



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:30 PM UTC

PDB ID : 2DYR / pdb\_00002dyr  
Title : Bovine heart cytochrome C oxidase at the fully oxidized state  
Authors : Shinzawa-Itoh, K.; Aoyama, H.; Muramoto, K.; Kurauchi, T.; Mizushima, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2006-09-16  
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

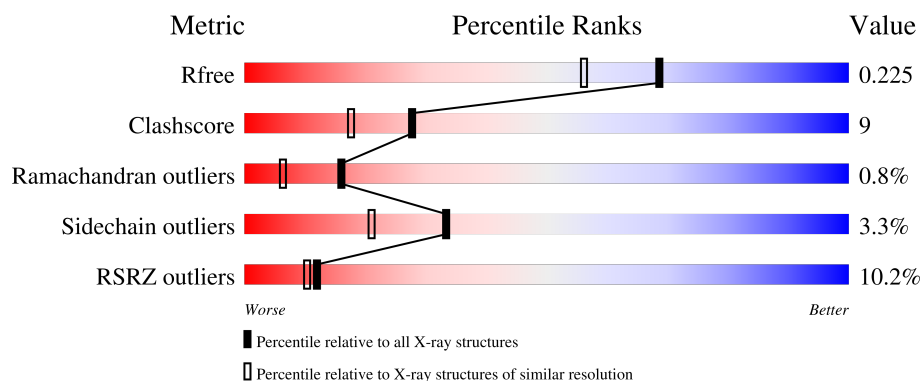
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 7662 (1.80-1.80)                                      |
| Clashscore            | 190562                      | 8479 (1.80-1.80)                                      |
| Ramachandran outliers | 187476                      | 8391 (1.80-1.80)                                      |
| Sidechain outliers    | 187428                      | 8390 (1.80-1.80)                                      |
| RSRZ outliers         | 180081                      | 7663 (1.80-1.80)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                                                 |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------------------------------|
| 1   | A     | 514    | <div> <div style="width: 81%;"></div> <div style="width: 17%;"></div> <div style="width: 2%;"></div> </div> <div>81% 17% .</div> |
| 1   | N     | 514    | <div> <div style="width: 79%;"></div> <div style="width: 19%;"></div> <div style="width: 2%;"></div> </div> <div>79% 19% .</div> |
| 2   | B     | 227    | <div> <div style="width: 78%;"></div> <div style="width: 19%;"></div> <div style="width: 3%;"></div> </div> <div>78% 19% .</div> |
| 2   | O     | 227    | <div> <div style="width: 73%;"></div> <div style="width: 25%;"></div> <div style="width: 2%;"></div> </div> <div>73% 25% .</div> |
| 3   | C     | 261    | <div> <div style="width: 87%;"></div> <div style="width: 12%;"></div> <div style="width: 1%;"></div> </div> <div>87% 12% .</div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 20  | TGL  | L     | 522 | -         | -        | X       | -                |
| 22  | CHD  | C     | 271 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22  | CHD  | J     | 60   | X         | -        | -       | -                |
| 22  | CHD  | P     | 1271 | X         | -        | -       | -                |
| 22  | CHD  | W     | 1060 | X         | -        | -       | -                |
| 23  | DMU  | C     | 272  | X         | -        | -       | -                |
| 23  | DMU  | M     | 526  | X         | -        | -       | -                |
| 23  | DMU  | P     | 1272 | X         | -        | -       | -                |
| 23  | DMU  | Z     | 1526 | X         | -        | -       | -                |
| 26  | CDL  | G     | 269  | -         | -        | X       | -                |
| 26  | CDL  | T     | 1269 | -         | -        | X       | -                |



## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32735 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       | 0       | 0     |
|     |       |          | 4027  | 2691 | 623 | 678 | 35 |         |         |       |
| 1   | N     | 514      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4027  | 2691 | 623 | 678 | 35 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 84       | Total | C   | N   | O   | P | S       | 0       | 0     |
|     |       |          | 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 VIb isoform 1.

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

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

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

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

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

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

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

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

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

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

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

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

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

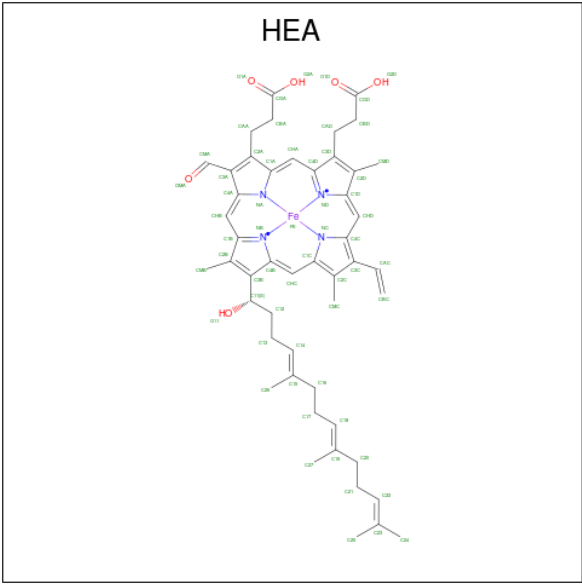
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

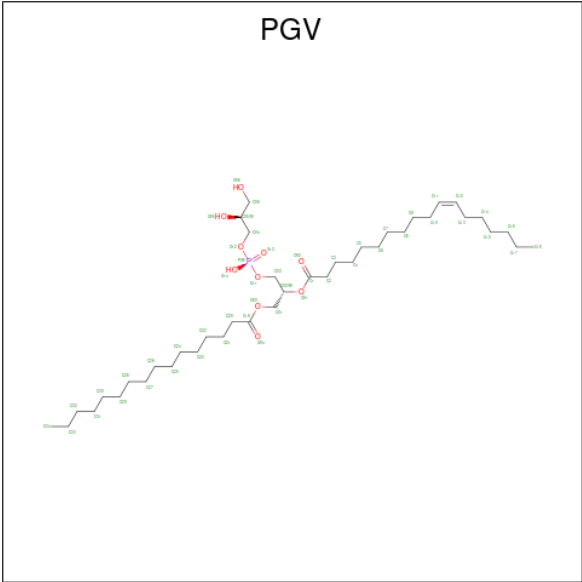
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16  | A     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | N     | 1        | Total | Na | 0       | 0       |
|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

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



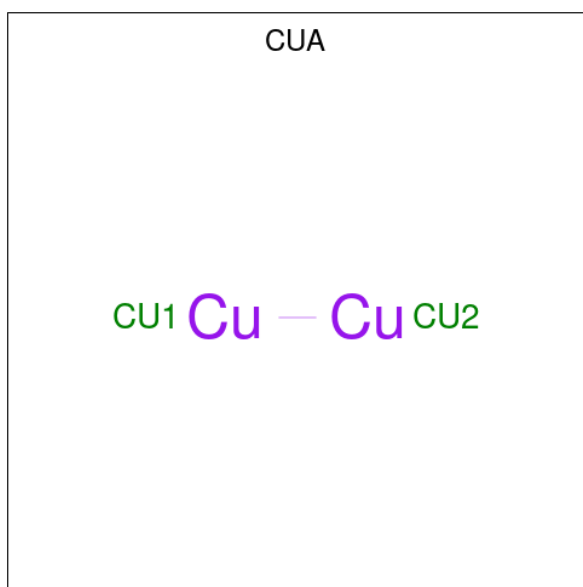
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17  | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |         |
| 17  | A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

- Molecule 18 is (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).



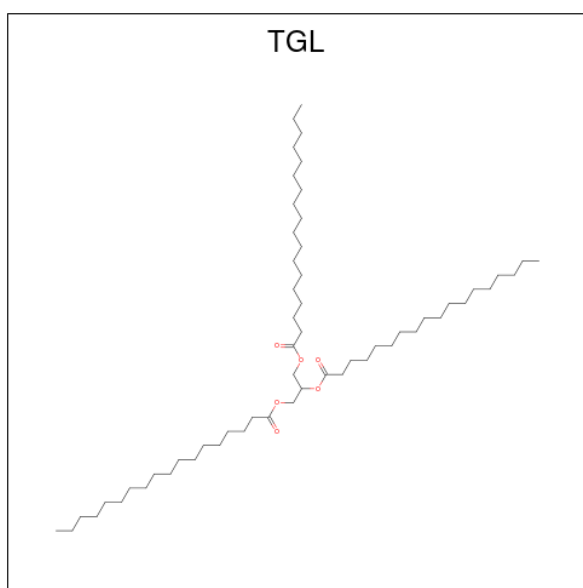
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 18  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 18  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 18  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 18  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 18  | N     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 18  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 18  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 18  | Z     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |

- Molecule 19 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 19  | B     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 19  | O     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula:  $C_{57}H_{110}O_6$ ).



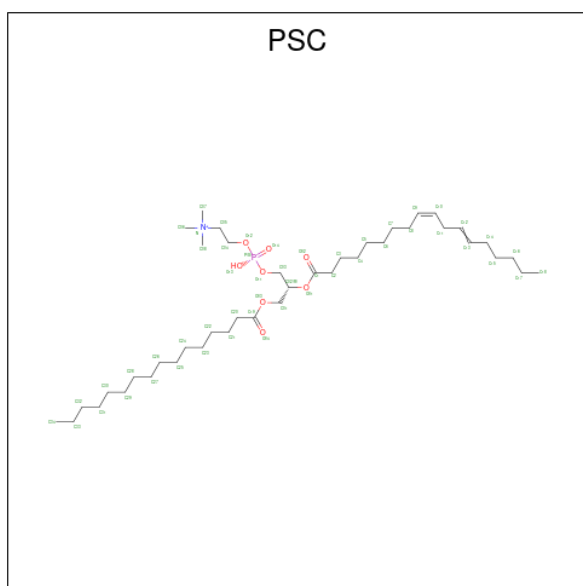
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 20  | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 20  | D     | 1        | Total | C  | O | 0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

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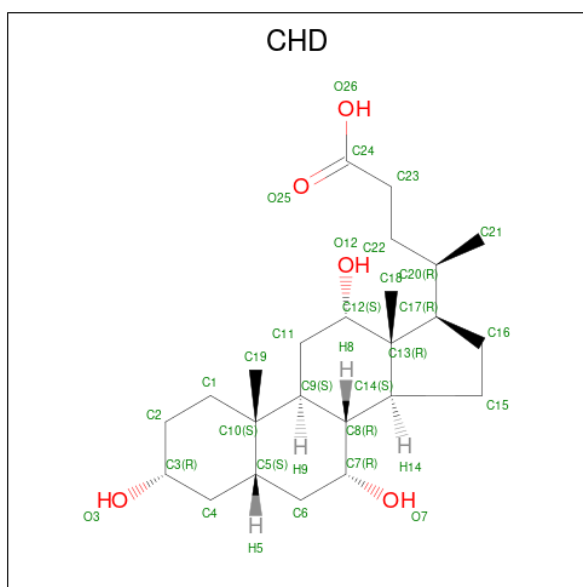
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 20  | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 20  | N     | 1        | Total | C  | O | 0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

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 21  | B     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |
| 21  | O     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |

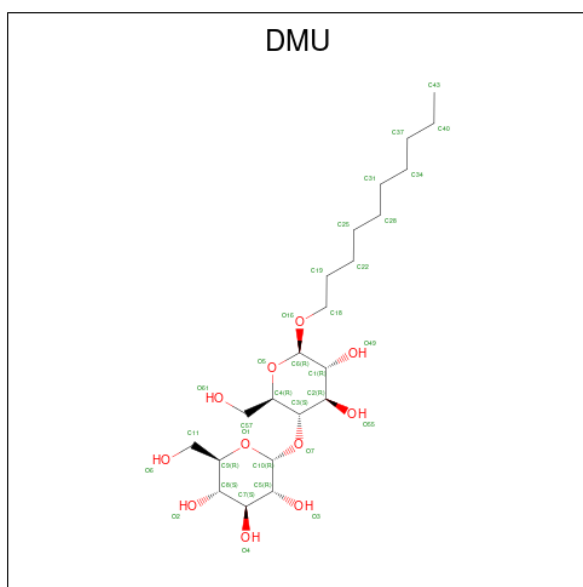
- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



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

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



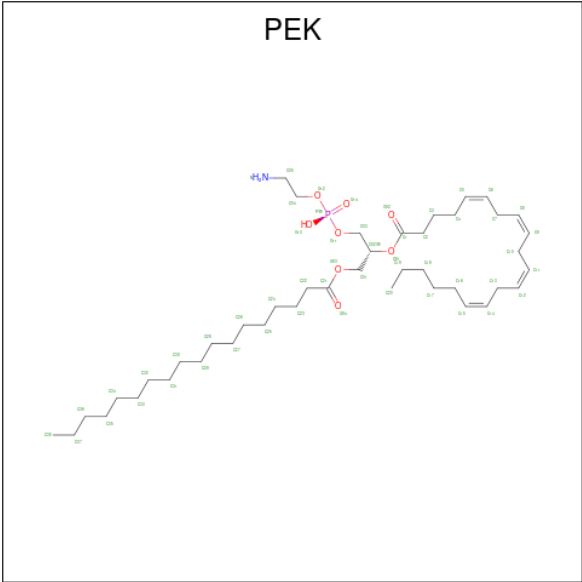


| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 23  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 23  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 23  | P     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 23  | Z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |

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

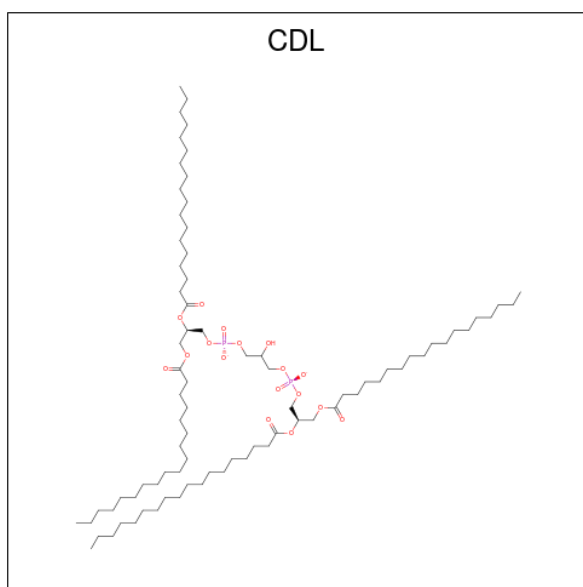
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 24  | C     | 1        | Total | X | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 24  | P     | 1        | Total | X | 0       | 0       |
|    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

- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 25  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 25  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 25  | G     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 25  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 25  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 25  | T     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |

- Molecule 26 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 |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 26  | G     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 26  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 26  | T     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |

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

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

- Molecule 28 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 28  | A     | 243      | Total | O   | 0       | 0       |
|     |       |          | 243   | 243 |         |         |
| 28  | B     | 186      | Total | O   | 0       | 0       |
|     |       |          | 186   | 186 |         |         |
| 28  | C     | 127      | Total | O   | 0       | 0       |
|     |       |          | 127   | 127 |         |         |

*Continued on next page...*

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 28  | D     | 109      | Total<br>109 | O<br>109 | 0       | 0       |
| 28  | E     | 67       | Total<br>67  | O<br>67  | 0       | 0       |
| 28  | F     | 85       | Total<br>85  | O<br>85  | 0       | 0       |
| 28  | G     | 57       | Total<br>57  | O<br>57  | 0       | 0       |
| 28  | H     | 66       | Total<br>66  | O<br>66  | 0       | 0       |
| 28  | I     | 58       | Total<br>58  | O<br>58  | 0       | 0       |
| 28  | J     | 21       | Total<br>21  | O<br>21  | 0       | 0       |
| 28  | K     | 38       | Total<br>38  | O<br>38  | 0       | 0       |
| 28  | L     | 22       | Total<br>22  | O<br>22  | 0       | 0       |
| 28  | M     | 27       | Total<br>27  | O<br>27  | 0       | 0       |
| 28  | N     | 212      | Total<br>212 | O<br>212 | 0       | 0       |
| 28  | O     | 152      | Total<br>152 | O<br>152 | 0       | 0       |
| 28  | P     | 120      | Total<br>120 | O<br>120 | 0       | 0       |
| 28  | Q     | 75       | Total<br>75  | O<br>75  | 0       | 0       |
| 28  | R     | 32       | Total<br>32  | O<br>32  | 0       | 0       |
| 28  | S     | 53       | Total<br>53  | O<br>53  | 0       | 0       |
| 28  | T     | 59       | Total<br>59  | O<br>59  | 0       | 0       |
| 28  | U     | 62       | Total<br>62  | O<br>62  | 0       | 0       |
| 28  | V     | 33       | Total<br>33  | O<br>33  | 0       | 0       |
| 28  | W     | 18       | Total<br>18  | O<br>18  | 0       | 0       |
| 28  | X     | 29       | Total<br>29  | O<br>29  | 0       | 0       |

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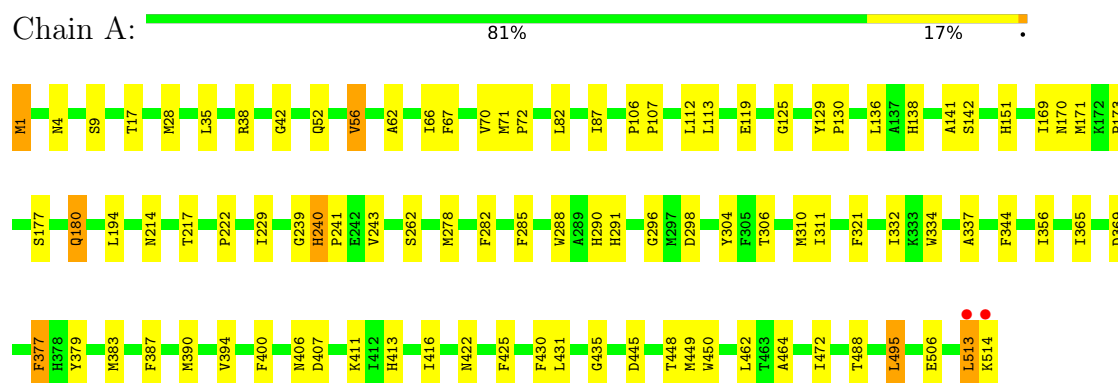
*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 28  | Y     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 28  | Z     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |

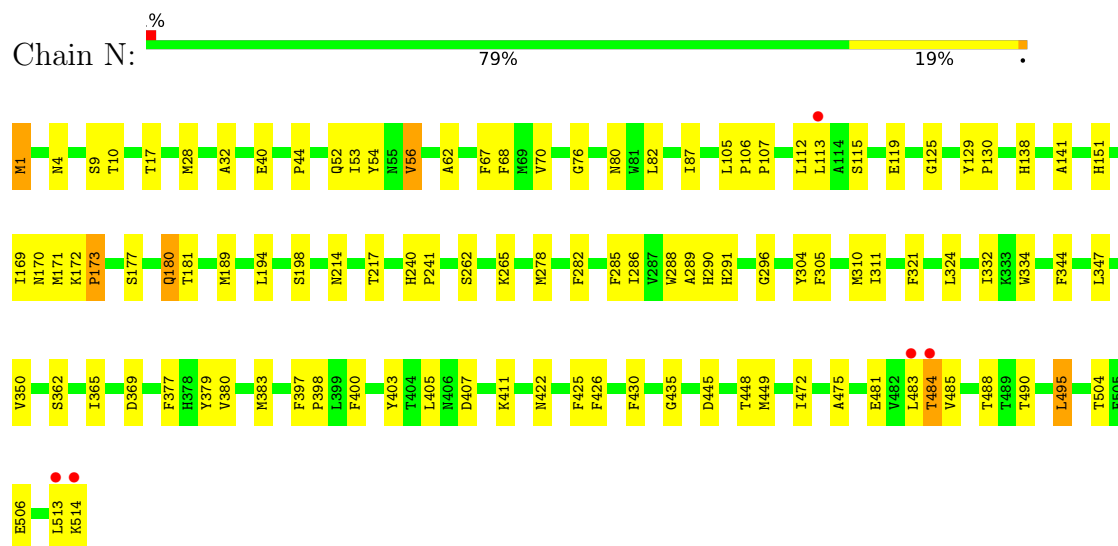
### 3 Residue-property plots

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.

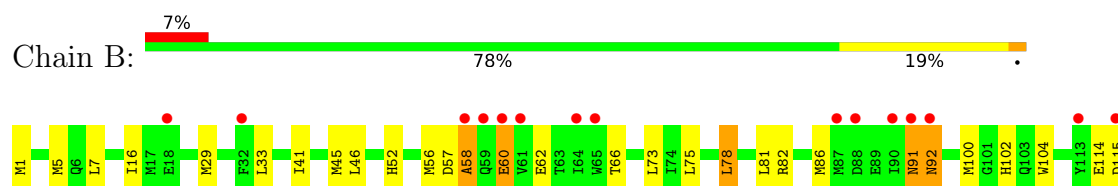
#### • Molecule 1: Cytochrome c oxidase subunit 1



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

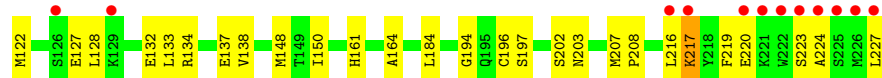
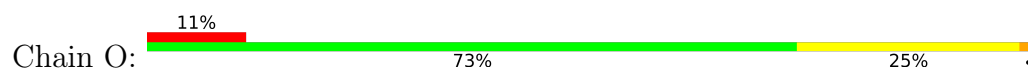


#### • Molecule 2: Cytochrome c oxidase subunit 2

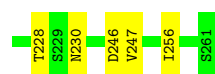
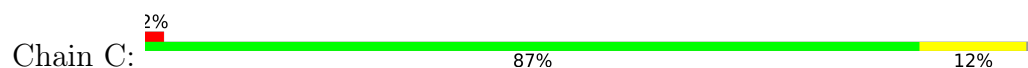




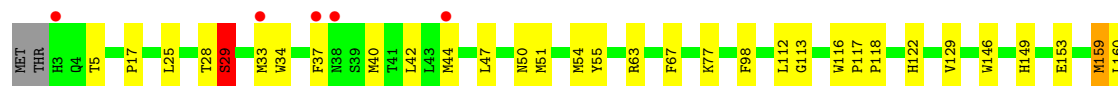
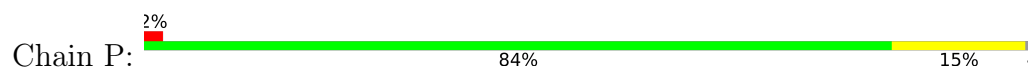
• Molecule 2: Cytochrome c oxidase subunit 2



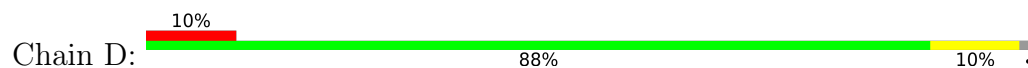
• Molecule 3: Cytochrome c oxidase subunit 3



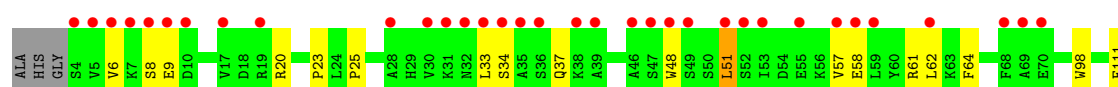
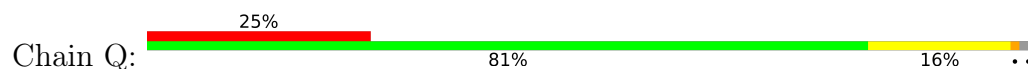
• Molecule 3: Cytochrome c oxidase subunit 3

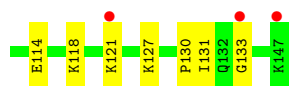


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

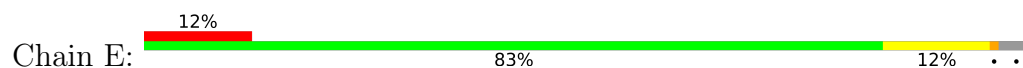


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

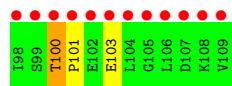




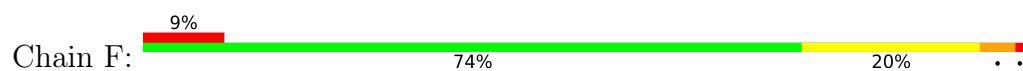
• Molecule 5: Cytochrome c oxidase polypeptide Va



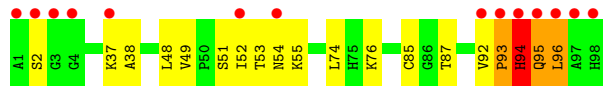
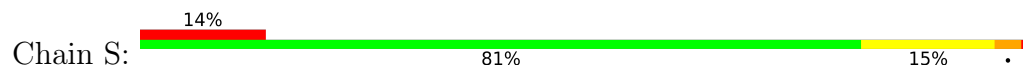
• Molecule 5: Cytochrome c oxidase polypeptide Va



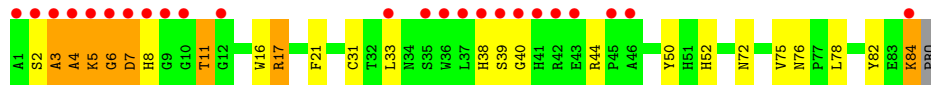
• Molecule 6: Cytochrome c oxidase polypeptide Vb



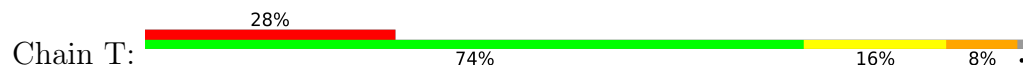
• Molecule 6: Cytochrome c oxidase polypeptide Vb



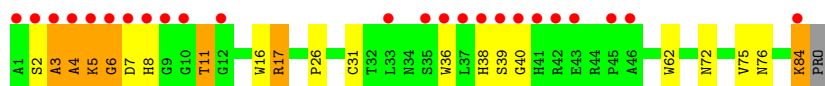
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



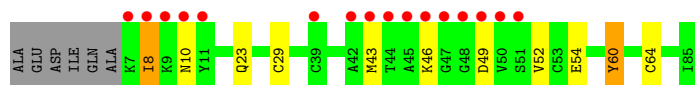
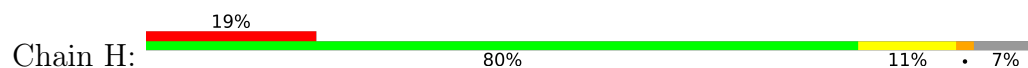
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



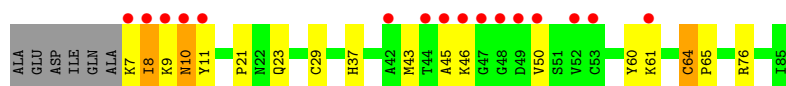




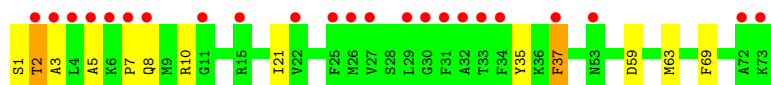
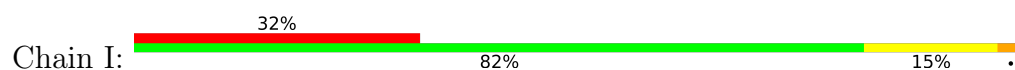
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



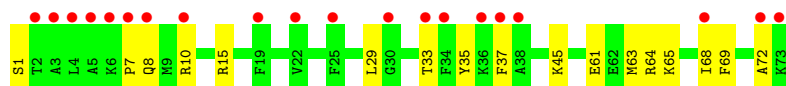
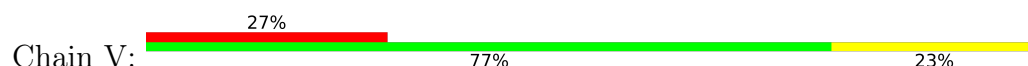
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



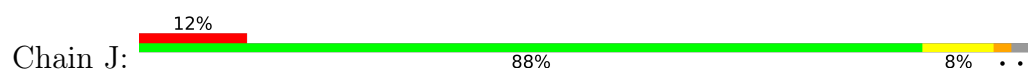
- Molecule 9: Cytochrome c oxidase polypeptide VIc



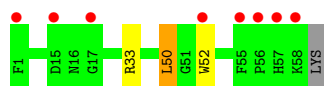
- Molecule 9: Cytochrome c oxidase polypeptide VIc



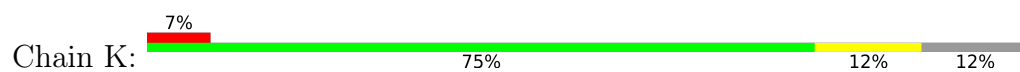
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



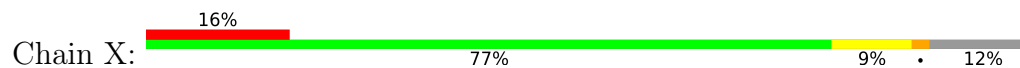
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



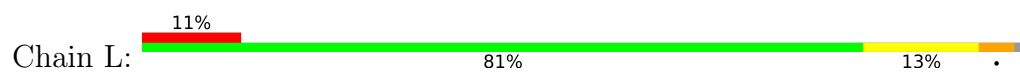
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



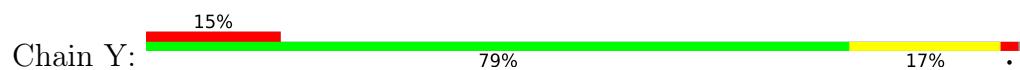
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



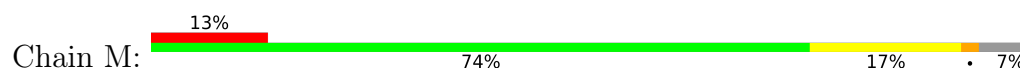
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 182.59Å 205.14Å 178.25Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 40.00 – 1.80<br>40.00 – 1.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (40.00-1.80)<br>99.2 (40.00-1.80)           | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.09 (at 1.80Å)                                             | Xtriage          |
| Refinement program                                                      | X-PLOR 3.851                                                | Depositor        |
| R, $R_{free}$                                                           | 0.202 , 0.227<br>0.202 , 0.225                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 22992 reflections (3.78%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 25.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.024                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 55.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | 0.009 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 32735                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 36.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: DMU, PEK, CUA, UNX, ZN, TGL, TPO, MG, CU, FME, PGV, CDL, NA, HEA, PSC, CHD, SAC

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 1   | A     | 0.63         | 1/4156 (0.0%)  | 1.05        | 28/5678 (0.5%)   |
| 1   | N     | 0.60         | 1/4156 (0.0%)  | 1.03        | 25/5678 (0.4%)   |
| 2   | B     | 0.59         | 0/1860         | 1.02        | 3/2534 (0.1%)    |
| 2   | O     | 0.61         | 0/1860         | 1.06        | 7/2534 (0.3%)    |
| 3   | C     | 0.56         | 0/2197         | 0.90        | 4/3005 (0.1%)    |
| 3   | P     | 0.55         | 0/2197         | 0.93        | 8/3005 (0.3%)    |
| 4   | D     | 0.54         | 0/1229         | 1.00        | 1/1658 (0.1%)    |
| 4   | Q     | 0.57         | 0/1229         | 1.02        | 1/1658 (0.1%)    |
| 5   | E     | 0.59         | 0/871          | 0.97        | 1/1182 (0.1%)    |
| 5   | R     | 0.55         | 0/871          | 1.07        | 6/1182 (0.5%)    |
| 6   | F     | 0.60         | 0/765          | 1.20        | 12/1038 (1.2%)   |
| 6   | S     | 0.62         | 0/765          | 1.22        | 7/1038 (0.7%)    |
| 7   | G     | 0.61         | 1/690 (0.1%)   | 1.01        | 3/937 (0.3%)     |
| 7   | T     | 0.63         | 1/690 (0.1%)   | 1.02        | 2/937 (0.2%)     |
| 8   | H     | 0.56         | 0/682          | 1.01        | 4/921 (0.4%)     |
| 8   | U     | 0.56         | 0/682          | 1.04        | 3/921 (0.3%)     |
| 9   | I     | 0.55         | 0/605          | 0.89        | 1/802 (0.1%)     |
| 9   | V     | 0.54         | 0/605          | 0.85        | 1/802 (0.1%)     |
| 10  | J     | 0.52         | 0/471          | 0.91        | 0/636            |
| 10  | W     | 0.51         | 0/471          | 0.97        | 0/636            |
| 11  | K     | 0.59         | 0/398          | 1.13        | 4/546 (0.7%)     |
| 11  | X     | 0.54         | 0/398          | 1.05        | 2/546 (0.4%)     |
| 12  | L     | 0.51         | 0/393          | 0.87        | 2/526 (0.4%)     |
| 12  | Y     | 0.54         | 0/393          | 0.90        | 1/526 (0.2%)     |
| 13  | M     | 0.54         | 0/345          | 0.96        | 1/470 (0.2%)     |
| 13  | Z     | 0.52         | 0/345          | 0.98        | 1/470 (0.2%)     |
| All | All   | 0.58         | 4/29324 (0.0%) | 1.01        | 128/39866 (0.3%) |

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

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | N     | 0                   | 1                   |
| 8   | U     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 7   | G     | 5   | LYS  | CA-C  | 5.40 | 1.56        | 1.53     |
| 1   | A     | 130 | PRO  | CA-C  | 5.21 | 1.57        | 1.52     |
| 1   | N     | 173 | PRO  | CA-C  | 5.21 | 1.54        | 1.51     |
| 7   | T     | 5   | LYS  | CA-C  | 5.03 | 1.56        | 1.53     |

All (128) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | D     | 133 | GLY  | N-CA-C | 12.74 | 127.28      | 112.50   |
| 4   | Q     | 133 | GLY  | N-CA-C | 12.61 | 127.12      | 112.50   |
| 6   | S     | 94  | HIS  | N-CA-C | 9.91  | 131.91      | 110.80   |
| 6   | F     | 93  | PRO  | N-CA-C | 9.66  | 126.31      | 111.34   |
| 6   | F     | 94  | HIS  | N-CA-C | 9.15  | 130.29      | 110.80   |
| 6   | S     | 93  | PRO  | N-CA-C | 8.89  | 125.12      | 111.34   |
| 1   | A     | 125 | GLY  | N-CA-C | -8.87 | 101.75      | 112.48   |
| 5   | R     | 42  | VAL  | N-CA-C | -8.80 | 97.91       | 107.77   |
| 1   | N     | 125 | GLY  | N-CA-C | -8.72 | 101.92      | 112.48   |
| 11  | X     | 36  | ILE  | N-CA-C | 7.92  | 119.72      | 112.43   |
| 11  | K     | 36  | ILE  | N-CA-C | 7.76  | 119.57      | 112.43   |
| 8   | U     | 64  | CYS  | N-CA-C | 7.71  | 119.36      | 109.65   |
| 1   | N     | 130 | PRO  | N-CA-C | -7.68 | 101.33      | 110.70   |
| 8   | H     | 64  | CYS  | N-CA-C | 7.51  | 119.12      | 109.65   |
| 1   | N     | 448 | THR  | N-CA-C | 7.40  | 118.99      | 111.07   |
| 5   | E     | 42  | VAL  | N-CA-C | -7.34 | 99.55       | 107.77   |
| 1   | N     | 56  | VAL  | N-CA-C | -7.04 | 103.60      | 110.72   |
| 1   | A     | 448 | THR  | N-CA-C | 7.03  | 118.60      | 111.07   |
| 1   | N     | 288 | TRP  | N-CA-C | 7.03  | 119.84      | 111.33   |
| 1   | A     | 130 | PRO  | N-CA-C | -7.01 | 102.14      | 110.70   |
| 1   | A     | 288 | TRP  | N-CA-C | 6.97  | 119.76      | 111.33   |
| 1   | A     | 141 | ALA  | N-CA-C | 6.81  | 120.85      | 112.54   |
| 3   | C     | 256 | ILE  | N-CA-C | 6.80  | 117.42      | 110.82   |
| 1   | N     | 262 | SER  | N-CA-C | -6.79 | 104.61      | 113.17   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | N     | 141 | ALA  | N-CA-C  | 6.78  | 120.81      | 112.54   |
| 3   | P     | 256 | ILE  | N-CA-C  | 6.74  | 117.36      | 110.82   |
| 6   | F     | 82  | CYS  | CA-C-N  | 6.73  | 126.42      | 119.56   |
| 6   | F     | 82  | CYS  | C-N-CA  | 6.73  | 126.42      | 119.56   |
| 1   | N     | 171 | MET  | N-CA-C  | 6.71  | 121.12      | 112.26   |
| 1   | A     | 56  | VAL  | N-CA-C  | -6.69 | 103.96      | 110.72   |
| 6   | S     | 49  | VAL  | N-CA-C  | 6.66  | 114.15      | 107.55   |
| 1   | A     | 82  | LEU  | N-CA-C  | 6.66  | 121.71      | 112.45   |
| 13  | Z     | 27  | LEU  | N-CA-C  | 6.60  | 118.55      | 111.36   |
| 13  | M     | 27  | LEU  | N-CA-C  | 6.60  | 118.55      | 111.36   |
| 1   | A     | 425 | PHE  | N-CA-C  | 6.59  | 121.53      | 112.90   |
| 2   | B     | 161 | HIS  | N-CA-C  | -6.58 | 99.59       | 108.86   |
| 1   | N     | 332 | ILE  | N-CA-C  | 6.55  | 117.77      | 108.93   |
| 6   | F     | 95  | GLN  | N-CA-C  | 6.53  | 124.70      | 110.80   |
| 1   | N     | 425 | PHE  | N-CA-C  | 6.45  | 121.44      | 113.50   |
| 1   | A     | 169 | ILE  | CB-CA-C | -6.44 | 103.61      | 112.24   |
| 6   | S     | 93  | PRO  | CA-C-N  | 6.43  | 133.83      | 121.54   |
| 6   | S     | 93  | PRO  | C-N-CA  | 6.43  | 133.83      | 121.54   |
| 1   | A     | 170 | ASN  | N-CA-C  | 6.41  | 121.38      | 113.50   |
| 1   | N     | 82  | LEU  | N-CA-C  | 6.38  | 121.32      | 112.45   |
| 1   | A     | 262 | SER  | N-CA-C  | -6.36 | 105.27      | 113.16   |
| 12  | Y     | 20  | ARG  | N-CA-C  | -6.35 | 104.44      | 111.36   |
| 7   | G     | 75  | VAL  | N-CA-C  | 6.25  | 119.78      | 113.47   |
| 1   | A     | 435 | GLY  | N-CA-C  | 6.23  | 124.73      | 115.64   |
| 1   | N     | 435 | GLY  | N-CA-C  | 6.18  | 124.66      | 115.64   |
| 3   | P     | 113 | GLY  | N-CA-C  | -6.16 | 106.65      | 115.64   |
| 5   | R     | 76  | GLY  | CA-C-N  | 6.13  | 125.83      | 119.64   |
| 5   | R     | 76  | GLY  | C-N-CA  | 6.13  | 125.83      | 119.64   |
| 11  | K     | 6   | ALA  | CA-C-N  | 6.11  | 126.42      | 119.83   |
| 11  | K     | 6   | ALA  | C-N-CA  | 6.11  | 126.42      | 119.83   |
| 1   | A     | 217 | THR  | N-CA-C  | -6.10 | 102.66      | 110.53   |
| 3   | C     | 113 | GLY  | N-CA-C  | -6.08 | 106.77      | 115.64   |
| 1   | A     | 171 | MET  | N-CA-C  | 6.08  | 120.28      | 112.26   |
| 7   | T     | 75  | VAL  | N-CA-C  | 6.05  | 119.58      | 113.47   |
| 3   | P     | 129 | VAL  | N-CA-CB | 6.00  | 114.28      | 110.50   |
| 1   | A     | 9   | SER  | N-CA-C  | 6.00  | 118.04      | 110.24   |
| 1   | A     | 332 | ILE  | N-CA-C  | 6.00  | 117.03      | 108.93   |
| 8   | H     | 10  | ASN  | CA-C-N  | 5.91  | 129.15      | 120.82   |
| 8   | H     | 10  | ASN  | C-N-CA  | 5.91  | 129.15      | 120.82   |
| 1   | N     | 445 | ASP  | N-CA-C  | 5.90  | 118.47      | 111.33   |
| 12  | L     | 20  | ARG  | N-CA-C  | -5.88 | 104.95      | 111.36   |
| 6   | F     | 49  | VAL  | N-CA-C  | 5.87  | 113.88      | 107.60   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 197 | SER  | N-CA-C  | 5.86  | 120.00      | 112.26   |
| 8   | H     | 54  | GLU  | N-CA-C  | 5.83  | 118.11      | 111.11   |
| 3   | P     | 122 | HIS  | CA-C-N  | 5.75  | 125.70      | 119.78   |
| 3   | P     | 122 | HIS  | C-N-CA  | 5.75  | 125.70      | 119.78   |
| 1   | A     | 506 | GLU  | N-CA-C  | -5.75 | 105.10      | 111.71   |
| 2   | O     | 58  | ALA  | N-CA-C  | 5.74  | 120.94      | 113.88   |
| 3   | P     | 228 | THR  | N-CA-C  | -5.70 | 102.02      | 110.46   |
| 1   | N     | 70  | VAL  | N-CA-C  | 5.68  | 115.81      | 110.30   |
| 1   | A     | 445 | ASP  | N-CA-C  | 5.65  | 118.17      | 111.33   |
| 1   | N     | 217 | THR  | N-CA-C  | -5.64 | 103.25      | 110.53   |
| 1   | N     | 506 | GLU  | N-CA-C  | -5.64 | 105.23      | 111.71   |
| 1   | A     | 70  | VAL  | N-CA-C  | 5.58  | 115.71      | 110.30   |
| 7   | G     | 6   | GLY  | N-CA-C  | 5.55  | 126.33      | 113.18   |
| 9   | V     | 69  | PHE  | N-CA-C  | 5.53  | 119.11      | 110.32   |
| 6   | F     | 54  | ASN  | N-CA-C  | 5.53  | 119.65      | 113.02   |
| 9   | I     | 69  | PHE  | N-CA-C  | 5.52  | 119.09      | 110.32   |
| 7   | T     | 6   | GLY  | N-CA-C  | 5.51  | 126.25      | 113.18   |
| 2   | O     | 161 | HIS  | N-CA-C  | -5.51 | 101.09      | 108.86   |
| 6   | F     | 12  | GLN  | N-CA-C  | 5.50  | 121.76      | 114.12   |
| 6   | F     | 94  | HIS  | CA-C-N  | 5.49  | 132.03      | 121.54   |
| 6   | F     | 94  | HIS  | C-N-CA  | 5.49  | 132.03      | 121.54   |
| 1   | A     | 495 | LEU  | N-CA-C  | 5.48  | 119.44      | 112.87   |
| 1   | N     | 129 | TYR  | N-CA-C  | 5.46  | 116.77      | 109.83   |
| 1   | A     | 67  | PHE  | N-CA-C  | 5.46  | 119.10      | 112.23   |
| 1   | N     | 170 | ASN  | N-CA-C  | 5.42  | 120.17      | 113.50   |
| 5   | R     | 100 | THR  | CA-C-N  | 5.42  | 125.50      | 119.32   |
| 5   | R     | 100 | THR  | C-N-CA  | 5.42  | 125.50      | 119.32   |
| 1   | N     | 119 | GLU  | CB-CA-C | -5.41 | 110.32      | 116.54   |
| 1   | A     | 142 | SER  | N-CA-C  | 5.36  | 117.56      | 111.02   |
| 1   | A     | 129 | TYR  | N-CA-C  | 5.34  | 116.62      | 109.83   |
| 2   | B     | 58  | ALA  | N-CA-C  | 5.34  | 120.45      | 113.88   |
| 1   | N     | 67  | PHE  | N-CA-C  | 5.34  | 118.96      | 112.23   |
| 2   | O     | 127 | GLU  | N-CA-C  | 5.28  | 119.82      | 113.17   |
| 6   | S     | 54  | ASN  | CB-CA-C | -5.24 | 99.69       | 110.38   |
| 2   | O     | 202 | SER  | N-CA-C  | 5.22  | 119.99      | 111.37   |
| 8   | U     | 10  | ASN  | CA-C-N  | 5.21  | 128.17      | 120.82   |
| 8   | U     | 10  | ASN  | C-N-CA  | 5.21  | 128.17      | 120.82   |
| 11  | X     | 7   | PRO  | N-CA-C  | 5.21  | 119.05      | 111.03   |
| 3   | P     | 29  | SER  | N-CA-C  | -5.20 | 105.61      | 111.28   |
| 12  | L     | 3   | TYR  | N-CA-C  | 5.16  | 118.16      | 110.52   |
| 1   | A     | 66  | ILE  | N-CA-C  | 5.16  | 115.44      | 110.74   |
| 2   | O     | 197 | SER  | N-CA-C  | 5.15  | 119.74      | 111.81   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 119 | GLU  | CB-CA-C | -5.14 | 110.63      | 116.54   |
| 3   | C     | 228 | THR  | N-CA-C  | -5.13 | 102.86      | 110.46   |
| 1   | A     | 239 | GLY  | N-CA-C  | 5.12  | 118.84      | 112.64   |
| 2   | O     | 92  | ASN  | CA-C-N  | 5.12  | 125.10      | 120.03   |
| 2   | O     | 92  | ASN  | C-N-CA  | 5.12  | 125.10      | 120.03   |
| 3   | C     | 198 | PHE  | N-CA-C  | 5.12  | 117.76      | 111.82   |
| 1   | A     | 214 | ASN  | N-CA-C  | 5.11  | 121.06      | 114.56   |
| 5   | R     | 16  | VAL  | N-CA-C  | -5.11 | 105.73      | 110.53   |
| 3   | P     | 159 | MET  | N-CA-C  | -5.09 | 105.64      | 111.14   |
| 1   | N     | 9   | SER  | N-CA-C  | 5.08  | 117.26      | 110.35   |
| 1   | N     | 214 | ASN  | N-CA-C  | 5.08  | 121.01      | 114.56   |
| 1   | A     | 377 | PHE  | N-CA-C  | 5.07  | 118.73      | 112.54   |
| 6   | S     | 2   | SER  | N-CA-C  | 5.07  | 116.52      | 108.96   |
| 7   | G     | 78  | LEU  | N-CA-C  | -5.06 | 104.31      | 110.13   |
| 1   | N     | 10  | THR  | N-CA-C  | -5.06 | 104.93      | 111.71   |
| 1   | N     | 495 | LEU  | N-CA-C  | 5.04  | 118.92      | 112.87   |
| 6   | F     | 32  | ASN  | N-CA-C  | 5.03  | 118.14      | 111.30   |
| 11  | K     | 13  | TYR  | N-CA-C  | 5.01  | 120.01      | 113.30   |
| 6   | F     | 39  | THR  | N-CA-C  | -5.00 | 102.21      | 109.31   |
| 1   | N     | 198 | SER  | N-CA-C  | 5.00  | 117.84      | 111.69   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 240 | HIS  | Sidechain |
| 1   | N     | 240 | HIS  | Sidechain |
| 8   | U     | 11  | TYR  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4027  | 0        | 4001     | 69      | 0            |
| 1   | N     | 4027  | 0        | 4001     | 77      | 0            |
| 2   | B     | 1824  | 0        | 1833     | 32      | 0            |
| 2   | O     | 1824  | 0        | 1833     | 42      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | C     | 2110  | 0        | 2027     | 30      | 0            |
| 3   | P     | 2110  | 0        | 2027     | 34      | 0            |
| 4   | D     | 1195  | 0        | 1183     | 10      | 0            |
| 4   | Q     | 1195  | 0        | 1183     | 18      | 0            |
| 5   | E     | 852   | 0        | 845      | 6       | 0            |
| 5   | R     | 852   | 0        | 845      | 15      | 0            |
| 6   | F     | 748   | 0        | 728      | 12      | 0            |
| 6   | S     | 748   | 0        | 728      | 15      | 0            |
| 7   | G     | 675   | 0        | 644      | 26      | 0            |
| 7   | T     | 675   | 0        | 644      | 28      | 0            |
| 8   | H     | 662   | 0        | 623      | 5       | 0            |
| 8   | U     | 662   | 0        | 623      | 10      | 0            |
| 9   | I     | 601   | 0        | 613      | 8       | 0            |
| 9   | V     | 601   | 0        | 613      | 9       | 0            |
| 10  | J     | 460   | 0        | 459      | 5       | 0            |
| 10  | W     | 460   | 0        | 459      | 3       | 0            |
| 11  | K     | 384   | 0        | 366      | 3       | 0            |
| 11  | X     | 384   | 0        | 366      | 6       | 0            |
| 12  | L     | 380   | 0        | 380      | 15      | 0            |
| 12  | Y     | 380   | 0        | 380      | 10      | 0            |
| 13  | M     | 335   | 0        | 352      | 5       | 0            |
| 13  | Z     | 335   | 0        | 352      | 6       | 0            |
| 14  | A     | 1     | 0        | 0        | 0       | 0            |
| 14  | N     | 1     | 0        | 0        | 0       | 0            |
| 15  | A     | 1     | 0        | 0        | 0       | 0            |
| 15  | N     | 1     | 0        | 0        | 0       | 0            |
| 16  | A     | 1     | 0        | 0        | 0       | 0            |
| 16  | N     | 1     | 0        | 0        | 0       | 0            |
| 17  | A     | 120   | 0        | 108      | 3       | 0            |
| 17  | N     | 120   | 0        | 108      | 3       | 0            |
| 18  | A     | 102   | 0        | 152      | 7       | 0            |
| 18  | C     | 102   | 0        | 152      | 8       | 0            |
| 18  | N     | 51    | 0        | 76       | 2       | 0            |
| 18  | P     | 102   | 0        | 152      | 8       | 0            |
| 18  | Z     | 51    | 0        | 76       | 4       | 0            |
| 19  | B     | 2     | 0        | 0        | 0       | 0            |
| 19  | O     | 2     | 0        | 0        | 0       | 0            |
| 20  | B     | 63    | 0        | 110      | 10      | 0            |
| 20  | D     | 63    | 0        | 110      | 5       | 0            |
| 20  | L     | 63    | 0        | 110      | 23      | 0            |
| 20  | N     | 126   | 0        | 220      | 30      | 0            |
| 20  | Q     | 63    | 0        | 110      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 21  | B     | 52    | 0        | 80       | 13      | 0            |
| 21  | O     | 52    | 0        | 80       | 12      | 0            |
| 22  | B     | 29    | 0        | 39       | 0       | 0            |
| 22  | C     | 58    | 0        | 78       | 2       | 0            |
| 22  | J     | 29    | 0        | 39       | 2       | 0            |
| 22  | O     | 29    | 0        | 39       | 1       | 0            |
| 22  | P     | 58    | 0        | 78       | 2       | 0            |
| 22  | W     | 29    | 0        | 39       | 2       | 0            |
| 23  | C     | 33    | 0        | 36       | 2       | 0            |
| 23  | M     | 33    | 0        | 36       | 0       | 0            |
| 23  | P     | 33    | 0        | 36       | 7       | 0            |
| 23  | Z     | 33    | 0        | 36       | 1       | 0            |
| 24  | C     | 1     | 0        | 0        | 0       | 0            |
| 24  | P     | 1     | 0        | 0        | 0       | 0            |
| 25  | C     | 106   | 0        | 154      | 11      | 0            |
| 25  | G     | 53    | 0        | 77       | 7       | 0            |
| 25  | P     | 106   | 0        | 154      | 12      | 0            |
| 25  | T     | 53    | 0        | 77       | 8       | 0            |
| 26  | C     | 100   | 0        | 156      | 17      | 0            |
| 26  | G     | 100   | 0        | 156      | 21      | 0            |
| 26  | P     | 100   | 0        | 156      | 15      | 0            |
| 26  | T     | 100   | 0        | 156      | 21      | 0            |
| 27  | F     | 1     | 0        | 0        | 0       | 0            |
| 27  | S     | 1     | 0        | 0        | 0       | 0            |
| 28  | A     | 243   | 0        | 0        | 4       | 0            |
| 28  | B     | 186   | 0        | 0        | 4       | 0            |
| 28  | C     | 127   | 0        | 0        | 2       | 0            |
| 28  | D     | 109   | 0        | 0        | 4       | 0            |
| 28  | E     | 67    | 0        | 0        | 0       | 0            |
| 28  | F     | 85    | 0        | 0        | 1       | 0            |
| 28  | G     | 57    | 0        | 0        | 2       | 0            |
| 28  | H     | 66    | 0        | 0        | 1       | 0            |
| 28  | I     | 58    | 0        | 0        | 3       | 0            |
| 28  | J     | 21    | 0        | 0        | 1       | 0            |
| 28  | K     | 38    | 0        | 0        | 0       | 0            |
| 28  | L     | 22    | 0        | 0        | 2       | 0            |
| 28  | M     | 27    | 0        | 0        | 1       | 0            |
| 28  | N     | 212   | 0        | 0        | 3       | 0            |
| 28  | O     | 152   | 0        | 0        | 2       | 0            |
| 28  | P     | 120   | 0        | 0        | 3       | 0            |
| 28  | Q     | 75    | 0        | 0        | 3       | 0            |
| 28  | R     | 32    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | S     | 53    | 0        | 0        | 1       | 0            |
| 28  | T     | 59    | 0        | 0        | 2       | 0            |
| 28  | U     | 62    | 0        | 0        | 3       | 0            |
| 28  | V     | 33    | 0        | 0        | 2       | 0            |
| 28  | W     | 18    | 0        | 0        | 0       | 0            |
| 28  | X     | 29    | 0        | 0        | 1       | 0            |
| 28  | Y     | 31    | 0        | 0        | 2       | 0            |
| 28  | Z     | 21    | 0        | 0        | 2       | 0            |
| All | All   | 32735 | 0        | 31294    | 557     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (557) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G:84:LYS:H       | 7:G:84:LYS:HD2     | 1.17                     | 1.05              |
| 7:T:84:LYS:HD2     | 7:T:84:LYS:H       | 1.19                     | 1.02              |
| 3:C:63:ARG:HE      | 26:C:270:CDL:HA22  | 1.24                     | 1.01              |
| 21:O:1230:PSC:H142 | 21:O:1230:PSC:H343 | 1.42                     | 1.01              |
| 21:B:230:PSC:H343  | 21:B:230:PSC:H142  | 1.42                     | 1.01              |
| 3:P:63:ARG:HE      | 26:P:1270:CDL:HA22 | 1.21                     | 0.98              |
| 7:T:72:ASN:H       | 7:T:76:ASN:HD22    | 1.16                     | 0.94              |
| 4:D:34:SER:H       | 4:D:37:GLN:HE21    | 1.14                     | 0.93              |
| 26:P:1270:CDL:H191 | 26:P:1270:CDL:H642 | 1.51                     | 0.92              |
| 26:C:270:CDL:H191  | 26:C:270:CDL:H642  | 1.51                     | 0.91              |
| 7:G:72:ASN:H       | 7:G:76:ASN:HD22    | 1.19                     | 0.90              |
| 10:W:33:ARG:HG2    | 22:W:1060:CHD:H152 | 1.53                     | 0.90              |
| 26:G:269:CDL:H541  | 26:G:269:CDL:H231  | 1.53                     | 0.90              |
| 2:O:224:ALA:O      | 2:O:227:LEU:HG     | 1.72                     | 0.89              |
| 7:T:5:LYS:HB2      | 25:T:263:PEK:H362  | 1.53                     | 0.89              |
| 20:B:521:TGL:H281  | 20:B:521:TGL:H102  | 1.55                     | 0.88              |
| 7:G:5:LYS:HB2      | 25:G:1263:PEK:H362 | 1.56                     | 0.88              |
| 20:N:1521:TGL:H281 | 20:N:1521:TGL:H102 | 1.54                     | 0.88              |
| 26:T:1269:CDL:H541 | 26:T:1269:CDL:H231 | 1.55                     | 0.88              |
| 6:F:85:CYS:SG      | 6:F:87:THR:HG23    | 2.14                     | 0.87              |
| 25:C:264:PEK:H161  | 25:C:264:PEK:H102  | 1.57                     | 0.86              |
| 7:T:31:CYS:SG      | 26:T:1269:CDL:H532 | 2.16                     | 0.85              |
| 1:N:472:ILE:HG21   | 20:N:1522:TGL:HA92 | 1.58                     | 0.85              |
| 7:G:5:LYS:HB3      | 1:N:278:MET:SD     | 2.16                     | 0.85              |
| 1:A:472:ILE:HG21   | 20:L:522:TGL:HA92  | 1.59                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:T:5:LYS:HG3      | 25:T:263:PEK:H383  | 1.59                     | 0.84              |
| 25:P:1264:PEK:H102 | 25:P:1264:PEK:H161 | 1.58                     | 0.83              |
| 2:O:41:ILE:HD13    | 21:O:1230:PSC:H342 | 1.60                     | 0.83              |
| 6:S:53:THR:HA      | 6:S:94:HIS:CE1     | 2.14                     | 0.83              |
| 12:L:20:ARG:HH22   | 20:L:522:TGL:HC61  | 1.45                     | 0.82              |
| 28:C:4863:HOH:O    | 6:F:1:ALA:HB2      | 1.79                     | 0.81              |
| 7:G:31:CYS:SG      | 26:G:269:CDL:H532  | 2.21                     | 0.80              |
| 12:L:24:MET:SD     | 20:L:522:TGL:H162  | 2.21                     | 0.80              |
| 20:L:522:TGL:HC62  | 20:L:522:TGL:HC22  | 1.64                     | 0.80              |
| 21:O:1230:PSC:H071 | 9:V:10:ARG:HE      | 1.47                     | 0.80              |
| 1:A:278:MET:SD     | 7:T:5:LYS:HB3      | 2.22                     | 0.79              |
| 20:N:1521:TGL:H102 | 20:N:1521:TGL:C28  | 2.12                     | 0.79              |
| 7:T:84:LYS:H       | 7:T:84:LYS:CD      | 1.95                     | 0.79              |
| 26:G:269:CDL:H622  | 18:P:1268:PGV:H152 | 1.64                     | 0.78              |
| 5:E:82:TYR:HB3     | 5:E:83:PRO:HD3     | 1.66                     | 0.77              |
| 20:B:521:TGL:H102  | 20:B:521:TGL:C28   | 2.15                     | 0.77              |
| 4:D:34:SER:H       | 4:D:37:GLN:NE2     | 1.84                     | 0.76              |
| 20:N:1522:TGL:HC62 | 20:N:1522:TGL:HC22 | 1.66                     | 0.76              |
| 5:R:43:PRO:HB2     | 5:R:48:ILE:HD11    | 1.68                     | 0.76              |
| 1:N:321:PHE:CD2    | 21:O:1230:PSC:H341 | 2.20                     | 0.75              |
| 20:B:521:TGL:H241  | 20:B:521:TGL:H201  | 1.69                     | 0.74              |
| 3:P:246:ASP:HB2    | 28:P:4502:HOH:O    | 1.87                     | 0.74              |
| 25:C:264:PEK:HN2   | 7:G:76:ASN:HD21    | 1.37                     | 0.73              |
| 20:N:1522:TGL:HC31 | 12:Y:13:PHE:HA     | 1.69                     | 0.73              |
| 12:L:13:PHE:HA     | 20:L:522:TGL:HC31  | 1.70                     | 0.73              |
| 20:N:1521:TGL:H241 | 20:N:1521:TGL:H201 | 1.68                     | 0.73              |
| 7:G:5:LYS:HG3      | 25:G:1263:PEK:H383 | 1.70                     | 0.73              |
| 26:G:269:CDL:H522  | 26:G:269:CDL:H202  | 1.70                     | 0.72              |
| 3:P:34:TRP:CZ2     | 23:P:1272:DMU:H29  | 2.25                     | 0.72              |
| 20:N:1522:TGL:H242 | 20:N:1522:TGL:H202 | 1.72                     | 0.71              |
| 12:L:20:ARG:HH12   | 20:L:522:TGL:HC61  | 1.55                     | 0.71              |
| 1:A:282:PHE:HA     | 7:T:4:ALA:HB3      | 1.72                     | 0.70              |
| 20:L:522:TGL:H242  | 20:L:522:TGL:H202  | 1.72                     | 0.70              |
| 3:P:29:SER:HB3     | 3:P:42:LEU:HD13    | 1.73                     | 0.70              |
| 1:N:334:TRP:CZ3    | 20:Q:1523:TGL:HA51 | 2.27                     | 0.70              |
| 2:B:41:ILE:HD13    | 21:B:230:PSC:H342  | 1.74                     | 0.70              |
| 1:A:1:FME:HE2      | 1:A:1:FME:HA       | 1.73                     | 0.69              |
| 18:C:268:PGV:H152  | 26:T:1269:CDL:H622 | 1.74                     | 0.69              |
| 13:M:42:LYS:HE3    | 13:M:42:LYS:HA     | 1.74                     | 0.69              |
| 1:A:321:PHE:CD2    | 21:B:230:PSC:H341  | 2.27                     | 0.69              |
| 25:P:1264:PEK:HN2  | 7:T:76:ASN:HD21    | 1.39                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:T:1269:CDL:H522 | 26:T:1269:CDL:H202 | 1.75                     | 0.69              |
| 18:Z:1524:PGV:H152 | 18:Z:1524:PGV:H321 | 1.74                     | 0.69              |
| 7:T:5:LYS:HD2      | 25:T:263:PEK:H371  | 1.75                     | 0.68              |
| 1:N:449:MET:SD     | 2:O:5:MET:HG2      | 2.33                     | 0.68              |
| 8:H:43:MET:HE1     | 8:U:43:MET:HE1     | 1.75                     | 0.68              |
| 21:B:230:PSC:C07   | 9:I:10:ARG:HH21    | 2.06                     | 0.67              |
| 10:J:33:ARG:HG2    | 22:J:60:CHD:H152   | 1.77                     | 0.67              |
| 4:Q:114:GLU:HG2    | 28:Q:4443:HOH:O    | 1.95                     | 0.67              |
| 1:N:1:FME:HCN      | 1:N:4:ASN:H        | 1.60                     | 0.67              |
| 7:G:72:ASN:H       | 7:G:76:ASN:ND2     | 1.93                     | 0.67              |
| 18:A:524:PGV:H152  | 18:A:524:PGV:H321  | 1.77                     | 0.67              |
| 7:G:5:LYS:HD2      | 25:G:1263:PEK:H371 | 1.76                     | 0.66              |
| 18:P:1267:PGV:H161 | 18:P:1267:PGV:H12  | 1.76                     | 0.66              |
| 6:S:52:ILE:O       | 6:S:94:HIS:NE2     | 2.29                     | 0.66              |
| 6:S:85:CYS:SG      | 6:S:87:THR:HG23    | 2.35                     | 0.66              |
| 5:R:89:LEU:O       | 5:R:93:LEU:HG      | 1.95                     | 0.66              |
| 21:O:1230:PSC:C07  | 9:V:10:ARG:HE      | 2.08                     | 0.66              |
| 26:P:1270:CDL:H642 | 26:P:1270:CDL:C19  | 2.26                     | 0.66              |
| 9:V:63:MET:HB3     | 9:V:68:ILE:HD11    | 1.78                     | 0.66              |
| 12:L:20:ARG:NH2    | 20:L:522:TGL:HC61  | 2.11                     | 0.65              |
| 4:Q:58:GLU:O       | 4:Q:62:LEU:HG      | 1.96                     | 0.65              |
| 5:R:12:ASP:HA      | 5:R:47:ILE:HD11    | 1.77                     | 0.65              |
| 13:Z:19:LEU:HD23   | 18:Z:1524:PGV:H322 | 1.78                     | 0.65              |
| 1:A:334:TRP:CZ3    | 20:D:523:TGL:HA51  | 2.31                     | 0.65              |
| 26:C:270:CDL:H642  | 26:C:270:CDL:C19   | 2.25                     | 0.65              |
| 1:A:472:ILE:HG21   | 20:L:522:TGL:CA9   | 2.26                     | 0.64              |
| 18:C:267:PGV:H12   | 18:C:267:PGV:H161  | 1.77                     | 0.64              |
| 1:A:194:LEU:HD22   | 1:A:285:PHE:HE2    | 1.62                     | 0.64              |
| 26:G:269:CDL:H541  | 26:G:269:CDL:C23   | 2.26                     | 0.64              |
| 26:P:1270:CDL:H112 | 28:P:5001:HOH:O    | 1.97                     | 0.64              |
| 7:G:84:LYS:HD2     | 7:G:84:LYS:N       | 2.01                     | 0.64              |
| 7:G:84:LYS:H       | 7:G:84:LYS:CD      | 2.00                     | 0.64              |
| 1:A:337:ALA:HB2    | 1:A:394:VAL:HG23   | 1.80                     | 0.64              |
| 3:C:34:TRP:CZ2     | 23:C:272:DMU:H29   | 2.33                     | 0.64              |
| 3:P:67:PHE:HE1     | 26:P:1270:CDL:H1   | 1.62                     | 0.63              |
| 18:C:267:PGV:H182  | 26:C:270:CDL:H673  | 1.79                     | 0.63              |
| 1:N:472:ILE:HG21   | 20:N:1522:TGL:CA9  | 2.26                     | 0.63              |
| 1:N:472:ILE:HD13   | 20:N:1522:TGL:HA91 | 1.80                     | 0.62              |
| 2:O:217:LYS:HA     | 2:O:217:LYS:HE2    | 1.80                     | 0.62              |
| 26:T:1269:CDL:H172 | 26:T:1269:CDL:H511 | 1.81                     | 0.62              |
| 18:P:1268:PGV:H062 | 28:U:4465:HOH:O    | 1.99                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:G:269:CDL:H511  | 26:G:269:CDL:H172  | 1.80                     | 0.62              |
| 6:S:52:ILE:O       | 6:S:94:HIS:CE1     | 2.52                     | 0.62              |
| 1:N:483:LEU:HD13   | 4:Q:6:VAL:HB       | 1.82                     | 0.62              |
| 2:B:92:ASN:HB3     | 28:B:5097:HOH:O    | 1.99                     | 0.61              |
| 1:N:194:LEU:HD22   | 1:N:285:PHE:HE2    | 1.65                     | 0.61              |
| 1:N:334:TRP:CH2    | 2:O:46:LEU:HD13    | 2.35                     | 0.61              |
| 7:G:5:LYS:HD3      | 1:N:278:MET:HB3    | 1.81                     | 0.61              |
| 1:N:28:MET:HE2     | 17:N:515:HEA:H271  | 1.83                     | 0.61              |
| 21:B:230:PSC:H072  | 9:I:10:ARG:HH21    | 1.65                     | 0.61              |
| 3:P:210:ILE:HG23   | 18:P:1267:PGV:H102 | 1.82                     | 0.61              |
| 20:B:521:TGL:HC22  | 28:I:2381:HOH:O    | 2.00                     | 0.61              |
| 26:T:1269:CDL:H541 | 26:T:1269:CDL:C23  | 2.28                     | 0.60              |
| 26:G:269:CDL:H231  | 26:G:269:CDL:C54   | 2.30                     | 0.60              |
| 1:A:17:THR:OG1     | 20:L:522:TGL:H281  | 2.01                     | 0.60              |
| 18:C:267:PGV:H172  | 26:C:270:CDL:H662  | 1.82                     | 0.60              |
| 20:N:1521:TGL:H161 | 2:O:7:LEU:HD11     | 1.84                     | 0.60              |
| 20:N:1521:TGL:HC92 | 28:O:4466:HOH:O    | 2.02                     | 0.60              |
| 2:B:78:LEU:HD12    | 26:T:1269:CDL:H351 | 1.83                     | 0.60              |
| 3:C:67:PHE:HE1     | 26:C:270:CDL:H1    | 1.67                     | 0.60              |
| 9:V:65:LYS:O       | 11:X:54:ARG:NH1    | 2.34                     | 0.60              |
| 1:A:282:PHE:HA     | 7:T:4:ALA:CB       | 2.32                     | 0.59              |
| 1:N:113:LEU:CD1    | 20:N:1522:TGL:H292 | 2.32                     | 0.59              |
| 1:A:296:GLY:HA2    | 8:H:23:GLN:OE1     | 2.02                     | 0.59              |
| 7:T:17:ARG:HD2     | 28:T:3307:HOH:O    | 2.02                     | 0.59              |
| 3:P:34:TRP:HZ2     | 23:P:1272:DMU:H29  | 1.67                     | 0.59              |
| 12:L:20:ARG:NH1    | 20:L:522:TGL:HC61  | 2.18                     | 0.59              |
| 4:Q:127:LYS:O      | 4:Q:130:PRO:HD3    | 2.02                     | 0.59              |
| 6:F:92:VAL:HG23    | 6:F:92:VAL:O       | 2.03                     | 0.58              |
| 21:B:230:PSC:H222  | 21:B:230:PSC:H21   | 1.85                     | 0.58              |
| 6:F:25:ARG:HD2     | 28:F:4173:HOH:O    | 2.03                     | 0.58              |
| 26:T:1269:CDL:H231 | 26:T:1269:CDL:C54  | 2.32                     | 0.58              |
| 1:A:430:PHE:HE1    | 20:B:521:TGL:HB21  | 1.69                     | 0.58              |
| 20:N:1522:TGL:H162 | 12:Y:24:MET:SD     | 2.43                     | 0.58              |
| 20:B:521:TGL:H222  | 20:B:521:TGL:HA82  | 1.86                     | 0.58              |
| 3:C:210:ILE:HG23   | 18:C:267:PGV:H102  | 1.86                     | 0.58              |
| 12:L:20:ARG:HH22   | 20:L:522:TGL:CC6   | 2.16                     | 0.58              |
| 8:U:50:VAL:HG21    | 28:U:5105:HOH:O    | 2.04                     | 0.58              |
| 18:A:525:PGV:H182  | 3:C:28:THR:HG22    | 1.84                     | 0.57              |
| 26:G:269:CDL:HB32  | 1:N:304:TYR:HD1    | 1.68                     | 0.57              |
| 3:P:168:THR:HG22   | 25:P:1265:PEK:H14  | 1.87                     | 0.57              |
| 6:S:53:THR:HA      | 6:S:94:HIS:HE1     | 1.65                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:41:ILE:CD1     | 21:O:1230:PSC:H342 | 2.34                     | 0.57              |
| 21:O:1230:PSC:H21  | 21:O:1230:PSC:H222 | 1.85                     | 0.57              |
| 25:C:265:PEK:C38   | 26:G:269:CDL:H273  | 2.35                     | 0.57              |
| 7:G:17:ARG:HD2     | 28:G:2307:HOH:O    | 2.04                     | 0.57              |
| 1:N:112:LEU:HG     | 28:N:3073:HOH:O    | 2.04                     | 0.57              |
| 20:Q:1523:TGL:HC21 | 20:Q:1523:TGL:HG11 | 1.85                     | 0.56              |
| 1:A:321:PHE:CZ     | 21:B:230:PSC:H171  | 2.40                     | 0.56              |
| 3:C:160:LEU:HD13   | 22:C:271:CHD:H181  | 1.86                     | 0.56              |
| 6:S:76:LYS:HE3     | 6:S:93:PRO:HG3     | 1.87                     | 0.56              |
| 12:Y:20:ARG:NH1    | 28:Y:4492:HOH:O    | 2.39                     | 0.56              |
| 9:I:5:ALA:O        | 9:I:7:PRO:HD3      | 2.04                     | 0.56              |
| 7:T:11:TPO:HG22    | 7:T:16:TRP:HE1     | 1.69                     | 0.56              |
| 1:N:321:PHE:CZ     | 21:O:1230:PSC:H171 | 2.41                     | 0.56              |
| 20:N:1521:TGL:H222 | 20:N:1521:TGL:HA82 | 1.87                     | 0.56              |
| 1:A:1:FME:HCN      | 1:A:4:ASN:H        | 1.70                     | 0.56              |
| 26:C:270:CDL:H431  | 28:J:5157:HOH:O    | 2.05                     | 0.56              |
| 10:J:56:PRO:HD3    | 12:L:46:LYS:HE3    | 1.87                     | 0.56              |
| 6:F:93:PRO:HB2     | 6:F:94:HIS:ND1     | 2.21                     | 0.56              |
| 1:A:229:ILE:HD11   | 2:B:175:ILE:HD13   | 1.88                     | 0.55              |
| 2:O:122:MET:HB2    | 2:O:208:PRO:HD2    | 1.89                     | 0.55              |
| 3:P:54:MET:HE3     | 26:P:1270:CDL:H612 | 1.88                     | 0.55              |
| 1:A:113:LEU:CD1    | 20:L:522:TGL:H292  | 2.37                     | 0.55              |
| 7:T:84:LYS:HD2     | 7:T:84:LYS:N       | 2.05                     | 0.55              |
| 13:Z:10:THR:HA     | 13:Z:14:GLU:OE2    | 2.05                     | 0.55              |
| 11:K:42:PRO:HG2    | 11:K:47:ARG:HE     | 1.72                     | 0.55              |
| 7:T:72:ASN:N       | 7:T:76:ASN:HD22    | 1.97                     | 0.55              |
| 18:A:524:PGV:H062  | 28:M:2158:HOH:O    | 2.05                     | 0.55              |
| 18:A:524:PGV:H311  | 13:M:16:ALA:HA     | 1.88                     | 0.55              |
| 26:G:269:CDL:H212  | 1:N:311:ILE:HD12   | 1.89                     | 0.55              |
| 3:P:160:LEU:HD13   | 22:P:1271:CHD:H181 | 1.88                     | 0.55              |
| 3:C:50:ASN:HD22    | 3:C:51:MET:HE2     | 1.72                     | 0.55              |
| 2:O:57:ASP:H       | 21:O:1230:PSC:H201 | 1.72                     | 0.55              |
| 1:N:87:ILE:O       | 1:N:173:PRO:HD3    | 2.07                     | 0.54              |
| 3:P:168:THR:CG2    | 25:P:1265:PEK:H14  | 2.37                     | 0.54              |
| 1:A:177:SER:H      | 1:A:180:GLN:HE21   | 1.54                     | 0.54              |
| 3:P:5:THR:HG22     | 6:S:96:LEU:HD13    | 1.90                     | 0.54              |
| 20:D:523:TGL:HC21  | 20:D:523:TGL:HG11  | 1.90                     | 0.54              |
| 20:L:522:TGL:HC21  | 20:L:522:TGL:OA1   | 2.06                     | 0.54              |
| 3:P:146:TRP:CZ2    | 7:T:17:ARG:HG3     | 2.42                     | 0.54              |
| 1:A:194:LEU:HD22   | 1:A:285:PHE:CE2    | 2.41                     | 0.54              |
| 21:B:230:PSC:H12   | 21:B:230:PSC:H322  | 1.89                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:C:265:PEK:H383  | 26:G:269:CDL:H273  | 1.88                     | 0.54              |
| 1:N:430:PHE:HE1    | 20:N:1521:TGL:HB21 | 1.73                     | 0.54              |
| 3:C:34:TRP:HZ2     | 23:C:272:DMU:H29   | 1.71                     | 0.54              |
| 4:D:58:GLU:HG3     | 28:D:4047:HOH:O    | 2.07                     | 0.54              |
| 1:A:151:HIS:CD2    | 25:C:264:PEK:H382  | 2.43                     | 0.54              |
| 2:B:56:MET:HG2     | 21:B:230:PSC:H211  | 1.88                     | 0.54              |
| 3:C:146:TRP:CZ2    | 7:G:17:ARG:HG3     | 2.42                     | 0.54              |
| 25:C:265:PEK:H231  | 7:G:21:PHE:CD2     | 2.43                     | 0.54              |
| 13:Z:16:ALA:HA     | 18:Z:1524:PGV:H311 | 1.90                     | 0.54              |
| 2:B:82:ARG:HH11    | 2:B:86:MET:HE1     | 1.73                     | 0.54              |
| 2:O:59:GLN:O       | 2:O:59:GLN:HG3     | 2.08                     | 0.54              |
| 26:T:1269:CDL:H322 | 26:T:1269:CDL:HA62 | 1.90                     | 0.54              |
| 18:N:1266:PGV:H182 | 3:P:28:THR:HG22    | 1.90                     | 0.54              |
| 25:P:1265:PEK:C38  | 26:T:1269:CDL:H273 | 2.37                     | 0.54              |
| 18:P:1267:PGV:H182 | 26:P:1270:CDL:H673 | 1.88                     | 0.54              |
| 3:C:50:ASN:ND2     | 3:C:54:MET:HE2     | 2.23                     | 0.53              |
| 20:N:1522:TGL:HC21 | 20:N:1522:TGL:OA1  | 2.09                     | 0.53              |
| 2:O:128:LEU:HD11   | 2:O:134:ARG:HA     | 1.91                     | 0.53              |
| 9:V:15:ARG:HD2     | 28:V:4894:HOH:O    | 2.08                     | 0.53              |
| 1:A:407:ASP:O      | 1:A:411:LYS:HG3    | 2.09                     | 0.53              |
| 3:C:213:THR:HG23   | 26:C:270:CDL:H762  | 1.90                     | 0.53              |
| 5:E:84:TYR:O       | 5:E:88:GLU:HG2     | 2.09                     | 0.53              |
| 1:A:406:ASN:HD21   | 18:A:524:PGV:C2    | 2.21                     | 0.53              |
| 18:P:1267:PGV:H172 | 26:P:1270:CDL:H662 | 1.91                     | 0.53              |
| 7:T:38:HIS:NE2     | 26:T:1269:CDL:H111 | 2.23                     | 0.53              |
| 2:B:196:CYS:HB2    | 2:B:207:MET:HG3    | 1.91                     | 0.53              |
| 26:G:269:CDL:H322  | 26:G:269:CDL:HA62  | 1.90                     | 0.52              |
| 7:G:4:ALA:HB3      | 1:N:282:PHE:HA     | 1.91                     | 0.52              |
| 6:S:51:SER:O       | 6:S:94:HIS:N       | 2.42                     | 0.52              |
| 6:S:52:ILE:C       | 6:S:94:HIS:CE1     | 2.88                     | 0.52              |
| 28:A:4756:HOH:O    | 8:H:23:GLN:HG3     | 2.08                     | 0.52              |
| 25:C:264:PEK:H102  | 25:C:264:PEK:C16   | 2.36                     | 0.52              |
| 1:N:151:HIS:CD2    | 25:P:1264:PEK:H382 | 2.44                     | 0.52              |
| 21:O:1230:PSC:H322 | 21:O:1230:PSC:H12  | 1.91                     | 0.52              |
| 2:B:122:MET:HB2    | 2:B:208:PRO:HD2    | 1.90                     | 0.52              |
| 7:G:3:ALA:O        | 7:G:4:ALA:HB2      | 2.10                     | 0.52              |
| 7:G:11:TPO:HG22    | 7:G:16:TRP:HE1     | 1.75                     | 0.52              |
| 1:N:68:PHE:HE2     | 1:N:112:LEU:HD13   | 1.74                     | 0.52              |
| 4:Q:34:SER:H       | 4:Q:37:GLN:HE21    | 1.57                     | 0.52              |
| 20:N:1521:TGL:HC22 | 28:Q:3381:HOH:O    | 2.09                     | 0.52              |
| 1:A:472:ILE:HD13   | 20:L:522:TGL:HA91  | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:81:LEU:HD13    | 26:T:1269:CDL:H122 | 1.92                     | 0.51              |
| 10:J:40:LEU:HD12   | 22:J:60:CHD:H183   | 1.90                     | 0.51              |
| 1:N:488:THR:HB     | 1:N:495:LEU:HD13   | 1.92                     | 0.51              |
| 20:N:1522:TGL:H202 | 20:N:1522:TGL:C24  | 2.40                     | 0.51              |
| 6:F:64:GLU:O       | 6:F:65:ASP:HB2     | 2.11                     | 0.51              |
| 20:N:1521:TGL:HB91 | 2:O:32:PHE:HE2     | 1.75                     | 0.51              |
| 3:P:51:MET:HB3     | 26:P:1270:CDL:H622 | 1.92                     | 0.51              |
| 1:N:347:LEU:HD13   | 1:N:383:MET:SD     | 2.49                     | 0.51              |
| 4:Q:48:TRP:HB2     | 5:R:96:LEU:O       | 2.10                     | 0.51              |
| 1:N:296:GLY:HA2    | 8:U:23:GLN:OE1     | 2.10                     | 0.51              |
| 8:H:49:ASP:O       | 8:H:52:VAL:HG22    | 2.11                     | 0.51              |
| 1:A:136:LEU:HB2    | 28:A:4733:HOH:O    | 2.11                     | 0.51              |
| 7:G:2:SER:O        | 25:G:1263:PEK:H322 | 2.10                     | 0.51              |
| 7:T:72:ASN:H       | 7:T:76:ASN:ND2     | 1.98                     | 0.51              |
| 25:P:1265:PEK:H383 | 26:T:1269:CDL:H273 | 1.93                     | 0.50              |
| 1:N:400:PHE:HB3    | 20:N:1522:TGL:H283 | 1.93                     | 0.50              |
| 1:N:407:ASP:O      | 1:N:411:LYS:HG3    | 2.12                     | 0.50              |
| 6:S:52:ILE:O       | 6:S:94:HIS:CD2     | 2.64                     | 0.50              |
| 12:L:24:MET:HG3    | 28:L:5077:HOH:O    | 2.11                     | 0.50              |
| 1:A:87:ILE:O       | 1:A:173:PRO:HD3    | 2.11                     | 0.50              |
| 3:C:51:MET:SD      | 26:C:270:CDL:C62   | 3.00                     | 0.50              |
| 1:N:481:GLU:HB2    | 13:Z:4:LYS:HE2     | 1.92                     | 0.50              |
| 12:Y:2:HIS:N       | 28:Y:5165:HOH:O    | 2.45                     | 0.50              |
| 28:B:4821:HOH:O    | 25:P:1265:PEK:H031 | 2.11                     | 0.50              |
| 2:O:49:LYS:O       | 4:Q:20:ARG:NH2     | 2.42                     | 0.50              |
| 1:N:52:GLN:O       | 1:N:56:VAL:HG23    | 2.12                     | 0.50              |
| 4:D:127:LYS:HD2    | 28:I:2389:HOH:O    | 2.11                     | 0.49              |
| 1:A:488:THR:HB     | 1:A:495:LEU:HD13   | 1.94                     | 0.49              |
| 7:G:2:SER:OG       | 25:G:1263:PEK:H301 | 2.12                     | 0.49              |
| 20:L:522:TGL:H202  | 20:L:522:TGL:C24   | 2.39                     | 0.49              |
| 1:N:106:PRO:HB2    | 1:N:107:PRO:HD3    | 1.94                     | 0.49              |
| 11:K:24:PHE:O      | 11:K:28:VAL:HG12   | 2.12                     | 0.49              |
| 7:T:3:ALA:O        | 7:T:4:ALA:HB2      | 2.12                     | 0.49              |
| 5:R:48:ILE:O       | 5:R:52:LEU:HG      | 2.12                     | 0.49              |
| 13:M:42:LYS:HA     | 13:M:42:LYS:CE     | 2.42                     | 0.49              |
| 1:A:449:MET:SD     | 2:B:5:MET:HG2      | 2.53                     | 0.49              |
| 3:P:34:TRP:CE2     | 23:P:1272:DMU:H29  | 2.46                     | 0.49              |
| 1:A:379:TYR:O      | 1:A:383:MET:HB2    | 2.12                     | 0.49              |
| 9:I:59:ASP:OD2     | 9:I:63:MET:HE3     | 2.13                     | 0.49              |
| 18:P:1268:PGV:H101 | 28:P:4808:HOH:O    | 2.13                     | 0.49              |
| 1:N:365:ILE:HD11   | 28:N:4705:HOH:O    | 2.12                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:R:37:VAL:HG11    | 5:R:70:VAL:HG21    | 1.93                     | 0.49              |
| 1:A:304:TYR:HD1    | 26:T:1269:CDL:HB32 | 1.78                     | 0.48              |
| 4:D:17:VAL:HG12    | 28:D:4051:HOH:O    | 2.13                     | 0.48              |
| 1:N:344:PHE:CD1    | 1:N:344:PHE:C      | 2.90                     | 0.48              |
| 2:B:82:ARG:HG2     | 2:B:86:MET:HE3     | 1.94                     | 0.48              |
| 1:N:290:HIS:CD2    | 1:N:291:HIS:CD2    | 3.01                     | 0.48              |
| 1:N:484:THR:HB     | 28:Z:5071:HOH:O    | 2.13                     | 0.48              |
| 2:B:58:ALA:O       | 2:B:62:GLU:HG3     | 2.13                     | 0.48              |
| 3:C:51:MET:SD      | 26:C:270:CDL:H622  | 2.53                     | 0.48              |
| 1:N:17:THR:OG1     | 20:N:1522:TGL:H281 | 2.13                     | 0.48              |
| 2:O:132:GLU:HB3    | 2:O:137:GLU:HG3    | 1.95                     | 0.48              |
| 1:A:390:MET:HE2    | 1:A:413:HIS:HE1    | 1.78                     | 0.48              |
| 5:R:81:ILE:HG12    | 9:V:7:PRO:HG2      | 1.94                     | 0.48              |
| 11:K:42:PRO:HG2    | 11:K:47:ARG:NE     | 2.29                     | 0.48              |
| 1:N:405:LEU:HD23   | 1:N:475:ALA:HB2    | 1.94                     | 0.48              |
| 6:F:51:SER:O       | 6:F:94:HIS:N       | 2.46                     | 0.48              |
| 1:N:44:PRO:HG2     | 4:Q:111:PHE:CZ     | 2.49                     | 0.48              |
| 1:N:324:LEU:HD13   | 2:O:41:ILE:CG2     | 2.44                     | 0.48              |
| 2:O:1:FME:SD       | 2:O:133:LEU:CD1    | 3.02                     | 0.48              |
| 2:B:164:ALA:O      | 2:B:194:GLY:HA3    | 2.13                     | 0.48              |
| 1:N:310:MET:HE1    | 2:O:76:ILE:HB      | 1.95                     | 0.48              |
| 25:C:265:PEK:H383  | 26:G:269:CDL:C27   | 2.44                     | 0.48              |
| 2:O:196:CYS:HB2    | 2:O:207:MET:HG3    | 1.95                     | 0.48              |
| 1:N:379:TYR:O      | 1:N:383:MET:HB2    | 2.14                     | 0.47              |
| 1:N:1:FME:HE2      | 12:Y:3:TYR:CE1     | 2.48                     | 0.47              |
| 20:N:1522:TGL:HG2  | 12:Y:12:PRO:HB2    | 1.95                     | 0.47              |
| 1:A:177:SER:H      | 1:A:180:GLN:NE2    | 2.12                     | 0.47              |
| 1:N:107:PRO:HB3    | 3:P:25:LEU:HB2     | 1.96                     | 0.47              |
| 1:N:112:LEU:HD23   | 1:N:112:LEU:C      | 2.39                     | 0.47              |
| 2:O:220:GLU:O      | 2:O:223:SER:HB2    | 2.14                     | 0.47              |
| 2:B:114:GLU:HB3    | 28:B:4063:HOH:O    | 2.13                     | 0.47              |
| 3:P:34:TRP:NE1     | 23:P:1272:DMU:H29  | 2.30                     | 0.47              |
| 3:P:213:THR:HG23   | 26:P:1270:CDL:H762 | 1.96                     | 0.47              |
| 6:S:92:VAL:O       | 6:S:92:VAL:HG23    | 2.14                     | 0.47              |
| 26:T:1269:CDL:H571 | 26:T:1269:CDL:H601 | 1.63                     | 0.47              |
| 1:A:290:HIS:CD2    | 1:A:291:HIS:CD2    | 3.02                     | 0.47              |
| 1:A:383:MET:O      | 1:A:387:PHE:HB2    | 2.15                     | 0.47              |
| 4:D:34:SER:N       | 4:D:37:GLN:HE21    | 1.96                     | 0.47              |
| 7:G:5:LYS:CD       | 1:N:278:MET:HB3    | 2.44                     | 0.47              |
| 2:O:56:MET:HG2     | 21:O:1230:PSC:H211 | 1.97                     | 0.47              |
| 18:Z:1524:PGV:H062 | 28:Z:3158:HOH:O    | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:222:PRO:HD2    | 28:B:4914:HOH:O    | 2.15                     | 0.47              |
| 1:A:52:GLN:O       | 1:A:56:VAL:HG23    | 2.15                     | 0.47              |
| 1:A:514:LYS:HA     | 6:F:38:ALA:HB3     | 1.97                     | 0.47              |
| 7:T:3:ALA:HB1      | 25:T:263:PEK:H382  | 1.97                     | 0.47              |
| 2:B:82:ARG:NH1     | 2:B:86:MET:HE1     | 2.30                     | 0.47              |
| 1:A:28:MET:HE2     | 17:A:515:HEA:H271  | 1.96                     | 0.46              |
| 1:A:406:ASN:HD21   | 18:A:524:PGV:H21   | 1.80                     | 0.46              |
| 10:W:50:LEU:O      | 10:W:50:LEU:HD22   | 2.16                     | 0.46              |
| 1:A:107:PRO:HB3    | 3:C:25:LEU:HB2     | 1.97                     | 0.46              |
| 25:C:264:PEK:H32   | 25:C:264:PEK:H71   | 1.98                     | 0.46              |
| 1:A:365:ILE:HD11   | 28:H:4750:HOH:O    | 2.16                     | 0.46              |
| 22:P:1271:CHD:H112 | 22:P:1271:CHD:H12A | 1.68                     | 0.46              |
| 1:A:311:ILE:HD12   | 26:T:1269:CDL:H212 | 1.98                     | 0.46              |
| 1:A:278:MET:HB3    | 7:T:5:LYS:HD3      | 1.98                     | 0.46              |
| 25:G:1263:PEK:H132 | 3:P:247:VAL:HG11   | 1.97                     | 0.46              |
| 1:N:28:MET:CE      | 17:N:515:HEA:H271  | 2.46                     | 0.46              |
| 2:O:216:LEU:O      | 2:O:219:PHE:HB3    | 2.16                     | 0.46              |
| 1:A:1:FME:HA       | 1:A:1:FME:CE       | 2.42                     | 0.46              |
| 3:C:5:THR:HG22     | 6:F:96:LEU:HD13    | 1.97                     | 0.46              |
| 6:F:55:LYS:HA      | 6:F:74:LEU:O       | 2.15                     | 0.46              |
| 3:P:37:PHE:CD1     | 10:W:52:TRP:HZ3    | 2.33                     | 0.46              |
| 18:P:1267:PGV:H12  | 18:P:1267:PGV:C16  | 2.43                     | 0.46              |
| 6:S:55:LYS:HA      | 6:S:74:LEU:O       | 2.15                     | 0.46              |
| 3:C:54:MET:HE1     | 18:C:267:PGV:H141  | 1.97                     | 0.46              |
| 26:G:269:CDL:H221  | 1:N:286:ILE:CD1    | 2.46                     | 0.46              |
| 6:S:87:THR:HG21    | 28:S:3337:HOH:O    | 2.16                     | 0.46              |
| 7:T:2:SER:OG       | 25:T:263:PEK:H301  | 2.15                     | 0.46              |
| 7:T:38:HIS:CE1     | 26:T:1269:CDL:H111 | 2.51                     | 0.46              |
| 1:A:35:LEU:HD11    | 1:A:462:LEU:HD13   | 1.98                     | 0.46              |
| 26:C:270:CDL:H352  | 26:C:270:CDL:H162  | 1.97                     | 0.46              |
| 7:G:4:ALA:CB       | 1:N:282:PHE:HA     | 2.46                     | 0.46              |
| 1:N:514:LYS:HA     | 6:S:38:ALA:HB3     | 1.98                     | 0.46              |
| 1:A:422:ASN:HB3    | 20:B:521:TGL:H242  | 1.98                     | 0.46              |
| 8:H:60:TYR:CD1     | 8:H:60:TYR:C       | 2.93                     | 0.46              |
| 9:I:5:ALA:N        | 28:I:4913:HOH:O    | 2.36                     | 0.46              |
| 2:O:41:ILE:O       | 2:O:45:MET:HG2     | 2.15                     | 0.46              |
| 4:Q:34:SER:H       | 4:Q:37:GLN:NE2     | 2.14                     | 0.46              |
| 26:T:1269:CDL:H382 | 28:T:5116:HOH:O    | 2.15                     | 0.46              |
| 1:A:42:GLY:HA3     | 4:D:104:TYR:OH     | 2.16                     | 0.45              |
| 7:G:7:ASP:O        | 1:N:169:ILE:HD12   | 2.16                     | 0.45              |
| 1:A:282:PHE:HZ     | 26:T:1269:CDL:H761 | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:52:HIS:HE1     | 21:B:230:PSC:H02   | 1.80                     | 0.45              |
| 3:C:177:GLN:HA     | 3:C:177:GLN:OE1    | 2.17                     | 0.45              |
| 1:N:62:ALA:HB2     | 17:N:515:HEA:HBD1  | 1.98                     | 0.45              |
| 2:O:46:LEU:HD12    | 20:Q:1523:TGL:H271 | 1.97                     | 0.45              |
| 9:V:35:TYR:C       | 9:V:37:PHE:H       | 2.25                     | 0.45              |
| 18:C:267:PGV:H12   | 18:C:267:PGV:C16   | 2.44                     | 0.45              |
| 1:N:172:LYS:HD2    | 1:N:181:THR:CG2    | 2.46                     | 0.45              |
| 1:A:240:HIS:O      | 1:A:243:VAL:HG22   | 2.16                     | 0.45              |
| 26:G:269:CDL:H761  | 1:N:282:PHE:HZ     | 1.81                     | 0.45              |
| 1:A:113:LEU:HD12   | 20:L:522:TGL:H292  | 1.98                     | 0.45              |
| 2:B:132:GLU:HB3    | 2:B:137:GLU:HG3    | 1.99                     | 0.45              |
| 1:N:54:TYR:HB2     | 28:N:3111:HOH:O    | 2.15                     | 0.45              |
| 20:N:1522:TGL:HB31 | 20:N:1522:TGL:HB61 | 1.80                     | 0.45              |
| 2:O:164:ALA:O      | 2:O:194:GLY:HA3    | 2.16                     | 0.45              |
| 3:P:55:TYR:CE1     | 26:P:1270:CDL:H161 | 2.52                     | 0.45              |
| 1:A:1:FME:HE3      | 12:L:3:TYR:HE1     | 1.81                     | 0.45              |
| 2:B:7:LEU:HD11     | 20:B:521:TGL:H161  | 1.99                     | 0.45              |
| 21:B:230:PSC:H062  | 21:B:230:PSC:H042  | 1.81                     | 0.45              |
| 3:C:246:ASP:HB2    | 28:C:4590:HOH:O    | 2.17                     | 0.45              |
| 20:D:523:TGL:H212  | 20:D:523:TGL:H242  | 1.66                     | 0.45              |
| 7:G:38:HIS:CE1     | 26:G:269:CDL:H111  | 2.52                     | 0.45              |
| 2:O:1:FME:SD       | 2:O:133:LEU:HD11   | 2.57                     | 0.45              |
| 26:P:1270:CDL:H352 | 26:P:1270:CDL:H162 | 1.99                     | 0.45              |
| 1:A:431:LEU:HD21   | 1:A:450:TRP:HB2    | 1.99                     | 0.45              |
| 10:J:50:LEU:HD22   | 10:J:50:LEU:O      | 2.17                     | 0.45              |
| 1:N:177:SER:H      | 1:N:180:GLN:NE2    | 2.15                     | 0.45              |
| 3:P:25:LEU:O       | 3:P:29:SER:HB2     | 2.17                     | 0.45              |
| 1:A:513:LEU:HD22   | 1:A:513:LEU:HA     | 1.79                     | 0.45              |
| 23:P:1272:DMU:H25  | 25:P:1264:PEK:H341 | 1.99                     | 0.45              |
| 28:O:4738:HOH:O    | 8:U:61:LYS:HD3     | 2.17                     | 0.45              |
| 25:P:1264:PEK:H102 | 25:P:1264:PEK:C16  | 2.38                     | 0.45              |
| 26:P:1270:CDL:H202 | 26:P:1270:CDL:H171 | 1.79                     | 0.45              |
| 7:T:84:LYS:CD      | 7:T:84:LYS:N       | 2.73                     | 0.44              |
| 11:X:54:ARG:NH2    | 11:X:54:ARG:HG3    | 2.32                     | 0.44              |
| 1:A:106:PRO:HB2    | 1:A:107:PRO:HD3    | 1.98                     | 0.44              |
| 5:E:71:VAL:HG11    | 5:E:85:VAL:HG11    | 2.00                     | 0.44              |
| 2:O:1:FME:HE1      | 2:O:133:LEU:HD22   | 1.99                     | 0.44              |
| 3:P:34:TRP:HE1     | 23:P:1272:DMU:H29  | 1.82                     | 0.44              |
| 26:G:269:CDL:H122  | 2:O:81:LEU:HD13    | 1.99                     | 0.44              |
| 12:L:20:ARG:CZ     | 20:L:522:TGL:HC61  | 2.47                     | 0.44              |
| 1:N:350:VAL:HG13   | 20:N:1521:TGL:HB81 | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:83:ILE:O       | 2:O:87:MET:HG3     | 2.18                     | 0.44              |
| 1:N:377:PHE:HA     | 1:N:380:VAL:HG22   | 1.99                     | 0.44              |
| 4:Q:33:LEU:HA      | 4:Q:37:GLN:NE2     | 2.32                     | 0.44              |
| 20:Q:1523:TGL:H212 | 20:Q:1523:TGL:H242 | 1.67                     | 0.44              |
| 8:U:37:HIS:CD2     | 8:U:76:ARG:CZ      | 3.00                     | 0.44              |
| 26:C:270:CDL:H672  | 26:C:270:CDL:H641  | 1.85                     | 0.44              |
| 2:O:102:HIS:O      | 2:O:104:TRP:HA     | 2.18                     | 0.44              |
| 3:P:116:TRP:HA     | 3:P:117:PRO:C      | 2.41                     | 0.44              |
| 25:P:1265:PEK:H383 | 26:T:1269:CDL:C27  | 2.47                     | 0.44              |
| 11:X:8:ASP:HB2     | 28:X:5081:HOH:O    | 2.17                     | 0.44              |
| 3:C:191:GLY:HA3    | 28:G:2161:HOH:O    | 2.17                     | 0.44              |
| 2:O:68:LEU:CB      | 2:O:69:PRO:HD3     | 2.48                     | 0.44              |
| 22:W:1060:CHD:H212 | 22:W:1060:CHD:H161 | 1.76                     | 0.44              |
| 5:R:31:LYS:HE2     | 5:R:35:THR:OG1     | 2.17                     | 0.44              |
| 1:A:377:PHE:CD1    | 17:A:516:HEA:HAD1  | 2.53                     | 0.44              |
| 2:B:100:MET:HE3    | 2:B:157:GLU:HG3    | 2.00                     | 0.44              |
| 2:B:151:ARG:CD     | 2:B:181:GLN:HE21   | 2.31                     | 0.44              |
| 2:O:56:MET:HA      | 21:O:1230:PSC:H202 | 1.99                     | 0.44              |
| 9:V:45:LYS:HB3     | 28:V:5052:HOH:O    | 2.17                     | 0.44              |
| 1:A:71:MET:HB2     | 1:A:72:PRO:HD3     | 2.00                     | 0.43              |
| 1:A:310:MET:HE2    | 1:A:356:ILE:HG23   | 1.99                     | 0.43              |
| 2:B:227:LEU:HD23   | 2:B:227:LEU:HA     | 1.76                     | 0.43              |
| 20:B:521:TGL:H201  | 20:B:521:TGL:C24   | 2.45                     | 0.43              |
| 5:E:5:HIS:HB3      | 5:E:6:GLU:H        | 1.56                     | 0.43              |
| 1:N:265:LYS:HB2    | 1:N:490:THR:HG21   | 2.00                     | 0.43              |
| 4:Q:131:ILE:HD12   | 4:Q:131:ILE:H      | 1.83                     | 0.43              |
| 2:B:41:ILE:O       | 2:B:45:MET:HG2     | 2.18                     | 0.43              |
| 4:Q:98:TRP:CD2     | 23:Z:1526:DMU:H10  | 2.53                     | 0.43              |
| 5:R:100:THR:HB     | 5:R:101:PRO:HD2    | 2.00                     | 0.43              |
| 8:U:7:LYS:O        | 8:U:8:ILE:HG22     | 2.17                     | 0.43              |
| 7:G:44:ARG:HD2     | 7:G:82:TYR:CE1     | 2.52                     | 0.43              |
| 7:T:2:SER:O        | 25:T:263:PEK:H322  | 2.18                     | 0.43              |
| 20:L:522:TGL:HB31  | 20:L:522:TGL:HB61  | 1.79                     | 0.43              |
| 2:B:91:ASN:HD22    | 2:B:92:ASN:N       | 2.17                     | 0.43              |
| 2:O:116:LEU:HD12   | 2:O:117:SER:N      | 2.34                     | 0.43              |
| 3:C:116:TRP:HA     | 3:C:117:PRO:C      | 2.43                     | 0.43              |
| 4:D:144:GLU:OE1    | 4:D:147:LYS:HE3    | 2.19                     | 0.43              |
| 9:I:35:TYR:C       | 9:I:37:PHE:H       | 2.26                     | 0.43              |
| 3:P:112:LEU:HD13   | 3:P:118:PRO:HG3    | 2.01                     | 0.43              |
| 7:T:31:CYS:HG      | 26:T:1269:CDL:H532 | 1.80                     | 0.43              |
| 1:A:334:TRP:CH2    | 2:B:46:LEU:HD13    | 2.54                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:390:MET:HE2    | 1:A:413:HIS:CE1    | 2.52                     | 0.43              |
| 13:M:17:ILE:O      | 13:M:21:VAL:HG23   | 2.18                     | 0.43              |
| 11:X:24:PHE:O      | 11:X:28:VAL:HG12   | 2.19                     | 0.43              |
| 26:C:270:CDL:H202  | 26:C:270:CDL:H171  | 1.79                     | 0.43              |
| 26:G:269:CDL:HB32  | 1:N:304:TYR:CD1    | 2.49                     | 0.43              |
| 12:Y:20:ARG:NH2    | 12:Y:24:MET:HG3    | 2.34                     | 0.43              |
| 3:C:168:THR:CG2    | 25:C:265:PEK:H14   | 2.49                     | 0.43              |
| 1:N:76:GLY:O       | 1:N:80:ASN:HB2     | 2.19                     | 0.43              |
| 1:N:449:MET:SD     | 2:O:5:MET:CG       | 3.06                     | 0.43              |
| 3:P:40:MET:O       | 3:P:44:MET:HG2     | 2.19                     | 0.43              |
| 4:Q:130:PRO:HG2    | 4:Q:131:ILE:HD12   | 2.01                     | 0.43              |
| 20:N:1522:TGL:H272 | 20:N:1522:TGL:H231 | 2.00                     | 0.42              |
| 5:R:82:TYR:N       | 5:R:83:PRO:CD      | 2.82                     | 0.42              |
| 5:R:86:ILE:HD13    | 5:R:86:ILE:HA      | 1.83                     | 0.42              |
| 3:C:51:MET:HB3     | 26:C:270:CDL:H622  | 2.00                     | 0.42              |
| 26:G:269:CDL:H571  | 26:G:269:CDL:H601  | 1.63                     | 0.42              |
| 20:L:522:TGL:H231  | 20:L:522:TGL:H272  | 2.01                     | 0.42              |
| 2:O:16:ILE:HD13    | 2:O:16:ILE:HA      | 1.86                     | 0.42              |
| 4:Q:23:PRO:O       | 4:Q:25:PRO:HD3     | 2.19                     | 0.42              |
| 1:A:298:ASP:HB3    | 28:A:2387:HOH:O    | 2.20                     | 0.42              |
| 20:D:523:TGL:HC31  | 28:D:4745:HOH:O    | 2.18                     | 0.42              |
| 12:Y:20:ARG:NH1    | 12:Y:20:ARG:HB3    | 2.34                     | 0.42              |
| 1:N:177:SER:H      | 1:N:180:GLN:HE21   | 1.67                     | 0.42              |
| 1:N:194:LEU:HD22   | 1:N:285:PHE:CE2    | 2.48                     | 0.42              |
| 3:P:149:HIS:O      | 3:P:153:GLU:HG3    | 2.19                     | 0.42              |
| 2:B:29:MET:HB2     | 9:I:35:TYR:CE2     | 2.55                     | 0.42              |
| 2:O:104:TRP:CG     | 2:O:203:ASN:HB2    | 2.55                     | 0.42              |
| 2:O:121:TYR:O      | 2:O:138:VAL:HA     | 2.19                     | 0.42              |
| 3:P:51:MET:SD      | 26:P:1270:CDL:C62  | 3.07                     | 0.42              |
| 4:Q:57:VAL:O       | 4:Q:61:ARG:HG2     | 2.19                     | 0.42              |
| 1:A:306:THR:O      | 1:A:310:MET:HG3    | 2.20                     | 0.42              |
| 3:C:210:ILE:HD13   | 18:C:267:PGV:H301  | 2.02                     | 0.42              |
| 12:L:20:ARG:HH22   | 20:L:522:TGL:HC32  | 1.85                     | 0.42              |
| 25:P:1264:PEK:H71  | 25:P:1264:PEK:H32  | 2.01                     | 0.42              |
| 2:B:151:ARG:HD3    | 2:B:181:GLN:HE21   | 1.84                     | 0.42              |
| 3:C:54:MET:HE3     | 26:C:270:CDL:H612  | 2.02                     | 0.42              |
| 5:E:12:ASP:OD1     | 5:E:44:GLU:HG3     | 2.20                     | 0.42              |
| 12:L:35:ALA:HB3    | 12:L:36:PRO:HD3    | 2.01                     | 0.42              |
| 1:N:400:PHE:HB3    | 20:N:1522:TGL:C28  | 2.50                     | 0.42              |
| 23:P:1272:DMU:H30  | 7:T:62:TRP:HB3     | 2.01                     | 0.42              |
| 1:A:400:PHE:HB3    | 20:L:522:TGL:H283  | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:B:230:PSC:H251  | 21:B:230:PSC:H221  | 1.77                     | 0.42              |
| 6:F:8:THR:OG1      | 6:F:11:GLU:HG3     | 2.20                     | 0.42              |
| 1:N:169:ILE:HD11   | 1:N:189:MET:SD     | 2.59                     | 0.42              |
| 1:N:426:PHE:CZ     | 20:N:1521:TGL:HA62 | 2.55                     | 0.42              |
| 2:O:92:ASN:HA      | 2:O:93:PRO:HD2     | 1.82                     | 0.42              |
| 7:G:50:TYR:HB3     | 7:G:52:HIS:CE1     | 2.54                     | 0.41              |
| 8:U:9:LYS:HB3      | 8:U:10:ASN:H       | 1.57                     | 0.41              |
| 22:C:271:CHD:H112  | 22:C:271:CHD:H12A  | 1.67                     | 0.41              |
| 9:V:64:ARG:HD3     | 9:V:72:ALA:HB1     | 2.01                     | 0.41              |
| 3:C:212:SER:O      | 3:C:216:ILE:HG13   | 2.21                     | 0.41              |
| 10:J:2:GLU:HB2     | 10:J:4:ARG:NH1     | 2.35                     | 0.41              |
| 1:N:422:ASN:HB3    | 20:N:1521:TGL:H242 | 2.02                     | 0.41              |
| 2:O:84:LEU:HA      | 2:O:87:MET:HE2     | 2.02                     | 0.41              |
| 1:A:344:PHE:CD1    | 1:A:344:PHE:C      | 2.98                     | 0.41              |
| 2:O:1:FME:SD       | 2:O:133:LEU:HD13   | 2.61                     | 0.41              |
| 3:P:50:ASN:ND2     | 3:P:54:MET:HE2     | 2.35                     | 0.41              |
| 13:M:37:LEU:HD23   | 13:M:37:LEU:HA     | 1.88                     | 0.41              |
| 5:R:84:TYR:O       | 5:R:87:GLN:HB3     | 2.21                     | 0.41              |
| 1:A:229:ILE:HD11   | 2:B:175:ILE:CD1    | 2.50                     | 0.41              |
| 3:C:127:LEU:HG     | 26:G:269:CDL:OB3   | 2.20                     | 0.41              |
| 28:D:4059:HOH:O    | 5:E:97:GLY:HA2     | 2.20                     | 0.41              |
| 6:F:51:SER:HB2     | 6:F:91:LEU:HD11    | 2.02                     | 0.41              |
| 8:U:64:CYS:HA      | 8:U:65:PRO:HD3     | 1.97                     | 0.41              |
| 11:X:54:ARG:HH21   | 11:X:54:ARG:CG     | 2.34                     | 0.41              |
| 1:A:406:ASN:HD21   | 18:A:524:PGV:H22   | 1.84                     | 0.41              |
| 2:B:168:LEU:HD13   | 2:B:184:LEU:HG     | 2.03                     | 0.41              |
| 25:G:1263:PEK:H182 | 3:P:98:PHE:CD2     | 2.56                     | 0.41              |
| 1:N:398:PRO:HA     | 1:N:403:TYR:O      | 2.20                     | 0.41              |
| 26:G:269:CDL:H762  | 26:G:269:CDL:H732  | 1.98                     | 0.41              |
| 1:N:40:GLU:HG2     | 1:N:54:TYR:CD2     | 2.56                     | 0.41              |
| 1:N:430:PHE:CE1    | 20:N:1521:TGL:HB21 | 2.54                     | 0.41              |
| 22:O:229:CHD:H12   | 22:O:229:CHD:H212  | 2.02                     | 0.41              |
| 3:P:173:PHE:CD2    | 3:P:173:PHE:C      | 2.99                     | 0.41              |
| 4:Q:64:PHE:CE1     | 5:R:66:ARG:HB2     | 2.56                     | 0.41              |
| 1:A:62:ALA:HB2     | 17:A:515:HEA:HBD1  | 2.03                     | 0.41              |
| 1:A:416:ILE:HG22   | 1:A:464:ALA:HB2    | 2.02                     | 0.41              |
| 2:B:57:ASP:H       | 21:B:230:PSC:H201  | 1.86                     | 0.41              |
| 2:B:102:HIS:O      | 2:B:104:TRP:HA     | 2.21                     | 0.41              |
| 3:C:22:LEU:O       | 3:C:26:LEU:HG      | 2.21                     | 0.41              |
| 3:C:168:THR:HG22   | 25:C:265:PEK:H14   | 2.03                     | 0.41              |
| 3:C:173:PHE:CD2    | 3:C:173:PHE:C      | 2.99                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:C:270:CDL:H602  | 26:C:270:CDL:H572  | 1.91                     | 0.41              |
| 4:D:126:MET:HG3    | 4:D:128:VAL:HG23   | 2.02                     | 0.41              |
| 1:N:105:LEU:HD23   | 1:N:105:LEU:HA     | 1.88                     | 0.41              |
| 3:P:54:MET:HE3     | 26:P:1270:CDL:C61  | 2.50                     | 0.41              |
| 4:Q:118:LYS:HE3    | 28:Q:4443:HOH:O    | 2.21                     | 0.41              |
| 1:A:112:LEU:HG     | 28:A:2073:HOH:O    | 2.19                     | 0.41              |
| 1:N:362:SER:HA     | 2:O:87:MET:HE1     | 2.03                     | 0.41              |
| 20:D:523:TGL:HC22  | 20:D:523:TGL:HC51  | 1.93                     | 0.40              |
| 12:L:20:ARG:HH12   | 20:L:522:TGL:CC6   | 2.30                     | 0.40              |
| 4:Q:48:TRP:O       | 4:Q:51:LEU:HB2     | 2.20                     | 0.40              |
| 25:T:263:PEK:H282  | 25:T:263:PEK:H312  | 1.84                     | 0.40              |
| 2:B:121:TYR:O      | 2:B:138:VAL:HA     | 2.21                     | 0.40              |
| 4:D:53:ILE:HD13    | 4:D:53:ILE:HA      | 1.88                     | 0.40              |
| 1:N:172:LYS:HB2    | 1:N:172:LYS:HE2    | 1.92                     | 0.40              |
| 5:R:100:THR:OG1    | 5:R:103:GLU:HG3    | 2.21                     | 0.40              |
| 8:U:50:VAL:O       | 8:U:50:VAL:HG12    | 2.21                     | 0.40              |
| 26:C:270:CDL:H602  | 26:C:270:CDL:H632  | 1.69                     | 0.40              |
| 9:I:2:THR:HG23     | 9:I:3:ALA:O        | 2.21                     | 0.40              |
| 3:P:47:LEU:O       | 3:P:51:MET:HG2     | 2.21                     | 0.40              |
| 20:Q:1523:TGL:HG11 | 20:Q:1523:TGL:CC2  | 2.49                     | 0.40              |
| 8:U:45:ALA:HB2     | 28:U:5144:HOH:O    | 2.20                     | 0.40              |
| 12:L:46:LYS:HG3    | 28:L:4932:HOH:O    | 2.22                     | 0.40              |
| 1:N:289:ALA:HB3    | 1:N:305:PHE:CD2    | 2.56                     | 0.40              |
| 20:N:1521:TGL:H201 | 20:N:1521:TGL:C24  | 2.44                     | 0.40              |
| 18:N:1266:PGV:H251 | 18:N:1266:PGV:H42  | 2.04                     | 0.40              |
| 6:S:53:THR:CA      | 6:S:94:HIS:CE1     | 2.96                     | 0.40              |
| 7:T:2:SER:O        | 7:T:3:ALA:HB3      | 2.21                     | 0.40              |
| 13:Z:28:LEU:HB2    | 13:Z:29:PRO:HD3    | 2.02                     | 0.40              |
| 1:A:310:MET:HB3    | 2:B:73:LEU:HD22    | 2.03                     | 0.40              |
| 1:A:430:PHE:CE1    | 20:B:521:TGL:HB21  | 2.52                     | 0.40              |
| 3:C:247:VAL:HG11   | 25:T:263:PEK:H132  | 2.02                     | 0.40              |
| 1:N:32:ALA:HB3     | 12:Y:36:PRO:HG2    | 2.02                     | 0.40              |
| 1:N:53:ILE:HD11    | 12:Y:40:VAL:HG13   | 2.03                     | 0.40              |
| 1:N:397:PHE:HB3    | 1:N:398:PRO:HD3    | 2.03                     | 0.40              |
| 2:O:59:GLN:O       | 2:O:59:GLN:CG      | 2.69                     | 0.40              |
| 2:O:150:ILE:HD12   | 2:O:184:LEU:HD22   | 2.04                     | 0.40              |
| 20:Q:1523:TGL:HC22 | 20:Q:1523:TGL:HC51 | 1.92                     | 0.40              |
| 5:R:5:HIS:HB3      | 5:R:6:GLU:H        | 1.57                     | 0.40              |
| 11:X:54:ARG:HG3    | 11:X:54:ARG:HH21   | 1.87                     | 0.40              |
| 13:Z:13:LYS:O      | 13:Z:17:ILE:HG13   | 2.20                     | 0.40              |

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed       | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 512/514 (100%) | 497 (97%)  | 15 (3%) | 0        | 100         | 100 |
| 1   | N     | 512/514 (100%) | 497 (97%)  | 15 (3%) | 0        | 100         | 100 |
| 2   | B     | 225/227 (99%)  | 211 (94%)  | 12 (5%) | 2 (1%)   | 14          | 5   |
| 2   | O     | 225/227 (99%)  | 208 (92%)  | 15 (7%) | 2 (1%)   | 14          | 5   |
| 3   | C     | 257/261 (98%)  | 252 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 3   | P     | 257/261 (98%)  | 251 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 4   | D     | 142/147 (97%)  | 138 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 4   | Q     | 142/147 (97%)  | 138 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 5   | E     | 103/109 (94%)  | 103 (100%) | 0       | 0        | 100         | 100 |
| 5   | R     | 103/109 (94%)  | 102 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 6   | F     | 96/98 (98%)    | 89 (93%)   | 5 (5%)  | 2 (2%)   | 5           | 1   |
| 6   | S     | 96/98 (98%)    | 90 (94%)   | 3 (3%)  | 3 (3%)   | 3           | 0   |
| 7   | G     | 81/85 (95%)    | 67 (83%)   | 7 (9%)  | 7 (9%)   | 0           | 0   |
| 7   | T     | 81/85 (95%)    | 65 (80%)   | 9 (11%) | 7 (9%)   | 0           | 0   |
| 8   | H     | 77/85 (91%)    | 70 (91%)   | 5 (6%)  | 2 (3%)   | 4           | 0   |
| 8   | U     | 77/85 (91%)    | 70 (91%)   | 5 (6%)  | 2 (3%)   | 4           | 0   |
| 9   | I     | 71/73 (97%)    | 67 (94%)   | 4 (6%)  | 0        | 100         | 100 |
| 9   | V     | 71/73 (97%)    | 66 (93%)   | 5 (7%)  | 0        | 100         | 100 |
| 10  | J     | 56/59 (95%)    | 55 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 10  | W     | 56/59 (95%)    | 54 (96%)   | 2 (4%)  | 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%)    | 43 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 12  | Y     | 44/47 (94%)    | 43 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 13  | M     | 41/46 (89%)    | 41 (100%)  | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 13  | Z     | 41/46 (89%)     | 41 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 3504/3614 (97%) | 3350 (96%) | 127 (4%) | 27 (1%)  | 16          | 6   |

All (27) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 426/426 (100%)  | 420 (99%)  | 6 (1%)   | 59          | 52  |
| 1   | N     | 426/426 (100%)  | 417 (98%)  | 9 (2%)   | 47          | 36  |
| 2   | B     | 210/210 (100%)  | 201 (96%)  | 9 (4%)   | 26          | 13  |
| 2   | O     | 210/210 (100%)  | 198 (94%)  | 12 (6%)  | 18          | 8   |
| 3   | C     | 224/226 (99%)   | 220 (98%)  | 4 (2%)   | 51          | 43  |
| 3   | P     | 224/226 (99%)   | 218 (97%)  | 6 (3%)   | 39          | 27  |
| 4   | D     | 128/129 (99%)   | 126 (98%)  | 2 (2%)   | 55          | 47  |
| 4   | Q     | 128/129 (99%)   | 124 (97%)  | 4 (3%)   | 35          | 23  |
| 5   | E     | 92/95 (97%)     | 89 (97%)   | 3 (3%)   | 33          | 21  |
| 5   | R     | 92/95 (97%)     | 89 (97%)   | 3 (3%)   | 33          | 21  |
| 6   | F     | 81/81 (100%)    | 78 (96%)   | 3 (4%)   | 30          | 18  |
| 6   | S     | 81/81 (100%)    | 78 (96%)   | 3 (4%)   | 30          | 18  |
| 7   | G     | 67/68 (98%)     | 64 (96%)   | 3 (4%)   | 24          | 12  |
| 7   | T     | 67/68 (98%)     | 63 (94%)   | 4 (6%)   | 17          | 7   |
| 8   | H     | 71/75 (95%)     | 68 (96%)   | 3 (4%)   | 26          | 14  |
| 8   | U     | 71/75 (95%)     | 68 (96%)   | 3 (4%)   | 26          | 14  |
| 9   | I     | 57/57 (100%)    | 53 (93%)   | 4 (7%)   | 14          | 4   |
| 9   | V     | 57/57 (100%)    | 53 (93%)   | 4 (7%)   | 14          | 4   |
| 10  | J     | 49/50 (98%)     | 48 (98%)   | 1 (2%)   | 48          | 38  |
| 10  | W     | 49/50 (98%)     | 48 (98%)   | 1 (2%)   | 48          | 38  |
| 11  | K     | 39/46 (85%)     | 39 (100%)  | 0        | 100         | 100 |
| 11  | X     | 39/46 (85%)     | 38 (97%)   | 1 (3%)   | 40          | 28  |
| 12  | L     | 39/40 (98%)     | 38 (97%)   | 1 (3%)   | 40          | 28  |
| 12  | Y     | 39/40 (98%)     | 37 (95%)   | 2 (5%)   | 21          | 9   |
| 13  | M     | 37/38 (97%)     | 33 (89%)   | 4 (11%)  | 6           | 1   |
| 13  | Z     | 37/38 (97%)     | 33 (89%)   | 4 (11%)  | 6           | 1   |
| All | All   | 3040/3082 (99%) | 2941 (97%) | 99 (3%)  | 33          | 21  |

All (99) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 38  | ARG  |
| 1   | A     | 138 | HIS  |
| 1   | A     | 180 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 241 | PRO  |
| 1   | A     | 369 | ASP  |
| 1   | A     | 513 | LEU  |
| 2   | B     | 16  | ILE  |
| 2   | B     | 33  | LEU  |
| 2   | B     | 60  | GLU  |
| 2   | B     | 66  | THR  |
| 2   | B     | 75  | LEU  |
| 2   | B     | 78  | LEU  |
| 2   | B     | 91  | ASN  |
| 2   | B     | 115 | ASP  |
| 2   | B     | 167 | SER  |
| 3   | C     | 77  | LYS  |
| 3   | C     | 127 | LEU  |
| 3   | C     | 179 | SER  |
| 3   | C     | 230 | ASN  |
| 4   | D     | 4   | SER  |
| 4   | D     | 51  | LEU  |
| 5   | E     | 5   | HIS  |
| 5   | E     | 70  | VAL  |
| 5   | E     | 90  | ARG  |
| 6   | F     | 48  | LEU  |
| 6   | F     | 87  | THR  |
| 6   | F     | 95  | GLN  |
| 7   | G     | 17  | ARG  |
| 7   | G     | 33  | LEU  |
| 7   | G     | 84  | LYS  |
| 8   | H     | 8   | ILE  |
| 8   | H     | 29  | CYS  |
| 8   | H     | 60  | TYR  |
| 9   | I     | 2   | THR  |
| 9   | I     | 8   | GLN  |
| 9   | I     | 21  | ILE  |
| 9   | I     | 37  | PHE  |
| 10  | J     | 50  | LEU  |
| 12  | L     | 26  | THR  |
| 13  | M     | 13  | LYS  |
| 13  | M     | 34  | LEU  |
| 13  | M     | 38  | ASP  |
| 13  | M     | 42  | LYS  |
| 1   | N     | 115 | SER  |
| 1   | N     | 138 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 180 | GLN  |
| 1   | N     | 241 | PRO  |
| 1   | N     | 369 | ASP  |
| 1   | N     | 484 | THR  |
| 1   | N     | 485 | VAL  |
| 1   | N     | 504 | THR  |
| 1   | N     | 513 | LEU  |
| 2   | O     | 16  | ILE  |
| 2   | O     | 33  | LEU  |
| 2   | O     | 60  | GLU  |
| 2   | O     | 66  | THR  |
| 2   | O     | 68  | LEU  |
| 2   | O     | 75  | LEU  |
| 2   | O     | 78  | LEU  |
| 2   | O     | 91  | ASN  |
| 2   | O     | 94  | SER  |
| 2   | O     | 115 | ASP  |
| 2   | O     | 148 | MET  |
| 2   | O     | 217 | LYS  |
| 3   | P     | 17  | PRO  |
| 3   | P     | 29  | SER  |
| 3   | P     | 33  | MET  |
| 3   | P     | 77  | LYS  |
| 3   | P     | 159 | MET  |
| 3   | P     | 230 | ASN  |
| 4   | Q     | 8   | SER  |
| 4   | Q     | 9   | GLU  |
| 4   | Q     | 51  | LEU  |
| 4   | Q     | 121 | LYS  |
| 5   | R     | 5   | HIS  |
| 5   | R     | 87  | GLN  |
| 5   | R     | 90  | ARG  |
| 6   | S     | 37  | LYS  |
| 6   | S     | 48  | LEU  |
| 6   | S     | 95  | GLN  |
| 7   | T     | 17  | ARG  |
| 7   | T     | 26  | PRO  |
| 7   | T     | 36  | TRP  |
| 7   | T     | 84  | LYS  |
| 8   | U     | 21  | PRO  |
| 8   | U     | 29  | CYS  |
| 8   | U     | 60  | TYR  |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 151 | HIS  |
| 1   | A     | 178 | GLN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 422 | ASN  |
| 1   | A     | 512 | ASN  |
| 2   | B     | 10  | GLN  |
| 2   | B     | 140 | ASN  |
| 2   | B     | 181 | GLN  |
| 3   | C     | 3   | HIS  |
| 3   | C     | 50  | ASN  |
| 3   | C     | 68  | GLN  |
| 3   | C     | 161 | GLN  |
| 4   | D     | 37  | GLN  |
| 4   | D     | 109 | HIS  |
| 4   | D     | 143 | ASN  |
| 5   | E     | 78  | HIS  |
| 5   | E     | 94  | ASN  |
| 7   | G     | 34  | ASN  |
| 7   | G     | 76  | ASN  |
| 8   | H     | 22  | ASN  |
| 8   | H     | 31  | GLN  |
| 10  | J     | 29  | ASN  |
| 11  | K     | 35  | GLN  |
| 1   | N     | 151 | HIS  |
| 1   | N     | 170 | ASN  |
| 1   | N     | 178 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 180 | GLN  |
| 1   | N     | 360 | ASN  |
| 1   | N     | 503 | HIS  |
| 1   | N     | 512 | ASN  |
| 2   | O     | 10  | GLN  |
| 3   | P     | 50  | ASN  |
| 3   | P     | 68  | GLN  |
| 4   | Q     | 37  | GLN  |
| 4   | Q     | 101 | HIS  |
| 5   | R     | 94  | ASN  |
| 7   | T     | 71  | HIS  |
| 7   | T     | 76  | ASN  |
| 8   | U     | 31  | GLN  |
| 10  | W     | 57  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 7   | TPO  | T     | 11  | 7    | 8,10,11      | 1.35 | 1 (12%)     | 10,14,16    | 1.13 | 0           |
| 1   | FME  | A     | 1   | 1    | 8,9,10       | 0.68 | 0           | 8,9,11      | 1.12 | 1 (12%)     |
| 2   | FME  | B     | 1   | 2    | 8,9,10       | 0.77 | 0           | 8,9,11      | 2.23 | 2 (25%)     |
| 9   | SAC  | V     | 1   | 9    | 7,8,9        | 2.68 | 2 (28%)     | 7,9,11      | 1.97 | 3 (42%)     |
| 7   | TPO  | G     | 11  | 7    | 8,10,11      | 1.59 | 1 (12%)     | 10,14,16    | 1.12 | 1 (10%)     |
| 1   | FME  | N     | 1   | 1    | 8,9,10       | 0.74 | 0           | 8,9,11      | 1.62 | 2 (25%)     |
| 2   | FME  | O     | 1   | 2    | 8,9,10       | 0.69 | 0           | 8,9,11      | 1.67 | 2 (25%)     |
| 9   | SAC  | I     | 1   | 9    | 7,8,9        | 2.50 | 2 (28%)     | 7,9,11      | 1.77 | 2 (28%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 7   | TPO  | T     | 11  | 7    | -       | 4/9/11/13 | -     |
| 1   | FME  | A     | 1   | 1    | -       | 3/7/9/11  | -     |
| 2   | FME  | B     | 1   | 2    | -       | 1/7/9/11  | -     |
| 9   | SAC  | V     | 1   | 9    | -       | 3/7/8/10  | -     |
| 7   | TPO  | G     | 11  | 7    | -       | 5/9/11/13 | -     |
| 1   | FME  | N     | 1   | 1    | -       | 4/7/9/11  | -     |
| 2   | FME  | O     | 1   | 2    | -       | 1/7/9/11  | -     |
| 9   | SAC  | I     | 1   | 9    | -       | 3/7/8/10  | -     |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 9   | V     | 1   | SAC  | OAC-C1A | 5.32 | 1.35        | 1.23     |
| 9   | I     | 1   | SAC  | OAC-C1A | 5.17 | 1.34        | 1.23     |
| 9   | V     | 1   | SAC  | CA-N    | 4.28 | 1.52        | 1.46     |
| 9   | I     | 1   | SAC  | CA-N    | 3.83 | 1.52        | 1.46     |
| 7   | G     | 11  | TPO  | CB-CA   | 3.11 | 1.60        | 1.53     |
| 7   | T     | 11  | TPO  | CB-CA   | 2.62 | 1.59        | 1.53     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 1   | FME  | CA-N-CN     | -4.41 | 116.05      | 122.82   |
| 2   | B     | 1   | FME  | C-CA-N      | 4.24  | 117.69      | 109.50   |
| 1   | N     | 1   | FME  | CA-N-CN     | -3.73 | 117.09      | 122.82   |
| 2   | O     | 1   | FME  | C-CA-N      | 3.56  | 116.37      | 109.50   |
| 9   | I     | 1   | SAC  | C-CA-N      | -3.28 | 103.16      | 109.50   |
| 9   | V     | 1   | SAC  | C2A-C1A-N   | 2.93  | 120.97      | 116.12   |
| 9   | V     | 1   | SAC  | C-CA-N      | -2.90 | 103.90      | 109.50   |
| 2   | O     | 1   | FME  | CA-N-CN     | -2.69 | 118.68      | 122.82   |
| 1   | A     | 1   | FME  | CA-N-CN     | -2.43 | 119.08      | 122.82   |
| 9   | V     | 1   | SAC  | OAC-C1A-C2A | -2.31 | 117.94      | 122.05   |
| 9   | I     | 1   | SAC  | C2A-C1A-N   | 2.19  | 119.75      | 116.12   |
| 1   | N     | 1   | FME  | O-C-CA      | -2.05 | 119.51      | 124.77   |
| 7   | G     | 11  | TPO  | O3P-P-OG1   | 2.02  | 113.72      | 105.85   |

There are no chirality outliers.



All (24) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | T     | 11  | TPO  | 1       | 0            |
| 1   | A     | 1   | FME  | 4       | 0            |
| 7   | G     | 11  | TPO  | 1       | 0            |
| 1   | N     | 1   | FME  | 2       | 0            |
| 2   | O     | 1   | FME  | 4       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 54 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 44 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  | DMU  | M     | 526  | -    | 34,34,34     | 3.25 | 8 (23%)  | 45,45,45    | 4.27 | 19 (42%) |
| 22  | CHD  | B     | 1086 | -    | 32,32,32     | 0.75 | 0        | 51,51,51    | 1.80 | 14 (27%) |
| 17  | HEA  | N     | 516  | 1    | 67,67,67     | 1.13 | 6 (8%)   | 81,103,103  | 1.24 | 9 (11%)  |
| 18  | PGV  | C     | 268  | -    | 50,50,50     | 1.25 | 3 (6%)   | 53,56,56    | 0.82 | 1 (1%)   |
| 20  | TGL  | B     | 521  | -    | 62,62,62     | 0.70 | 0        | 65,65,65    | 1.43 | 11 (16%) |
| 23  | DMU  | P     | 1272 | -    | 34,34,34     | 3.03 | 8 (23%)  | 45,45,45    | 4.07 | 19 (42%) |
| 25  | PEK  | P     | 1264 | -    | 52,52,52     | 1.43 | 4 (7%)   | 55,57,57    | 1.05 | 3 (5%)   |
| 26  | CDL  | T     | 1269 | -    | 99,99,99     | 0.89 | 4 (4%)   | 105,111,111 | 0.98 | 7 (6%)   |
| 20  | TGL  | L     | 522  | -    | 62,62,62     | 1.14 | 4 (6%)   | 65,65,65    | 1.73 | 13 (20%) |
| 22  | CHD  | C     | 525  | -    | 32,32,32     | 0.87 | 1 (3%)   | 51,51,51    | 1.65 | 12 (23%) |
| 17  | HEA  | N     | 515  | 1    | 67,67,67     | 1.04 | 3 (4%)   | 81,103,103  | 1.11 | 6 (7%)   |
| 22  | CHD  | J     | 60   | -    | 32,32,32     | 0.91 | 1 (3%)   | 51,51,51    | 3.19 | 25 (49%) |
| 17  | HEA  | A     | 516  | 1    | 67,67,67     | 1.13 | 4 (5%)   | 81,103,103  | 1.15 | 4 (4%)   |
| 18  | PGV  | P     | 1267 | -    | 50,50,50     | 0.85 | 1 (2%)   | 53,56,56    | 0.83 | 1 (1%)   |
| 20  | TGL  | N     | 1521 | -    | 62,62,62     | 0.74 | 1 (1%)   | 65,65,65    | 1.42 | 10 (15%) |
| 19  | CUA  | B     | 228  | 2    | 0,1,1        | -    | -        | -           | -    | -        |
| 22  | CHD  | P     | 1525 | -    | 32,32,32     | 0.88 | 0        | 51,51,51    | 1.59 | 9 (17%)  |
| 23  | DMU  | C     | 272  | -    | 34,34,34     | 3.03 | 8 (23%)  | 45,45,45    | 4.07 | 19 (42%) |
| 25  | PEK  | G     | 1263 | -    | 52,52,52     | 1.83 | 12 (23%) | 55,57,57    | 1.22 | 4 (7%)   |
| 18  | PGV  | A     | 524  | -    | 50,50,50     | 1.08 | 3 (6%)   | 53,56,56    | 0.95 | 2 (3%)   |
| 17  | HEA  | A     | 515  | 1    | 67,67,67     | 1.09 | 4 (5%)   | 81,103,103  | 1.11 | 6 (7%)   |
| 18  | PGV  | C     | 267  | -    | 50,50,50     | 0.84 | 1 (2%)   | 53,56,56    | 0.85 | 2 (3%)   |
| 18  | PGV  | P     | 1268 | -    | 50,50,50     | 1.28 | 4 (8%)   | 53,56,56    | 0.84 | 1 (1%)   |
| 22  | CHD  | O     | 229  | -    | 32,32,32     | 0.85 | 0        | 51,51,51    | 1.83 | 13 (25%) |
| 18  | PGV  | A     | 525  | -    | 50,50,50     | 0.90 | 2 (4%)   | 53,56,56    | 0.75 | 2 (3%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CHD  | W     | 1060 | -    | 32,32,32     | 0.98 | 2 (6%)   | 51,51,51    | 3.17 | 26 (50%) |
| 21  | PSC  | O     | 1230 | -    | 51,51,51     | 1.16 | 3 (5%)   | 57,59,59    | 0.88 | 1 (1%)   |
| 25  | PEK  | C     | 265  | -    | 52,52,52     | 1.62 | 10 (19%) | 55,57,57    | 1.10 | 5 (9%)   |
| 21  | PSC  | B     | 230  | -    | 51,51,51     | 1.19 | 3 (5%)   | 57,59,59    | 0.87 | 1 (1%)   |
| 25  | PEK  | P     | 1265 | -    | 52,52,52     | 1.66 | 11 (21%) | 55,57,57    | 1.08 | 5 (9%)   |
| 23  | DMU  | Z     | 1526 | -    | 34,34,34     | 3.20 | 8 (23%)  | 45,45,45    | 4.22 | 19 (42%) |
| 18  | PGV  | Z     | 1524 | -    | 50,50,50     | 1.05 | 3 (6%)   | 53,56,56    | 0.92 | 2 (3%)   |
| 22  | CHD  | P     | 1271 | -    | 32,32,32     | 0.82 | 0        | 51,51,51    | 3.54 | 22 (43%) |
| 18  | PGV  | N     | 1266 | -    | 50,50,50     | 0.93 | 2 (4%)   | 53,56,56    | 0.78 | 3 (5%)   |
| 20  | TGL  | N     | 1522 | -    | 62,62,62     | 1.17 | 4 (6%)   | 65,65,65    | 1.71 | 13 (20%) |
| 25  | PEK  | C     | 264  | -    | 52,52,52     | 1.44 | 4 (7%)   | 55,57,57    | 1.02 | 3 (5%)   |
| 25  | PEK  | T     | 263  | -    | 52,52,52     | 1.85 | 12 (23%) | 55,57,57    | 1.22 | 4 (7%)   |
| 26  | CDL  | C     | 270  | -    | 99,99,99     | 0.80 | 3 (3%)   | 105,111,111 | 0.99 | 6 (5%)   |
| 19  | CUA  | O     | 228  | 2    | 0,1,1        | -    | -        | -           | -    | -        |
| 26  | CDL  | P     | 1270 | -    | 99,99,99     | 0.83 | 3 (3%)   | 105,111,111 | 0.97 | 6 (5%)   |
| 20  | TGL  | D     | 523  | -    | 62,62,62     | 0.79 | 1 (1%)   | 65,65,65    | 1.30 | 9 (13%)  |
| 26  | CDL  | G     | 269  | -    | 99,99,99     | 0.93 | 6 (6%)   | 105,111,111 | 0.97 | 7 (6%)   |
| 20  | TGL  | Q     | 1523 | -    | 62,62,62     | 0.82 | 2 (3%)   | 65,65,65    | 1.27 | 9 (13%)  |
| 22  | CHD  | C     | 271  | -    | 32,32,32     | 0.84 | 0        | 51,51,51    | 3.60 | 22 (43%) |

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  | DMU  | M     | 526  | -    | 5/5/10/10 | 8/19/59/59     | 0/2/2/2 |
| 22  | CHD  | B     | 1086 | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 17  | HEA  | N     | 516  | 1    | -         | 5/36/76/76     | -       |
| 18  | PGV  | C     | 268  | -    | -         | 34/55/55/55    | -       |
| 20  | TGL  | B     | 521  | -    | -         | 14/65/65/65    | -       |
| 23  | DMU  | P     | 1272 | -    | 6/6/10/10 | 9/19/59/59     | 0/2/2/2 |
| 25  | PEK  | P     | 1264 | -    | -         | 21/56/56/56    | -       |
| 26  | CDL  | T     | 1269 | -    | -         | 61/110/110/110 | -       |
| 20  | TGL  | L     | 522  | -    | -         | 16/65/65/65    | -       |
| 22  | CHD  | C     | 525  | -    | -         | 2/9/74/74      | 0/4/4/4 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions       | Rings   |
|-----|------|-------|------|------|-----------|----------------|---------|
| 17  | HEA  | N     | 515  | 1    | -         | 7/36/76/76     | -       |
| 22  | CHD  | J     | 60   | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |
| 17  | HEA  | A     | 516  | 1    | -         | 6/36/76/76     | -       |
| 18  | PGV  | P     | 1267 | -    | -         | 17/55/55/55    | -       |
| 20  | TGL  | N     | 1521 | -    | -         | 14/65/65/65    | -       |
| 22  | CHD  | P     | 1525 | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 23  | DMU  | C     | 272  | -    | 6/6/10/10 | 9/19/59/59     | 0/2/2/2 |
| 25  | PEK  | G     | 1263 | -    | -         | 28/56/56/56    | -       |
| 18  | PGV  | A     | 524  | -    | -         | 31/55/55/55    | -       |
| 17  | HEA  | A     | 515  | 1    | -         | 8/36/76/76     | -       |
| 18  | PGV  | C     | 267  | -    | -         | 17/55/55/55    | -       |
| 18  | PGV  | P     | 1268 | -    | -         | 34/55/55/55    | -       |
| 22  | CHD  | O     | 229  | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 18  | PGV  | A     | 525  | -    | -         | 13/55/55/55    | -       |
| 22  | CHD  | W     | 1060 | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |
| 21  | PSC  | O     | 1230 | -    | -         | 39/55/55/55    | -       |
| 25  | PEK  | C     | 265  | -    | -         | 20/56/56/56    | -       |
| 21  | PSC  | B     | 230  | -    | -         | 39/55/55/55    | -       |
| 25  | PEK  | P     | 1265 | -    | -         | 21/56/56/56    | -       |
| 23  | DMU  | Z     | 1526 | -    | 5/5/10/10 | 8/19/59/59     | 0/2/2/2 |
| 18  | PGV  | Z     | 1524 | -    | -         | 30/55/55/55    | -       |
| 22  | CHD  | P     | 1271 | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |
| 18  | PGV  | N     | 1266 | -    | -         | 14/55/55/55    | -       |
| 20  | TGL  | N     | 1522 | -    | -         | 16/65/65/65    | -       |
| 25  | PEK  | C     | 264  | -    | -         | 21/56/56/56    | -       |
| 25  | PEK  | T     | 263  | -    | -         | 28/56/56/56    | -       |
| 26  | CDL  | C     | 270  | -    | -         | 68/110/110/110 | -       |
| 26  | CDL  | P     | 1270 | -    | -         | 69/110/110/110 | -       |
| 20  | TGL  | D     | 523  | -    | -         | 14/65/65/65    | -       |
| 26  | CDL  | G     | 269  | -    | -         | 61/110/110/110 | -       |
| 20  | TGL  | Q     | 1523 | -    | -         | 14/65/65/65    | -       |
| 22  | CHD  | C     | 271  | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |

All (159) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | Z     | 1526 | DMU  | O7-C3   | -8.20 | 1.23        | 1.43     |
| 23  | M     | 526  | DMU  | O7-C3   | -8.15 | 1.23        | 1.43     |
| 23  | M     | 526  | DMU  | O16-C6  | -7.56 | 1.27        | 1.40     |
| 23  | Z     | 1526 | DMU  | O16-C6  | -7.49 | 1.27        | 1.40     |
| 23  | M     | 526  | DMU  | O1-C9   | -7.19 | 1.26        | 1.44     |
| 23  | C     | 272  | DMU  | O16-C6  | -7.19 | 1.28        | 1.40     |
| 23  | P     | 1272 | DMU  | O1-C9   | -7.12 | 1.27        | 1.44     |
| 23  | P     | 1272 | DMU  | O16-C6  | -7.05 | 1.28        | 1.40     |
| 23  | Z     | 1526 | DMU  | O1-C9   | -6.92 | 1.27        | 1.44     |
| 23  | C     | 272  | DMU  | O1-C9   | -6.81 | 1.27        | 1.44     |
| 23  | P     | 1272 | DMU  | O7-C3   | -6.78 | 1.26        | 1.43     |
| 23  | C     | 272  | DMU  | O7-C3   | -6.74 | 1.26        | 1.43     |
| 23  | C     | 272  | DMU  | O16-C18 | -6.62 | 1.25        | 1.43     |
| 23  | P     | 1272 | DMU  | O16-C18 | -6.58 | 1.25        | 1.43     |
| 23  | M     | 526  | DMU  | O5-C4   | -6.50 | 1.28        | 1.44     |
| 23  | Z     | 1526 | DMU  | O5-C4   | -6.44 | 1.28        | 1.44     |
| 23  | M     | 526  | DMU  | O16-C18 | -6.29 | 1.25        | 1.43     |
| 23  | Z     | 1526 | DMU  | O16-C18 | -6.00 | 1.26        | 1.43     |
| 23  | Z     | 1526 | DMU  | O7-C10  | -5.98 | 1.24        | 1.41     |
| 23  | M     | 526  | DMU  | O7-C10  | -5.97 | 1.25        | 1.41     |
| 23  | M     | 526  | DMU  | O1-C10  | -5.78 | 1.27        | 1.41     |
| 23  | Z     | 1526 | DMU  | O1-C10  | -5.73 | 1.27        | 1.41     |
| 23  | C     | 272  | DMU  | O5-C4   | -5.34 | 1.31        | 1.44     |
| 23  | P     | 1272 | DMU  | O5-C4   | -5.24 | 1.31        | 1.44     |
| 23  | C     | 272  | DMU  | O1-C10  | -5.15 | 1.28        | 1.41     |
| 23  | C     | 272  | DMU  | O7-C10  | -5.15 | 1.27        | 1.41     |
| 23  | P     | 1272 | DMU  | O1-C10  | -5.12 | 1.28        | 1.41     |
| 23  | P     | 1272 | DMU  | O7-C10  | -5.11 | 1.27        | 1.41     |
| 20  | N     | 1522 | TGL  | OG2-CB1 | 5.05  | 1.48        | 1.34     |
| 20  | L     | 522  | TGL  | OG2-CB1 | 4.94  | 1.48        | 1.34     |
| 25  | G     | 1263 | PEK  | C12-C11 | 4.79  | 1.58        | 1.31     |
| 23  | C     | 272  | DMU  | O5-C6   | -4.75 | 1.29        | 1.41     |
| 25  | C     | 264  | PEK  | C15-C14 | 4.73  | 1.58        | 1.31     |
| 25  | P     | 1264 | PEK  | C12-C11 | 4.73  | 1.58        | 1.31     |
| 25  | T     | 263  | PEK  | C12-C11 | 4.63  | 1.58        | 1.31     |
| 23  | P     | 1272 | DMU  | O5-C6   | -4.62 | 1.29        | 1.41     |
| 25  | P     | 1264 | PEK  | C15-C14 | 4.61  | 1.57        | 1.31     |
| 25  | T     | 263  | PEK  | C6-C5   | 4.60  | 1.57        | 1.31     |
| 25  | G     | 1263 | PEK  | C6-C5   | 4.59  | 1.57        | 1.31     |
| 25  | C     | 264  | PEK  | C12-C11 | 4.59  | 1.57        | 1.31     |
| 23  | M     | 526  | DMU  | O5-C6   | -4.54 | 1.30        | 1.41     |
| 18  | P     | 1268 | PGV  | C12-C11 | 4.50  | 1.57        | 1.31     |
| 25  | P     | 1265 | PEK  | C12-C11 | 4.47  | 1.57        | 1.31     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | C     | 268  | PGV  | C12-C11 | 4.45  | 1.57        | 1.31     |
| 25  | C     | 265  | PEK  | C9-C8   | 4.43  | 1.56        | 1.31     |
| 25  | C     | 265  | PEK  | C12-C11 | 4.41  | 1.56        | 1.31     |
| 25  | T     | 263  | PEK  | O03-C21 | 4.40  | 1.46        | 1.33     |
| 25  | C     | 265  | PEK  | C15-C14 | 4.36  | 1.56        | 1.31     |
| 21  | O     | 1230 | PSC  | C10-C9  | 4.35  | 1.56        | 1.31     |
| 23  | Z     | 1526 | DMU  | O5-C6   | -4.31 | 1.30        | 1.41     |
| 25  | P     | 1265 | PEK  | C15-C14 | 4.30  | 1.56        | 1.31     |
| 25  | P     | 1265 | PEK  | C9-C8   | 4.29  | 1.56        | 1.31     |
| 25  | G     | 1263 | PEK  | C15-C14 | 4.29  | 1.56        | 1.31     |
| 21  | B     | 230  | PSC  | C10-C9  | 4.28  | 1.56        | 1.31     |
| 25  | G     | 1263 | PEK  | O03-C21 | 4.27  | 1.45        | 1.33     |
| 25  | T     | 263  | PEK  | C15-C14 | 4.22  | 1.55        | 1.31     |
| 25  | P     | 1265 | PEK  | C6-C5   | 4.22  | 1.55        | 1.31     |
| 21  | O     | 1230 | PSC  | C13-C12 | 4.21  | 1.55        | 1.31     |
| 21  | B     | 230  | PSC  | C13-C12 | 4.18  | 1.55        | 1.31     |
| 25  | C     | 264  | PEK  | C6-C5   | 4.17  | 1.55        | 1.31     |
| 25  | C     | 264  | PEK  | C9-C8   | 4.17  | 1.55        | 1.31     |
| 25  | T     | 263  | PEK  | C9-C8   | 4.17  | 1.55        | 1.31     |
| 18  | P     | 1268 | PGV  | O01-C1  | 4.17  | 1.46        | 1.34     |
| 25  | P     | 1264 | PEK  | C9-C8   | 4.14  | 1.55        | 1.31     |
| 25  | P     | 1264 | PEK  | C6-C5   | 4.14  | 1.55        | 1.31     |
| 25  | G     | 1263 | PEK  | C9-C8   | 4.11  | 1.55        | 1.31     |
| 18  | N     | 1266 | PGV  | C12-C11 | 4.09  | 1.54        | 1.31     |
| 25  | C     | 265  | PEK  | C6-C5   | 4.07  | 1.54        | 1.31     |
| 18  | Z     | 1524 | PGV  | C12-C11 | 4.04  | 1.54        | 1.31     |
| 18  | A     | 524  | PGV  | C12-C11 | 3.95  | 1.54        | 1.31     |
| 20  | N     | 1522 | TGL  | OG1-CA1 | 3.93  | 1.44        | 1.33     |
| 18  | A     | 525  | PGV  | C12-C11 | 3.91  | 1.53        | 1.31     |
| 17  | A     | 516  | HEA  | FE-NC   | 3.71  | 2.07        | 1.95     |
| 17  | A     | 515  | HEA  | FE-NA   | 3.66  | 2.07        | 1.95     |
| 17  | N     | 516  | HEA  | FE-NA   | 3.62  | 2.07        | 1.95     |
| 18  | C     | 268  | PGV  | O01-C1  | 3.61  | 1.44        | 1.34     |
| 25  | G     | 1263 | PEK  | C01-C02 | 3.56  | 1.61        | 1.50     |
| 26  | T     | 1269 | CDL  | CB6-CB4 | 3.54  | 1.61        | 1.50     |
| 25  | G     | 1263 | PEK  | C03-C02 | 3.43  | 1.61        | 1.50     |
| 18  | A     | 524  | PGV  | O03-C19 | 3.42  | 1.43        | 1.33     |
| 25  | T     | 263  | PEK  | C01-C02 | 3.32  | 1.61        | 1.50     |
| 18  | P     | 1267 | PGV  | C12-C11 | 3.29  | 1.50        | 1.31     |
| 18  | C     | 267  | PGV  | C12-C11 | 3.27  | 1.50        | 1.31     |
| 26  | G     | 269  | CDL  | CB6-CB4 | 3.27  | 1.61        | 1.50     |
| 25  | T     | 263  | PEK  | C03-C02 | 3.25  | 1.61        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | W     | 1060 | CHD  | C13-C17 | 3.11  | 1.60        | 1.55     |
| 20  | L     | 522  | TGL  | OG1-CA1 | 3.07  | 1.42        | 1.33     |
| 25  | T     | 263  | PEK  | O01-C1  | 3.00  | 1.42        | 1.34     |
| 17  | N     | 515  | HEA  | CMA-C3A | -2.99 | 1.38        | 1.45     |
| 18  | Z     | 1524 | PGV  | O03-C19 | 2.93  | 1.41        | 1.33     |
| 25  | T     | 263  | PEK  | P-O11   | 2.91  | 1.70        | 1.59     |
| 25  | T     | 263  | PEK  | C2-C1   | 2.88  | 1.59        | 1.50     |
| 25  | P     | 1265 | PEK  | O03-C21 | 2.84  | 1.41        | 1.33     |
| 17  | N     | 516  | HEA  | CMA-C3A | -2.81 | 1.39        | 1.45     |
| 20  | L     | 522  | TGL  | CG1-CG2 | 2.81  | 1.59        | 1.50     |
| 22  | J     | 60   | CHD  | C13-C17 | 2.70  | 1.60        | 1.55     |
| 26  | P     | 1270 | CDL  | CA6-CA4 | 2.69  | 1.59        | 1.50     |
| 26  | G     | 269  | CDL  | OA6-CA5 | 2.66  | 1.41        | 1.34     |
| 25  | G     | 1263 | PEK  | P-O11   | 2.65  | 1.69        | 1.59     |
| 25  | P     | 1265 | PEK  | C22-C21 | 2.60  | 1.58        | 1.50     |
| 17  | A     | 515  | HEA  | CMA-C3A | -2.59 | 1.39        | 1.45     |
| 20  | N     | 1522 | TGL  | CG1-CG2 | 2.58  | 1.58        | 1.50     |
| 25  | C     | 265  | PEK  | C03-C02 | 2.56  | 1.58        | 1.50     |
| 17  | N     | 516  | HEA  | FE-ND   | -2.55 | 1.87        | 1.94     |
| 25  | C     | 265  | PEK  | C22-C21 | 2.55  | 1.58        | 1.50     |
| 25  | G     | 1263 | PEK  | O01-C1  | 2.54  | 1.41        | 1.34     |
| 17  | A     | 515  | HEA  | FE-ND   | 2.52  | 2.02        | 1.94     |
| 18  | C     | 268  | PGV  | C04-C05 | 2.50  | 1.59        | 1.51     |
| 21  | B     | 230  | PSC  | C2-C1   | 2.50  | 1.58        | 1.50     |
| 20  | N     | 1521 | TGL  | OG2-CB1 | 2.48  | 1.41        | 1.34     |
| 25  | P     | 1265 | PEK  | C03-C02 | 2.47  | 1.58        | 1.50     |
| 25  | P     | 1265 | PEK  | P-O11   | 2.47  | 1.69        | 1.59     |
| 26  | G     | 269  | CDL  | CB3-CB4 | 2.45  | 1.58        | 1.50     |
| 18  | P     | 1268 | PGV  | C2-C1   | 2.45  | 1.57        | 1.50     |
| 17  | A     | 516  | HEA  | C20-C19 | 2.42  | 1.56        | 1.51     |
| 26  | T     | 1269 | CDL  | C11-CA5 | 2.42  | 1.57        | 1.50     |
| 26  | C     | 270  | CDL  | CA6-CA4 | 2.42  | 1.58        | 1.50     |
| 20  | Q     | 1523 | TGL  | OG2-CB1 | 2.41  | 1.41        | 1.34     |
| 25  | C     | 265  | PEK  | O03-C21 | 2.37  | 1.40        | 1.33     |
| 25  | T     | 263  | PEK  | C22-C21 | 2.37  | 1.57        | 1.50     |
| 25  | G     | 1263 | PEK  | C22-C21 | 2.33  | 1.57        | 1.50     |
| 17  | A     | 516  | HEA  | FE-NA   | 2.33  | 2.02        | 1.95     |
| 26  | G     | 269  | CDL  | CA6-CA4 | 2.32  | 1.58        | 1.50     |
| 25  | C     | 265  | PEK  | P-O11   | 2.32  | 1.68        | 1.59     |
| 26  | P     | 1270 | CDL  | OA8-CA7 | 2.31  | 1.40        | 1.33     |
| 25  | P     | 1265 | PEK  | C01-C02 | 2.28  | 1.57        | 1.50     |
| 26  | T     | 1269 | CDL  | CB3-CB4 | 2.27  | 1.57        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | P     | 1265 | PEK  | P-O12   | 2.27  | 1.68        | 1.59     |
| 17  | N     | 515  | HEA  | CMC-C2C | 2.27  | 1.55        | 1.50     |
| 22  | C     | 525  | CHD  | C10-C9  | -2.27 | 1.52        | 1.56     |
| 21  | O     | 1230 | PSC  | C2-C1   | 2.26  | 1.57        | 1.50     |
| 25  | P     | 1265 | PEK  | O01-C1  | 2.26  | 1.40        | 1.34     |
| 26  | P     | 1270 | CDL  | CA3-CA4 | 2.25  | 1.57        | 1.50     |
| 25  | C     | 265  | PEK  | C01-C02 | 2.24  | 1.57        | 1.50     |
| 26  | G     | 269  | CDL  | C11-CA5 | 2.20  | 1.57        | 1.50     |
| 26  | C     | 270  | CDL  | CA3-CA4 | 2.19  | 1.57        | 1.50     |
| 26  | T     | 1269 | CDL  | OA6-CA5 | 2.18  | 1.40        | 1.34     |
| 17  | N     | 515  | HEA  | C1C-C2C | 2.18  | 1.48        | 1.43     |
| 18  | P     | 1268 | PGV  | C04-C05 | 2.17  | 1.58        | 1.51     |
| 25  | T     | 263  | PEK  | P-O12   | 2.17  | 1.67        | 1.59     |
| 18  | A     | 524  | PGV  | C20-C19 | 2.16  | 1.57        | 1.50     |
| 25  | G     | 1263 | PEK  | C2-C1   | 2.15  | 1.57        | 1.50     |
| 26  | C     | 270  | CDL  | OA8-CA7 | 2.15  | 1.39        | 1.33     |
| 22  | W     | 1060 | CHD  | C20-C17 | 2.13  | 1.58        | 1.54     |
| 17  | A     | 515  | HEA  | CMB-C2B | 2.13  | 1.55        | 1.50     |
| 17  | A     | 516  | HEA  | CMA-C3A | -2.12 | 1.40        | 1.45     |
| 20  | N     | 1522 | TGL  | CC2-CC1 | 2.10  | 1.56        | 1.50     |
| 20  | D     | 523  | TGL  | OG1-CA1 | 2.08  | 1.39        | 1.33     |
| 25  | C     | 265  | PEK  | P-O12   | 2.07  | 1.67        | 1.59     |
| 17  | N     | 516  | HEA  | FE-NC   | 2.06  | 2.02        | 1.95     |
| 18  | Z     | 1524 | PGV  | C20-C19 | 2.06  | 1.56        | 1.50     |
| 26  | G     | 269  | CDL  | CB2-C1  | 2.06  | 1.58        | 1.51     |
| 17  | N     | 516  | HEA  | C4D-ND  | 2.06  | 1.42        | 1.38     |
| 17  | N     | 516  | HEA  | C3C-C4C | 2.05  | 1.48        | 1.42     |
| 18  | N     | 1266 | PGV  | C01-C02 | 2.05  | 1.57        | 1.50     |
| 20  | L     | 522  | TGL  | CG3-CG2 | 2.05  | 1.57        | 1.50     |
| 20  | Q     | 1523 | TGL  | OG1-CA1 | 2.04  | 1.39        | 1.33     |
| 18  | A     | 525  | PGV  | C20-C19 | 2.04  | 1.56        | 1.50     |
| 25  | G     | 1263 | PEK  | P-O12   | 2.03  | 1.67        | 1.59     |

All (375) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 271  | CHD  | C17-C13-C14 | 10.49 | 110.64      | 100.11   |
| 23  | C     | 272  | DMU  | C1-C2-C3    | 10.11 | 132.62      | 109.68   |
| 23  | P     | 1272 | DMU  | C1-C2-C3    | 9.99  | 132.34      | 109.68   |
| 22  | P     | 1271 | CHD  | C17-C13-C14 | 9.97  | 110.12      | 100.11   |
| 22  | P     | 1271 | CHD  | C10-C9-C8   | 9.84  | 122.80      | 111.84   |
| 23  | Z     | 1526 | DMU  | C1-C2-C3    | 9.74  | 131.80      | 109.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | M     | 526  | DMU  | C1-C2-C3    | 9.68  | 131.64      | 109.68   |
| 22  | P     | 1271 | CHD  | C17-C13-C12 | -9.67 | 108.97      | 117.67   |
| 22  | C     | 271  | CHD  | C17-C13-C12 | -9.61 | 109.02      | 117.67   |
| 22  | J     | 60   | CHD  | C17-C13-C14 | 9.49  | 109.63      | 100.11   |
| 23  | M     | 526  | DMU  | C10-C5-C7   | 9.41  | 129.80      | 110.01   |
| 22  | C     | 271  | CHD  | C10-C9-C8   | 9.40  | 122.32      | 111.84   |
| 23  | Z     | 1526 | DMU  | C10-C5-C7   | 9.28  | 129.53      | 110.01   |
| 22  | W     | 1060 | CHD  | C17-C13-C14 | 9.15  | 109.29      | 100.11   |
| 23  | P     | 1272 | DMU  | O16-C6-C1   | 9.14  | 122.16      | 108.27   |
| 23  | C     | 272  | DMU  | O16-C6-C1   | 9.05  | 122.02      | 108.27   |
| 23  | C     | 272  | DMU  | C6-O5-C4    | 8.71  | 130.74      | 113.72   |
| 22  | C     | 271  | CHD  | C19-C10-C9  | -8.61 | 99.61       | 111.18   |
| 23  | C     | 272  | DMU  | O5-C4-C3    | 8.54  | 127.38      | 109.72   |
| 23  | P     | 1272 | DMU  | O5-C4-C3    | 8.53  | 127.36      | 109.72   |
| 23  | P     | 1272 | DMU  | C6-O5-C4    | 8.48  | 130.29      | 113.72   |
| 23  | M     | 526  | DMU  | C6-O5-C4    | 8.17  | 129.67      | 113.72   |
| 23  | C     | 272  | DMU  | O1-C9-C11   | 8.14  | 126.62      | 106.44   |
| 23  | Z     | 1526 | DMU  | C6-O5-C4    | 8.03  | 129.41      | 113.72   |
| 22  | P     | 1271 | CHD  | C19-C10-C9  | -7.96 | 100.48      | 111.18   |
| 23  | C     | 272  | DMU  | O7-C3-C4    | 7.79  | 129.92      | 109.48   |
| 23  | P     | 1272 | DMU  | O1-C9-C11   | 7.77  | 125.70      | 106.44   |
| 23  | Z     | 1526 | DMU  | O5-C4-C3    | 7.72  | 125.69      | 109.72   |
| 23  | M     | 526  | DMU  | O1-C9-C8    | 7.68  | 123.54      | 109.70   |
| 23  | P     | 1272 | DMU  | O7-C3-C4    | 7.59  | 129.39      | 109.48   |
| 23  | M     | 526  | DMU  | O5-C4-C3    | 7.35  | 124.92      | 109.72   |
| 23  | Z     | 1526 | DMU  | O1-C9-C11   | 7.33  | 124.61      | 106.44   |
| 23  | Z     | 1526 | DMU  | O1-C9-C8    | 7.27  | 122.80      | 109.70   |
| 23  | M     | 526  | DMU  | O7-C3-C2    | 7.18  | 125.48      | 107.23   |
| 23  | M     | 526  | DMU  | C8-C7-C5    | -7.12 | 98.34       | 110.83   |
| 22  | W     | 1060 | CHD  | C13-C17-C20 | 7.03  | 128.00      | 119.48   |
| 23  | M     | 526  | DMU  | O5-C4-C57   | 6.97  | 123.72      | 106.44   |
| 23  | M     | 526  | DMU  | O1-C9-C11   | 6.97  | 123.70      | 106.44   |
| 23  | Z     | 1526 | DMU  | C8-C7-C5    | -6.88 | 98.76       | 110.83   |
| 22  | J     | 60   | CHD  | C13-C17-C20 | 6.80  | 127.72      | 119.48   |
| 23  | Z     | 1526 | DMU  | O7-C3-C2    | 6.74  | 124.35      | 107.23   |
| 23  | M     | 526  | DMU  | C7-C8-C9    | 6.73  | 122.44      | 110.23   |
| 23  | Z     | 1526 | DMU  | O5-C4-C57   | 6.69  | 123.02      | 106.44   |
| 23  | Z     | 1526 | DMU  | C7-C8-C9    | 6.63  | 122.25      | 110.23   |
| 23  | M     | 526  | DMU  | C18-O16-C6  | 6.45  | 124.69      | 113.68   |
| 23  | P     | 1272 | DMU  | O1-C9-C8    | 6.37  | 121.18      | 109.70   |
| 22  | P     | 1271 | CHD  | C1-C10-C5   | 6.33  | 116.84      | 107.75   |
| 22  | C     | 271  | CHD  | C1-C10-C5   | 6.30  | 116.79      | 107.75   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | P     | 1272 | DMU  | C18-O16-C6  | 6.30  | 124.44      | 113.68   |
| 22  | J     | 60   | CHD  | C10-C9-C8   | 6.07  | 118.60      | 111.84   |
| 22  | W     | 1060 | CHD  | C10-C9-C8   | 6.05  | 118.58      | 111.84   |
| 23  | C     | 272  | DMU  | O1-C9-C8    | 5.96  | 120.44      | 109.70   |
| 23  | Z     | 1526 | DMU  | C18-O16-C6  | 5.92  | 123.79      | 113.68   |
| 23  | Z     | 1526 | DMU  | O5-C6-O16   | 5.89  | 123.97      | 110.04   |
| 23  | C     | 272  | DMU  | C18-O16-C6  | 5.89  | 123.73      | 113.68   |
| 22  | W     | 1060 | CHD  | C6-C5-C10   | 5.77  | 118.80      | 112.66   |
| 22  | W     | 1060 | CHD  | C15-C14-C8  | -5.73 | 110.50      | 118.36   |
| 22  | J     | 60   | CHD  | C6-C5-C10   | 5.70  | 118.73      | 112.66   |
| 22  | J     | 60   | CHD  | C15-C14-C8  | -5.59 | 110.69      | 118.36   |
| 23  | P     | 1272 | DMU  | O5-C4-C57   | 5.57  | 120.25      | 106.44   |
| 23  | P     | 1272 | DMU  | O7-C3-C2    | 5.56  | 121.37      | 107.23   |
| 23  | C     | 272  | DMU  | O5-C4-C57   | 5.56  | 120.21      | 106.44   |
| 23  | C     | 272  | DMU  | O7-C3-C2    | 5.48  | 121.15      | 107.23   |
| 22  | J     | 60   | CHD  | C4-C3-C2    | 5.43  | 117.24      | 110.62   |
| 23  | M     | 526  | DMU  | O5-C6-C1    | 5.42  | 121.50      | 110.37   |
| 22  | J     | 60   | CHD  | C1-C10-C5   | 5.40  | 115.49      | 107.75   |
| 22  | C     | 271  | CHD  | C9-C8-C7    | 5.38  | 118.63      | 111.86   |
| 23  | C     | 272  | DMU  | O7-C10-C5   | 5.36  | 121.28      | 108.09   |
| 22  | P     | 1271 | CHD  | C9-C8-C7    | 5.30  | 118.53      | 111.86   |
| 23  | Z     | 1526 | DMU  | O5-C6-C1    | 5.29  | 121.25      | 110.37   |
| 23  | P     | 1272 | DMU  | O7-C10-C5   | 5.29  | 121.11      | 108.09   |
| 22  | P     | 1271 | CHD  | C15-C14-C8  | -5.23 | 111.19      | 118.36   |
| 23  | M     | 526  | DMU  | O5-C6-O16   | 5.23  | 122.39      | 110.04   |
| 22  | C     | 271  | CHD  | C15-C14-C8  | -5.16 | 111.28      | 118.36   |
| 22  | W     | 1060 | CHD  | C4-C3-C2    | 5.15  | 116.90      | 110.62   |
| 22  | C     | 271  | CHD  | C19-C10-C1  | -5.13 | 100.14      | 108.31   |
| 22  | P     | 1525 | CHD  | C13-C17-C20 | 5.09  | 125.65      | 119.48   |
| 22  | W     | 1060 | CHD  | C1-C10-C5   | 5.08  | 115.04      | 107.75   |
| 22  | W     | 1060 | CHD  | C9-C8-C7    | 5.07  | 118.25      | 111.86   |
| 22  | J     | 60   | CHD  | C9-C8-C7    | 5.06  | 118.23      | 111.86   |
| 22  | P     | 1271 | CHD  | C19-C10-C1  | -5.02 | 100.32      | 108.31   |
| 23  | M     | 526  | DMU  | O16-C6-C1   | 4.99  | 115.85      | 108.27   |
| 20  | L     | 522  | TGL  | C12-C11-C10 | -4.77 | 90.25       | 114.37   |
| 23  | Z     | 1526 | DMU  | O7-C3-C4    | 4.77  | 121.98      | 109.48   |
| 22  | C     | 271  | CHD  | C14-C13-C12 | 4.77  | 111.77      | 107.42   |
| 20  | L     | 522  | TGL  | CB9-CB8-CB7 | -4.75 | 90.36       | 114.37   |
| 20  | N     | 1522 | TGL  | CB9-CB8-CB7 | -4.74 | 90.40       | 114.37   |
| 23  | M     | 526  | DMU  | O7-C10-C5   | 4.68  | 119.59      | 108.09   |
| 22  | C     | 271  | CHD  | C4-C5-C10   | 4.67  | 117.63      | 112.66   |
| 20  | N     | 1522 | TGL  | C12-C11-C10 | -4.63 | 90.97       | 114.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | J     | 60   | CHD  | C18-C13-C14 | -4.61 | 103.98      | 111.20   |
| 22  | C     | 525  | CHD  | C13-C17-C20 | 4.59  | 125.04      | 119.48   |
| 22  | P     | 1271 | CHD  | C14-C13-C12 | 4.45  | 111.48      | 107.42   |
| 23  | Z     | 1526 | DMU  | O7-C10-C5   | 4.42  | 118.97      | 108.09   |
| 22  | W     | 1060 | CHD  | C18-C13-C14 | -4.37 | 104.36      | 111.20   |
| 23  | C     | 272  | DMU  | O7-C10-O1   | 4.37  | 122.18      | 110.69   |
| 20  | B     | 521  | TGL  | CG2-OG2-CB1 | 4.35  | 128.21      | 117.80   |
| 22  | W     | 1060 | CHD  | C11-C12-C13 | 4.33  | 115.67      | 111.26   |
| 20  | N     | 1521 | TGL  | CG2-OG2-CB1 | 4.29  | 128.07      | 117.80   |
| 23  | P     | 1272 | DMU  | O7-C10-O1   | 4.26  | 121.89      | 110.69   |
| 22  | P     | 1271 | CHD  | C4-C5-C10   | 4.25  | 117.18      | 112.66   |
| 20  | B     | 521  | TGL  | CG1-OG1-CA1 | -4.24 | 101.61      | 117.12   |
| 23  | C     | 272  | DMU  | C2-C3-C4    | -4.23 | 101.55      | 110.93   |
| 22  | C     | 271  | CHD  | C4-C3-C2    | 4.22  | 115.77      | 110.62   |
| 20  | N     | 1521 | TGL  | CG1-OG1-CA1 | -4.21 | 101.72      | 117.12   |
| 20  | L     | 522  | TGL  | C15-CC9-CC8 | 4.21  | 135.65      | 114.37   |
| 23  | P     | 1272 | DMU  | C10-O1-C9   | 4.21  | 121.94      | 113.72   |
| 23  | P     | 1272 | DMU  | O5-C6-C1    | 4.19  | 118.99      | 110.37   |
| 23  | C     | 272  | DMU  | C10-O1-C9   | 4.18  | 121.88      | 113.72   |
| 23  | M     | 526  | DMU  | O7-C3-C4    | 4.16  | 120.40      | 109.48   |
| 20  | N     | 1522 | TGL  | C15-CC9-CC8 | 4.15  | 135.36      | 114.37   |
| 22  | J     | 60   | CHD  | C11-C12-C13 | 4.14  | 115.47      | 111.26   |
| 23  | Z     | 1526 | DMU  | O16-C6-C1   | 4.13  | 114.55      | 108.27   |
| 25  | T     | 263  | PEK  | O03-C01-C02 | 4.09  | 120.19      | 108.40   |
| 23  | C     | 272  | DMU  | O5-C6-C1    | 4.09  | 118.77      | 110.37   |
| 25  | G     | 1263 | PEK  | O03-C01-C02 | 4.06  | 120.11      | 108.40   |
| 23  | P     | 1272 | DMU  | C2-C3-C4    | -4.06 | 101.93      | 110.93   |
| 22  | C     | 525  | CHD  | C14-C13-C12 | -4.04 | 103.73      | 107.42   |
| 25  | G     | 1263 | PEK  | C02-O01-C1  | 3.98  | 127.32      | 117.80   |
| 25  | T     | 263  | PEK  | P-O11-C03   | 3.92  | 143.84      | 121.35   |
| 22  | W     | 1060 | CHD  | C5-C6-C7    | 3.91  | 119.05      | 114.40   |
| 20  | L     | 522  | TGL  | CC3-CC2-CC1 | 3.91  | 128.02      | 113.69   |
| 25  | G     | 1263 | PEK  | P-O11-C03   | 3.88  | 143.57      | 121.35   |
| 22  | O     | 229  | CHD  | C10-C9-C8   | 3.84  | 116.12      | 111.84   |
| 22  | B     | 1086 | CHD  | C16-C17-C13 | -3.82 | 99.84       | 103.54   |
| 20  | N     | 1522 | TGL  | C16-C15-CC9 | 3.81  | 133.62      | 114.37   |
| 22  | P     | 1271 | CHD  | C4-C3-C2    | 3.80  | 115.25      | 110.62   |
| 22  | W     | 1060 | CHD  | C2-C1-C10   | 3.79  | 119.14      | 112.74   |
| 25  | T     | 263  | PEK  | C02-O01-C1  | 3.79  | 126.86      | 117.80   |
| 20  | L     | 522  | TGL  | C16-C15-CC9 | 3.78  | 133.48      | 114.37   |
| 22  | P     | 1271 | CHD  | C1-C10-C9   | 3.74  | 117.15      | 111.34   |
| 22  | C     | 271  | CHD  | C1-C10-C9   | 3.73  | 117.14      | 111.34   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | J     | 60   | CHD  | C5-C6-C7    | 3.73  | 118.83      | 114.40   |
| 22  | J     | 60   | CHD  | C17-C13-C12 | -3.73 | 114.31      | 117.67   |
| 22  | W     | 1060 | CHD  | C17-C13-C12 | -3.73 | 114.31      | 117.67   |
| 20  | N     | 1522 | TGL  | CC3-CC2-CC1 | 3.72  | 127.34      | 113.69   |
| 22  | P     | 1525 | CHD  | C15-C14-C8  | -3.71 | 113.27      | 118.36   |
| 23  | M     | 526  | DMU  | C10-O7-C3   | 3.70  | 126.76      | 117.98   |
| 20  | D     | 523  | TGL  | CG3-OG3-CC1 | 3.62  | 130.36      | 117.12   |
| 22  | B     | 1086 | CHD  | C15-C14-C8  | -3.59 | 113.44      | 118.36   |
| 23  | C     | 272  | DMU  | O5-C6-O16   | 3.58  | 118.51      | 110.04   |
| 20  | N     | 1522 | TGL  | C11-C10-CB9 | 3.58  | 132.47      | 114.37   |
| 22  | O     | 229  | CHD  | C14-C13-C12 | -3.57 | 104.15      | 107.42   |
| 22  | J     | 60   | CHD  | C2-C1-C10   | 3.57  | 118.77      | 112.74   |
| 22  | B     | 1086 | CHD  | C14-C13-C12 | -3.56 | 104.16      | 107.42   |
| 22  | O     | 229  | CHD  | C5-C4-C3    | 3.55  | 118.06      | 112.71   |
| 22  | O     | 229  | CHD  | C5-C6-C7    | 3.54  | 118.61      | 114.40   |
| 22  | O     | 229  | CHD  | C15-C14-C8  | -3.54 | 113.51      | 118.36   |
| 25  | C     | 265  | PEK  | P-O11-C03   | 3.54  | 141.61      | 121.35   |
| 23  | P     | 1272 | DMU  | O5-C6-O16   | 3.50  | 118.32      | 110.04   |
| 18  | A     | 524  | PGV  | C02-O01-C1  | 3.49  | 126.14      | 117.80   |
| 22  | P     | 1271 | CHD  | C5-C4-C3    | 3.48  | 117.96      | 112.71   |
| 22  | O     | 229  | CHD  | C16-C17-C13 | -3.48 | 100.17      | 103.54   |
| 22  | W     | 1060 | CHD  | C5-C4-C3    | 3.48  | 117.96      | 112.71   |
| 25  | P     | 1265 | PEK  | P-O11-C03   | 3.46  | 141.16      | 121.35   |
| 20  | L     | 522  | TGL  | C11-C10-CB9 | 3.43  | 131.71      | 114.37   |
| 22  | C     | 525  | CHD  | C15-C14-C8  | -3.42 | 113.67      | 118.36   |
| 22  | C     | 271  | CHD  | C18-C13-C14 | -3.41 | 105.85      | 111.20   |
| 20  | Q     | 1523 | TGL  | CG3-OG3-CC1 | 3.40  | 129.54      | 117.12   |
| 22  | J     | 60   | CHD  | C19-C10-C9  | -3.39 | 106.62      | 111.18   |
| 26  | P     | 1270 | CDL  | PA1-OA5-CA3 | 3.36  | 140.59      | 121.35   |
| 20  | D     | 523  | TGL  | OG1-CG1-CG2 | 3.32  | 117.97      | 108.40   |
| 22  | J     | 60   | CHD  | C11-C9-C10  | 3.31  | 117.07      | 113.70   |
| 22  | B     | 1086 | CHD  | C1-C2-C3    | 3.29  | 114.84      | 110.48   |
| 22  | B     | 1086 | CHD  | C15-C14-C13 | -3.29 | 100.35      | 103.54   |
| 22  | J     | 60   | CHD  | C5-C4-C3    | 3.26  | 117.62      | 112.71   |
| 18  | Z     | 1524 | PGV  | C02-O01-C1  | 3.25  | 125.58      | 117.80   |
| 22  | P     | 1271 | CHD  | C5-C6-C7    | 3.22  | 118.23      | 114.40   |
| 22  | B     | 1086 | CHD  | O3-C3-C4    | -3.22 | 103.44      | 109.84   |
| 17  | N     | 516  | HEA  | C3C-C4C-NC  | 3.21  | 112.50      | 109.80   |
| 26  | C     | 270  | CDL  | PA1-OA5-CA3 | 3.20  | 139.69      | 121.35   |
| 22  | W     | 1060 | CHD  | C11-C9-C10  | 3.20  | 116.95      | 113.70   |
| 22  | C     | 271  | CHD  | C5-C4-C3    | 3.15  | 117.46      | 112.71   |
| 22  | W     | 1060 | CHD  | C19-C10-C9  | -3.15 | 106.95      | 111.18   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | C     | 272  | DMU  | C8-C7-C5    | 3.14  | 116.34      | 110.83   |
| 23  | P     | 1272 | DMU  | C8-C7-C5    | 3.13  | 116.32      | 110.83   |
| 22  | B     | 1086 | CHD  | C1-C10-C5   | 3.12  | 112.22      | 107.75   |
| 20  | Q     | 1523 | TGL  | CG1-OG1-CA1 | -3.06 | 105.94      | 117.12   |
| 22  | B     | 1086 | CHD  | C19-C10-C1  | -3.04 | 103.47      | 108.31   |
| 23  | Z     | 1526 | DMU  | C2-C3-C4    | -3.03 | 104.21      | 110.93   |
| 22  | P     | 1525 | CHD  | C14-C8-C9   | -3.01 | 105.55      | 109.75   |
| 22  | O     | 229  | CHD  | C1-C10-C5   | 3.00  | 112.06      | 107.75   |
| 26  | G     | 269  | CDL  | C22-C21-C20 | 3.00  | 129.53      | 114.37   |
| 22  | P     | 1271 | CHD  | C18-C13-C14 | -2.99 | 106.52      | 111.20   |
| 22  | P     | 1525 | CHD  | C14-C13-C12 | -2.99 | 104.68      | 107.42   |
| 23  | Z     | 1526 | DMU  | O7-C10-O1   | 2.99  | 118.55      | 110.69   |
| 22  | J     | 60   | CHD  | C1-C2-C3    | 2.98  | 114.43      | 110.48   |
| 26  | T     | 1269 | CDL  | C22-C21-C20 | 2.98  | 129.44      | 114.37   |
| 20  | L     | 522  | TGL  | CG2-OG2-CB1 | 2.95  | 124.85      | 117.80   |
| 17  | A     | 515  | HEA  | C27-C19-C18 | -2.95 | 116.06      | 123.63   |
| 22  | C     | 271  | CHD  | C6-C5-C10   | 2.95  | 115.80      | 112.66   |
| 22  | W     | 1060 | CHD  | C16-C15-C14 | 2.94  | 110.89      | 105.14   |
| 22  | B     | 1086 | CHD  | C10-C9-C8   | 2.94  | 115.11      | 111.84   |
| 23  | Z     | 1526 | DMU  | C10-O7-C3   | 2.93  | 124.93      | 117.98   |
| 17  | N     | 515  | HEA  | C27-C19-C18 | -2.92 | 116.14      | 123.63   |
| 22  | W     | 1060 | CHD  | C14-C13-C12 | 2.89  | 110.06      | 107.42   |
| 22  | C     | 525  | CHD  | C2-C1-C10   | 2.89  | 117.62      | 112.74   |
| 22  | P     | 1271 | CHD  | C6-C5-C10   | 2.89  | 115.74      | 112.66   |
| 22  | C     | 271  | CHD  | C5-C6-C7    | 2.89  | 117.84      | 114.40   |
| 22  | J     | 60   | CHD  | C16-C15-C14 | 2.89  | 110.80      | 105.14   |
| 23  | P     | 1272 | DMU  | O1-C10-C5   | 2.88  | 116.29      | 110.37   |
| 20  | N     | 1522 | TGL  | CG2-OG2-CB1 | 2.88  | 124.68      | 117.80   |
| 22  | W     | 1060 | CHD  | C1-C2-C3    | 2.87  | 114.29      | 110.48   |
| 20  | D     | 523  | TGL  | CG1-OG1-CA1 | -2.87 | 106.63      | 117.12   |
| 17  | N     | 516  | HEA  | C27-C19-C20 | 2.86  | 120.20      | 115.23   |
| 22  | J     | 60   | CHD  | C15-C16-C17 | 2.86  | 110.75      | 105.14   |
| 26  | C     | 270  | CDL  | OB6-CB5-C51 | -2.86 | 105.29      | 111.48   |
| 22  | J     | 60   | CHD  | C14-C13-C12 | 2.85  | 110.02      | 107.42   |
| 20  | Q     | 1523 | TGL  | OG2-CG2-CG3 | 2.84  | 118.52      | 108.34   |
| 20  | Q     | 1523 | TGL  | OG1-CG1-CG2 | 2.83  | 116.56      | 108.40   |
| 22  | J     | 60   | CHD  | C4-C5-C10   | 2.83  | 115.67      | 112.66   |
| 20  | B     | 521  | TGL  | CG3-CG2-CG1 | 2.82  | 118.36      | 111.78   |
| 23  | M     | 526  | DMU  | C2-C3-C4    | -2.81 | 104.71      | 110.93   |
| 21  | B     | 230  | PSC  | C01-O03-C19 | -2.80 | 106.89      | 117.12   |
| 22  | P     | 1525 | CHD  | C5-C6-C7    | 2.79  | 117.72      | 114.40   |
| 22  | C     | 525  | CHD  | C10-C9-C8   | 2.79  | 114.95      | 111.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | T     | 1269 | CDL  | C23-C22-C21 | 2.79  | 128.48      | 114.37   |
| 22  | C     | 525  | CHD  | C5-C6-C7    | 2.78  | 117.71      | 114.40   |
| 22  | W     | 1060 | CHD  | C15-C16-C17 | 2.78  | 110.59      | 105.14   |
| 17  | A     | 515  | HEA  | C12-C11-C3B | 2.78  | 116.47      | 112.12   |
| 22  | C     | 271  | CHD  | C15-C16-C17 | 2.78  | 110.58      | 105.14   |
| 22  | W     | 1060 | CHD  | C4-C5-C10   | 2.75  | 115.59      | 112.66   |
| 17  | A     | 516  | HEA  | C27-C19-C20 | 2.75  | 120.00      | 115.23   |
| 22  | P     | 1271 | CHD  | C15-C16-C17 | 2.74  | 110.51      | 105.14   |
| 21  | O     | 1230 | PSC  | C01-O03-C19 | -2.74 | 107.11      | 117.12   |
| 26  | G     | 269  | CDL  | C23-C22-C21 | 2.73  | 128.19      | 114.37   |
| 17  | N     | 515  | HEA  | C17-C18-C19 | -2.71 | 121.42      | 127.62   |
| 22  | C     | 271  | CHD  | O12-C12-C13 | 2.71  | 115.59      | 111.02   |
| 20  | L     | 522  | TGL  | CC4-CC3-CC2 | 2.70  | 123.07      | 113.13   |
| 18  | P     | 1267 | PGV  | C9-C10-C11  | -2.70 | 97.48       | 112.60   |
| 20  | D     | 523  | TGL  | CB3-CB2-CB1 | 2.70  | 123.59      | 113.69   |
| 22  | C     | 271  | CHD  | C16-C15-C14 | 2.70  | 110.42      | 105.14   |
| 22  | O     | 229  | CHD  | C15-C14-C13 | -2.70 | 100.93      | 103.54   |
| 23  | C     | 272  | DMU  | C10-O7-C3   | 2.69  | 124.36      | 117.98   |
| 22  | P     | 1525 | CHD  | C1-C2-C3    | 2.69  | 114.05      | 110.48   |
| 23  | P     | 1272 | DMU  | C10-O7-C3   | 2.69  | 124.34      | 117.98   |
| 22  | C     | 525  | CHD  | C14-C8-C9   | -2.68 | 106.00      | 109.75   |
| 20  | N     | 1522 | TGL  | C10-CB9-CB8 | 2.68  | 127.89      | 114.37   |
| 25  | C     | 265  | PEK  | C24-C23-C22 | 2.68  | 122.96      | 113.13   |
| 17  | A     | 516  | HEA  | CMB-C2B-C3B | -2.67 | 125.11      | 130.28   |
| 25  | P     | 1264 | PEK  | C3-C2-C1    | -2.67 | 103.91      | 113.69   |
| 18  | C     | 267  | PGV  | C9-C10-C11  | -2.67 | 97.65       | 112.60   |
| 23  | C     | 272  | DMU  | O1-C10-C5   | 2.67  | 115.85      | 110.37   |
| 25  | C     | 265  | PEK  | C11-C10-C9  | 2.65  | 125.05      | 112.02   |
| 25  | P     | 1265 | PEK  | C11-C10-C9  | 2.64  | 125.04      | 112.02   |
| 20  | L     | 522  | TGL  | C10-CB9-CB8 | 2.64  | 127.72      | 114.37   |
| 20  | N     | 1522 | TGL  | CC4-CC3-CC2 | 2.64  | 122.82      | 113.13   |
| 25  | C     | 264  | PEK  | O03-C21-C22 | -2.64 | 103.80      | 111.83   |
| 20  | N     | 1521 | TGL  | CG3-CG2-CG1 | 2.62  | 117.90      | 111.78   |
| 17  | N     | 516  | HEA  | CHA-C4D-C3D | -2.62 | 120.95      | 124.77   |
| 26  | C     | 270  | CDL  | OB6-CB5-OB7 | 2.60  | 129.78      | 123.70   |
| 26  | C     | 270  | CDL  | OA8-CA6-CA4 | 2.59  | 115.88      | 108.40   |
| 22  | O     | 229  | CHD  | C19-C10-C1  | -2.59 | 104.19      | 108.31   |
| 18  | P     | 1268 | PGV  | O03-C01-C02 | 2.59  | 115.86      | 108.40   |
| 26  | G     | 269  | CDL  | C20-C19-C18 | 2.58  | 127.43      | 114.37   |
| 22  | O     | 229  | CHD  | C1-C2-C3    | 2.57  | 113.89      | 110.48   |
| 25  | P     | 1265 | PEK  | P-O12-C04   | 2.57  | 133.48      | 121.26   |
| 22  | P     | 1271 | CHD  | C16-C15-C14 | 2.56  | 110.16      | 105.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | C     | 525  | CHD  | C16-C17-C13 | -2.56 | 101.06      | 103.54   |
| 18  | C     | 268  | PGV  | O03-C01-C02 | 2.55  | 115.75      | 108.40   |
| 22  | C     | 271  | CHD  | C1-C2-C3    | 2.55  | 113.86      | 110.48   |
| 20  | N     | 1522 | TGL  | C13-C12-C11 | 2.55  | 127.24      | 114.37   |
| 22  | O     | 229  | CHD  | O3-C3-C4    | -2.54 | 104.79      | 109.84   |
| 25  | P     | 1264 | PEK  | O03-C21-C22 | -2.53 | 104.12      | 111.83   |
| 22  | P     | 1271 | CHD  | C1-C2-C3    | 2.52  | 113.83      | 110.48   |
| 20  | D     | 523  | TGL  | OG2-CG2-CG3 | 2.51  | 117.36      | 108.34   |
| 22  | J     | 60   | CHD  | C14-C8-C7   | 2.51  | 115.19      | 111.85   |
| 22  | P     | 1525 | CHD  | C1-C10-C5   | 2.51  | 111.35      | 107.75   |
| 25  | C     | 264  | PEK  | C3-C2-C1    | -2.51 | 104.49      | 113.69   |
| 20  | B     | 521  | TGL  | CA8-CA7-CA6 | -2.51 | 101.70      | 114.37   |
| 26  | T     | 1269 | CDL  | C20-C19-C18 | 2.50  | 127.01      | 114.37   |
| 22  | W     | 1060 | CHD  | C14-C8-C7   | 2.49  | 115.16      | 111.85   |
| 26  | C     | 270  | CDL  | C52-C51-CB5 | -2.49 | 104.57      | 113.69   |
| 25  | C     | 265  | PEK  | P-O12-C04   | 2.48  | 133.06      | 121.26   |
| 22  | B     | 1086 | CHD  | C9-C11-C12  | 2.48  | 117.53      | 114.29   |
| 17  | N     | 515  | HEA  | C13-C14-C15 | -2.47 | 121.97      | 127.62   |
| 26  | P     | 1270 | CDL  | OB6-CB5-C51 | -2.47 | 106.14      | 111.48   |
| 22  | P     | 1271 | CHD  | O12-C12-C13 | 2.46  | 115.17      | 111.02   |
| 18  | N     | 1266 | PGV  | C01-O03-C19 | -2.46 | 108.14      | 117.12   |
| 25  | P     | 1265 | PEK  | C24-C23-C22 | 2.45  | 122.13      | 113.13   |
| 26  | P     | 1270 | CDL  | CB6-OB8-CB7 | -2.45 | 108.16      | 117.12   |
| 20  | Q     | 1523 | TGL  | CB3-CB2-CB1 | 2.45  | 122.67      | 113.69   |
| 17  | A     | 515  | HEA  | C13-C14-C15 | -2.45 | 122.03      | 127.62   |
| 25  | T     | 263  | PEK  | P-O12-C04   | 2.44  | 132.90      | 121.26   |
| 20  | D     | 523  | TGL  | OG2-CG2-CG1 | 2.44  | 117.08      | 108.34   |
| 22  | O     | 229  | CHD  | C14-C8-C9   | -2.44 | 106.35      | 109.75   |
| 22  | B     | 1086 | CHD  | C14-C8-C9   | -2.43 | 106.35      | 109.75   |
| 23  | M     | 526  | DMU  | O7-C10-O1   | 2.43  | 117.09      | 110.69   |
| 26  | P     | 1270 | CDL  | OA8-CA6-CA4 | 2.42  | 115.39      | 108.40   |
| 20  | N     | 1521 | TGL  | CA8-CA7-CA6 | -2.42 | 102.13      | 114.37   |
| 17  | N     | 515  | HEA  | C12-C11-C3B | 2.42  | 115.90      | 112.12   |
| 22  | B     | 1086 | CHD  | C5-C4-C3    | 2.40  | 116.32      | 112.71   |
| 22  | J     | 60   | CHD  | C19-C10-C1  | -2.39 | 104.50      | 108.31   |
| 20  | L     | 522  | TGL  | C20-CA9-CA8 | 2.38  | 126.41      | 114.37   |
| 17  | N     | 516  | HEA  | CHA-C4D-ND  | 2.38  | 126.98      | 124.42   |
| 20  | N     | 1522 | TGL  | C20-CA9-CA8 | 2.37  | 126.37      | 114.37   |
| 17  | A     | 516  | HEA  | C3C-C4C-NC  | 2.37  | 111.80      | 109.80   |
| 26  | P     | 1270 | CDL  | OB6-CB5-OB7 | 2.37  | 129.25      | 123.70   |
| 26  | P     | 1270 | CDL  | C52-C51-CB5 | -2.37 | 105.01      | 113.69   |
| 20  | D     | 523  | TGL  | CG2-OG2-CB1 | 2.37  | 123.47      | 117.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | B     | 521  | TGL  | CA3-CA2-CA1 | -2.37 | 105.02      | 113.69   |
| 20  | L     | 522  | TGL  | C13-C12-C11 | 2.37  | 126.33      | 114.37   |
| 20  | Q     | 1523 | TGL  | OG2-CG2-CG1 | 2.35  | 116.77      | 108.34   |
| 26  | C     | 270  | CDL  | CB6-OB8-CB7 | -2.35 | 108.54      | 117.12   |
| 20  | L     | 522  | TGL  | OG1-CG1-CG2 | 2.32  | 115.10      | 108.40   |
| 26  | T     | 1269 | CDL  | OB8-CB6-CB4 | 2.31  | 115.07      | 108.40   |
| 25  | P     | 1264 | PEK  | O03-C21-O04 | 2.31  | 129.41      | 123.63   |
| 20  | D     | 523  | TGL  | CB4-CB3-CB2 | 2.31  | 121.60      | 113.13   |
| 22  | C     | 525  | CHD  | C19-C10-C9  | -2.30 | 108.09      | 111.18   |
| 20  | N     | 1521 | TGL  | CG3-OG3-CC1 | 2.30  | 125.51      | 117.12   |
| 26  | T     | 1269 | CDL  | C19-C18-C17 | 2.30  | 125.97      | 114.37   |
| 18  | N     | 1266 | PGV  | O03-C01-C02 | 2.29  | 115.00      | 108.40   |
| 22  | W     | 1060 | CHD  | C18-C13-C12 | -2.29 | 106.76      | 109.06   |
| 20  | N     | 1521 | TGL  | CA3-CA2-CA1 | -2.29 | 105.31      | 113.69   |
| 20  | B     | 521  | TGL  | CG3-OG3-CC1 | 2.29  | 125.47      | 117.12   |
| 20  | Q     | 1523 | TGL  | CB4-CB3-CB2 | 2.28  | 121.50      | 113.13   |
| 25  | G     | 1263 | PEK  | P-O12-C04   | 2.27  | 132.08      | 121.26   |
| 20  | N     | 1522 | TGL  | OG1-CG1-CG2 | 2.26  | 114.91      | 108.40   |
| 20  | L     | 522  | TGL  | CC7-CC6-CC5 | 2.25  | 125.75      | 114.37   |
| 26  | G     | 269  | CDL  | C19-C18-C17 | 2.25  | 125.73      | 114.37   |
| 22  | W     | 1060 | CHD  | C19-C10-C5  | -2.23 | 106.70      | 110.44   |
| 17  | A     | 516  | HEA  | C21-C20-C19 | 2.23  | 120.58      | 113.19   |
| 17  | N     | 516  | HEA  | C21-C20-C19 | 2.23  | 120.57      | 113.19   |
| 20  | N     | 1521 | TGL  | OG2-CG2-CG3 | 2.22  | 116.32      | 108.34   |
| 18  | A     | 525  | PGV  | O01-C1-C2   | -2.22 | 106.67      | 111.48   |
| 17  | A     | 515  | HEA  | C17-C18-C19 | -2.22 | 122.54      | 127.62   |
| 22  | O     | 229  | CHD  | C9-C11-C12  | 2.21  | 117.19      | 114.29   |
| 20  | Q     | 1523 | TGL  | CG2-OG2-CB1 | 2.21  | 123.09      | 117.80   |
| 26  | G     | 269  | CDL  | OB8-CB6-CB4 | 2.21  | 114.77      | 108.40   |
| 25  | C     | 265  | PEK  | O03-C01-C02 | 2.20  | 114.75      | 108.40   |
| 25  | C     | 264  | PEK  | O03-C21-O04 | 2.20  | 129.13      | 123.63   |
| 26  | T     | 1269 | CDL  | OB8-CB7-C71 | -2.19 | 105.15      | 111.83   |
| 20  | N     | 1521 | TGL  | C10-CB9-CB8 | 2.19  | 125.42      | 114.37   |
| 22  | C     | 525  | CHD  | C1-C10-C5   | 2.19  | 110.88      | 107.75   |
| 22  | J     | 60   | CHD  | C19-C10-C5  | -2.18 | 106.79      | 110.44   |
| 18  | C     | 267  | PGV  | O01-C1-C2   | -2.18 | 106.77      | 111.48   |
| 22  | C     | 525  | CHD  | C15-C14-C13 | -2.18 | 101.43      | 103.54   |
| 25  | P     | 1265 | PEK  | O03-C01-C02 | 2.17  | 114.65      | 108.40   |
| 26  | G     | 269  | CDL  | OB8-CB7-C71 | -2.16 | 105.24      | 111.83   |
| 17  | A     | 515  | HEA  | C2D-C1D-ND  | 2.16  | 112.33      | 109.84   |
| 17  | N     | 516  | HEA  | C2D-C1D-ND  | 2.15  | 112.31      | 109.84   |
| 20  | N     | 1521 | TGL  | CA6-CA5-CA4 | -2.15 | 103.50      | 114.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | B     | 521  | TGL  | OG1-CG1-CG2 | 2.15  | 114.58      | 108.40   |
| 22  | W     | 1060 | CHD  | C19-C10-C1  | -2.14 | 104.91      | 108.31   |
| 22  | J     | 60   | CHD  | C9-C11-C12  | 2.14  | 117.09      | 114.29   |
| 18  | N     | 1266 | PGV  | O01-C1-C2   | -2.13 | 106.87      | 111.48   |
| 17  | N     | 516  | HEA  | C26-C15-C16 | 2.13  | 118.92      | 115.23   |
| 22  | P     | 1271 | CHD  | C11-C12-C13 | 2.12  | 113.42      | 111.26   |
| 22  | P     | 1525 | CHD  | C2-C1-C10   | 2.12  | 116.31      | 112.74   |
| 20  | B     | 521  | TGL  | CA6-CA5-CA4 | -2.11 | 103.69      | 114.37   |
| 20  | D     | 523  | TGL  | CA3-CA2-CA1 | -2.11 | 105.97      | 113.69   |
| 20  | B     | 521  | TGL  | C10-CB9-CB8 | 2.11  | 125.02      | 114.37   |
| 18  | A     | 524  | PGV  | P-O12-C04   | 2.11  | 133.42      | 121.35   |
| 20  | B     | 521  | TGL  | OG2-CG2-CG3 | 2.11  | 115.90      | 108.34   |
| 20  | Q     | 1523 | TGL  | CA3-CA2-CA1 | -2.09 | 106.03      | 113.69   |
| 17  | A     | 515  | HEA  | C27-C19-C20 | 2.09  | 118.86      | 115.23   |
| 18  | A     | 525  | PGV  | C01-O03-C19 | -2.09 | 109.47      | 117.12   |
| 17  | N     | 516  | HEA  | C1D-ND-C4D  | -2.08 | 102.74      | 105.21   |
| 17  | N     | 516  | HEA  | C3B-C4B-NB  | 2.08  | 112.23      | 109.84   |
| 26  | T     | 1269 | CDL  | C83-C82-C81 | 2.06  | 124.79      | 114.37   |
| 20  | B     | 521  | TGL  | CB9-CB8-CB7 | -2.06 | 103.95      | 114.37   |
| 22  | B     | 1086 | CHD  | C5-C6-C7    | 2.06  | 116.84      | 114.40   |
| 17  | N     | 515  | HEA  | C3C-C2C-C1C | -2.05 | 104.75      | 107.17   |
| 20  | N     | 1521 | TGL  | OG1-CG1-CG2 | 2.05  | 114.31      | 108.40   |
| 20  | N     | 1522 | TGL  | CC7-CC6-CC5 | 2.05  | 124.72      | 114.37   |
| 22  | C     | 271  | CHD  | C14-C8-C7   | 2.04  | 114.56      | 111.85   |
| 22  | C     | 271  | CHD  | C9-C10-C5   | 2.04  | 111.35      | 108.51   |
| 22  | W     | 1060 | CHD  | C9-C11-C12  | 2.03  | 116.95      | 114.29   |
| 26  | G     | 269  | CDL  | C80-C79-C78 | 2.03  | 124.64      | 114.37   |
| 22  | P     | 1525 | CHD  | C9-C11-C12  | 2.02  | 116.94      | 114.29   |
| 22  | B     | 1086 | CHD  | C17-C13-C14 | 2.02  | 102.14      | 100.11   |
| 22  | C     | 525  | CHD  | C1-C2-C3    | 2.01  | 113.14      | 110.48   |
| 18  | Z     | 1524 | PGV  | P-O12-C04   | 2.01  | 132.86      | 121.35   |
| 17  | N     | 515  | HEA  | C2D-C1D-ND  | 2.00  | 112.14      | 109.84   |
| 22  | P     | 1271 | CHD  | C2-C1-C10   | 2.00  | 116.12      | 112.74   |

All (42) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | C     | 271 | CHD  | C8   |
| 22  | C     | 271 | CHD  | C12  |
| 22  | C     | 271 | CHD  | C9   |
| 22  | C     | 271 | CHD  | C3   |
| 22  | C     | 271 | CHD  | C14  |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 22  | J     | 60   | CHD  | C8   |
| 22  | J     | 60   | CHD  | C12  |
| 22  | J     | 60   | CHD  | C9   |
| 22  | J     | 60   | CHD  | C14  |
| 22  | J     | 60   | CHD  | C17  |
| 22  | P     | 1271 | CHD  | C8   |
| 22  | P     | 1271 | CHD  | C12  |
| 22  | P     | 1271 | CHD  | C9   |
| 22  | P     | 1271 | CHD  | C3   |
| 22  | P     | 1271 | CHD  | C14  |
| 22  | W     | 1060 | CHD  | C8   |
| 22  | W     | 1060 | CHD  | C12  |
| 22  | W     | 1060 | CHD  | C9   |
| 22  | W     | 1060 | CHD  | C14  |
| 22  | W     | 1060 | CHD  | C17  |
| 23  | C     | 272  | DMU  | C5   |
| 23  | C     | 272  | DMU  | C6   |
| 23  | C     | 272  | DMU  | C10  |
| 23  | C     | 272  | DMU  | C4   |
| 23  | C     | 272  | DMU  | C2   |
| 23  | C     | 272  | DMU  | C9   |
| 23  | M     | 526  | DMU  | C5   |
| 23  | M     | 526  | DMU  | C6   |
| 23  | M     | 526  | DMU  | C4   |
| 23  | M     | 526  | DMU  | C2   |
| 23  | M     | 526  | DMU  | C9   |
| 23  | P     | 1272 | DMU  | C5   |
| 23  | P     | 1272 | DMU  | C6   |
| 23  | P     | 1272 | DMU  | C10  |
| 23  | P     | 1272 | DMU  | C4   |
| 23  | P     | 1272 | DMU  | C2   |
| 23  | P     | 1272 | DMU  | C9   |
| 23  | Z     | 1526 | DMU  | C5   |
| 23  | Z     | 1526 | DMU  | C6   |
| 23  | Z     | 1526 | DMU  | C4   |
| 23  | Z     | 1526 | DMU  | C2   |
| 23  | Z     | 1526 | DMU  | C9   |

All (854) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 18  | A     | 524 | PGV  | C04-O12-P-O11 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | A     | 524  | PGV  | C04-O12-P-O13   |
| 18  | A     | 524  | PGV  | C04-O12-P-O14   |
| 18  | A     | 524  | PGV  | C02-C03-O11-P   |
| 18  | A     | 524  | PGV  | C05-C04-O12-P   |
| 18  | A     | 524  | PGV  | O02-C1-O01-C02  |
| 18  | A     | 524  | PGV  | C20-C19-O03-C01 |
| 18  | C     | 268  | PGV  | C04-O12-P-O11   |
| 18  | C     | 268  | PGV  | C04-O12-P-O13   |
| 18  | C     | 268  | PGV  | C04-O12-P-O14   |
| 18  | P     | 1268 | PGV  | C04-O12-P-O11   |
| 18  | P     | 1268 | PGV  | C04-O12-P-O13   |
| 18  | P     | 1268 | PGV  | C04-O12-P-O14   |
| 18  | Z     | 1524 | PGV  | C04-O12-P-O11   |
| 18  | Z     | 1524 | PGV  | C04-O12-P-O13   |
| 18  | Z     | 1524 | PGV  | C04-O12-P-O14   |
| 18  | Z     | 1524 | PGV  | C02-C03-O11-P   |
| 18  | Z     | 1524 | PGV  | C05-C04-O12-P   |
| 18  | Z     | 1524 | PGV  | O02-C1-O01-C02  |
| 18  | Z     | 1524 | PGV  | C20-C19-O03-C01 |
| 21  | B     | 230  | PSC  | C03-O11-P-O12   |
| 21  | B     | 230  | PSC  | C03-O11-P-O14   |
| 21  | B     | 230  | PSC  | C04-O12-P-O11   |
| 21  | B     | 230  | PSC  | C04-O12-P-O14   |
| 21  | B     | 230  | PSC  | O02-C1-O01-C02  |
| 21  | O     | 1230 | PSC  | C03-O11-P-O12   |
| 21  | O     | 1230 | PSC  | C03-O11-P-O14   |
| 21  | O     | 1230 | PSC  | C04-O12-P-O11   |
| 21  | O     | 1230 | PSC  | C04-O12-P-O14   |
| 22  | J     | 60   | CHD  | C16-C17-C20-C21 |
| 22  | J     | 60   | CHD  | C16-C17-C20-C22 |
| 22  | W     | 1060 | CHD  | C16-C17-C20-C21 |
| 22  | W     | 1060 | CHD  | C16-C17-C20-C22 |
| 23  | M     | 526  | DMU  | O5-C6-O16-C18   |
| 23  | Z     | 1526 | DMU  | O5-C6-O16-C18   |
| 25  | C     | 265  | PEK  | C03-O11-P-O13   |
| 25  | C     | 265  | PEK  | C04-O12-P-O11   |
| 25  | C     | 265  | PEK  | C04-O12-P-O13   |
| 25  | C     | 265  | PEK  | C04-O12-P-O14   |
| 25  | G     | 1263 | PEK  | C03-O11-P-O12   |
| 25  | G     | 1263 | PEK  | C03-O11-P-O14   |
| 25  | G     | 1263 | PEK  | O12-C04-C05-N   |
| 25  | P     | 1265 | PEK  | C03-O11-P-O13   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | P     | 1265 | PEK  | C04-O12-P-O11   |
| 25  | P     | 1265 | PEK  | C04-O12-P-O13   |
| 25  | P     | 1265 | PEK  | C04-O12-P-O14   |
| 25  | T     | 263  | PEK  | C03-O11-P-O12   |
| 25  | T     | 263  | PEK  | C03-O11-P-O14   |
| 25  | T     | 263  | PEK  | O12-C04-C05-N   |
| 26  | C     | 270  | CDL  | CA2-C1-CB2-OB2  |
| 26  | C     | 270  | CDL  | CA2-OA2-PA1-OA3 |
| 26  | C     | 270  | CDL  | CA2-OA2-PA1-OA4 |
| 26  | C     | 270  | CDL  | CA2-OA2-PA1-OA5 |
| 26  | C     | 270  | CDL  | CA4-CA3-OA5-PA1 |
| 26  | C     | 270  | CDL  | C11-CA5-OA6-CA4 |
| 26  | C     | 270  | CDL  | CB2-OB2-PB2-OB3 |
| 26  | C     | 270  | CDL  | CB2-OB2-PB2-OB4 |
| 26  | G     | 269  | CDL  | CA2-OA2-PA1-OA3 |
| 26  | G     | 269  | CDL  | C1-CB2-OB2-PB2  |
| 26  | G     | 269  | CDL  | CB3-OB5-PB2-OB2 |
| 26  | G     | 269  | CDL  | CB3-OB5-PB2-OB3 |
| 26  | G     | 269  | CDL  | CB3-OB5-PB2-OB4 |
| 26  | G     | 269  | CDL  | OB6-CB4-CB6-OB8 |
| 26  | P     | 1270 | CDL  | CA2-C1-CB2-OB2  |
| 26  | P     | 1270 | CDL  | CA2-OA2-PA1-OA3 |
| 26  | P     | 1270 | CDL  | CA2-OA2-PA1-OA4 |
| 26  | P     | 1270 | CDL  | CA2-OA2-PA1-OA5 |
| 26  | P     | 1270 | CDL  | CA4-CA3-OA5-PA1 |
| 26  | P     | 1270 | CDL  | C11-CA5-OA6-CA4 |
| 26  | P     | 1270 | CDL  | CB2-OB2-PB2-OB3 |
| 26  | P     | 1270 | CDL  | CB2-OB2-PB2-OB4 |
| 26  | T     | 1269 | CDL  | CA2-OA2-PA1-OA3 |
| 26  | T     | 1269 | CDL  | C1-CB2-OB2-PB2  |
| 26  | T     | 1269 | CDL  | CB3-OB5-PB2-OB2 |
| 26  | T     | 1269 | CDL  | CB3-OB5-PB2-OB3 |
| 26  | T     | 1269 | CDL  | CB3-OB5-PB2-OB4 |
| 26  | T     | 1269 | CDL  | OB6-CB4-CB6-OB8 |
| 18  | A     | 524  | PGV  | O04-C19-O03-C01 |
| 18  | Z     | 1524 | PGV  | O04-C19-O03-C01 |
| 20  | D     | 523  | TGL  | OC1-CC1-OG3-CG3 |
| 20  | Q     | 1523 | TGL  | OC1-CC1-OG3-CG3 |
| 20  | B     | 521  | TGL  | OB1-CB1-OG2-CG2 |
| 20  | N     | 1521 | TGL  | OB1-CB1-OG2-CG2 |
| 21  | O     | 1230 | PSC  | O02-C1-O01-C02  |
| 26  | C     | 270  | CDL  | OA7-CA5-OA6-CA4 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | A     | 524  | PGV  | C2-C1-O01-C02   |
| 18  | Z     | 1524 | PGV  | C2-C1-O01-C02   |
| 20  | D     | 523  | TGL  | CC2-CC1-OG3-CG3 |
| 20  | Q     | 1523 | TGL  | CC2-CC1-OG3-CG3 |
| 26  | G     | 269  | CDL  | C31-CA7-OA8-CA6 |
| 26  | T     | 1269 | CDL  | C31-CA7-OA8-CA6 |
| 26  | G     | 269  | CDL  | C77-C78-C79-C80 |
| 26  | T     | 1269 | CDL  | C77-C78-C79-C80 |
| 23  | C     | 272  | DMU  | O6-C11-C9-O1    |
| 23  | P     | 1272 | DMU  | O6-C11-C9-O1    |
| 20  | B     | 521  | TGL  | OA1-CA1-OG1-CG1 |
| 20  | N     | 1521 | TGL  | OA1-CA1-OG1-CG1 |
| 20  | N     | 1522 | TGL  | OA1-CA1-OG1-CG1 |
| 26  | G     | 269  | CDL  | OA9-CA7-OA8-CA6 |
| 26  | T     | 1269 | CDL  | OA9-CA7-OA8-CA6 |
| 26  | P     | 1270 | CDL  | OA7-CA5-OA6-CA4 |
| 26  | C     | 270  | CDL  | C40-C41-C42-C43 |
| 26  | C     | 270  | CDL  | C57-C58-C59-C60 |
| 26  | C     | 270  | CDL  | C60-C61-C62-C63 |
| 26  | C     | 270  | CDL  | C80-C81-C82-C83 |
| 26  | G     | 269  | CDL  | C17-C18-C19-C20 |
| 26  | G     | 269  | CDL  | C20-C21-C22-C23 |
| 26  | G     | 269  | CDL  | C40-C41-C42-C43 |
| 26  | G     | 269  | CDL  | C57-C58-C59-C60 |
| 26  | P     | 1270 | CDL  | C40-C41-C42-C43 |
| 26  | P     | 1270 | CDL  | C60-C61-C62-C63 |
| 26  | P     | 1270 | CDL  | C80-C81-C82-C83 |
| 26  | T     | 1269 | CDL  | C20-C21-C22-C23 |
| 26  | T     | 1269 | CDL  | C57-C58-C59-C60 |
| 20  | N     | 1521 | TGL  | C16-C15-CC9-CC8 |
| 26  | C     | 270  | CDL  | C20-C21-C22-C23 |
| 26  | C     | 270  | CDL  | C77-C78-C79-C80 |
| 26  | P     | 1270 | CDL  | C20-C21-C22-C23 |
| 26  | P     | 1270 | CDL  | C57-C58-C59-C60 |
| 26  | P     | 1270 | CDL  | C77-C78-C79-C80 |
| 26  | T     | 1269 | CDL  | C17-C18-C19-C20 |
| 26  | T     | 1269 | CDL  | C40-C41-C42-C43 |
| 18  | P     | 1268 | PGV  | O12-C04-C05-O05 |
| 26  | G     | 269  | CDL  | O1-C1-CA2-OA2   |
| 26  | T     | 1269 | CDL  | O1-C1-CA2-OA2   |
| 20  | L     | 522  | TGL  | OA1-CA1-OG1-CG1 |
| 26  | T     | 1269 | CDL  | C60-C61-C62-C63 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | M     | 526  | DMU  | O6-C11-C9-C8    |
| 20  | B     | 521  | TGL  | C16-C15-CC9-CC8 |
| 20  | B     | 521  | TGL  | CB2-CB1-OG2-CG2 |
| 20  | N     | 1521 | TGL  | CB2-CB1-OG2-CG2 |
| 23  | Z     | 1526 | DMU  | O6-C11-C9-C8    |
| 26  | G     | 269  | CDL  | C80-C81-C82-C83 |
| 26  | G     | 269  | CDL  | C37-C38-C39-C40 |
| 26  | T     | 1269 | CDL  | C80-C81-C82-C83 |
| 20  | B     | 521  | TGL  | CA2-CA1-OG1-CG1 |
| 20  | N     | 1521 | TGL  | CA2-CA1-OG1-CG1 |
| 26  | G     | 269  | CDL  | C60-C61-C62-C63 |
| 26  | T     | 1269 | CDL  | C37-C38-C39-C40 |
| 20  | N     | 1522 | TGL  | C21-C20-CA9-CA8 |
| 26  | C     | 270  | CDL  | C37-C38-C39-C40 |
| 26  | P     | 1270 | CDL  | C37-C38-C39-C40 |
| 20  | L     | 522  | TGL  | C21-C20-CA9-CA8 |
| 26  | C     | 270  | CDL  | C17-C18-C19-C20 |
| 26  | P     | 1270 | CDL  | C17-C18-C19-C20 |
| 20  | N     | 1522 | TGL  | CA2-CA1-OG1-CG1 |
| 20  | D     | 523  | TGL  | C21-C20-CA9-CA8 |
| 20  | D     | 523  | TGL  | C11-C10-CB9-CB8 |
| 20  | Q     | 1523 | TGL  | C21-C20-CA9-CA8 |
| 20  | Q     | 1523 | TGL  | C16-C15-CC9-CC8 |
| 20  | B     | 521  | TGL  | C21-C20-CA9-CA8 |
| 20  | N     | 1521 | TGL  | C21-C20-CA9-CA8 |
| 20  | Q     | 1523 | TGL  | C11-C10-CB9-CB8 |
| 20  | D     | 523  | TGL  | C16-C15-CC9-CC8 |
| 20  | L     | 522  | TGL  | C16-C15-CC9-CC8 |
| 20  | N     | 1522 | TGL  | C16-C15-CC9-CC8 |
| 18  | A     | 524  | PGV  | O12-C04-C05-C06 |
| 18  | Z     | 1524 | PGV  | O12-C04-C05-C06 |
| 26  | G     | 269  | CDL  | CB2-C1-CA2-OA2  |
| 26  | T     | 1269 | CDL  | CB2-C1-CA2-OA2  |
| 20  | D     | 523  | TGL  | CA2-CA1-OG1-CG1 |
| 20  | L     | 522  | TGL  | CA2-CA1-OG1-CG1 |
| 20  | Q     | 1523 | TGL  | CA2-CA1-OG1-CG1 |
| 21  | B     | 230  | PSC  | C20-C19-O03-C01 |
| 21  | O     | 1230 | PSC  | C20-C19-O03-C01 |
| 20  | N     | 1522 | TGL  | C11-C10-CB9-CB8 |
| 20  | B     | 521  | TGL  | C11-C10-CB9-CB8 |
| 20  | L     | 522  | TGL  | C11-C10-CB9-CB8 |
| 20  | N     | 1521 | TGL  | C11-C10-CB9-CB8 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | C     | 272  | DMU  | C1-C6-O16-C18   |
| 23  | P     | 1272 | DMU  | C1-C6-O16-C18   |
| 26  | C     | 270  | CDL  | O1-C1-CB2-OB2   |
| 26  | G     | 269  | CDL  | O1-C1-CB2-OB2   |
| 26  | P     | 1270 | CDL  | O1-C1-CB2-OB2   |
| 26  | T     | 1269 | CDL  | O1-C1-CB2-OB2   |
| 22  | W     | 1060 | CHD  | C21-C20-C22-C23 |
| 23  | M     | 526  | DMU  | O5-C4-C57-O61   |
| 18  | P     | 1268 | PGV  | O05-C05-C06-O06 |
| 22  | J     | 60   | CHD  | C13-C17-C20-C22 |
| 22  | W     | 1060 | CHD  | C13-C17-C20-C22 |
| 23  | P     | 1272 | DMU  | O5-C4-C57-O61   |
| 21  | B     | 230  | PSC  | C1-C2-C3-C4     |
| 25  | C     | 265  | PEK  | C21-C22-C23-C24 |
| 25  | P     | 1265 | PEK  | C21-C22-C23-C24 |
| 23  | Z     | 1526 | DMU  | O5-C4-C57-O61   |
| 18  | Z     | 1524 | PGV  | C19-C20-C21-C22 |
| 21  | O     | 1230 | PSC  | C1-C2-C3-C4     |
| 20  | D     | 523  | TGL  | OA1-CA1-OG1-CG1 |
| 20  | Q     | 1523 | TGL  | OA1-CA1-OG1-CG1 |
| 21  | B     | 230  | PSC  | C2-C1-O01-C02   |
| 21  | O     | 1230 | PSC  | C2-C1-O01-C02   |
| 23  | C     | 272  | DMU  | O5-C4-C57-O61   |
| 18  | A     | 524  | PGV  | C19-C20-C21-C22 |
| 21  | B     | 230  | PSC  | O04-C19-O03-C01 |
| 25  | T     | 263  | PEK  | C28-C29-C30-C31 |
| 25  | G     | 1263 | PEK  | C28-C29-C30-C31 |
| 18  | C     | 268  | PGV  | O12-C04-C05-O05 |
| 21  | O     | 1230 | PSC  | O04-C19-O03-C01 |
| 22  | C     | 271  | CHD  | C21-C20-C22-C23 |
| 22  | J     | 60   | CHD  | C21-C20-C22-C23 |
| 22  | P     | 1271 | CHD  | C21-C20-C22-C23 |
| 23  | Z     | 1526 | DMU  | O16-C18-C19-C22 |
| 26  | P     | 1270 | CDL  | CB7-C71-C72-C73 |
| 21  | B     | 230  | PSC  | C20-C21-C22-C23 |
| 21  | O     | 1230 | PSC  | C20-C21-C22-C23 |
| 23  | M     | 526  | DMU  | O16-C18-C19-C22 |
| 26  | T     | 1269 | CDL  | C11-CA5-OA6-CA4 |
| 26  | C     | 270  | CDL  | CB7-C71-C72-C73 |
| 22  | P     | 1271 | CHD  | C17-C20-C22-C23 |
| 22  | W     | 1060 | CHD  | C17-C20-C22-C23 |
| 26  | G     | 269  | CDL  | OA7-CA5-OA6-CA4 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | T     | 1269 | CDL  | OA7-CA5-OA6-CA4 |
| 18  | C     | 268  | PGV  | O12-C04-C05-C06 |
| 18  | P     | 1268 | PGV  | O12-C04-C05-C06 |
| 26  | G     | 269  | CDL  | CA2-C1-CB2-OB2  |
| 26  | T     | 1269 | CDL  | CA2-C1-CB2-OB2  |
| 20  | L     | 522  | TGL  | CC3-CC4-CC5-CC6 |
| 18  | P     | 1268 | PGV  | C1-C2-C3-C4     |
| 23  | C     | 272  | DMU  | C3-C4-C57-O61   |
| 22  | C     | 271  | CHD  | C17-C20-C22-C23 |
| 22  | J     | 60   | CHD  | C17-C20-C22-C23 |
| 23  | P     | 1272 | DMU  | C3-C4-C57-O61   |
| 18  | C     | 268  | PGV  | C2-C1-O01-C02   |
| 18  | P     | 1268 | PGV  | C2-C1-O01-C02   |
| 26  | G     | 269  | CDL  | C11-CA5-OA6-CA4 |
| 22  | J     | 60   | CHD  | C13-C17-C20-C21 |
| 22  | W     | 1060 | CHD  | C13-C17-C20-C21 |
| 18  | C     | 268  | PGV  | C1-C2-C3-C4     |
| 26  | G     | 269  | CDL  | CA5-C11-C12-C13 |
| 18  | A     | 524  | PGV  | O12-C04-C05-O05 |
| 18  | Z     | 1524 | PGV  | O12-C04-C05-O05 |
| 25  | T     | 263  | PEK  | C1-C2-C3-C4     |
| 20  | N     | 1522 | TGL  | CC3-CC4-CC5-CC6 |
| 18  | C     | 268  | PGV  | C04-C05-C06-O06 |
| 18  | P     | 1268 | PGV  | C04-C05-C06-O06 |
| 21  | B     | 230  | PSC  | C22-C23-C24-C25 |
| 18  | P     | 1268 | PGV  | O02-C1-O01-C02  |
| 23  | C     | 272  | DMU  | O5-C6-O16-C18   |
| 23  | P     | 1272 | DMU  | O5-C6-O16-C18   |
| 25  | C     | 264  | PEK  | C22-C21-O03-C01 |
| 26  | T     | 1269 | CDL  | CA5-C11-C12-C13 |
| 26  | G     | 269  | CDL  | C73-C74-C75-C76 |
| 18  | A     | 525  | PGV  | C6-C7-C8-C9     |
| 21  | B     | 230  | PSC  | C2-C3-C4-C5     |
| 26  | P     | 1270 | CDL  | C51-C52-C53-C54 |
| 18  | A     | 524  | PGV  | C4-C5-C6-C7     |
| 18  | C     | 268  | PGV  | C22-C23-C24-C25 |
| 18  | N     | 1266 | PGV  | C6-C7-C8-C9     |
| 26  | C     | 270  | CDL  | C13-C14-C15-C16 |
| 18  | P     | 1268 | PGV  | C22-C23-C24-C25 |
| 18  | Z     | 1524 | PGV  | C4-C5-C6-C7     |
| 21  | O     | 1230 | PSC  | C2-C3-C4-C5     |
| 25  | P     | 1265 | PEK  | C25-C26-C27-C28 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | C     | 270  | CDL  | C51-C52-C53-C54 |
| 26  | T     | 1269 | CDL  | C73-C74-C75-C76 |
| 21  | B     | 230  | PSC  | C29-C30-C31-C32 |
| 21  | O     | 1230 | PSC  | C29-C30-C31-C32 |
| 26  | C     | 270  | CDL  | C59-C60-C61-C62 |
| 26  | P     | 1270 | CDL  | C13-C14-C15-C16 |
| 18  | C     | 268  | PGV  | O02-C1-O01-C02  |
| 18  | C     | 268  | PGV  | O05-C05-C06-O06 |
| 18  | C     | 268  | PGV  | C13-C14-C15-C16 |
| 26  | P     | 1270 | CDL  | C59-C60-C61-C62 |
| 26  | T     | 1269 | CDL  | C58-C59-C60-C61 |
| 21  | O     | 1230 | PSC  | C22-C23-C24-C25 |
| 26  | G     | 269  | CDL  | C58-C59-C60-C61 |
| 18  | P     | 1268 | PGV  | C13-C14-C15-C16 |
| 25  | C     | 265  | PEK  | C25-C26-C27-C28 |
| 25  | T     | 263  | PEK  | C29-C30-C31-C32 |
| 18  | C     | 268  | PGV  | C24-C25-C26-C27 |
| 18  | P     | 1268 | PGV  | C24-C25-C26-C27 |
| 25  | C     | 264  | PEK  | C23-C24-C25-C26 |
| 25  | C     | 264  | PEK  | C1-C2-C3-C4     |
| 25  | G     | 1263 | PEK  | C1-C2-C3-C4     |
| 25  | P     | 1264 | PEK  | C1-C2-C3-C4     |
| 23  | Z     | 1526 | DMU  | C25-C28-C31-C34 |
| 25  | G     | 1263 | PEK  | C29-C30-C31-C32 |
| 25  | P     | 1264 | PEK  | C23-C24-C25-C26 |
| 26  | C     | 270  | CDL  | C55-C56-C57-C58 |
| 26  | P     | 1270 | CDL  | C16-C17-C18-C19 |
| 26  | T     | 1269 | CDL  | C72-C73-C74-C75 |
| 20  | B     | 521  | TGL  | OC1-CC1-OG3-CG3 |
| 18  | N     | 1266 | PGV  | C29-C30-C31-C32 |
| 18  | A     | 525  | PGV  | C23-C24-C25-C26 |
| 26  | C     | 270  | CDL  | C16-C17-C18-C19 |
| 26  | G     | 269  | CDL  | C72-C73-C74-C75 |
| 26  | P     | 1270 | CDL  | CA5-C11-C12-C13 |
| 20  | N     | 1521 | TGL  | OC1-CC1-OG3-CG3 |
| 25  | P     | 1264 | PEK  | O04-C21-O03-C01 |
| 26  | P     | 1270 | CDL  | C55-C56-C57-C58 |
| 25  | P     | 1264 | PEK  | C22-C21-O03-C01 |
| 25  | C     | 264  | PEK  | O03-C01-C02-C03 |
| 25  | P     | 1264 | PEK  | O03-C01-C02-C03 |
| 18  | N     | 1266 | PGV  | C23-C24-C25-C26 |
| 23  | M     | 526  | DMU  | C25-C28-C31-C34 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | C     | 270  | CDL  | CA5-C11-C12-C13 |
| 18  | A     | 525  | PGV  | C29-C30-C31-C32 |
| 18  | C     | 268  | PGV  | C3-C4-C5-C6     |
| 18  | P     | 1268 | PGV  | C3-C4-C5-C6     |
| 20  | L     | 522  | TGL  | CB4-CB5-CB6-CB7 |
| 26  | C     | 270  | CDL  | C74-C75-C76-C77 |
| 25  | C     | 264  | PEK  | O04-C21-O03-C01 |
| 26  | G     | 269  | CDL  | C13-C14-C15-C16 |
| 26  | P     | 1270 | CDL  | C72-C73-C74-C75 |
| 21  | O     | 1230 | PSC  | C04-C05-N-C08   |
| 20  | N     | 1522 | TGL  | CB4-CB5-CB6-CB7 |
| 26  | C     | 270  | CDL  | C72-C73-C74-C75 |
| 26  | P     | 1270 | CDL  | C74-C75-C76-C77 |
| 26  | T     | 1269 | CDL  | C13-C14-C15-C16 |
| 26  | P     | 1270 | CDL  | C51-CB5-OB6-CB4 |
| 26  | G     | 269  | CDL  | C79-C80-C81-C82 |
| 26  | T     | 1269 | CDL  | C79-C80-C81-C82 |
| 18  | C     | 267  | PGV  | C7-C8-C9-C10    |
| 18  | P     | 1267 | PGV  | C7-C8-C9-C10    |
| 18  | A     | 525  | PGV  | C5-C6-C7-C8     |
| 25  | C     | 265  | PEK  | C31-C32-C33-C34 |
| 25  | T     | 263  | PEK  | C27-C28-C29-C30 |
| 18  | N     | 1266 | PGV  | C5-C6-C7-C8     |
| 25  | G     | 1263 | PEK  | C25-C26-C27-C28 |
| 25  | G     | 1263 | PEK  | C27-C28-C29-C30 |
| 26  | P     | 1270 | CDL  | C73-C74-C75-C76 |
| 25  | P     | 1265 | PEK  | C31-C32-C33-C34 |
| 25  | T     | 263  | PEK  | C25-C26-C27-C28 |
| 26  | C     | 270  | CDL  | C73-C74-C75-C76 |
| 18  | C     | 268  | PGV  | C27-C28-C29-C30 |
| 18  | P     | 1268 | PGV  | C27-C28-C29-C30 |
| 26  | T     | 1269 | CDL  | C56-C57-C58-C59 |
| 18  | C     | 267  | PGV  | C22-C23-C24-C25 |
| 26  | G     | 269  | CDL  | C56-C57-C58-C59 |
| 18  | P     | 1267 | PGV  | C22-C23-C24-C25 |
| 25  | P     | 1265 | PEK  | C16-C17-C18-C19 |
| 26  | C     | 270  | CDL  | C51-CB5-OB6-CB4 |
| 26  | C     | 270  | CDL  | OB7-CB5-OB6-CB4 |
| 26  | P     | 1270 | CDL  | OB7-CB5-OB6-CB4 |
| 26  | C     | 270  | CDL  | C36-C37-C38-C39 |
| 21  | B     | 230  | PSC  | C13-C14-C15-C16 |
| 21  | O     | 1230 | PSC  | C13-C14-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | Z     | 1524 | PGV  | C24-C25-C26-C27 |
| 26  | P     | 1270 | CDL  | C36-C37-C38-C39 |
| 18  | A     | 524  | PGV  | C24-C25-C26-C27 |
| 25  | C     | 265  | PEK  | C16-C17-C18-C19 |
| 18  | A     | 524  | PGV  | C22-C23-C24-C25 |
| 18  | Z     | 1524 | PGV  | C28-C29-C30-C31 |
| 21  | B     | 230  | PSC  | C04-C05-N-C08   |
| 18  | N     | 1266 | PGV  | C7-C8-C9-C10    |
| 26  | P     | 1270 | CDL  | C75-C76-C77-C78 |
| 18  | A     | 525  | PGV  | C7-C8-C9-C10    |
| 18  | Z     | 1524 | PGV  | C22-C23-C24-C25 |
| 18  | A     | 524  | PGV  | C28-C29-C30-C31 |
| 26  | G     | 269  | CDL  | CB5-C51-C52-C53 |
| 26  | T     | 1269 | CDL  | CB5-C51-C52-C53 |
| 25  | P     | 1264 | PEK  | C22-C23-C24-C25 |
| 26  | P     | 1270 | CDL  | C11-C12-C13-C14 |
| 26  | C     | 270  | CDL  | C75-C76-C77-C78 |
| 20  | B     | 521  | TGL  | CB6-CB7-CB8-CB9 |
| 20  | N     | 1522 | TGL  | CC2-CC3-CC4-CC5 |
| 25  | C     | 264  | PEK  | C22-C23-C24-C25 |
| 25  | P     | 1264 | PEK  | C31-C32-C33-C34 |
| 18  | C     | 268  | PGV  | C12-C13-C14-C15 |
| 18  | P     | 1268 | PGV  | C12-C13-C14-C15 |
| 25  | G     | 1263 | PEK  | O03-C01-C02-O01 |
| 25  | T     | 263  | PEK  | O03-C01-C02-O01 |
| 20  | N     | 1522 | TGL  | CC2-CC1-OG3-CG3 |
| 25  | C     | 264  | PEK  | C31-C32-C33-C34 |
| 25  | P     | 1264 | PEK  | C16-C17-C18-C19 |
| 25  | T     | 263  | PEK  | C26-C27-C28-C29 |
| 26  | T     | 1269 | CDL  | C43-C44-C45-C46 |
| 23  | C     | 272  | DMU  | C25-C28-C31-C34 |
| 25  | G     | 1263 | PEK  | C26-C27-C28-C29 |
| 26  | G     | 269  | CDL  | C43-C44-C45-C46 |
| 20  | L     | 522  | TGL  | CC2-CC3-CC4-CC5 |
| 23  | P     | 1272 | DMU  | C25-C28-C31-C34 |
| 25  | C     | 264  | PEK  | C16-C17-C18-C19 |
| 17  | A     | 515  | HEA  | C21-C22-C23-C25 |
| 26  | C     | 270  | CDL  | C11-C12-C13-C14 |
| 26  | C     | 270  | CDL  | C18-C19-C20-C21 |
| 26  | C     | 270  | CDL  | C71-C72-C73-C74 |
| 26  | P     | 1270 | CDL  | C71-C72-C73-C74 |
| 26  | P     | 1270 | CDL  | C18-C19-C20-C21 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | P     | 1267 | PGV  | C25-C26-C27-C28 |
| 18  | A     | 524  | PGV  | C5-C6-C7-C8     |
| 21  | B     | 230  | PSC  | C24-C25-C26-C27 |
| 26  | G     | 269  | CDL  | C53-C54-C55-C56 |
| 18  | C     | 267  | PGV  | C25-C26-C27-C28 |
| 21  | O     | 1230 | PSC  | C24-C25-C26-C27 |
| 23  | Z     | 1526 | DMU  | C3-C4-C57-O61   |
| 25  | C     | 264  | PEK  | C35-C36-C37-C38 |
| 18  | C     | 268  | PGV  | C25-C26-C27-C28 |
| 18  | A     | 524  | PGV  | C12-C13-C14-C15 |
| 18  | C     | 268  | PGV  | C11-C10-C9-C8   |
| 18  | P     | 1268 | PGV  | C11-C10-C9-C8   |
| 25  | G     | 1263 | PEK  | C2-C3-C4-C5     |
| 25  | G     | 1263 | PEK  | C15-C16-C17-C18 |
| 26  | P     | 1270 | CDL  | C64-C65-C66-C67 |
| 18  | P     | 1268 | PGV  | C25-C26-C27-C28 |
| 25  | G     | 1263 | PEK  | C01-C02-C03-O11 |
| 25  | T     | 263  | PEK  | C01-C02-C03-O11 |
| 26  | C     | 270  | CDL  | OB5-CB3-CB4-CB6 |
| 26  | P     | 1270 | CDL  | OB5-CB3-CB4-CB6 |
| 26  | T     | 1269 | CDL  | OA5-CA3-CA4-CA6 |
| 26  | C     | 270  | CDL  | C64-C65-C66-C67 |
| 18  | P     | 1268 | PGV  | C28-C29-C30-C31 |
| 18  | Z     | 1524 | PGV  | C5-C6-C7-C8     |
| 26  | G     | 269  | CDL  | C21-C22-C23-C24 |
| 18  | C     | 268  | PGV  | C28-C29-C30-C31 |
| 20  | N     | 1521 | TGL  | CB6-CB7-CB8-CB9 |
| 26  | T     | 1269 | CDL  | C53-C54-C55-C56 |
| 26  | T     | 1269 | CDL  | C21-C22-C23-C24 |
| 20  | B     | 521  | TGL  | CC2-CC1-OG3-CG3 |
| 20  | N     | 1521 | TGL  | CC2-CC1-OG3-CG3 |
| 25  | C     | 265  | PEK  | C29-C30-C31-C32 |
| 21  | B     | 230  | PSC  | O03-C01-C02-C03 |
| 21  | O     | 1230 | PSC  | O03-C01-C02-C03 |
| 25  | G     | 1263 | PEK  | O03-C01-C02-C03 |
| 25  | T     | 263  | PEK  | O03-C01-C02-C03 |
| 26  | C     | 270  | CDL  | CB3-CB4-CB6-OB8 |
| 26  | G     | 269  | CDL  | CB3-CB4-CB6-OB8 |
| 26  | P     | 1270 | CDL  | CB3-CB4-CB6-OB8 |
| 26  | T     | 1269 | CDL  | CB3-CB4-CB6-OB8 |
| 23  | Z     | 1526 | DMU  | C22-C25-C28-C31 |
| 26  | P     | 1270 | CDL  | C32-C33-C34-C35 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | Z     | 1524 | PGV  | C12-C13-C14-C15 |
| 25  | T     | 263  | PEK  | C2-C3-C4-C5     |
| 26  | G     | 269  | CDL  | C82-C83-C84-C85 |
| 21  | B     | 230  | PSC  | C14-C15-C16-C17 |
| 21  | O     | 1230 | PSC  | C14-C15-C16-C17 |
| 20  | L     | 522  | TGL  | CC2-CC1-OG3-CG3 |
| 21  | B     | 230  | PSC  | C27-C28-C29-C30 |
| 26  | C     | 270  | CDL  | C32-C33-C34-C35 |
| 23  | M     | 526  | DMU  | C22-C25-C28-C31 |
| 18  | P     | 1267 | PGV  | C23-C24-C25-C26 |
| 21  | O     | 1230 | PSC  | C27-C28-C29-C30 |
| 18  | C     | 267  | PGV  | C23-C24-C25-C26 |
| 26  | C     | 270  | CDL  | C61-C62-C63-C64 |
| 26  | C     | 270  | CDL  | C63-C64-C65-C66 |
| 26  | P     | 1270 | CDL  | C63-C64-C65-C66 |
| 26  | T     | 1269 | CDL  | C33-C34-C35-C36 |
| 26  | T     | 1269 | CDL  | C82-C83-C84-C85 |
| 25  | P     | 1265 | PEK  | C29-C30-C31-C32 |
| 26  | P     | 1270 | CDL  | C61-C62-C63-C64 |
| 18  | A     | 524  | PGV  | C03-C02-O01-C1  |
| 18  | Z     | 1524 | PGV  | C03-C02-O01-C1  |
| 18  | C     | 267  | PGV  | C11-C10-C9-C8   |
| 18  | P     | 1267 | PGV  | C11-C10-C9-C8   |
| 21  | O     | 1230 | PSC  | C23-C24-C25-C26 |
| 26  | G     | 269  | CDL  | C33-C34-C35-C36 |
| 21  | B     | 230  | PSC  | C23-C24-C25-C26 |
| 26  | C     | 270  | CDL  | OA5-CA3-CA4-OA6 |
| 26  | P     | 1270 | CDL  | OA5-CA3-CA4-OA6 |
| 25  | G     | 1263 | PEK  | C22-C21-O03-C01 |
| 18  | C     | 267  | PGV  | C15-C16-C17-C18 |
| 18  | C     | 268  | PGV  | C30-C31-C32-C33 |
| 18  | P     | 1268 | PGV  | C30-C31-C32-C33 |
| 18  | P     | 1267 | PGV  | C15-C16-C17-C18 |
| 18  | P     | 1267 | PGV  | C13-C14-C15-C16 |
| 25  | P     | 1265 | PEK  | C32-C33-C34-C35 |
| 21  | B     | 230  | PSC  | O03-C01-C02-O01 |
| 18  | C     | 268  | PGV  | C31-C32-C33-C34 |
| 18  | C     | 267  | PGV  | C13-C14-C15-C16 |
| 21  | O     | 1230 | PSC  | C04-C05-N-C07   |
| 18  | C     | 268  | PGV  | C14-C15-C16-C17 |
| 23  | C     | 272  | DMU  | C34-C37-C40-C43 |
| 23  | P     | 1272 | DMU  | C34-C37-C40-C43 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | G     | 269  | CDL  | C52-C53-C54-C55 |
| 26  | P     | 1270 | CDL  | C44-C45-C46-C47 |
| 18  | P     | 1268 | PGV  | C14-C15-C16-C17 |
| 25  | C     | 265  | PEK  | C32-C33-C34-C35 |
| 25  | G     | 1263 | PEK  | C16-C17-C18-C19 |
| 25  | P     | 1264 | PEK  | C24-C25-C26-C27 |
| 18  | P     | 1268 | PGV  | C31-C32-C33-C34 |
| 26  | C     | 270  | CDL  | C44-C45-C46-C47 |
| 26  | C     | 270  | CDL  | C84-C85-C86-C87 |
| 26  | P     | 1270 | CDL  | C84-C85-C86-C87 |
| 18  | C     | 268  | PGV  | C26-C27-C28-C29 |
| 26  | T     | 1269 | CDL  | C52-C53-C54-C55 |
| 17  | N     | 515  | HEA  | C21-C22-C23-C25 |
| 25  | T     | 263  | PEK  | C22-C21-O03-C01 |
| 26  | C     | 270  | CDL  | C38-C39-C40-C41 |
| 26  | G     | 269  | CDL  | C35-C36-C37-C38 |
| 26  | T     | 1269 | CDL  | C35-C36-C37-C38 |
| 18  | P     | 1268 | PGV  | C26-C27-C28-C29 |
| 26  | P     | 1270 | CDL  | C34-C35-C36-C37 |
| 26  | P     | 1270 | CDL  | C38-C39-C40-C41 |
| 26  | P     | 1270 | CDL  | C78-C79-C80-C81 |
| 18  | P     | 1268 | PGV  | C5-C6-C7-C8     |
| 25  | T     | 263  | PEK  | C34-C35-C36-C37 |
| 26  | C     | 270  | CDL  | C34-C35-C36-C37 |
| 26  | G     | 269  | CDL  | OA5-CA3-CA4-CA6 |
| 25  | G     | 1263 | PEK  | O04-C21-O03-C01 |
| 26  | P     | 1270 | CDL  | C42-C43-C44-C45 |
| 18  | C     | 268  | PGV  | C5-C6-C7-C8     |
| 18  | N     | 1266 | PGV  | C30-C31-C32-C33 |
| 26  | G     | 269  | CDL  | C44-C45-C46-C47 |
| 26  | T     | 1269 | CDL  | C44-C45-C46-C47 |
| 25  | C     | 264  | PEK  | C25-C26-C27-C28 |
| 25  | G     | 1263 | PEK  | C34-C35-C36-C37 |
| 26  | C     | 270  | CDL  | C78-C79-C80-C81 |
| 25  | T     | 263  | PEK  | O04-C21-O03-C01 |
| 21  | B     | 230  | PSC  | C3-C4-C5-C6     |
| 18  | C     | 268  | PGV  | C20-C19-O03-C01 |
| 25  | T     | 263  | PEK  | C16-C17-C18-C19 |
| 26  | G     | 269  | CDL  | C41-C42-C43-C44 |
| 25  | P     | 1264 | PEK  | C25-C26-C27-C28 |
| 25  | C     | 264  | PEK  | C24-C25-C26-C27 |
| 26  | T     | 1269 | CDL  | C19-C20-C21-C22 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | T     | 1269 | CDL  | C71-C72-C73-C74 |
| 26  | T     | 1269 | CDL  | C31-C32-C33-C34 |
| 25  | P     | 1264 | PEK  | C17-C18-C19-C20 |
| 26  | G     | 269  | CDL  | C31-C32-C33-C34 |
| 18  | Z     | 1524 | PGV  | O03-C01-C02-C03 |
| 26  | G     | 269  | CDL  | CA3-CA4-CA6-OA8 |
| 26  | T     | 1269 | CDL  | CA3-CA4-CA6-OA8 |
| 21  | O     | 1230 | PSC  | C3-C4-C5-C6     |
| 25  | C     | 264  | PEK  | C17-C18-C19-C20 |
| 26  | C     | 270  | CDL  | C42-C43-C44-C45 |
| 26  | G     | 269  | CDL  | C71-C72-C73-C74 |
| 26  | T     | 1269 | CDL  | C41-C42-C43-C44 |
| 18  | A     | 525  | PGV  | C30-C31-C32-C33 |
| 25  | T     | 263  | PEK  | C15-C16-C17-C18 |
| 26  | C     | 270  | CDL  | C39-C40-C41-C42 |
| 26  | G     | 269  | CDL  | C19-C20-C21-C22 |
| 26  | C     | 270  | CDL  | C43-C44-C45-C46 |
| 21  | O     | 1230 | PSC  | O03-C01-C02-O01 |
| 26  | C     | 270  | CDL  | OB6-CB4-CB6-OB8 |
| 18  | C     | 268  | PGV  | O04-C19-O03-C01 |
| 25  | C     | 264  | PEK  | C5-C6-C7-C8     |
| 25  | C     | 264  | PEK  | C9-C10-C11-C12  |
| 25  | C     | 265  | PEK  | C11-C12-C13-C14 |
| 25  | G     | 1263 | PEK  | C6-C7-C8-C9     |
| 25  | P     | 1264 | PEK  | C5-C6-C7-C8     |
| 25  | P     | 1264 | PEK  | C9-C10-C11-C12  |
| 25  | P     | 1265 | PEK  | C11-C12-C13-C14 |
| 25  | T     | 263  | PEK  | C6-C7-C8-C9     |
| 26  | P     | 1270 | CDL  | C39-C40-C41-C42 |
| 23  | M     | 526  | DMU  | C3-C4-C57-O61   |
| 18  | C     | 268  | PGV  | C15-C16-C17-C18 |
| 20  | N     | 1522 | TGL  | OB1-CB1-OG2-CG2 |
| 18  | P     | 1268 | PGV  | C4-C5-C6-C7     |
| 26  | P     | 1270 | CDL  | C43-C44-C45-C46 |
| 25  | P     | 1264 | PEK  | C35-C36-C37-C38 |
| 18  | C     | 268  | PGV  | C4-C5-C6-C7     |
| 18  | A     | 524  | PGV  | C20-C21-C22-C23 |
| 18  | P     | 1268 | PGV  | C15-C16-C17-C18 |
| 18  | P     | 1268 | PGV  | C20-C19-O03-C01 |
| 18  | C     | 268  | PGV  | C23-C24-C25-C26 |
| 18  | P     | 1268 | PGV  | C23-C24-C25-C26 |
| 18  | P     | 1268 | PGV  | O04-C19-O03-C01 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | L     | 522  | TGL  | OB1-CB1-OG2-CG2 |
| 22  | C     | 271  | CHD  | C13-C17-C20-C21 |
| 26  | G     | 269  | CDL  | C14-C15-C16-C17 |
| 22  | P     | 1271 | CHD  | C13-C17-C20-C21 |
| 26  | C     | 270  | CDL  | OB5-CB3-CB4-OB6 |
| 26  | P     | 1270 | CDL  | OB5-CB3-CB4-OB6 |
| 18  | A     | 524  | PGV  | O03-C01-C02-C03 |
| 18  | P     | 1267 | PGV  | C31-C32-C33-C34 |
| 18  | C     | 267  | PGV  | C20-C21-C22-C23 |
| 18  | P     | 1267 | PGV  | C20-C21-C22-C23 |
| 25  | G     | 1263 | PEK  | C30-C31-C32-C33 |
| 25  | P     | 1264 | PEK  | C26-C27-C28-C29 |
| 26  | P     | 1270 | CDL  | OB6-CB4-CB6-OB8 |
| 25  | C     | 264  | PEK  | C26-C27-C28-C29 |
| 21  | B     | 230  | PSC  | C04-C05-N-C07   |
| 18  | A     | 525  | PGV  | C25-C26-C27-C28 |
| 25  | T     | 263  | PEK  | C30-C31-C32-C33 |
| 18  | C     | 267  | PGV  | C31-C32-C33-C34 |
| 26  | T     | 1269 | CDL  | C14-C15-C16-C17 |
| 18  | N     | 1266 | PGV  | C25-C26-C27-C28 |
| 26  | G     | 269  | CDL  | C24-C25-C26-C27 |
| 22  | C     | 271  | CHD  | C13-C17-C20-C22 |
| 20  | B     | 521  | TGL  | C12-C13-C14-C29 |
| 21  | B     | 230  | PSC  | C31-C32-C33-C34 |
| 20  | B     | 521  | TGL  | CG2-CG3-OG3-CC1 |
| 18  | Z     | 1524 | PGV  | C20-C21-C22-C23 |
| 21  | O     | 1230 | PSC  | C04-C05-N-C06   |
| 23  | P     | 1272 | DMU  | C22-C25-C28-C31 |
| 26  | T     | 1269 | CDL  | C36-C37-C38-C39 |
| 22  | P     | 1271 | CHD  | C13-C17-C20-C22 |
| 17  | N     | 515  | HEA  | C17-C18-C19-C27 |
| 21  | O     | 1230 | PSC  | C31-C32-C33-C34 |
| 25  | C     | 265  | PEK  | C30-C31-C32-C33 |
| 25  | P     | 1265 | PEK  | C30-C31-C32-C33 |
| 26  | G     | 269  | CDL  | C36-C37-C38-C39 |
| 26  | T     | 1269 | CDL  | CB4-CB3-OB5-PB2 |
| 20  | N     | 1521 | TGL  | C12-C13-C14-C29 |
| 25  | T     | 263  | PEK  | O01-C02-C03-O11 |
| 21  | B     | 230  | PSC  | C04-C05-N-C06   |
| 20  | N     | 1522 | TGL  | CC5-CC6-CC7-CC8 |
| 20  | Q     | 1523 | TGL  | CA9-C20-C21-C22 |
| 23  | C     | 272  | DMU  | C22-C25-C28-C31 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | C     | 270  | CDL  | C52-C53-C54-C55 |
| 18  | Z     | 1524 | PGV  | C26-C27-C28-C29 |
| 20  | N     | 1522 | TGL  | CC7-CC8-CC9-C15 |
| 18  | A     | 524  | PGV  | O03-C01-C02-O01 |
| 18  | Z     | 1524 | PGV  | O03-C01-C02-O01 |
| 20  | D     | 523  | TGL  | OG2-CG2-CG3-OG3 |
| 20  | Q     | 1523 | TGL  | OG2-CG2-CG3-OG3 |
| 25  | C     | 264  | PEK  | O03-C01-C02-O01 |
| 25  | P     | 1264 | PEK  | O03-C01-C02-O01 |
| 26  | G     | 269  | CDL  | OA6-CA4-CA6-OA8 |
| 26  | T     | 1269 | CDL  | OA6-CA4-CA6-OA8 |
| 18  | C     | 267  | PGV  | C24-C25-C26-C27 |
| 26  | G     | 269  | CDL  | C64-C65-C66-C67 |
| 18  | N     | 1266 | PGV  | C26-C27-C28-C29 |
| 26  | T     | 1269 | CDL  | C64-C65-C66-C67 |
| 20  | D     | 523  | TGL  | CA9-C20-C21-C22 |
| 18  | P     | 1267 | PGV  | C24-C25-C26-C27 |
| 26  | T     | 1269 | CDL  | C12-C13-C14-C15 |
| 18  | A     | 524  | PGV  | C03-O11-P-O13   |
| 18  | Z     | 1524 | PGV  | C03-O11-P-O13   |
| 21  | B     | 230  | PSC  | C03-O11-P-O13   |
| 21  | B     | 230  | PSC  | C04-O12-P-O13   |
| 21  | O     | 1230 | PSC  | C03-O11-P-O13   |
| 21  | O     | 1230 | PSC  | C04-O12-P-O13   |
| 25  | C     | 265  | PEK  | C03-O11-P-O12   |
| 25  | C     | 265  | PEK  | C03-O11-P-O14   |
| 25  | G     | 1263 | PEK  | C03-O11-P-O13   |
| 25  | P     | 1265 | PEK  | C03-O11-P-O12   |
| 25  | P     | 1265 | PEK  | C03-O11-P-O14   |
| 25  | T     | 263  | PEK  | C03-O11-P-O13   |
| 26  | C     | 270  | CDL  | CB2-OB2-PB2-OB5 |
| 26  | P     | 1270 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | C     | 264  | PEK  | C32-C33-C34-C35 |
| 22  | P     | 1271 | CHD  | C16-C17-C20-C22 |
| 18  | C     | 267  | PGV  | C02-C03-O11-P   |
| 18  | P     | 1267 | PGV  | C02-C03-O11-P   |
| 25  | G     | 1263 | PEK  | C02-C03-O11-P   |
| 25  | T     | 263  | PEK  | C02-C03-O11-P   |
| 26  | G     | 269  | CDL  | CB4-CB3-OB5-PB2 |
| 26  | C     | 270  | CDL  | C24-C25-C26-C27 |
| 26  | P     | 1270 | CDL  | C24-C25-C26-C27 |
| 26  | G     | 269  | CDL  | C12-C13-C14-C15 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | A     | 524  | PGV  | C26-C27-C28-C29 |
| 18  | A     | 525  | PGV  | C9-C10-C11-C12  |
| 18  | N     | 1266 | PGV  | C9-C10-C11-C12  |
| 20  | Q     | 1523 | TGL  | CG1-CG2-OG2-CB1 |
| 21  | B     | 230  | PSC  | C03-C02-O01-C1  |
| 21  | O     | 1230 | PSC  | C03-C02-O01-C1  |
| 20  | L     | 522  | TGL  | CC7-CC8-CC9-C15 |
| 22  | C     | 271  | CHD  | C16-C17-C20-C22 |
| 17  | N     | 515  | HEA  | C15-C16-C17-C18 |
| 26  | C     | 270  | CDL  | OA5-CA3-CA4-CA6 |
| 26  | P     | 1270 | CDL  | OA5-CA3-CA4-CA6 |
| 25  | C     | 265  | PEK  | C17-C18-C19-C20 |
| 26  | T     | 1269 | CDL  | C24-C25-C26-C27 |
| 25  | C     | 264  | PEK  | C27-C28-C29-C30 |
| 25  | P     | 1264 | PEK  | C27-C28-C29-C30 |
| 25  | G     | 1263 | PEK  | O01-C02-C03-O11 |
| 26  | T     | 1269 | CDL  | OA5-CA3-CA4-OA6 |
| 25  | P     | 1265 | PEK  | C17-C18-C19-C20 |
| 20  | N     | 1521 | TGL  | CG2-CG3-OG3-CC1 |
| 22  | P     | 1271 | CHD  | C16-C17-C20-C21 |
| 26  | P     | 1270 | CDL  | C52-C53-C54-C55 |
| 26  | G     | 269  | CDL  | C38-C39-C40-C41 |
| 25  | G     | 1263 | PEK  | C21-C22-C23-C24 |
| 25  | T     | 263  | PEK  | C21-C22-C23-C24 |
| 18  | A     | 525  | PGV  | C26-C27-C28-C29 |
| 18  | Z     | 1524 | PGV  | C11-C10-C9-C8   |
| 17  | A     | 515  | HEA  | C15-C16-C17-C18 |
| 22  | C     | 271  | CHD  | C16-C17-C20-C21 |
| 18  | A     | 524  | PGV  | C11-C10-C9-C8   |
| 21  | O     | 1230 | PSC  | C4-C5-C6-C7     |
| 26  | G     | 269  | CDL  | CB7-C71-C72-C73 |
| 20  | L     | 522  | TGL  | CC5-CC6-CC7-CC8 |
| 21  | B     | 230  | PSC  | C4-C5-C6-C7     |
| 21  | B     | 230  | PSC  | C15-C16-C17-C18 |
| 18  | P     | 1267 | PGV  | C11-C12-C13-C14 |
| 26  | G     | 269  | CDL  | C11-C12-C13-C14 |
| 26  | T     | 1269 | CDL  | C59-C60-C61-C62 |
| 25  | T     | 263  | PEK  | C32-C33-C34-C35 |
| 25  | G     | 1263 | PEK  | C32-C33-C34-C35 |
| 25  | P     | 1264 | PEK  | C32-C33-C34-C35 |
| 18  | P     | 1268 | PGV  | O03-C01-C02-O01 |
| 26  | T     | 1269 | CDL  | C38-C39-C40-C41 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | C     | 271  | CHD  | C22-C23-C24-O25 |
| 17  | A     | 516  | HEA  | CAD-CBD-CGD-O1D |
| 17  | N     | 516  | HEA  | CAD-CBD-CGD-O1D |
| 26  | T     | 1269 | CDL  | C11-C12-C13-C14 |
| 17  | N     | 516  | HEA  | CAD-CBD-CGD-O2D |
| 18  | C     | 267  | PGV  | C14-C15-C16-C17 |
| 25  | C     | 265  | PEK  | C3-C4-C5-C6     |
| 25  | P     | 1265 | PEK  | C3-C4-C5-C6     |
| 21  | O     | 1230 | PSC  | C15-C16-C17-C18 |
| 18  | P     | 1267 | PGV  | C14-C15-C16-C17 |
| 22  | P     | 1271 | CHD  | C22-C23-C24-O25 |
| 20  | D     | 523  | TGL  | CG1-CG2-OG2-CB1 |
| 26  | G     | 269  | CDL  | C59-C60-C61-C62 |
| 18  | P     | 1268 | PGV  | C7-C8-C9-C10    |
| 18  | A     | 525  | PGV  | O03-C19-C20-C21 |
| 17  | A     | 516  | HEA  | CAD-CBD-CGD-O2D |
| 22  | C     | 271  | CHD  | C22-C23-C24-O26 |
| 22  | P     | 1271 | CHD  | C22-C23-C24-O26 |
| 18  | A     | 525  | PGV  | C19-C20-C21-C22 |
| 18  | C     | 267  | PGV  | C11-C12-C13-C14 |
| 25  | C     | 264  | PEK  | C3-C4-C5-C6     |
| 18  | C     | 267  | PGV  | C05-C04-O12-P   |
| 18  | A     | 524  | PGV  | C25-C26-C27-C28 |
| 22  | B     | 1086 | CHD  | C22-C23-C24-O26 |
| 18  | P     | 1268 | PGV  | C01-C02-C03-O11 |
| 20  | N     | 1522 | TGL  | OC1-CC1-OG3-CG3 |
| 22  | O     | 229  | CHD  | C22-C23-C24-O25 |
| 18  | C     | 268  | PGV  | O03-C01-C02-O01 |
| 25  | C     | 265  | PEK  | O03-C01-C02-O01 |
| 25  | P     | 1265 | PEK  | O03-C01-C02-O01 |
| 22  | O     | 229  | CHD  | C22-C23-C24-O26 |
| 18  | C     | 268  | PGV  | C7-C8-C9-C10    |
| 21  | B     | 230  | PSC  | C9-C10-C11-C12  |
| 21  | O     | 1230 | PSC  | C9-C10-C11-C12  |
| 25  | C     | 265  | PEK  | C5-C6-C7-C8     |
| 25  | C     | 265  | PEK  | C12-C13-C14-C15 |
| 25  | P     | 1265 | PEK  | C5-C6-C7-C8     |
| 25  | P     | 1265 | PEK  | C12-C13-C14-C15 |
| 17  | A     | 516  | HEA  | CAA-CBA-CGA-O1A |
| 26  | C     | 270  | CDL  | C41-C42-C43-C44 |
| 22  | B     | 1086 | CHD  | C22-C23-C24-O25 |
| 17  | N     | 516  | HEA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | N     | 516  | HEA  | CAA-CBA-CGA-O1A |
| 26  | P     | 1270 | CDL  | C22-C23-C24-C25 |
| 18  | A     | 524  | PGV  | C7-C8-C9-C10    |
| 26  | G     | 269  | CDL  | C15-C16-C17-C18 |
| 18  | Z     | 1524 | PGV  | C7-C8-C9-C10    |
| 18  | C     | 267  | PGV  | C1-C2-C3-C4     |
| 26  | G     | 269  | CDL  | OA5-CA3-CA4-OA6 |
| 18  | N     | 1266 | PGV  | O03-C19-C20-C21 |
| 17  | A     | 516  | HEA  | CAA-CBA-CGA-O2A |
| 26  | T     | 1269 | CDL  | CB7-C71-C72-C73 |
| 21  | B     | 230  | PSC  | C11-C12-C13-C14 |
| 21  | O     | 1230 | PSC  | C11-C12-C13-C14 |
| 18  | A     | 525  | PGV  | C31-C32-C33-C34 |
| 18  | C     | 268  | PGV  | C01-C02-C03-O11 |
| 23  | Z     | 1526 | DMU  | C34-C37-C40-C43 |
| 20  | L     | 522  | TGL  | OG2-CB1-CB2-CB3 |
| 20  | N     | 1522 | TGL  | OG2-CB1-CB2-CB3 |
| 21  | O     | 1230 | PSC  | C7-C8-C9-C10    |
| 25  | P     | 1264 | PEK  | C3-C4-C5-C6     |
| 26  | T     | 1269 | CDL  | C22-C23-C24-C25 |
| 26  | C     | 270  | CDL  | C1-CA2-OA2-PA1  |
| 17  | A     | 515  | HEA  | CAD-CBD-CGD-O1D |
| 17  | N     | 516  | HEA  | C2D-C3D-CAD-CBD |
| 26  | T     | 1269 | CDL  | C39-C40-C41-C42 |
| 18  | A     | 525  | PGV  | C11-C12-C13-C14 |
| 18  | C     | 267  | PGV  | C9-C10-C11-C12  |
| 25  | G     | 1263 | PEK  | C14-C15-C16-C17 |
| 25  | T     | 263  | PEK  | C3-C4-C5-C6     |
| 18  | N     | 1266 | PGV  | C19-C20-C21-C22 |
| 26  | C     | 270  | CDL  | C22-C23-C24-C25 |
| 18  | Z     | 1524 | PGV  | C25-C26-C27-C28 |
| 26  | G     | 269  | CDL  | C22-C23-C24-C25 |
| 26  | G     | 269  | CDL  | C39-C40-C41-C42 |
| 26  | P     | 1270 | CDL  | C41-C42-C43-C44 |
| 20  | B     | 521  | TGL  | CG1-CG2-OG2-CB1 |
| 18  | N     | 1266 | PGV  | C11-C12-C13-C14 |
| 18  | P     | 1267 | PGV  | C9-C10-C11-C12  |
| 25  | G     | 1263 | PEK  | C3-C4-C5-C6     |
| 22  | C     | 525  | CHD  | C22-C23-C24-O26 |
| 20  | L     | 522  | TGL  | CB5-CB6-CB7-CB8 |
| 22  | P     | 1525 | CHD  | C22-C23-C24-O26 |
| 20  | N     | 1522 | TGL  | CB5-CB6-CB7-CB8 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 21  | B     | 230  | PSC  | C7-C8-C9-C10    |
| 21  | B     | 230  | PSC  | C12-C13-C14-C15 |
| 25  | T     | 263  | PEK  | C14-C15-C16-C17 |
| 26  | P     | 1270 | CDL  | C1-CA2-OA2-PA1  |
| 26  | P     | 1270 | CDL  | C56-C57-C58-C59 |
| 18  | N     | 1266 | PGV  | C31-C32-C33-C34 |
| 20  | Q     | 1523 | TGL  | C21-C22-C23-C24 |
| 25  | P     | 1265 | PEK  | C35-C36-C37-C38 |
| 26  | P     | 1270 | CDL  | C52-C51-CB5-OB6 |
| 17  | N     | 515  | HEA  | CAD-CBD-CGD-O1D |
| 25  | C     | 264  | PEK  | O01-C1-C2-C3    |
| 25  | P     | 1264 | PEK  | O01-C1-C2-C3    |
| 26  | C     | 270  | CDL  | C76-C77-C78-C79 |
| 21  | O     | 1230 | PSC  | C12-C13-C14-C15 |
| 18  | Z     | 1524 | PGV  | O01-C1-C2-C3    |
| 21  | B     | 230  | PSC  | O03-C19-C20-C21 |
| 21  | O     | 1230 | PSC  | O03-C19-C20-C21 |
| 20  | D     | 523  | TGL  | C21-C22-C23-C24 |
| 18  | A     | 524  | PGV  | C01-C02-C03-O11 |
| 17  | A     | 515  | HEA  | C21-C22-C23-C24 |
| 26  | T     | 1269 | CDL  | CA7-C31-C32-C33 |
| 26  | P     | 1270 | CDL  | C76-C77-C78-C79 |
| 17  | A     | 515  | HEA  | C17-C18-C19-C27 |
| 26  | P     | 1270 | CDL  | C83-C84-C85-C86 |
| 26  | C     | 270  | CDL  | C52-C51-CB5-OB6 |
| 21  | B     | 230  | PSC  | C26-C27-C28-C29 |
| 22  | P     | 1525 | CHD  | C22-C23-C24-O25 |
| 18  | Z     | 1524 | PGV  | C9-C10-C11-C12  |
| 25  | C     | 265  | PEK  | C35-C36-C37-C38 |
| 18  | A     | 524  | PGV  | O01-C1-C2-C3    |
| 26  | C     | 270  | CDL  | C56-C57-C58-C59 |
| 26  | T     | 1269 | CDL  | C15-C16-C17-C18 |
| 26  | P     | 1270 | CDL  | C32-C31-CA7-OA8 |
| 17  | A     | 516  | HEA  | C2D-C3D-CAD-CBD |
| 26  | C     | 270  | CDL  | C32-C31-CA7-OA8 |
| 22  | C     | 525  | CHD  | C22-C23-C24-O25 |
| 20  | L     | 522  | TGL  | OG3-CC1-CC2-CC3 |
| 21  | O     | 1230 | PSC  | C26-C27-C28-C29 |
| 22  | J     | 60   | CHD  | C22-C23-C24-O26 |
| 22  | W     | 1060 | CHD  | C22-C23-C24-O26 |
| 18  | P     | 1268 | PGV  | C2-C3-C4-C5     |
| 26  | P     | 1270 | CDL  | C82-C83-C84-C85 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | N     | 1522 | TGL  | OG3-CC1-CC2-CC3 |
| 22  | J     | 60   | CHD  | C22-C23-C24-O25 |
| 22  | W     | 1060 | CHD  | C22-C23-C24-O25 |
| 26  | C     | 270  | CDL  | C82-C83-C84-C85 |
| 23  | M     | 526  | DMU  | C34-C37-C40-C43 |
| 20  | D     | 523  | TGL  | OG2-CB1-CB2-CB3 |
| 23  | P     | 1272 | DMU  | C4-C3-O7-C10    |
| 17  | A     | 515  | HEA  | CAD-CBD-CGD-O2D |
| 20  | L     | 522  | TGL  | OC1-CC1-OG3-CG3 |
| 20  | Q     | 1523 | TGL  | OG2-CB1-CB2-CB3 |
| 26  | P     | 1270 | CDL  | C12-C11-CA5-OA6 |
| 18  | N     | 1266 | PGV  | C24-C25-C26-C27 |
| 20  | N     | 1521 | TGL  | CG1-CG2-OG2-CB1 |
| 18  | C     | 267  | PGV  | C29-C30-C31-C32 |
| 17  | A     | 515  | HEA  | CAA-CBA-CGA-O1A |
| 17  | N     | 515  | HEA  | CAA-CBA-CGA-O1A |
| 23  | C     | 272  | DMU  | C4-C3-O7-C10    |
| 18  | P     | 1267 | PGV  | C29-C30-C31-C32 |
| 25  | P     | 1265 | PEK  | C34-C35-C36-C37 |
| 18  | C     | 268  | PGV  | C02-C03-O11-P   |
| 18  | P     | 1267 | PGV  | C05-C04-O12-P   |
| 18  | P     | 1268 | PGV  | C02-C03-O11-P   |
| 17  | A     | 516  | HEA  | C26-C15-C16-C17 |
| 26  | C     | 270  | CDL  | C83-C84-C85-C86 |
| 26  | C     | 270  | CDL  | C19-C20-C21-C22 |
| 21  | B     | 230  | PSC  | O01-C1-C2-C3    |
| 26  | C     | 270  | CDL  | C12-C11-CA5-OA6 |
| 18  | A     | 524  | PGV  | C9-C10-C11-C12  |
| 26  | C     | 270  | CDL  | C32-C31-CA7-OA9 |
| 17  | N     | 515  | HEA  | CAD-CBD-CGD-O2D |
| 18  | A     | 524  | PGV  | O02-C1-C2-C3    |
| 25  | P     | 1264 | PEK  | O02-C1-C2-C3    |
| 26  | P     | 1270 | CDL  | C32-C31-CA7-OA9 |
| 26  | G     | 269  | CDL  | CA7-C31-C32-C33 |
| 21  | O     | 1230 | PSC  | O04-C19-C20-C21 |
| 20  | N     | 1521 | TGL  | OG1-CA1-CA2-CA3 |
| 20  | D     | 523  | TGL  | OC1-CC1-CC2-CC3 |
| 20  | Q     | 1523 | TGL  | OB1-CB1-CB2-CB3 |
| 20  | Q     | 1523 | TGL  | OC1-CC1-CC2-CC3 |
| 21  | B     | 230  | PSC  | O04-C19-C20-C21 |
| 18  | Z     | 1524 | PGV  | O02-C1-C2-C3    |
| 20  | D     | 523  | TGL  | OB1-CB1-CB2-CB3 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | C     | 264  | PEK  | O02-C1-C2-C3    |
| 20  | B     | 521  | TGL  | OG1-CA1-CA2-CA3 |
| 18  | C     | 268  | PGV  | C2-C3-C4-C5     |
| 21  | O     | 1230 | PSC  | O01-C1-C2-C3    |
| 21  | B     | 230  | PSC  | O02-C1-C2-C3    |
| 21  | O     | 1230 | PSC  | O02-C1-C2-C3    |
| 18  | P     | 1267 | PGV  | C21-C22-C23-C24 |
| 26  | P     | 1270 | CDL  | C52-C51-CB5-OB7 |
| 26  | P     | 1270 | CDL  | C19-C20-C21-C22 |
| 25  | G     | 1263 | PEK  | C33-C34-C35-C36 |
| 17  | A     | 515  | HEA  | CAA-CBA-CGA-O2A |
| 25  | T     | 263  | PEK  | C33-C34-C35-C36 |
| 17  | N     | 515  | HEA  | CAA-CBA-CGA-O2A |

There are no ring outliers.

37 monomers are involved in 252 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 18  | C     | 268  | PGV  | 1       | 0            |
| 20  | B     | 521  | TGL  | 10      | 0            |
| 23  | P     | 1272 | DMU  | 7       | 0            |
| 25  | P     | 1264 | PEK  | 6       | 0            |
| 26  | T     | 1269 | CDL  | 21      | 0            |
| 20  | L     | 522  | TGL  | 23      | 0            |
| 17  | N     | 515  | HEA  | 3       | 0            |
| 22  | J     | 60   | CHD  | 2       | 0            |
| 17  | A     | 516  | HEA  | 1       | 0            |
| 18  | P     | 1267 | PGV  | 5       | 0            |
| 20  | N     | 1521 | TGL  | 14      | 0            |
| 23  | C     | 272  | DMU  | 2       | 0            |
| 25  | G     | 1263 | PEK  | 7       | 0            |
| 18  | A     | 524  | PGV  | 6       | 0            |
| 17  | A     | 515  | HEA  | 2       | 0            |
| 18  | C     | 267  | PGV  | 7       | 0            |
| 18  | P     | 1268 | PGV  | 3       | 0            |
| 22  | O     | 229  | CHD  | 1       | 0            |
| 18  | A     | 525  | PGV  | 1       | 0            |
| 22  | W     | 1060 | CHD  | 2       | 0            |
| 21  | O     | 1230 | PSC  | 12      | 0            |
| 25  | C     | 265  | PEK  | 6       | 0            |
| 21  | B     | 230  | PSC  | 13      | 0            |
| 25  | P     | 1265 | PEK  | 6       | 0            |

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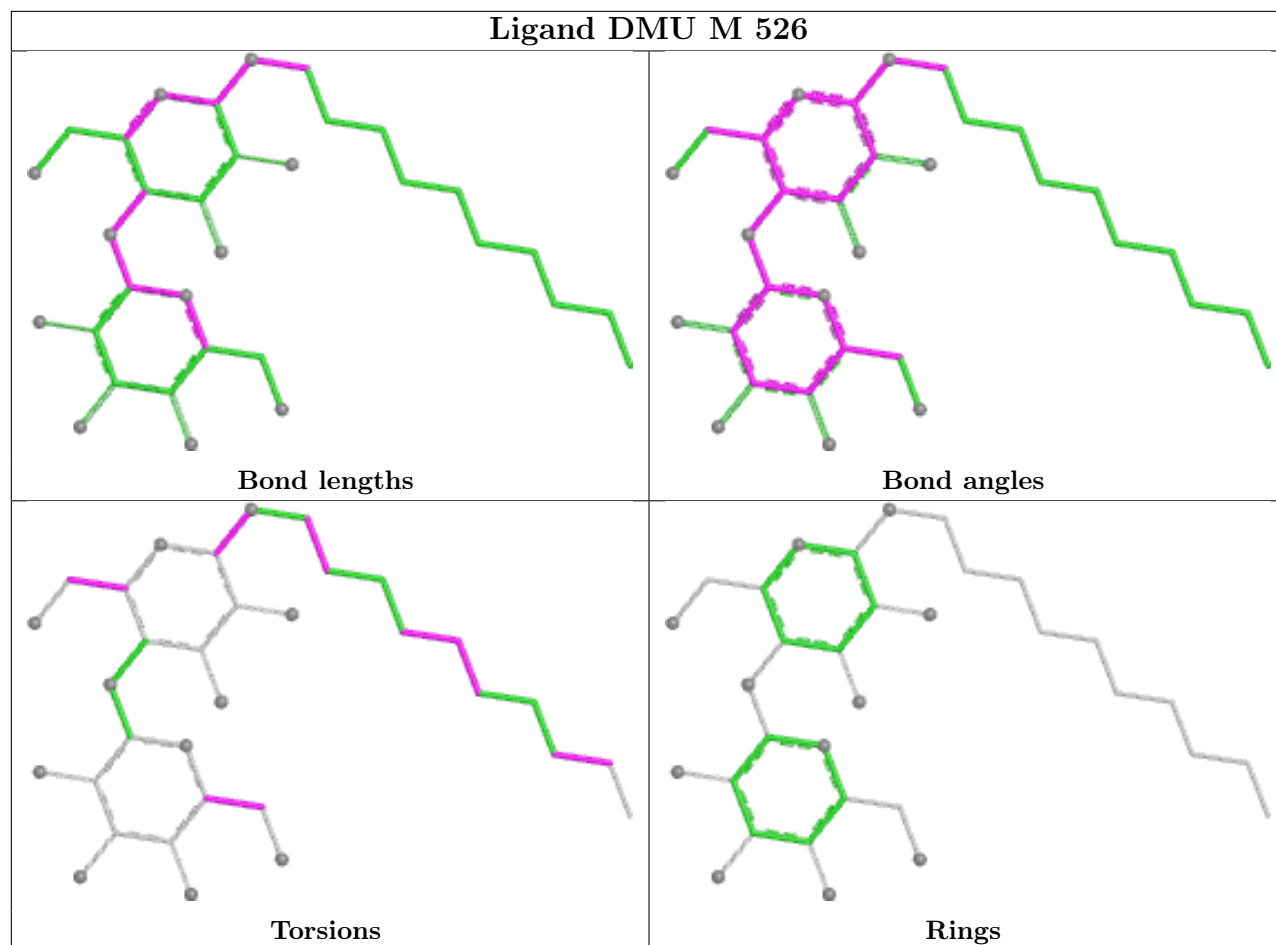
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 23  | Z     | 1526 | DMU  | 1       | 0            |
| 18  | Z     | 1524 | PGV  | 4       | 0            |
| 22  | P     | 1271 | CHD  | 2       | 0            |
| 18  | N     | 1266 | PGV  | 2       | 0            |
| 20  | N     | 1522 | TGL  | 16      | 0            |
| 25  | C     | 264  | PEK  | 5       | 0            |
| 25  | T     | 263  | PEK  | 8       | 0            |
| 26  | C     | 270  | CDL  | 17      | 0            |
| 26  | P     | 1270 | CDL  | 15      | 0            |
| 20  | D     | 523  | TGL  | 5       | 0            |
| 26  | G     | 269  | CDL  | 21      | 0            |
| 20  | Q     | 1523 | TGL  | 6       | 0            |
| 22  | C     | 271  | CHD  | 2       | 0            |

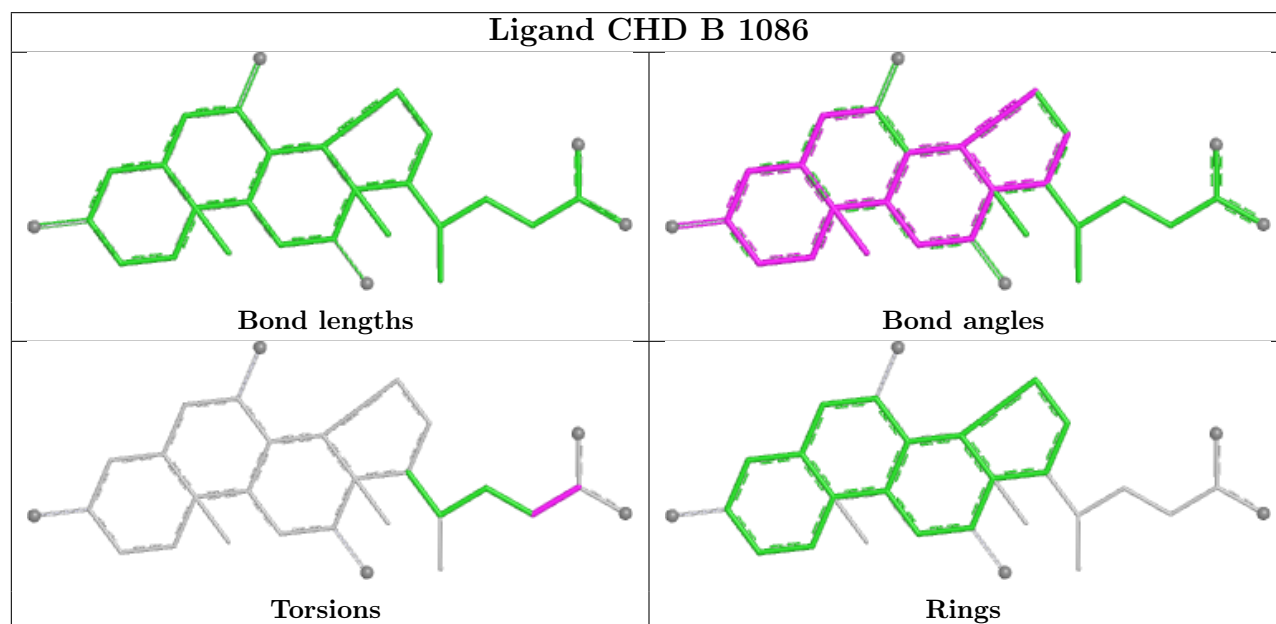
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

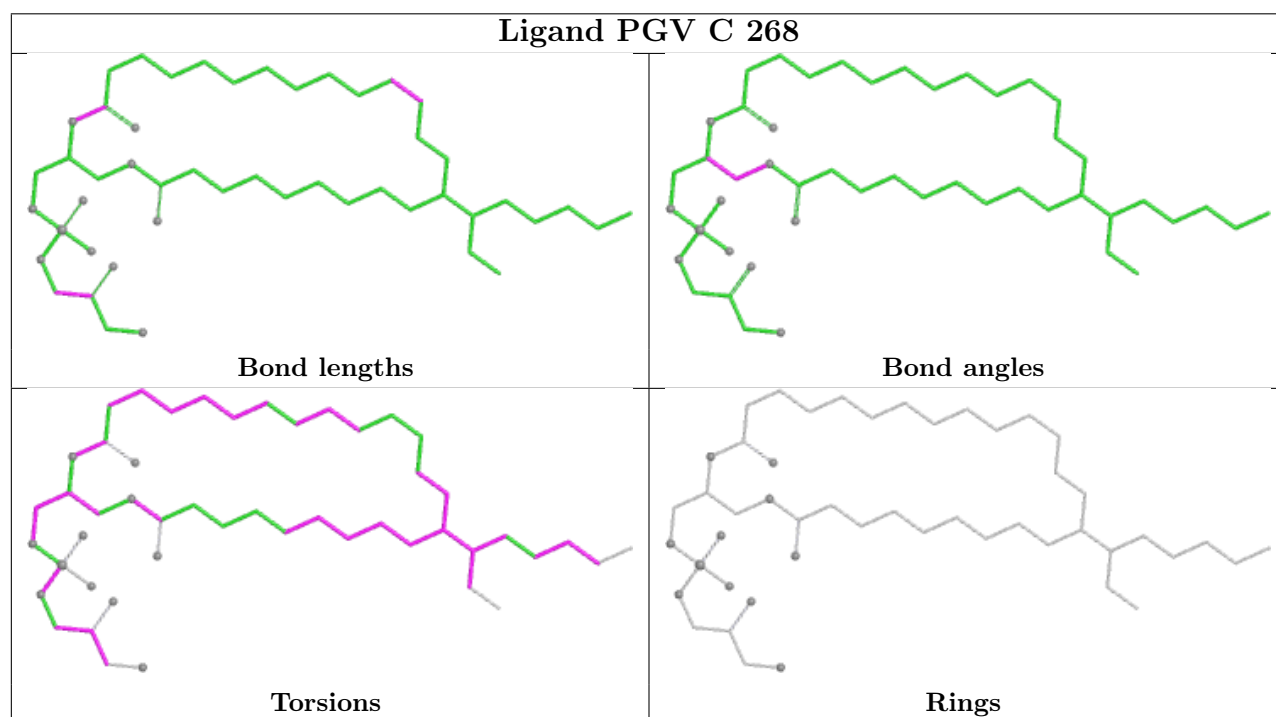
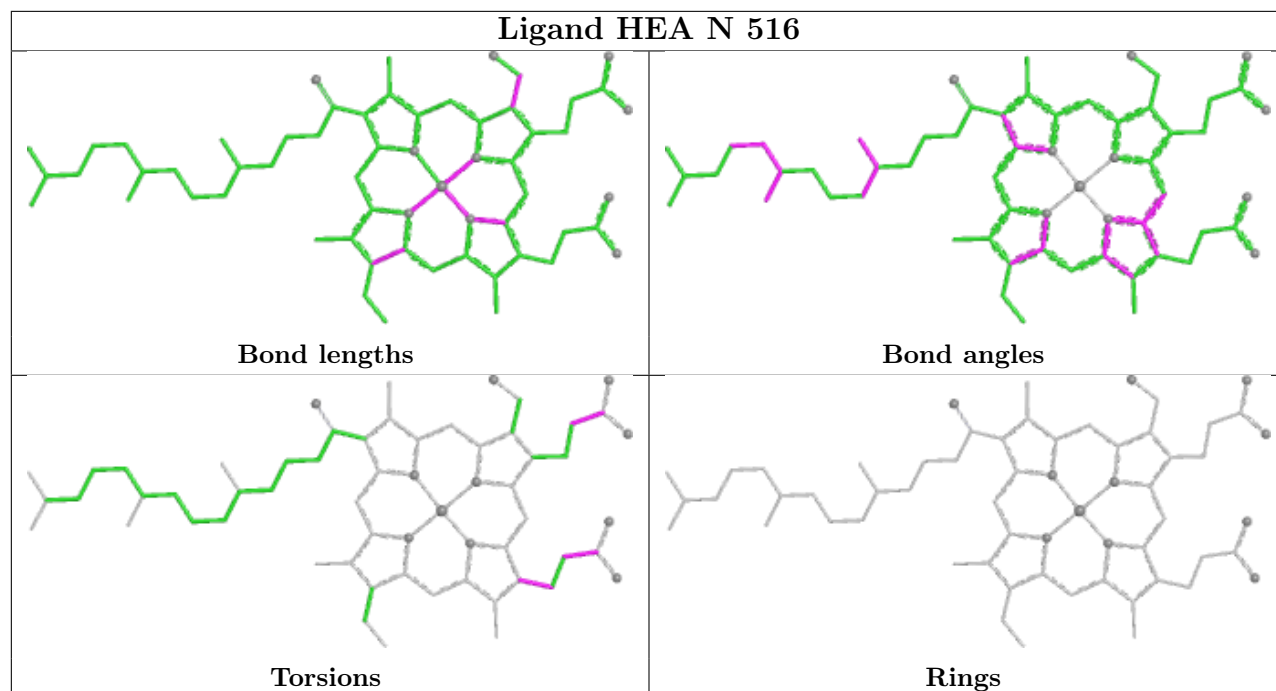


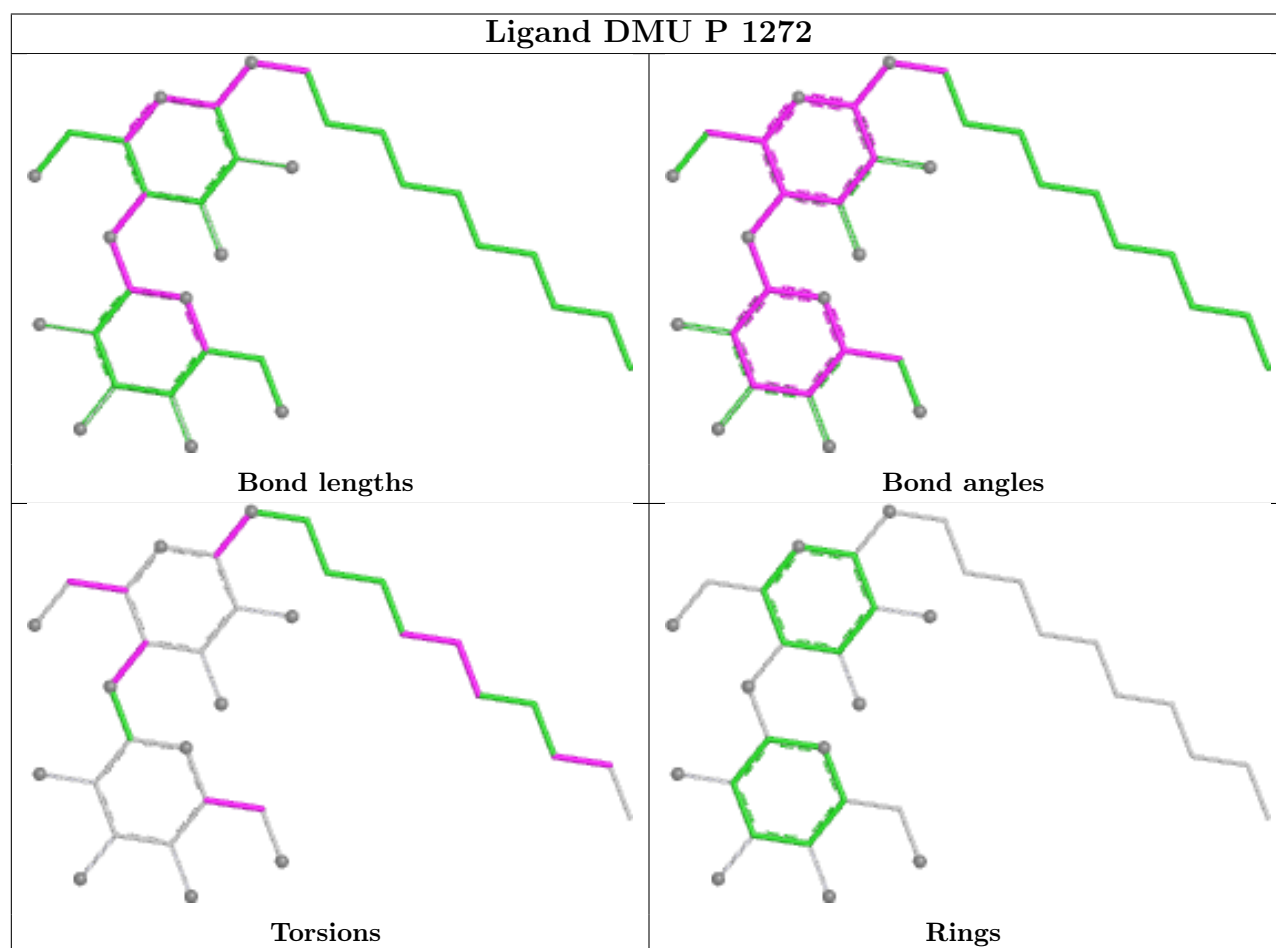
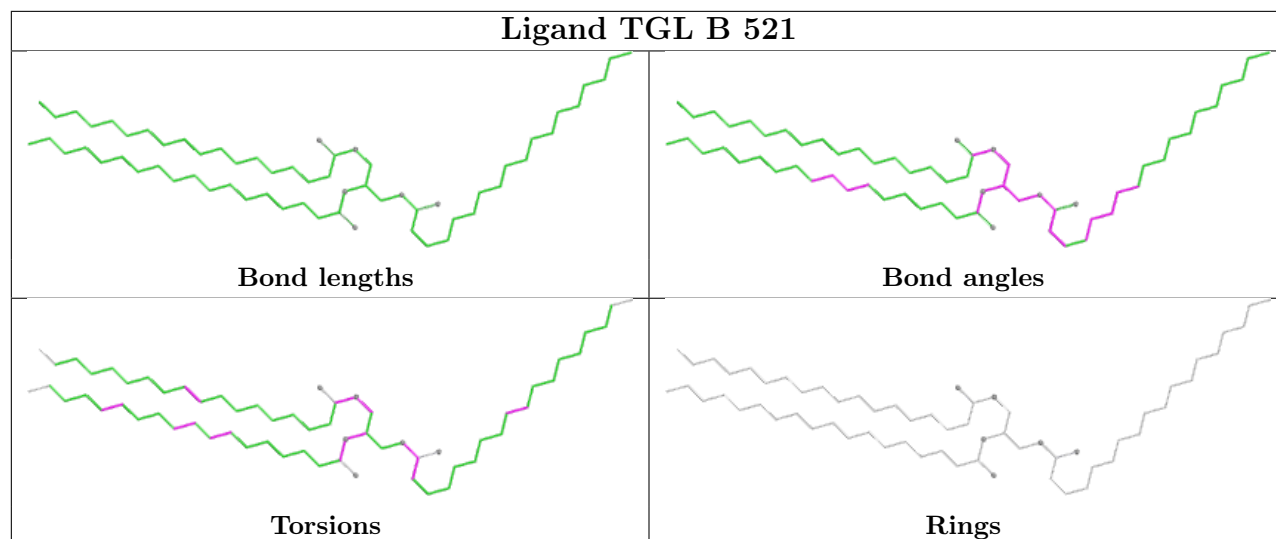
## Ligand DMU M 526

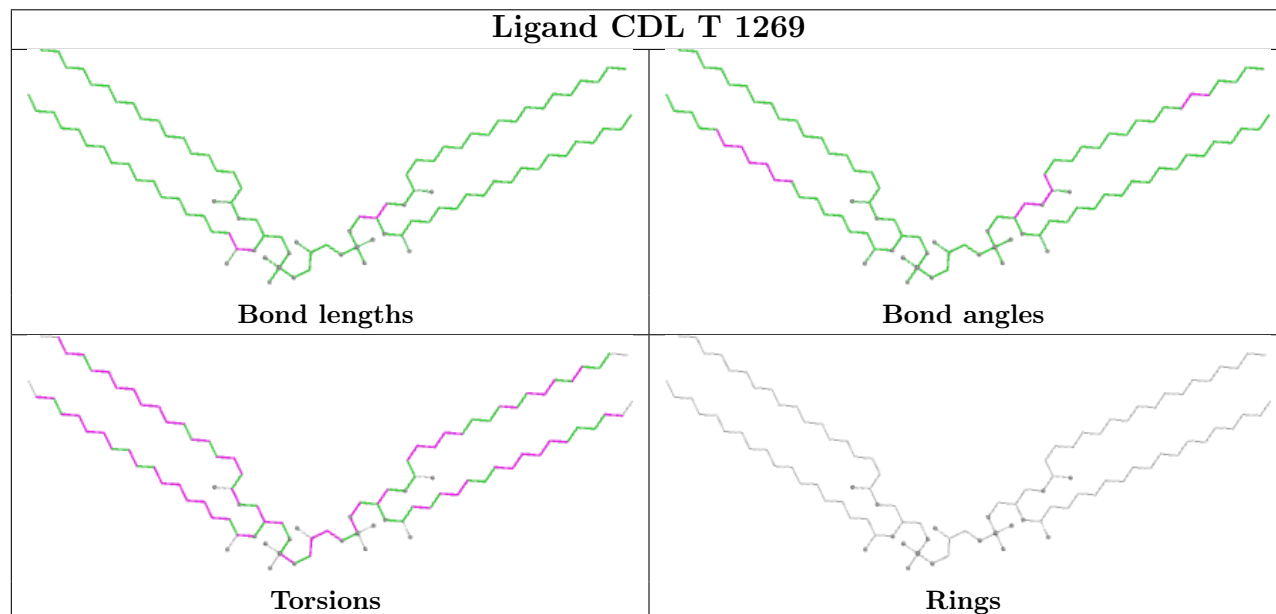
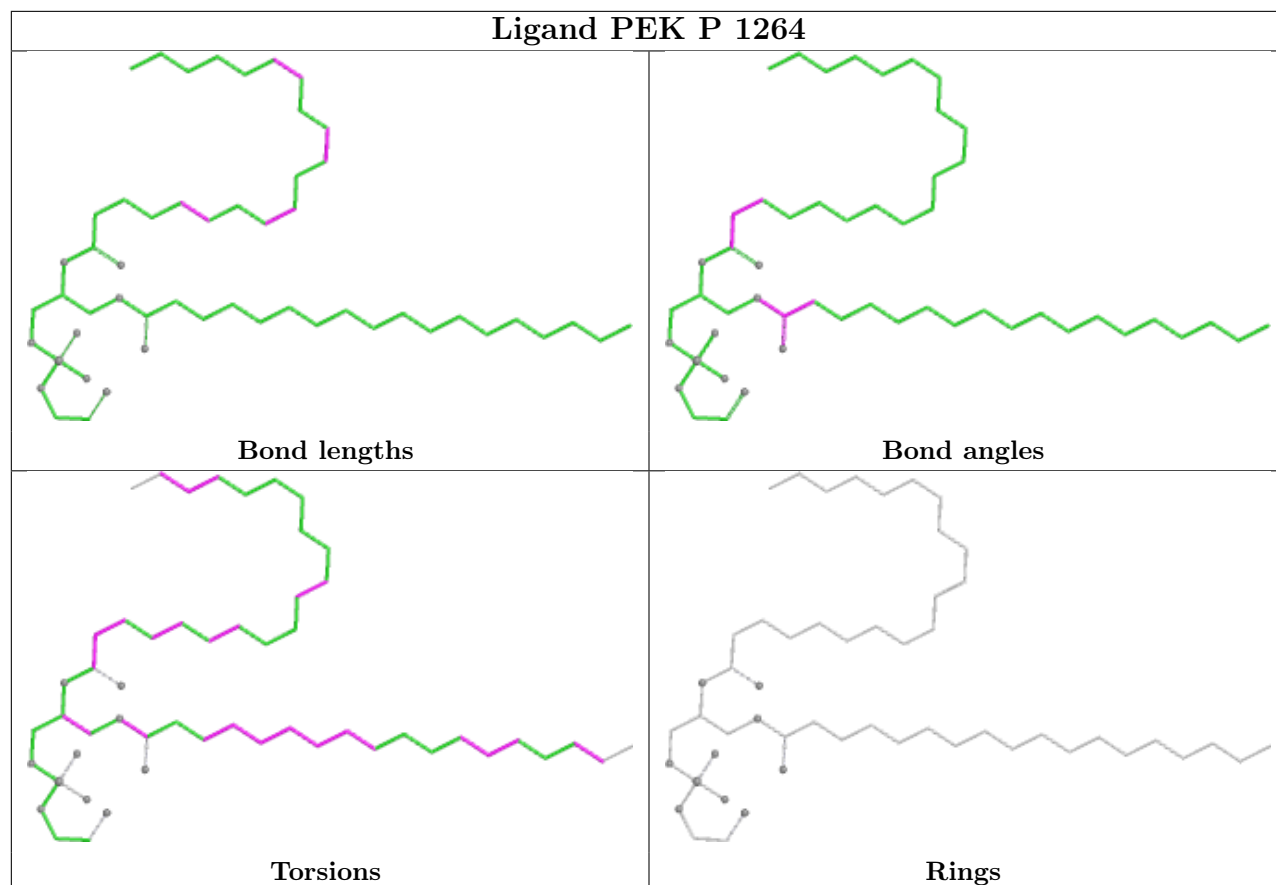


## Ligand CHD B 1086

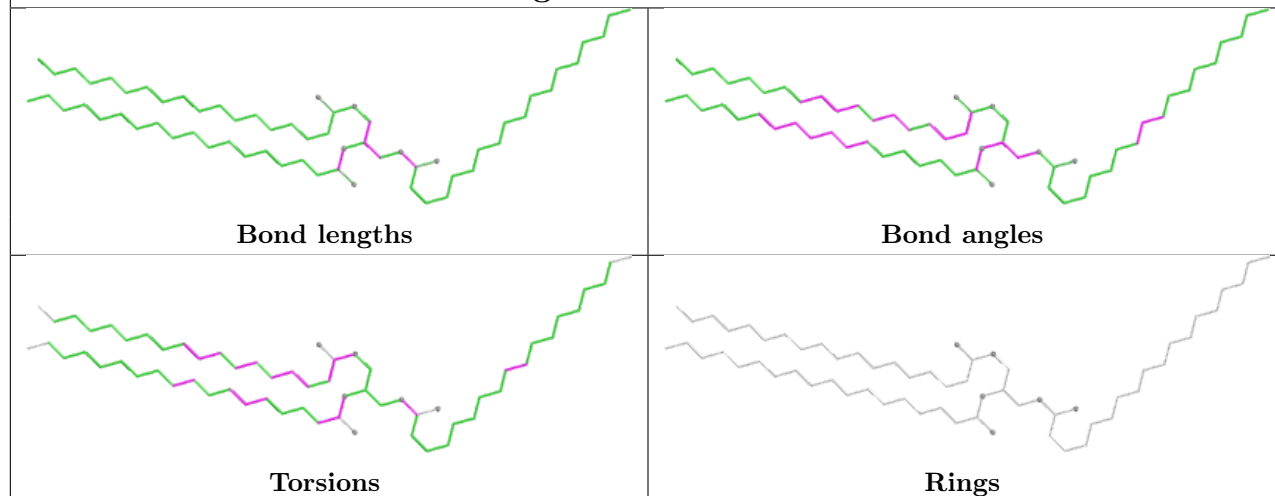




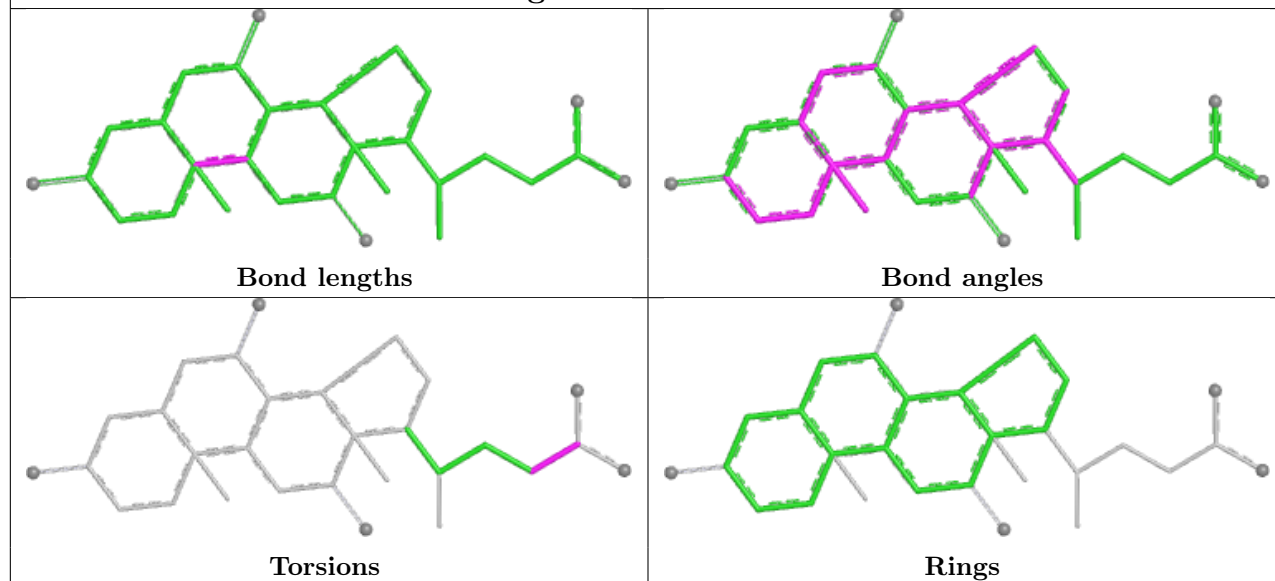


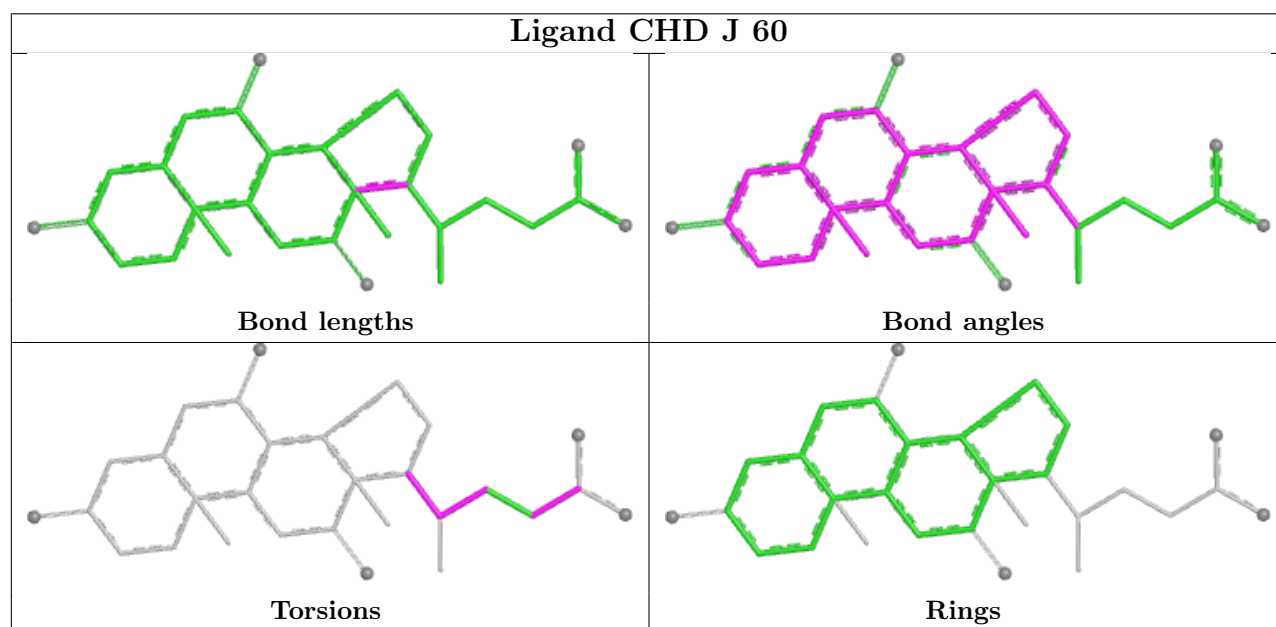
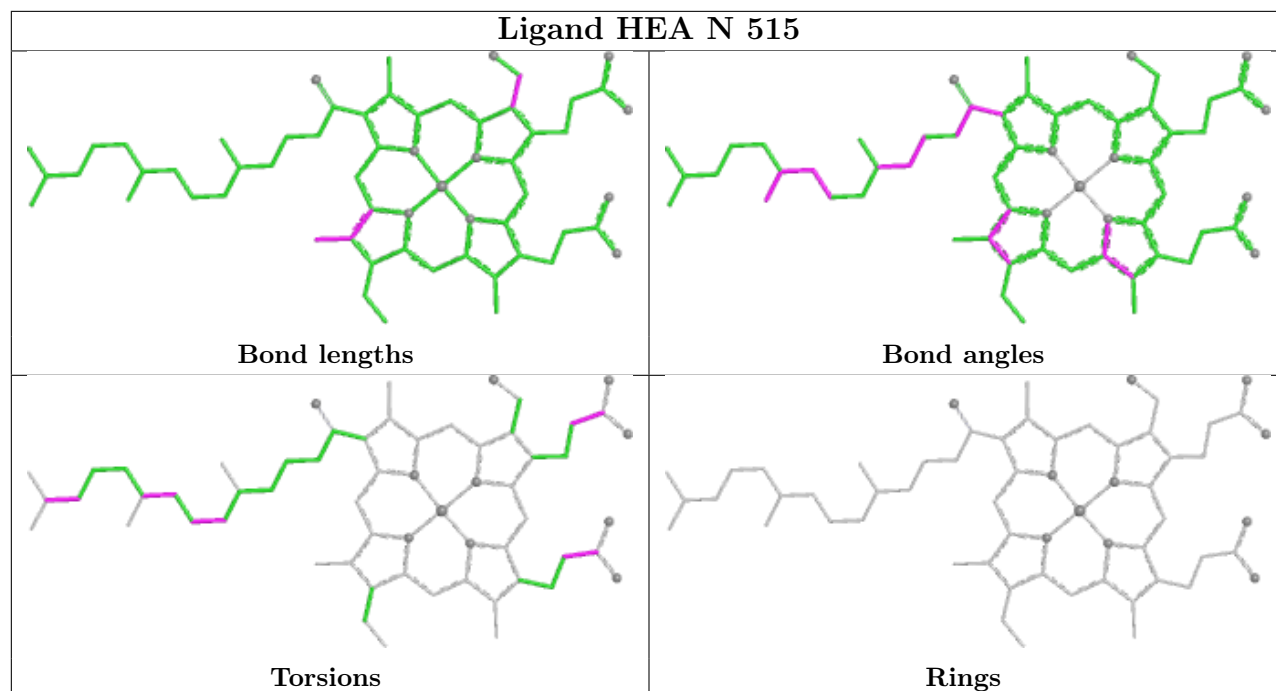


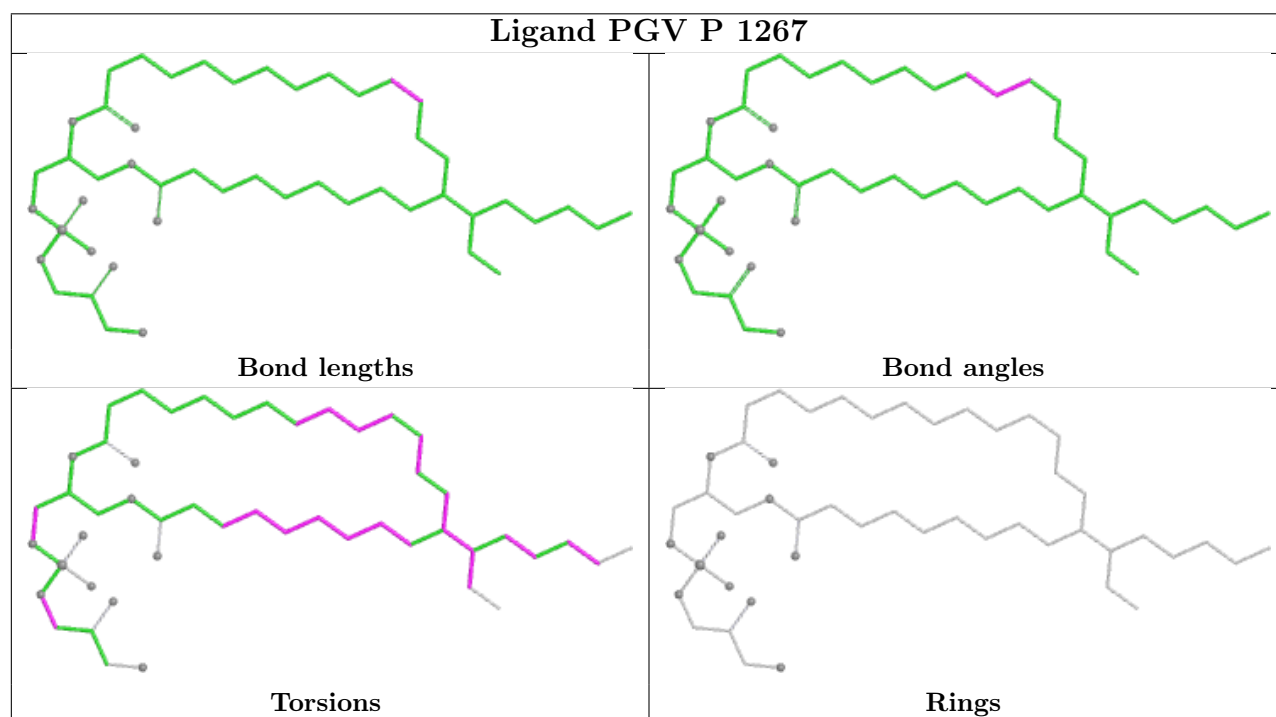
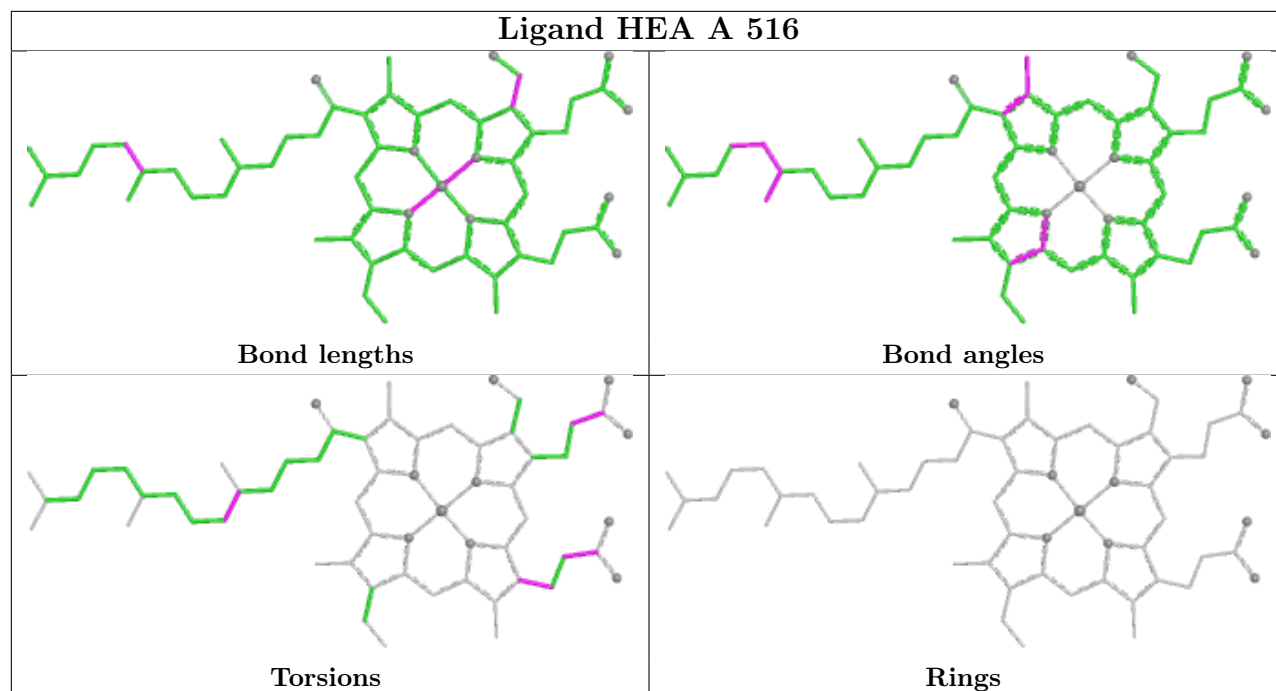
## Ligand TGL L 522

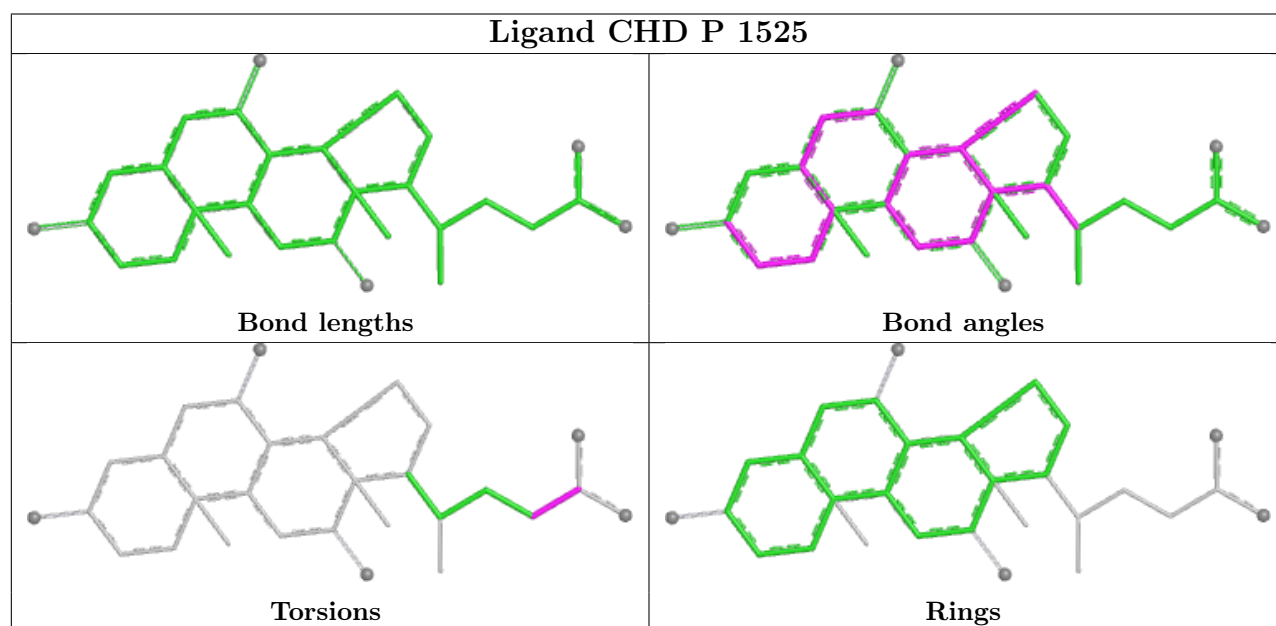
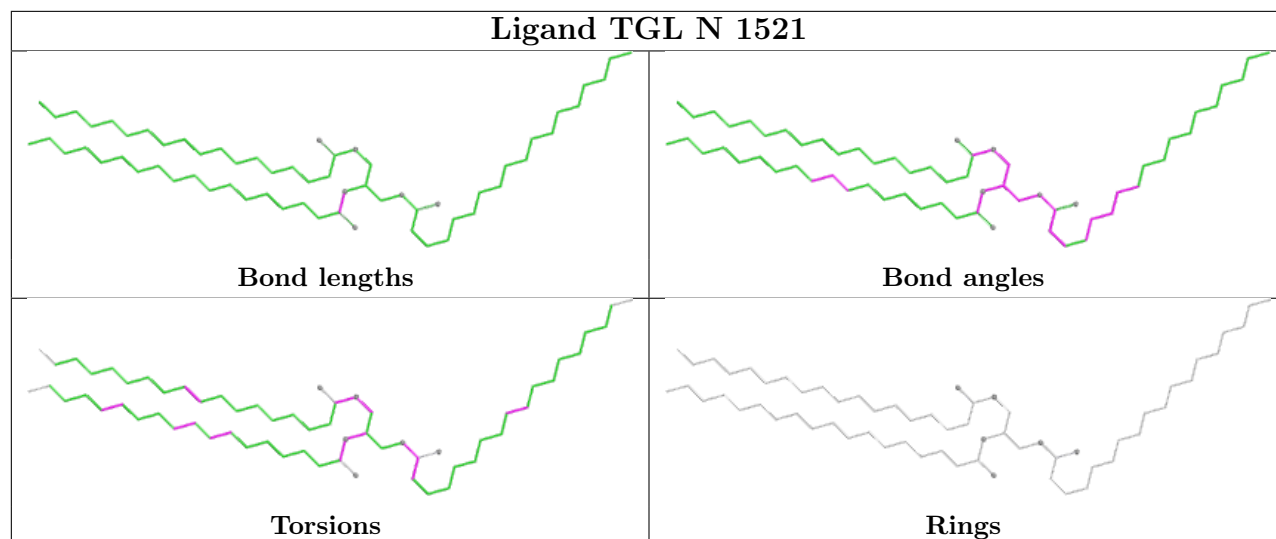


## Ligand CHD C 525

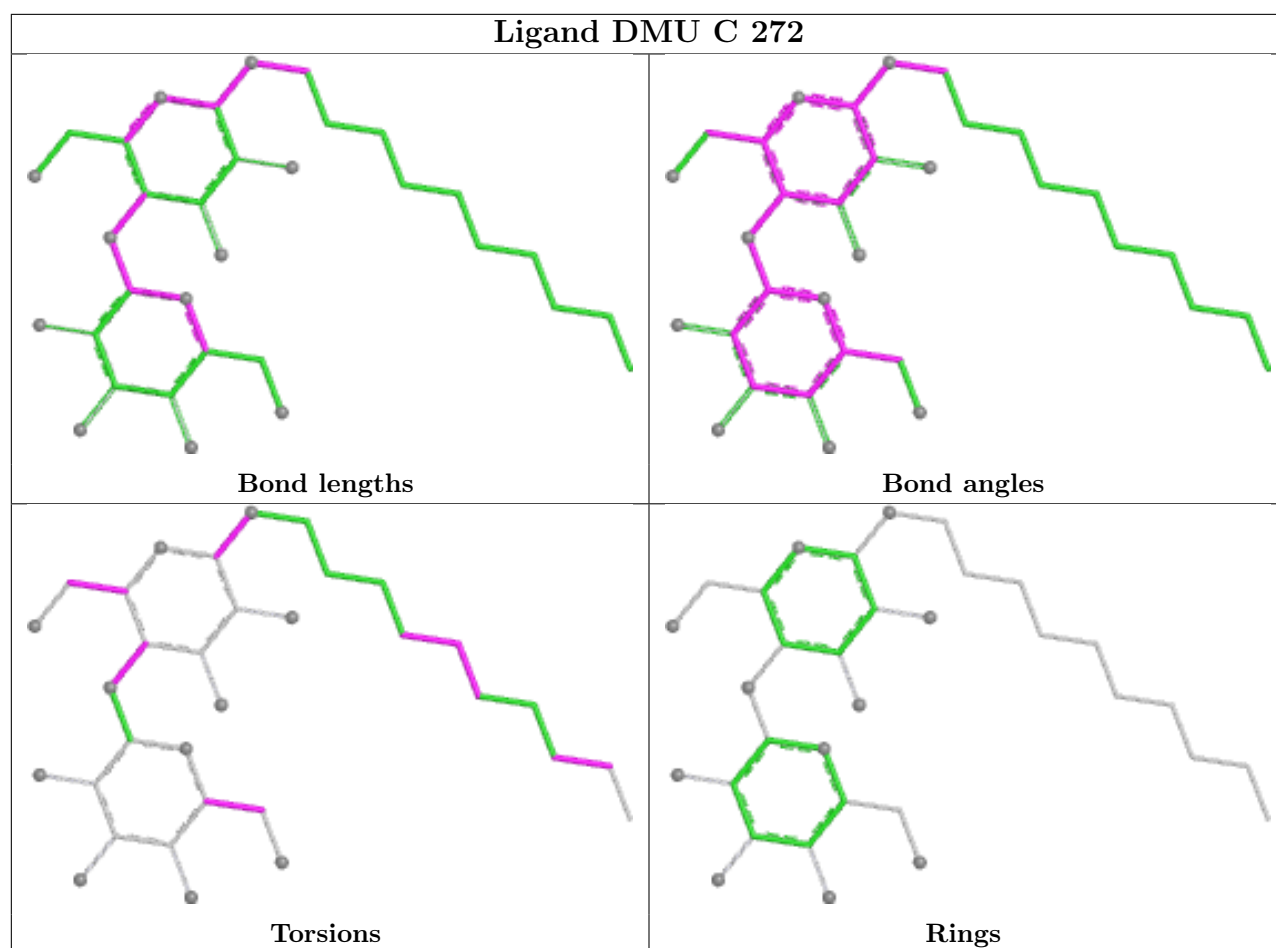




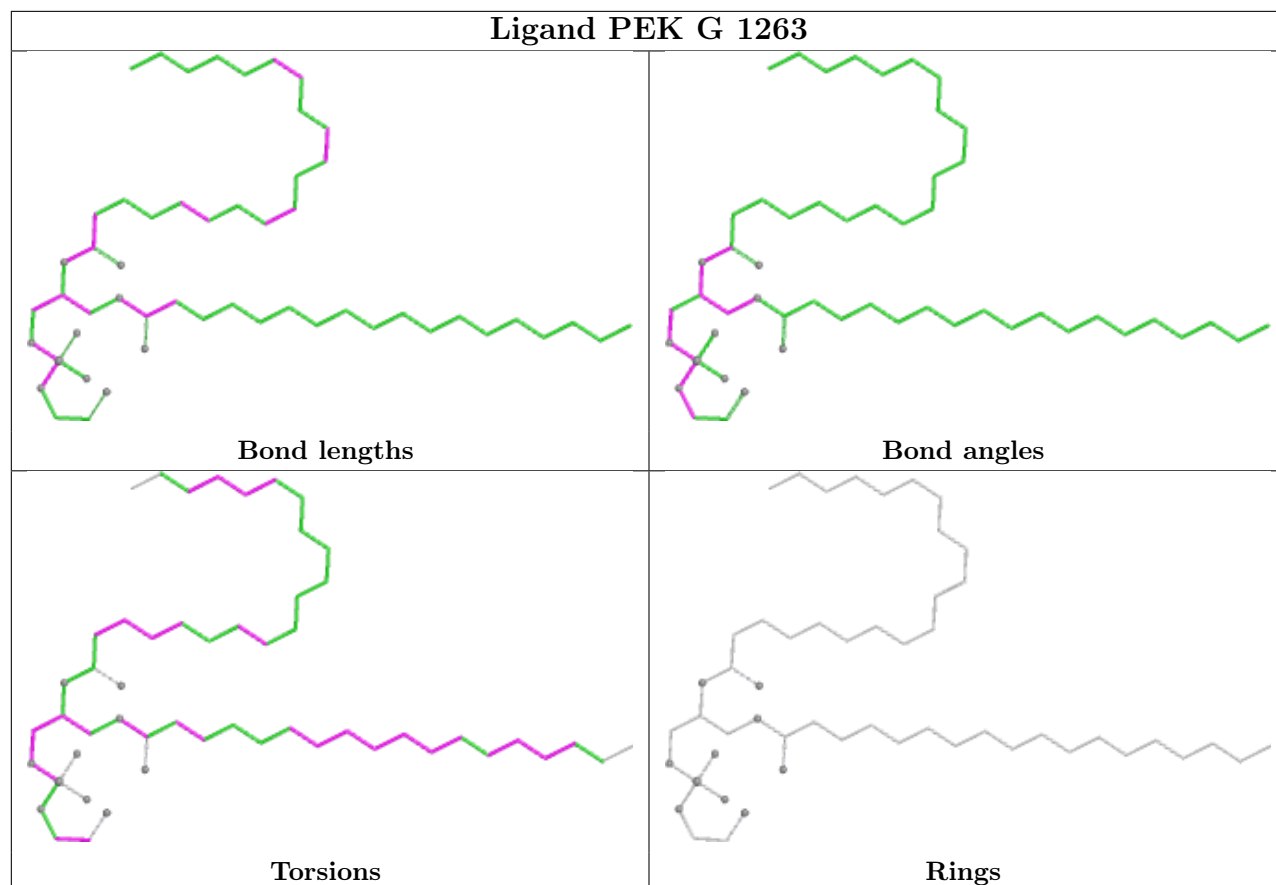




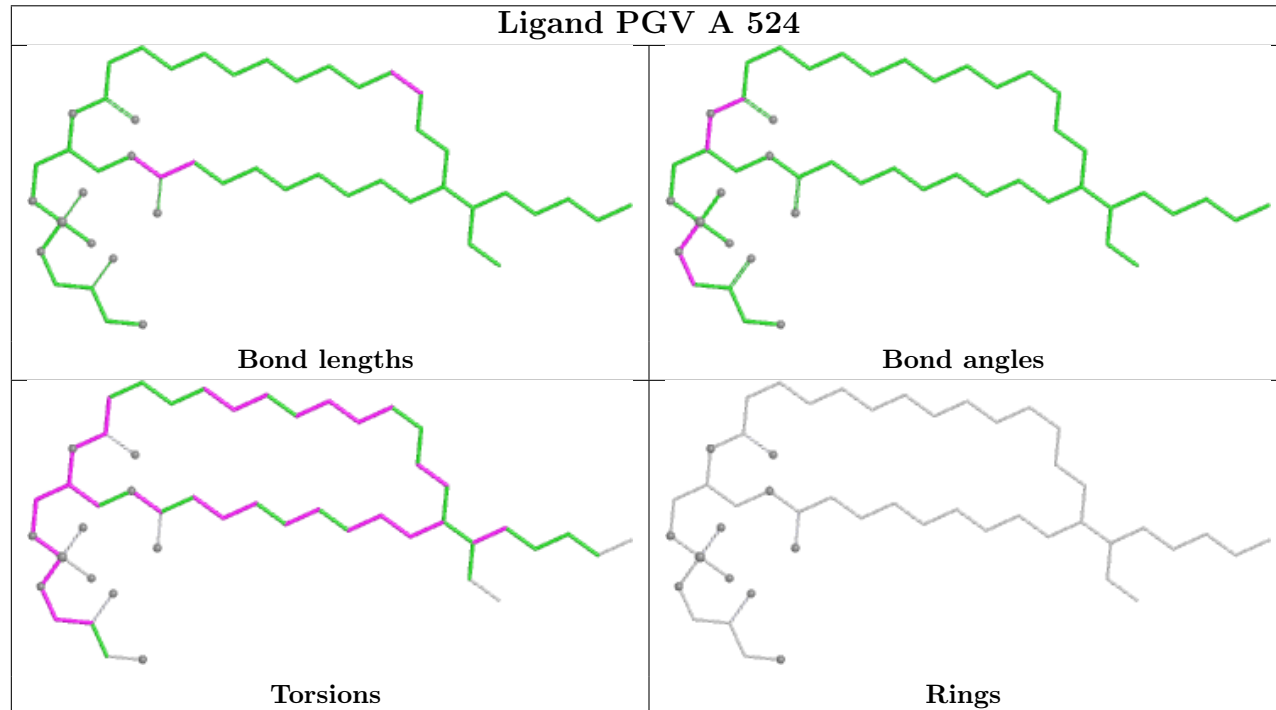


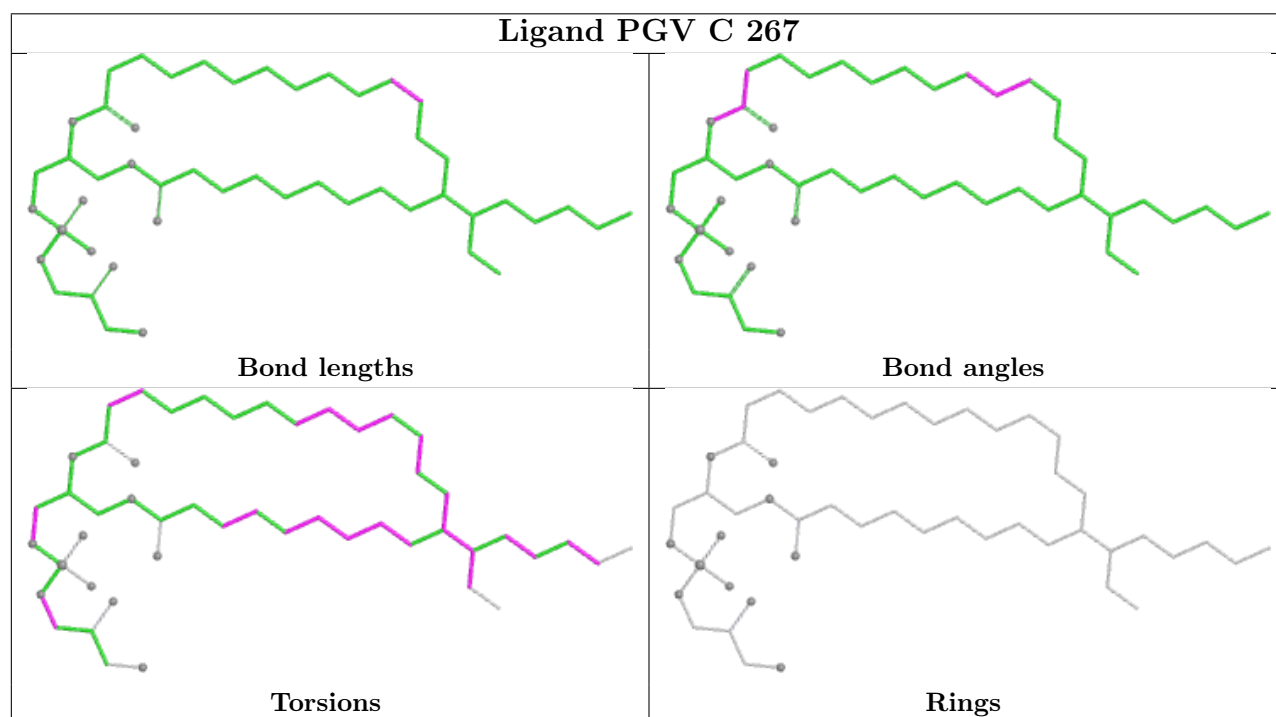
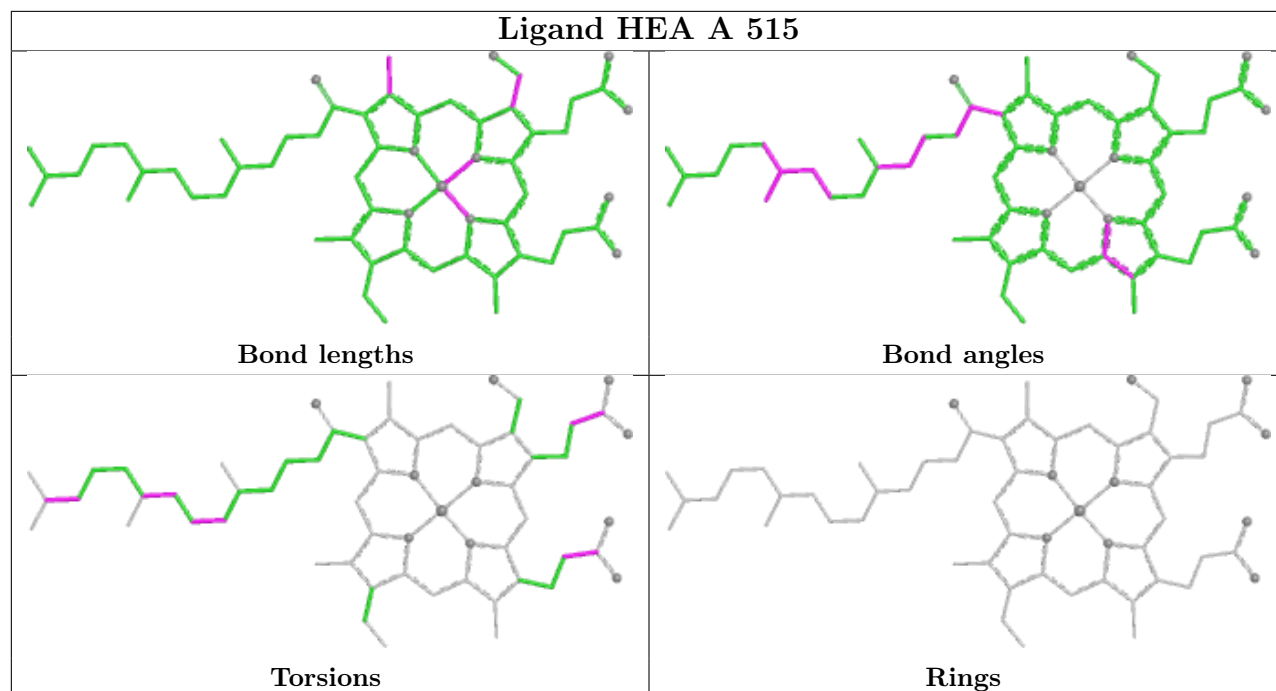


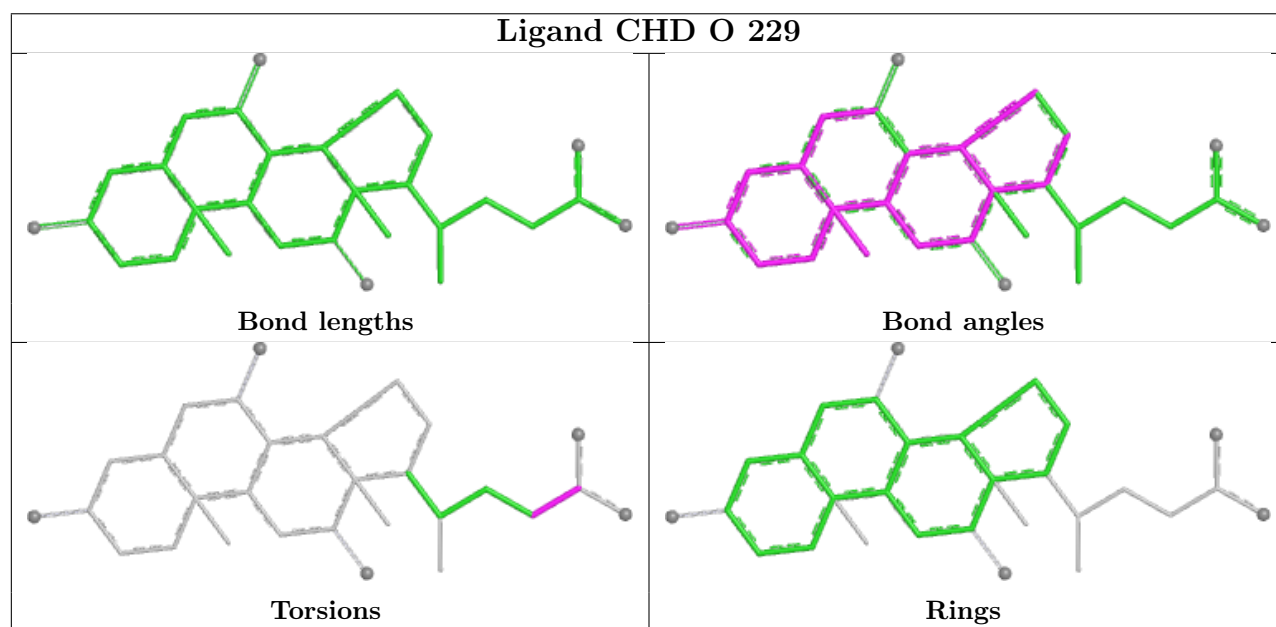
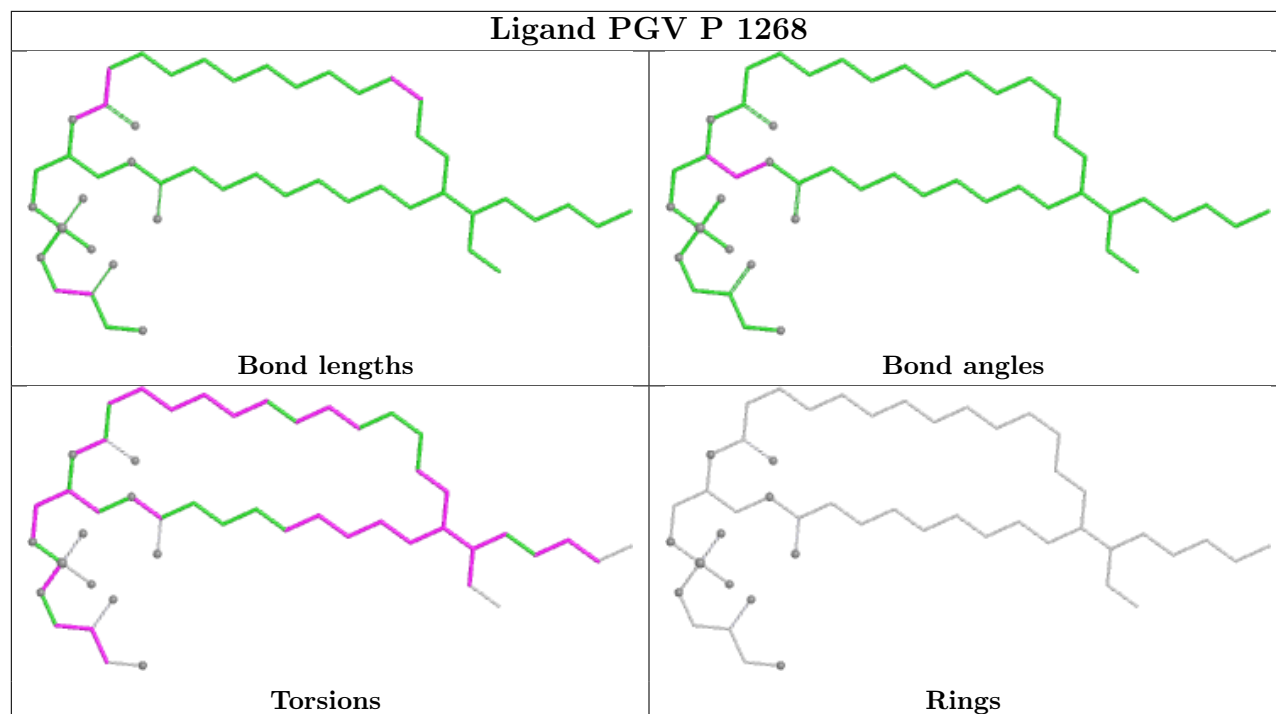
## Ligand PEK G 1263

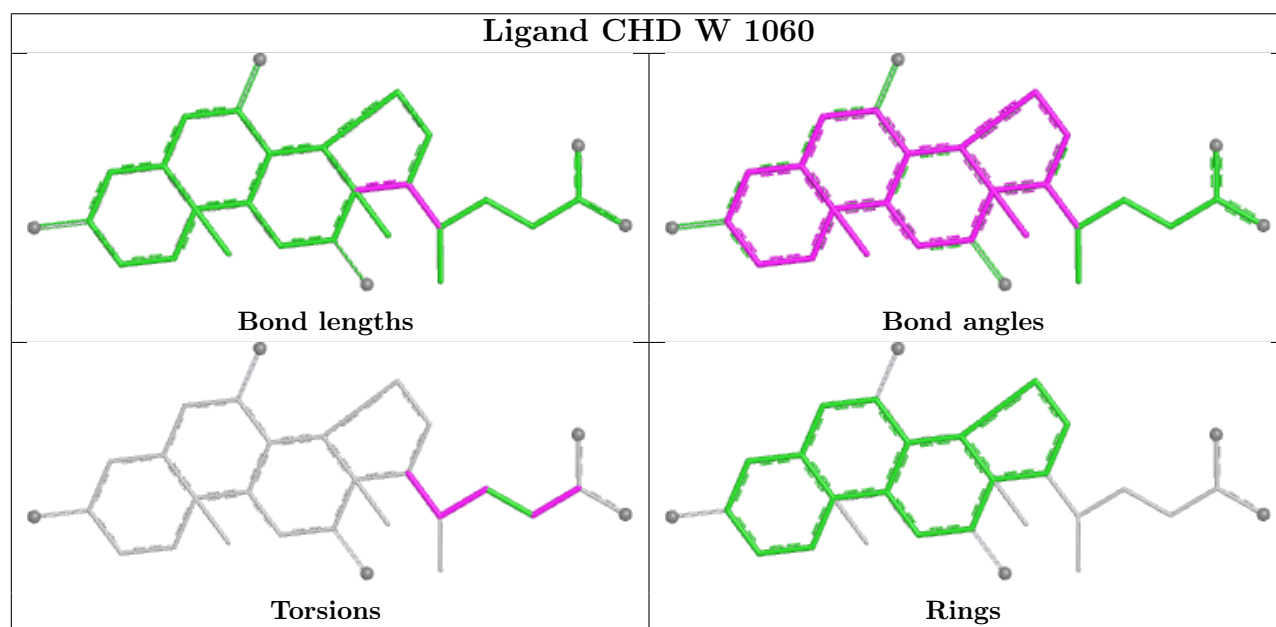
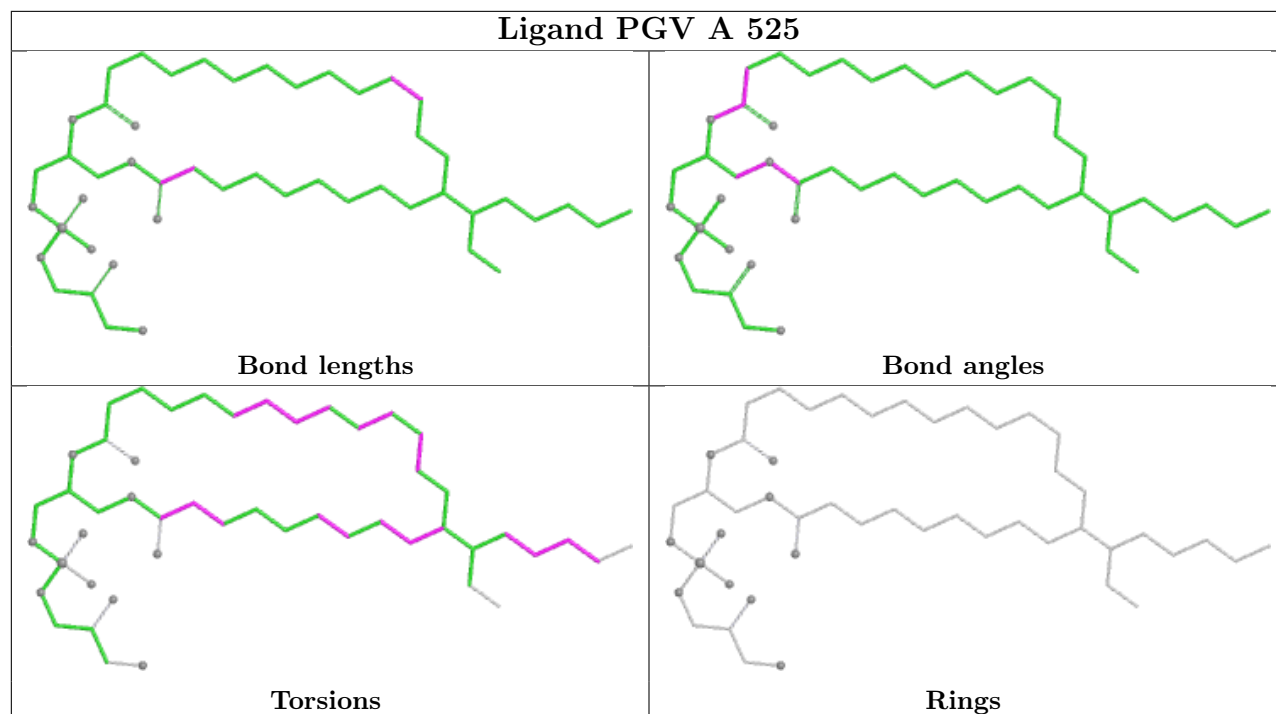


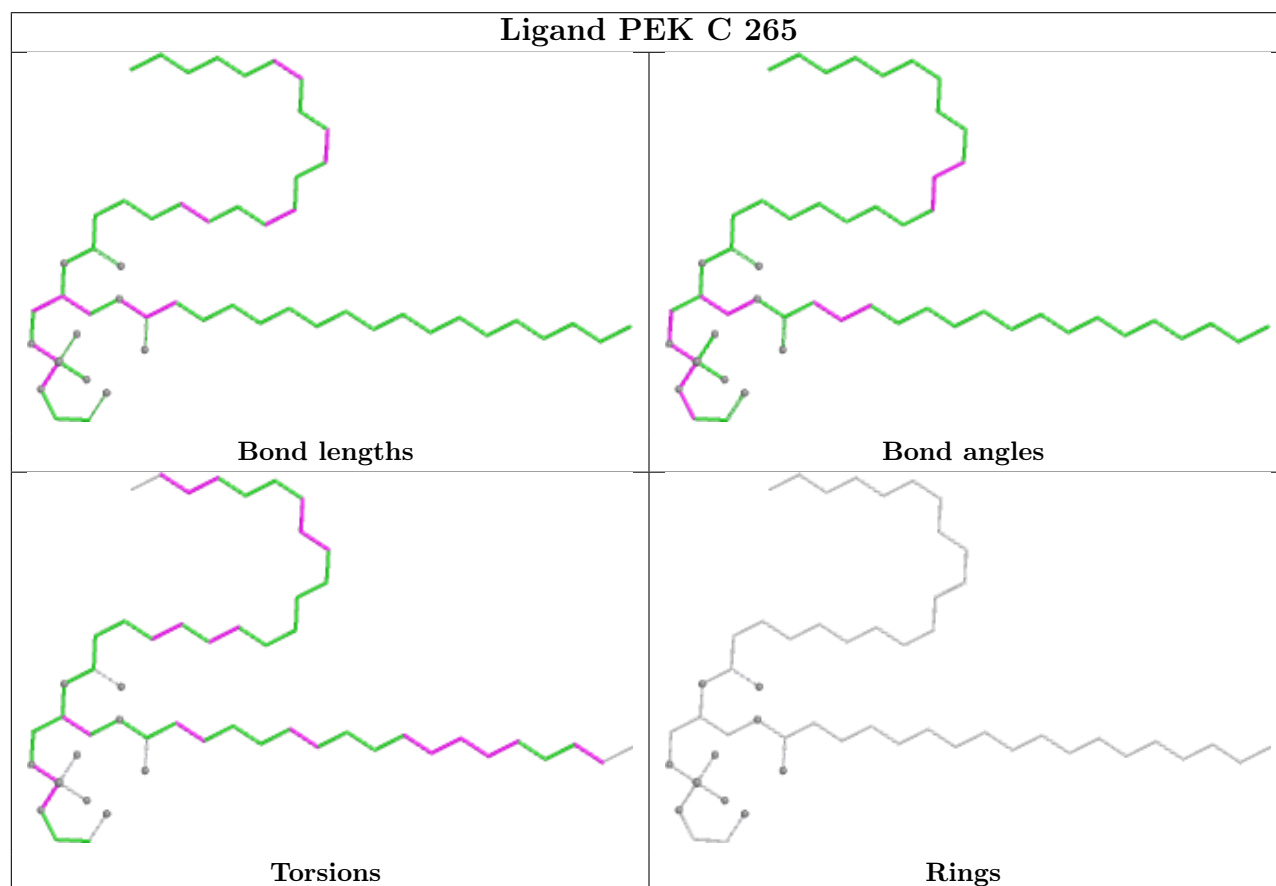
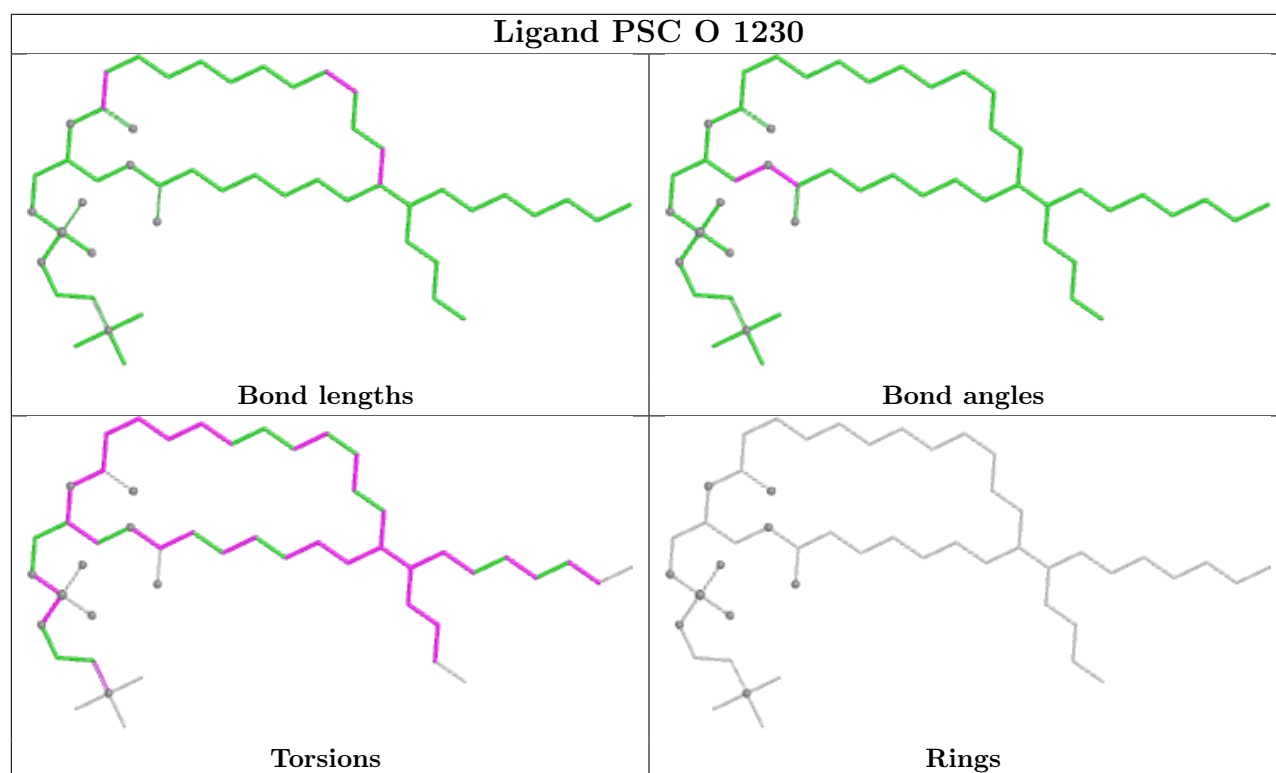
## Ligand PGV A 524



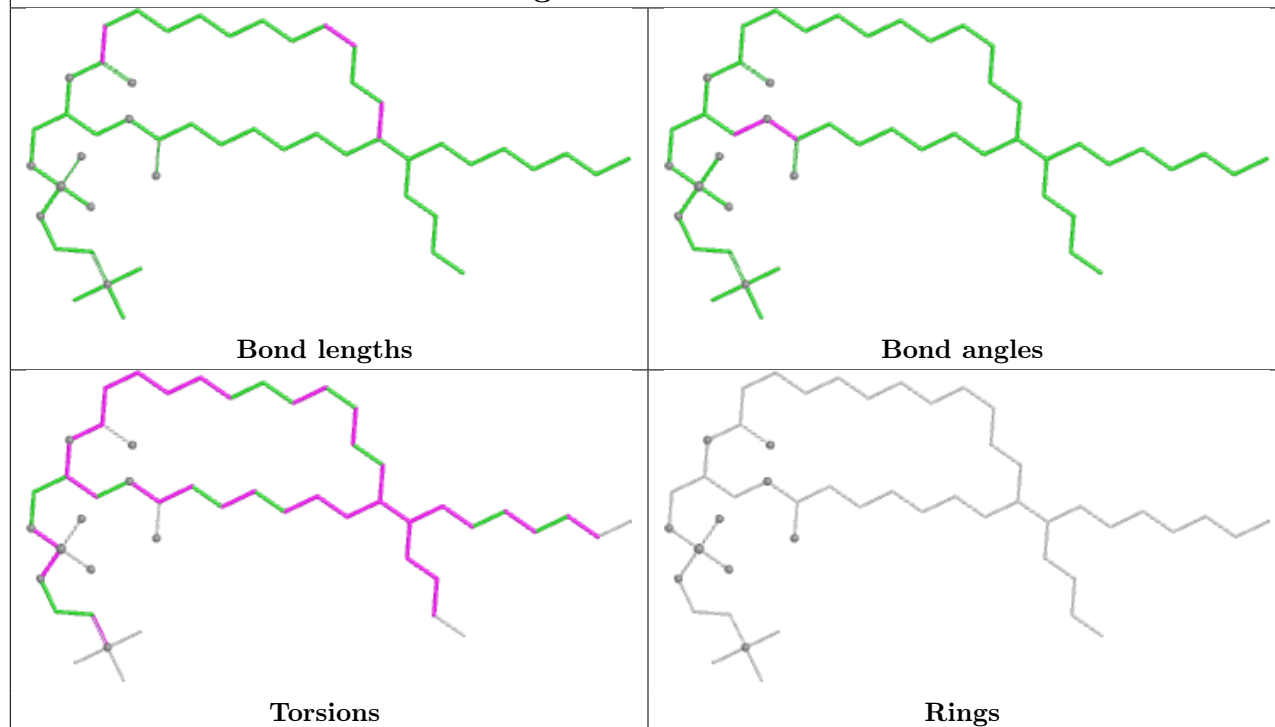




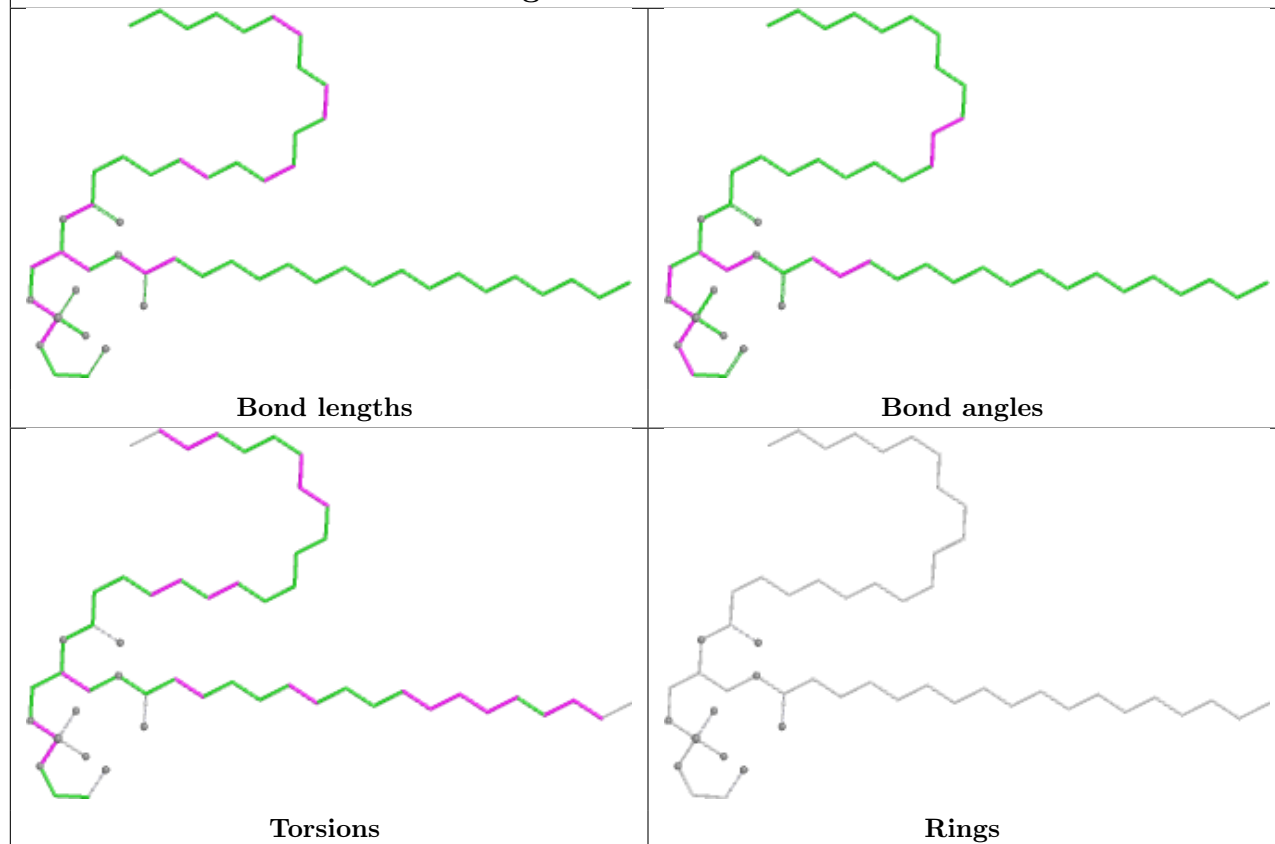




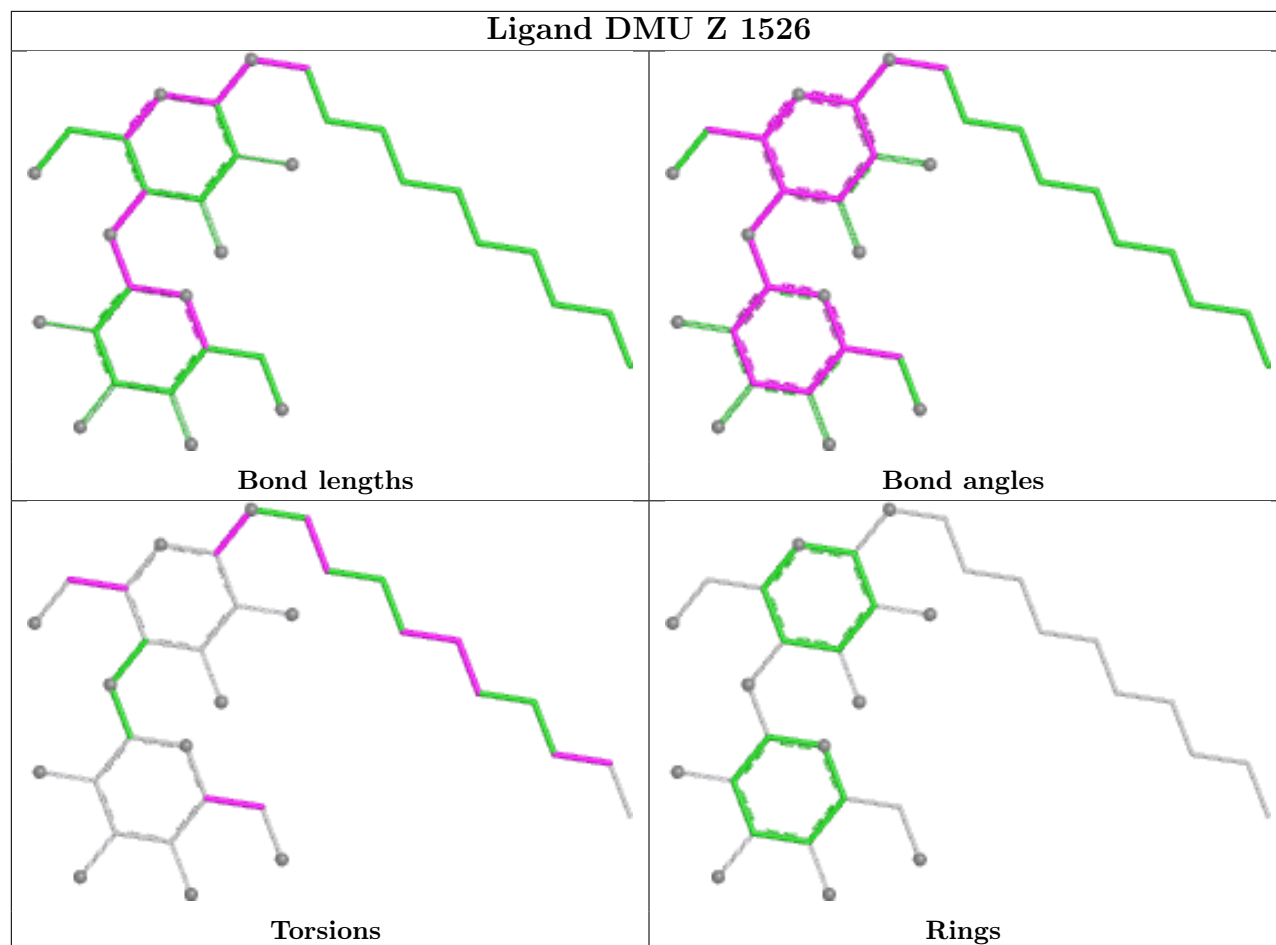
## Ligand PSC B 230



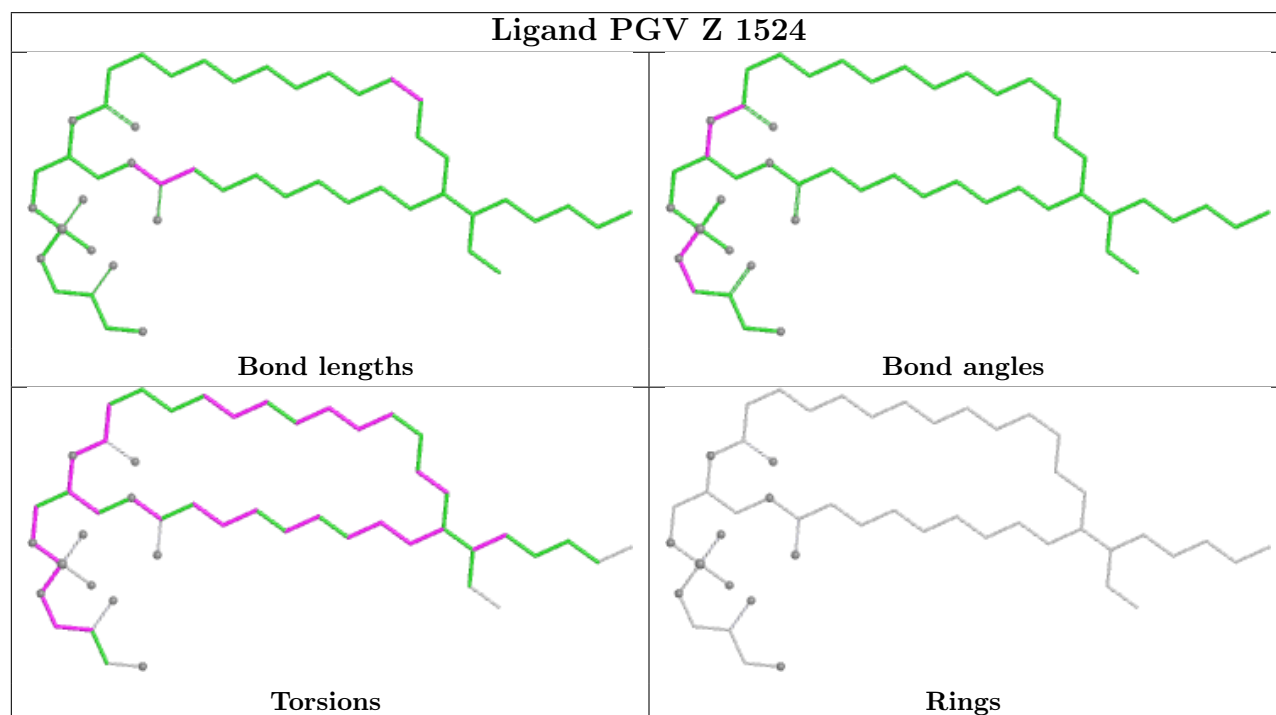
## Ligand PEK P 1265



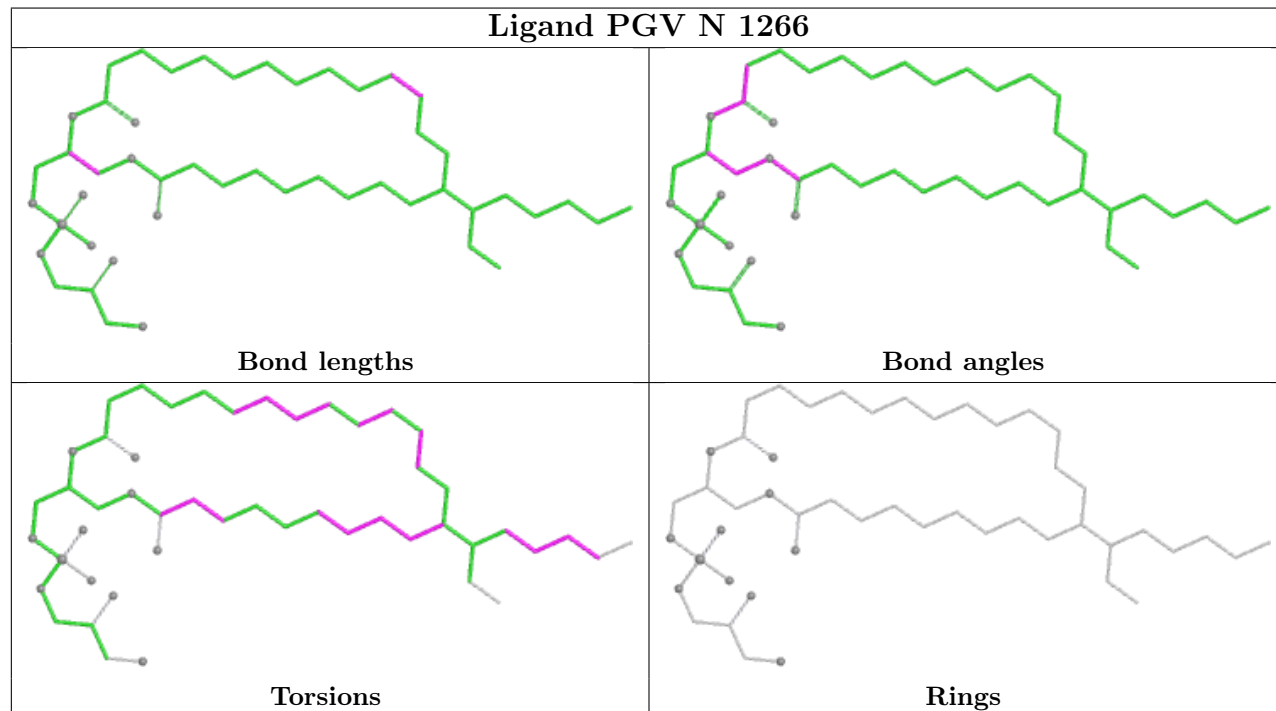
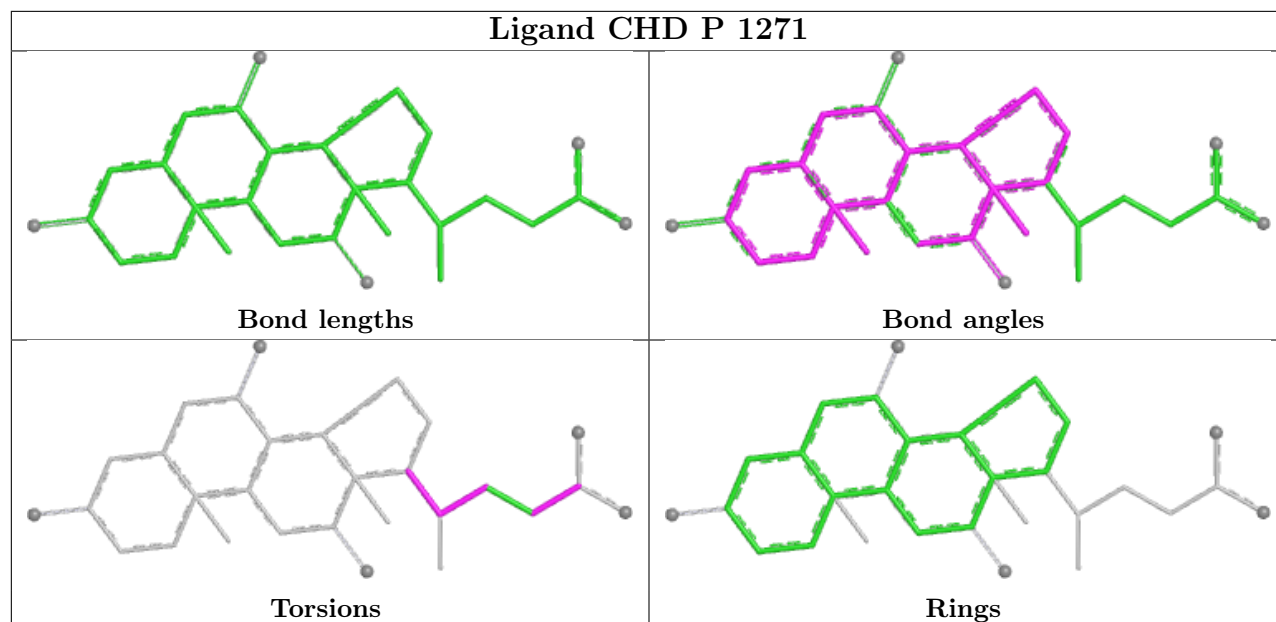
## Ligand DMU Z 1526

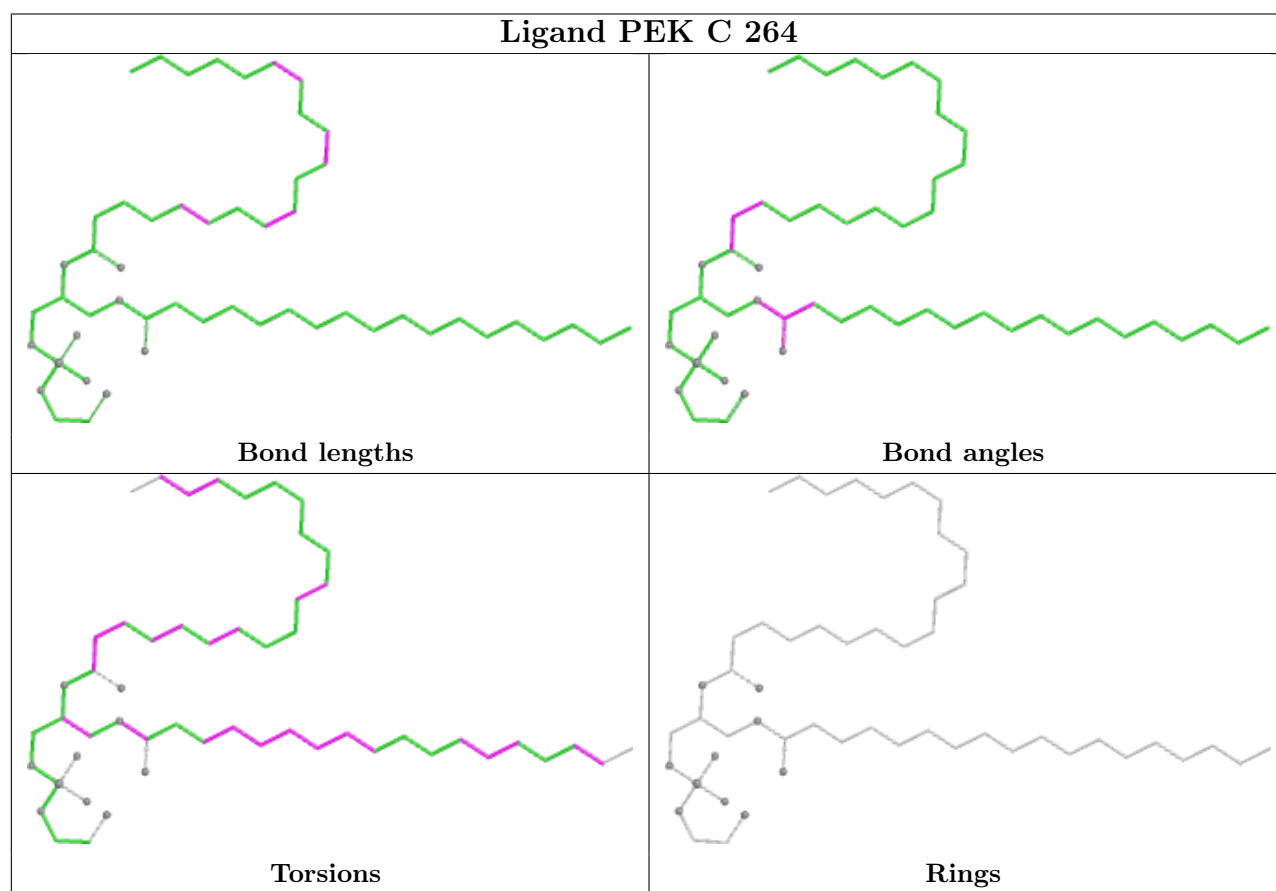
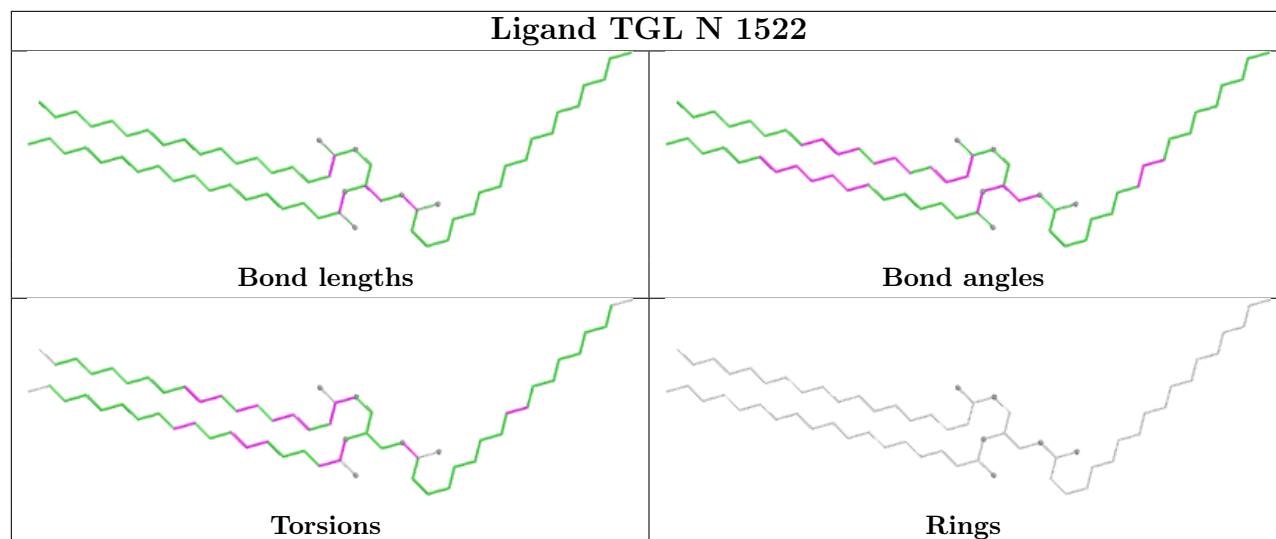


## Ligand PGV Z 1524

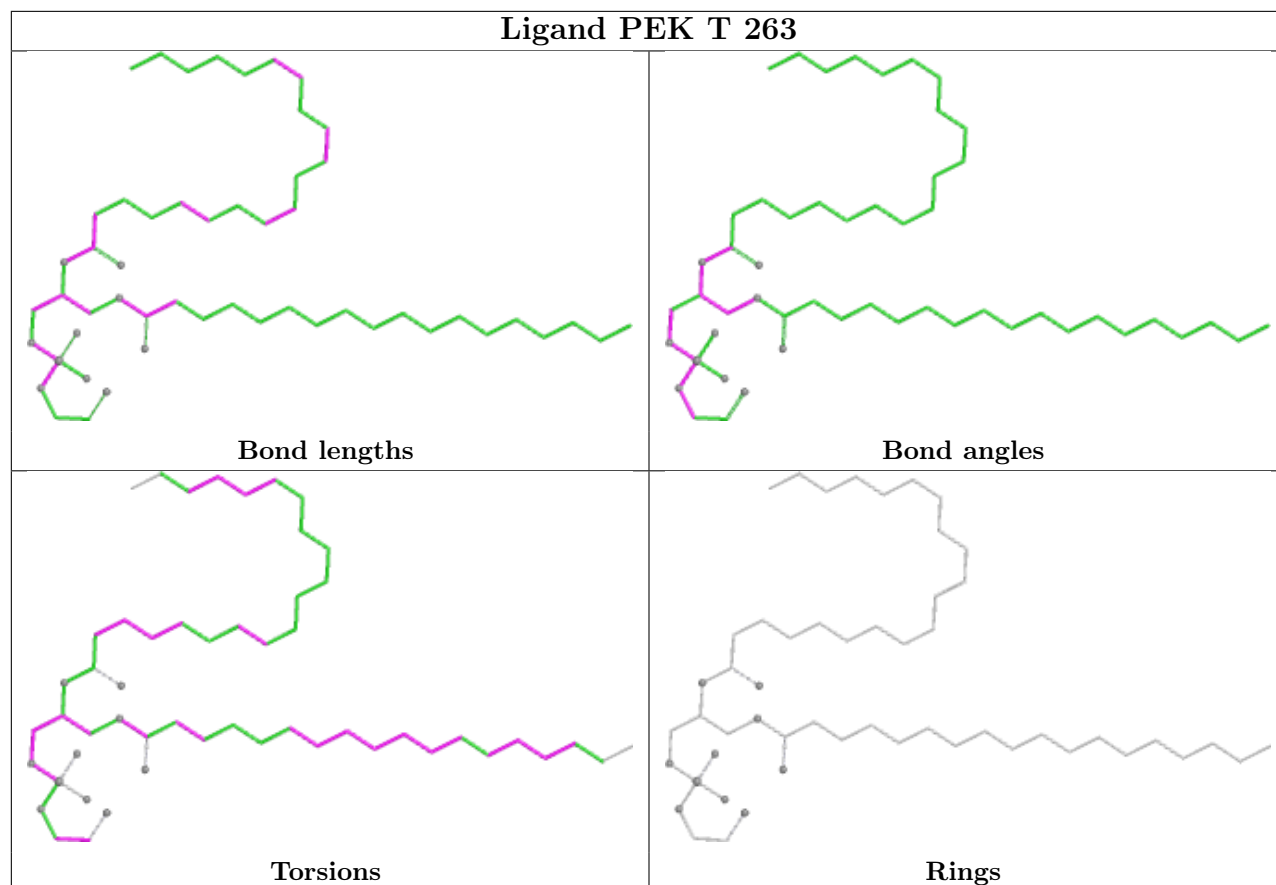




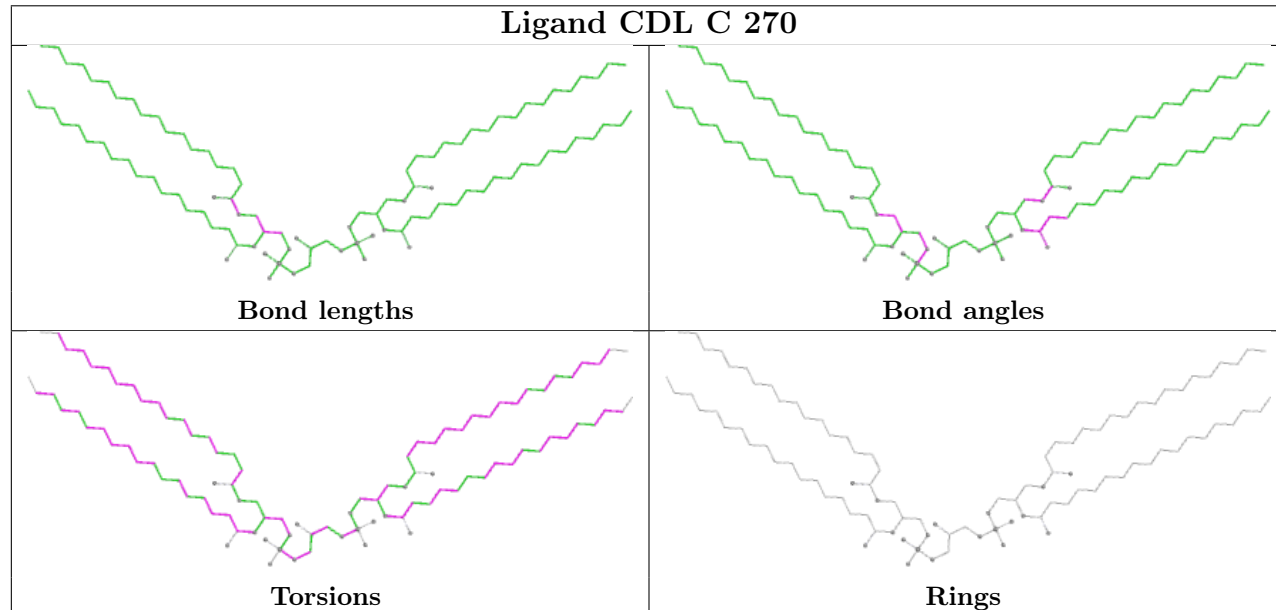


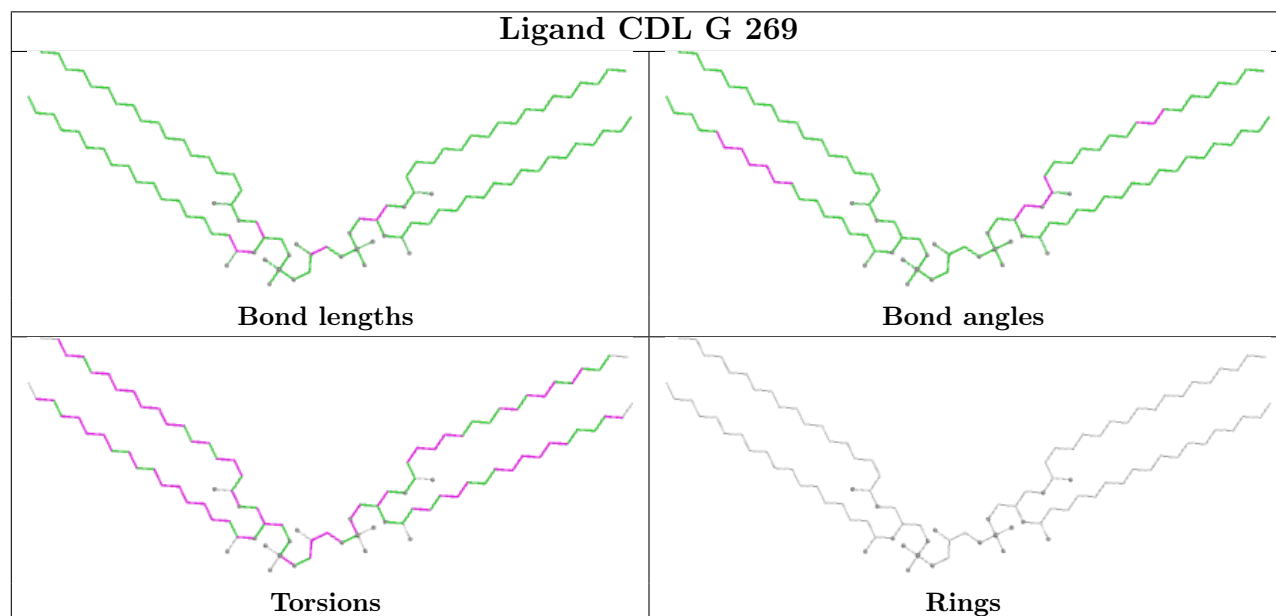
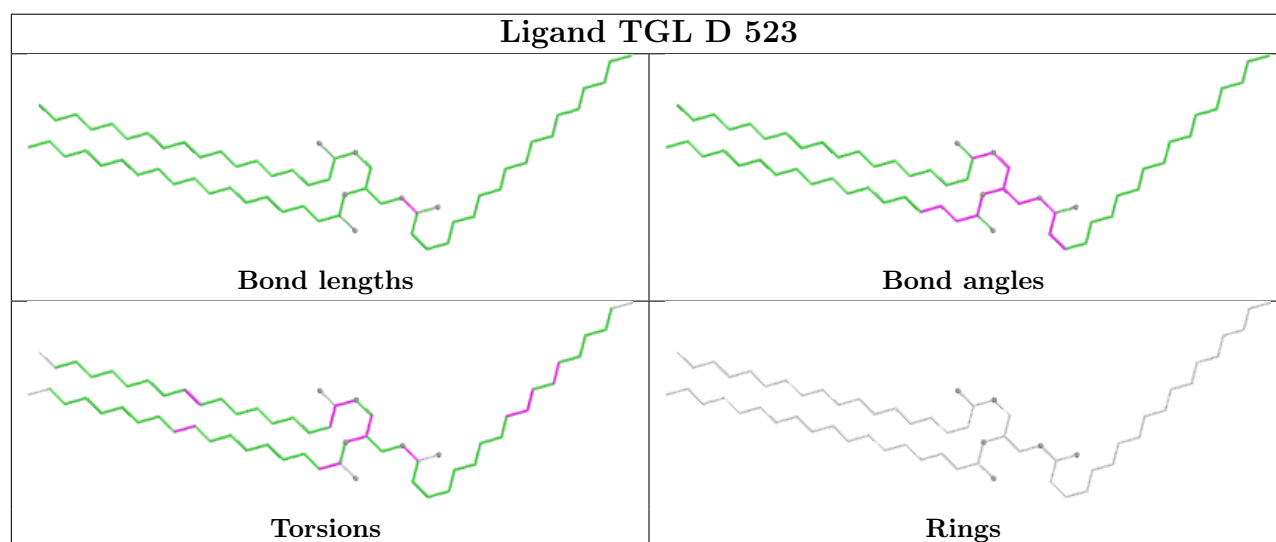
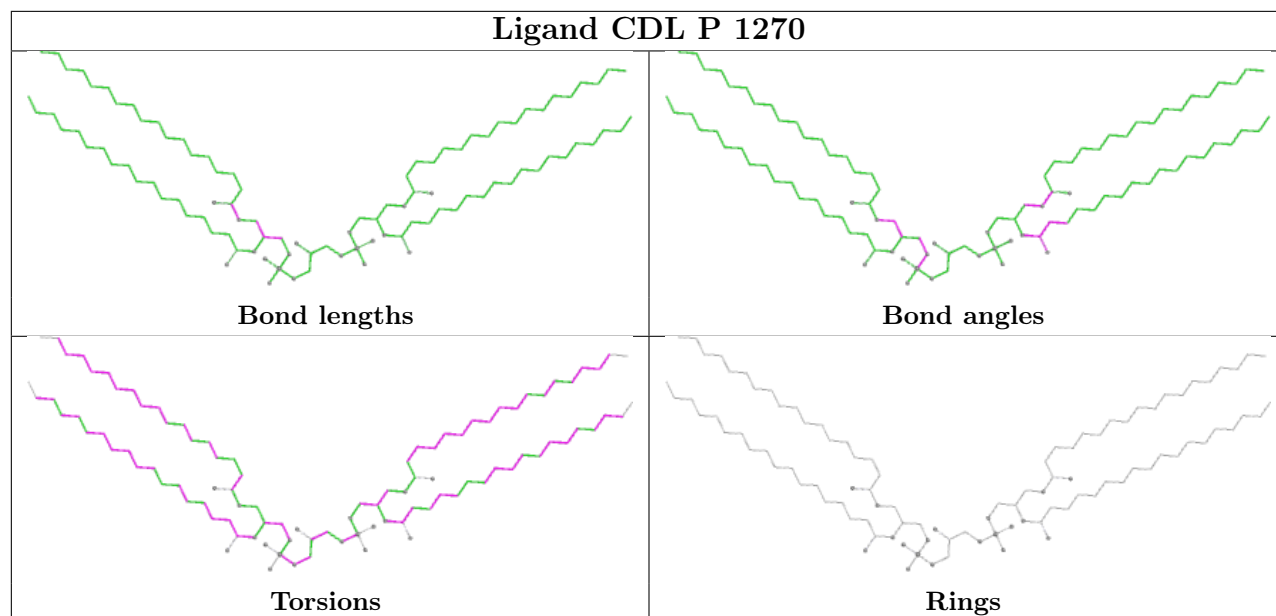


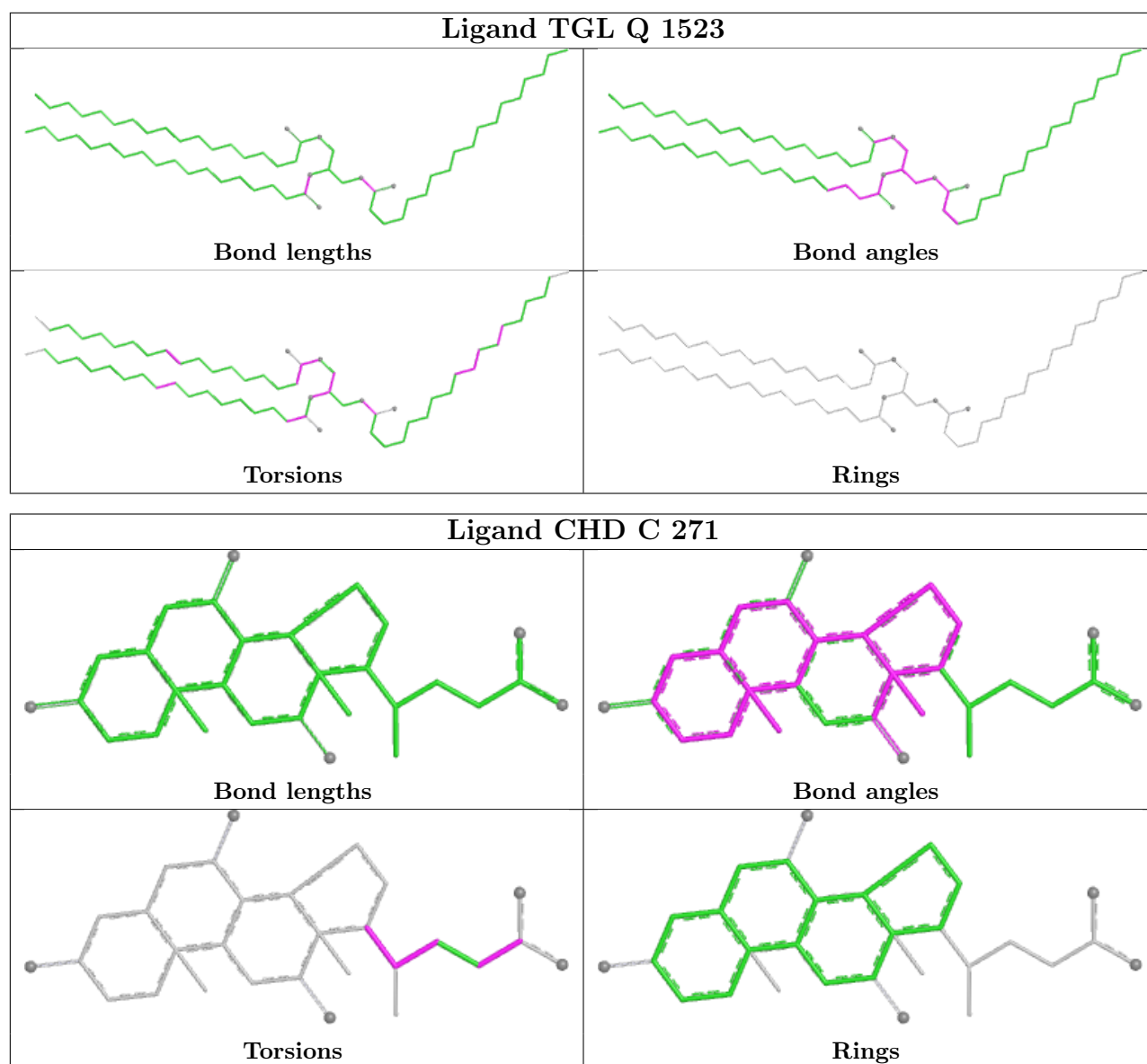
## Ligand PEK T 263



## Ligand CDL C 270







## 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%) | -0.56  | 2 (0%) 88 89  | 16, 22, 31, 72        | 0     |
| 1   | N     | 513/514 (99%) | -0.33  | 5 (0%) 79 80  | 17, 24, 34, 66        | 0     |
| 2   | B     | 226/227 (99%) | 0.18   | 15 (6%) 24 23 | 18, 29, 52, 90        | 0     |
| 2   | O     | 226/227 (99%) | 0.64   | 24 (10%) 11 9 | 22, 32, 61, 84        | 0     |
| 3   | C     | 259/261 (99%) | -0.26  | 4 (1%) 72 72  | 19, 25, 39, 70        | 0     |
| 3   | P     | 259/261 (99%) | -0.13  | 5 (1%) 66 66  | 19, 26, 40, 74        | 0     |
| 4   | D     | 144/147 (97%) | 0.58   | 14 (9%) 13 11 | 21, 31, 57, 86        | 0     |
| 4   | Q     | 144/147 (97%) | 1.62   | 37 (25%) 1 1  | 28, 42, 65, 100       | 0     |
| 5   | E     | 105/109 (96%) | 0.70   | 13 (12%) 8 6  | 22, 31, 59, 101       | 0     |
| 5   | R     | 105/109 (96%) | 1.87   | 42 (40%) 1 0  | 25, 39, 71, 102       | 0     |
| 6   | F     | 98/98 (100%)  | 0.63   | 9 (9%) 14 12  | 20, 32, 88, 110       | 0     |
| 6   | S     | 98/98 (100%)  | 0.99   | 14 (14%) 6 5  | 20, 31, 93, 106       | 0     |
| 7   | G     | 83/85 (97%)   | 1.45   | 24 (28%) 1 1  | 23, 34, 99, 107       | 0     |
| 7   | T     | 83/85 (97%)   | 1.66   | 24 (28%) 1 1  | 23, 36, 102, 109      | 0     |
| 8   | H     | 79/85 (92%)   | 0.97   | 16 (20%) 3 2  | 23, 35, 90, 108       | 0     |
| 8   | U     | 79/85 (92%)   | 1.22   | 16 (20%) 3 2  | 27, 39, 91, 110       | 0     |
| 9   | I     | 72/73 (98%)   | 1.46   | 23 (31%) 1 1  | 25, 44, 65, 85        | 0     |
| 9   | V     | 72/73 (98%)   | 1.76   | 20 (27%) 1 1  | 24, 49, 68, 94        | 0     |
| 10  | J     | 58/59 (98%)   | 0.84   | 7 (12%) 8 7   | 26, 36, 72, 99        | 0     |
| 10  | W     | 58/59 (98%)   | 1.24   | 8 (13%) 6 5   | 26, 38, 75, 106       | 0     |
| 11  | K     | 49/56 (87%)   | 0.89   | 4 (8%) 17 15  | 26, 36, 50, 66        | 0     |
| 11  | X     | 49/56 (87%)   | 1.30   | 9 (18%) 3 2   | 35, 41, 60, 76        | 0     |
| 12  | L     | 46/47 (97%)   | 0.31   | 5 (10%) 10 9  | 22, 28, 52, 87        | 0     |
| 12  | Y     | 46/47 (97%)   | 0.79   | 7 (15%) 5 4   | 26, 34, 65, 88        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------------|-----------------------|-------|
| 13  | M     | 43/46 (93%)     | 0.55   | 6 (13%) 6 5     | 23, 28, 75, 103       | 0     |
| 13  | Z     | 43/46 (93%)     | 1.11   | 8 (18%) 3 2     | 31, 36, 80, 106       | 0     |
| All | All   | 3550/3614 (98%) | 0.39   | 361 (10%) 12 10 | 16, 29, 64, 110       | 0     |

All (361) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 6   | S     | 1   | ALA  | 17.3 |
| 6   | F     | 1   | ALA  | 15.7 |
| 4   | Q     | 6   | VAL  | 12.8 |
| 9   | V     | 3   | ALA  | 12.7 |
| 6   | S     | 97  | ALA  | 11.3 |
| 6   | S     | 96  | LEU  | 10.5 |
| 7   | T     | 3   | ALA  | 10.5 |
| 7   | G     | 4   | ALA  | 9.6  |
| 6   | S     | 94  | HIS  | 9.5  |
| 4   | Q     | 5   | VAL  | 9.0  |
| 7   | G     | 5   | LYS  | 8.9  |
| 4   | Q     | 4   | SER  | 8.9  |
| 4   | D     | 5   | VAL  | 8.5  |
| 2   | O     | 227 | LEU  | 8.5  |
| 6   | F     | 97  | ALA  | 8.5  |
| 8   | U     | 8   | ILE  | 8.4  |
| 9   | V     | 5   | ALA  | 8.4  |
| 6   | F     | 96  | LEU  | 8.3  |
| 7   | T     | 5   | LYS  | 7.8  |
| 7   | T     | 4   | ALA  | 7.6  |
| 9   | I     | 3   | ALA  | 7.6  |
| 7   | T     | 36  | TRP  | 7.6  |
| 8   | H     | 8   | ILE  | 7.5  |
| 7   | G     | 36  | TRP  | 7.5  |
| 4   | D     | 6   | VAL  | 7.4  |
| 5   | R     | 79  | LYS  | 7.3  |
| 2   | O     | 226 | MET  | 7.1  |
| 1   | N     | 513 | LEU  | 7.1  |
| 4   | Q     | 8   | SER  | 7.1  |
| 6   | S     | 95  | GLN  | 7.0  |
| 6   | S     | 98  | HIS  | 6.9  |
| 2   | O     | 59  | GLN  | 6.8  |
| 7   | G     | 3   | ALA  | 6.8  |
| 7   | T     | 2   | SER  | 6.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7   | T     | 6   | GLY  | 6.8  |
| 11  | X     | 6   | ALA  | 6.6  |
| 5   | R     | 109 | VAL  | 6.5  |
| 7   | T     | 9   | GLY  | 6.5  |
| 7   | G     | 6   | GLY  | 6.3  |
| 6   | F     | 2   | SER  | 6.2  |
| 9   | I     | 2   | THR  | 6.2  |
| 9   | V     | 2   | THR  | 6.2  |
| 11  | K     | 6   | ALA  | 6.1  |
| 7   | G     | 1   | ALA  | 6.0  |
| 7   | G     | 7   | ASP  | 5.9  |
| 2   | O     | 224 | ALA  | 5.9  |
| 8   | H     | 47  | GLY  | 5.7  |
| 5   | R     | 83  | PRO  | 5.7  |
| 4   | D     | 4   | SER  | 5.7  |
| 4   | Q     | 7   | LYS  | 5.6  |
| 6   | F     | 3   | GLY  | 5.6  |
| 2   | B     | 59  | GLN  | 5.6  |
| 2   | O     | 113 | TYR  | 5.6  |
| 7   | T     | 39  | SER  | 5.5  |
| 12  | L     | 2   | HIS  | 5.5  |
| 7   | G     | 37  | LEU  | 5.5  |
| 4   | Q     | 58  | GLU  | 5.5  |
| 6   | F     | 94  | HIS  | 5.5  |
| 7   | T     | 8   | HIS  | 5.5  |
| 7   | T     | 10  | GLY  | 5.4  |
| 10  | W     | 58  | LYS  | 5.4  |
| 9   | I     | 4   | LEU  | 5.4  |
| 9   | I     | 37  | PHE  | 5.3  |
| 5   | R     | 105 | GLY  | 5.3  |
| 7   | T     | 7   | ASP  | 5.2  |
| 7   | T     | 37  | LEU  | 5.2  |
| 9   | V     | 4   | LEU  | 5.2  |
| 10  | W     | 57  | HIS  | 5.2  |
| 4   | Q     | 35  | ALA  | 5.1  |
| 13  | M     | 39  | ASN  | 5.0  |
| 7   | T     | 38  | HIS  | 5.0  |
| 9   | V     | 37  | PHE  | 5.0  |
| 6   | S     | 93  | PRO  | 4.9  |
| 7   | G     | 9   | GLY  | 4.9  |
| 10  | W     | 1   | PHE  | 4.9  |
| 7   | G     | 12  | GLY  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8   | U     | 48  | GLY  | 4.8  |
| 5   | R     | 108 | LYS  | 4.8  |
| 7   | G     | 2   | SER  | 4.8  |
| 2   | B     | 61  | VAL  | 4.8  |
| 3   | P     | 3   | HIS  | 4.7  |
| 6   | S     | 3   | GLY  | 4.7  |
| 7   | G     | 10  | GLY  | 4.7  |
| 5   | R     | 86  | ILE  | 4.7  |
| 6   | F     | 95  | GLN  | 4.6  |
| 5   | E     | 109 | VAL  | 4.6  |
| 10  | W     | 52  | TRP  | 4.6  |
| 13  | M     | 40  | TYR  | 4.6  |
| 13  | Z     | 41  | LYS  | 4.6  |
| 6   | S     | 2   | SER  | 4.6  |
| 2   | O     | 58  | ALA  | 4.6  |
| 8   | H     | 9   | LYS  | 4.6  |
| 7   | T     | 40  | GLY  | 4.6  |
| 7   | T     | 42  | ARG  | 4.5  |
| 4   | Q     | 51  | LEU  | 4.5  |
| 6   | F     | 98  | HIS  | 4.5  |
| 13  | Z     | 43  | SER  | 4.5  |
| 8   | U     | 47  | GLY  | 4.4  |
| 9   | V     | 7   | PRO  | 4.4  |
| 7   | G     | 38  | HIS  | 4.4  |
| 7   | T     | 1   | ALA  | 4.4  |
| 7   | G     | 39  | SER  | 4.3  |
| 8   | H     | 10  | ASN  | 4.3  |
| 7   | T     | 84  | LYS  | 4.3  |
| 4   | D     | 8   | SER  | 4.3  |
| 2   | B     | 90  | ILE  | 4.3  |
| 8   | U     | 44  | THR  | 4.2  |
| 2   | B     | 60  | GLU  | 4.2  |
| 8   | H     | 7   | LYS  | 4.2  |
| 11  | K     | 47  | ARG  | 4.2  |
| 2   | B     | 65  | TRP  | 4.2  |
| 8   | U     | 9   | LYS  | 4.2  |
| 8   | U     | 46  | LYS  | 4.2  |
| 5   | R     | 89  | LEU  | 4.2  |
| 10  | J     | 1   | PHE  | 4.1  |
| 5   | R     | 85  | VAL  | 4.1  |
| 5   | R     | 9   | GLU  | 4.1  |
| 4   | Q     | 10  | ASP  | 4.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | R     | 76  | GLY  | 4.1  |
| 2   | O     | 60  | GLU  | 4.1  |
| 2   | O     | 223 | SER  | 4.1  |
| 13  | M     | 43  | SER  | 4.1  |
| 7   | G     | 40  | GLY  | 4.1  |
| 9   | I     | 5   | ALA  | 4.1  |
| 5   | R     | 84  | TYR  | 4.1  |
| 3   | C     | 3   | HIS  | 4.1  |
| 9   | V     | 8   | GLN  | 4.1  |
| 5   | R     | 90  | ARG  | 4.0  |
| 4   | Q     | 53  | ILE  | 4.0  |
| 10  | J     | 58  | LYS  | 4.0  |
| 2   | O     | 225 | SER  | 4.0  |
| 2   | O     | 90  | ILE  | 4.0  |
| 10  | J     | 55  | PHE  | 4.0  |
| 7   | G     | 8   | HIS  | 4.0  |
| 8   | U     | 7   | LYS  | 4.0  |
| 5   | R     | 77  | PRO  | 4.0  |
| 8   | H     | 50  | VAL  | 4.0  |
| 2   | B     | 113 | TYR  | 3.9  |
| 1   | N     | 514 | LYS  | 3.9  |
| 4   | Q     | 33  | LEU  | 3.9  |
| 13  | Z     | 40  | TYR  | 3.9  |
| 5   | R     | 80  | GLU  | 3.9  |
| 4   | Q     | 39  | ALA  | 3.9  |
| 4   | Q     | 57  | VAL  | 3.9  |
| 7   | T     | 12  | GLY  | 3.8  |
| 10  | W     | 56  | PRO  | 3.8  |
| 8   | U     | 10  | ASN  | 3.8  |
| 2   | O     | 65  | TRP  | 3.7  |
| 4   | D     | 9   | GLU  | 3.7  |
| 2   | O     | 217 | LYS  | 3.7  |
| 5   | R     | 93  | LEU  | 3.7  |
| 4   | Q     | 69  | ALA  | 3.7  |
| 1   | A     | 514 | LYS  | 3.7  |
| 8   | U     | 50  | VAL  | 3.6  |
| 10  | J     | 56  | PRO  | 3.6  |
| 12  | Y     | 45  | LEU  | 3.6  |
| 7   | G     | 42  | ARG  | 3.6  |
| 13  | Z     | 42  | LYS  | 3.6  |
| 5   | R     | 106 | LEU  | 3.6  |
| 12  | Y     | 16  | GLU  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9   | I     | 33  | THR  | 3.5  |
| 12  | L     | 47  | LYS  | 3.5  |
| 8   | U     | 45  | ALA  | 3.5  |
| 10  | J     | 57  | HIS  | 3.5  |
| 12  | Y     | 2   | HIS  | 3.5  |
| 13  | M     | 41  | LYS  | 3.5  |
| 5   | E     | 5   | HIS  | 3.5  |
| 5   | R     | 5   | HIS  | 3.5  |
| 8   | H     | 48  | GLY  | 3.4  |
| 9   | I     | 25  | PHE  | 3.4  |
| 9   | I     | 30  | GLY  | 3.4  |
| 5   | R     | 101 | PRO  | 3.4  |
| 11  | X     | 47  | ARG  | 3.4  |
| 7   | G     | 41  | HIS  | 3.4  |
| 5   | R     | 99  | SER  | 3.4  |
| 12  | Y     | 20  | ARG  | 3.4  |
| 5   | R     | 100 | THR  | 3.4  |
| 8   | H     | 42  | ALA  | 3.3  |
| 4   | Q     | 38  | LYS  | 3.3  |
| 5   | R     | 7   | THR  | 3.3  |
| 9   | I     | 73  | LYS  | 3.2  |
| 2   | O     | 115 | ASP  | 3.2  |
| 9   | I     | 29  | LEU  | 3.2  |
| 4   | Q     | 9   | GLU  | 3.2  |
| 7   | T     | 41  | HIS  | 3.2  |
| 4   | D     | 19  | ARG  | 3.2  |
| 5   | R     | 91  | PRO  | 3.2  |
| 2   | B     | 91  | ASN  | 3.2  |
| 4   | Q     | 32  | ASN  | 3.2  |
| 2   | O     | 129 | LYS  | 3.2  |
| 10  | W     | 55  | PHE  | 3.2  |
| 5   | R     | 14  | ARG  | 3.2  |
| 5   | R     | 82  | TYR  | 3.2  |
| 5   | R     | 87  | GLN  | 3.2  |
| 3   | C     | 38  | ASN  | 3.1  |
| 4   | Q     | 31  | LYS  | 3.1  |
| 7   | T     | 35  | SER  | 3.1  |
| 11  | X     | 7   | PRO  | 3.1  |
| 10  | W     | 17  | GLY  | 3.1  |
| 9   | V     | 36  | LYS  | 3.1  |
| 11  | X     | 52  | GLU  | 3.1  |
| 10  | J     | 52  | TRP  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 10  | W     | 15  | ASP  | 3.1  |
| 4   | D     | 7   | LYS  | 3.0  |
| 8   | U     | 42  | ALA  | 3.0  |
| 8   | H     | 46  | LYS  | 3.0  |
| 4   | Q     | 59  | LEU  | 3.0  |
| 12  | Y     | 44  | LEU  | 3.0  |
| 5   | R     | 104 | LEU  | 2.9  |
| 5   | R     | 94  | ASN  | 2.9  |
| 5   | R     | 81  | ILE  | 2.9  |
| 4   | D     | 74  | SER  | 2.9  |
| 3   | P     | 33  | MET  | 2.9  |
| 5   | E     | 7   | THR  | 2.9  |
| 4   | Q     | 52  | SER  | 2.9  |
| 4   | Q     | 34  | SER  | 2.9  |
| 8   | H     | 49  | ASP  | 2.9  |
| 5   | R     | 6   | GLU  | 2.9  |
| 5   | R     | 88  | GLU  | 2.9  |
| 1   | N     | 113 | LEU  | 2.9  |
| 9   | I     | 53  | ASN  | 2.8  |
| 5   | E     | 83  | PRO  | 2.8  |
| 7   | G     | 45  | PRO  | 2.8  |
| 11  | X     | 13  | TYR  | 2.8  |
| 2   | B     | 32  | PHE  | 2.8  |
| 11  | X     | 20  | SER  | 2.8  |
| 8   | H     | 44  | THR  | 2.8  |
| 8   | H     | 11  | TYR  | 2.8  |
| 9   | I     | 32  | ALA  | 2.8  |
| 13  | Z     | 39  | ASN  | 2.8  |
| 1   | A     | 513 | LEU  | 2.8  |
| 2   | B     | 115 | ASP  | 2.8  |
| 9   | V     | 34  | PHE  | 2.8  |
| 6   | S     | 54  | ASN  | 2.8  |
| 13  | M     | 42  | LYS  | 2.8  |
| 9   | I     | 27  | VAL  | 2.8  |
| 13  | Z     | 3   | ALA  | 2.7  |
| 7   | G     | 84  | LYS  | 2.7  |
| 8   | U     | 53  | CYS  | 2.7  |
| 5   | R     | 78  | HIS  | 2.7  |
| 5   | R     | 102 | GLU  | 2.7  |
| 9   | I     | 11  | GLY  | 2.7  |
| 8   | H     | 51  | SER  | 2.7  |
| 9   | I     | 34  | PHE  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9   | V     | 33  | THR  | 2.7  |
| 7   | T     | 33  | LEU  | 2.7  |
| 4   | Q     | 30  | VAL  | 2.7  |
| 2   | O     | 216 | LEU  | 2.7  |
| 4   | Q     | 55  | GLU  | 2.7  |
| 9   | I     | 6   | LYS  | 2.7  |
| 9   | V     | 6   | LYS  | 2.7  |
| 9   | I     | 8   | GLN  | 2.6  |
| 8   | U     | 52  | VAL  | 2.6  |
| 7   | T     | 43  | GLU  | 2.6  |
| 3   | P     | 44  | MET  | 2.6  |
| 6   | S     | 4   | GLY  | 2.6  |
| 8   | H     | 45  | ALA  | 2.6  |
| 2   | O     | 91  | ASN  | 2.6  |
| 4   | D     | 51  | LEU  | 2.6  |
| 4   | D     | 31  | LYS  | 2.6  |
| 6   | S     | 92  | VAL  | 2.6  |
| 5   | E     | 108 | LYS  | 2.5  |
| 9   | V     | 73  | LYS  | 2.5  |
| 4   | Q     | 17  | VAL  | 2.5  |
| 4   | Q     | 48  | TRP  | 2.5  |
| 1   | N     | 484 | THR  | 2.5  |
| 2   | B     | 92  | ASN  | 2.5  |
| 2   | O     | 126 | SER  | 2.5  |
| 4   | Q     | 28  | ALA  | 2.5  |
| 3   | P     | 38  | ASN  | 2.4  |
| 6   | S     | 37  | LYS  | 2.4  |
| 8   | U     | 61  | LYS  | 2.4  |
| 12  | Y     | 47  | LYS  | 2.4  |
| 9   | V     | 10  | ARG  | 2.4  |
| 7   | G     | 33  | LEU  | 2.4  |
| 5   | R     | 62  | ALA  | 2.4  |
| 9   | I     | 22  | VAL  | 2.4  |
| 13  | Z     | 32  | TRP  | 2.4  |
| 2   | O     | 116 | LEU  | 2.4  |
| 9   | V     | 25  | PHE  | 2.4  |
| 6   | S     | 52  | ILE  | 2.4  |
| 9   | V     | 38  | ALA  | 2.4  |
| 7   | G     | 35  | SER  | 2.4  |
| 5   | R     | 107 | ASP  | 2.3  |
| 4   | Q     | 62  | LEU  | 2.3  |
| 5   | R     | 96  | LEU  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | E     | 81  | ILE  | 2.3  |
| 5   | R     | 75  | ALA  | 2.3  |
| 4   | D     | 147 | LYS  | 2.3  |
| 2   | O     | 61  | VAL  | 2.3  |
| 2   | O     | 220 | GLU  | 2.3  |
| 12  | Y     | 4   | GLU  | 2.3  |
| 9   | V     | 19  | PHE  | 2.3  |
| 2   | O     | 221 | LYS  | 2.3  |
| 4   | Q     | 133 | GLY  | 2.3  |
| 6   | F     | 4   | GLY  | 2.3  |
| 4   | Q     | 47  | SER  | 2.3  |
| 11  | K     | 54  | ARG  | 2.3  |
| 4   | Q     | 70  | GLU  | 2.3  |
| 8   | H     | 39  | CYS  | 2.3  |
| 9   | I     | 26  | MET  | 2.3  |
| 4   | Q     | 147 | LYS  | 2.3  |
| 2   | B     | 58  | ALA  | 2.3  |
| 5   | E     | 14  | ARG  | 2.3  |
| 9   | I     | 15  | ARG  | 2.3  |
| 11  | X     | 54  | ARG  | 2.3  |
| 5   | E     | 9   | GLU  | 2.3  |
| 2   | O     | 222 | TRP  | 2.2  |
| 2   | O     | 32  | PHE  | 2.2  |
| 3   | P     | 37  | PHE  | 2.2  |
| 8   | U     | 11  | TYR  | 2.2  |
| 9   | I     | 7   | PRO  | 2.2  |
| 9   | V     | 72  | ALA  | 2.2  |
| 7   | G     | 43  | GLU  | 2.2  |
| 5   | R     | 8   | ASP  | 2.2  |
| 5   | R     | 13  | ALA  | 2.2  |
| 7   | T     | 46  | ALA  | 2.2  |
| 13  | M     | 38  | ASP  | 2.2  |
| 4   | Q     | 68  | PHE  | 2.2  |
| 9   | V     | 68  | ILE  | 2.2  |
| 8   | H     | 43  | MET  | 2.2  |
| 5   | R     | 65  | VAL  | 2.2  |
| 5   | R     | 70  | VAL  | 2.2  |
| 10  | J     | 17  | GLY  | 2.2  |
| 11  | K     | 7   | PRO  | 2.2  |
| 9   | I     | 31  | PHE  | 2.2  |
| 12  | L     | 3   | TYR  | 2.2  |
| 4   | D     | 73  | ARG  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7   | G     | 46  | ALA  | 2.2  |
| 11  | X     | 16  | ALA  | 2.2  |
| 11  | X     | 48  | VAL  | 2.1  |
| 4   | Q     | 19  | ARG  | 2.1  |
| 3   | C     | 44  | MET  | 2.1  |
| 4   | Q     | 46  | ALA  | 2.1  |
| 4   | D     | 53  | ILE  | 2.1  |
| 2   | B     | 88  | ASP  | 2.1  |
| 4   | Q     | 36  | SER  | 2.1  |
| 5   | E     | 85  | VAL  | 2.1  |
| 7   | T     | 45  | PRO  | 2.1  |
| 12  | L     | 44  | LEU  | 2.1  |
| 9   | I     | 72  | ALA  | 2.1  |
| 8   | U     | 49  | ASP  | 2.1  |
| 4   | Q     | 121 | LYS  | 2.0  |
| 5   | E     | 80  | GLU  | 2.0  |
| 5   | R     | 98  | ILE  | 2.0  |
| 5   | E     | 39  | TYR  | 2.0  |
| 5   | E     | 84  | TYR  | 2.0  |
| 2   | B     | 87  | MET  | 2.0  |
| 3   | C     | 33  | MET  | 2.0  |
| 9   | V     | 30  | GLY  | 2.0  |
| 2   | O     | 92  | ASN  | 2.0  |
| 9   | V     | 22  | VAL  | 2.0  |
| 1   | N     | 483 | LEU  | 2.0  |
| 12  | L     | 45  | LEU  | 2.0  |
| 13  | Z     | 37  | LEU  | 2.0  |
| 4   | D     | 39  | ALA  | 2.0  |
| 5   | E     | 13  | ALA  | 2.0  |
| 2   | B     | 18  | GLU  | 2.0  |
| 5   | R     | 103 | GLU  | 2.0  |
| 4   | Q     | 49  | SER  | 2.0  |
| 2   | B     | 64  | ILE  | 2.0  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 9   | SAC  | V     | 1   | 9/10  | 0.18 | 0.23 | 99,100,104,104              | 0     |
| 7   | TPO  | G     | 11  | 11/12 | 0.46 | 0.31 | 77,85,107,108               | 0     |
| 7   | TPO  | T     | 11  | 11/12 | 0.55 | 0.31 | 76,84,110,112               | 0     |
| 9   | SAC  | I     | 1   | 9/10  | 0.60 | 0.27 | 93,97,99,99                 | 0     |
| 1   | FME  | A     | 1   | 10/11 | 0.84 | 0.15 | 40,45,66,72                 | 0     |
| 1   | FME  | N     | 1   | 10/11 | 0.84 | 0.18 | 39,43,65,69                 | 0     |
| 2   | FME  | O     | 1   | 10/11 | 0.90 | 0.15 | 37,38,47,53                 | 0     |
| 2   | FME  | B     | 1   | 10/11 | 0.93 | 0.13 | 23,31,39,50                 | 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|---------|------|------|-----------------------------|-------|
| 23  | DMU  | P     | 1272 | 33/33   | 0.66 | 0.23 | 73,96,104,105               | 0     |
| 25  | PEK  | T     | 263  | 53/53   | 0.66 | 0.28 | 45,83,100,103               | 0     |
| 22  | CHD  | W     | 1060 | 29/29   | 0.69 | 0.28 | 98,104,106,108              | 0     |
| 23  | DMU  | C     | 272  | 33/33   | 0.70 | 0.22 | 71,97,102,104               | 0     |
| 25  | PEK  | G     | 1263 | 53/53   | 0.71 | 0.27 | 46,83,99,101                | 0     |
| 18  | PGV  | P     | 1268 | 51/51   | 0.71 | 0.27 | 65,84,104,106               | 0     |
| 26  | CDL  | T     | 1269 | 100/100 | 0.71 | 0.26 | 54,84,97,105                | 0     |
| 22  | CHD  | J     | 60   | 29/29   | 0.72 | 0.28 | 98,104,107,109              | 0     |
| 25  | PEK  | C     | 265  | 53/53   | 0.74 | 0.28 | 44,88,103,104               | 0     |
| 20  | TGL  | N     | 1522 | 63/63   | 0.74 | 0.28 | 42,67,79,82                 | 0     |
| 21  | PSC  | B     | 230  | 52/52   | 0.74 | 0.25 | 48,84,113,116               | 0     |
| 26  | CDL  | G     | 269  | 100/100 | 0.74 | 0.27 | 61,83,101,105               | 0     |
| 20  | TGL  | D     | 523  | 63/63   | 0.74 | 0.26 | 47,65,79,82                 | 0     |
| 20  | TGL  | B     | 521  | 63/63   | 0.75 | 0.26 | 49,64,85,90                 | 0     |
| 25  | PEK  | P     | 1265 | 53/53   | 0.75 | 0.29 | 46,89,107,109               | 0     |
| 20  | TGL  | Q     | 1523 | 63/63   | 0.75 | 0.26 | 45,70,80,84                 | 0     |
| 18  | PGV  | C     | 268  | 51/51   | 0.75 | 0.28 | 65,84,103,106               | 0     |
| 26  | CDL  | P     | 1270 | 100/100 | 0.75 | 0.27 | 42,88,101,105               | 0     |
| 20  | TGL  | N     | 1521 | 63/63   | 0.75 | 0.24 | 49,67,84,86                 | 0     |
| 22  | CHD  | C     | 271  | 29/29   | 0.76 | 0.23 | 87,95,96,97                 | 0     |
| 18  | PGV  | A     | 524  | 51/51   | 0.76 | 0.26 | 35,71,101,104               | 0     |

*Continued on next page...*



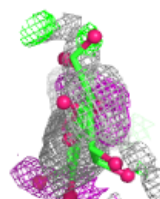
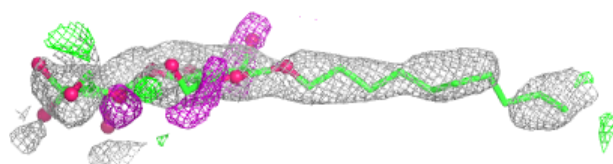
*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms   | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|---------|------|------|-----------------------------|-------|
| 21  | PSC  | O     | 1230 | 52/52   | 0.76 | 0.28 | 48,80,111,116               | 0     |
| 26  | CDL  | C     | 270  | 100/100 | 0.77 | 0.25 | 44,87,100,106               | 0     |
| 18  | PGV  | Z     | 1524 | 51/51   | 0.77 | 0.23 | 38,71,101,104               | 0     |
| 22  | CHD  | P     | 1271 | 29/29   | 0.78 | 0.22 | 89,95,98,101                | 0     |
| 20  | TGL  | L     | 522  | 63/63   | 0.78 | 0.27 | 34,65,79,81                 | 0     |
| 24  | UNX  | P     | 1262 | 1/1     | 0.87 | 0.42 | 43,43,43,43                 | 0     |
| 23  | DMU  | Z     | 1526 | 33/33   | 0.88 | 0.12 | 40,49,61,64                 | 0     |
| 24  | UNX  | C     | 262  | 1/1     | 0.92 | 0.31 | 47,47,47,47                 | 0     |
| 23  | DMU  | M     | 526  | 33/33   | 0.92 | 0.11 | 32,42,55,58                 | 0     |
| 16  | NA   | N     | 1519 | 1/1     | 0.93 | 0.08 | 30,30,30,30                 | 0     |
| 25  | PEK  | P     | 1264 | 53/53   | 0.94 | 0.13 | 25,44,68,72                 | 0     |
| 25  | PEK  | C     | 264  | 53/53   | 0.95 | 0.12 | 10,44,70,73                 | 0     |
| 18  | PGV  | C     | 267  | 51/51   | 0.96 | 0.10 | 20,34,58,62                 | 0     |
| 15  | MG   | N     | 1518 | 1/1     | 0.96 | 0.06 | 26,26,26,26                 | 0     |
| 22  | CHD  | C     | 525  | 29/29   | 0.96 | 0.06 | 21,27,30,33                 | 0     |
| 18  | PGV  | N     | 1266 | 51/51   | 0.96 | 0.11 | 20,38,55,64                 | 0     |
| 18  | PGV  | P     | 1267 | 51/51   | 0.96 | 0.11 | 23,34,59,61                 | 0     |
| 22  | CHD  | P     | 1525 | 29/29   | 0.96 | 0.06 | 20,27,31,34                 | 0     |
| 16  | NA   | A     | 519  | 1/1     | 0.96 | 0.08 | 27,27,27,27                 | 0     |
| 18  | PGV  | A     | 525  | 51/51   | 0.96 | 0.11 | 21,36,56,63                 | 0     |
| 22  | CHD  | O     | 229  | 29/29   | 0.97 | 0.05 | 19,22,28,32                 | 0     |
| 22  | CHD  | B     | 1086 | 29/29   | 0.97 | 0.06 | 20,24,30,37                 | 0     |
| 19  | CUA  | O     | 228  | 2/2     | 0.98 | 0.04 | 26,26,26,27                 | 0     |
| 15  | MG   | A     | 518  | 1/1     | 0.98 | 0.03 | 20,20,20,20                 | 0     |
| 17  | HEA  | N     | 515  | 60/60   | 0.98 | 0.06 | 18,24,41,43                 | 0     |
| 17  | HEA  | A     | 516  | 60/60   | 0.99 | 0.05 | 15,18,29,29                 | 0     |
| 17  | HEA  | A     | 515  | 60/60   | 0.99 | 0.06 | 12,20,44,45                 | 0     |
| 19  | CUA  | B     | 228  | 2/2     | 0.99 | 0.02 | 19,19,19,22                 | 0     |
| 17  | HEA  | N     | 516  | 60/60   | 0.99 | 0.05 | 17,20,29,31                 | 0     |
| 27  | ZN   | F     | 99   | 1/1     | 0.99 | 0.02 | 25,25,25,25                 | 0     |
| 27  | ZN   | S     | 99   | 1/1     | 0.99 | 0.02 | 27,27,27,27                 | 0     |
| 14  | CU   | A     | 517  | 1/1     | 1.00 | 0.01 | 20,20,20,20                 | 0     |
| 14  | CU   | N     | 517  | 1/1     | 1.00 | 0.01 | 21,21,21,21                 | 0     |

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

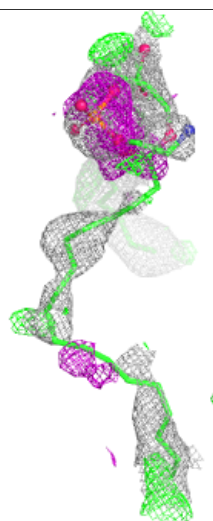
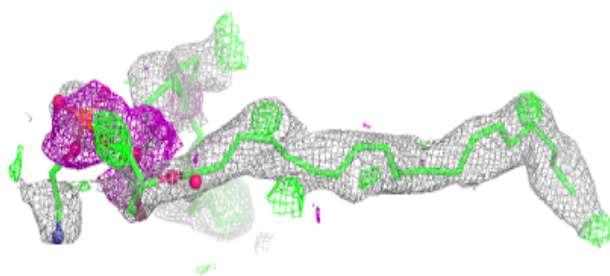
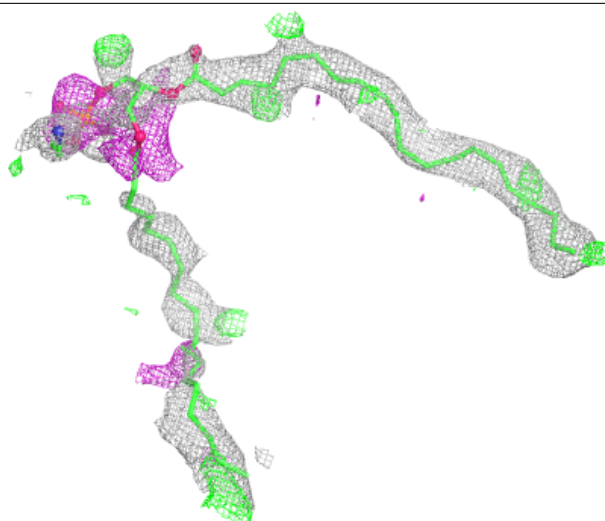
**Electron density around DMU P 1272:**

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



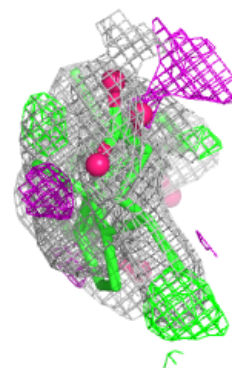
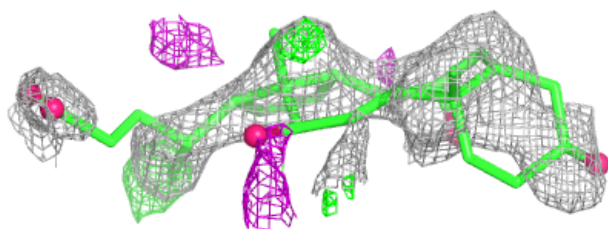
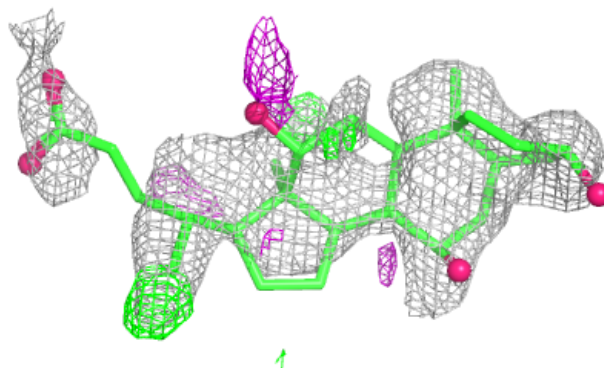
**Electron density around PEK T 263:**

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

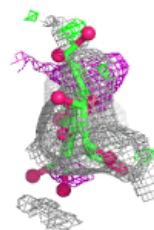
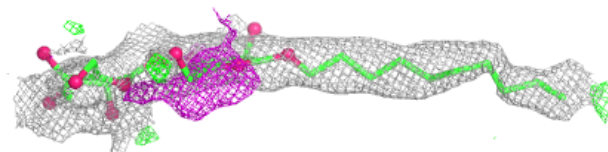
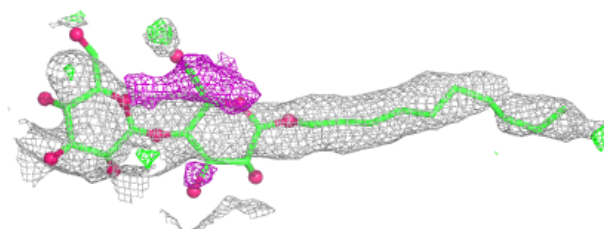


**Electron density around CHD W 1060:**

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

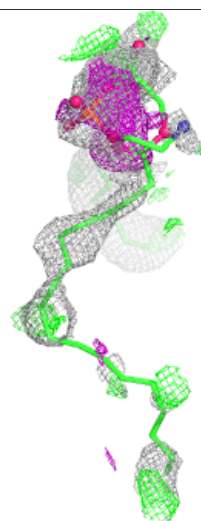
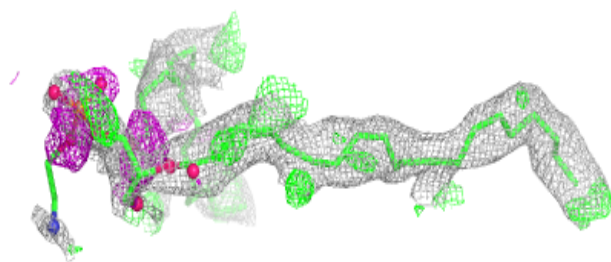
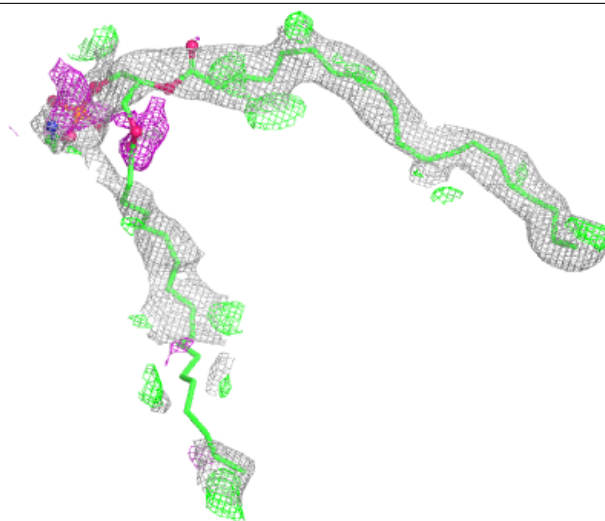
**Electron density around DMU C 272:**

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



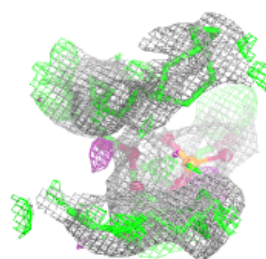
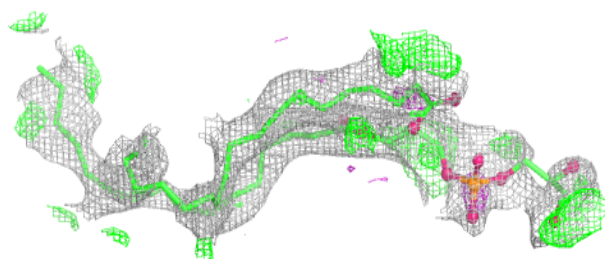
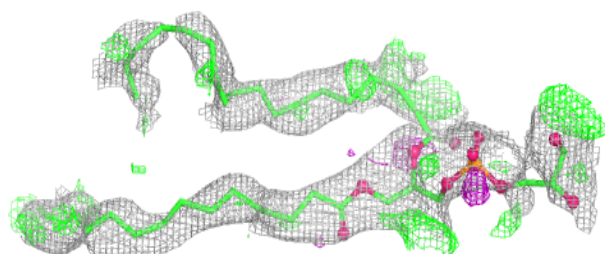
**Electron density around PEK G 1263:**

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

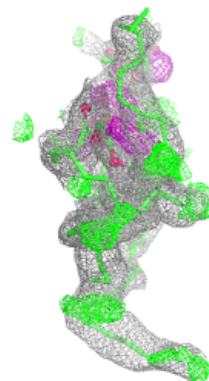
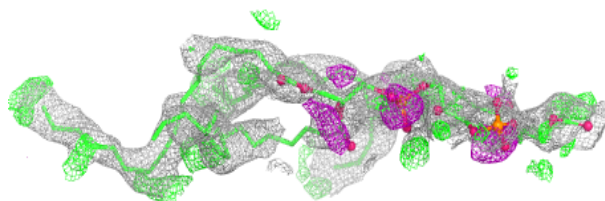
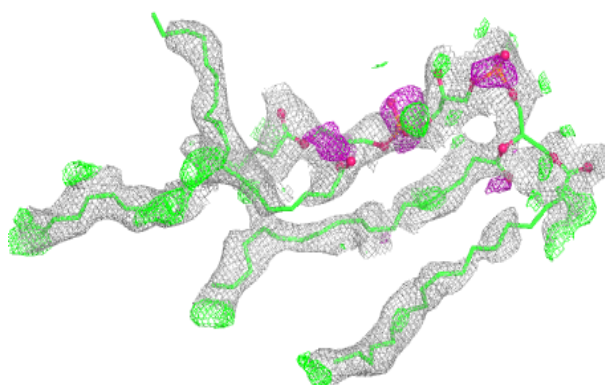


**Electron density around PGV P 1268:**

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

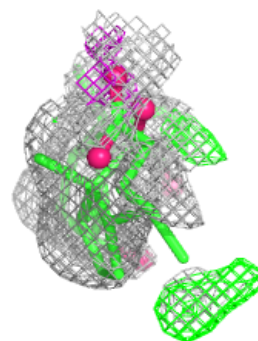
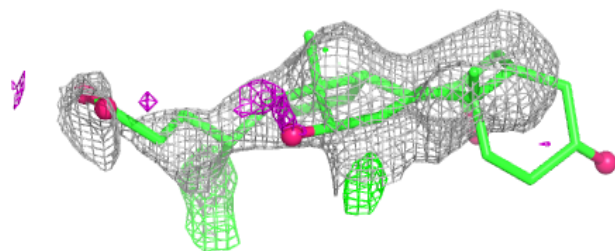
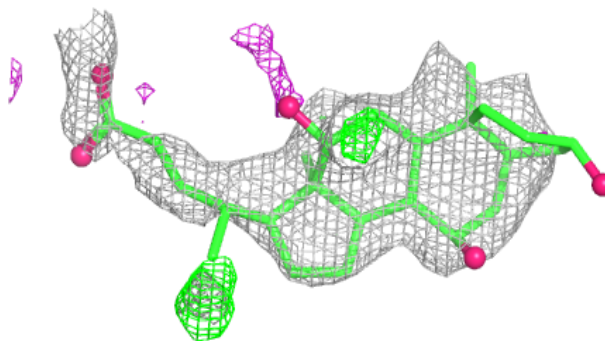
**Electron density around CDL T 1269:**

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



**Electron density around CHD J 60:**

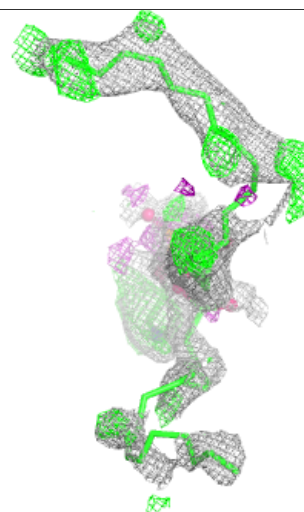
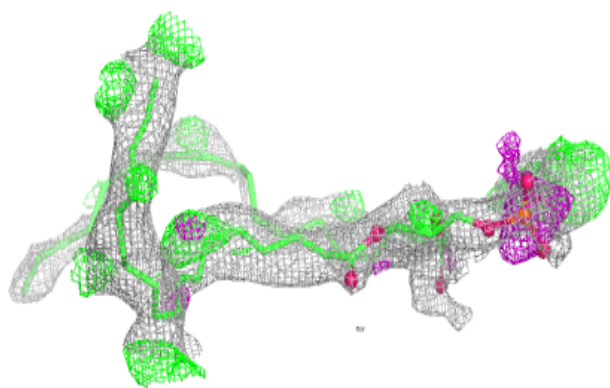
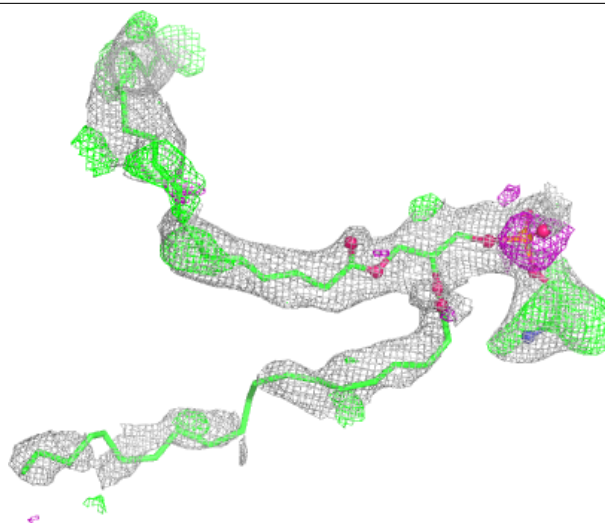
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PEK C 265:**

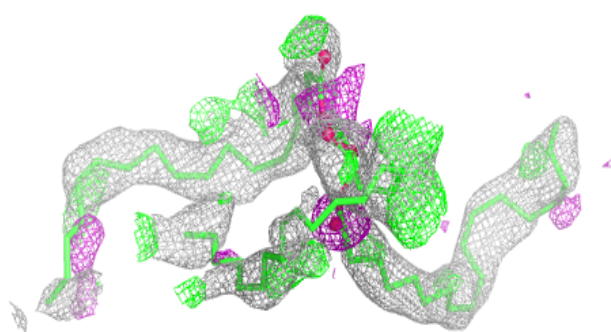
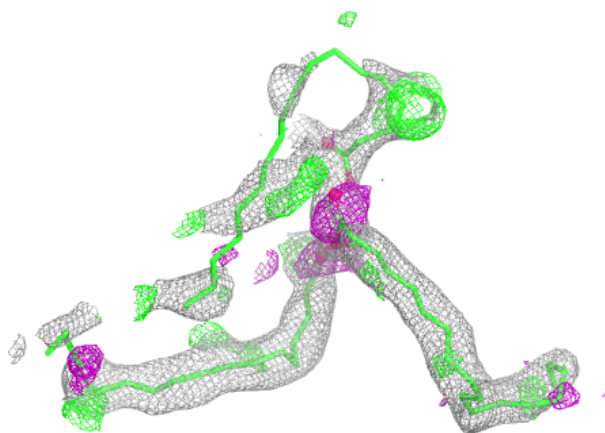
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



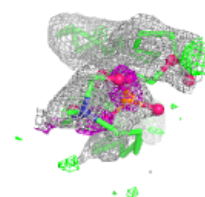
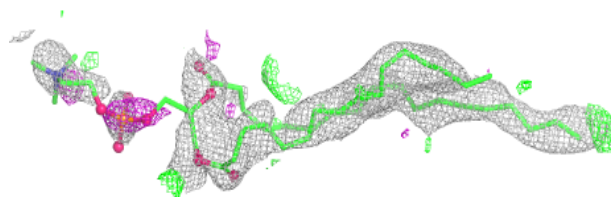
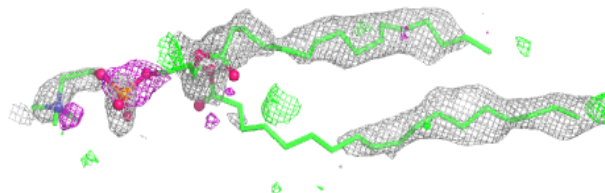


**Electron density around TGL N 1522:**

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

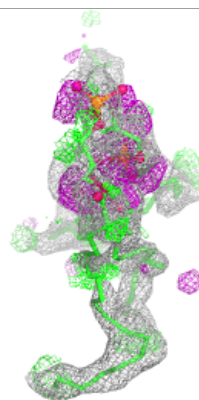
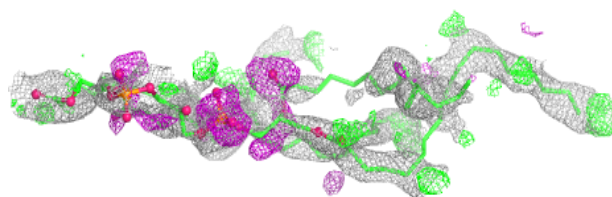
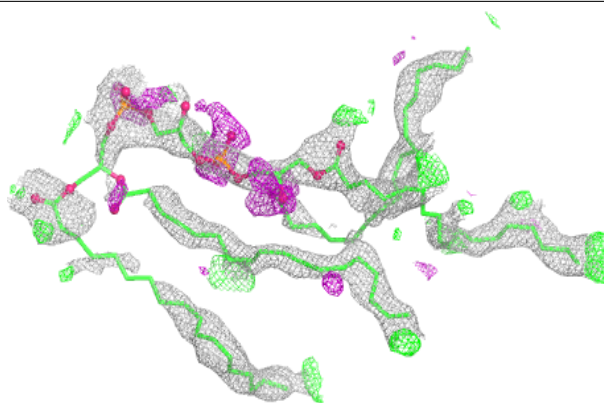
**Electron density around PSC B 230:**

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

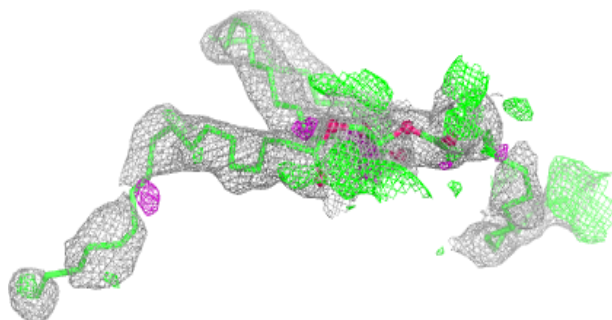
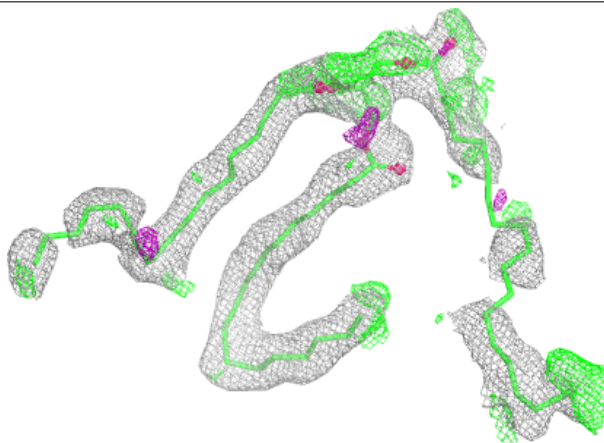


**Electron density around CDL G 269:**

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and green (positive)

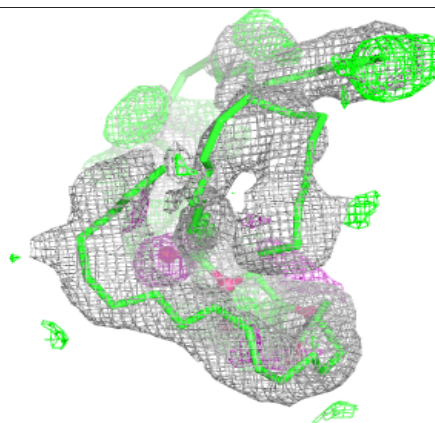
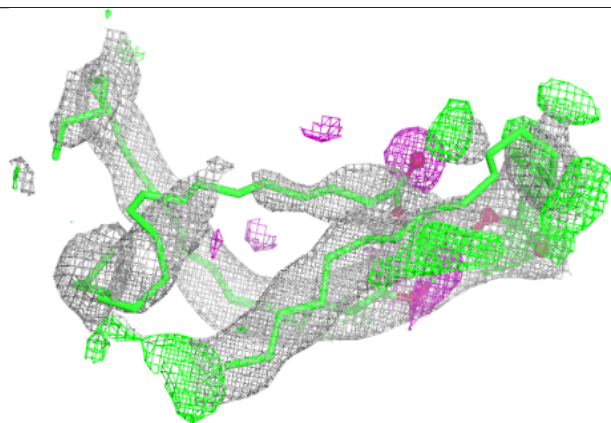
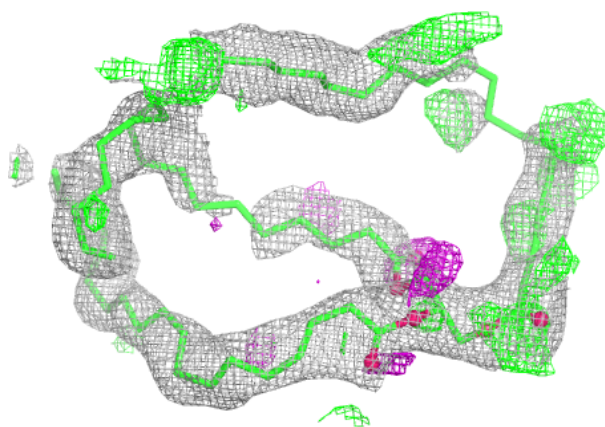
**Electron density around TGL D 523:**

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



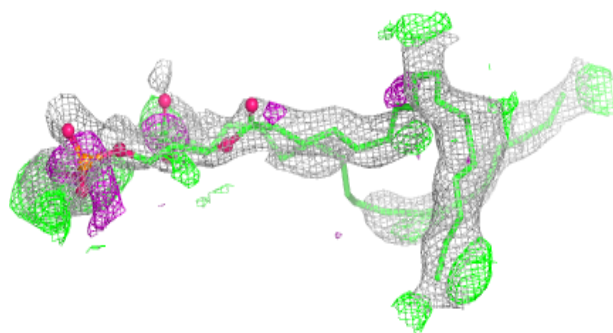
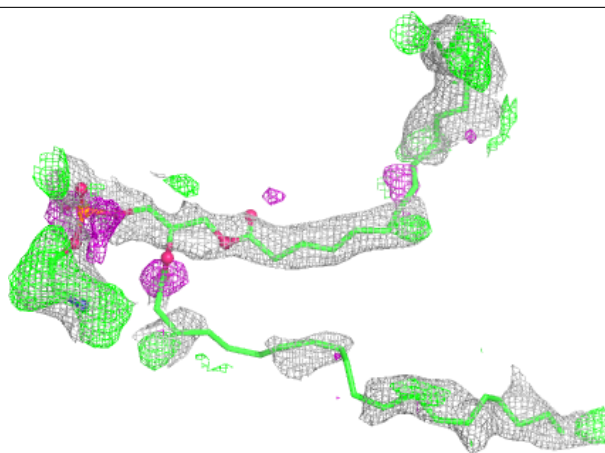
**Electron density around TGL B 521:**

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



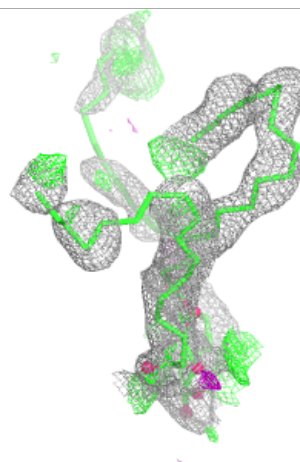
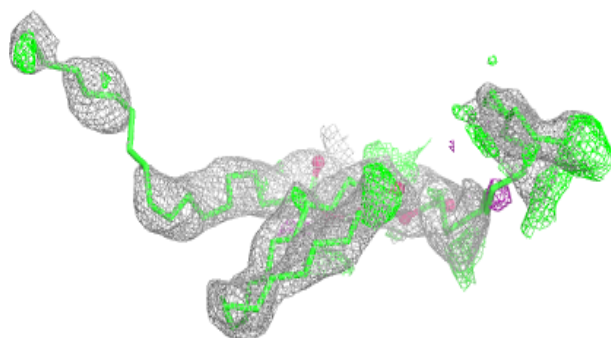
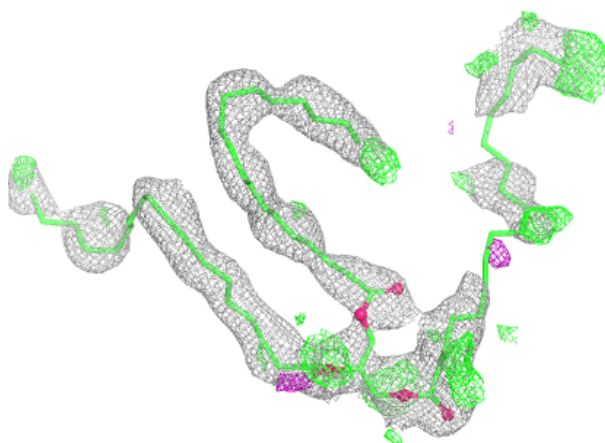
**Electron density around PEK P 1265:**

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



**Electron density around TGL Q 1523:**

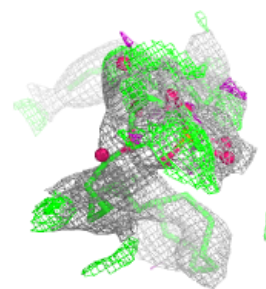
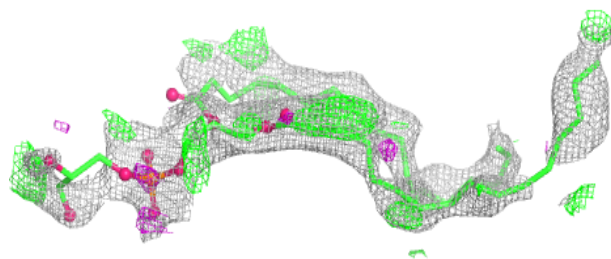
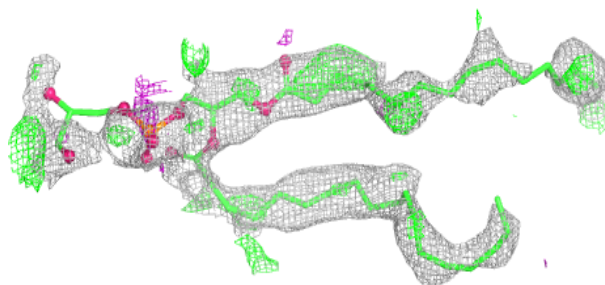
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



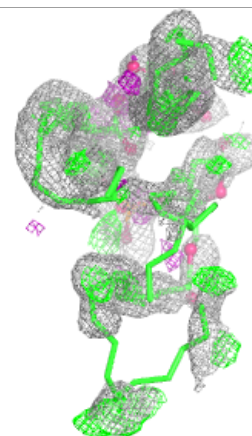
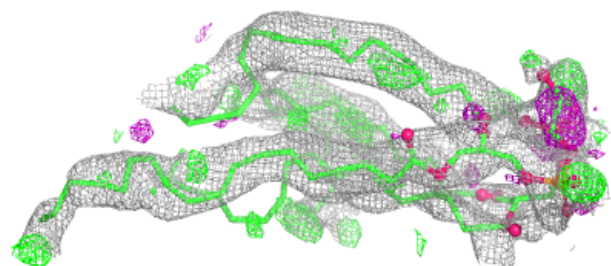
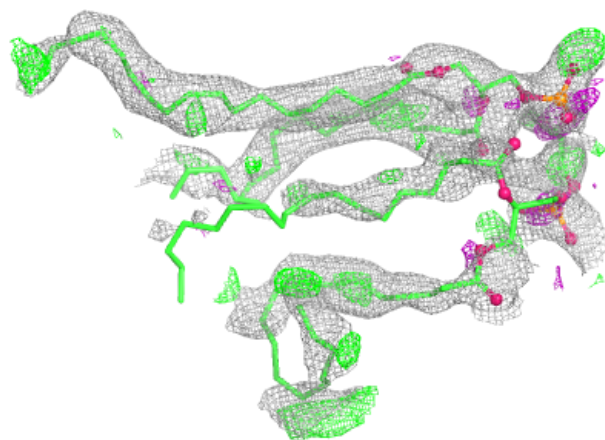


**Electron density around PGV C 268:**

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

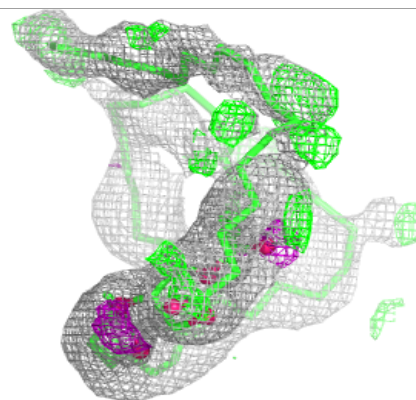
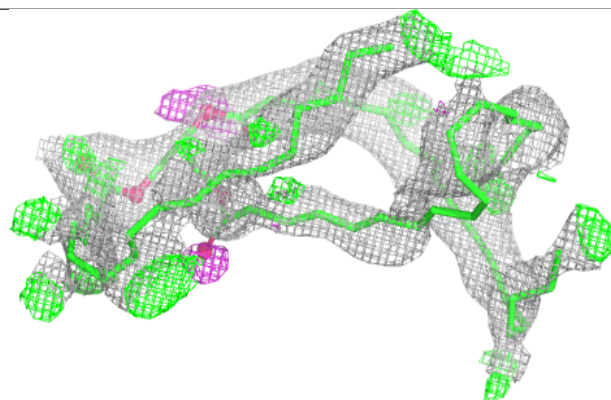
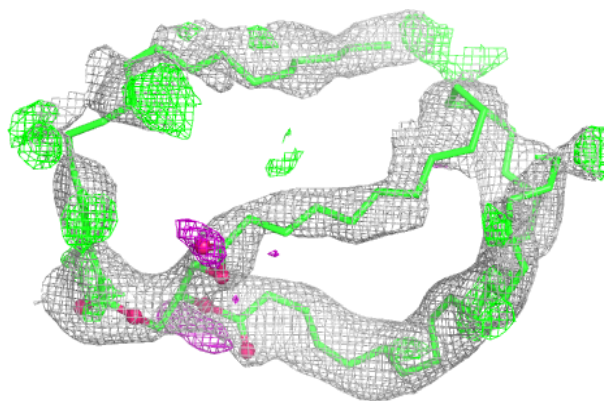
**Electron density around CDL P 1270:**

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

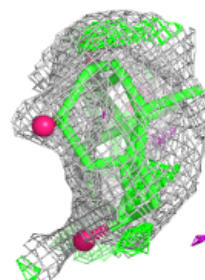
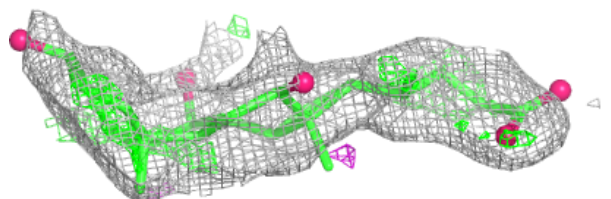
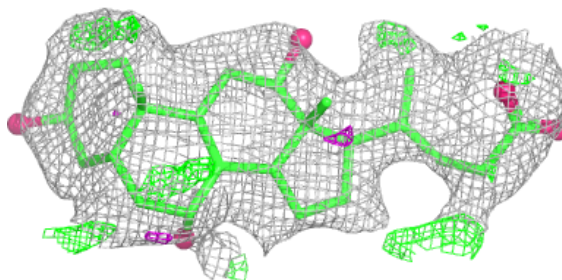


**Electron density around TGL N 1521:**

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

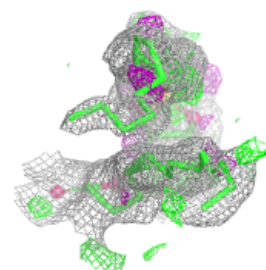
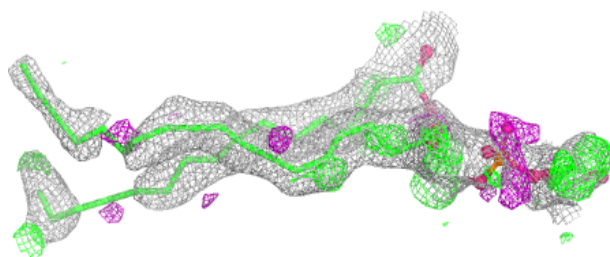
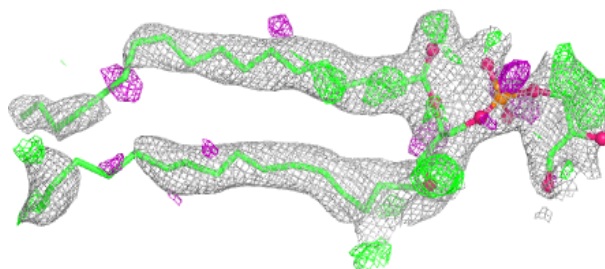
**Electron density around CHD C 271:**

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

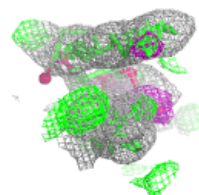
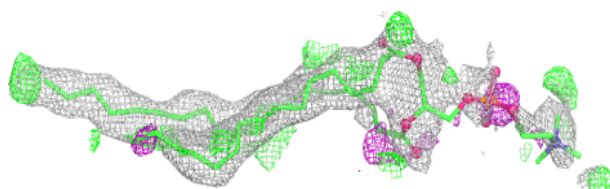
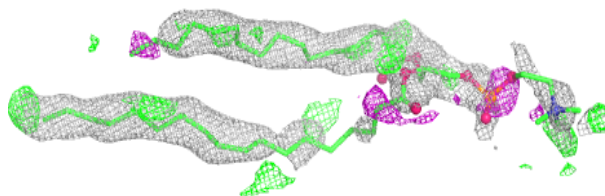


**Electron density around PGV A 524:**

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

**Electron density around PSC O 1230:**

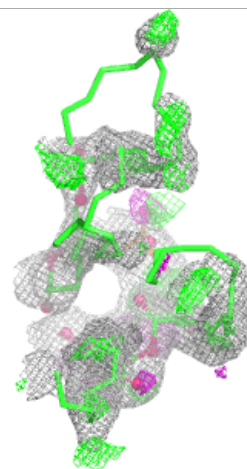
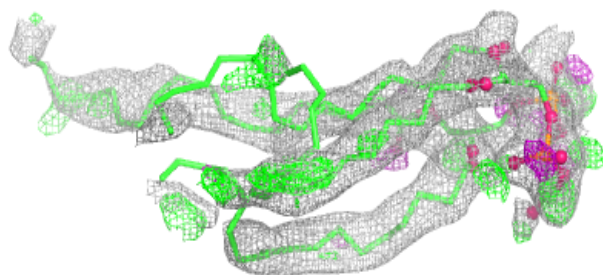
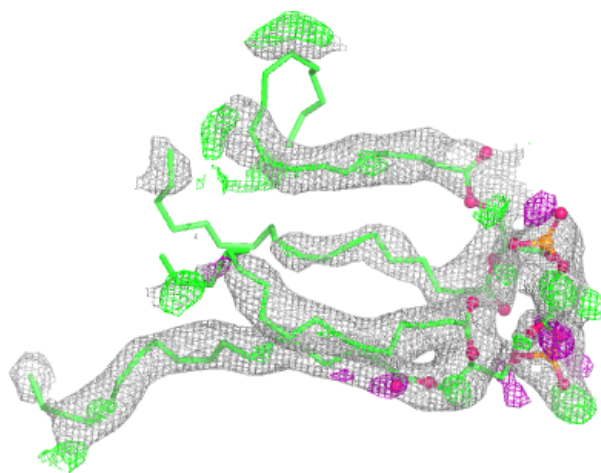
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





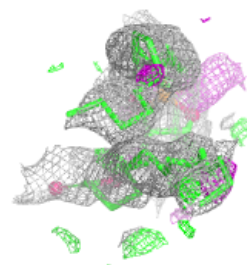
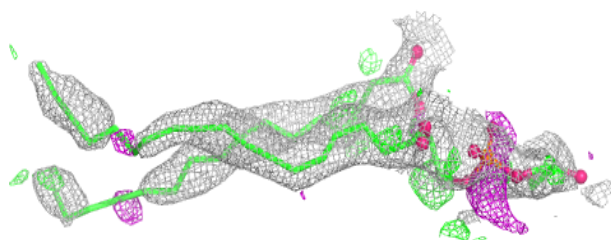
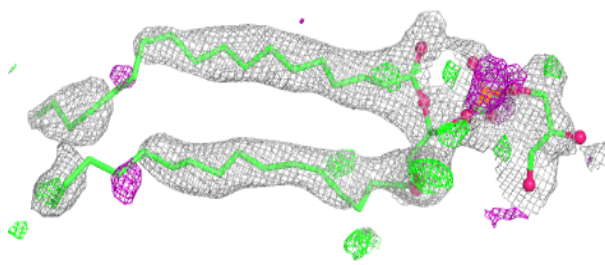
**Electron density around CDL C 270:**

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

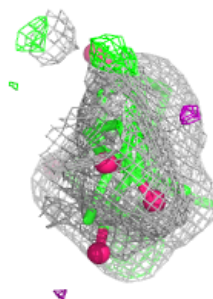
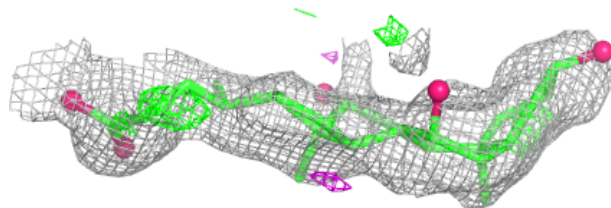
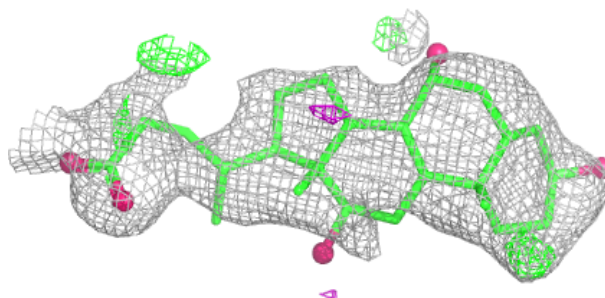


**Electron density around PGV Z 1524:**

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

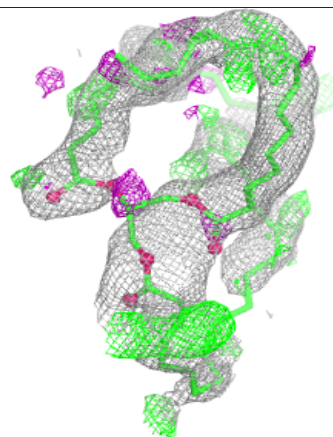
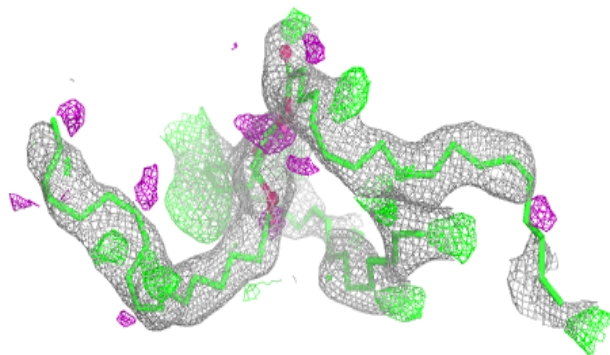
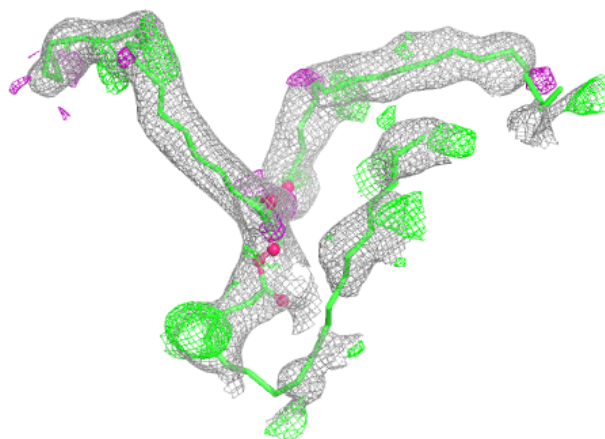
**Electron density around CHD P 1271:**

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



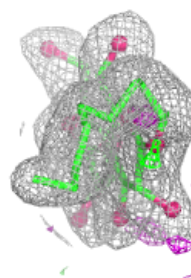
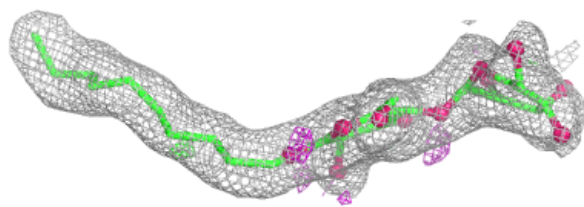
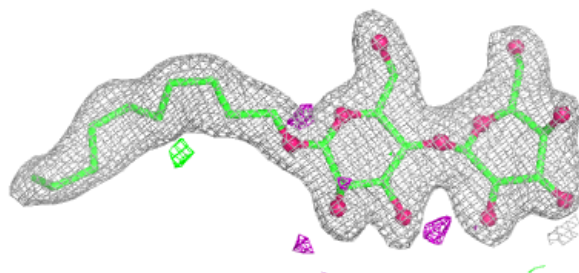
**Electron density around TGL L 522:**

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

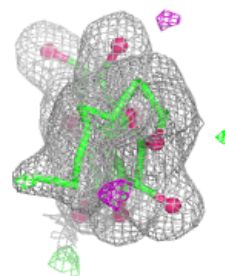
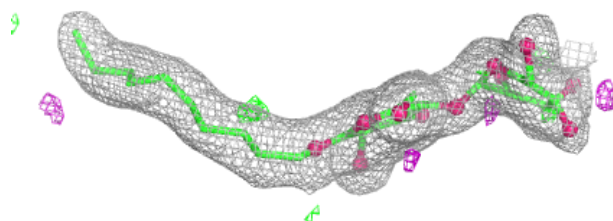
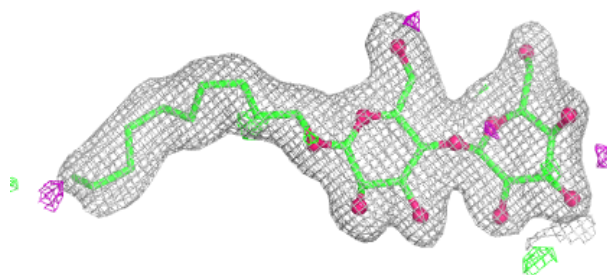


**Electron density around DMU Z 1526:**

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

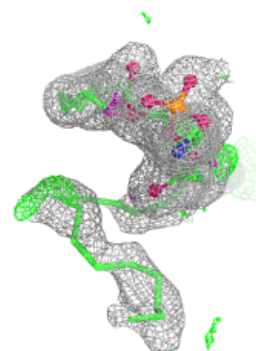
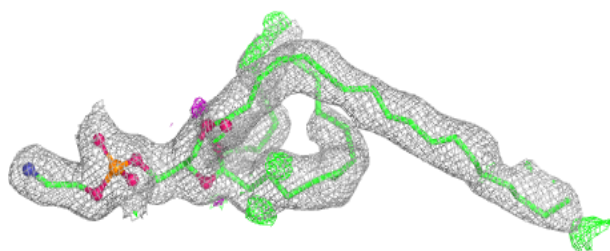
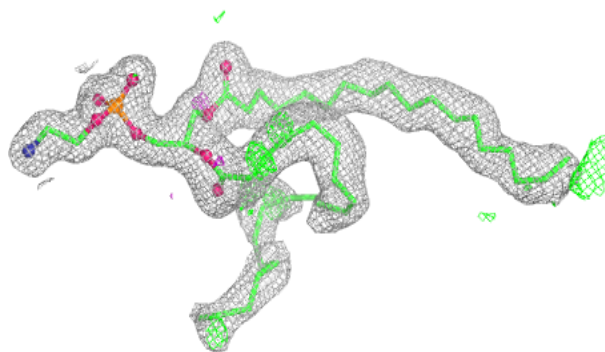
**Electron density around DMU M 526:**

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

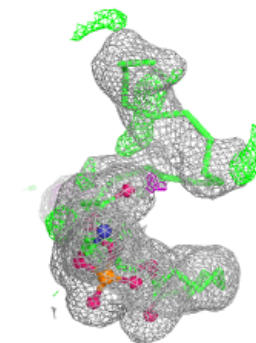
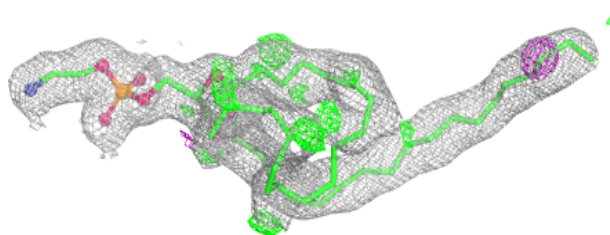
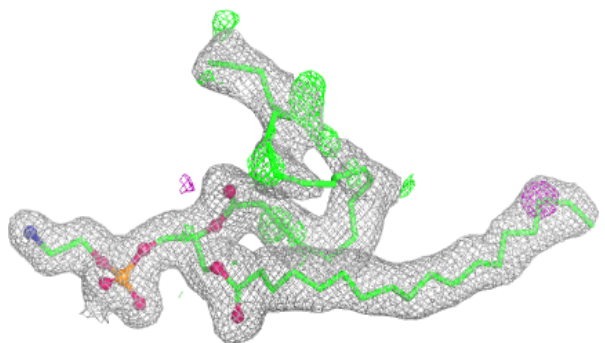


**Electron density around PEK P 1264:**

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

**Electron density around PEK C 264:**

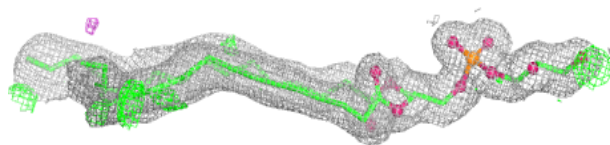
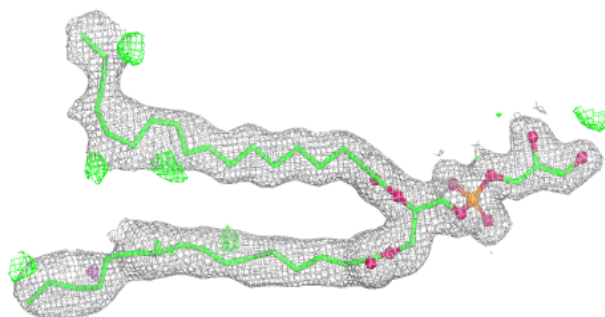
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



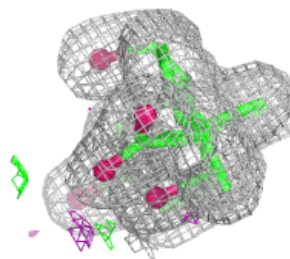
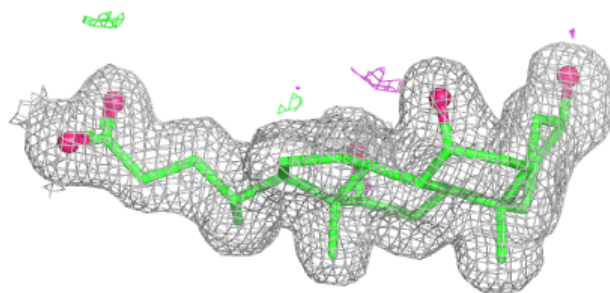
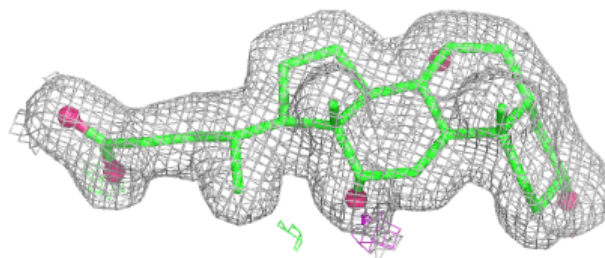


**Electron density around PGV C 267:**

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

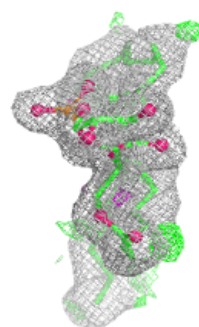
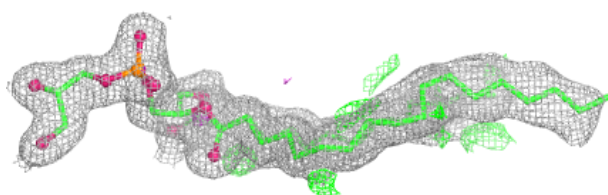
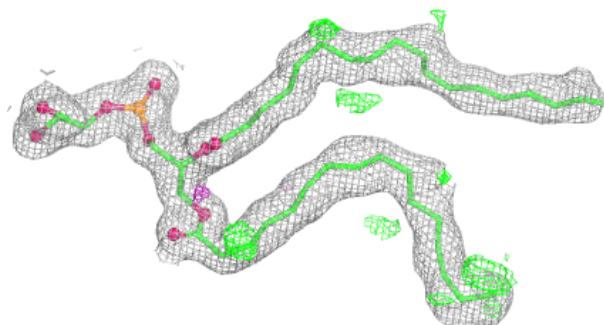
**Electron density around CHD C 525:**

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

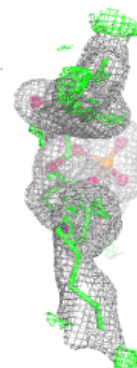
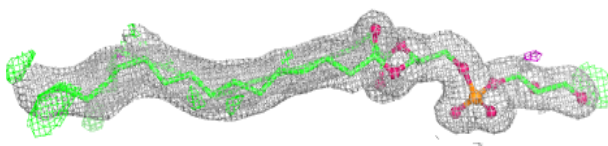
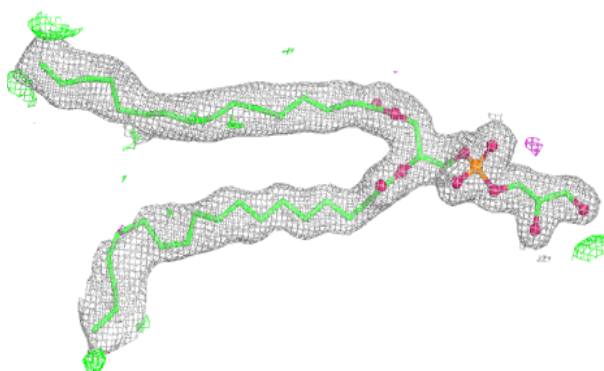


**Electron density around PGV N 1266:**

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

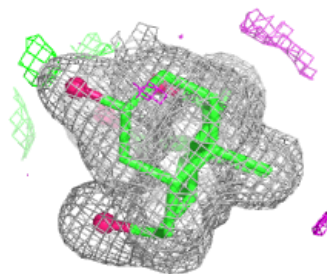
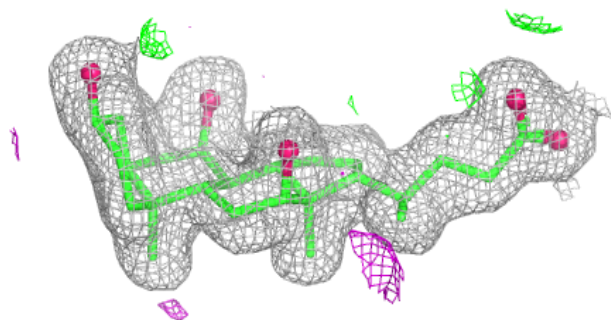
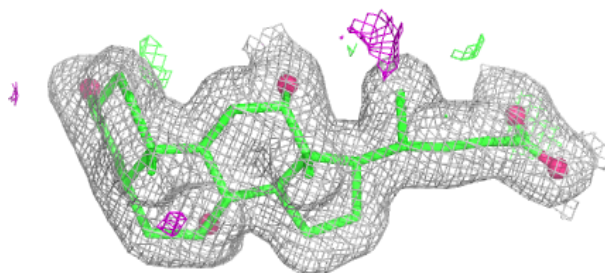
**Electron density around PGV P 1267:**

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

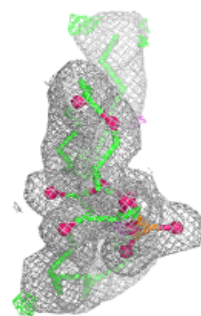
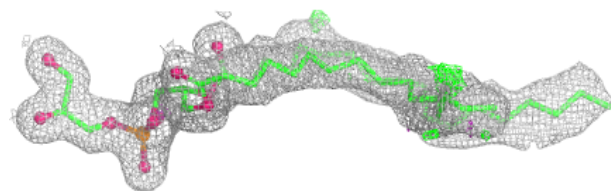
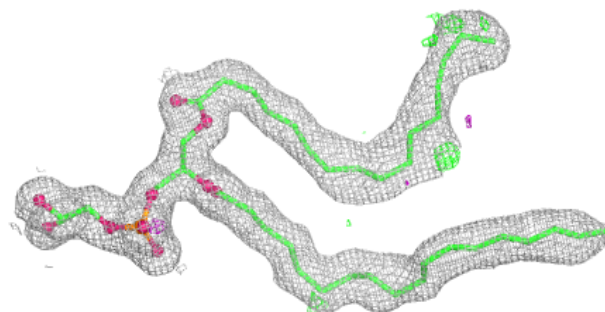


**Electron density around CHD P 1525:**

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

**Electron density around PGV A 525:**

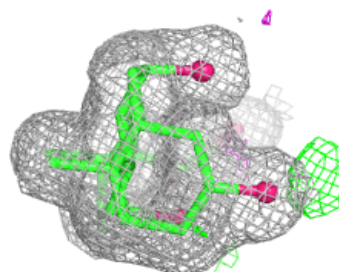
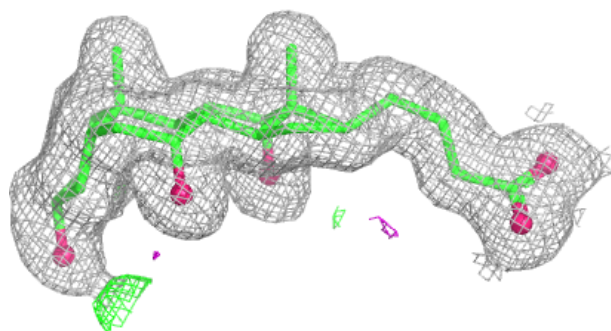
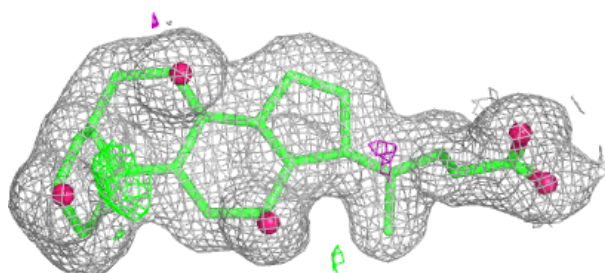
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



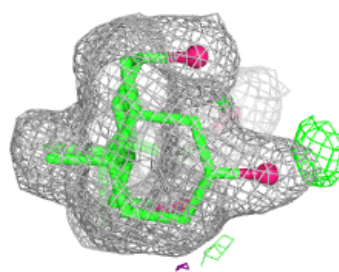
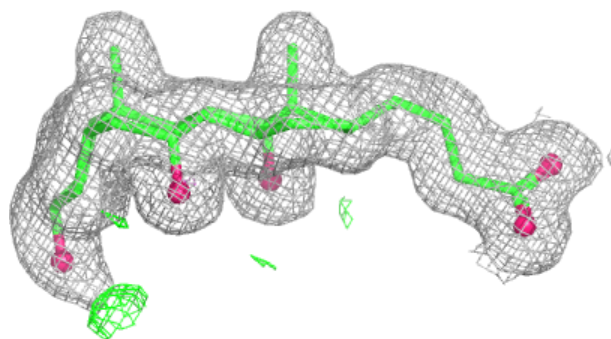
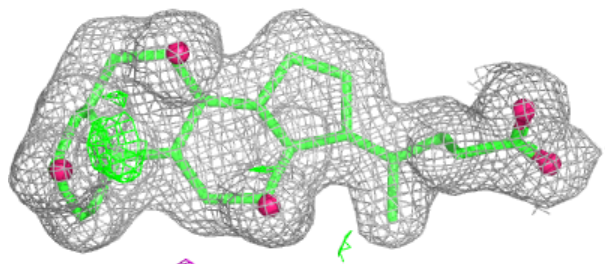


**Electron density around CHD O 229:**

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

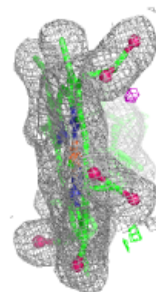
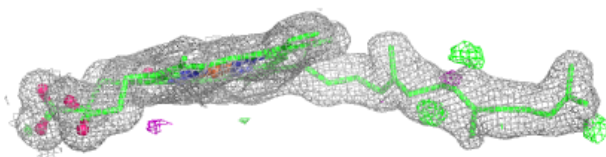
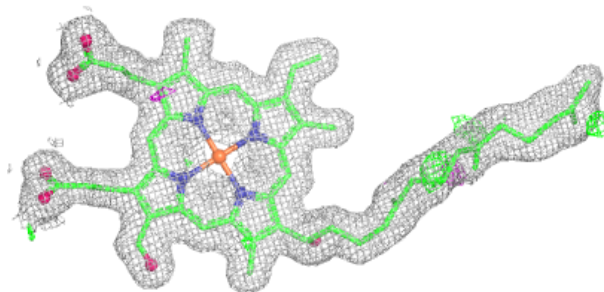
**Electron density around CHD B 1086:**

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

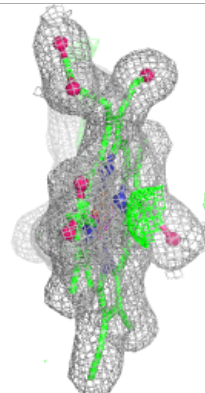
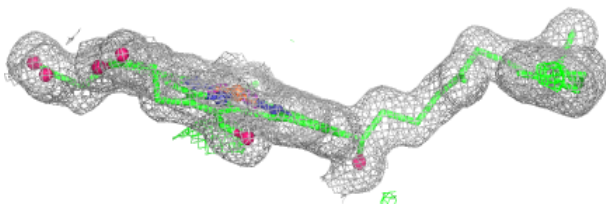
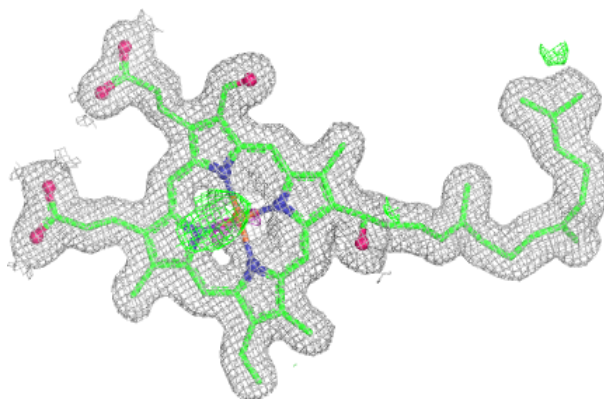


**Electron density around HEA N 515:**

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

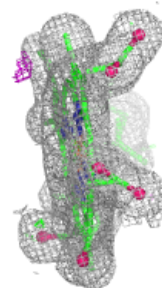
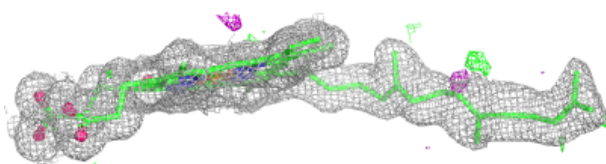
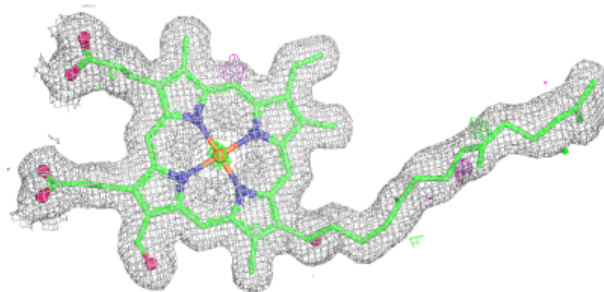
**Electron density around HEA A 516:**

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

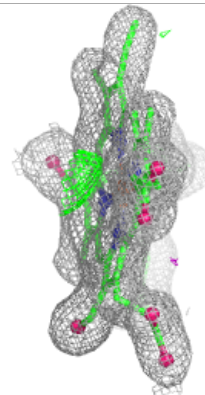
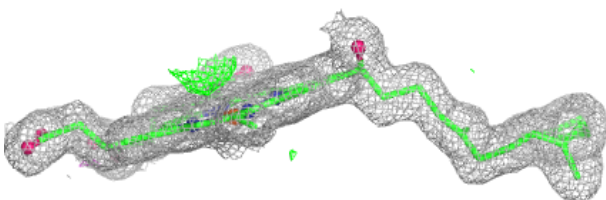
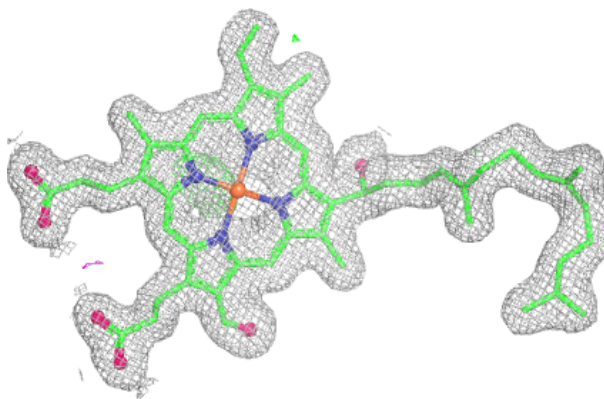


**Electron density around HEA A 515:**

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

**Electron density around HEA N 516:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.