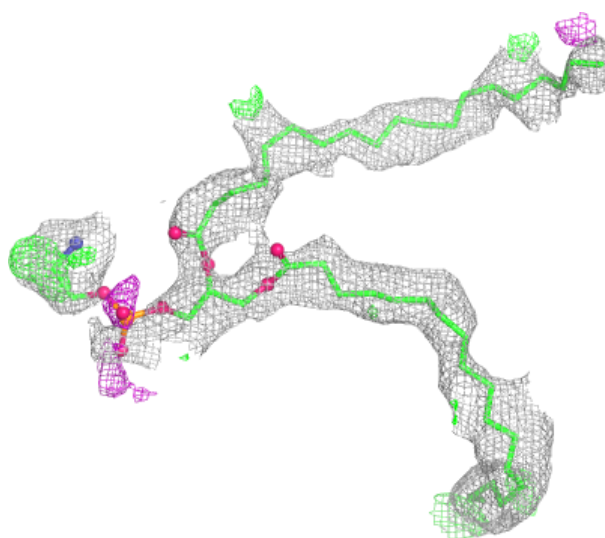
**Electron density around PGV P 301:**

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



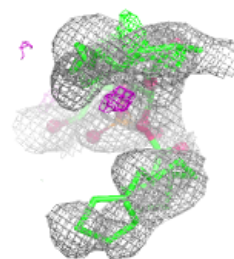
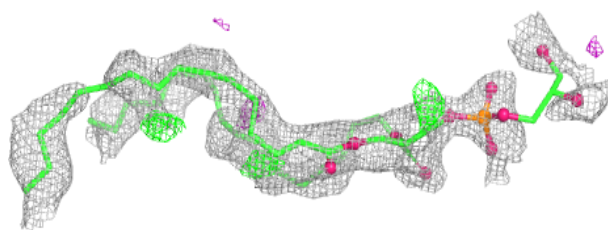
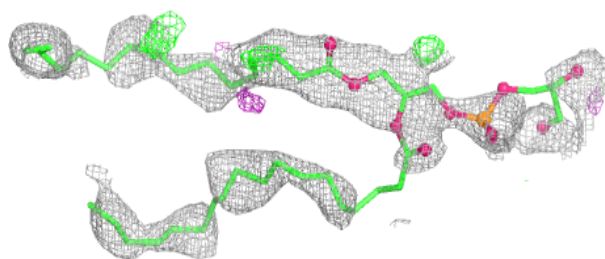
**Electron density around PEK C 307:**

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



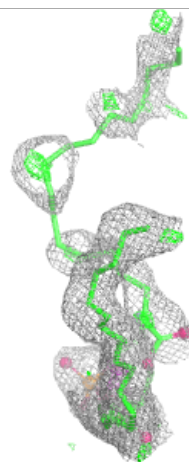
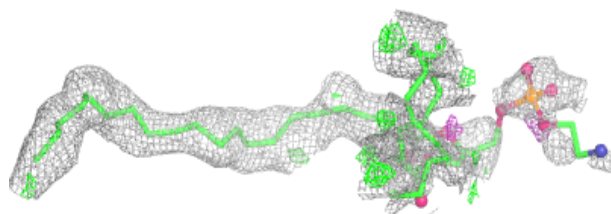
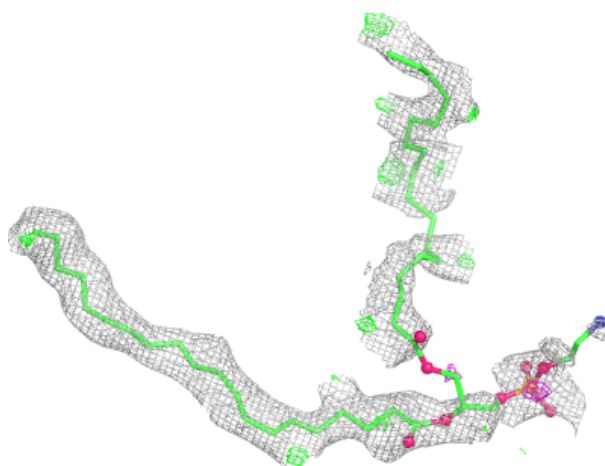
**Electron density around PGV C 308:**

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



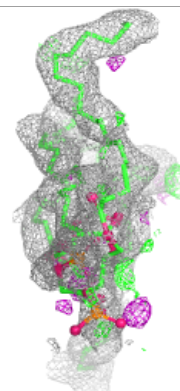
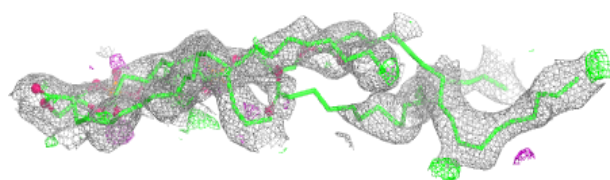
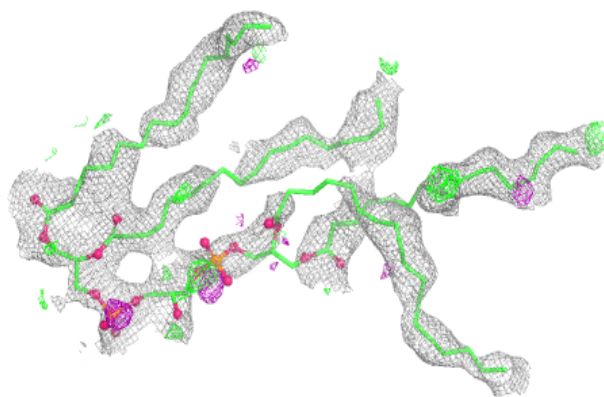
**Electron density around PEK G 102:**

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

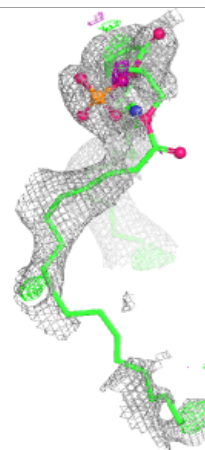
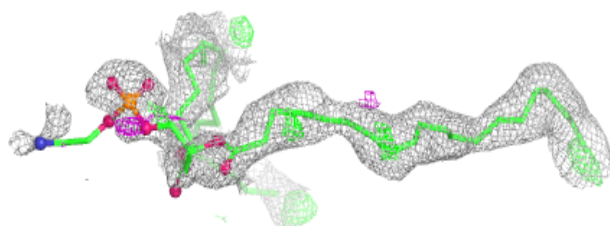
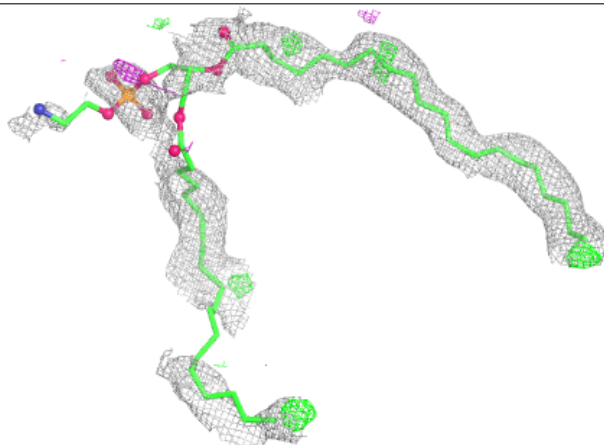


**Electron density around CDL T 102:**

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

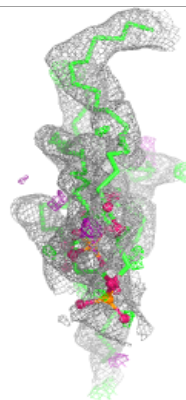
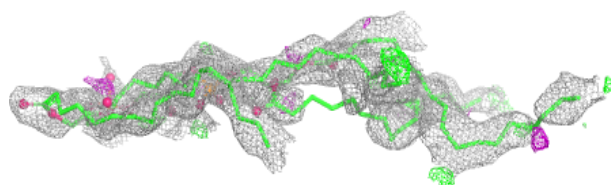
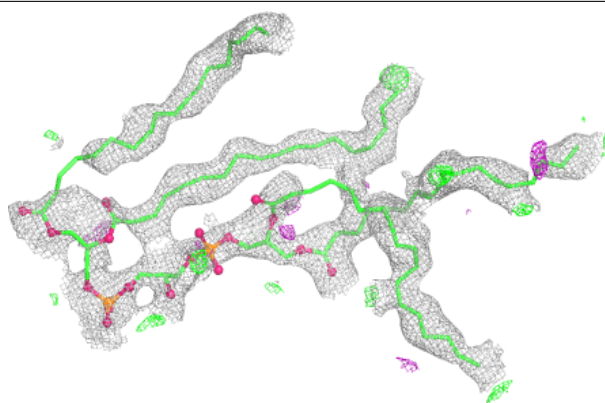
**Electron density around PEK T 101:**

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

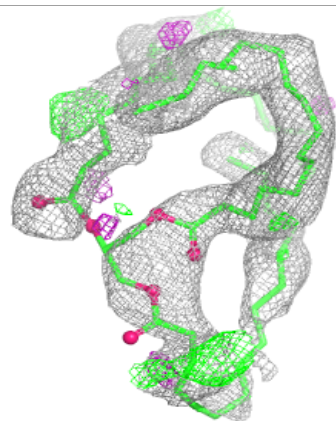
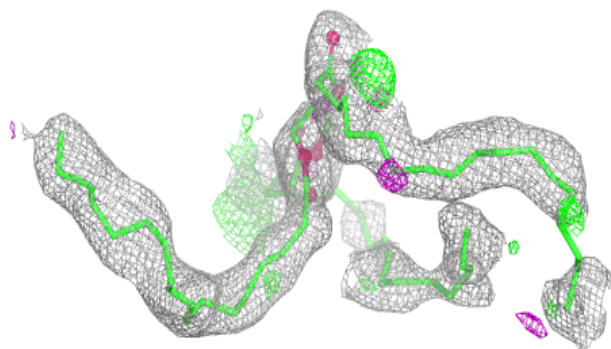
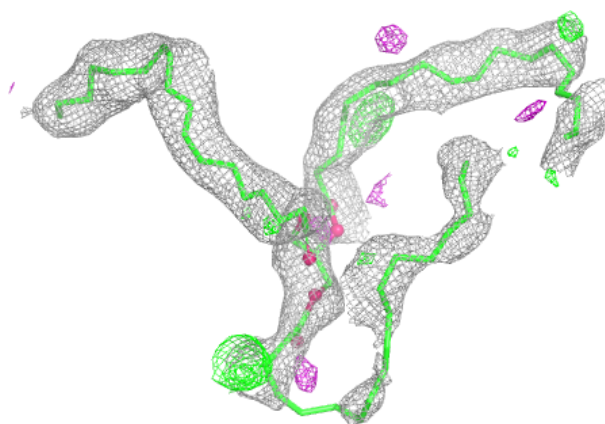


**Electron density around CDL G 101:**

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

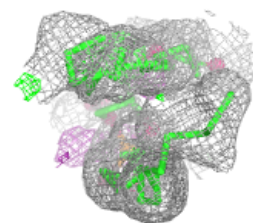
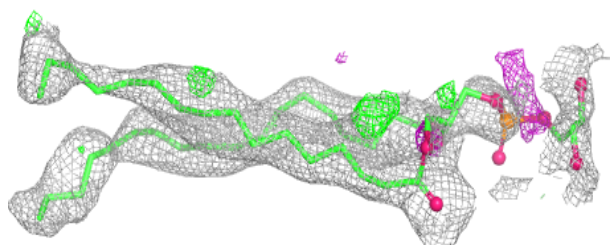
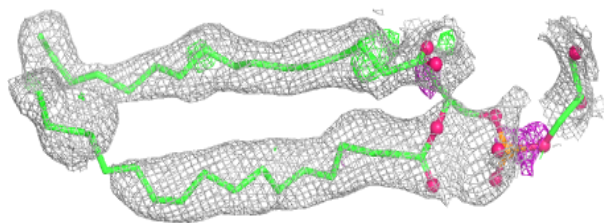
**Electron density around TGL Y 101:**

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

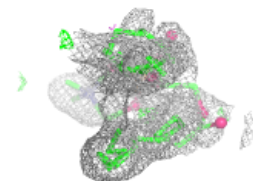
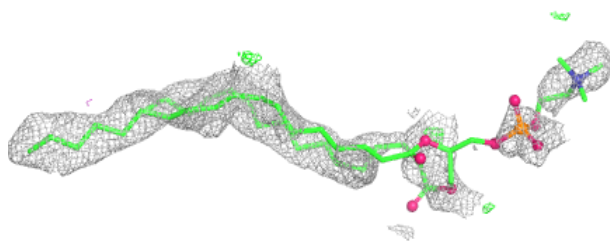
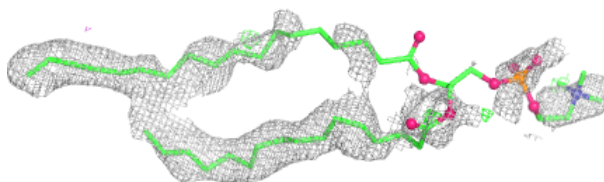


**Electron density around PGV N 607:**

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

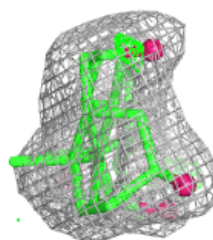
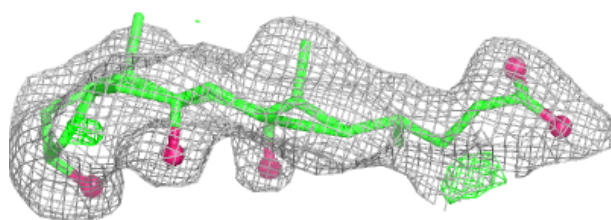
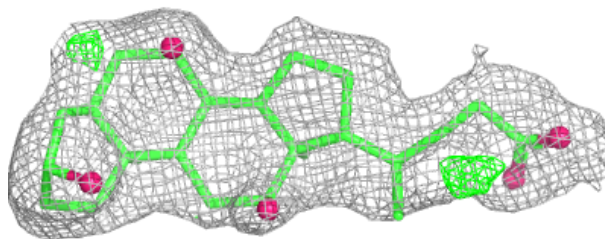
**Electron density around PSC B 304:**

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



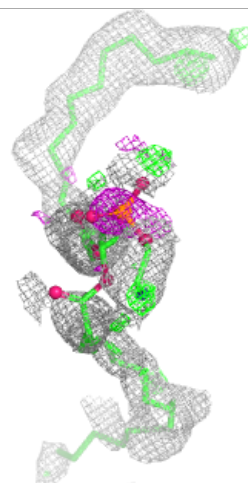
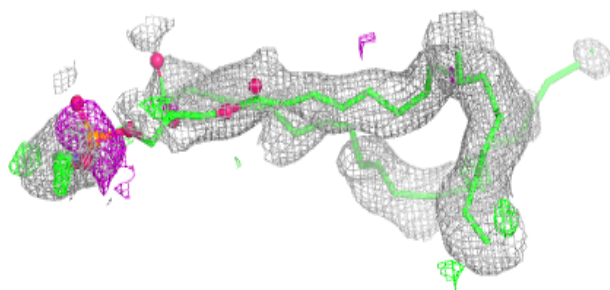
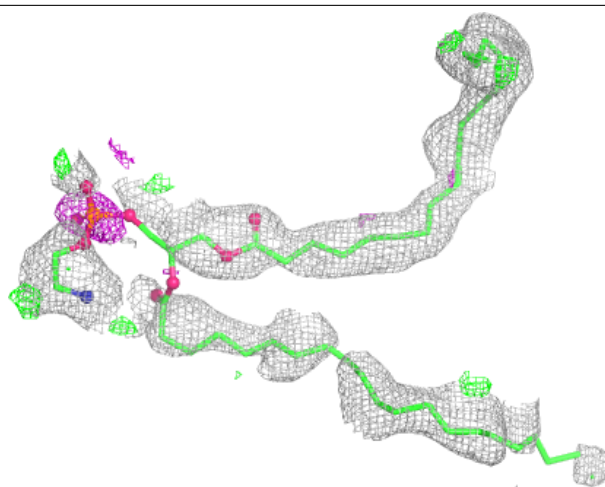
**Electron density around CHD P 306:**

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



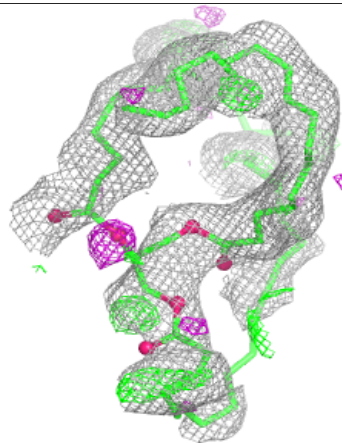
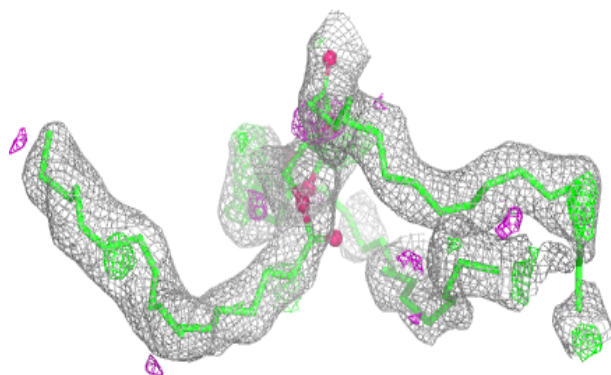
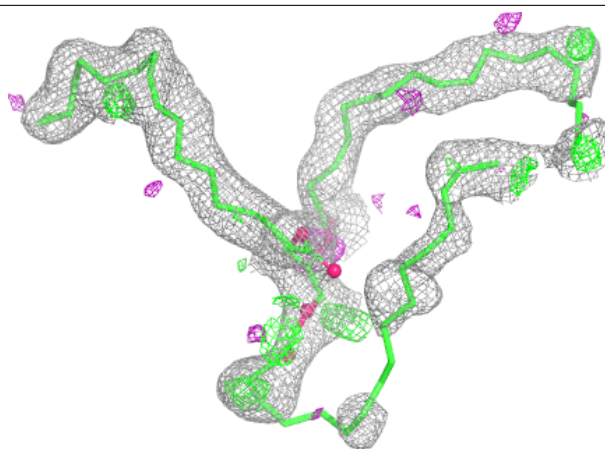
**Electron density around PEK P 308:**

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

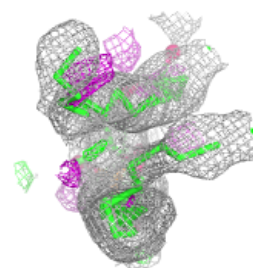
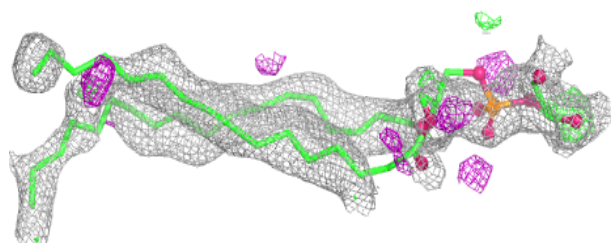
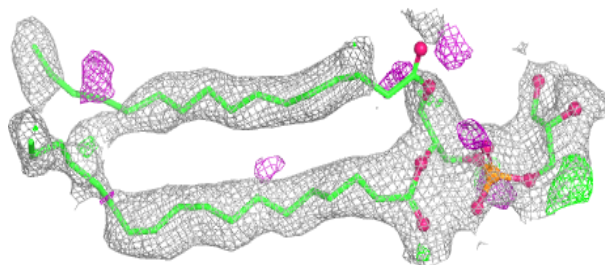


**Electron density around TGL L 101:**

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

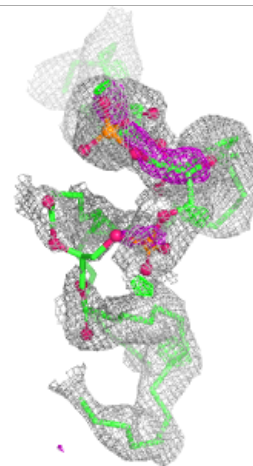
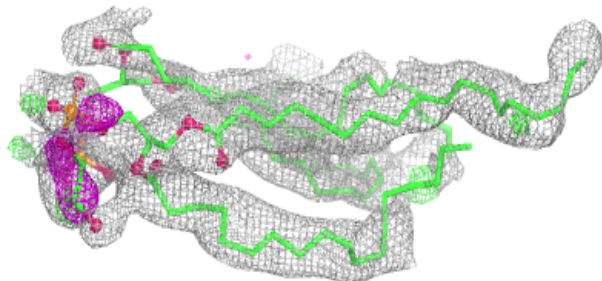
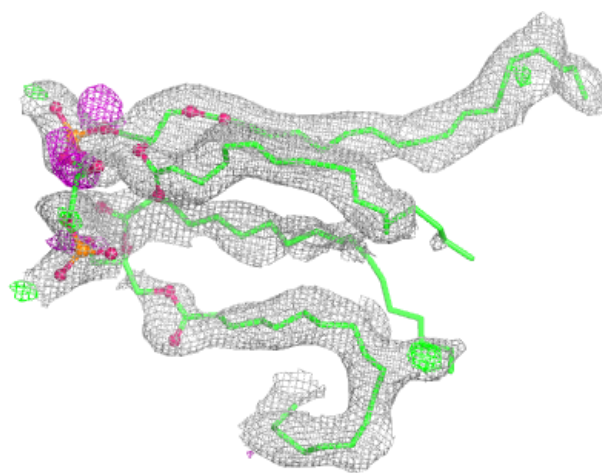
**Electron density around PGV A 608:**

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



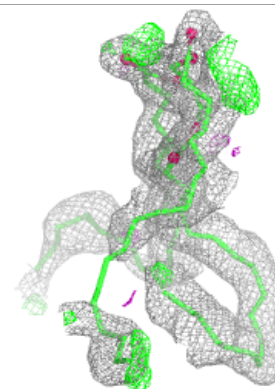
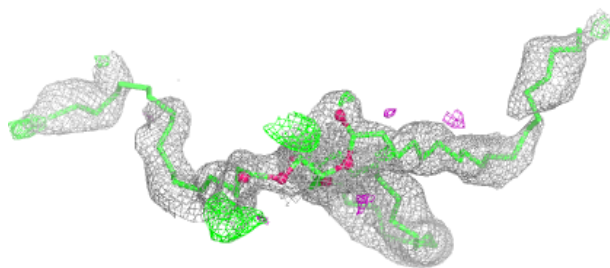
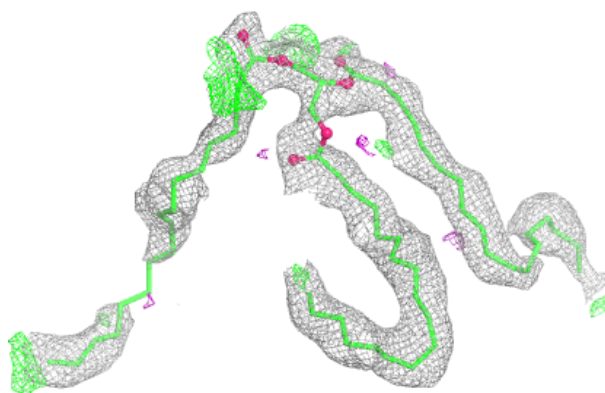
**Electron density around CDL P 305:**

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

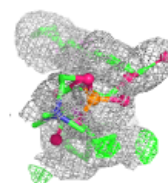
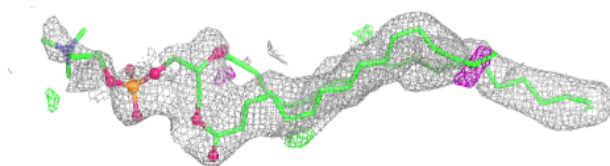
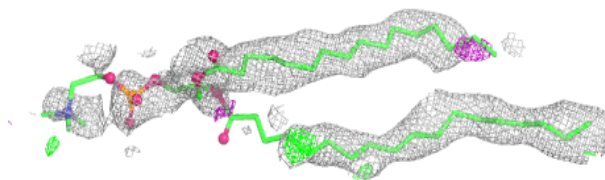


**Electron density around TGL D 201:**

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

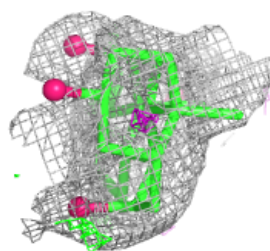
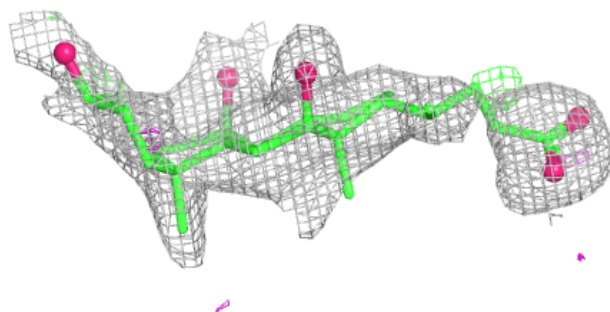
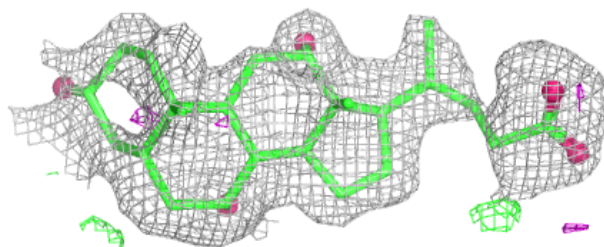
**Electron density around PSC N 610:**

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



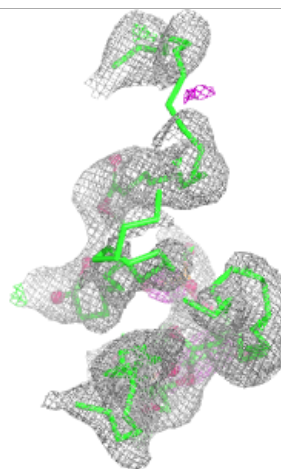
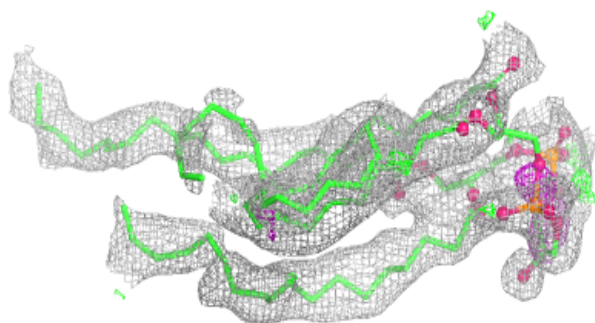
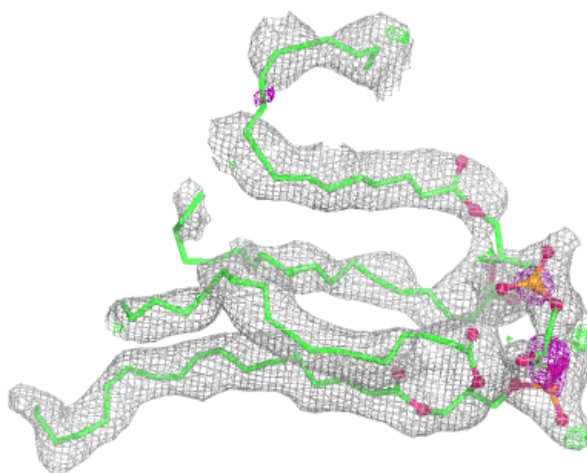
**Electron density around CHD C 305:**

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



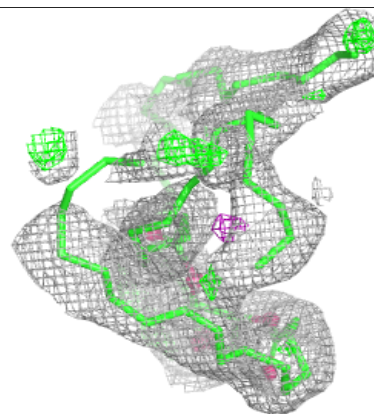
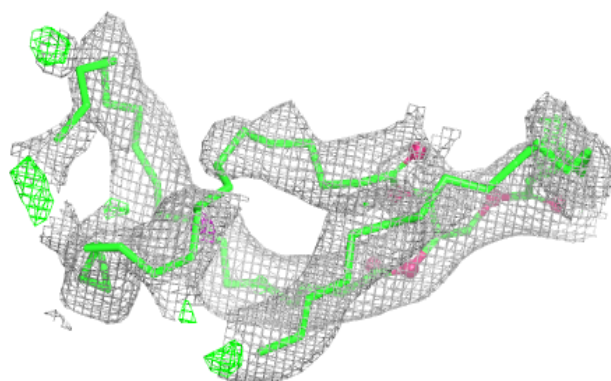
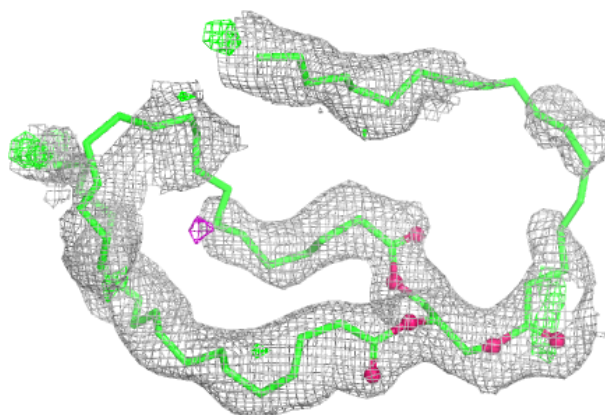
**Electron density around CDL C 304:**

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

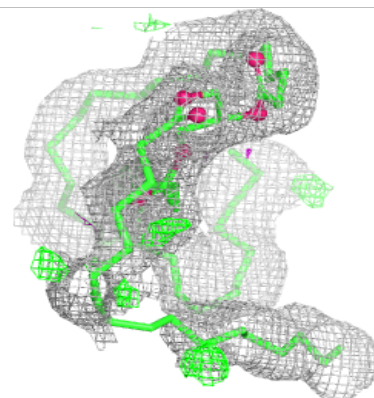
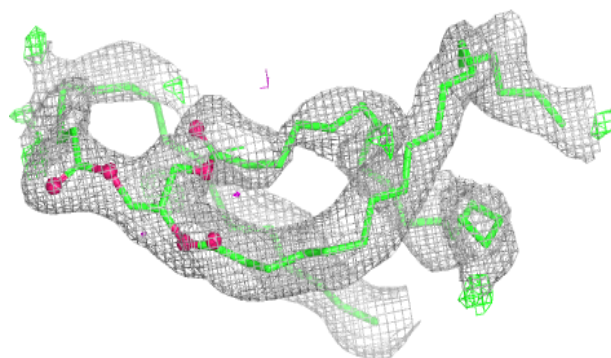
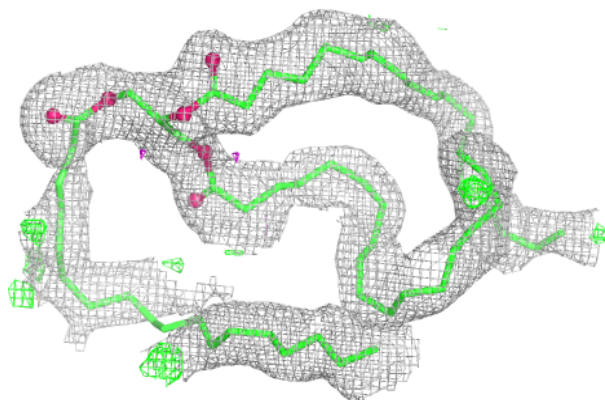


**Electron density around TGL N 609:**

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

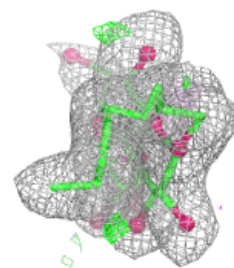
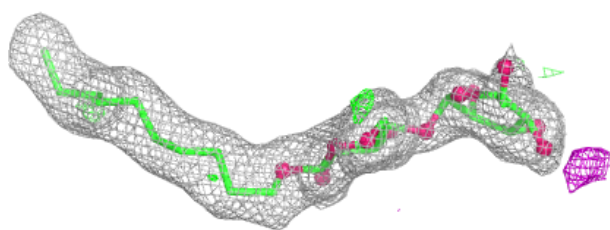
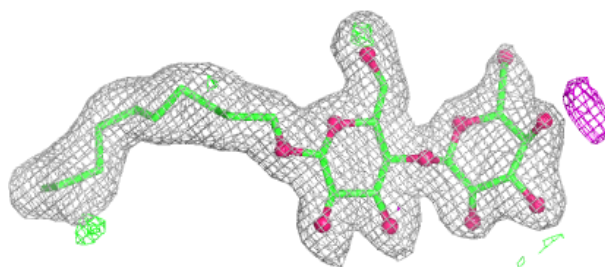
**Electron density around TGL B 301:**

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

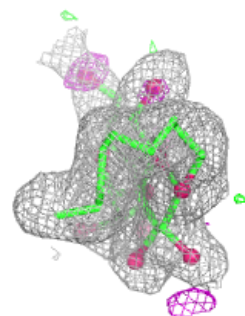
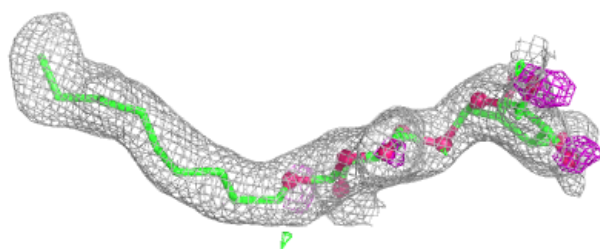
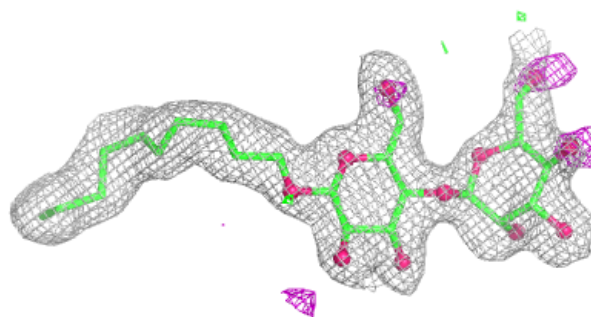


**Electron density around DMU M 101:**

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

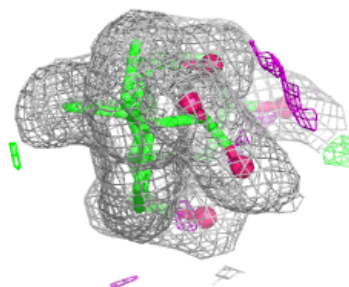
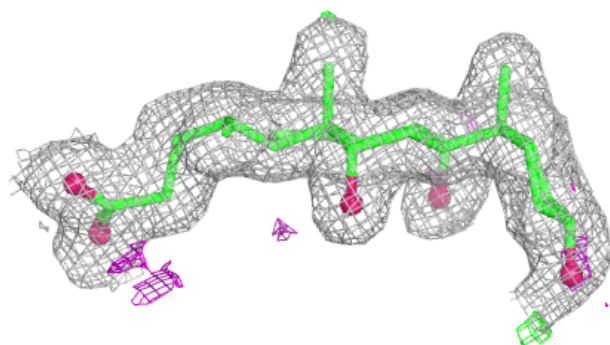
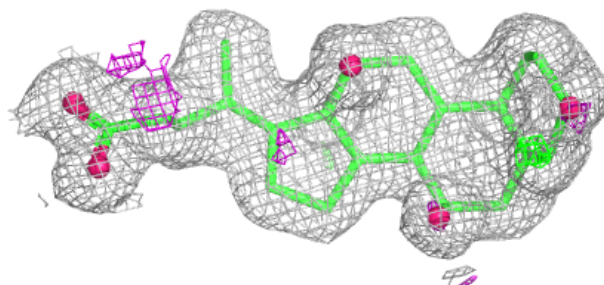
**Electron density around DMU Z 101:**

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

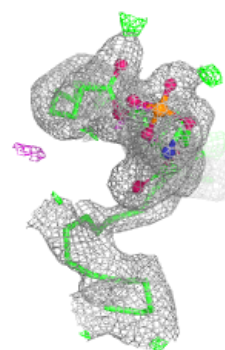
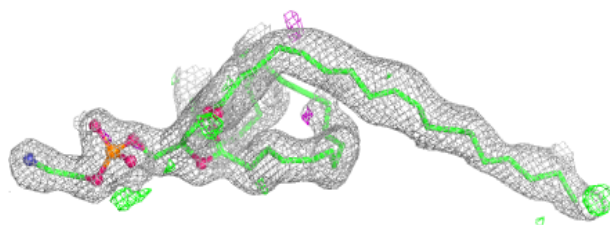
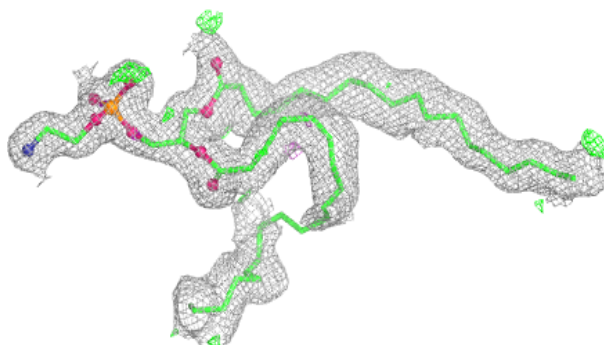


**Electron density around CHD B 303:**

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

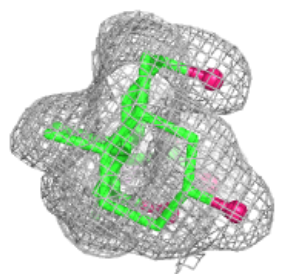
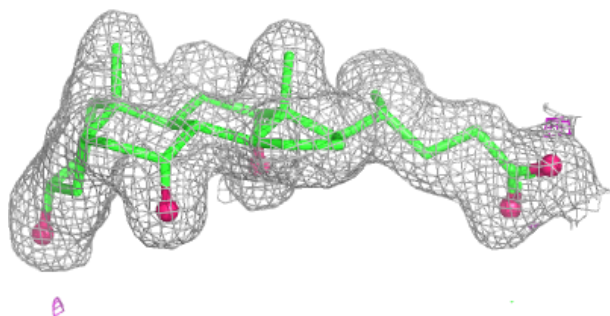
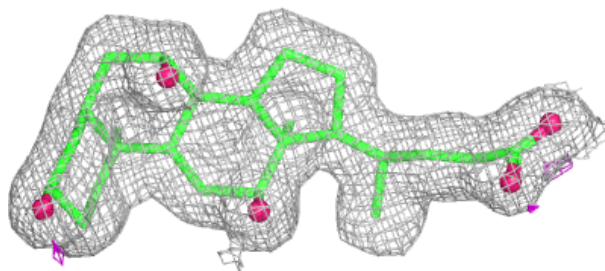
**Electron density around PEK P 303:**

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

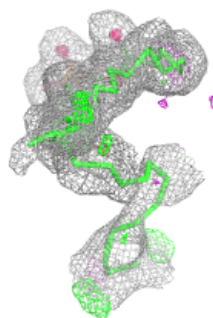
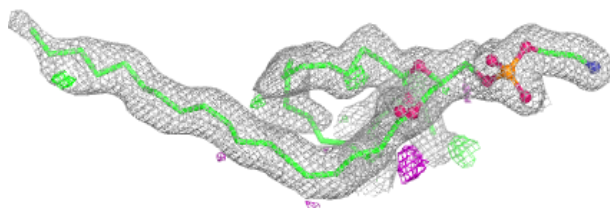
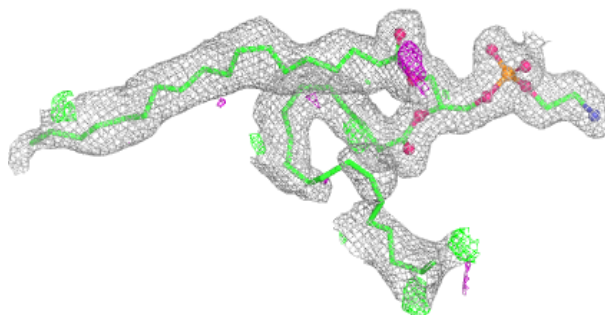


**Electron density around CHD P 307:**

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

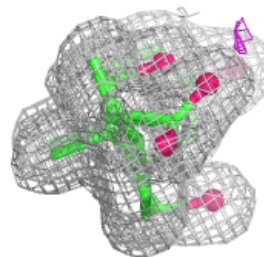
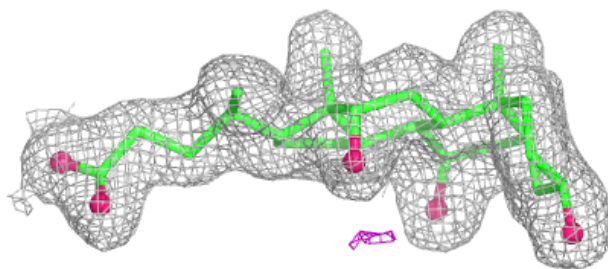
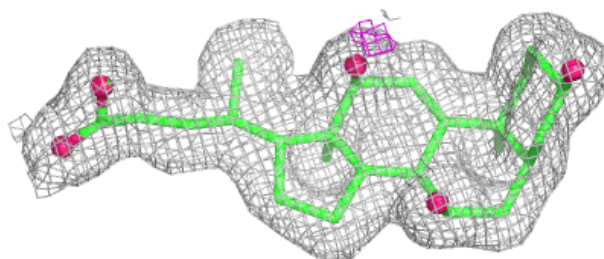
**Electron density around PEK C 302:**

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

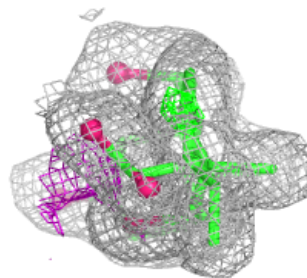
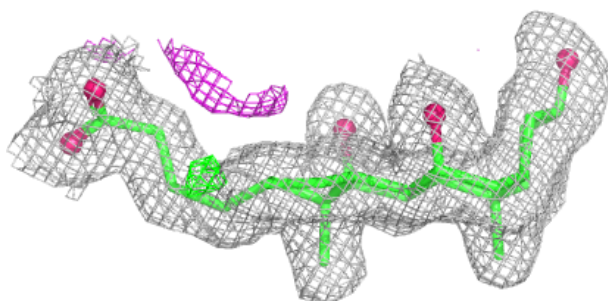
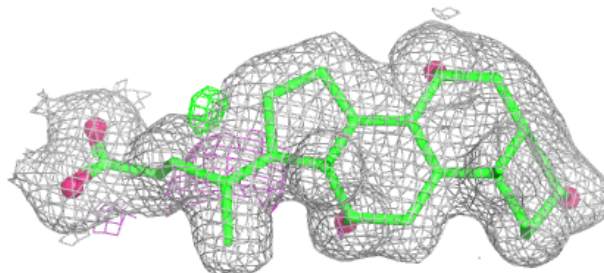


**Electron density around CHD C 306:**

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

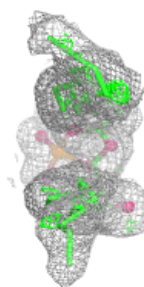
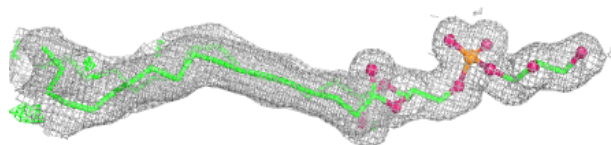
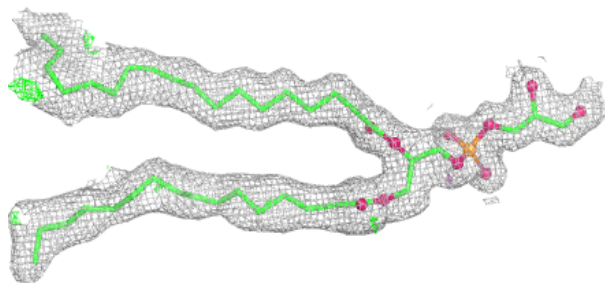
**Electron density around CHD G 103:**

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

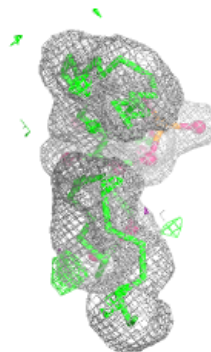
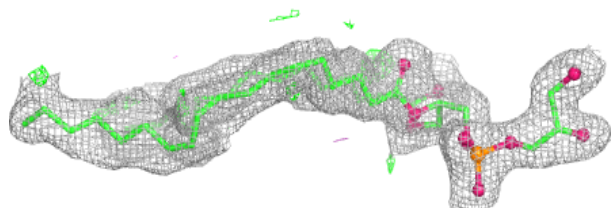
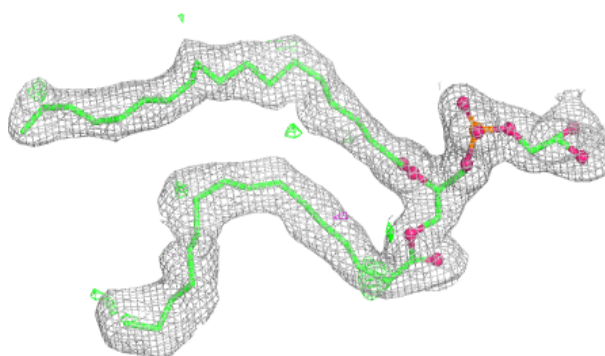


**Electron density around PGV C 303:**

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

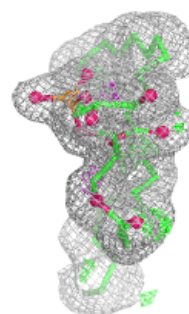
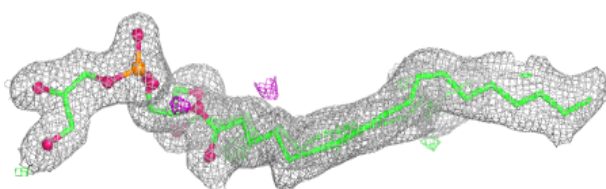
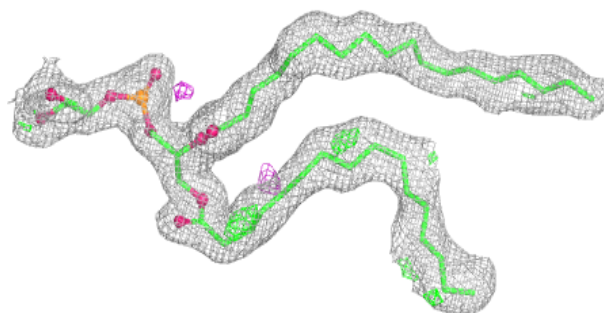
**Electron density around PGV N 608:**

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

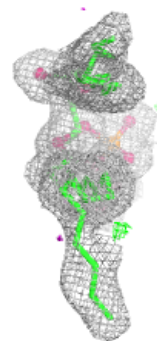
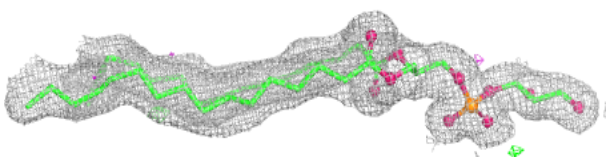
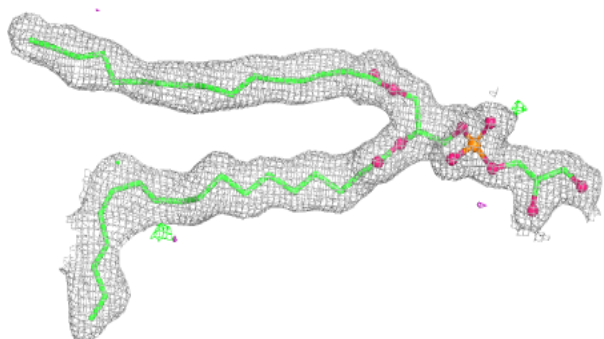


**Electron density around PGV A 607:**

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

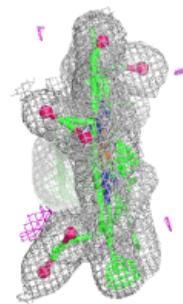
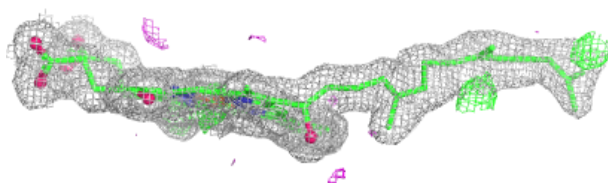
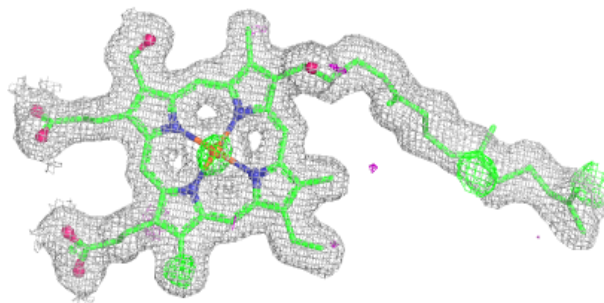
**Electron density around PGV P 304:**

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

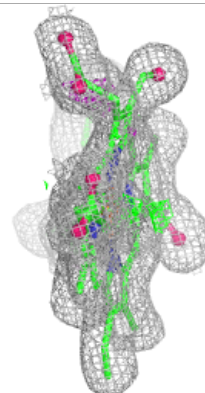
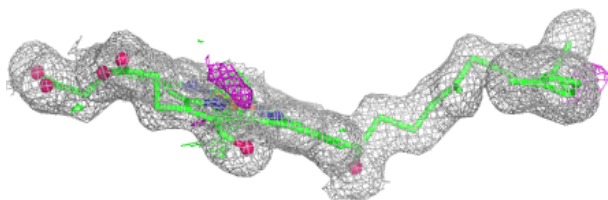
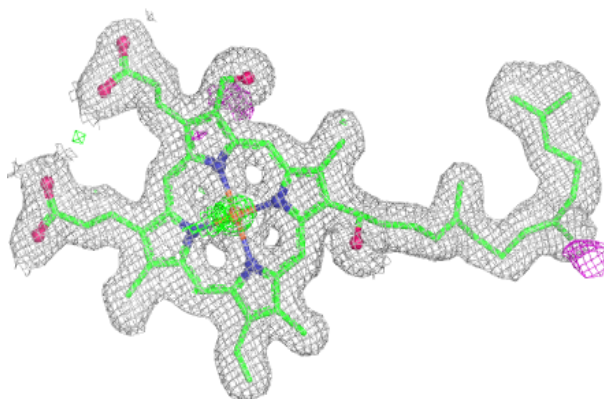


**Electron density around HEA A 601:**

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

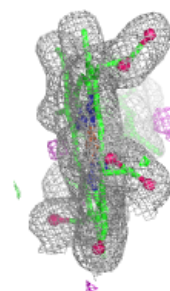
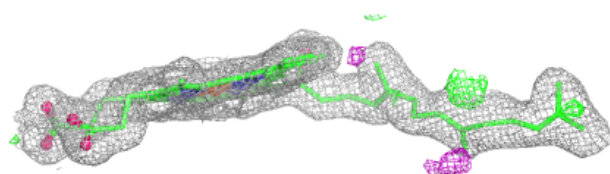
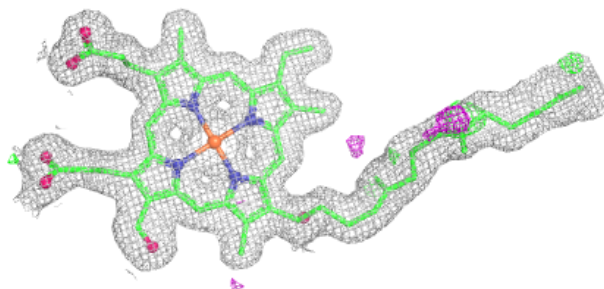
**Electron density around HEA A 602:**

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

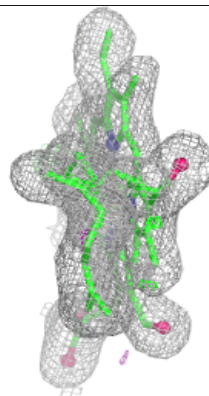
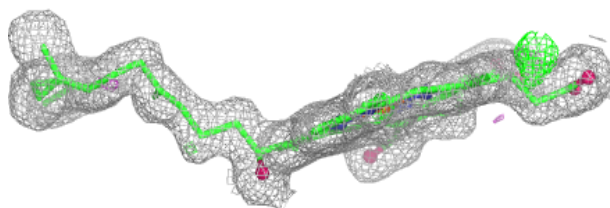
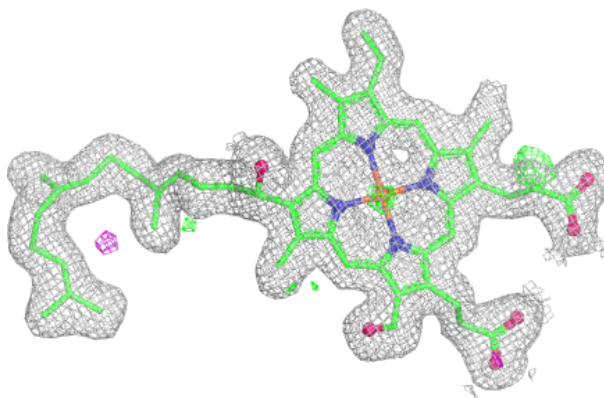


**Electron density around HEA N 601:**

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

**Electron density around HEA N 602:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.