



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:38 PM BST

PDB ID : 1PPJ  
Title : Bovine cytochrome bc1 complex with stigmatellin and antimycin  
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.  
Deposited on : 2003-06-16  
Resolution : 2.10 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

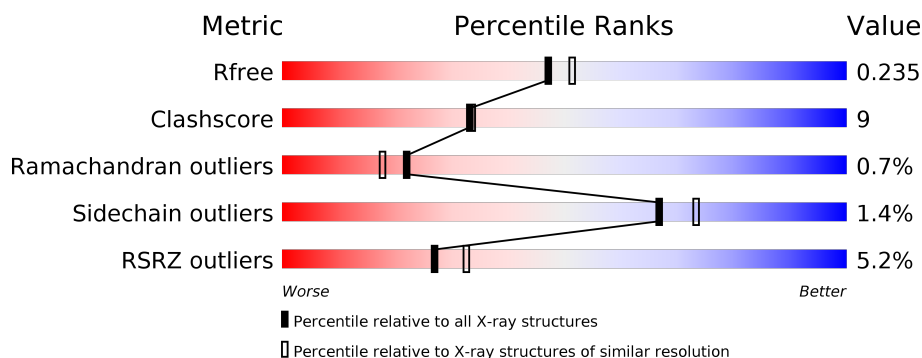
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 5197 (2.10-2.10)                                      |
| Clashscore            | 141614                      | 5710 (2.10-2.10)                                      |
| Ramachandran outliers | 138981                      | 5647 (2.10-2.10)                                      |
| Sidechain outliers    | 138945                      | 5648 (2.10-2.10)                                      |
| RSRZ outliers         | 127900                      | 5083 (2.10-2.10)                                      |

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 on 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     | 446    | <div> <div>2%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div> |
| 1   | N     | 446    | <div> <div>5%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div> |
| 2   | B     | 439    | <div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>.</div> </div> </div>  |
| 2   | O     | 439    | <div> <div>3%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>.</div> </div> </div>  |
| 3   | C     | 379    | <div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>  |
| 3   | P     | 379    | <div> <div>%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | D     | 241    |                  |
| 4   | Q     | 241    |                  |
| 5   | E     | 196    |                  |
| 5   | R     | 196    |                  |
| 6   | F     | 110    |                  |
| 6   | S     | 110    |                  |
| 7   | G     | 81     |                  |
| 7   | T     | 81     |                  |
| 8   | H     | 78     |                  |
| 8   | U     | 78     |                  |
| 9   | I     | 78     |                  |
| 9   | V     | 78     |                  |
| 10  | J     | 62     |                  |
| 10  | W     | 62     |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 11  | JZR  | C     | 4002 | -         | -        | -       | X                |
| 11  | JZR  | D     | 4003 | -         | -        | -       | X                |
| 11  | JZR  | F     | 3011 | -         | -        | -       | X                |
| 11  | JZR  | F     | 4001 | -         | -        | -       | X                |
| 11  | JZR  | S     | 2011 | -         | -        | -       | X                |
| 13  | AZI  | A     | 4011 | -         | -        | -       | X                |
| 13  | AZI  | O     | 4010 | -         | -        | -       | X                |
| 14  | GOL  | B     | 2009 | -         | -        | -       | X                |
| 14  | GOL  | C     | 4006 | -         | -        | -       | X                |
| 14  | GOL  | O     | 3009 | -         | -        | -       | X                |
| 18  | ANY  | P     | 3002 | X         | -        | -       | -                |

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 33549 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 Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 442      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 3396  | 2117 | 601 | 658 | 20 |         |         |       |
| 1   | N     | 442      | Total | C    | N   | O   | S  | 10      | 0       | 1     |
|     |       |          | 3396  | 2117 | 601 | 658 | 20 |         |         |       |

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 424      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 3178  | 1997 | 562 | 612 | 7 |         |         |       |
| 2   | O     | 424      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 3156  | 1984 | 558 | 607 | 7 |         |         |       |

- Molecule 3 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 365      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2892  | 1940 | 450 | 485 | 17 |         |         |       |
| 3   | P     | 365      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2891  | 1940 | 449 | 485 | 17 |         |         |       |

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 241      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1919  | 1225 | 330 | 349 | 15 |         |         |       |
| 4   | Q     | 241      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1919  | 1225 | 330 | 349 | 15 |         |         |       |

- Molecule 5 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1510  | 954 | 263 | 285 | 8 |         |         |       |
| 5   | R     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1517  | 956 | 263 | 290 | 8 |         |         |       |

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 861   | 545 | 155 | 159 | 2 |         |         |       |
| 6   | S     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 861   | 545 | 155 | 159 | 2 |         |         |       |

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 7   | G     | 75       | Total | C   | N   | O  | S | 0       | 0       | 2     |
|     |       |          | 621   | 406 | 117 | 97 | 1 |         |         |       |
| 7   | T     | 76       | Total | C   | N   | O  | S | 0       | 0       | 2     |
|     |       |          | 626   | 409 | 118 | 98 | 1 |         |         |       |

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

| Mol | Chain | Residues | Atoms |     |    |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 8   | H     | 66       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 539   | 327 | 98 | 109 | 5 |         |         |       |
| 8   | U     | 66       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 539   | 327 | 98 | 109 | 5 |         |         |       |

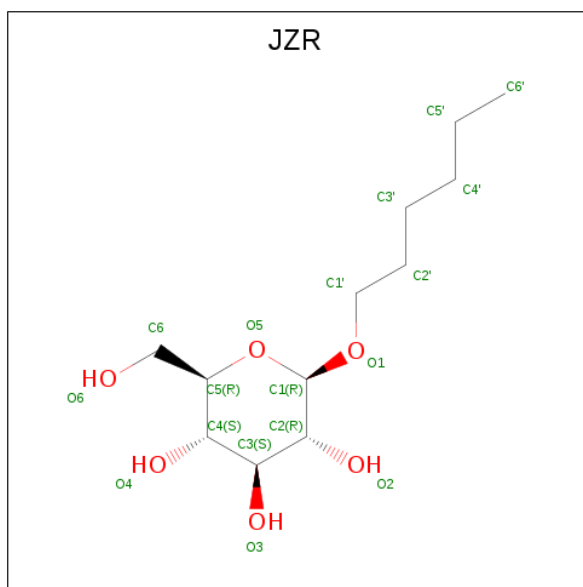
- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | I     | 43       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 285   | 175 | 53 | 56 | 1 |         |         |       |
| 9   | V     | 43       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 285   | 175 | 53 | 56 | 1 |         |         |       |

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10  | J     | 33       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 284   | 185 | 50 | 49 |         |         |       |
| 10  | W     | 62       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 506   | 332 | 88 | 86 |         |         |       |

- Molecule 11 is hexyl beta-D-glucopyranoside (three-letter code: JZR) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>6</sub>).



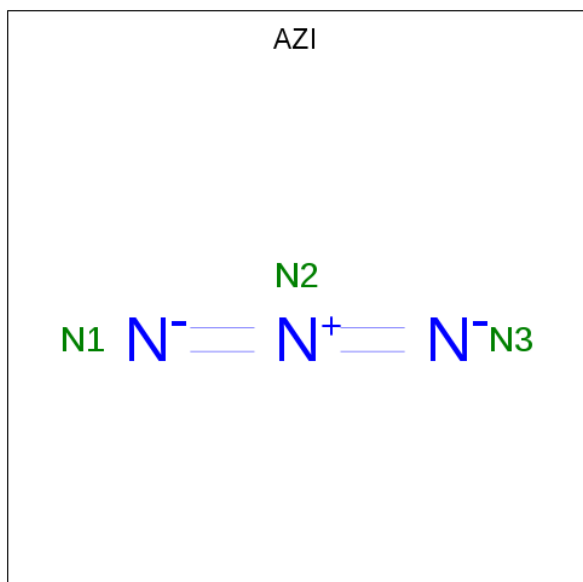
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 11  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 12 | 6 |         |         |
| 11  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 12 | 6 |         |         |
| 11  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 12 | 6 |         |         |
| 11  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 12 | 6 |         |         |
| 11  | F     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 12 | 6 |         |         |
| 11  | F     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 12 | 6 |         |         |
| 11  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 12 | 6 |         |         |
| 11  | R     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 12 | 6 |         |         |
| 11  | S     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 12 | 6 |         |         |

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



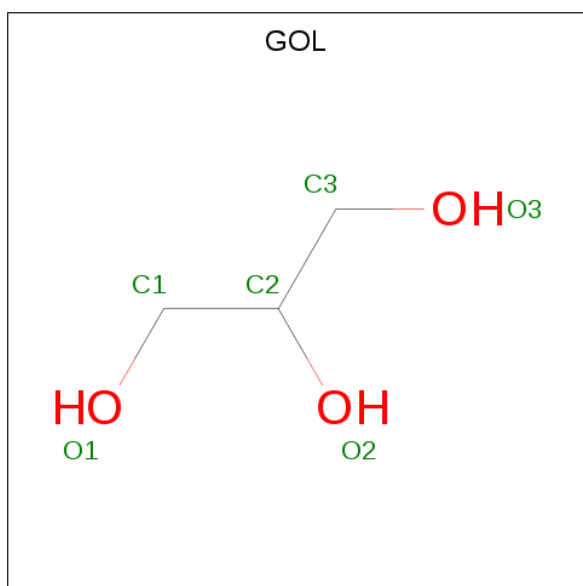
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 12  | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 12  | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 12  | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 12  | P     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 12  | S     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 13 is AZIDE ION (three-letter code: AZI) (formula:  $N_3$ ).



| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 13  | A     | 1        | Total N<br>3 3 | 0       | 0       |
| 13  | C     | 1        | Total N<br>3 3 | 0       | 0       |
| 13  | G     | 1        | Total N<br>3 3 | 0       | 0       |
| 13  | O     | 1        | Total N<br>3 3 | 0       | 0       |
| 13  | P     | 1        | Total N<br>3 3 | 0       | 0       |

- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

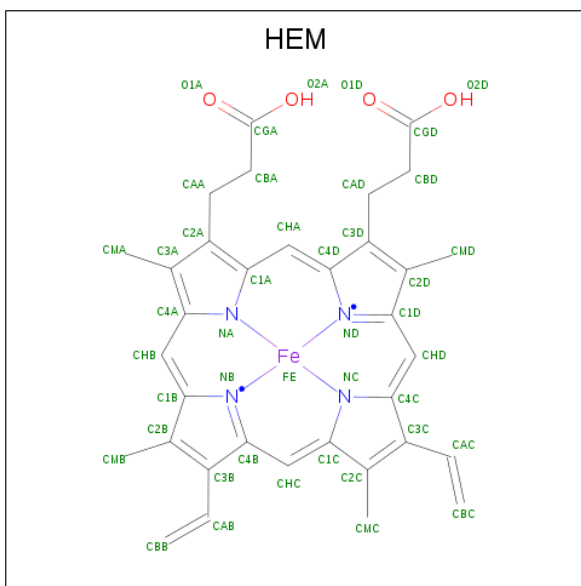


| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 14  | B     | 1        | Total C O<br>6 3 3 | 0       | 0       |
| 14  | C     | 1        | Total C O<br>6 3 3 | 0       | 0       |
| 14  | C     | 1        | Total C O<br>6 3 3 | 0       | 0       |
| 14  | O     | 1        | Total C O<br>6 3 3 | 0       | 0       |
| 14  | P     | 1        | Total C O<br>6 3 3 | 0       | 0       |
| 14  | R     | 1        | Total C O<br>6 3 3 | 0       | 0       |

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

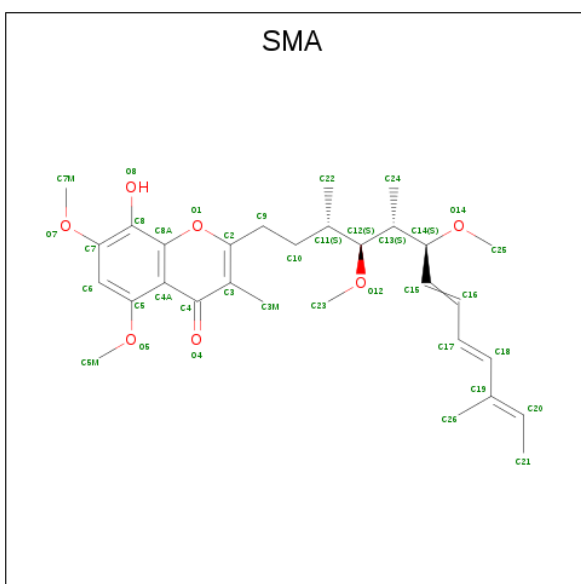


mula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



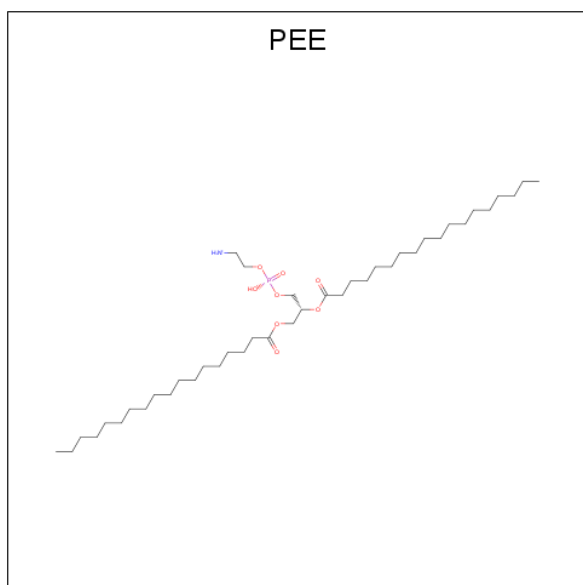
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 15  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 15  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 15  | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 15  | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 16 is STIGMATELLIN A (three-letter code: SMA) (formula:  $\text{C}_{30}\text{H}_{42}\text{O}_7$ ).



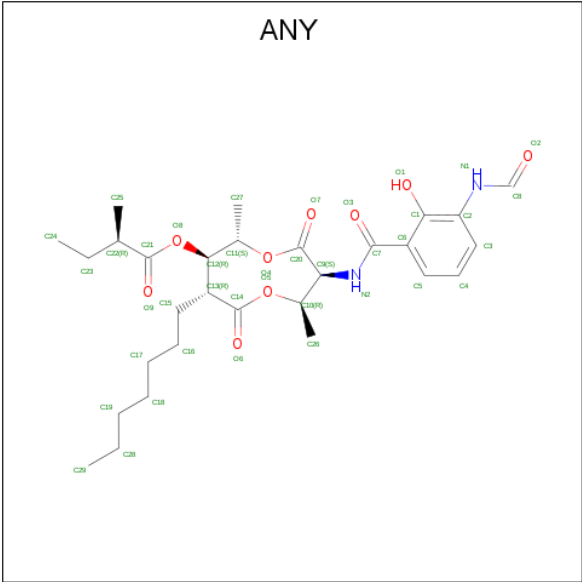
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 16  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 30 | 7 |         |         |
| 16  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 30 | 7 |         |         |

- Molecule 17 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C<sub>41</sub>H<sub>83</sub>NO<sub>8</sub>P).



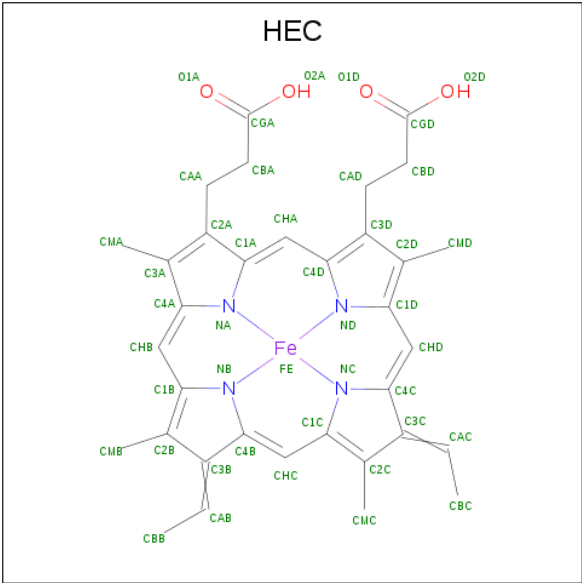
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 17  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |         |
| 17  | D     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 26    | 16 | 1 | 8 | 1 |         |         |
| 17  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |         |
| 17  | Q     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |

- Molecule 18 is 2-METHYL-BUTYRIC ACID 3-(3-FORMYLAMINO-2-HYDROXY-BENZ OYLAMINO)-8-HEPTYL-2,6-DIMETHYL-4,9-DIOXO-[1,5]DIOXONAN-7-YL ESTER (three-letter code: ANY) (formula: C<sub>29</sub>H<sub>42</sub>N<sub>2</sub>O<sub>9</sub>).



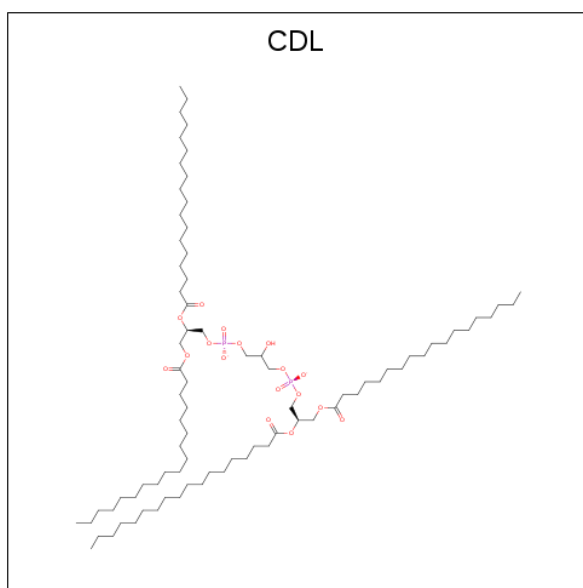
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 18  | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 37    | 26 | 2 | 9 |         |         |
| 18  | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 37    | 26 | 2 | 9 |         |         |

- Molecule 19 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



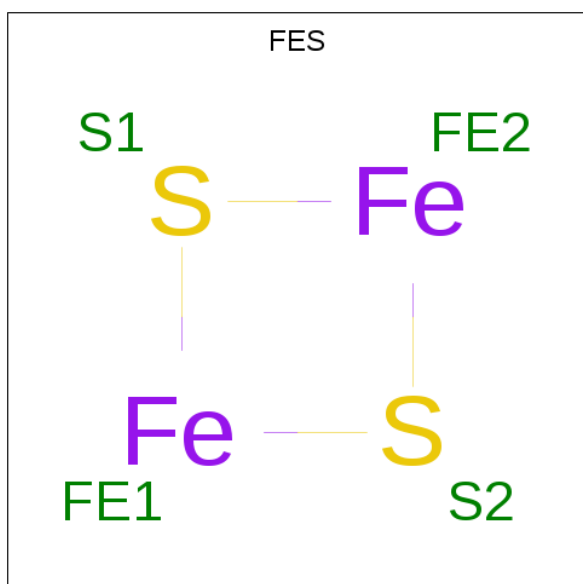
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19  | D     | 1        | Total | C  | Fe | N | O       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |
| 19  | Q     | 1        | Total | C  | Fe | N | O       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |

- Molecule 20 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 20  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 24 | 13 | 2 |         |         |
| 20  | G     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 44    | 25 | 17 | 2 |         |         |
| 20  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 24 | 13 | 2 |         |         |
| 20  | T     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 30 | 17 | 2 |         |         |

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21  | E     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 21  | R     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

- Molecule 22 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 22  | A     | 219      | Total | O   | 0       | 0       |
|     |       |          | 219   | 219 |         |         |
| 22  | B     | 167      | Total | O   | 0       | 0       |
|     |       |          | 167   | 167 |         |         |
| 22  | C     | 123      | Total | O   | 0       | 0       |
|     |       |          | 123   | 123 |         |         |
| 22  | D     | 96       | Total | O   | 0       | 0       |
|     |       |          | 96    | 96  |         |         |
| 22  | E     | 50       | Total | O   | 0       | 0       |
|     |       |          | 50    | 50  |         |         |
| 22  | F     | 63       | Total | O   | 0       | 0       |
|     |       |          | 63    | 63  |         |         |
| 22  | G     | 17       | Total | O   | 0       | 0       |
|     |       |          | 17    | 17  |         |         |
| 22  | H     | 17       | Total | O   | 0       | 0       |
|     |       |          | 17    | 17  |         |         |
| 22  | I     | 16       | Total | O   | 0       | 0       |
|     |       |          | 16    | 16  |         |         |
| 22  | J     | 4        | Total | O   | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 22  | N     | 98       | Total | O   | 0       | 0       |
|     |       |          | 98    | 98  |         |         |
| 22  | O     | 127      | Total | O   | 0       | 0       |
|     |       |          | 127   | 127 |         |         |
| 22  | P     | 115      | Total | O   | 0       | 0       |
|     |       |          | 115   | 115 |         |         |
| 22  | Q     | 89       | Total | O   | 0       | 0       |
|     |       |          | 89    | 89  |         |         |
| 22  | R     | 63       | Total | O   | 0       | 0       |
|     |       |          | 63    | 63  |         |         |
| 22  | S     | 63       | Total | O   | 0       | 0       |
|     |       |          | 63    | 63  |         |         |
| 22  | T     | 20       | Total | O   | 0       | 0       |
|     |       |          | 20    | 20  |         |         |
| 22  | U     | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |

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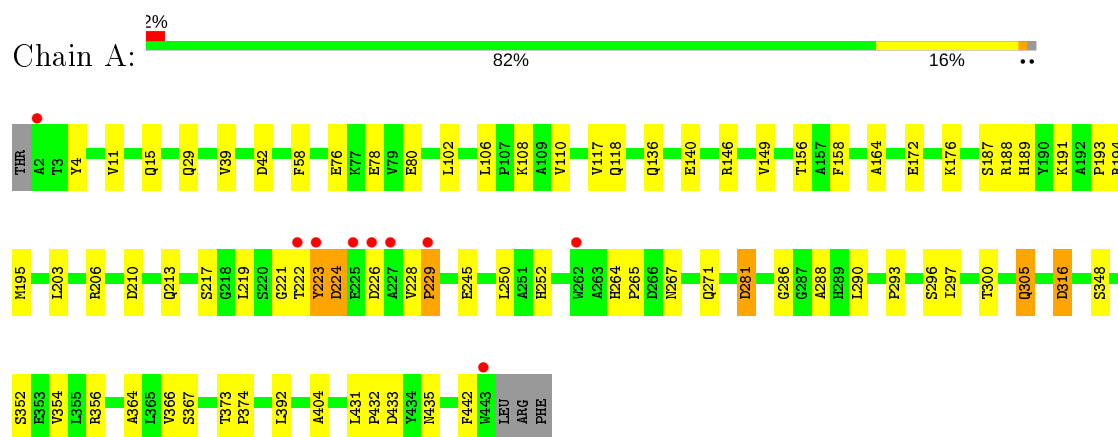
*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 22  | V     | 8        | Total | O | 0       | 0       |
|     |       |          | 8     | 8 |         |         |
| 22  | W     | 9        | Total | O | 0       | 0       |
|     |       |          | 9     | 9 |         |         |

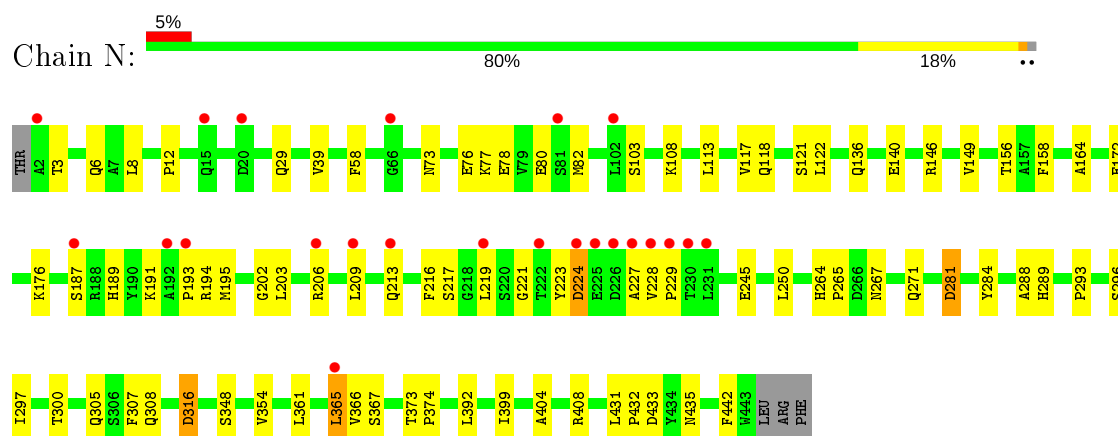
### 3 Residue-property plots [i](#)

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

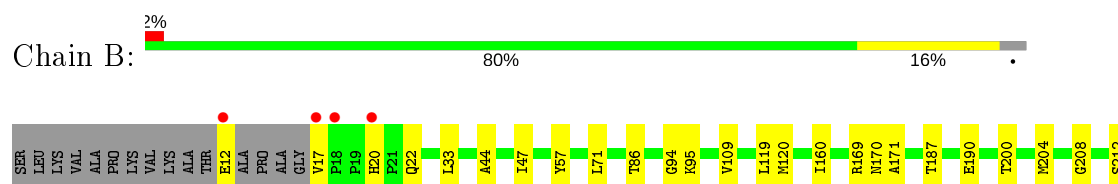
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

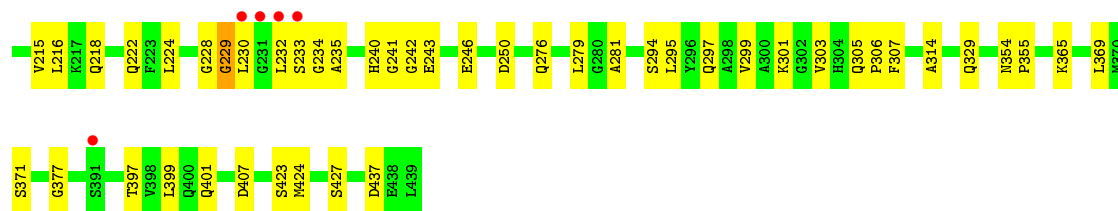


- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

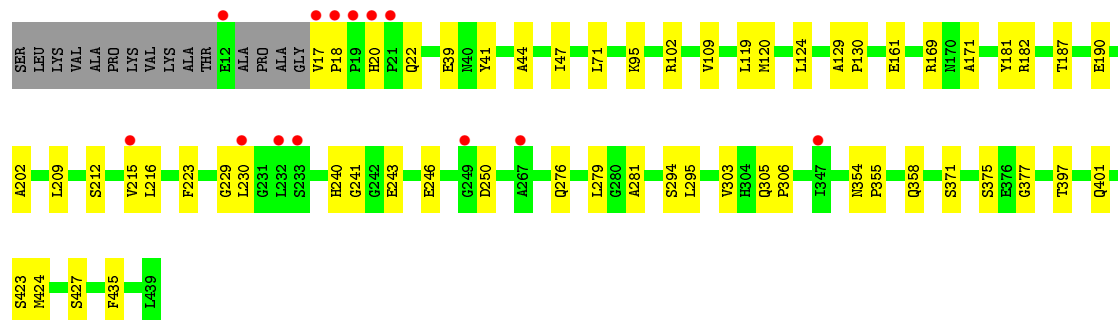
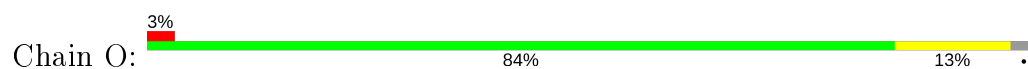


- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

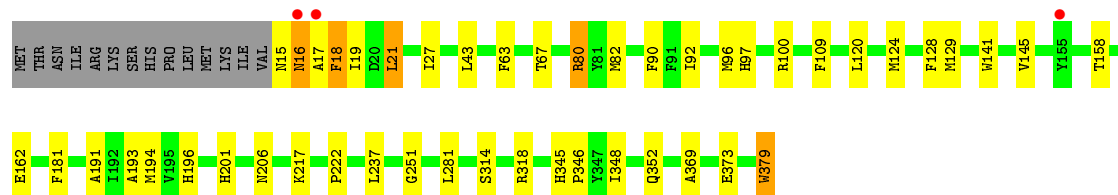
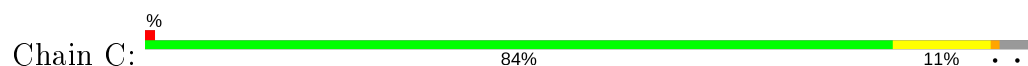




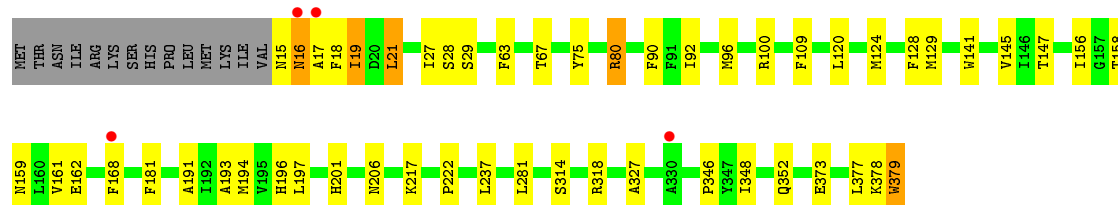
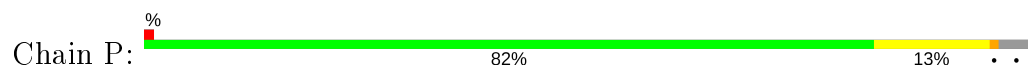
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial



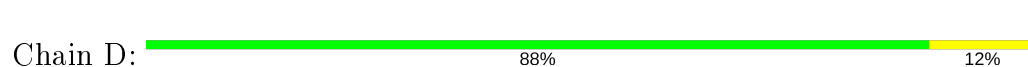
- Molecule 3: Cytochrome b



- Molecule 3: Cytochrome b

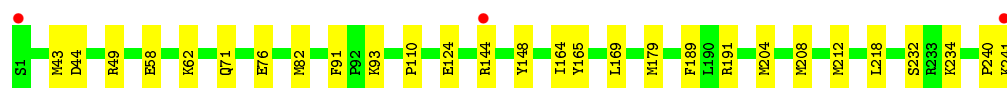
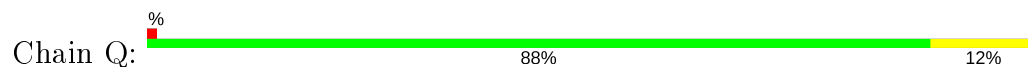


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

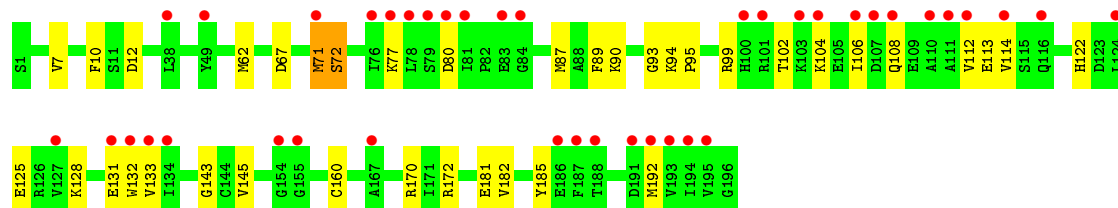
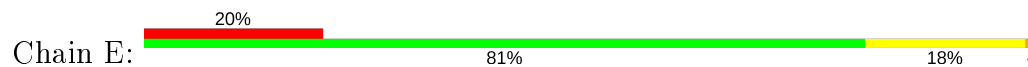




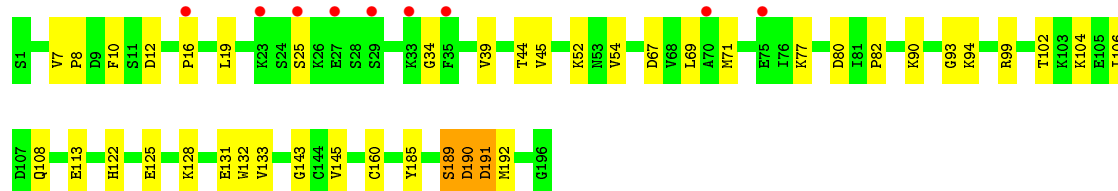
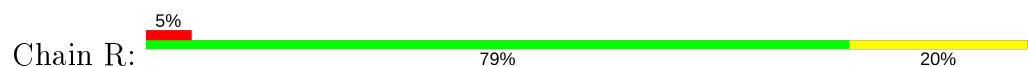
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



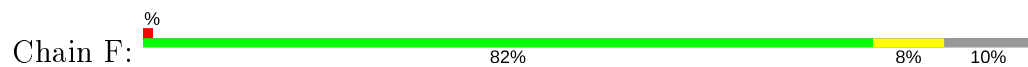
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



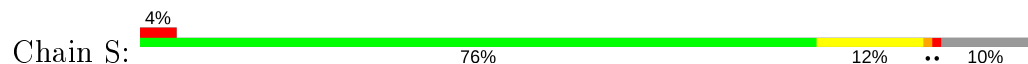
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

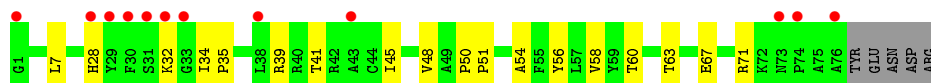
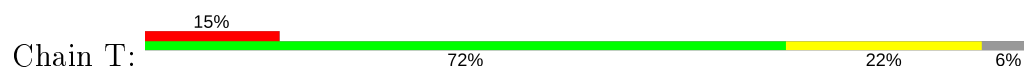


- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C





- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C



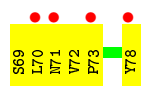
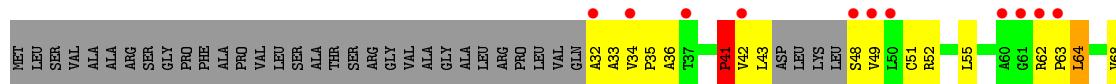
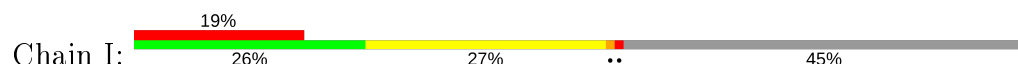
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein



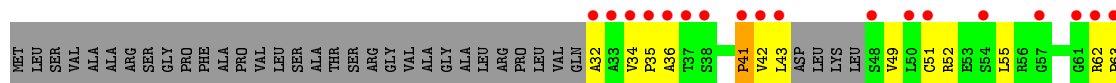
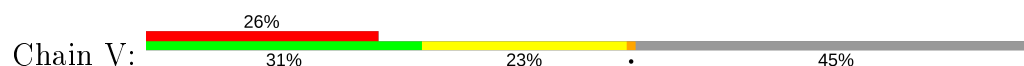
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein



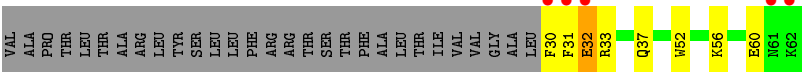
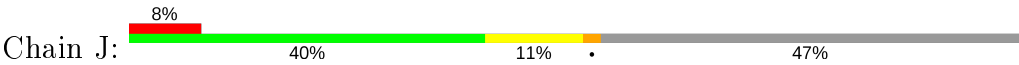
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



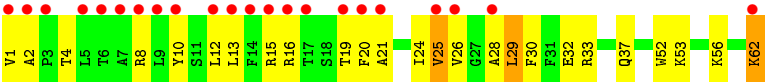
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein



● Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 128.53Å 168.75Å 231.53Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 93.53 – 2.10<br>93.53 – 2.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.7 (93.53-2.10)<br>97.8 (93.53-2.10)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.15  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.03 (at 2.10Å)   | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.224 , 0.260<br>0.219 , 0.235                              | Depositor<br>DCC |
| $R_{free}$ test set   | 14181 reflections (4.97%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 41.8  | Xtriage          |
| Anisotropy  | 0.314   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.37 , 65.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 33549   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 50.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, CDL, PO4, JZR, FES, HEC, HEM, PEE, ANY, SMA

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     | 0.33         | 0/3465  | 0.64        | 0/4704         |
| 1   | N     | 0.30         | 0/3465  | 0.63        | 1/4704 (0.0%)  |
| 2   | B     | 0.32         | 0/3236  | 0.63        | 0/4388         |
| 2   | O     | 0.31         | 0/3213  | 0.62        | 0/4354         |
| 3   | C     | 0.34         | 0/2986  | 0.64        | 1/4089 (0.0%)  |
| 3   | P     | 0.33         | 0/2985  | 0.64        | 1/4087 (0.0%)  |
| 4   | D     | 0.30         | 0/1978  | 0.61        | 0/2684         |
| 4   | Q     | 0.29         | 0/1978  | 0.59        | 0/2684         |
| 5   | E     | 0.29         | 0/1544  | 0.64        | 1/2087 (0.0%)  |
| 5   | R     | 0.30         | 0/1551  | 0.66        | 1/2097 (0.0%)  |
| 6   | F     | 0.32         | 0/878   | 0.63        | 0/1175         |
| 6   | S     | 0.30         | 0/878   | 0.61        | 0/1175         |
| 7   | G     | 0.31         | 0/642   | 0.61        | 0/869          |
| 7   | T     | 0.31         | 0/647   | 0.61        | 0/876          |
| 8   | H     | 0.30         | 0/544   | 0.56        | 0/729          |
| 8   | U     | 0.27         | 0/544   | 0.55        | 0/729          |
| 9   | I     | 0.35         | 0/286   | 0.87        | 2/387 (0.5%)   |
| 9   | V     | 0.34         | 0/286   | 0.84        | 1/387 (0.3%)   |
| 10  | J     | 0.33         | 0/292   | 0.53        | 0/386          |
| 10  | W     | 0.31         | 0/518   | 0.55        | 0/696          |
| All | All   | 0.31         | 0/31916 | 0.63        | 8/43287 (0.0%) |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 9   | I     | 35  | PRO  | N-CA-CB  | 5.84 | 110.31      | 103.30   |
| 9   | I     | 64  | LEU  | CA-CB-CG | 5.72 | 128.47      | 115.30   |
| 5   | R     | 143 | GLY  | N-CA-C   | 5.70 | 127.35      | 113.10   |
| 1   | N     | 365 | LEU  | CA-CB-CG | 5.68 | 128.36      | 115.30   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | E     | 143 | GLY  | N-CA-C  | 5.58  | 127.06      | 113.10   |
| 9   | V     | 35  | PRO  | N-CA-CB | 5.36  | 109.73      | 103.30   |
| 3   | C     | 109 | PHE  | N-CA-C  | -5.26 | 96.79       | 111.00   |
| 3   | P     | 109 | PHE  | N-CA-C  | -5.12 | 97.17       | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 3396  | 0        | 3292     | 65      | 0            |
| 1   | N     | 3396  | 0        | 3292     | 57      | 0            |
| 2   | B     | 3178  | 0        | 3153     | 72      | 0            |
| 2   | O     | 3156  | 0        | 3123     | 44      | 0            |
| 3   | C     | 2892  | 0        | 2938     | 36      | 0            |
| 3   | P     | 2891  | 0        | 2937     | 43      | 0            |
| 4   | D     | 1919  | 0        | 1868     | 27      | 0            |
| 4   | Q     | 1919  | 0        | 1868     | 28      | 0            |
| 5   | E     | 1510  | 0        | 1495     | 30      | 0            |
| 5   | R     | 1517  | 0        | 1499     | 33      | 0            |
| 6   | F     | 861   | 0        | 854      | 12      | 0            |
| 6   | S     | 861   | 0        | 854      | 19      | 0            |
| 7   | G     | 621   | 0        | 626      | 15      | 0            |
| 7   | T     | 626   | 0        | 631      | 15      | 0            |
| 8   | H     | 539   | 0        | 524      | 11      | 0            |
| 8   | U     | 539   | 0        | 524      | 10      | 0            |
| 9   | I     | 285   | 0        | 280      | 50      | 0            |
| 9   | V     | 285   | 0        | 280      | 24      | 0            |
| 10  | J     | 284   | 0        | 264      | 5       | 0            |
| 10  | W     | 506   | 0        | 512      | 30      | 0            |
| 11  | A     | 18    | 0        | 24       | 0       | 0            |
| 11  | C     | 36    | 0        | 48       | 2       | 0            |
| 11  | D     | 18    | 0        | 24       | 3       | 0            |
| 11  | F     | 36    | 0        | 48       | 3       | 0            |
| 11  | P     | 18    | 0        | 24       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | R     | 18    | 0        | 24       | 1       | 0            |
| 11  | S     | 18    | 0        | 24       | 3       | 0            |
| 12  | A     | 5     | 0        | 0        | 0       | 0            |
| 12  | C     | 5     | 0        | 0        | 0       | 0            |
| 12  | F     | 5     | 0        | 0        | 0       | 0            |
| 12  | P     | 5     | 0        | 0        | 0       | 0            |
| 12  | S     | 5     | 0        | 0        | 0       | 0            |
| 13  | A     | 3     | 0        | 0        | 0       | 0            |
| 13  | C     | 3     | 0        | 0        | 0       | 0            |
| 13  | G     | 3     | 0        | 0        | 0       | 0            |
| 13  | O     | 3     | 0        | 0        | 0       | 0            |
| 13  | P     | 3     | 0        | 0        | 0       | 0            |
| 14  | B     | 6     | 0        | 8        | 0       | 0            |
| 14  | C     | 12    | 0        | 16       | 1       | 0            |
| 14  | O     | 6     | 0        | 8        | 0       | 0            |
| 14  | P     | 6     | 0        | 8        | 0       | 0            |
| 14  | R     | 6     | 0        | 8        | 1       | 0            |
| 15  | C     | 86    | 0        | 60       | 3       | 0            |
| 15  | P     | 86    | 0        | 60       | 2       | 0            |
| 16  | C     | 37    | 0        | 42       | 2       | 0            |
| 16  | P     | 37    | 0        | 42       | 2       | 0            |
| 17  | C     | 49    | 0        | 72       | 0       | 0            |
| 17  | D     | 26    | 0        | 26       | 3       | 0            |
| 17  | P     | 49    | 0        | 72       | 1       | 0            |
| 17  | Q     | 51    | 0        | 82       | 3       | 0            |
| 18  | C     | 37    | 0        | 28       | 1       | 0            |
| 18  | P     | 37    | 0        | 29       | 2       | 0            |
| 19  | D     | 43    | 0        | 30       | 3       | 0            |
| 19  | Q     | 43    | 0        | 30       | 1       | 0            |
| 20  | D     | 39    | 0        | 39       | 0       | 0            |
| 20  | G     | 44    | 0        | 32       | 0       | 0            |
| 20  | P     | 39    | 0        | 39       | 2       | 0            |
| 20  | T     | 49    | 0        | 42       | 2       | 0            |
| 21  | E     | 4     | 0        | 0        | 0       | 0            |
| 21  | R     | 4     | 0        | 0        | 0       | 0            |
| 22  | A     | 219   | 0        | 0        | 7       | 0            |
| 22  | B     | 167   | 0        | 0        | 5       | 0            |
| 22  | C     | 123   | 0        | 0        | 1       | 0            |
| 22  | D     | 96    | 0        | 0        | 0       | 0            |
| 22  | E     | 50    | 0        | 0        | 0       | 0            |
| 22  | F     | 63    | 0        | 0        | 0       | 0            |
| 22  | G     | 17    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | H     | 17    | 0        | 0        | 0       | 0            |
| 22  | I     | 16    | 0        | 0        | 2       | 0            |
| 22  | J     | 4     | 0        | 0        | 0       | 0            |
| 22  | N     | 98    | 0        | 0        | 1       | 0            |
| 22  | O     | 127   | 0        | 0        | 2       | 0            |
| 22  | P     | 115   | 0        | 0        | 5       | 0            |
| 22  | Q     | 89    | 0        | 0        | 0       | 0            |
| 22  | R     | 63    | 0        | 0        | 5       | 0            |
| 22  | S     | 63    | 0        | 0        | 1       | 0            |
| 22  | T     | 20    | 0        | 0        | 0       | 0            |
| 22  | U     | 6     | 0        | 0        | 0       | 0            |
| 22  | V     | 8     | 0        | 0        | 1       | 0            |
| 22  | W     | 9     | 0        | 0        | 0       | 0            |
| All | All   | 33549 | 0        | 31803    | 551     | 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 (551) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:95:LYS:HE2   | 9:I:32:ALA:HB3   | 1.47                     | 0.94              |
| 10:W:16:ARG:HB2  | 10:W:19:THR:HG22 | 1.48                     | 0.94              |
| 2:O:95:LYS:HE2   | 9:V:32:ALA:N     | 1.82                     | 0.94              |
| 1:A:136:GLN:HE21 | 9:I:51:CYS:HB3   | 1.30                     | 0.93              |
| 1:A:146:ARG:HA   | 22:A:4191:HOH:O  | 1.69                     | 0.92              |
| 9:I:32:ALA:HA    | 9:I:71:ASN:CB    | 1.99                     | 0.91              |
| 6:S:13:LEU:H     | 6:S:13:LEU:HD23  | 1.32                     | 0.91              |
| 2:B:200:THR:HG21 | 2:B:228:GLY:HA3  | 1.51                     | 0.90              |
| 1:N:136:GLN:HE21 | 9:V:51:CYS:HB3   | 1.38                     | 0.88              |
| 2:O:47:ILE:HG21  | 2:O:120:MET:HE1  | 1.56                     | 0.88              |
| 8:H:25:GLU:HB2   | 8:H:34:ARG:HH22  | 1.38                     | 0.88              |
| 2:B:95:LYS:HE2   | 9:I:32:ALA:CB    | 2.03                     | 0.88              |
| 8:U:25:GLU:HB2   | 8:U:34:ARG:HH22  | 1.37                     | 0.87              |
| 1:N:136:GLN:NE2  | 9:V:51:CYS:HB3   | 1.93                     | 0.83              |
| 2:B:204:MET:HE1  | 2:B:224:LEU:HD22 | 1.58                     | 0.83              |
| 2:B:47:ILE:HG21  | 2:B:120:MET:HE1  | 1.57                     | 0.83              |
| 1:N:39:VAL:HG11  | 1:N:195:MET:HE3  | 1.60                     | 0.81              |
| 9:V:49:VAL:HG11  | 9:V:55:LEU:HD13  | 1.62                     | 0.81              |
| 9:V:36:ALA:HB2   | 9:V:73:PRO:HD2   | 1.63                     | 0.81              |
| 6:F:13:LEU:O     | 6:F:16:ILE:HG12  | 1.80                     | 0.80              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:O:20:HIS:HB2   | 2:O:22:GLN:HG2    | 1.62                     | 0.80              |
| 1:A:136:GLN:NE2  | 9:I:51:CYS:HB3    | 1.96                     | 0.80              |
| 5:R:44:THR:HG21  | 10:W:24:ILE:HD13  | 1.65                     | 0.78              |
| 9:I:49:VAL:HG11  | 9:I:55:LEU:HD13   | 1.65                     | 0.77              |
| 2:B:71:LEU:HD23  | 9:I:68:VAL:HG21   | 1.68                     | 0.74              |
| 6:F:95:LYS:HB2   | 6:F:95:LYS:NZ     | 2.02                     | 0.74              |
| 5:R:34:GLY:CA    | 10:W:10:TYR:HB2   | 2.17                     | 0.74              |
| 10:W:21:ALA:O    | 10:W:25:VAL:HG23  | 1.88                     | 0.74              |
| 5:R:34:GLY:HA2   | 10:W:10:TYR:HB2   | 1.70                     | 0.74              |
| 2:O:71:LEU:HD23  | 9:V:68:VAL:HG21   | 1.70                     | 0.74              |
| 4:D:110:PRO:HG3  | 19:D:501:HEC:HMD3 | 1.71                     | 0.73              |
| 6:S:95:LYS:HB2   | 6:S:95:LYS:NZ     | 2.04                     | 0.72              |
| 7:T:63:THR:O     | 7:T:67:GLU:HG2    | 1.90                     | 0.72              |
| 8:U:28:GLU:O     | 8:U:31:VAL:HG22   | 1.91                     | 0.71              |
| 5:E:112:VAL:HG21 | 5:E:170:ARG:NH2   | 2.05                     | 0.71              |
| 8:H:28:GLU:O     | 8:H:31:VAL:HG22   | 1.91                     | 0.71              |
| 3:P:17:ALA:HA    | 3:P:201:HIS:HE1   | 1.55                     | 0.70              |
| 3:C:129:MET:CE   | 3:C:181:PHE:HD2   | 2.05                     | 0.70              |
| 7:G:63:THR:O     | 7:G:67:GLU:HG2    | 1.91                     | 0.70              |
| 3:C:17:ALA:HA    | 3:C:201:HIS:HE1   | 1.57                     | 0.69              |
| 9:I:62:ARG:HB3   | 9:I:63:PRO:HD2    | 1.74                     | 0.69              |
| 9:I:72:VAL:HG13  | 9:I:73:PRO:HD2    | 1.74                     | 0.69              |
| 3:P:129:MET:CE   | 3:P:181:PHE:HD2   | 2.05                     | 0.69              |
| 1:N:209:LEU:O    | 1:N:213:GLN:HG3   | 1.93                     | 0.69              |
| 5:R:104:LYS:O    | 5:R:108:GLN:HG3   | 1.91                     | 0.69              |
| 9:V:62:ARG:HB3   | 9:V:63:PRO:HD2    | 1.74                     | 0.69              |
| 2:B:204:MET:CE   | 2:B:224:LEU:HD22  | 2.23                     | 0.68              |
| 5:E:104:LYS:O    | 5:E:108:GLN:HG3   | 1.92                     | 0.68              |
| 1:A:293:PRO:O    | 1:A:297:ILE:HG12  | 1.93                     | 0.68              |
| 2:B:200:THR:CG2  | 2:B:228:GLY:HA3   | 2.23                     | 0.68              |
| 1:N:293:PRO:O    | 1:N:297:ILE:HG12  | 1.94                     | 0.68              |
| 9:I:32:ALA:HA    | 9:I:71:ASN:HB3    | 1.76                     | 0.68              |
| 2:B:20:HIS:HB2   | 2:B:22:GLN:HG2    | 1.74                     | 0.67              |
| 8:U:25:GLU:CB    | 8:U:34:ARG:HH22   | 2.08                     | 0.67              |
| 22:A:4203:HOH:O  | 9:I:73:PRO:HG3    | 1.94                     | 0.67              |
| 8:U:28:GLU:O     | 8:U:32:LYS:HG2    | 1.95                     | 0.67              |
| 8:H:25:GLU:CB    | 8:H:34:ARG:HH22   | 2.07                     | 0.67              |
| 1:A:39:VAL:HG11  | 1:A:195:MET:HE3   | 1.75                     | 0.67              |
| 2:B:95:LYS:HE2   | 9:I:32:ALA:N      | 2.10                     | 0.67              |
| 7:G:34:ILE:HB    | 7:G:35:PRO:HD3    | 1.77                     | 0.66              |
| 8:H:28:GLU:O     | 8:H:32:LYS:HG2    | 1.95                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:O:358:GLN:HB2   | 22:O:4120:HOH:O   | 1.95                     | 0.66              |
| 3:C:129:MET:HE1   | 3:C:181:PHE:HD2   | 1.61                     | 0.66              |
| 8:H:21:ARG:O      | 8:H:25:GLU:HG2    | 1.96                     | 0.66              |
| 3:P:379:TRP:CZ3   | 6:S:33:ARG:HD3    | 2.29                     | 0.66              |
| 6:F:95:LYS:HB2    | 6:F:95:LYS:HZ2    | 1.61                     | 0.66              |
| 1:A:316:ASP:OD1   | 1:A:316:ASP:N     | 2.26                     | 0.66              |
| 4:Q:110:PRO:HG3   | 19:Q:501:HEC:HMD3 | 1.78                     | 0.66              |
| 3:P:129:MET:HE1   | 3:P:181:PHE:HD2   | 1.60                     | 0.65              |
| 10:W:33:ARG:O     | 10:W:37:GLN:HG3   | 1.96                     | 0.65              |
| 5:R:189:SER:O     | 5:R:190:ASP:C     | 2.33                     | 0.65              |
| 3:C:16:ASN:HD22   | 3:C:16:ASN:N      | 1.93                     | 0.65              |
| 1:A:136:GLN:O     | 1:A:140:GLU:HG3   | 1.97                     | 0.65              |
| 7:T:34:ILE:HB     | 7:T:35:PRO:HD3    | 1.79                     | 0.65              |
| 9:I:32:ALA:N      | 9:I:72:VAL:HG23   | 2.13                     | 0.64              |
| 4:Q:144:ARG:HH11  | 4:Q:144:ARG:HG2   | 1.62                     | 0.64              |
| 3:C:379:TRP:CZ3   | 6:F:33:ARG:HD3    | 2.32                     | 0.64              |
| 1:N:113:LEU:O     | 1:N:117:VAL:HG12  | 1.97                     | 0.64              |
| 2:O:306:PRO:HA    | 9:V:52:ARG:HG3    | 1.80                     | 0.64              |
| 10:W:16:ARG:HH11  | 10:W:19:THR:HG21  | 1.63                     | 0.64              |
| 9:I:36:ALA:HB2    | 9:I:73:PRO:HD2    | 1.79                     | 0.64              |
| 9:V:72:VAL:HG13   | 9:V:73:PRO:HD2    | 1.78                     | 0.64              |
| 1:A:172:GLU:OE2   | 1:A:176:LYS:HE3   | 1.98                     | 0.64              |
| 5:E:112:VAL:HG21  | 5:E:170:ARG:HH22  | 1.61                     | 0.64              |
| 4:D:144:ARG:HG2   | 4:D:144:ARG:HH11  | 1.64                     | 0.63              |
| 4:D:71:GLN:HA     | 4:D:82:MET:HE2    | 1.81                     | 0.63              |
| 1:A:305:GLN:HA    | 1:A:305:GLN:HE21  | 1.62                     | 0.63              |
| 2:B:94:GLY:O      | 9:I:32:ALA:HB2    | 1.99                     | 0.63              |
| 8:U:21:ARG:O      | 8:U:25:GLU:HG2    | 1.98                     | 0.62              |
| 9:I:32:ALA:CA     | 9:I:71:ASN:CB     | 2.74                     | 0.62              |
| 2:B:299:VAL:HG12  | 2:B:303:VAL:CG1   | 2.30                     | 0.62              |
| 1:N:136:GLN:O     | 1:N:140:GLU:HG3   | 2.00                     | 0.62              |
| 1:A:352:SER:HB3   | 6:S:110:LYS:OXT   | 1.99                     | 0.62              |
| 2:B:95:LYS:CE     | 9:I:32:ALA:HB3    | 2.25                     | 0.61              |
| 1:N:316:ASP:N     | 1:N:316:ASP:OD1   | 2.33                     | 0.61              |
| 15:P:501:HEM:HMC1 | 15:P:501:HEM:HBC2 | 1.83                     | 0.61              |
| 1:N:224:ASP:OD1   | 1:N:227:ALA:HB3   | 1.99                     | 0.61              |
| 5:R:44:THR:CG2    | 10:W:24:ILE:HG21  | 2.30                     | 0.61              |
| 2:O:202:ALA:HB3   | 2:O:229:GLY:O     | 2.00                     | 0.61              |
| 9:I:32:ALA:N      | 9:I:71:ASN:HB2    | 2.16                     | 0.61              |
| 4:Q:218:LEU:HD13  | 22:R:4057:HOH:O   | 1.99                     | 0.61              |
| 1:N:172:GLU:OE2   | 1:N:176:LYS:HE3   | 2.00                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:O:250:ASP:HB3   | 22:O:4111:HOH:O   | 1.99                     | 0.60              |
| 1:A:288:ALA:HB2   | 1:A:300:THR:HG22  | 1.84                     | 0.60              |
| 22:A:4157:HOH:O   | 9:I:41:PRO:HB3    | 2.00                     | 0.60              |
| 15:C:501:HEM:HBC2 | 15:C:501:HEM:HMC1 | 1.82                     | 0.60              |
| 6:F:13:LEU:HD12   | 6:F:16:ILE:HD11   | 1.84                     | 0.60              |
| 3:P:16:ASN:HD22   | 3:P:16:ASN:N      | 1.99                     | 0.60              |
| 5:E:71:MET:O      | 5:E:72:SER:HB3    | 2.01                     | 0.60              |
| 6:S:95:LYS:HB2    | 6:S:95:LYS:HZ2    | 1.66                     | 0.60              |
| 5:E:94:LYS:HE3    | 3:P:168:PHE:O     | 2.01                     | 0.59              |
| 1:N:193:PRO:HD3   | 1:N:221:GLY:HA2   | 1.84                     | 0.59              |
| 9:I:32:ALA:HA     | 9:I:71:ASN:HB2    | 1.84                     | 0.59              |
| 9:V:36:ALA:CB     | 9:V:73:PRO:HD2    | 2.32                     | 0.59              |
| 1:N:288:ALA:HB2   | 1:N:300:THR:HG22  | 1.85                     | 0.59              |
| 6:S:13:LEU:N      | 6:S:13:LEU:HD23   | 2.12                     | 0.59              |
| 10:W:15:ARG:HG3   | 10:W:15:ARG:HH11  | 1.67                     | 0.59              |
| 2:B:33:LEU:HD12   | 2:B:204:MET:HE2   | 1.85                     | 0.58              |
| 5:R:39:VAL:HG13   | 22:R:4057:HOH:O   | 2.02                     | 0.58              |
| 4:Q:218:LEU:HD22  | 22:R:4057:HOH:O   | 2.01                     | 0.58              |
| 1:N:117:VAL:HG13  | 1:N:118:GLN:HG3   | 1.85                     | 0.58              |
| 1:A:305:GLN:HB3   | 9:I:41:PRO:HA     | 1.85                     | 0.58              |
| 1:A:252:HIS:ND1   | 22:A:4191:HOH:O   | 2.32                     | 0.58              |
| 5:R:131:GLU:HG2   | 5:R:132:TRP:CD1   | 2.38                     | 0.58              |
| 2:O:169:ARG:HG3   | 2:O:240:HIS:HB2   | 1.85                     | 0.58              |
| 3:P:15:ASN:OD1    | 3:P:19:ILE:HB     | 2.03                     | 0.58              |
| 5:E:131:GLU:HG2   | 5:E:132:TRP:CD1   | 2.39                     | 0.57              |
| 2:B:276:GLN:HG2   | 2:B:281:ALA:HB2   | 1.86                     | 0.57              |
| 9:I:42:VAL:HG12   | 9:I:43:LEU:CG     | 2.35                     | 0.57              |
| 2:B:12:GLU:HG2    | 2:B:17:VAL:N      | 2.19                     | 0.57              |
| 3:C:129:MET:HE1   | 3:C:181:PHE:CD2   | 2.40                     | 0.57              |
| 4:D:145:GLU:HA    | 11:D:4003:JZR:H2  | 1.87                     | 0.57              |
| 3:C:251:GLY:HA2   | 14:C:2008:GOL:H11 | 1.87                     | 0.56              |
| 4:Q:165:TYR:HA    | 4:Q:179:MET:HE2   | 1.86                     | 0.56              |
| 10:W:13:LEU:O     | 10:W:19:THR:HG23  | 2.05                     | 0.56              |
| 2:B:299:VAL:O     | 2:B:303:VAL:HG12  | 2.05                     | 0.56              |
| 2:B:354:ASN:HB2   | 2:B:355:PRO:HD3   | 1.85                     | 0.56              |
| 7:T:71:ARG:HH22   | 8:U:60:ASP:CG     | 2.08                     | 0.56              |
| 1:A:118:GLN:HG2   | 1:A:219:LEU:HD13  | 1.88                     | 0.56              |
| 1:A:188:ARG:NH1   | 1:A:229:PRO:HD3   | 2.20                     | 0.56              |
| 2:B:299:VAL:HG12  | 2:B:303:VAL:HG12  | 1.87                     | 0.56              |
| 1:N:3:THR:OG1     | 1:N:6:GLN:HG3     | 2.05                     | 0.56              |
| 7:G:42:ARG:HG3    | 7:G:42:ARG:HH11   | 1.71                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:I:32:ALA:HA     | 9:I:71:ASN:CG    | 2.25                     | 0.56              |
| 10:J:56:LYS:HG2   | 10:J:60:GLU:CD   | 2.26                     | 0.56              |
| 2:O:276:GLN:HG2   | 2:O:281:ALA:HB2  | 1.88                     | 0.56              |
| 4:Q:44:ASP:OD1    | 4:Q:93:LYS:HE2   | 2.05                     | 0.56              |
| 1:N:228:VAL:HG13  | 1:N:228:VAL:O    | 2.06                     | 0.56              |
| 1:A:191:LYS:HE2   | 1:A:223:TYR:CB   | 2.36                     | 0.56              |
| 17:Q:3006:PEE:H18 | 5:R:54:VAL:HG22  | 1.88                     | 0.56              |
| 5:R:128:LYS:HE3   | 5:R:185:TYR:O    | 2.05                     | 0.56              |
| 11:F:3011:JZR:H1  | 1:N:289:HIS:NE2  | 2.21                     | 0.55              |
| 2:B:305:GLN:HB3   | 2:B:329:GLN:OE1  | 2.06                     | 0.55              |
| 10:J:32:GLU:HG3   | 10:J:33:ARG:N    | 2.20                     | 0.55              |
| 5:R:44:THR:HG22   | 10:W:24:ILE:HG21 | 1.89                     | 0.55              |
| 1:N:39:VAL:CG1    | 1:N:195:MET:HE3  | 2.33                     | 0.55              |
| 1:N:361:LEU:O     | 1:N:365:LEU:HG   | 2.07                     | 0.55              |
| 2:B:212:SER:O     | 2:B:215:VAL:HG22 | 2.07                     | 0.55              |
| 2:O:202:ALA:HB1   | 2:O:230:LEU:HD23 | 1.89                     | 0.55              |
| 1:N:281:ASP:OD2   | 9:V:73:PRO:HG3   | 2.07                     | 0.55              |
| 1:A:193:PRO:HD3   | 1:A:221:GLY:HA2  | 1.88                     | 0.54              |
| 1:A:267:ASN:O     | 1:A:271:GLN:HG2  | 2.07                     | 0.54              |
| 4:D:44:ASP:OD1    | 4:D:93:LYS:HE2   | 2.07                     | 0.54              |
| 1:A:228:VAL:O     | 1:A:228:VAL:HG13 | 2.06                     | 0.54              |
| 3:P:100:ARG:C     | 3:P:100:ARG:HD2  | 2.27                     | 0.54              |
| 5:R:44:THR:CG2    | 10:W:24:ILE:HD13 | 2.37                     | 0.54              |
| 9:V:42:VAL:HG12   | 9:V:43:LEU:CG    | 2.38                     | 0.54              |
| 1:A:136:GLN:NE2   | 9:I:51:CYS:CB    | 2.70                     | 0.54              |
| 3:P:18:PHE:O      | 3:P:21:LEU:HB2   | 2.07                     | 0.54              |
| 3:P:314:SER:O     | 3:P:318:ARG:HD3  | 2.08                     | 0.54              |
| 10:W:10:TYR:OH    | 10:W:15:ARG:NH1  | 2.41                     | 0.54              |
| 1:A:296:SER:O     | 1:A:300:THR:HG23 | 2.08                     | 0.54              |
| 1:N:78:GLU:OE2    | 1:N:108:LYS:HD3  | 2.08                     | 0.54              |
| 9:V:36:ALA:HB3    | 9:V:73:PRO:HG2   | 1.90                     | 0.54              |
| 10:W:15:ARG:HG3   | 10:W:15:ARG:NH1  | 2.23                     | 0.54              |
| 1:A:78:GLU:OE2    | 1:A:108:LYS:HD3  | 2.08                     | 0.53              |
| 3:C:17:ALA:HA     | 3:C:201:HIS:CE1  | 2.42                     | 0.53              |
| 4:D:144:ARG:NH1   | 4:D:144:ARG:HG2  | 2.23                     | 0.53              |
| 4:D:165:TYR:HA    | 4:D:179:MET:HE2  | 1.90                     | 0.53              |
| 6:F:95:LYS:NZ     | 6:F:95:LYS:CB    | 2.69                     | 0.53              |
| 9:I:32:ALA:CA     | 9:I:71:ASN:HB3   | 2.38                     | 0.53              |
| 1:N:373:THR:HB    | 1:N:374:PRO:HD3  | 1.90                     | 0.53              |
| 3:P:129:MET:HE1   | 3:P:181:PHE:CD2  | 2.41                     | 0.53              |
| 6:S:106:GLU:HG2   | 22:S:3048:HOH:O  | 2.06                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:33:ARG:O    | 10:J:37:GLN:HG3   | 2.09                     | 0.53              |
| 7:T:71:ARG:NH2   | 8:U:60:ASP:OD1    | 2.42                     | 0.53              |
| 3:C:158:THR:O    | 3:C:162:GLU:HG3   | 2.09                     | 0.53              |
| 3:C:18:PHE:O     | 3:C:21:LEU:HB2    | 2.08                     | 0.53              |
| 5:E:95:PRO:HG2   | 5:E:145:VAL:HG22  | 1.90                     | 0.53              |
| 4:Q:208:MET:HA   | 17:Q:3006:PEE:H49 | 1.88                     | 0.53              |
| 2:O:279:LEU:HB3  | 2:O:295:LEU:HG    | 1.89                     | 0.53              |
| 4:Q:144:ARG:NH1  | 4:Q:144:ARG:HG2   | 2.21                     | 0.53              |
| 2:B:20:HIS:HB2   | 2:B:22:GLN:CG     | 2.39                     | 0.53              |
| 9:I:70:LEU:HB3   | 22:I:1016:HOH:O   | 2.09                     | 0.53              |
| 1:N:195:MET:SD   | 1:N:219:LEU:HD21  | 2.49                     | 0.53              |
| 2:O:305:GLN:N    | 2:O:306:PRO:HD3   | 2.23                     | 0.53              |
| 1:A:366:VAL:HG21 | 2:B:44:ALA:HB2    | 1.89                     | 0.52              |
| 1:N:146:ARG:NH2  | 1:N:308:GLN:HE22  | 2.06                     | 0.52              |
| 2:B:169:ARG:HG3  | 2:B:240:HIS:HB2   | 1.91                     | 0.52              |
| 10:W:4:THR:O     | 10:W:8:ARG:HG2    | 2.09                     | 0.52              |
| 1:N:267:ASN:O    | 1:N:271:GLN:HG2   | 2.09                     | 0.52              |
| 1:N:365:LEU:HD11 | 1:N:399:ILE:HD11  | 1.91                     | 0.52              |
| 2:O:212:SER:O    | 2:O:215:VAL:HG22  | 2.08                     | 0.52              |
| 9:I:32:ALA:CA    | 9:I:71:ASN:HB2    | 2.40                     | 0.52              |
| 7:T:41:THR:O     | 7:T:45:ILE:HG12   | 2.09                     | 0.52              |
| 1:A:4:TYR:HB2    | 22:B:2124:HOH:O   | 2.10                     | 0.52              |
| 7:G:41:THR:O     | 7:G:45:ILE:HG12   | 2.09                     | 0.52              |
| 4:Q:164:ILE:O    | 4:Q:179:MET:HE2   | 2.10                     | 0.52              |
| 4:D:148:TYR:OH   | 11:D:4003:JZR:H6  | 2.08                     | 0.52              |
| 9:I:36:ALA:HB3   | 9:I:73:PRO:HG2    | 1.90                     | 0.52              |
| 2:B:86:THR:HG23  | 9:I:70:LEU:HD11   | 1.92                     | 0.52              |
| 1:N:158:PHE:O    | 1:N:164:ALA:HB2   | 2.10                     | 0.52              |
| 10:W:52:TRP:O    | 10:W:56:LYS:HB2   | 2.09                     | 0.52              |
| 2:B:187:THR:OG1  | 2:B:190:GLU:HG3   | 2.10                     | 0.52              |
| 3:P:206:ASN:HB3  | 15:P:502:HEM:O2D  | 2.10                     | 0.52              |
| 5:R:94:LYS:HE3   | 14:R:4005:GOL:O3  | 2.09                     | 0.52              |
| 8:U:19:THR:O     | 8:U:23:GLN:HG3    | 2.10                     | 0.52              |
| 1:A:364:ALA:HB2  | 9:I:33:ALA:HB1    | 1.92                     | 0.52              |
| 6:F:19:TRP:CD1   | 11:F:4001:JZR:H1  | 2.46                     | 0.51              |
| 4:Q:71:GLN:HA    | 4:Q:82:MET:HE2    | 1.90                     | 0.51              |
| 7:G:50:PRO:HB2   | 7:G:51:PRO:HD3    | 1.92                     | 0.51              |
| 1:N:354:VAL:HG21 | 1:N:404:ALA:HA    | 1.92                     | 0.51              |
| 3:P:158:THR:O    | 3:P:162:GLU:HG3   | 2.11                     | 0.51              |
| 3:P:80:ARG:C     | 3:P:80:ARG:HD3    | 2.31                     | 0.51              |
| 1:A:191:LYS:HZ3  | 1:A:223:TYR:HA    | 1.75                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:99:ARG:HB3   | 5:E:133:VAL:CG1   | 2.41                     | 0.51              |
| 2:B:208:GLY:HA3  | 2:B:216:LEU:HD11  | 1.91                     | 0.51              |
| 1:N:296:SER:O    | 1:N:300:THR:HG23  | 2.10                     | 0.51              |
| 3:P:17:ALA:HA    | 3:P:201:HIS:CE1   | 2.42                     | 0.51              |
| 7:T:32:LYS:C     | 7:T:35:PRO:HD2    | 2.31                     | 0.51              |
| 5:E:114:VAL:O    | 5:E:114:VAL:HG12  | 2.10                     | 0.51              |
| 7:G:48:VAL:O     | 7:G:51:PRO:HD2    | 2.10                     | 0.51              |
| 2:B:397:THR:O    | 2:B:401:GLN:HG3   | 2.11                     | 0.51              |
| 3:C:16:ASN:ND2   | 3:C:16:ASN:N      | 2.59                     | 0.51              |
| 3:C:206:ASN:HB3  | 15:C:502:HEM:O2D  | 2.11                     | 0.51              |
| 4:D:2:ASP:OD1    | 7:G:70:LYS:HE3    | 2.11                     | 0.51              |
| 2:O:202:ALA:HB3  | 2:O:229:GLY:C     | 2.30                     | 0.51              |
| 9:I:36:ALA:CB    | 9:I:73:PRO:HD2    | 2.41                     | 0.50              |
| 7:T:50:PRO:HB2   | 7:T:51:PRO:HD3    | 1.92                     | 0.50              |
| 2:B:94:GLY:O     | 9:I:32:ALA:CB     | 2.59                     | 0.50              |
| 6:S:12:TRP:N     | 6:S:13:LEU:HD23   | 2.27                     | 0.50              |
| 6:S:95:LYS:CB    | 6:S:95:LYS:NZ     | 2.72                     | 0.50              |
| 4:D:116:ILE:HG12 | 19:D:501:HEC:HMA3 | 1.92                     | 0.50              |
| 2:B:95:LYS:NZ    | 9:I:34:VAL:HG22   | 2.27                     | 0.50              |
| 7:T:48:VAL:O     | 7:T:51:PRO:HD2    | 2.12                     | 0.50              |
| 10:J:52:TRP:O    | 10:J:56:LYS:HB2   | 2.12                     | 0.50              |
| 1:N:366:VAL:HG21 | 2:O:44:ALA:HB2    | 1.94                     | 0.50              |
| 6:F:13:LEU:O     | 6:F:16:ILE:CG1    | 2.56                     | 0.50              |
| 9:I:32:ALA:HA    | 9:I:71:ASN:ND2    | 2.26                     | 0.50              |
| 2:B:279:LEU:HB3  | 2:B:295:LEU:HG    | 1.93                     | 0.49              |
| 8:H:19:THR:O     | 8:H:23:GLN:HG3    | 2.11                     | 0.49              |
| 7:G:71:ARG:HH22  | 8:H:60:ASP:CG     | 2.15                     | 0.49              |
| 3:C:15:ASN:C     | 3:C:17:ALA:H      | 2.15                     | 0.49              |
| 5:R:25:SER:HA    | 22:R:4016:HOH:O   | 2.12                     | 0.49              |
| 2:O:95:LYS:NZ    | 9:V:34:VAL:HG22   | 2.26                     | 0.49              |
| 5:R:45:VAL:HG13  | 10:W:28:ALA:HA    | 1.94                     | 0.49              |
| 1:A:158:PHE:O    | 1:A:164:ALA:HB2   | 2.12                     | 0.49              |
| 2:B:71:LEU:CD2   | 9:I:68:VAL:HG21   | 2.38                     | 0.49              |
| 3:C:129:MET:HE2  | 3:C:181:PHE:HD2   | 1.78                     | 0.49              |
| 5:R:90:LYS:HE3   | 5:R:93:GLY:O      | 2.12                     | 0.49              |
| 1:A:140:GLU:HB3  | 9:I:48:SER:O      | 2.12                     | 0.49              |
| 1:N:433:ASP:OD2  | 1:N:435:ASN:HB2   | 2.12                     | 0.49              |
| 3:C:80:ARG:C     | 3:C:80:ARG:HD3    | 2.33                     | 0.49              |
| 5:E:71:MET:O     | 5:E:72:SER:CB     | 2.60                     | 0.49              |
| 3:P:378:LYS:HE3  | 6:S:17:ARG:HD3    | 1.95                     | 0.49              |
| 2:B:246:GLU:O    | 2:B:427:SER:HA    | 2.13                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G:56:TYR:O       | 7:G:60:THR:HG23    | 2.12                     | 0.49              |
| 4:D:234:LYS:HE2    | 5:E:10:PHE:CE1     | 2.48                     | 0.49              |
| 7:G:32:LYS:C       | 7:G:35:PRO:HD2     | 2.32                     | 0.49              |
| 10:W:16:ARG:NH1    | 10:W:19:THR:HG21   | 2.25                     | 0.49              |
| 20:P:3003:CDL:H721 | 20:P:3003:CDL:H511 | 1.95                     | 0.49              |
| 5:E:102:THR:O      | 5:E:106:ILE:HG13   | 2.12                     | 0.48              |
| 2:O:215:VAL:HG23   | 2:O:216:LEU:N      | 2.28                     | 0.48              |
| 1:N:408:ARG:HD2    | 22:N:522:HOH:O     | 2.12                     | 0.48              |
| 2:O:39:GLU:OE2     | 2:O:41:TYR:N       | 2.44                     | 0.48              |
| 1:A:431:LEU:HD12   | 1:A:432:PRO:HD2    | 1.96                     | 0.48              |
| 4:D:165:TYR:HA     | 4:D:179:MET:CE     | 2.44                     | 0.48              |
| 3:P:29:SER:HB3     | 20:P:3003:CDL:H722 | 1.94                     | 0.48              |
| 1:A:281:ASP:OD2    | 9:I:73:PRO:HG3     | 2.13                     | 0.48              |
| 4:Q:124:GLU:OE2    | 4:Q:191:ARG:CD     | 2.62                     | 0.48              |
| 9:V:32:ALA:HB1     | 22:V:1505:HOH:O    | 2.13                     | 0.48              |
| 2:B:297:GLN:O      | 2:B:301:LYS:HG3    | 2.14                     | 0.48              |
| 6:F:72:GLN:HA      | 6:F:72:GLN:OE1     | 2.14                     | 0.48              |
| 1:N:76:GLU:HG2     | 1:N:80:GLU:OE2     | 2.14                     | 0.48              |
| 1:A:76:GLU:HG2     | 1:A:80:GLU:OE2     | 2.13                     | 0.48              |
| 3:C:191:ALA:HA     | 3:C:194:MET:CE     | 2.43                     | 0.47              |
| 3:C:217:LYS:HE3    | 22:C:4101:HOH:O    | 2.14                     | 0.47              |
| 4:D:124:GLU:OE2    | 4:D:191:ARG:HD3    | 2.13                     | 0.47              |
| 1:N:366:VAL:HG23   | 1:N:367:SER:N      | 2.28                     | 0.47              |
| 5:R:99:ARG:HB3     | 5:R:133:VAL:CG1    | 2.44                     | 0.47              |
| 6:S:100:GLU:HB3    | 11:S:2011:JZR:H6A  | 1.94                     | 0.47              |
| 3:C:27:ILE:HD12    | 18:C:2002:ANY:H3   | 1.96                     | 0.47              |
| 3:C:63:PHE:O       | 3:C:67:THR:HG23    | 2.14                     | 0.47              |
| 2:B:95:LYS:HE2     | 9:I:32:ALA:CA      | 2.45                     | 0.47              |
| 3:C:120:LEU:O      | 3:C:124:MET:HG3    | 2.13                     | 0.47              |
| 2:O:187:THR:OG1    | 2:O:190:GLU:HG3    | 2.14                     | 0.47              |
| 5:E:62:MET:HG2     | 22:P:3114:HOH:O    | 2.14                     | 0.47              |
| 2:O:279:LEU:HA     | 2:O:294:SER:HB3    | 1.97                     | 0.47              |
| 7:T:39:ARG:HH11    | 7:T:39:ARG:HG2     | 1.79                     | 0.47              |
| 7:G:39:ARG:HG2     | 7:G:39:ARG:HH11    | 1.78                     | 0.47              |
| 5:R:77:LYS:HA      | 5:R:192:MET:HG2    | 1.96                     | 0.47              |
| 2:O:95:LYS:NZ      | 9:V:34:VAL:CG2     | 2.78                     | 0.47              |
| 1:A:102:LEU:CD2    | 2:B:369:LEU:HD12   | 2.45                     | 0.47              |
| 10:W:62:LYS:HD2    | 10:W:62:LYS:C      | 2.35                     | 0.47              |
| 1:A:223:TYR:O      | 1:A:224:ASP:HB3    | 2.14                     | 0.47              |
| 9:I:72:VAL:HG13    | 9:I:73:PRO:CD      | 2.43                     | 0.47              |
| 9:I:72:VAL:CG1     | 9:I:73:PRO:HD2     | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:T:56:TYR:O     | 7:T:60:THR:HG23  | 2.14                     | 0.47              |
| 2:B:250:ASP:HB3  | 22:B:2139:HOH:O  | 2.14                     | 0.47              |
| 3:C:314:SER:O    | 3:C:318:ARG:HD3  | 2.14                     | 0.47              |
| 2:O:209:LEU:HD23 | 2:O:375:SER:HB2  | 1.96                     | 0.47              |
| 3:P:156:ILE:HA   | 3:P:159:ASN:HD22 | 1.80                     | 0.47              |
| 1:A:11:VAL:HG21  | 1:A:392:LEU:HD12 | 1.97                     | 0.47              |
| 1:A:433:ASP:OD2  | 1:A:435:ASN:HB2  | 2.14                     | 0.47              |
| 1:N:250:LEU:HD13 | 1:N:305:GLN:HG3  | 1.98                     | 0.47              |
| 2:O:241:GLY:HA2  | 2:O:423:SER:OG   | 2.14                     | 0.47              |
| 5:E:112:VAL:CG2  | 5:E:170:ARG:HH22 | 2.28                     | 0.46              |
| 4:Q:165:TYR:HA   | 4:Q:179:MET:CE   | 2.44                     | 0.46              |
| 5:R:44:THR:HG21  | 10:W:24:ILE:HG21 | 1.97                     | 0.46              |
| 1:A:213:GLN:O    | 1:A:217:SER:OG   | 2.25                     | 0.46              |
| 6:S:72:GLN:OE1   | 6:S:72:GLN:HA    | 2.15                     | 0.46              |
| 10:W:20:PHE:CE1  | 10:W:24:ILE:HD11 | 2.51                     | 0.46              |
| 3:P:237:LEU:HD13 | 4:Q:212:MET:HG3  | 1.98                     | 0.46              |
| 2:B:306:PRO:HA   | 9:I:52:ARG:HG3   | 1.96                     | 0.46              |
| 2:B:95:LYS:CE    | 9:I:32:ALA:N     | 2.76                     | 0.46              |
| 1:N:189:HIS:ND1  | 1:N:194:ARG:NH2  | 2.64                     | 0.46              |
| 1:N:206:ARG:HH11 | 1:N:206:ARG:HG3  | 1.80                     | 0.46              |
| 1:N:29:GLN:O     | 2:O:18:PRO:HG3   | 2.15                     | 0.46              |
| 5:E:160:CYS:HB3  | 16:P:3001:SMA:H4 | 1.95                     | 0.46              |
| 2:B:187:THR:HB   | 22:B:2093:HOH:O  | 2.14                     | 0.46              |
| 2:O:305:GLN:N    | 2:O:305:GLN:C    | 2.68                     | 0.46              |
| 4:Q:124:GLU:OE2  | 4:Q:191:ARG:HD3  | 2.15                     | 0.46              |
| 6:S:16:ILE:HG13  | 6:S:17:ARG:N     | 2.30                     | 0.46              |
| 1:A:354:VAL:HG21 | 1:A:404:ALA:HA   | 1.97                     | 0.46              |
| 4:D:138:PRO:HG2  | 4:D:141:VAL:CG2  | 2.46                     | 0.46              |
| 9:I:69:SER:HB2   | 22:I:1441:HOH:O  | 2.14                     | 0.46              |
| 3:P:191:ALA:HA   | 3:P:194:MET:CE   | 2.46                     | 0.46              |
| 1:A:195:MET:HE2  | 1:A:195:MET:HB3  | 1.79                     | 0.46              |
| 1:N:224:ASP:OD2  | 1:N:227:ALA:N    | 2.49                     | 0.46              |
| 16:C:2001:SMA:H4 | 5:R:160:CYS:HB3  | 1.97                     | 0.46              |
| 3:P:120:LEU:O    | 3:P:124:MET:HG3  | 2.16                     | 0.46              |
| 3:P:348:ILE:O    | 3:P:352:GLN:HG3  | 2.16                     | 0.46              |
| 7:T:28:HIS:CG    | 7:T:32:LYS:HE2   | 2.51                     | 0.46              |
| 1:A:189:HIS:ND1  | 1:A:194:ARG:NH2  | 2.63                     | 0.45              |
| 1:A:373:THR:HB   | 1:A:374:PRO:HD3  | 1.96                     | 0.45              |
| 3:C:379:TRP:CE3  | 6:F:33:ARG:HD3   | 2.50                     | 0.45              |
| 1:A:366:VAL:HG23 | 1:A:367:SER:N    | 2.31                     | 0.45              |
| 3:C:43:LEU:HD11  | 3:C:82:MET:HE2   | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:97:HIS:CD2    | 15:C:502:HEM:NC   | 2.83                     | 0.45              |
| 2:O:71:LEU:CD2    | 9:V:68:VAL:HG21   | 2.44                     | 0.45              |
| 10:W:8:ARG:O      | 10:W:12:LEU:HB2   | 2.16                     | 0.45              |
| 3:C:345:HIS:NE2   | 11:C:4002:JZR:H3  | 2.32                     | 0.45              |
| 3:P:158:THR:HB    | 22:P:3127:HOH:O   | 2.17                     | 0.45              |
| 4:Q:240:PRO:O     | 4:Q:241:LYS:HB2   | 2.16                     | 0.45              |
| 1:A:29:GLN:HB3    | 2:B:12:GLU:O      | 2.17                     | 0.45              |
| 1:A:102:LEU:HD21  | 2:B:369:LEU:HD12  | 1.98                     | 0.45              |
| 4:D:207:LYS:HZ2   | 17:D:2006:PEE:H11 | 1.81                     | 0.45              |
| 4:Q:204:MET:HE3   | 17:Q:3006:PEE:C10 | 2.46                     | 0.45              |
| 7:G:28:HIS:CG     | 7:G:32:LYS:HE2    | 2.51                     | 0.45              |
| 1:A:206:ARG:HG3   | 1:A:206:ARG:HH11  | 1.80                     | 0.45              |
| 5:R:52:LYS:HE3    | 10:W:32:GLU:OE2   | 2.17                     | 0.45              |
| 6:S:49:ARG:HH22   | 11:S:2011:JZR:H4  | 1.81                     | 0.45              |
| 9:V:72:VAL:HG13   | 9:V:73:PRO:CD     | 2.46                     | 0.45              |
| 2:O:102:ARG:HH22  | 2:O:161:GLU:CD    | 2.20                     | 0.45              |
| 3:P:281:LEU:HD23  | 3:P:281:LEU:C     | 2.37                     | 0.45              |
| 6:S:13:LEU:H      | 6:S:13:LEU:CD2    | 2.07                     | 0.45              |
| 9:V:64:LEU:HB3    | 9:V:78:TYR:OXT    | 2.17                     | 0.45              |
| 9:I:32:ALA:N      | 9:I:71:ASN:CB     | 2.79                     | 0.45              |
| 2:O:109:VAL:HB    | 2:O:119:LEU:HD12  | 1.98                     | 0.45              |
| 2:B:240:HIS:CE1   | 2:O:435:PHE:CD1   | 3.05                     | 0.45              |
| 5:R:102:THR:O     | 5:R:106:ILE:HG13  | 2.17                     | 0.45              |
| 3:C:191:ALA:HA    | 3:C:194:MET:HE2   | 1.98                     | 0.45              |
| 3:C:145:VAL:HG21  | 16:C:2001:SMA:H6  | 1.98                     | 0.45              |
| 3:P:129:MET:HE2   | 3:P:181:PHE:HD2   | 1.78                     | 0.45              |
| 1:A:108:LYS:HE3   | 1:A:108:LYS:HA    | 1.99                     | 0.44              |
| 1:A:206:ARG:NH1   | 1:A:206:ARG:HG3   | 2.31                     | 0.44              |
| 2:B:241:GLY:HA2   | 2:B:423:SER:OG    | 2.17                     | 0.44              |
| 3:C:141:TRP:CH2   | 5:R:145:VAL:HG23  | 2.52                     | 0.44              |
| 3:C:281:LEU:HD23  | 3:C:281:LEU:C     | 2.37                     | 0.44              |
| 1:N:206:ARG:NH1   | 1:N:206:ARG:HG3   | 2.32                     | 0.44              |
| 3:P:327:ALA:HA    | 7:T:51:PRO:HB3    | 1.98                     | 0.44              |
| 1:A:213:GLN:HG2   | 22:A:4063:HOH:O   | 2.16                     | 0.44              |
| 2:B:160:ILE:HG22  | 22:B:2146:HOH:O   | 2.16                     | 0.44              |
| 2:O:246:GLU:O     | 2:O:427:SER:HA    | 2.17                     | 0.44              |
| 19:D:501:HEC:HMB1 | 19:D:501:HEC:HBB3 | 1.99                     | 0.44              |
| 2:O:354:ASN:HB3   | 2:O:355:PRO:HD3   | 2.00                     | 0.44              |
| 2:O:181:TYR:CE1   | 2:O:182:ARG:HG2   | 2.53                     | 0.44              |
| 10:W:25:VAL:O     | 10:W:28:ALA:HB3   | 2.17                     | 0.44              |
| 4:D:124:GLU:OE2   | 4:D:191:ARG:CD    | 2.65                     | 0.44              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:C:237:LEU:HD13 | 4:D:212:MET:HG3    | 1.99                     | 0.44              |
| 5:E:145:VAL:HG23 | 3:P:141:TRP:CH2    | 2.52                     | 0.44              |
| 3:P:197:LEU:CD1  | 18:P:3002:ANY:H12  | 2.48                     | 0.44              |
| 1:N:431:LEU:HD12 | 1:N:432:PRO:HD2    | 1.99                     | 0.44              |
| 4:Q:43:MET:CE    | 4:Q:91:PHE:HE2     | 2.31                     | 0.44              |
| 7:G:71:ARG:NH2   | 8:H:60:ASP:OD1     | 2.50                     | 0.44              |
| 1:N:103:SER:HB3  | 1:N:202:GLY:O      | 2.18                     | 0.44              |
| 2:O:397:THR:O    | 2:O:401:GLN:HG3    | 2.18                     | 0.44              |
| 3:P:145:VAL:HG21 | 16:P:3001:SMA:H6   | 1.99                     | 0.44              |
| 3:P:191:ALA:HA   | 3:P:194:MET:HE2    | 1.99                     | 0.44              |
| 1:A:15:GLN:NE2   | 2:B:12:GLU:HB2     | 2.33                     | 0.43              |
| 2:B:218:GLN:O    | 2:B:222:GLN:HG3    | 2.18                     | 0.43              |
| 3:C:100:ARG:C    | 3:C:100:ARG:HD2    | 2.37                     | 0.43              |
| 5:E:77:LYS:HA    | 5:E:192:MET:HG2    | 1.99                     | 0.43              |
| 2:B:437:ASP:OD2  | 2:O:240:HIS:CD2    | 2.71                     | 0.43              |
| 4:Q:148:TYR:CD1  | 4:Q:148:TYR:N      | 2.86                     | 0.43              |
| 1:A:195:MET:SD   | 1:A:219:LEU:HD21   | 2.58                     | 0.43              |
| 1:A:223:TYR:O    | 1:A:224:ASP:CB     | 2.66                     | 0.43              |
| 6:F:104:ARG:HH21 | 11:F:3011:JZR:H6'B | 1.83                     | 0.43              |
| 2:B:279:LEU:HA   | 2:B:294:SER:HB3    | 2.00                     | 0.43              |
| 1:N:82:MET:CE    | 1:N:108:LYS:HG2    | 2.48                     | 0.43              |
| 1:N:213:GLN:O    | 1:N:217:SER:OG     | 2.29                     | 0.43              |
| 1:A:222:THR:O    | 1:A:223:TYR:CB     | 2.66                     | 0.43              |
| 1:A:356:ARG:NH1  | 22:A:4058:HOH:O    | 2.51                     | 0.43              |
| 4:D:49:ARG:NH2   | 5:E:67:ASP:HB3     | 2.33                     | 0.43              |
| 1:N:8:LEU:HD22   | 1:N:392:LEU:HB3    | 2.01                     | 0.43              |
| 3:P:21:LEU:HD13  | 22:P:3100:HOH:O    | 2.18                     | 0.43              |
| 5:R:69:LEU:O     | 5:R:71:MET:HG3     | 2.18                     | 0.43              |
| 2:B:299:VAL:HG12 | 2:B:303:VAL:HG11   | 1.98                     | 0.43              |
| 5:E:90:LYS:HE2   | 5:E:93:GLY:HA2     | 2.00                     | 0.43              |
| 2:B:12:GLU:CG    | 2:B:17:VAL:N       | 2.82                     | 0.43              |
| 2:O:305:GLN:N    | 2:O:306:PRO:CD     | 2.82                     | 0.43              |
| 5:R:16:PRO:HA    | 5:R:19:LEU:HD12    | 2.00                     | 0.43              |
| 22:B:2146:HOH:O  | 9:I:64:LEU:CG      | 2.66                     | 0.43              |
| 9:I:64:LEU:HB3   | 9:I:78:TYR:OXT     | 2.18                     | 0.43              |
| 1:N:288:ALA:CB   | 1:N:300:THR:HG22   | 2.48                     | 0.43              |
| 1:A:149:VAL:CG1  | 22:A:4191:HOH:O    | 2.66                     | 0.42              |
| 1:A:281:ASP:HA   | 1:A:305:GLN:O      | 2.18                     | 0.42              |
| 3:C:92:ILE:O     | 3:C:96:MET:HG2     | 2.19                     | 0.42              |
| 4:D:145:GLU:HG2  | 11:D:4003:JZR:O3   | 2.19                     | 0.42              |
| 6:S:95:LYS:HB2   | 6:S:95:LYS:HZ3     | 1.82                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:V:34:VAL:O     | 9:V:34:VAL:HG23   | 2.19                     | 0.42              |
| 1:A:187:SER:O    | 1:A:191:LYS:HD3   | 2.18                     | 0.42              |
| 2:B:232:LEU:HB3  | 2:B:235:ALA:CB    | 2.49                     | 0.42              |
| 1:A:288:ALA:CB   | 1:A:300:THR:HG22  | 2.48                     | 0.42              |
| 5:E:122:HIS:HB3  | 5:E:125:GLU:HG3   | 2.02                     | 0.42              |
| 6:F:40:ASN:O     | 6:F:44:LYS:HG3    | 2.19                     | 0.42              |
| 10:W:1:VAL:O     | 10:W:2:ALA:HB2    | 2.19                     | 0.42              |
| 1:A:286:GLY:HA3  | 1:A:290:LEU:HD21  | 2.01                     | 0.42              |
| 2:B:305:GLN:NE2  | 2:B:305:GLN:HA    | 2.35                     | 0.42              |
| 4:D:211:MET:HE1  | 10:J:31:PHE:CZ    | 2.54                     | 0.42              |
| 7:G:39:ARG:HG2   | 7:G:39:ARG:NH1    | 2.34                     | 0.42              |
| 8:H:31:VAL:HG23  | 8:H:32:LYS:N      | 2.33                     | 0.42              |
| 4:D:175:THR:HG23 | 8:H:78:LYS:HE3    | 2.01                     | 0.42              |
| 3:P:217:LYS:HG3  | 7:T:7:LEU:HD13    | 2.01                     | 0.42              |
| 4:D:43:MET:HE1   | 4:D:189:PHE:HZ    | 1.84                     | 0.42              |
| 1:A:156:THR:HA   | 5:E:7:VAL:HG21    | 2.00                     | 0.42              |
| 1:N:156:THR:HA   | 5:R:7:VAL:HG21    | 2.01                     | 0.42              |
| 1:N:264:HIS:HA   | 1:N:265:PRO:HD3   | 1.81                     | 0.42              |
| 3:P:92:ILE:O     | 3:P:96:MET:HG2    | 2.19                     | 0.42              |
| 9:V:42:VAL:HG12  | 9:V:43:LEU:N      | 2.34                     | 0.42              |
| 1:A:42:ASP:O     | 1:A:194:ARG:CZ    | 2.68                     | 0.42              |
| 4:D:203:ARG:HD2  | 17:D:2006:PEE:N   | 2.34                     | 0.42              |
| 7:G:33:GLY:O     | 7:G:37:VAL:HG23   | 2.20                     | 0.42              |
| 2:O:202:ALA:HB3  | 2:O:230:LEU:HA    | 2.01                     | 0.42              |
| 2:O:371:SER:O    | 2:O:377:GLY:HA3   | 2.20                     | 0.42              |
| 3:P:193:ALA:O    | 3:P:196:HIS:HB3   | 2.19                     | 0.42              |
| 4:Q:43:MET:HE1   | 4:Q:91:PHE:HE2    | 1.85                     | 0.42              |
| 8:U:31:VAL:HG23  | 8:U:32:LYS:N      | 2.34                     | 0.42              |
| 1:A:117:VAL:HG11 | 1:A:195:MET:CE    | 2.50                     | 0.42              |
| 2:B:57:TYR:HD1   | 2:B:233:SER:HA    | 1.85                     | 0.42              |
| 2:B:303:VAL:O    | 2:B:303:VAL:HG13  | 2.20                     | 0.42              |
| 3:C:193:ALA:O    | 3:C:196:HIS:HB3   | 2.19                     | 0.42              |
| 4:D:207:LYS:NZ   | 17:D:2006:PEE:H11 | 2.35                     | 0.42              |
| 5:E:99:ARG:HB3   | 5:E:133:VAL:HG12  | 2.01                     | 0.42              |
| 3:P:147:THR:HG22 | 3:P:161:VAL:HG13  | 2.00                     | 0.42              |
| 4:Q:43:MET:HE1   | 4:Q:189:PHE:HZ    | 1.83                     | 0.42              |
| 2:B:230:LEU:N    | 2:B:230:LEU:HD12  | 2.35                     | 0.42              |
| 3:C:345:HIS:CD2  | 11:C:4002:JZR:H3  | 2.55                     | 0.42              |
| 10:W:8:ARG:HG2   | 10:W:8:ARG:HH11   | 1.84                     | 0.42              |
| 5:E:77:LYS:HD3   | 5:E:80:ASP:OD1    | 2.20                     | 0.42              |
| 2:O:17:VAL:HA    | 2:O:18:PRO:HD3    | 1.78                     | 0.42              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:243:GLU:HA   | 2:B:424:MET:O      | 2.20                     | 0.41              |
| 3:C:369:ALA:O    | 3:C:373:GLU:HG3    | 2.20                     | 0.41              |
| 5:E:77:LYS:HB2   | 5:E:192:MET:HE3    | 2.02                     | 0.41              |
| 1:N:117:VAL:HG11 | 1:N:216:PHE:HE2    | 1.85                     | 0.41              |
| 2:O:243:GLU:HA   | 2:O:424:MET:O      | 2.21                     | 0.41              |
| 8:U:26:GLN:HA    | 8:U:26:GLN:OE1     | 2.19                     | 0.41              |
| 9:V:72:VAL:CG1   | 9:V:73:PRO:HD2     | 2.48                     | 0.41              |
| 8:H:25:GLU:HB2   | 8:H:34:ARG:NH2     | 2.20                     | 0.41              |
| 1:A:264:HIS:HA   | 1:A:265:PRO:HD3    | 1.83                     | 0.41              |
| 2:B:200:THR:O    | 2:B:204:MET:HG3    | 2.20                     | 0.41              |
| 2:B:371:SER:O    | 2:B:377:GLY:HA3    | 2.20                     | 0.41              |
| 5:E:172:ARG:HH11 | 5:E:172:ARG:HB3    | 1.85                     | 0.41              |
| 3:P:63:PHE:O     | 3:P:67:THR:HG23    | 2.21                     | 0.41              |
| 4:Q:218:LEU:HB3  | 22:R:4057:HOH:O    | 2.19                     | 0.41              |
| 6:S:49:ARG:NH2   | 11:S:2011:JZR:H4   | 2.35                     | 0.41              |
| 2:B:229:GLY:C    | 2:B:230:LEU:HD12   | 2.41                     | 0.41              |
| 5:E:87:MET:CG    | 5:E:89:PHE:CZ      | 3.03                     | 0.41              |
| 1:N:117:VAL:HG11 | 1:N:216:PHE:CE2    | 2.56                     | 0.41              |
| 1:N:187:SER:O    | 1:N:191:LYS:HD3    | 2.20                     | 0.41              |
| 5:R:122:HIS:HB3  | 5:R:125:GLU:HG3    | 2.01                     | 0.41              |
| 6:S:77:LYS:HA    | 6:S:80:TRP:CE2     | 2.56                     | 0.41              |
| 5:R:34:GLY:HA3   | 10:W:10:TYR:HB2    | 1.97                     | 0.41              |
| 9:I:62:ARG:CB    | 9:I:63:PRO:HD2     | 2.49                     | 0.41              |
| 2:O:95:LYS:O     | 2:O:109:VAL:HA     | 2.20                     | 0.41              |
| 3:P:28:SER:HB2   | 20:T:3004:CDL:HA21 | 2.01                     | 0.41              |
| 1:N:12:PRO:HG3   | 2:O:18:PRO:HA      | 2.02                     | 0.41              |
| 3:P:377:LEU:HD11 | 22:P:3086:HOH:O    | 2.21                     | 0.41              |
| 4:Q:58:GLU:O     | 4:Q:62:LYS:HG3     | 2.21                     | 0.41              |
| 4:Q:43:MET:CE    | 4:Q:91:PHE:CE2     | 3.04                     | 0.41              |
| 5:E:87:MET:HG2   | 5:E:89:PHE:CZ      | 2.56                     | 0.41              |
| 4:Q:43:MET:CE    | 4:Q:189:PHE:HZ     | 2.34                     | 0.41              |
| 4:D:43:MET:HE1   | 4:D:91:PHE:HE2     | 1.85                     | 0.41              |
| 9:I:36:ALA:HB3   | 9:I:73:PRO:CG      | 2.51                     | 0.41              |
| 2:O:124:LEU:HD13 | 2:O:223:PHE:CB     | 2.50                     | 0.41              |
| 2:B:354:ASN:ND2  | 2:B:407:ASP:OD2    | 2.54                     | 0.41              |
| 1:N:73:ASN:O     | 1:N:77:LYS:HG3     | 2.20                     | 0.41              |
| 5:R:80:ASP:O     | 5:R:82:PRO:HD3     | 2.20                     | 0.41              |
| 1:N:284:TYR:HE1  | 9:V:73:PRO:HG3     | 1.85                     | 0.41              |
| 1:A:250:LEU:HD13 | 1:A:305:GLN:HG3    | 2.03                     | 0.41              |
| 2:O:129:ALA:N    | 2:O:130:PRO:CD     | 2.84                     | 0.41              |
| 3:P:379:TRP:CE3  | 6:S:33:ARG:HD3     | 2.55                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:348:ILE:O    | 3:C:352:GLN:HG3   | 2.20                     | 0.41              |
| 4:D:164:ILE:O    | 4:D:179:MET:HE2   | 2.21                     | 0.41              |
| 2:B:314:ALA:HA   | 9:I:63:PRO:HD3    | 2.02                     | 0.41              |
| 1:N:264:HIS:ND1  | 1:N:265:PRO:HD2   | 2.36                     | 0.41              |
| 4:Q:232:SER:O    | 5:R:10:PHE:HE1    | 2.04                     | 0.41              |
| 4:Q:71:GLN:HG3   | 4:Q:82:MET:CE     | 2.51                     | 0.41              |
| 5:E:128:LYS:HE3  | 5:E:185:TYR:O     | 2.21                     | 0.40              |
| 7:T:39:ARG:HG2   | 7:T:39:ARG:NH1    | 2.35                     | 0.40              |
| 10:W:26:VAL:O    | 10:W:30:PHE:HD1   | 2.04                     | 0.40              |
| 1:A:15:GLN:HE21  | 2:B:12:GLU:HB2    | 1.86                     | 0.40              |
| 2:B:170:ASN:HD22 | 2:B:232:LEU:HD23  | 1.86                     | 0.40              |
| 4:D:91:PHE:HA    | 4:D:92:PRO:HD3    | 1.97                     | 0.40              |
| 3:P:159:ASN:ND2  | 22:P:3127:HOH:O   | 2.54                     | 0.40              |
| 17:P:3007:PEE:H2 | 20:T:3004:CDL:OB3 | 2.21                     | 0.40              |
| 1:A:106:LEU:O    | 1:A:110:VAL:HG23  | 2.20                     | 0.40              |
| 2:B:109:VAL:HB   | 2:B:119:LEU:HD12  | 2.03                     | 0.40              |
| 2:B:242:GLY:O    | 2:B:423:SER:HA    | 2.21                     | 0.40              |
| 2:B:365:LYS:HB3  | 2:B:399:LEU:HD22  | 2.03                     | 0.40              |
| 1:N:121:SER:O    | 1:N:122:LEU:HB2   | 2.22                     | 0.40              |
| 1:N:307:PHE:CD1  | 1:N:307:PHE:C     | 2.94                     | 0.40              |
| 4:Q:49:ARG:NH2   | 5:R:67:ASP:HB3    | 2.36                     | 0.40              |
| 5:R:77:LYS:HB2   | 5:R:192:MET:HE3   | 2.02                     | 0.40              |
| 2:B:120:MET:HA   | 2:B:120:MET:HE2   | 2.04                     | 0.40              |
| 2:B:232:LEU:HB3  | 2:B:235:ALA:HB3   | 2.04                     | 0.40              |
| 2:B:307:PHE:CD1  | 2:B:307:PHE:C     | 2.94                     | 0.40              |
| 5:E:112:VAL:O    | 5:E:114:VAL:N     | 2.54                     | 0.40              |
| 2:B:95:LYS:HB2   | 9:I:32:ALA:HB2    | 2.02                     | 0.40              |
| 3:P:318:ARG:HB3  | 3:P:373:GLU:OE2   | 2.21                     | 0.40              |
| 9:V:76:VAL:HG13  | 9:V:76:VAL:O      | 2.21                     | 0.40              |
| 1:A:224:ASP:OD2  | 1:A:226:ASP:OD1   | 2.40                     | 0.40              |
| 2:B:95:LYS:O     | 2:B:109:VAL:HA    | 2.21                     | 0.40              |
| 5:E:181:GLU:HG2  | 5:E:182:VAL:N     | 2.36                     | 0.40              |
| 1:N:146:ARG:O    | 1:N:149:VAL:HG12  | 2.21                     | 0.40              |
| 3:P:27:ILE:HD12  | 18:P:3002:ANY:H3  | 2.03                     | 0.40              |
| 3:P:75:TYR:CE2   | 11:R:4007:JZR:H6  | 2.56                     | 0.40              |
| 4:Q:234:LYS:HD2  | 5:R:8:PRO:HB2     | 2.04                     | 0.40              |
| 7:T:54:ALA:O     | 7:T:58:VAL:HG23   | 2.22                     | 0.40              |
| 10:W:29:LEU:HD12 | 10:W:29:LEU:HA    | 1.86                     | 0.40              |
| 10:W:53:LYS:HE3  | 10:W:53:LYS:HB2   | 1.90                     | 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     | 440/446 (99%)   | 425 (97%)  | 11 (2%)  | 4 (1%)   | 17          | 12  |
| 1   | N     | 440/446 (99%)   | 425 (97%)  | 11 (2%)  | 4 (1%)   | 17          | 12  |
| 2   | B     | 418/439 (95%)   | 405 (97%)  | 10 (2%)  | 3 (1%)   | 22          | 18  |
| 2   | O     | 419/439 (95%)   | 404 (96%)  | 13 (3%)  | 2 (0%)   | 29          | 26  |
| 3   | C     | 363/379 (96%)   | 352 (97%)  | 9 (2%)   | 2 (1%)   | 25          | 21  |
| 3   | P     | 363/379 (96%)   | 352 (97%)  | 10 (3%)  | 1 (0%)   | 41          | 41  |
| 4   | D     | 239/241 (99%)   | 233 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 4   | Q     | 239/241 (99%)   | 232 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 5   | E     | 194/196 (99%)   | 181 (93%)  | 10 (5%)  | 3 (2%)   | 10          | 5   |
| 5   | R     | 194/196 (99%)   | 183 (94%)  | 8 (4%)   | 3 (2%)   | 10          | 5   |
| 6   | F     | 97/110 (88%)    | 96 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 6   | S     | 97/110 (88%)    | 94 (97%)   | 1 (1%)   | 2 (2%)   | 7           | 3   |
| 7   | G     | 73/81 (90%)     | 70 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 7   | T     | 74/81 (91%)     | 69 (93%)   | 5 (7%)   | 0        | 100         | 100 |
| 8   | H     | 64/78 (82%)     | 63 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 8   | U     | 64/78 (82%)     | 64 (100%)  | 0        | 0        | 100         | 100 |
| 9   | I     | 39/78 (50%)     | 37 (95%)   | 1 (3%)   | 1 (3%)   | 5           | 2   |
| 9   | V     | 39/78 (50%)     | 36 (92%)   | 2 (5%)   | 1 (3%)   | 5           | 2   |
| 10  | J     | 30/62 (48%)     | 28 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 10  | W     | 59/62 (95%)     | 54 (92%)   | 4 (7%)   | 1 (2%)   | 9           | 4   |
| All | All   | 3945/4220 (94%) | 3803 (96%) | 115 (3%) | 27 (1%)  | 22          | 18  |

All (27) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 224 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 19  | ILE  |
| 5   | E     | 71  | MET  |
| 5   | E     | 72  | SER  |
| 9   | I     | 41  | PRO  |
| 1   | N     | 224 | ASP  |
| 2   | O     | 171 | ALA  |
| 2   | O     | 303 | VAL  |
| 3   | P     | 19  | ILE  |
| 5   | R     | 191 | ASP  |
| 9   | V     | 41  | PRO  |
| 2   | B     | 171 | ALA  |
| 2   | B     | 229 | GLY  |
| 5   | E     | 113 | GLU  |
| 5   | R     | 189 | SER  |
| 5   | R     | 190 | ASP  |
| 6   | S     | 13  | LEU  |
| 1   | A     | 223 | TYR  |
| 3   | C     | 18  | PHE  |
| 1   | N     | 223 | TYR  |
| 1   | A     | 229 | PRO  |
| 1   | A     | 442 | PHE  |
| 1   | N     | 229 | PRO  |
| 1   | N     | 442 | PHE  |
| 6   | S     | 14  | GLU  |
| 10  | W     | 25  | VAL  |
| 2   | B     | 234 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 363/370 (98%) | 355 (98%)  | 8 (2%)   | 52          | 57  |
| 1   | N     | 363/370 (98%) | 357 (98%)  | 6 (2%)   | 60          | 67  |
| 2   | B     | 332/343 (97%) | 332 (100%) | 0        | 100         | 100 |
| 2   | O     | 328/343 (96%) | 328 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 3   | C     | 312/327 (95%)   | 304 (97%)  | 8 (3%)   | 46          | 50  |
| 3   | P     | 311/327 (95%)   | 303 (97%)  | 8 (3%)   | 46          | 50  |
| 4   | D     | 206/206 (100%)  | 206 (100%) | 0        | 100         | 100 |
| 4   | Q     | 206/206 (100%)  | 204 (99%)  | 2 (1%)   | 76          | 82  |
| 5   | E     | 165/168 (98%)   | 164 (99%)  | 1 (1%)   | 86          | 90  |
| 5   | R     | 167/168 (99%)   | 164 (98%)  | 3 (2%)   | 59          | 65  |
| 6   | F     | 90/98 (92%)     | 90 (100%)  | 0        | 100         | 100 |
| 6   | S     | 90/98 (92%)     | 87 (97%)   | 3 (3%)   | 38          | 40  |
| 7   | G     | 66/71 (93%)     | 66 (100%)  | 0        | 100         | 100 |
| 7   | T     | 66/71 (93%)     | 66 (100%)  | 0        | 100         | 100 |
| 8   | H     | 63/74 (85%)     | 63 (100%)  | 0        | 100         | 100 |
| 8   | U     | 63/74 (85%)     | 61 (97%)   | 2 (3%)   | 39          | 41  |
| 9   | I     | 27/60 (45%)     | 26 (96%)   | 1 (4%)   | 34          | 35  |
| 9   | V     | 27/60 (45%)     | 26 (96%)   | 1 (4%)   | 34          | 35  |
| 10  | J     | 27/52 (52%)     | 25 (93%)   | 2 (7%)   | 13          | 10  |
| 10  | W     | 51/52 (98%)     | 49 (96%)   | 2 (4%)   | 32          | 33  |
| All | All   | 3323/3538 (94%) | 3276 (99%) | 47 (1%)  | 67          | 73  |

All (47) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 58  | PHE  |
| 1   | A     | 203 | LEU  |
| 1   | A     | 210 | ASP  |
| 1   | A     | 245 | GLU  |
| 1   | A     | 281 | ASP  |
| 1   | A     | 305 | GLN  |
| 1   | A     | 316 | ASP  |
| 1   | A     | 348 | SER  |
| 3   | C     | 16  | ASN  |
| 3   | C     | 21  | LEU  |
| 3   | C     | 80  | ARG  |
| 3   | C     | 90  | PHE  |
| 3   | C     | 128 | PHE  |
| 3   | C     | 222 | PRO  |
| 3   | C     | 346 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 379 | TRP  |
| 5   | E     | 12  | ASP  |
| 9   | I     | 41  | PRO  |
| 10  | J     | 30  | PHE  |
| 10  | J     | 32  | GLU  |
| 1   | N     | 58  | PHE  |
| 1   | N     | 203 | LEU  |
| 1   | N     | 245 | GLU  |
| 1   | N     | 281 | ASP  |
| 1   | N     | 316 | ASP  |
| 1   | N     | 348 | SER  |
| 3   | P     | 16  | ASN  |
| 3   | P     | 21  | LEU  |
| 3   | P     | 80  | ARG  |
| 3   | P     | 90  | PHE  |
| 3   | P     | 128 | PHE  |
| 3   | P     | 222 | PRO  |
| 3   | P     | 346 | PRO  |
| 3   | P     | 379 | TRP  |
| 4   | Q     | 76  | GLU  |
| 4   | Q     | 169 | LEU  |
| 5   | R     | 12  | ASP  |
| 5   | R     | 113 | GLU  |
| 5   | R     | 191 | ASP  |
| 6   | S     | 13  | LEU  |
| 6   | S     | 33  | ARG  |
| 6   | S     | 58  | ARG  |
| 8   | U     | 42  | GLU  |
| 8   | U     | 78  | LYS  |
| 9   | V     | 41  | PRO  |
| 10  | W     | 29  | LEU  |
| 10  | W     | 62  | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | GLN  |
| 1   | A     | 136 | GLN  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 213 | GLN  |
| 1   | A     | 271 | GLN  |
| 1   | A     | 289 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 305 | GLN  |
| 2   | B     | 22  | GLN  |
| 2   | B     | 104 | ASN  |
| 2   | B     | 240 | HIS  |
| 2   | B     | 305 | GLN  |
| 2   | B     | 412 | ASN  |
| 3   | C     | 16  | ASN  |
| 3   | C     | 159 | ASN  |
| 3   | C     | 201 | HIS  |
| 3   | C     | 341 | GLN  |
| 5   | E     | 57  | GLN  |
| 6   | F     | 79  | GLN  |
| 9   | I     | 71  | ASN  |
| 1   | N     | 136 | GLN  |
| 1   | N     | 165 | GLN  |
| 1   | N     | 215 | HIS  |
| 1   | N     | 271 | GLN  |
| 1   | N     | 311 | ASN  |
| 2   | O     | 104 | ASN  |
| 2   | O     | 218 | GLN  |
| 2   | O     | 240 | HIS  |
| 2   | O     | 412 | ASN  |
| 3   | P     | 16  | ASN  |
| 3   | P     | 159 | ASN  |
| 3   | P     | 201 | HIS  |
| 4   | Q     | 225 | HIS  |
| 5   | R     | 57  | GLN  |
| 6   | S     | 38  | HIS  |
| 6   | S     | 79  | GLN  |
| 8   | U     | 71  | HIS  |
| 8   | U     | 75  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

45 ligands 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 |
| 12  | PO4  | A     | 2013 | -    | 4,4,4        | 1.36 | 1 (25%)  | 6,6,6       | 0.86 | 0        |
| 16  | SMA  | P     | 3001 | -    | 35,38,38     | 1.62 | 9 (25%)  | 46,52,52    | 1.70 | 6 (13%)  |
| 20  | CDL  | T     | 3004 | -    | 48,48,99     | 1.13 | 4 (8%)   | 54,60,111   | 1.15 | 3 (5%)   |
| 13  | AZI  | C     | 2005 | -    | 0,2,2        | 0.00 | -        | 0,1,1       | 0.00 | -        |
| 12  | PO4  | F     | 2012 | -    | 4,4,4        | 1.28 | 1 (25%)  | 6,6,6       | 0.86 | 0        |
| 14  | GOL  | R     | 4005 | -    | 5,5,5        | 1.26 | 0        | 5,5,5       | 0.55 | 0        |
| 11  | JZR  | F     | 3011 | -    | 18,18,18     | 1.79 | 5 (27%)  | 23,23,23    | 0.66 | 0        |
| 19  | HEC  | Q     | 501  | 4    | 26,50,50     | 1.99 | 3 (11%)  | 18,82,82    | 0.82 | 0        |
| 20  | CDL  | G     | 2004 | -    | 43,43,99     | 1.11 | 3 (6%)   | 49,55,111   | 1.21 | 5 (10%)  |
| 18  | ANY  | P     | 3002 | -    | 38,38,41     | 1.84 | 11 (28%) | 34,52,55    | 1.58 | 7 (20%)  |
| 19  | HEC  | D     | 501  | 4    | 26,50,50     | 1.84 | 5 (19%)  | 18,82,82    | 0.94 | 1 (5%)   |
| 17  | PEE  | Q     | 3006 | -    | 50,50,50     | 1.23 | 5 (10%)  | 53,55,55    | 0.84 | 4 (7%)   |
| 12  | PO4  | S     | 3012 | -    | 4,4,4        | 1.33 | 1 (25%)  | 6,6,6       | 0.85 | 0        |
| 13  | AZI  | A     | 4011 | -    | 0,2,2        | 0.00 | -        | 0,1,1       | 0.00 | -        |
| 13  | AZI  | P     | 3005 | -    | 0,2,2        | 0.00 | -        | 0,1,1       | 0.00 | -        |
| 13  | AZI  | O     | 4010 | -    | 0,2,2        | 0.00 | -        | 0,1,1       | 0.00 | -        |
| 13  | AZI  | G     | 4009 | -    | 0,2,2        | 0.00 | -        | 0,1,1       | 0.00 | -        |
| 14  | GOL  | C     | 2008 | -    | 5,5,5        | 1.40 | 0        | 5,5,5       | 0.74 | 0        |
| 16  | SMA  | C     | 2001 | -    | 35,38,38     | 1.67 | 7 (20%)  | 46,52,52    | 1.67 | 6 (13%)  |
| 20  | CDL  | D     | 2003 | -    | 38,38,99     | 1.05 | 1 (2%)   | 43,47,111   | 1.04 | 3 (6%)   |
| 15  | HEM  | P     | 501  | 3    | 27,50,50     | 1.94 | 7 (25%)  | 17,82,82    | 1.29 | 3 (17%)  |
| 15  | HEM  | C     | 501  | 3    | 27,50,50     | 1.89 | 5 (18%)  | 17,82,82    | 1.16 | 1 (5%)   |
| 21  | FES  | R     | 501  | 5    | 0,4,4        | 0.00 | -        | -           | -    | -        |
| 14  | GOL  | O     | 3009 | -    | 5,5,5        | 1.12 | 0        | 5,5,5       | 0.49 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | FES  | E     | 501  | 5    | 0,4,4        | 0.00 | -        | -           |      |          |
| 15  | HEM  | C     | 502  | 3    | 27,50,50     | 1.92 | 9 (33%)  | 17,82,82    | 1.34 | 3 (17%)  |
| 20  | CDL  | P     | 3003 | -    | 38,38,99     | 1.02 | 1 (2%)   | 43,47,111   | 1.03 | 3 (6%)   |
| 18  | ANY  | C     | 2002 | -    | 38,38,41     | 1.84 | 11 (28%) | 34,52,55    | 1.70 | 6 (17%)  |
| 17  | PEE  | D     | 2006 | -    | 25,25,50     | 1.49 | 6 (24%)  | 28,30,55    | 0.75 | 0        |
| 11  | JZR  | A     | 4004 | -    | 18,18,18     | 1.58 | 3 (16%)  | 23,23,23    | 0.62 | 0        |
| 11  | JZR  | P     | 3010 | -    | 18,18,18     | 1.81 | 6 (33%)  | 23,23,23    | 0.69 | 0        |
| 11  | JZR  | S     | 2011 | -    | 18,18,18     | 1.78 | 3 (16%)  | 23,23,23    | 0.72 | 0        |
| 11  | JZR  | D     | 4003 | -    | 18,18,18     | 1.83 | 5 (27%)  | 23,23,23    | 0.71 | 0        |
| 14  | GOL  | B     | 2009 | -    | 5,5,5        | 1.17 | 0        | 5,5,5       | 0.55 | 0        |
| 12  | PO4  | P     | 3013 | -    | 4,4,4        | 1.35 | 1 (25%)  | 6,6,6       | 0.83 | 0        |
| 14  | GOL  | P     | 3008 | -    | 5,5,5        | 1.24 | 0        | 5,5,5       | 0.55 | 0        |
| 11  | JZR  | C     | 2010 | -    | 18,18,18     | 1.80 | 5 (27%)  | 23,23,23    | 0.68 | 0        |
| 11  | JZR  | R     | 4007 | -    | 18,18,18     | 1.84 | 5 (27%)  | 23,23,23    | 0.70 | 0        |
| 15  | HEM  | P     | 502  | 3    | 27,50,50     | 2.05 | 7 (25%)  | 17,82,82    | 1.33 | 4 (23%)  |
| 11  | JZR  | F     | 4001 | -    | 18,18,18     | 1.84 | 5 (27%)  | 23,23,23    | 0.70 | 0        |
| 14  | GOL  | C     | 4006 | -    | 5,5,5        | 1.27 | 0        | 5,5,5       | 0.60 | 0        |
| 17  | PEE  | P     | 3007 | -    | 48,48,50     | 1.20 | 5 (10%)  | 51,53,55    | 0.85 | 4 (7%)   |
| 12  | PO4  | C     | 4008 | -    | 4,4,4        | 1.40 | 1 (25%)  | 6,6,6       | 0.85 | 0        |
| 11  | JZR  | C     | 4002 | -    | 18,18,18     | 1.86 | 4 (22%)  | 23,23,23    | 0.76 | 1 (4%)   |
| 17  | PEE  | C     | 2007 | -    | 48,48,50     | 1.18 | 5 (10%)  | 51,53,55    | 0.85 | 4 (7%)   |

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

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 16  | SMA  | P     | 3001 | -    | -         | 0/33/34/34   | 0/2/2/2 |
| 20  | CDL  | T     | 3004 | -    | -         | 28/57/57/110 | -       |
| 15  | HEM  | P     | 501  | 3    | -         | 0/6/54/54    | -       |
| 14  | GOL  | R     | 4005 | -    | -         | 2/4/4/4      | -       |
| 11  | JZR  | F     | 3011 | -    | -         | 3/9/29/29    | 0/1/1/1 |
| 19  | HEC  | Q     | 501  | 4    | -         | 0/6/54/54    | -       |
| 20  | CDL  | G     | 2004 | -    | -         | 36/52/52/110 | -       |
| 18  | ANY  | P     | 3002 | -    | 1/1/10/13 | 3/37/52/56   | 0/1/2/2 |
| 19  | HEC  | D     | 501  | 4    | -         | 0/6/54/54    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|------|------|---------|--------------|---------|
| 17  | PEE  | Q     | 3006 | -    | -       | 26/54/54/54  | -       |
| 14  | GOL  | C     | 2008 | -    | -       | 4/4/4/4      | -       |
| 16  | SMA  | C     | 2001 | -    | -       | 2/33/34/34   | 0/2/2/2 |
| 20  | CDL  | D     | 2003 | -    | -       | 19/43/43/110 | -       |
| 18  | ANY  | C     | 2002 | -    | -       | 2/37/52/56   | 0/1/2/2 |
| 15  | HEM  | C     | 501  | 3    | -       | 0/6/54/54    | -       |
| 21  | FES  | R     | 501  | 5    | -       | -            | 0/1/1/1 |
| 14  | GOL  | O     | 3009 | -    | -       | 4/4/4/4      | -       |
| 15  | HEM  | C     | 502  | 3    | -       | 0/6/54/54    | -       |
| 20  | CDL  | P     | 3003 | -    | -       | 26/43/43/110 | -       |
| 17  | PEE  | D     | 2006 | -    | -       | 19/29/29/54  | -       |
| 11  | JZR  | A     | 4004 | -    | -       | 0/9/29/29    | 0/1/1/1 |
| 11  | JZR  | P     | 3010 | -    | -       | 4/9/29/29    | 0/1/1/1 |
| 11  | JZR  | S     | 2011 | -    | -       | 5/9/29/29    | 0/1/1/1 |
| 11  | JZR  | D     | 4003 | -    | -       | 4/9/29/29    | 0/1/1/1 |
| 14  | GOL  | B     | 2009 | -    | -       | 2/4/4/4      | -       |
| 14  | GOL  | P     | 3008 | -    | -       | 2/4/4/4      | -       |
| 11  | JZR  | C     | 2010 | -    | -       | 4/9/29/29    | 0/1/1/1 |
| 11  | JZR  | R     | 4007 | -    | -       | 2/9/29/29    | 0/1/1/1 |
| 15  | HEM  | P     | 502  | 3    | -       | 0/6/54/54    | -       |
| 11  | JZR  | F     | 4001 | -    | -       | 2/9/29/29    | 0/1/1/1 |
| 14  | GOL  | C     | 4006 | -    | -       | 3/4/4/4      | -       |
| 17  | PEE  | P     | 3007 | -    | -       | 17/52/52/54  | -       |
| 21  | FES  | E     | 501  | 5    | -       | -            | 0/1/1/1 |
| 11  | JZR  | C     | 4002 | -    | -       | 3/9/29/29    | 0/1/1/1 |
| 17  | PEE  | C     | 2007 | -    | -       | 18/52/52/54  | -       |

All (150) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 19  | Q     | 501  | HEC  | C3C-C2C | -6.52 | 1.33        | 1.40     |
| 19  | Q     | 501  | HEC  | C3B-C2B | -5.66 | 1.34        | 1.40     |
| 18  | P     | 3002 | ANY  | C8-N1   | 4.94  | 1.40        | 1.34     |
| 19  | D     | 501  | HEC  | C3C-C2C | -4.90 | 1.35        | 1.40     |
| 19  | D     | 501  | HEC  | C3B-C2B | -4.84 | 1.35        | 1.40     |
| 11  | C     | 4002 | JZR  | O1-C1   | 4.81  | 1.48        | 1.40     |
| 11  | S     | 2011 | JZR  | O1-C1   | 4.80  | 1.48        | 1.40     |
| 15  | P     | 502  | HEM  | C3B-CAB | -4.78 | 1.38        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | D     | 4003 | JZR  | O1-C1   | 4.76  | 1.48        | 1.40     |
| 11  | F     | 4001 | JZR  | O1-C1   | 4.70  | 1.48        | 1.40     |
| 11  | C     | 2010 | JZR  | O1-C1   | 4.66  | 1.48        | 1.40     |
| 11  | R     | 4007 | JZR  | O1-C1   | 4.66  | 1.48        | 1.40     |
| 18  | C     | 2002 | ANY  | C2-C1   | 4.54  | 1.47        | 1.40     |
| 11  | P     | 3010 | JZR  | O1-C1   | 4.53  | 1.47        | 1.40     |
| 11  | F     | 3011 | JZR  | O1-C1   | 4.50  | 1.47        | 1.40     |
| 18  | C     | 2002 | ANY  | C8-N1   | 4.27  | 1.40        | 1.34     |
| 18  | P     | 3002 | ANY  | C2-C1   | 4.24  | 1.46        | 1.40     |
| 15  | P     | 502  | HEM  | C3C-CAC | -4.18 | 1.39        | 1.47     |
| 15  | P     | 501  | HEM  | C3B-CAB | -4.16 | 1.39        | 1.47     |
| 15  | P     | 502  | HEM  | CBB-CAB | 4.13  | 1.56        | 1.29     |
| 15  | P     | 501  | HEM  | CBB-CAB | 4.09  | 1.56        | 1.29     |
| 15  | C     | 501  | HEM  | C3B-CAB | -4.08 | 1.39        | 1.47     |
| 16  | P     | 3001 | SMA  | O1-C2   | 4.07  | 1.41        | 1.35     |
| 15  | C     | 501  | HEM  | CBC-CAC | 4.02  | 1.56        | 1.29     |
| 16  | C     | 2001 | SMA  | O1-C2   | 4.00  | 1.40        | 1.35     |
| 15  | C     | 501  | HEM  | C3C-CAC | -3.91 | 1.39        | 1.47     |
| 15  | P     | 501  | HEM  | C3C-CAC | -3.90 | 1.39        | 1.47     |
| 15  | P     | 501  | HEM  | CBC-CAC | 3.78  | 1.54        | 1.29     |
| 15  | C     | 502  | HEM  | CBC-CAC | 3.78  | 1.54        | 1.29     |
| 15  | P     | 502  | HEM  | CBC-CAC | 3.75  | 1.54        | 1.29     |
| 15  | C     | 502  | HEM  | C3B-CAB | -3.71 | 1.40        | 1.47     |
| 15  | C     | 502  | HEM  | CBB-CAB | 3.56  | 1.52        | 1.29     |
| 18  | C     | 2002 | ANY  | C3-C2   | 3.56  | 1.45        | 1.39     |
| 18  | P     | 3002 | ANY  | C12-C11 | 3.51  | 1.60        | 1.52     |
| 18  | C     | 2002 | ANY  | C12-C11 | 3.51  | 1.60        | 1.52     |
| 16  | C     | 2001 | SMA  | C4A-C8A | 3.49  | 1.46        | 1.41     |
| 19  | D     | 501  | HEC  | C3C-C4C | 3.49  | 1.49        | 1.43     |
| 18  | P     | 3002 | ANY  | C3-C2   | 3.49  | 1.45        | 1.39     |
| 15  | C     | 501  | HEM  | CBB-CAB | 3.45  | 1.52        | 1.29     |
| 15  | C     | 502  | HEM  | C3C-CAC | -3.41 | 1.40        | 1.47     |
| 11  | S     | 2011 | JZR  | O5-C1   | 3.41  | 1.50        | 1.41     |
| 11  | F     | 3011 | JZR  | O5-C1   | 3.40  | 1.50        | 1.41     |
| 16  | P     | 3001 | SMA  | C4-C3   | 3.40  | 1.51        | 1.41     |
| 15  | P     | 501  | HEM  | C3B-C2B | -3.38 | 1.35        | 1.40     |
| 16  | C     | 2001 | SMA  | C7-C8   | 3.34  | 1.44        | 1.40     |
| 11  | R     | 4007 | JZR  | O5-C1   | 3.34  | 1.50        | 1.41     |
| 11  | D     | 4003 | JZR  | O5-C1   | 3.32  | 1.50        | 1.41     |
| 11  | A     | 4004 | JZR  | O1-C1   | 3.31  | 1.45        | 1.40     |
| 11  | C     | 4002 | JZR  | O5-C1   | 3.26  | 1.50        | 1.41     |
| 11  | F     | 4001 | JZR  | O5-C1   | 3.26  | 1.50        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 16  | P     | 3001 | SMA  | C7-C8   | 3.25  | 1.44        | 1.40     |
| 11  | C     | 2010 | JZR  | O5-C1   | 3.22  | 1.50        | 1.41     |
| 17  | C     | 2007 | PEE  | O3-C30  | 3.16  | 1.42        | 1.33     |
| 11  | A     | 4004 | JZR  | O5-C1   | 3.09  | 1.49        | 1.41     |
| 18  | P     | 3002 | ANY  | C13-C12 | 3.09  | 1.59        | 1.53     |
| 11  | P     | 3010 | JZR  | O5-C1   | 3.09  | 1.49        | 1.41     |
| 16  | C     | 2001 | SMA  | C4-C3   | 3.07  | 1.50        | 1.41     |
| 17  | Q     | 3006 | PEE  | C19-C18 | -3.07 | 1.34        | 1.51     |
| 19  | Q     | 501  | HEC  | C3C-C4C | 3.07  | 1.48        | 1.43     |
| 16  | P     | 3001 | SMA  | C6-C7   | 3.05  | 1.44        | 1.38     |
| 16  | C     | 2001 | SMA  | C6-C7   | 3.05  | 1.44        | 1.38     |
| 17  | Q     | 3006 | PEE  | O3-C30  | 3.03  | 1.42        | 1.33     |
| 17  | P     | 3007 | PEE  | C19-C18 | -3.02 | 1.34        | 1.51     |
| 17  | Q     | 3006 | PEE  | C22-C21 | -2.99 | 1.34        | 1.51     |
| 17  | P     | 3007 | PEE  | O3-C30  | 2.98  | 1.42        | 1.33     |
| 17  | D     | 2006 | PEE  | P-O1P   | 2.97  | 1.61        | 1.50     |
| 17  | C     | 2007 | PEE  | C22-C21 | -2.97 | 1.34        | 1.51     |
| 17  | C     | 2007 | PEE  | C19-C18 | -2.96 | 1.35        | 1.51     |
| 18  | C     | 2002 | ANY  | C10-C9  | 2.96  | 1.60        | 1.53     |
| 17  | P     | 3007 | PEE  | C22-C21 | -2.95 | 1.35        | 1.51     |
| 17  | Q     | 3006 | PEE  | P-O1P   | 2.95  | 1.61        | 1.50     |
| 17  | P     | 3007 | PEE  | P-O1P   | 2.94  | 1.61        | 1.50     |
| 17  | P     | 3007 | PEE  | O2-C10  | 2.91  | 1.42        | 1.34     |
| 15  | P     | 502  | HEM  | C1A-NA  | 2.90  | 1.42        | 1.36     |
| 17  | D     | 2006 | PEE  | O2-C10  | 2.90  | 1.42        | 1.34     |
| 17  | Q     | 3006 | PEE  | O2-C10  | 2.83  | 1.42        | 1.34     |
| 18  | C     | 2002 | ANY  | C13-C12 | 2.74  | 1.58        | 1.53     |
| 18  | P     | 3002 | ANY  | C7-N2   | 2.74  | 1.40        | 1.34     |
| 11  | A     | 4004 | JZR  | C4-C5   | 2.73  | 1.58        | 1.53     |
| 16  | C     | 2001 | SMA  | C20-C19 | 2.72  | 1.35        | 1.33     |
| 17  | C     | 2007 | PEE  | O2-C10  | 2.71  | 1.42        | 1.34     |
| 16  | P     | 3001 | SMA  | O1-C8A  | 2.70  | 1.40        | 1.36     |
| 17  | D     | 2006 | PEE  | O3-C30  | 2.67  | 1.41        | 1.33     |
| 11  | C     | 4002 | JZR  | C4-C5   | 2.64  | 1.58        | 1.53     |
| 18  | C     | 2002 | ANY  | O8-C21  | 2.62  | 1.40        | 1.34     |
| 18  | C     | 2002 | ANY  | O5-C14  | 2.61  | 1.40        | 1.34     |
| 11  | P     | 3010 | JZR  | C4-C5   | 2.60  | 1.58        | 1.53     |
| 16  | P     | 3001 | SMA  | C4A-C8A | 2.58  | 1.44        | 1.41     |
| 11  | R     | 4007 | JZR  | C4-C5   | 2.57  | 1.58        | 1.53     |
| 15  | C     | 502  | HEM  | C3C-C2C | -2.54 | 1.36        | 1.40     |
| 17  | C     | 2007 | PEE  | P-O1P   | 2.47  | 1.59        | 1.50     |
| 11  | F     | 4001 | JZR  | C4-C5   | 2.47  | 1.58        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | C     | 502  | HEM  | C3B-C2B | -2.44 | 1.37        | 1.40     |
| 12  | C     | 4008 | PO4  | P-O1    | 2.44  | 1.56        | 1.50     |
| 16  | P     | 3001 | SMA  | C20-C19 | 2.44  | 1.35        | 1.33     |
| 16  | C     | 2001 | SMA  | O1-C8A  | 2.43  | 1.40        | 1.36     |
| 15  | C     | 501  | HEM  | C4D-C3D | 2.42  | 1.48        | 1.42     |
| 11  | F     | 3011 | JZR  | C4-C5   | 2.40  | 1.58        | 1.53     |
| 15  | P     | 501  | HEM  | C4A-NA  | 2.40  | 1.41        | 1.36     |
| 11  | D     | 4003 | JZR  | C4-C5   | 2.39  | 1.58        | 1.53     |
| 18  | C     | 2002 | ANY  | C5-C6   | 2.39  | 1.43        | 1.39     |
| 20  | T     | 3004 | CDL  | O1-C1   | 2.38  | 1.50        | 1.43     |
| 20  | T     | 3004 | CDL  | OB8-CB6 | -2.36 | 1.39        | 1.45     |
| 15  | P     | 501  | HEM  | C4D-C3D | 2.35  | 1.47        | 1.42     |
| 20  | G     | 2004 | CDL  | O1-C1   | 2.35  | 1.50        | 1.43     |
| 18  | P     | 3002 | ANY  | O5-C14  | 2.34  | 1.39        | 1.34     |
| 18  | P     | 3002 | ANY  | O8-C21  | 2.33  | 1.39        | 1.34     |
| 12  | A     | 2013 | PO4  | P-O1    | 2.33  | 1.56        | 1.50     |
| 11  | C     | 4002 | JZR  | O5-C5   | 2.32  | 1.50        | 1.44     |
| 17  | D     | 2006 | PEE  | C3-C2   | 2.32  | 1.57        | 1.50     |
| 18  | P     | 3002 | ANY  | C5-C6   | 2.32  | 1.43        | 1.39     |
| 11  | S     | 2011 | JZR  | O5-C5   | 2.32  | 1.50        | 1.44     |
| 12  | S     | 3012 | PO4  | P-O1    | 2.31  | 1.56        | 1.50     |
| 11  | R     | 4007 | JZR  | O5-C5   | 2.31  | 1.49        | 1.44     |
| 12  | P     | 3013 | PO4  | P-O1    | 2.30  | 1.56        | 1.50     |
| 18  | P     | 3002 | ANY  | C10-C9  | 2.28  | 1.58        | 1.53     |
| 11  | D     | 4003 | JZR  | O5-C5   | 2.28  | 1.49        | 1.44     |
| 18  | C     | 2002 | ANY  | C7-N2   | 2.27  | 1.39        | 1.34     |
| 20  | D     | 2003 | CDL  | O1-C1   | 2.24  | 1.50        | 1.43     |
| 16  | P     | 3001 | SMA  | C6-C5   | 2.24  | 1.44        | 1.37     |
| 12  | F     | 2012 | PO4  | P-O1    | 2.22  | 1.56        | 1.50     |
| 11  | F     | 4001 | JZR  | O5-C5   | 2.21  | 1.49        | 1.44     |
| 20  | T     | 3004 | CDL  | OA8-CA6 | -2.19 | 1.40        | 1.45     |
| 15  | C     | 502  | HEM  | C1D-ND  | 2.19  | 1.40        | 1.36     |
| 19  | D     | 501  | HEC  | C3B-C4B | 2.19  | 1.47        | 1.43     |
| 15  | P     | 502  | HEM  | C1B-C2B | 2.18  | 1.47        | 1.42     |
| 11  | C     | 2010 | JZR  | C4-C5   | 2.18  | 1.57        | 1.53     |
| 19  | D     | 501  | HEC  | C4A-C3A | 2.15  | 1.47        | 1.42     |
| 11  | F     | 3011 | JZR  | O5-C5   | 2.14  | 1.49        | 1.44     |
| 18  | P     | 3002 | ANY  | C6-C1   | 2.14  | 1.45        | 1.41     |
| 20  | P     | 3003 | CDL  | O1-C1   | 2.14  | 1.49        | 1.43     |
| 11  | C     | 2010 | JZR  | O5-C5   | 2.14  | 1.49        | 1.44     |
| 11  | P     | 3010 | JZR  | C1-C2   | 2.12  | 1.58        | 1.52     |
| 11  | P     | 3010 | JZR  | O5-C5   | 2.10  | 1.49        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | P     | 502  | HEM  | C4D-C3D | 2.10  | 1.47        | 1.42     |
| 17  | D     | 2006 | PEE  | C1-C2   | 2.10  | 1.57        | 1.50     |
| 20  | G     | 2004 | CDL  | OA8-CA6 | -2.09 | 1.40        | 1.45     |
| 15  | C     | 502  | HEM  | CAD-C3D | 2.08  | 1.55        | 1.52     |
| 16  | P     | 3001 | SMA  | O5-C5   | 2.07  | 1.40        | 1.36     |
| 20  | G     | 2004 | CDL  | OB8-CB6 | -2.07 | 1.40        | 1.45     |
| 11  | F     | 3011 | JZR  | C1-C2   | 2.07  | 1.58        | 1.52     |
| 17  | D     | 2006 | PEE  | C31-C30 | 2.07  | 1.56        | 1.50     |
| 11  | F     | 4001 | JZR  | C1-C2   | 2.05  | 1.58        | 1.52     |
| 11  | P     | 3010 | JZR  | C4-C3   | 2.04  | 1.57        | 1.52     |
| 11  | C     | 2010 | JZR  | C1-C2   | 2.03  | 1.58        | 1.52     |
| 18  | C     | 2002 | ANY  | C6-C1   | 2.03  | 1.44        | 1.41     |
| 11  | R     | 4007 | JZR  | C1-C2   | 2.02  | 1.58        | 1.52     |
| 20  | T     | 3004 | CDL  | CB3-CB4 | 2.02  | 1.56        | 1.50     |
| 15  | C     | 502  | HEM  | C1A-NA  | 2.01  | 1.40        | 1.36     |
| 11  | D     | 4003 | JZR  | C1-C2   | 2.00  | 1.58        | 1.52     |

All (64) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 16  | C     | 2001 | SMA  | C3-C4-C4A   | -5.76 | 114.79      | 120.58   |
| 16  | P     | 3001 | SMA  | C9-C2-C3    | 5.56  | 128.27      | 120.39   |
| 16  | P     | 3001 | SMA  | C3-C4-C4A   | -5.30 | 115.25      | 120.58   |
| 18  | C     | 2002 | ANY  | C25-C22-C23 | 5.11  | 133.03      | 111.69   |
| 16  | C     | 2001 | SMA  | C9-C2-C3    | 5.04  | 127.53      | 120.39   |
| 16  | P     | 3001 | SMA  | C9-C10-C11  | -4.50 | 108.65      | 114.72   |
| 20  | T     | 3004 | CDL  | CB4-OB6-CB5 | -4.33 | 109.82      | 117.90   |
| 16  | C     | 2001 | SMA  | C4-C3-C2    | 4.16  | 121.19      | 116.63   |
| 16  | C     | 2001 | SMA  | C9-C10-C11  | -4.07 | 109.23      | 114.72   |
| 18  | P     | 3002 | ANY  | C23-C22-C21 | 3.97  | 123.05      | 111.02   |
| 20  | G     | 2004 | CDL  | CB4-OB6-CB5 | -3.82 | 110.77      | 117.90   |
| 16  | P     | 3001 | SMA  | C4-C3-C2    | 3.72  | 120.71      | 116.63   |
| 18  | C     | 2002 | ANY  | O5-C14-O6   | -3.58 | 119.58      | 124.08   |
| 18  | P     | 3002 | ANY  | O5-C14-O6   | -3.49 | 119.69      | 124.08   |
| 18  | C     | 2002 | ANY  | O2-C8-N1    | -3.12 | 121.82      | 125.80   |
| 16  | P     | 3001 | SMA  | O1-C2-C9    | -3.00 | 108.35      | 111.91   |
| 20  | T     | 3004 | CDL  | CA4-OA6-CA5 | -3.00 | 110.42      | 117.79   |
| 18  | P     | 3002 | ANY  | O2-C8-N1    | -2.98 | 121.99      | 125.80   |
| 17  | Q     | 3006 | PEE  | C20-C19-C18 | 2.77  | 128.49      | 114.42   |
| 18  | C     | 2002 | ANY  | C25-C22-C21 | 2.76  | 119.39      | 111.02   |
| 20  | G     | 2004 | CDL  | CA4-OA6-CA5 | -2.74 | 111.06      | 117.79   |
| 18  | P     | 3002 | ANY  | C25-C22-C23 | 2.72  | 123.05      | 111.69   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | P     | 3007 | PEE  | C19-C18-C17 | 2.67  | 127.97      | 114.42   |
| 15  | P     | 502  | HEM  | CMD-C2D-C1D | -2.66 | 124.38      | 128.46   |
| 20  | G     | 2004 | CDL  | CA6-CA4-CA3 | -2.66 | 105.50      | 111.79   |
| 15  | C     | 501  | HEM  | C4A-C3A-C2A | -2.65 | 105.15      | 107.00   |
| 17  | C     | 2007 | PEE  | C19-C18-C17 | 2.65  | 127.86      | 114.42   |
| 19  | D     | 501  | HEC  | CMB-C2B-C3B | -2.64 | 122.72      | 125.82   |
| 17  | C     | 2007 | PEE  | C20-C19-C18 | 2.63  | 127.78      | 114.42   |
| 17  | C     | 2007 | PEE  | C23-C22-C21 | 2.62  | 127.74      | 114.42   |
| 17  | P     | 3007 | PEE  | C20-C19-C18 | 2.62  | 127.72      | 114.42   |
| 17  | P     | 3007 | PEE  | C23-C22-C21 | 2.61  | 127.67      | 114.42   |
| 15  | P     | 501  | HEM  | C4A-C3A-C2A | -2.60 | 105.19      | 107.00   |
| 20  | P     | 3003 | CDL  | CB6-CB4-CB3 | -2.58 | 105.68      | 111.79   |
| 20  | D     | 2003 | CDL  | CB4-OB6-CB5 | -2.58 | 111.44      | 117.79   |
| 17  | Q     | 3006 | PEE  | C22-C21-C20 | 2.54  | 127.32      | 114.42   |
| 20  | D     | 2003 | CDL  | CB6-CB4-CB3 | -2.49 | 105.89      | 111.79   |
| 17  | Q     | 3006 | PEE  | C19-C18-C17 | 2.49  | 127.07      | 114.42   |
| 16  | C     | 2001 | SMA  | O1-C2-C9    | -2.44 | 109.01      | 111.91   |
| 20  | P     | 3003 | CDL  | CB4-OB6-CB5 | -2.39 | 111.90      | 117.79   |
| 18  | P     | 3002 | ANY  | O4-C20-O7   | -2.37 | 121.09      | 124.08   |
| 17  | P     | 3007 | PEE  | C22-C21-C20 | 2.37  | 126.44      | 114.42   |
| 16  | P     | 3001 | SMA  | C10-C9-C2   | 2.35  | 118.64      | 113.59   |
| 17  | C     | 2007 | PEE  | C22-C21-C20 | 2.34  | 126.32      | 114.42   |
| 18  | C     | 2002 | ANY  | O8-C21-O9   | -2.29 | 119.67      | 123.94   |
| 20  | D     | 2003 | CDL  | OA4-PA1-OA2 | 2.28  | 112.81      | 106.73   |
| 18  | P     | 3002 | ANY  | O8-C21-O9   | -2.26 | 119.72      | 123.94   |
| 11  | C     | 4002 | JZR  | C1'-O1-C1   | 2.26  | 117.58      | 113.84   |
| 20  | G     | 2004 | CDL  | CB6-CB4-CB3 | -2.25 | 106.47      | 111.79   |
| 17  | Q     | 3006 | PEE  | C23-C22-C21 | 2.23  | 125.74      | 114.42   |
| 15  | C     | 502  | HEM  | C3B-C4B-NB  | 2.22  | 112.09      | 109.21   |
| 15  | P     | 502  | HEM  | C3B-C4B-NB  | 2.22  | 112.08      | 109.21   |
| 15  | C     | 502  | HEM  | CBD-CAD-C3D | -2.21 | 108.42      | 112.48   |
| 20  | T     | 3004 | CDL  | CB6-OB8-CB7 | -2.20 | 111.57      | 117.10   |
| 18  | C     | 2002 | ANY  | C23-C22-C21 | -2.17 | 104.43      | 111.02   |
| 15  | P     | 501  | HEM  | CMB-C2B-C3B | 2.17  | 128.73      | 124.68   |
| 15  | P     | 501  | HEM  | C3B-C4B-NB  | 2.13  | 111.96      | 109.21   |
| 20  | G     | 2004 | CDL  | CB6-OB8-CB7 | -2.13 | 111.76      | 117.10   |
| 15  | P     | 502  | HEM  | CMB-C2B-C3B | 2.13  | 128.65      | 124.68   |
| 15  | P     | 502  | HEM  | CBD-CAD-C3D | -2.11 | 108.60      | 112.48   |
| 20  | P     | 3003 | CDL  | OA4-PA1-OA2 | 2.09  | 112.30      | 106.73   |
| 18  | P     | 3002 | ANY  | O7-C20-C9   | 2.04  | 130.37      | 124.72   |
| 15  | C     | 502  | HEM  | CMB-C2B-C3B | 2.02  | 128.46      | 124.68   |
| 16  | C     | 2001 | SMA  | O8-C8-C8A   | 2.00  | 123.29      | 119.62   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 18  | P     | 3002 | ANY  | C22  |

All (240) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | T     | 3004 | CDL  | O1-C1-CA2-OA2   |
| 20  | T     | 3004 | CDL  | O1-C1-CB2-OB2   |
| 20  | T     | 3004 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | T     | 3004 | CDL  | CB2-OB2-PB2-OB5 |
| 14  | R     | 4005 | GOL  | O1-C1-C2-C3     |
| 20  | G     | 2004 | CDL  | O1-C1-CB2-OB2   |
| 20  | G     | 2004 | CDL  | CA2-C1-CB2-OB2  |
| 20  | G     | 2004 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | G     | 2004 | CDL  | CA2-OA2-PA1-OA4 |
| 20  | G     | 2004 | CDL  | CA2-OA2-PA1-OA5 |
| 20  | G     | 2004 | CDL  | C11-CA5-OA6-CA4 |
| 20  | G     | 2004 | CDL  | C51-CB5-OB6-CB4 |
| 17  | Q     | 3006 | PEE  | O4P-C4-C5-N     |
| 17  | Q     | 3006 | PEE  | C4-O4P-P-O1P    |
| 17  | Q     | 3006 | PEE  | C4-O4P-P-O2P    |
| 17  | Q     | 3006 | PEE  | C4-O4P-P-O3P    |
| 14  | C     | 2008 | GOL  | C1-C2-C3-O3     |
| 20  | D     | 2003 | CDL  | CA2-OA2-PA1-OA4 |
| 20  | D     | 2003 | CDL  | CA2-OA2-PA1-OA5 |
| 20  | D     | 2003 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | D     | 2003 | CDL  | CB2-OB2-PB2-OB4 |
| 20  | D     | 2003 | CDL  | OB5-CB3-CB4-OB6 |
| 14  | O     | 3009 | GOL  | O1-C1-C2-C3     |
| 14  | O     | 3009 | GOL  | C1-C2-C3-O3     |
| 20  | P     | 3003 | CDL  | CA2-C1-CB2-OB2  |
| 20  | P     | 3003 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | P     | 3003 | CDL  | CA2-OA2-PA1-OA5 |
| 20  | P     | 3003 | CDL  | OB6-CB4-CB6-OB8 |
| 17  | D     | 2006 | PEE  | C2-C1-O3P-P     |
| 17  | D     | 2006 | PEE  | C4-O4P-P-O1P    |
| 17  | D     | 2006 | PEE  | C4-O4P-P-O2P    |
| 17  | D     | 2006 | PEE  | C4-O4P-P-O3P    |
| 17  | P     | 3007 | PEE  | C4-O4P-P-O1P    |
| 14  | P     | 3008 | GOL  | O1-C1-C2-C3     |
| 17  | C     | 2007 | PEE  | C4-O4P-P-O1P    |
| 20  | T     | 3004 | CDL  | C51-CB5-OB6-CB4 |
| 20  | G     | 2004 | CDL  | C71-CB7-OB8-CB6 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | T     | 3004 | CDL  | OB7-CB5-OB6-CB4 |
| 20  | G     | 2004 | CDL  | OA7-CA5-OA6-CA4 |
| 20  | T     | 3004 | CDL  | OA9-CA7-OA8-CA6 |
| 20  | G     | 2004 | CDL  | OB7-CB5-OB6-CB4 |
| 20  | G     | 2004 | CDL  | OB9-CB7-OB8-CB6 |
| 17  | D     | 2006 | PEE  | O5-C30-O3-C3    |
| 20  | P     | 3003 | CDL  | O1-C1-CB2-OB2   |
| 20  | T     | 3004 | CDL  | C31-CA7-OA8-CA6 |
| 17  | D     | 2006 | PEE  | C31-C30-O3-C3   |
| 20  | T     | 3004 | CDL  | C71-CB7-OB8-CB6 |
| 20  | G     | 2004 | CDL  | C31-CA7-OA8-CA6 |
| 11  | S     | 2011 | JZR  | C4-C5-C6-O6     |
| 17  | C     | 2007 | PEE  | C21-C22-C23-C24 |
| 17  | P     | 3007 | PEE  | C21-C22-C23-C24 |
| 20  | G     | 2004 | CDL  | CA7-C31-C32-C33 |
| 20  | T     | 3004 | CDL  | C11-CA5-OA6-CA4 |
| 17  | P     | 3007 | PEE  | C10-C11-C12-C13 |
| 17  | C     | 2007 | PEE  | C10-C11-C12-C13 |
| 20  | T     | 3004 | CDL  | OB9-CB7-OB8-CB6 |
| 14  | O     | 3009 | GOL  | O1-C1-C2-O2     |
| 14  | O     | 3009 | GOL  | O2-C2-C3-O3     |
| 20  | T     | 3004 | CDL  | CA5-C11-C12-C13 |
| 17  | Q     | 3006 | PEE  | C10-C11-C12-C13 |
| 17  | Q     | 3006 | PEE  | C30-C31-C32-C33 |
| 11  | F     | 3011 | JZR  | O1-C1'-C2'-C3'  |
| 11  | D     | 4003 | JZR  | O5-C5-C6-O6     |
| 11  | P     | 3010 | JZR  | O1-C1'-C2'-C3'  |
| 20  | G     | 2004 | CDL  | OA9-CA7-OA8-CA6 |
| 11  | D     | 4003 | JZR  | O1-C1'-C2'-C3'  |
| 11  | S     | 2011 | JZR  | O5-C5-C6-O6     |
| 20  | G     | 2004 | CDL  | CB2-OB2-PB2-OB5 |
| 20  | D     | 2003 | CDL  | CB2-OB2-PB2-OB5 |
| 20  | T     | 3004 | CDL  | CB2-C1-CA2-OA2  |
| 20  | T     | 3004 | CDL  | CA2-C1-CB2-OB2  |
| 20  | T     | 3004 | CDL  | OA7-CA5-OA6-CA4 |
| 17  | C     | 2007 | PEE  | C37-C38-C39-C40 |
| 11  | P     | 3010 | JZR  | O5-C5-C6-O6     |
| 20  | T     | 3004 | CDL  | C11-C12-C13-C14 |
| 17  | Q     | 3006 | PEE  | C35-C36-C37-C38 |
| 17  | Q     | 3006 | PEE  | C38-C39-C40-C41 |
| 17  | P     | 3007 | PEE  | C12-C13-C14-C15 |
| 17  | P     | 3007 | PEE  | C19-C20-C21-C22 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | P     | 3007 | PEE  | C37-C38-C39-C40 |
| 17  | C     | 2007 | PEE  | C12-C13-C14-C15 |
| 17  | C     | 2007 | PEE  | C19-C20-C21-C22 |
| 11  | D     | 4003 | JZR  | C2'-C3'-C4'-C5' |
| 20  | D     | 2003 | CDL  | C78-C79-C80-C81 |
| 17  | C     | 2007 | PEE  | C41-C42-C43-C44 |
| 20  | T     | 3004 | CDL  | C13-C14-C15-C16 |
| 17  | Q     | 3006 | PEE  | C43-C44-C45-C46 |
| 17  | P     | 3007 | PEE  | C41-C42-C43-C44 |
| 20  | T     | 3004 | CDL  | C32-C33-C34-C35 |
| 20  | P     | 3003 | CDL  | C77-C78-C79-C80 |
| 17  | P     | 3007 | PEE  | C18-C19-C20-C21 |
| 17  | C     | 2007 | PEE  | C18-C19-C20-C21 |
| 17  | Q     | 3006 | PEE  | C18-C19-C20-C21 |
| 14  | C     | 2008 | GOL  | O1-C1-C2-C3     |
| 14  | B     | 2009 | GOL  | C1-C2-C3-O3     |
| 14  | C     | 4006 | GOL  | O1-C1-C2-C3     |
| 14  | C     | 4006 | GOL  | C1-C2-C3-O3     |
| 20  | D     | 2003 | CDL  | C51-CB5-OB6-CB4 |
| 17  | C     | 2007 | PEE  | C20-C21-C22-C23 |
| 17  | Q     | 3006 | PEE  | C15-C16-C17-C18 |
| 17  | Q     | 3006 | PEE  | C42-C43-C44-C45 |
| 20  | D     | 2003 | CDL  | C73-C74-C75-C76 |
| 11  | C     | 4002 | JZR  | C2'-C3'-C4'-C5' |
| 17  | P     | 3007 | PEE  | C20-C21-C22-C23 |
| 17  | Q     | 3006 | PEE  | C17-C18-C19-C20 |
| 17  | Q     | 3006 | PEE  | C40-C41-C42-C43 |
| 20  | T     | 3004 | CDL  | C31-C32-C33-C34 |
| 20  | D     | 2003 | CDL  | CB3-CB4-CB6-OB8 |
| 17  | Q     | 3006 | PEE  | C13-C14-C15-C16 |
| 17  | C     | 2007 | PEE  | C33-C34-C35-C36 |
| 14  | R     | 4005 | GOL  | O1-C1-C2-O2     |
| 14  | C     | 2008 | GOL  | O1-C1-C2-O2     |
| 14  | C     | 2008 | GOL  | O2-C2-C3-O3     |
| 14  | B     | 2009 | GOL  | O2-C2-C3-O3     |
| 14  | C     | 4006 | GOL  | O2-C2-C3-O3     |
| 17  | Q     | 3006 | PEE  | C22-C23-C24-C25 |
| 20  | P     | 3003 | CDL  | C73-C74-C75-C76 |
| 20  | D     | 2003 | CDL  | OB7-CB5-OB6-CB4 |
| 20  | T     | 3004 | CDL  | C34-C35-C36-C37 |
| 17  | Q     | 3006 | PEE  | C34-C35-C36-C37 |
| 20  | P     | 3003 | CDL  | C72-C73-C74-C75 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | P     | 3007 | PEE  | C33-C34-C35-C36 |
| 17  | Q     | 3006 | PEE  | C37-C38-C39-C40 |
| 17  | P     | 3007 | PEE  | C22-C23-C24-C25 |
| 17  | C     | 2007 | PEE  | C22-C23-C24-C25 |
| 20  | P     | 3003 | CDL  | CB5-C51-C52-C53 |
| 20  | P     | 3003 | CDL  | CB7-C71-C72-C73 |
| 20  | P     | 3003 | CDL  | C78-C79-C80-C81 |
| 17  | Q     | 3006 | PEE  | C23-C24-C25-C26 |
| 20  | D     | 2003 | CDL  | CB7-C71-C72-C73 |
| 11  | D     | 4003 | JZR  | C1'-C2'-C3'-C4' |
| 11  | C     | 2010 | JZR  | C1'-C2'-C3'-C4' |
| 11  | R     | 4007 | JZR  | C1'-C2'-C3'-C4' |
| 17  | P     | 3007 | PEE  | C13-C14-C15-C16 |
| 17  | D     | 2006 | PEE  | C11-C10-O2-C2   |
| 17  | C     | 2007 | PEE  | C13-C14-C15-C16 |
| 17  | D     | 2006 | PEE  | O4-C10-O2-C2    |
| 11  | C     | 4002 | JZR  | O5-C5-C6-O6     |
| 17  | C     | 2007 | PEE  | C35-C36-C37-C38 |
| 11  | F     | 4001 | JZR  | C1'-C2'-C3'-C4' |
| 20  | G     | 2004 | CDL  | CA3-OA5-PA1-OA2 |
| 11  | P     | 3010 | JZR  | C1'-C2'-C3'-C4' |
| 20  | G     | 2004 | CDL  | OA5-CA3-CA4-CA6 |
| 20  | G     | 2004 | CDL  | OB5-CB3-CB4-CB6 |
| 20  | P     | 3003 | CDL  | OB5-CB3-CB4-CB6 |
| 11  | S     | 2011 | JZR  | C1'-C2'-C3'-C4' |
| 17  | Q     | 3006 | PEE  | C20-C21-C22-C23 |
| 17  | P     | 3007 | PEE  | C35-C36-C37-C38 |
| 20  | P     | 3003 | CDL  | CB3-CB4-CB6-OB8 |
| 14  | P     | 3008 | GOL  | O1-C1-C2-O2     |
| 11  | C     | 4002 | JZR  | C3'-C4'-C5'-C6' |
| 20  | P     | 3003 | CDL  | C51-C52-C53-C54 |
| 20  | D     | 2003 | CDL  | CA2-OA2-PA1-OA3 |
| 17  | D     | 2006 | PEE  | C33-C34-C35-C36 |
| 20  | D     | 2003 | CDL  | C72-C73-C74-C75 |
| 11  | P     | 3010 | JZR  | C2'-C3'-C4'-C5' |
| 17  | P     | 3007 | PEE  | C23-C24-C25-C26 |
| 20  | D     | 2003 | CDL  | OB5-CB3-CB4-CB6 |
| 17  | C     | 2007 | PEE  | C23-C24-C25-C26 |
| 17  | Q     | 3006 | PEE  | C39-C40-C41-C42 |
| 20  | G     | 2004 | CDL  | C35-C36-C37-C38 |
| 20  | G     | 2004 | CDL  | C34-C35-C36-C37 |
| 20  | T     | 3004 | CDL  | CA3-CA4-CA6-OA8 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | D     | 2006 | PEE  | C32-C33-C34-C35 |
| 20  | T     | 3004 | CDL  | OB5-CB3-CB4-OB6 |
| 20  | P     | 3003 | CDL  | OB5-CB3-CB4-OB6 |
| 18  | P     | 3002 | ANY  | C16-C17-C18-C19 |
| 20  | D     | 2003 | CDL  | C76-C77-C78-C79 |
| 11  | C     | 2010 | JZR  | C4-C5-C6-O6     |
| 20  | G     | 2004 | CDL  | OA6-CA4-CA6-OA8 |
| 18  | P     | 3002 | ANY  | C15-C16-C17-C18 |
| 17  | Q     | 3006 | PEE  | C44-C45-C46-C47 |
| 20  | G     | 2004 | CDL  | CA3-CA4-CA6-OA8 |
| 20  | G     | 2004 | CDL  | OA5-CA3-CA4-OA6 |
| 20  | G     | 2004 | CDL  | OB5-CB3-CB4-OB6 |
| 17  | Q     | 3006 | PEE  | O3P-C1-C2-O2    |
| 17  | D     | 2006 | PEE  | C10-C11-C12-C13 |
| 20  | P     | 3003 | CDL  | OB7-CB5-OB6-CB4 |
| 11  | F     | 3011 | JZR  | C1'-C2'-C3'-C4' |
| 17  | D     | 2006 | PEE  | C1-O3P-P-O4P    |
| 20  | T     | 3004 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | G     | 2004 | CDL  | CA3-OA5-PA1-OA3 |
| 20  | G     | 2004 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | G     | 2004 | CDL  | CB3-OB5-PB2-OB3 |
| 17  | D     | 2006 | PEE  | C1-O3P-P-O2P    |
| 20  | T     | 3004 | CDL  | OB5-CB3-CB4-CB6 |
| 17  | D     | 2006 | PEE  | O3P-C1-C2-C3    |
| 20  | P     | 3003 | CDL  | C51-CB5-OB6-CB4 |
| 20  | G     | 2004 | CDL  | C33-C34-C35-C36 |
| 17  | D     | 2006 | PEE  | O3P-C1-C2-O2    |
| 20  | T     | 3004 | CDL  | OA6-CA4-CA6-OA8 |
| 20  | D     | 2003 | CDL  | OB6-CB4-CB6-OB8 |
| 20  | G     | 2004 | CDL  | CA4-CA3-OA5-PA1 |
| 11  | S     | 2011 | JZR  | O1-C1'-C2'-C3'  |
| 20  | P     | 3003 | CDL  | C75-C76-C77-C78 |
| 17  | D     | 2006 | PEE  | C3-C2-O2-C10    |
| 11  | F     | 3011 | JZR  | C3'-C4'-C5'-C6' |
| 20  | P     | 3003 | CDL  | CB2-OB2-PB2-OB5 |
| 20  | P     | 3003 | CDL  | CB3-OB5-PB2-OB2 |
| 17  | C     | 2007 | PEE  | C4-O4P-P-O3P    |
| 20  | D     | 2003 | CDL  | CB5-C51-C52-C53 |
| 20  | G     | 2004 | CDL  | C12-C11-CA5-OA6 |
| 17  | Q     | 3006 | PEE  | O3P-C1-C2-C3    |
| 20  | D     | 2003 | CDL  | C71-C72-C73-C74 |
| 11  | C     | 2010 | JZR  | O5-C5-C6-O6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | C     | 2007 | PEE  | C42-C43-C44-C45 |
| 16  | C     | 2001 | SMA  | C9-C10-C11-C22  |
| 20  | G     | 2004 | CDL  | O1-C1-CA2-OA2   |
| 11  | F     | 4001 | JZR  | C2'-C3'-C4'-C5' |
| 17  | P     | 3007 | PEE  | C42-C43-C44-C45 |
| 20  | G     | 2004 | CDL  | C12-C11-CA5-OA7 |
| 17  | D     | 2006 | PEE  | C30-C31-C32-C33 |
| 11  | S     | 2011 | JZR  | C2'-C3'-C4'-C5' |
| 11  | C     | 2010 | JZR  | C2'-C3'-C4'-C5' |
| 11  | R     | 4007 | JZR  | C3'-C4'-C5'-C6' |
| 20  | P     | 3003 | CDL  | CA2-OA2-PA1-OA4 |
| 20  | G     | 2004 | CDL  | C32-C31-CA7-OA8 |
| 17  | C     | 2007 | PEE  | O3-C30-C31-C32  |
| 18  | P     | 3002 | ANY  | C9-C10-O5-C14   |
| 18  | C     | 2002 | ANY  | C9-C10-O5-C14   |
| 20  | T     | 3004 | CDL  | C32-C31-CA7-OA8 |
| 20  | P     | 3003 | CDL  | C72-C71-CB7-OB8 |
| 17  | P     | 3007 | PEE  | O3-C30-C31-C32  |
| 17  | Q     | 3006 | PEE  | C16-C17-C18-C19 |
| 18  | C     | 2002 | ANY  | C16-C17-C18-C19 |
| 20  | T     | 3004 | CDL  | C12-C13-C14-C15 |
| 20  | P     | 3003 | CDL  | C71-C72-C73-C74 |
| 20  | G     | 2004 | CDL  | C32-C31-CA7-OA9 |
| 17  | Q     | 3006 | PEE  | C31-C32-C33-C34 |
| 20  | G     | 2004 | CDL  | CA3-OA5-PA1-OA4 |
| 20  | G     | 2004 | CDL  | CB2-OB2-PB2-OB4 |
| 20  | P     | 3003 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | P     | 3003 | CDL  | CB3-OB5-PB2-OB3 |
| 17  | D     | 2006 | PEE  | C1-O3P-P-O1P    |
| 17  | C     | 2007 | PEE  | O5-C30-C31-C32  |
| 16  | C     | 2001 | SMA  | C16-C17-C18-C19 |
| 17  | D     | 2006 | PEE  | C5-C4-O4P-P     |
| 17  | P     | 3007 | PEE  | O5-C30-C31-C32  |
| 20  | P     | 3003 | CDL  | C72-C71-CB7-OB9 |
| 20  | T     | 3004 | CDL  | C32-C31-CA7-OA9 |

There are no ring outliers.

23 monomers are involved in 40 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 16  | P     | 3001 | SMA  | 2       | 0            |
| 20  | T     | 3004 | CDL  | 2       | 0            |

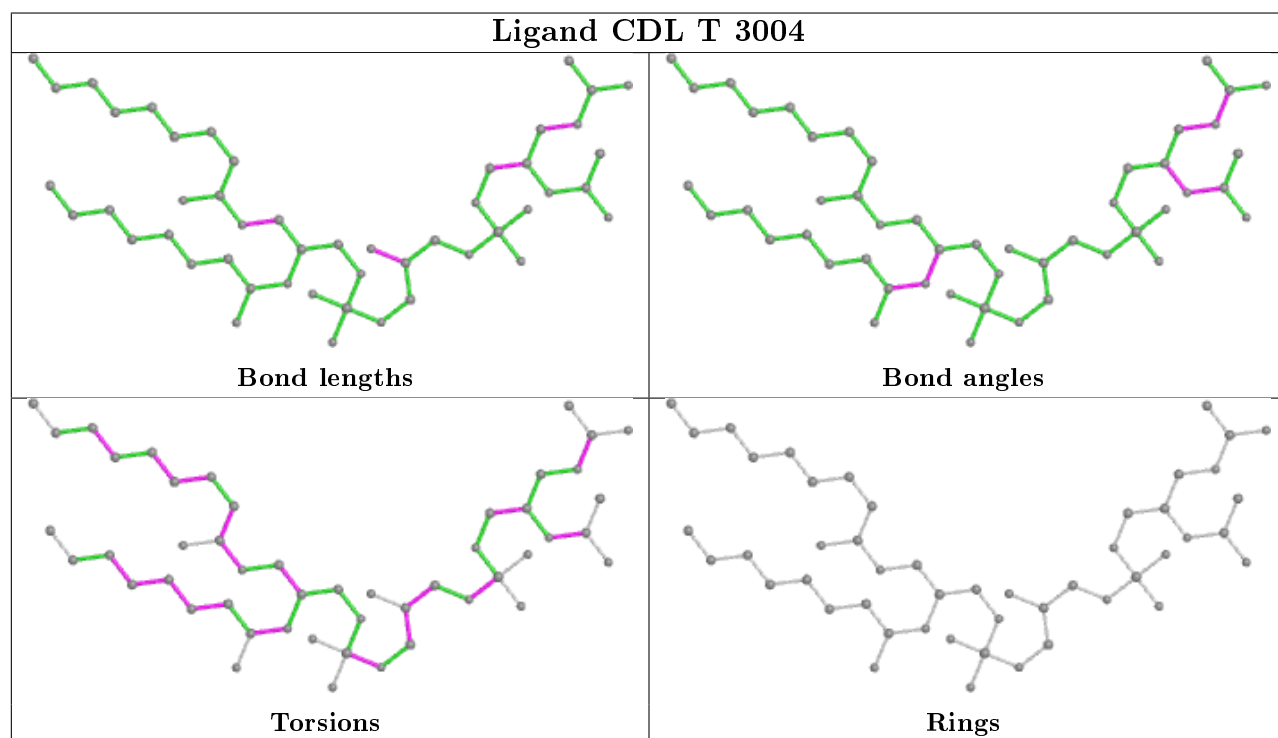
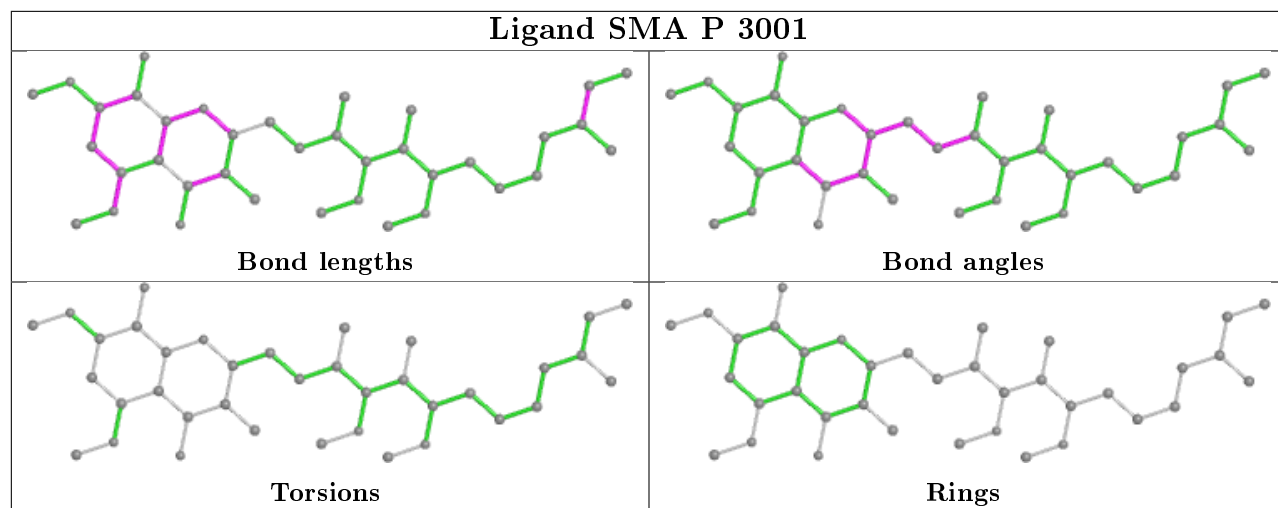
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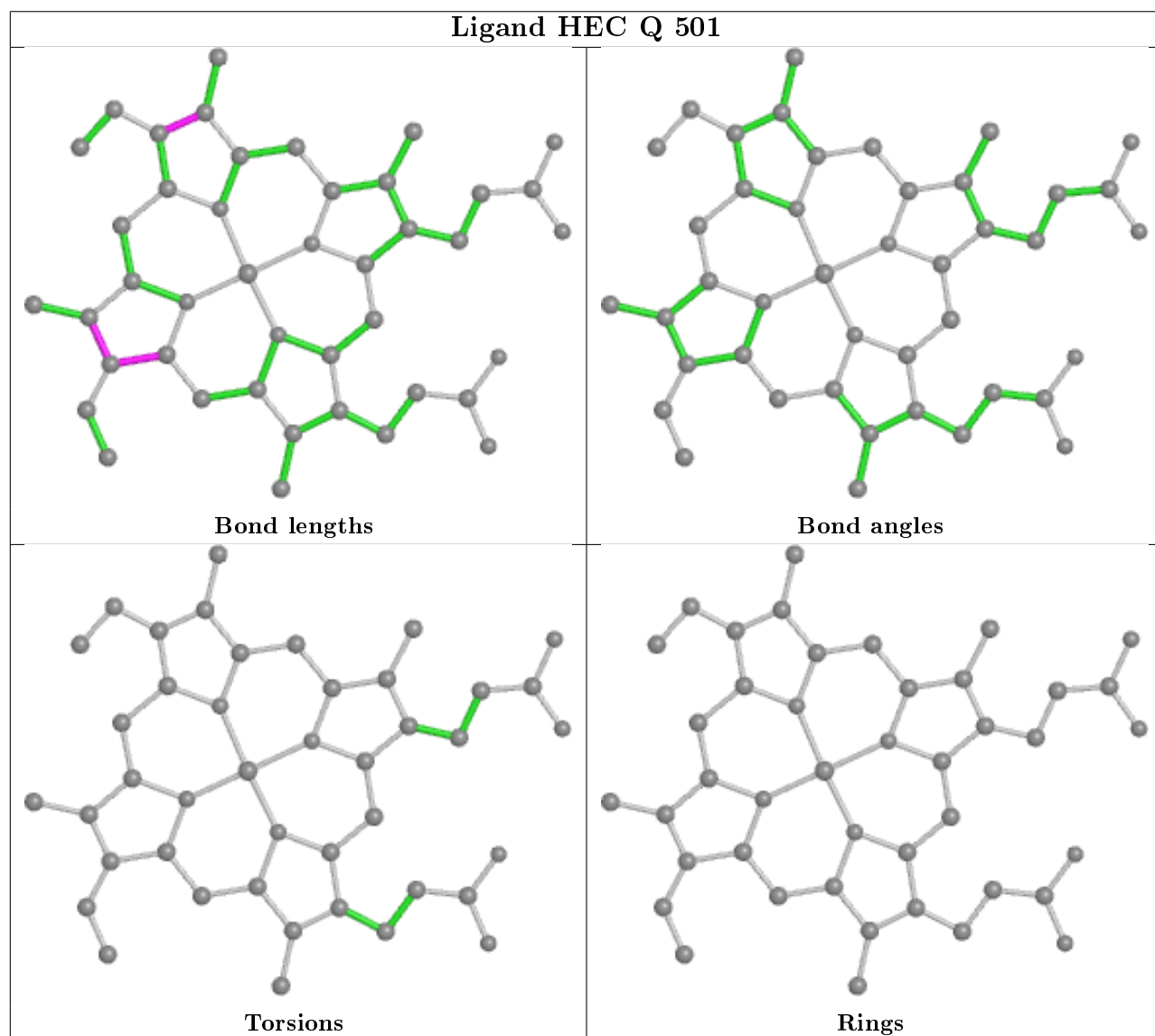
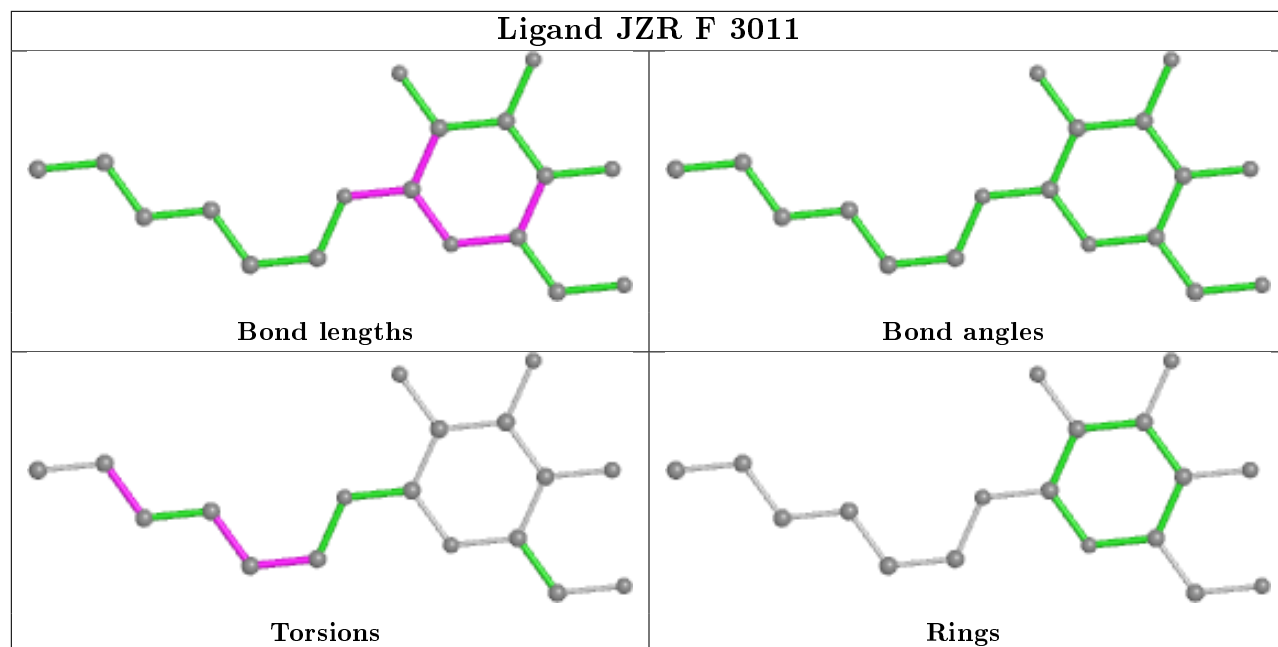


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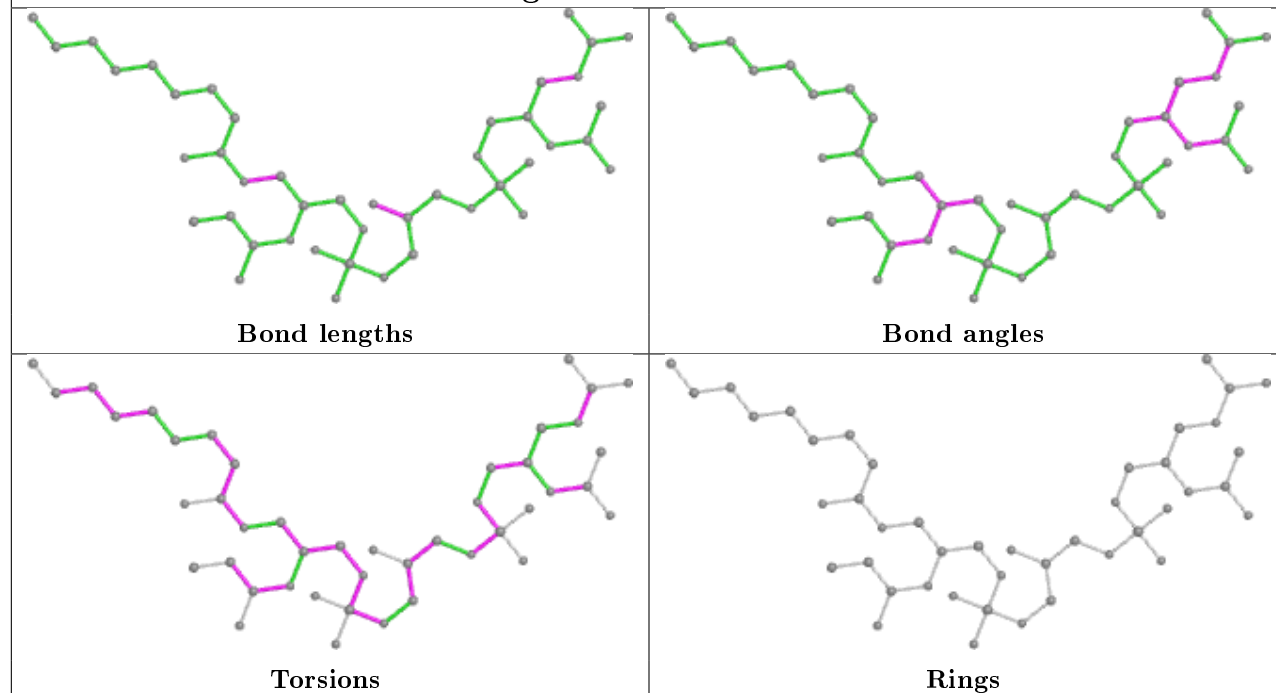
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | R     | 4005 | GOL  | 1       | 0            |
| 11  | F     | 3011 | JZR  | 2       | 0            |
| 19  | Q     | 501  | HEC  | 1       | 0            |
| 18  | P     | 3002 | ANY  | 2       | 0            |
| 19  | D     | 501  | HEC  | 3       | 0            |
| 17  | Q     | 3006 | PEE  | 3       | 0            |
| 14  | C     | 2008 | GOL  | 1       | 0            |
| 16  | C     | 2001 | SMA  | 2       | 0            |
| 15  | P     | 501  | HEM  | 1       | 0            |
| 15  | C     | 501  | HEM  | 1       | 0            |
| 15  | C     | 502  | HEM  | 2       | 0            |
| 20  | P     | 3003 | CDL  | 2       | 0            |
| 18  | C     | 2002 | ANY  | 1       | 0            |
| 17  | D     | 2006 | PEE  | 3       | 0            |
| 11  | S     | 2011 | JZR  | 3       | 0            |
| 11  | D     | 4003 | JZR  | 3       | 0            |
| 11  | R     | 4007 | JZR  | 1       | 0            |
| 15  | P     | 502  | HEM  | 1       | 0            |
| 11  | F     | 4001 | JZR  | 1       | 0            |
| 17  | P     | 3007 | PEE  | 1       | 0            |
| 11  | C     | 4002 | JZR  | 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.

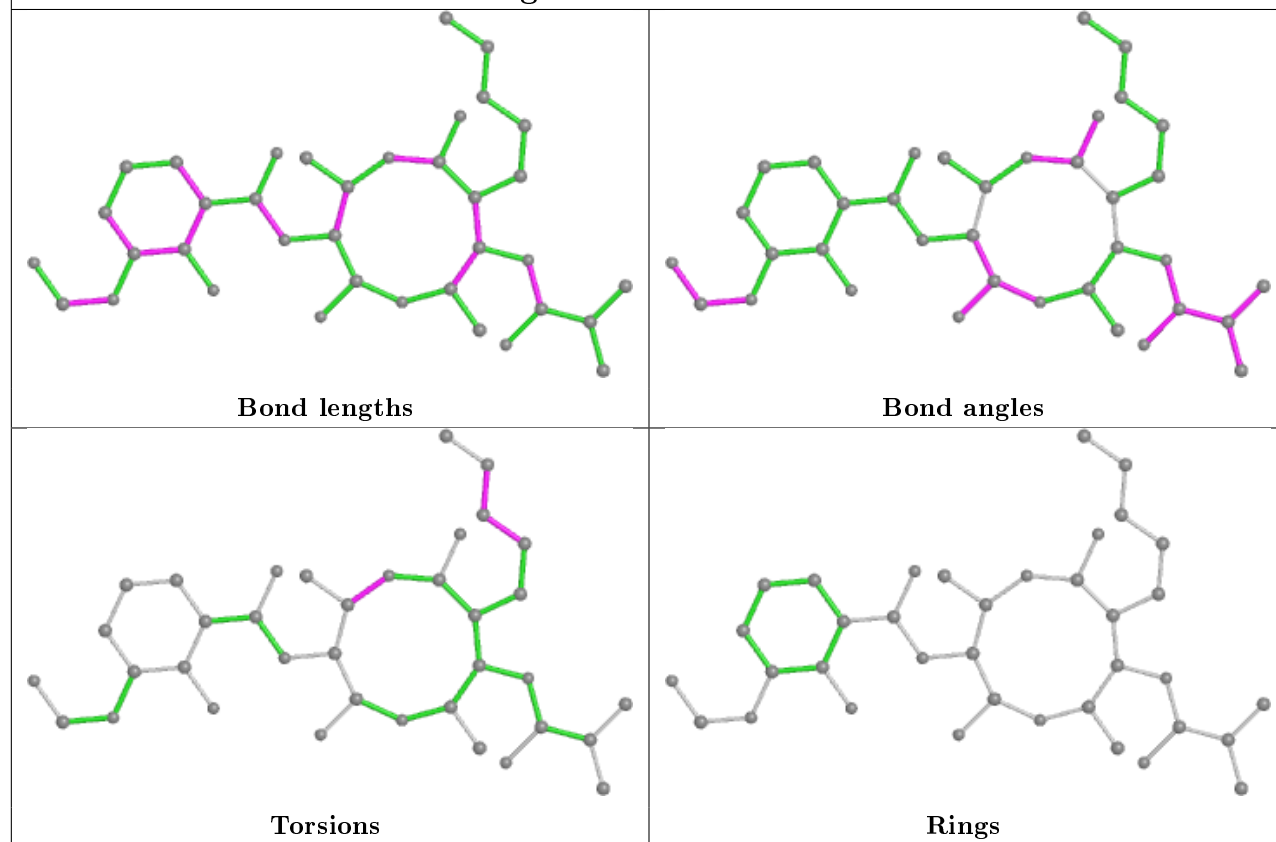


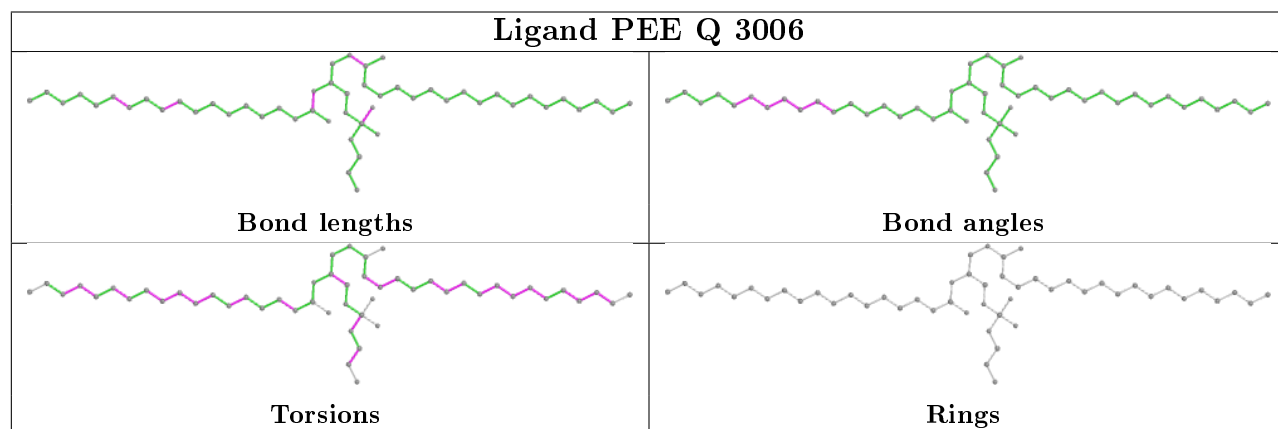
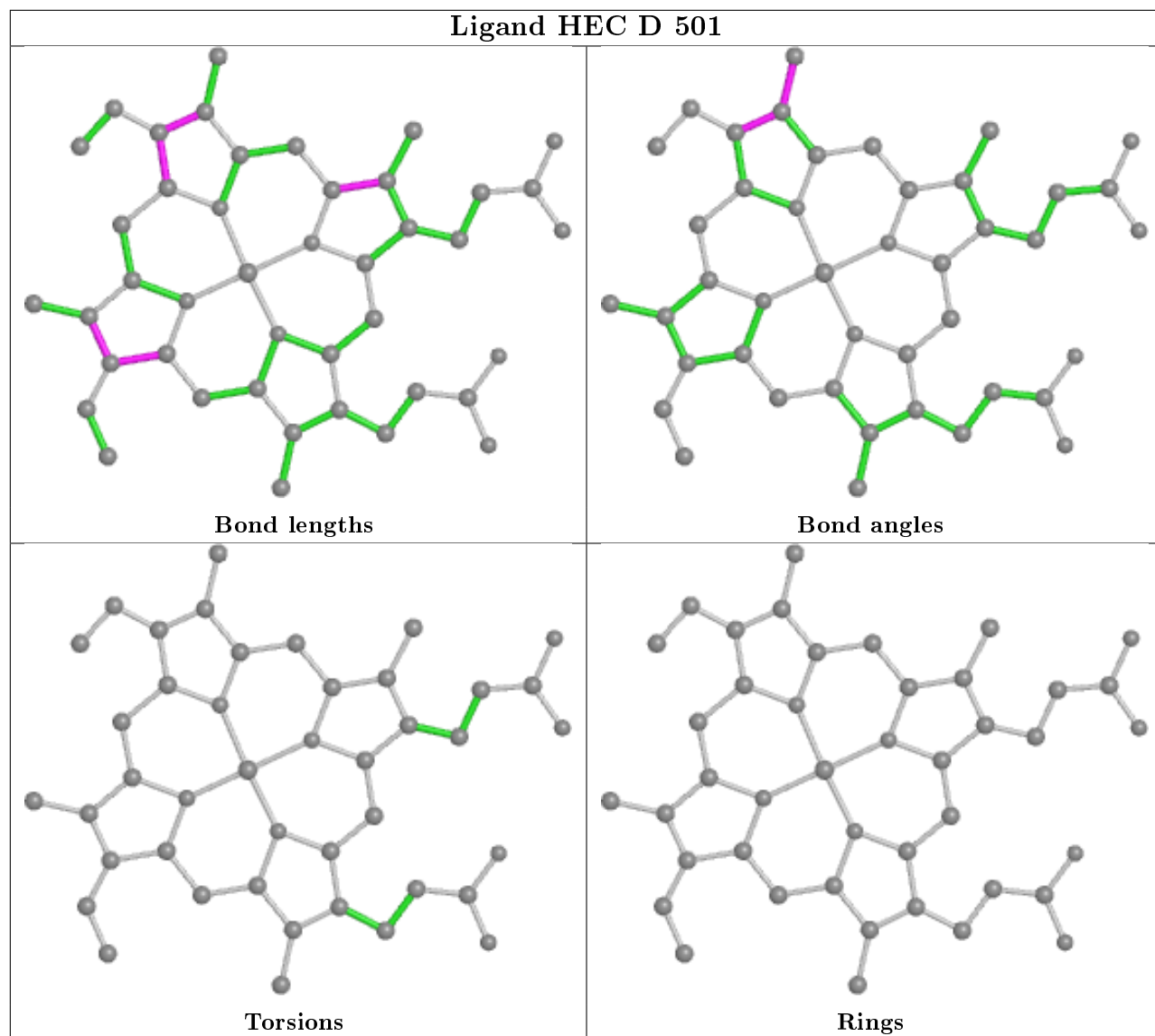


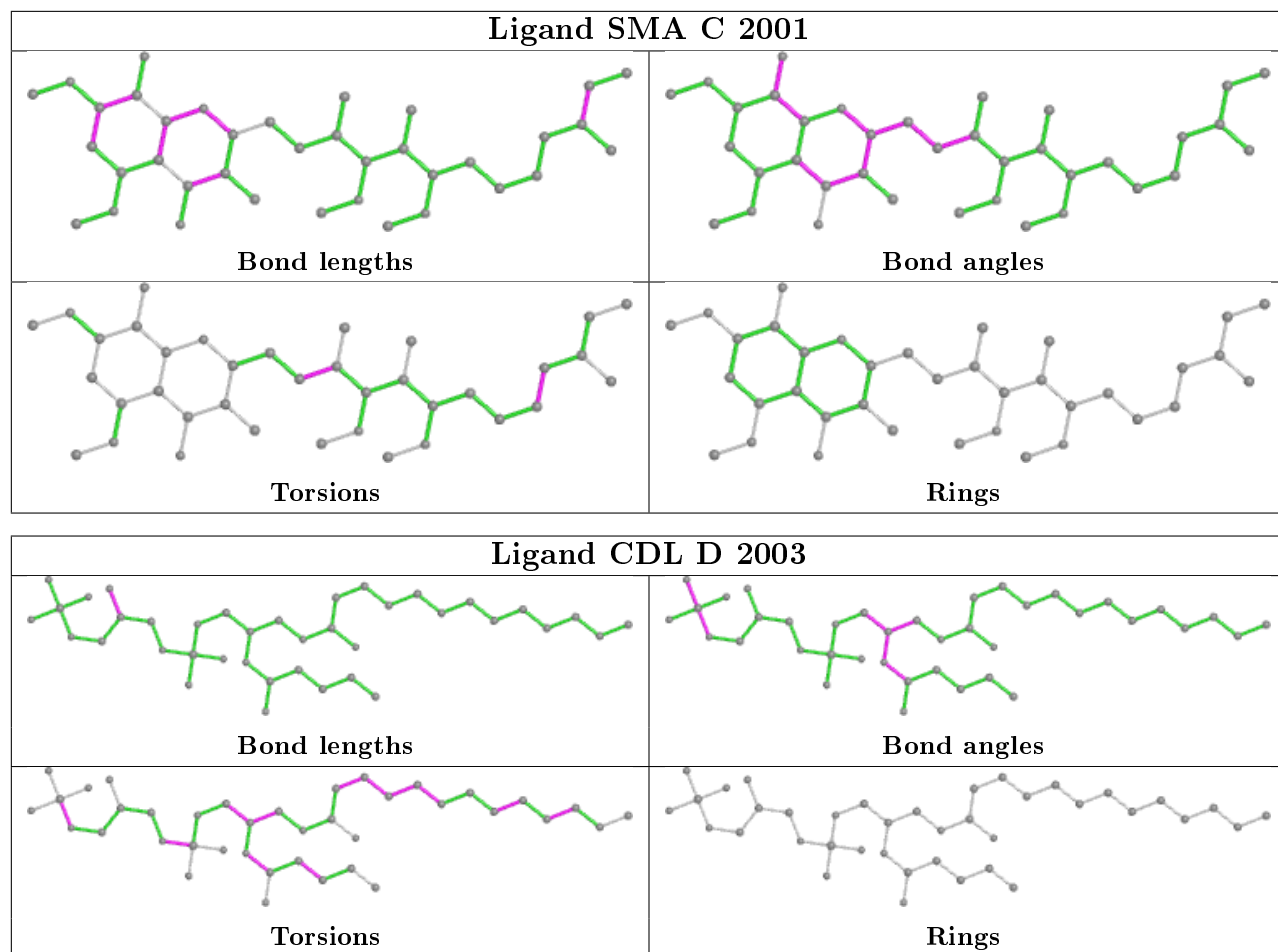
## Ligand CDL G 2004

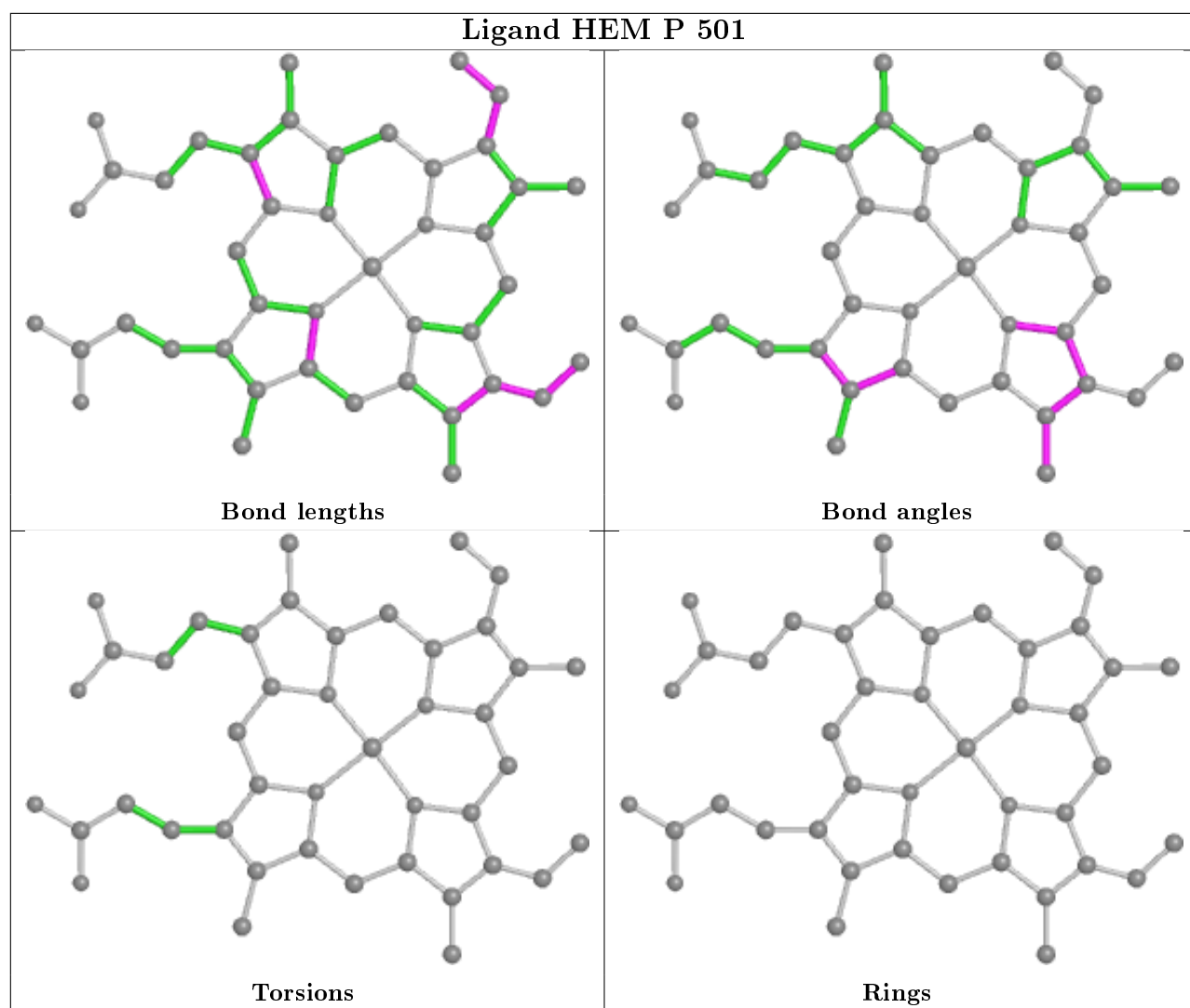


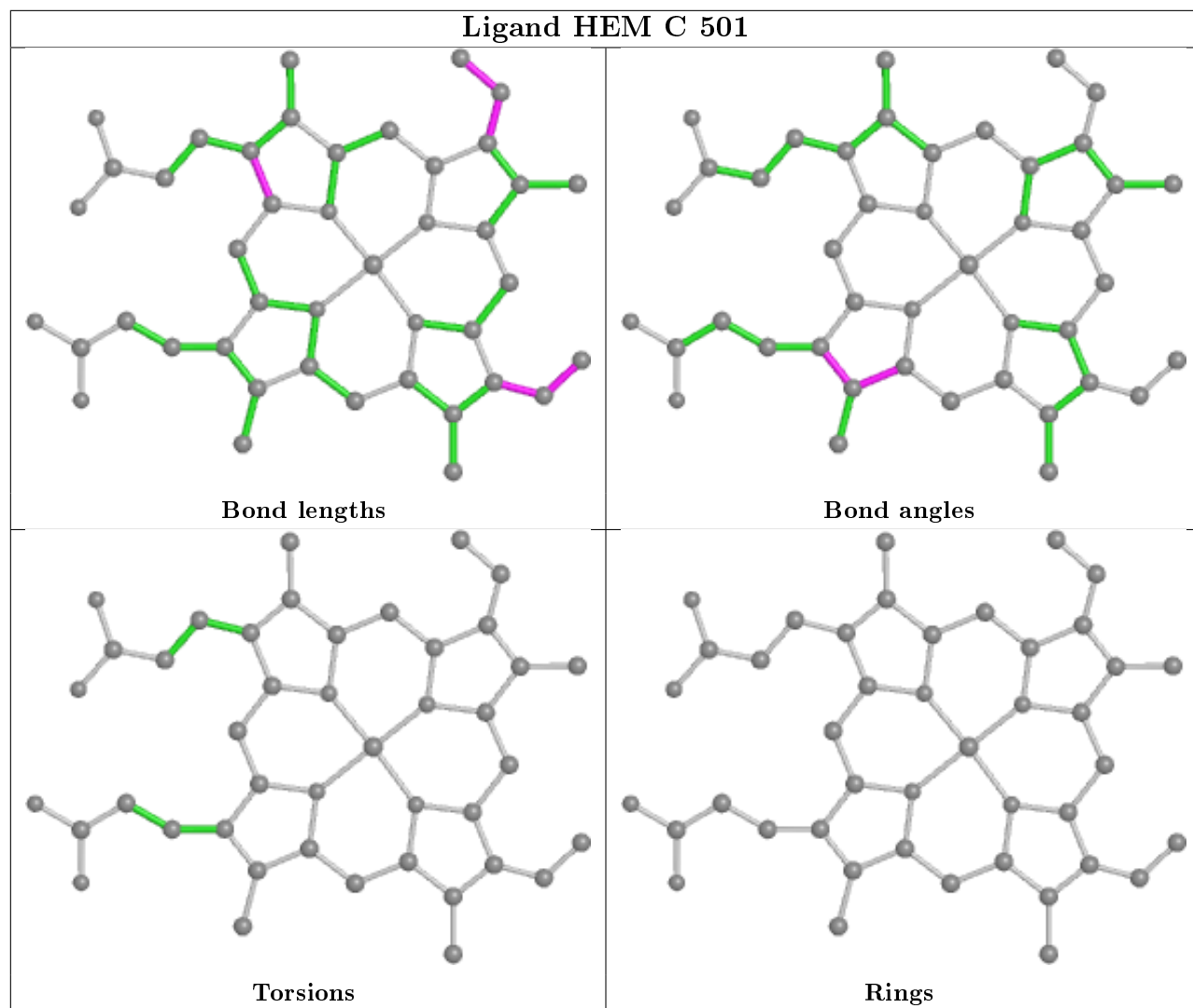
## Ligand ANY P 3002



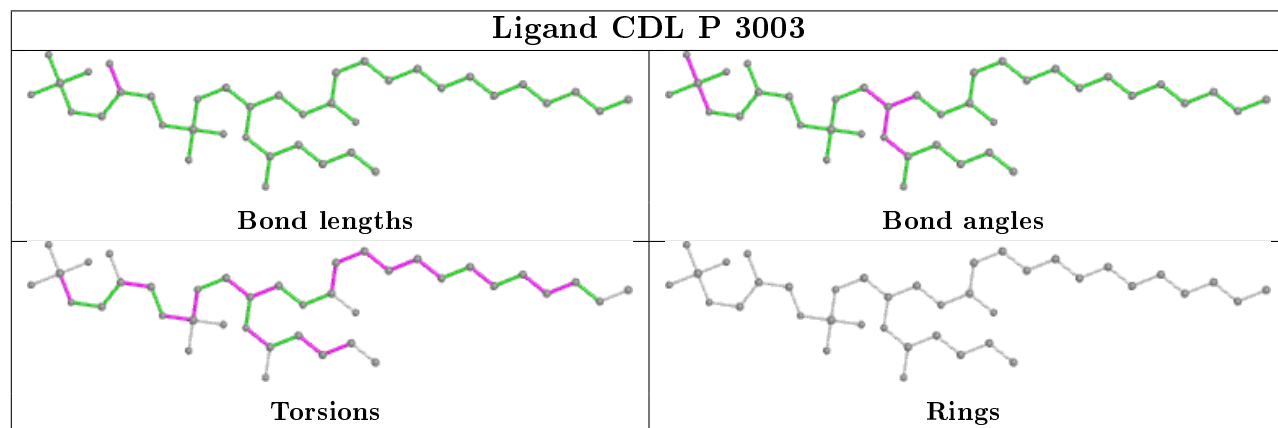
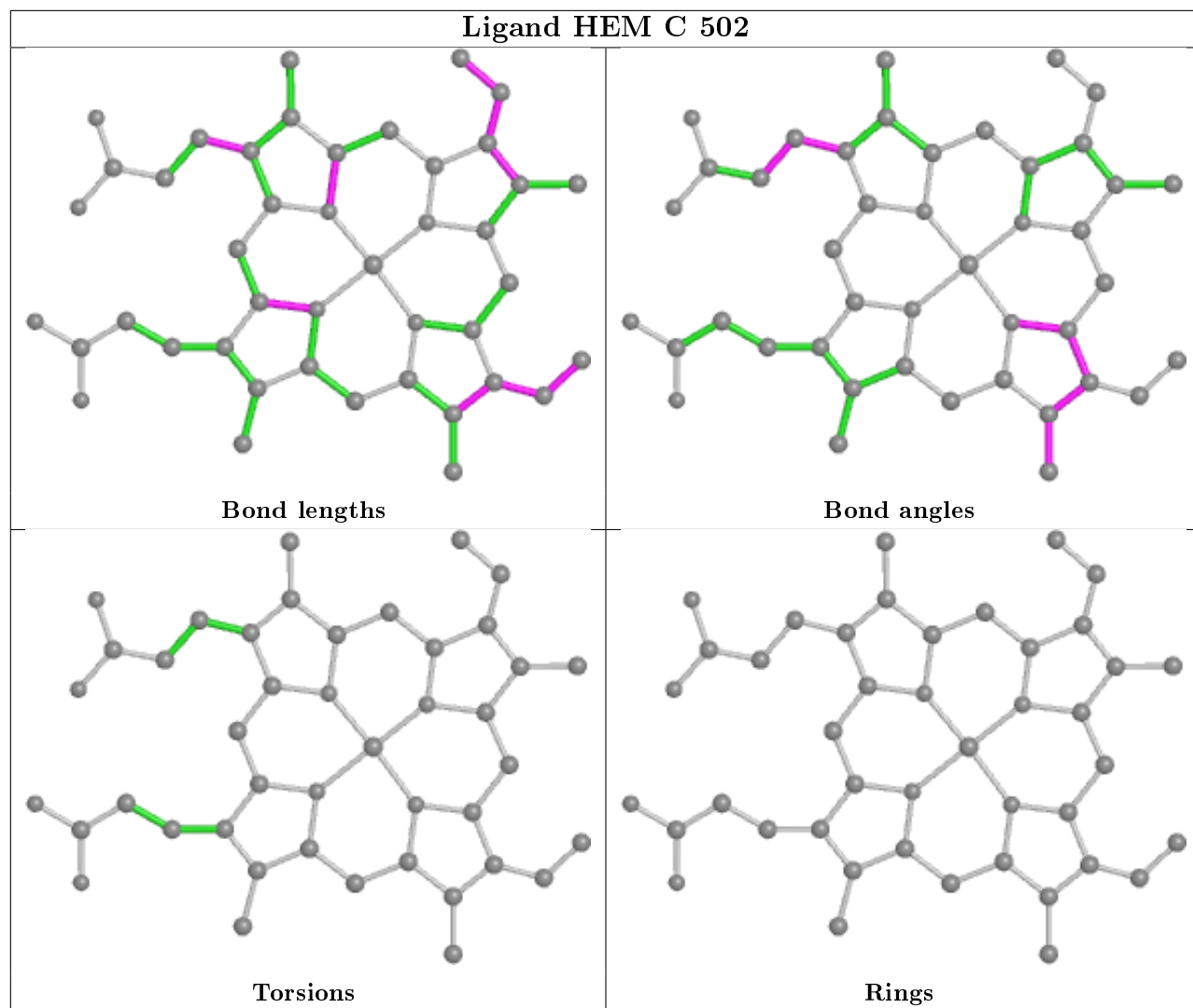


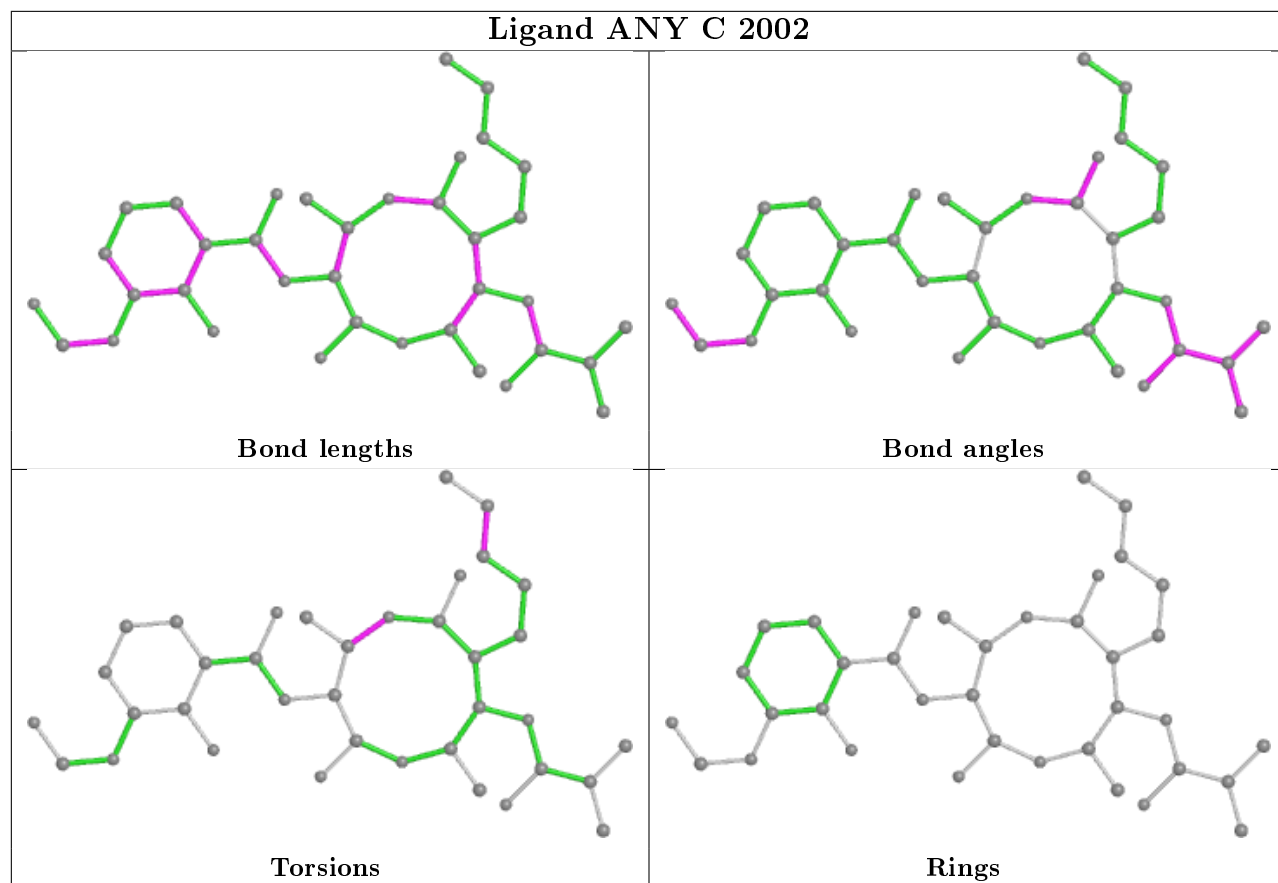




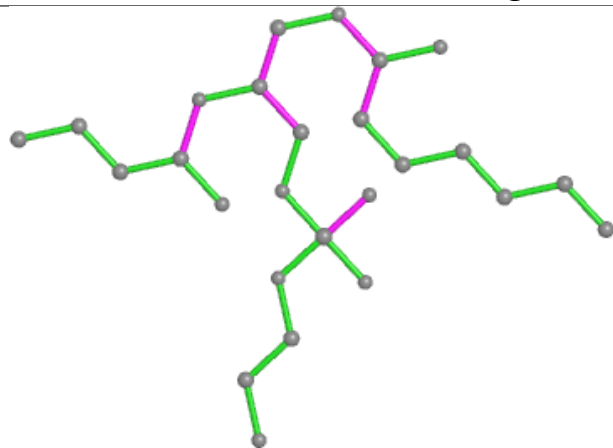




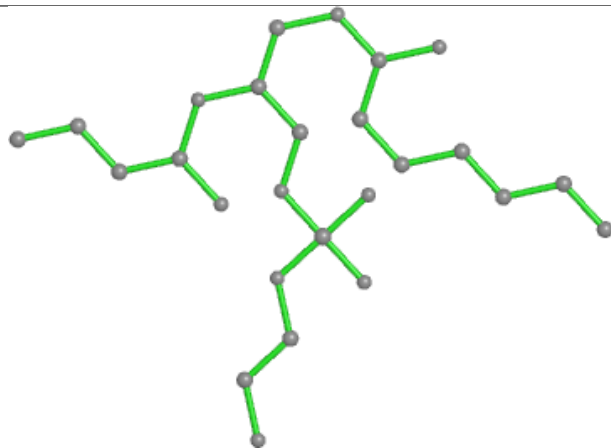




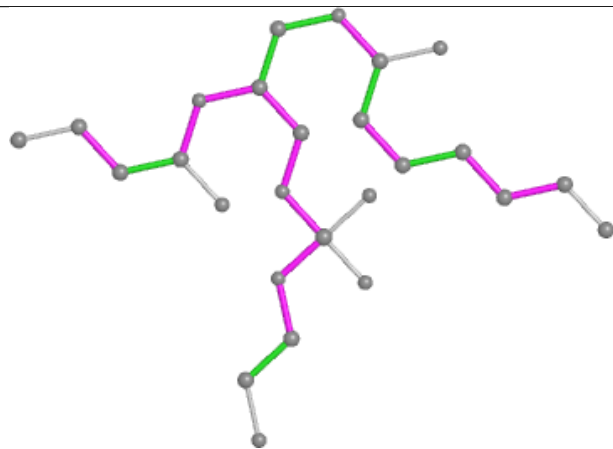
## Ligand PEE D 2006



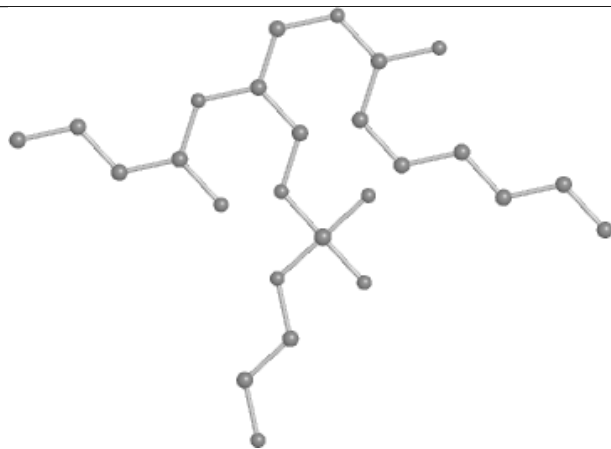
Bond lengths



Bond angles

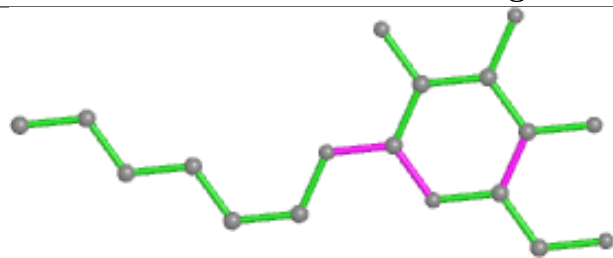


Torsions

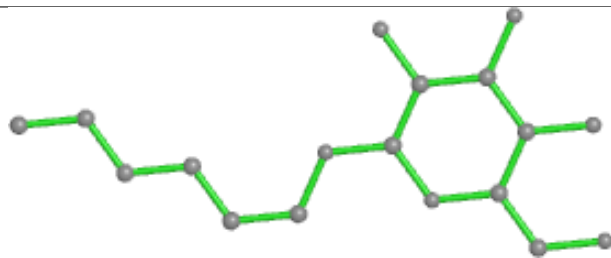


Rings

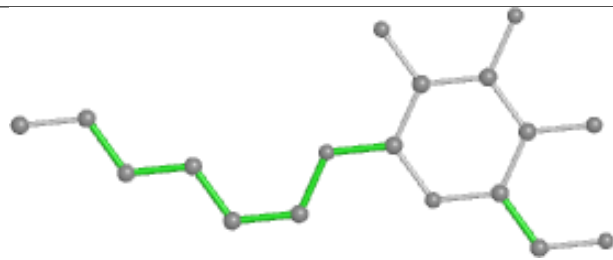
## Ligand JZR A 4004



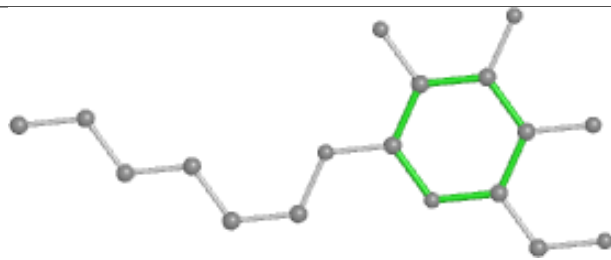
Bond lengths



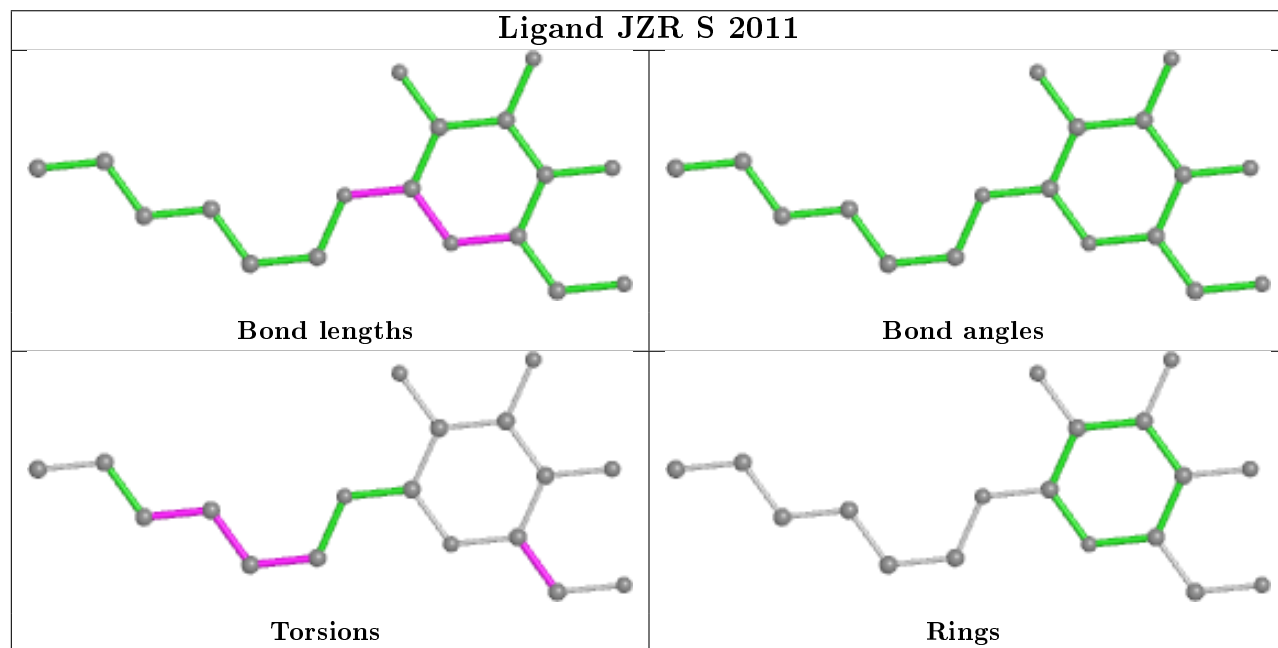
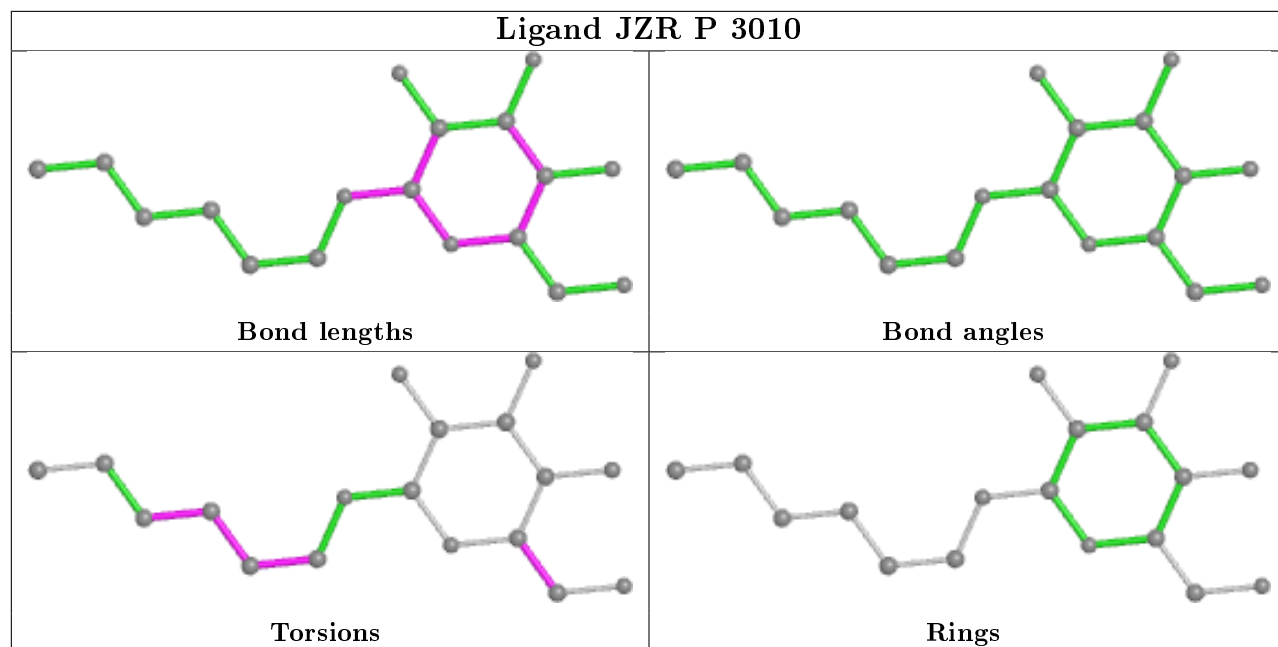
Bond angles

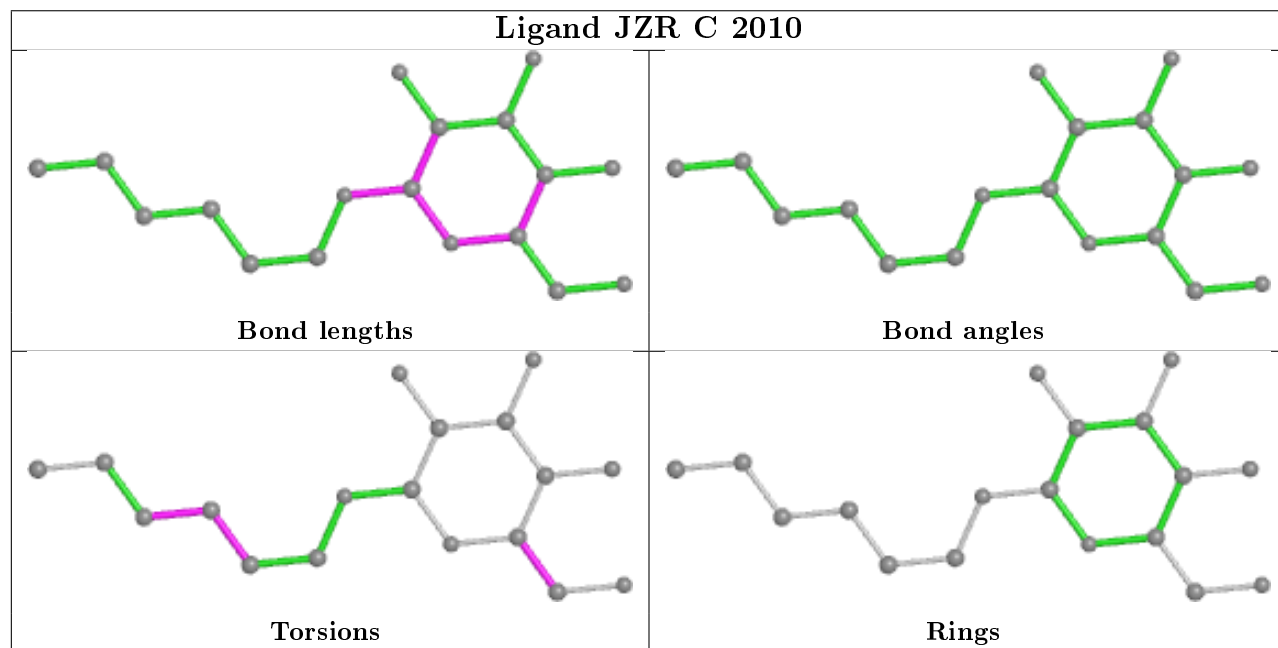
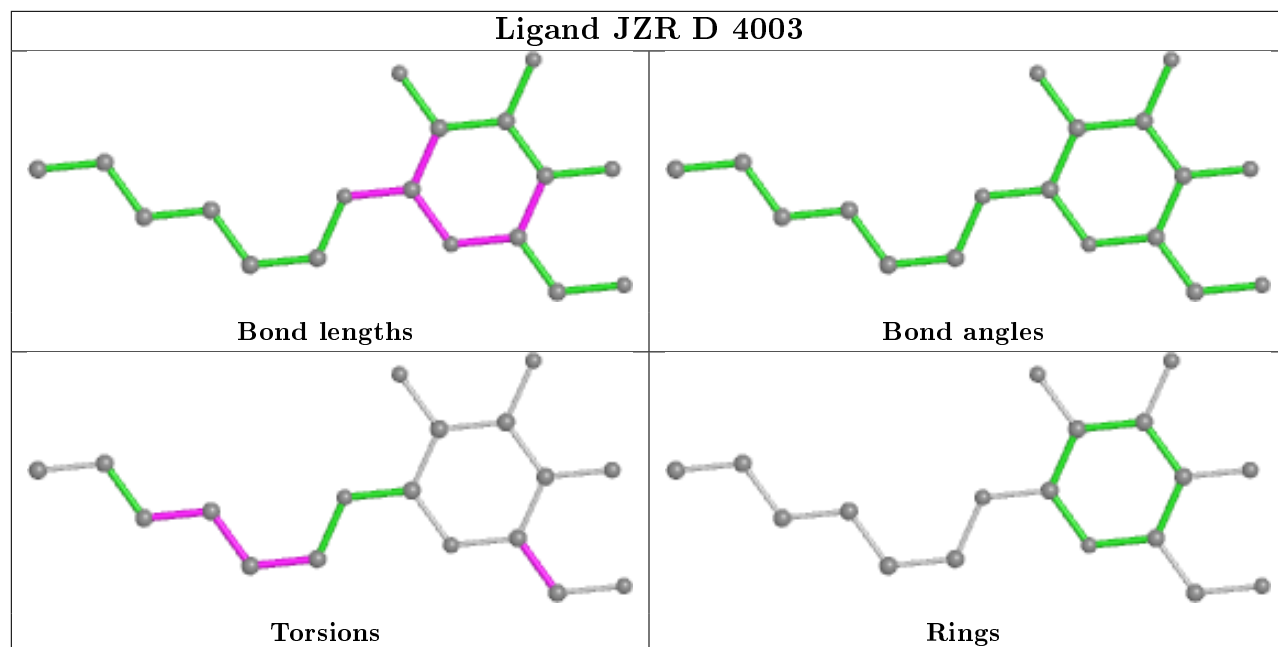


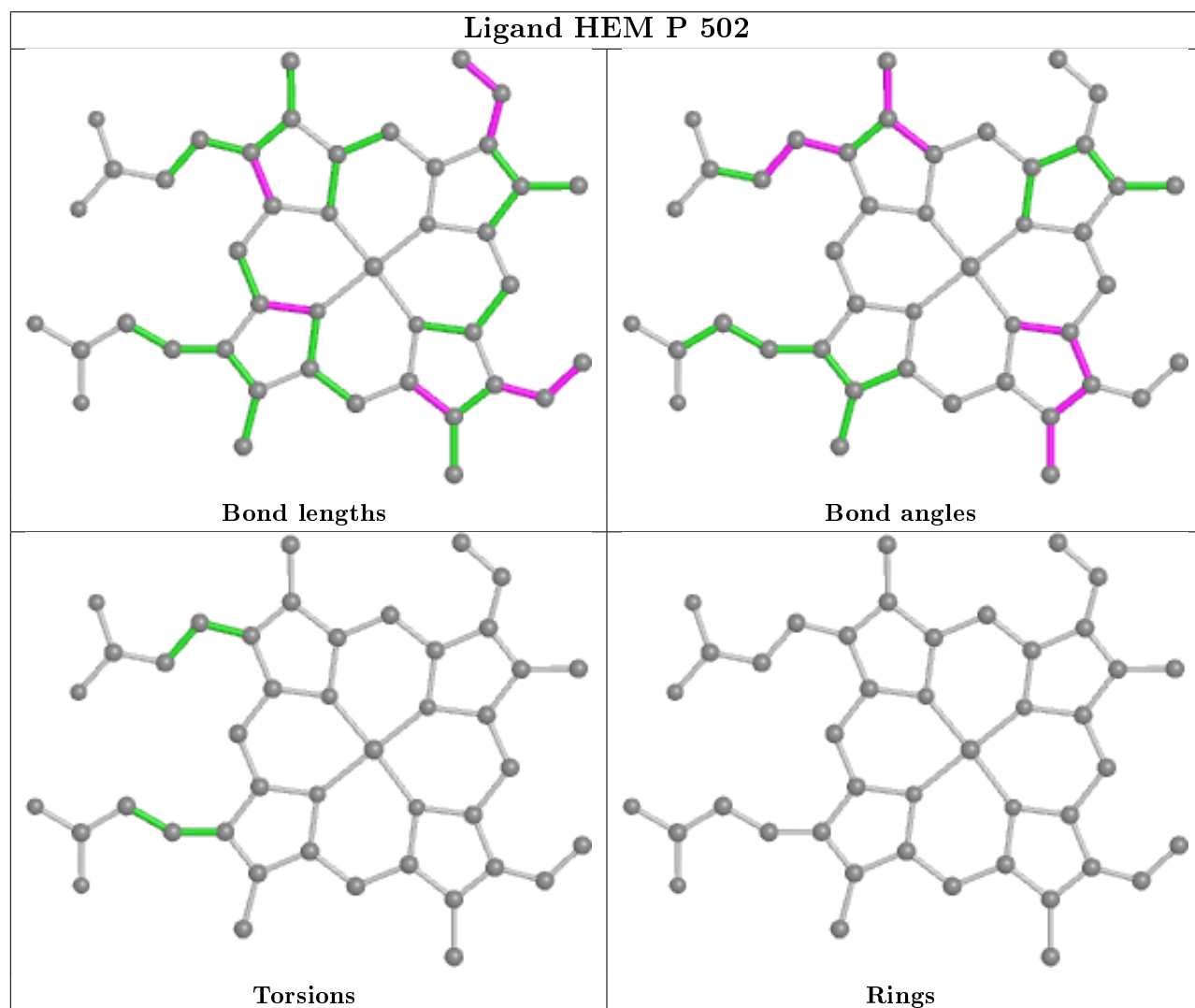
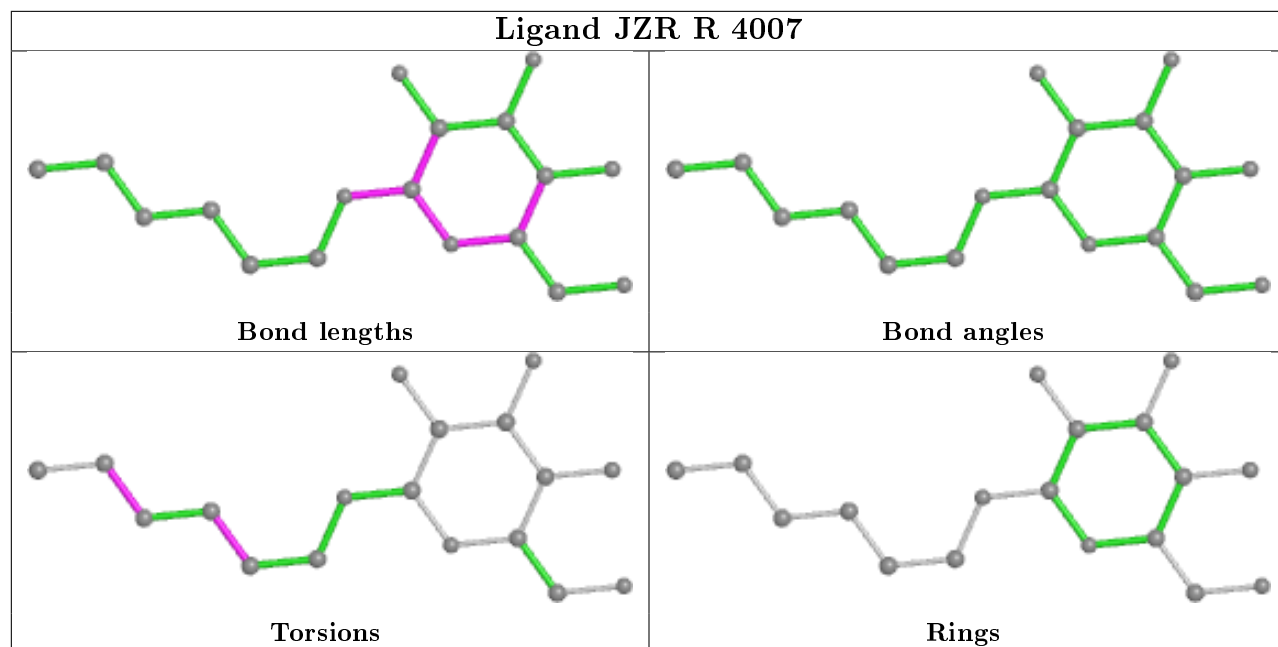
Torsions

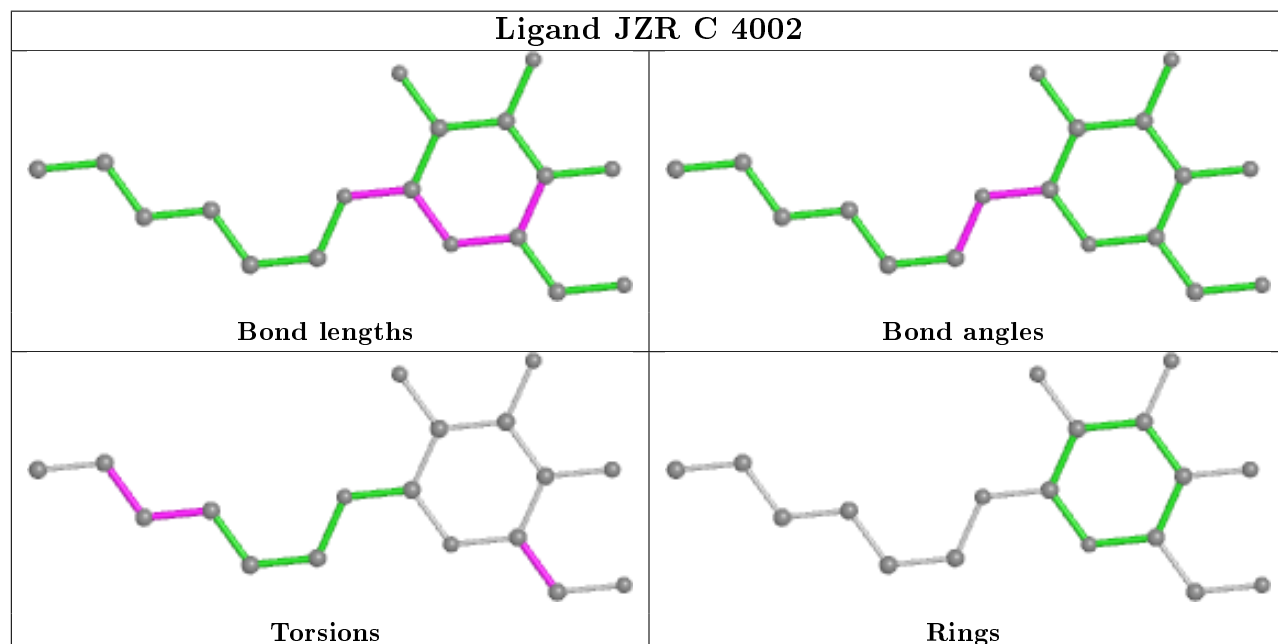
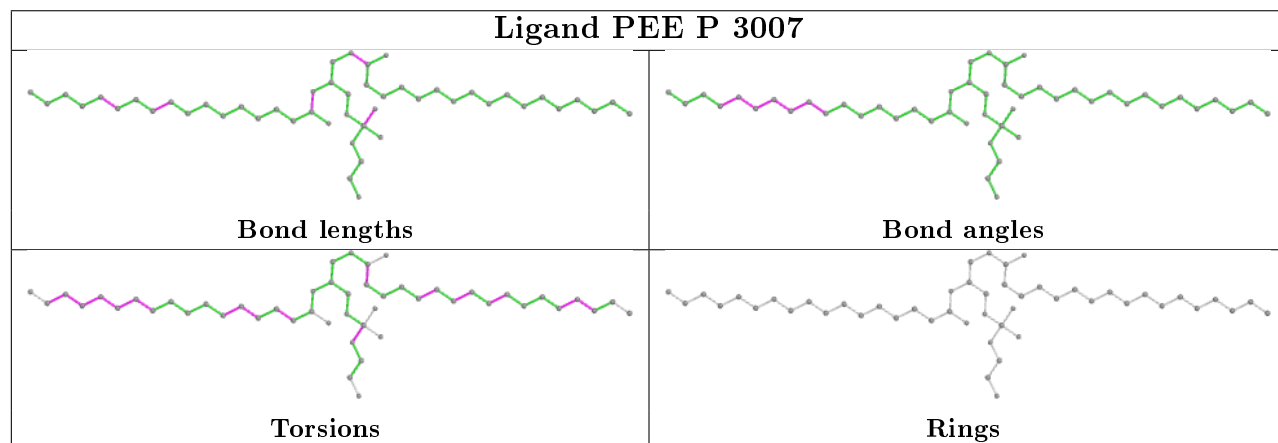
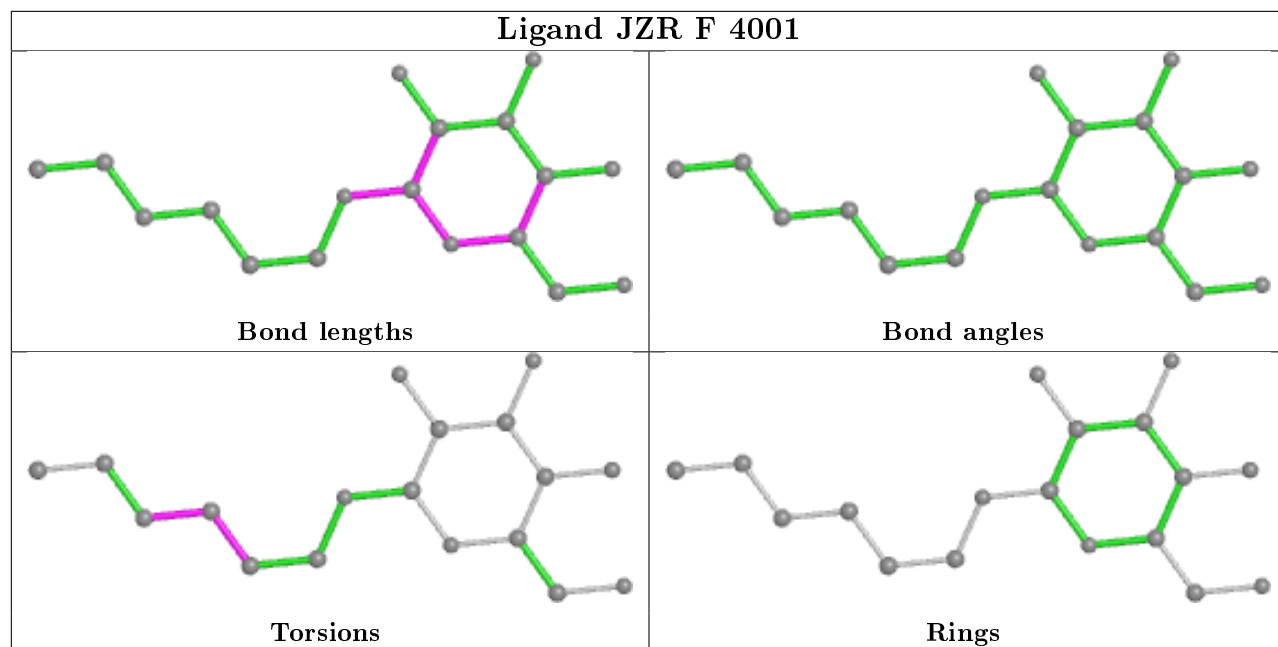


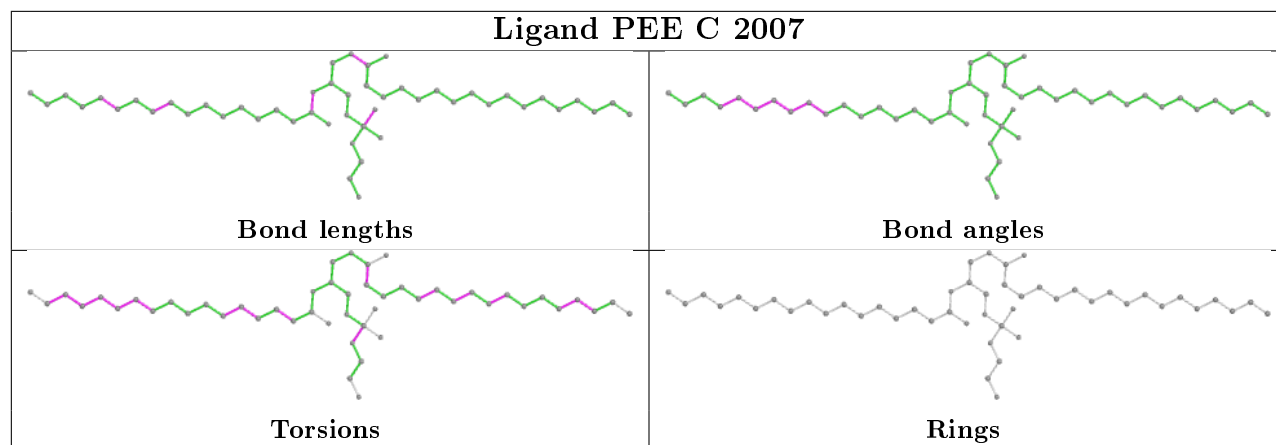
Rings











## 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     | 442/446 (99%)   | 0.28   | 9 (2%) 65 69   | 25, 39, 60, 115       | 0      |
| 1   | N     | 441/446 (98%)   | 0.41   | 23 (5%) 27 32  | 33, 52, 76, 139       | 1 (0%) |
| 2   | B     | 424/439 (96%)   | 0.20   | 9 (2%) 63 68   | 29, 42, 66, 94        | 0      |
| 2   | O     | 424/439 (96%)   | 0.26   | 13 (3%) 49 55  | 30, 47, 70, 124       | 0      |
| 3   | C     | 365/379 (96%)   | 0.00   | 3 (0%) 86 88   | 23, 36, 53, 108       | 0      |
| 3   | P     | 365/379 (96%)   | 0.02   | 4 (1%) 80 84   | 29, 39, 53, 106       | 0      |
| 4   | D     | 241/241 (100%)  | 0.02   | 1 (0%) 92 93   | 31, 44, 64, 82        | 0      |
| 4   | Q     | 241/241 (100%)  | 0.11   | 3 (1%) 79 82   | 35, 48, 67, 89        | 0      |
| 5   | E     | 196/196 (100%)  | 1.04   | 40 (20%) 1 1   | 35, 62, 106, 111      | 0      |
| 5   | R     | 196/196 (100%)  | 0.37   | 9 (4%) 32 38   | 34, 51, 77, 95        | 0      |
| 6   | F     | 99/110 (90%)    | 0.04   | 1 (1%) 82 85   | 27, 40, 69, 79        | 0      |
| 6   | S     | 99/110 (90%)    | 0.24   | 4 (4%) 38 44   | 33, 42, 80, 102       | 0      |
| 7   | G     | 75/81 (92%)     | 0.54   | 5 (6%) 17 22   | 29, 53, 76, 89        | 0      |
| 7   | T     | 76/81 (93%)     | 0.80   | 12 (15%) 2 2   | 37, 63, 93, 95        | 0      |
| 8   | H     | 66/78 (84%)     | 0.32   | 2 (3%) 50 56   | 43, 59, 77, 81        | 0      |
| 8   | U     | 66/78 (84%)     | 0.95   | 9 (13%) 3 4    | 50, 66, 89, 104       | 0      |
| 9   | I     | 43/78 (55%)     | 1.60   | 15 (34%) 0 0   | 34, 65, 84, 89        | 0      |
| 9   | V     | 43/78 (55%)     | 2.22   | 20 (46%) 0 0   | 38, 72, 86, 91        | 0      |
| 10  | J     | 33/62 (53%)     | 1.03   | 5 (15%) 2 3    | 37, 54, 115, 130      | 0      |
| 10  | W     | 62/62 (100%)    | 1.70   | 22 (35%) 0 0   | 44, 74, 129, 144      | 0      |
| All | All   | 3997/4220 (94%) | 0.33   | 209 (5%) 27 32 | 23, 45, 81, 144       | 1 (0%) |

All (209) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 227 | ALA  | 18.5 |
| 7   | G     | 75  | ALA  | 11.6 |
| 10  | J     | 62  | LYS  | 10.2 |
| 10  | W     | 2   | ALA  | 9.8  |
| 10  | W     | 1   | VAL  | 9.4  |
| 1   | N     | 226 | ASP  | 7.9  |
| 2   | O     | 12  | GLU  | 7.8  |
| 2   | B     | 232 | LEU  | 7.6  |
| 10  | J     | 31  | PHE  | 7.5  |
| 10  | J     | 32  | GLU  | 7.3  |
| 10  | W     | 12  | LEU  | 7.2  |
| 9   | V     | 41  | PRO  | 6.7  |
| 1   | N     | 229 | PRO  | 6.7  |
| 2   | O     | 17  | VAL  | 6.6  |
| 2   | B     | 233 | SER  | 6.2  |
| 10  | J     | 30  | PHE  | 5.8  |
| 5   | E     | 187 | PHE  | 5.8  |
| 1   | N     | 2   | ALA  | 5.7  |
| 7   | T     | 76  | ALA  | 5.7  |
| 10  | W     | 5   | LEU  | 5.6  |
| 9   | V     | 36  | ALA  | 5.6  |
| 5   | E     | 83  | GLU  | 5.5  |
| 5   | E     | 104 | LYS  | 5.5  |
| 10  | W     | 25  | VAL  | 5.5  |
| 2   | B     | 12  | GLU  | 5.4  |
| 1   | A     | 2   | ALA  | 5.4  |
| 9   | V     | 33  | ALA  | 5.3  |
| 9   | V     | 78  | TYR  | 5.3  |
| 9   | I     | 78  | TYR  | 5.3  |
| 1   | N     | 222 | THR  | 5.2  |
| 7   | T     | 1   | GLY  | 5.2  |
| 2   | O     | 19  | PRO  | 5.2  |
| 2   | O     | 21  | PRO  | 5.1  |
| 3   | C     | 16  | ASN  | 5.1  |
| 2   | B     | 230 | LEU  | 5.1  |
| 4   | Q     | 241 | LYS  | 5.1  |
| 5   | E     | 112 | VAL  | 4.9  |
| 1   | N     | 225 | GLU  | 4.9  |
| 10  | W     | 62  | LYS  | 4.9  |
| 10  | W     | 3   | PRO  | 4.9  |
| 5   | E     | 76  | ILE  | 4.8  |
| 5   | E     | 132 | TRP  | 4.7  |
| 5   | E     | 78  | LEU  | 4.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | R     | 27  | GLU  | 4.7  |
| 1   | A     | 225 | GLU  | 4.6  |
| 9   | V     | 38  | SER  | 4.6  |
| 1   | N     | 228 | VAL  | 4.6  |
| 5   | E     | 192 | MET  | 4.4  |
| 10  | W     | 19  | THR  | 4.4  |
| 1   | N     | 365 | LEU  | 4.4  |
| 5   | E     | 107 | ASP  | 4.4  |
| 7   | T     | 30  | PHE  | 4.4  |
| 9   | V     | 50  | LEU  | 4.4  |
| 5   | E     | 194 | ILE  | 4.4  |
| 2   | B     | 231 | GLY  | 4.3  |
| 10  | W     | 21  | ALA  | 4.3  |
| 5   | E     | 167 | ALA  | 4.2  |
| 1   | A     | 227 | ALA  | 4.2  |
| 7   | T     | 29  | TYR  | 4.2  |
| 7   | T     | 31  | SER  | 4.2  |
| 5   | E     | 80  | ASP  | 4.2  |
| 3   | C     | 17  | ALA  | 4.2  |
| 8   | U     | 51  | GLU  | 4.1  |
| 5   | E     | 195 | VAL  | 4.0  |
| 5   | E     | 84  | GLY  | 4.0  |
| 9   | I     | 63  | PRO  | 4.0  |
| 10  | W     | 13  | LEU  | 4.0  |
| 9   | V     | 63  | PRO  | 3.9  |
| 4   | Q     | 1   | SER  | 3.9  |
| 5   | E     | 127 | VAL  | 3.9  |
| 1   | A     | 226 | ASP  | 3.9  |
| 10  | W     | 9   | LEU  | 3.8  |
| 5   | E     | 103 | LYS  | 3.8  |
| 1   | A     | 223 | TYR  | 3.8  |
| 10  | W     | 14  | PHE  | 3.8  |
| 2   | O     | 20  | HIS  | 3.8  |
| 8   | U     | 49  | GLN  | 3.7  |
| 1   | A     | 222 | THR  | 3.7  |
| 5   | E     | 71  | MET  | 3.7  |
| 6   | S     | 12  | TRP  | 3.7  |
| 5   | E     | 108 | GLN  | 3.7  |
| 9   | V     | 42  | VAL  | 3.7  |
| 1   | N     | 20  | ASP  | 3.6  |
| 5   | R     | 70  | ALA  | 3.6  |
| 5   | E     | 101 | ARG  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8   | U     | 47  | ARG  | 3.6  |
| 9   | I     | 50  | LEU  | 3.5  |
| 9   | V     | 48  | SER  | 3.5  |
| 10  | W     | 16  | ARG  | 3.5  |
| 5   | E     | 81  | ILE  | 3.4  |
| 5   | E     | 111 | ALA  | 3.4  |
| 9   | I     | 37  | THR  | 3.3  |
| 5   | E     | 79  | SER  | 3.3  |
| 10  | W     | 17  | THR  | 3.3  |
| 9   | I     | 49  | VAL  | 3.3  |
| 2   | O     | 233 | SER  | 3.2  |
| 10  | J     | 61  | ASN  | 3.2  |
| 7   | G     | 30  | PHE  | 3.2  |
| 9   | V     | 54  | SER  | 3.2  |
| 5   | E     | 77  | LYS  | 3.2  |
| 8   | U     | 34  | ARG  | 3.2  |
| 8   | U     | 48  | SER  | 3.2  |
| 5   | E     | 114 | VAL  | 3.2  |
| 10  | W     | 20  | PHE  | 3.2  |
| 5   | R     | 16  | PRO  | 3.1  |
| 2   | B     | 20  | HIS  | 3.1  |
| 1   | A     | 443 | TRP  | 3.1  |
| 7   | G     | 29  | TYR  | 3.1  |
| 9   | I     | 70  | LEU  | 3.1  |
| 2   | B     | 18  | PRO  | 3.1  |
| 9   | I     | 42  | VAL  | 3.1  |
| 5   | E     | 186 | GLU  | 3.0  |
| 9   | I     | 62  | ARG  | 3.0  |
| 2   | O     | 230 | LEU  | 3.0  |
| 5   | E     | 188 | THR  | 2.9  |
| 8   | U     | 71  | HIS  | 2.9  |
| 9   | V     | 37  | THR  | 2.9  |
| 6   | S     | 16  | ILE  | 2.9  |
| 5   | R     | 29  | SER  | 2.9  |
| 8   | U     | 44  | VAL  | 2.9  |
| 5   | E     | 110 | ALA  | 2.9  |
| 5   | R     | 25  | SER  | 2.9  |
| 3   | C     | 155 | TYR  | 2.8  |
| 2   | O     | 18  | PRO  | 2.8  |
| 9   | V     | 72  | VAL  | 2.8  |
| 9   | V     | 32  | ALA  | 2.8  |
| 7   | T     | 43  | ALA  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | P     | 168 | PHE  | 2.8  |
| 5   | E     | 131 | GLU  | 2.7  |
| 9   | V     | 43  | LEU  | 2.7  |
| 5   | E     | 193 | VAL  | 2.7  |
| 9   | V     | 35  | PRO  | 2.7  |
| 4   | Q     | 144 | ARG  | 2.6  |
| 1   | N     | 192 | ALA  | 2.6  |
| 9   | I     | 60  | ALA  | 2.6  |
| 7   | T     | 32  | LYS  | 2.6  |
| 10  | W     | 6   | THR  | 2.6  |
| 1   | N     | 206 | ARG  | 2.6  |
| 2   | O     | 215 | VAL  | 2.6  |
| 3   | P     | 16  | ASN  | 2.6  |
| 5   | E     | 100 | HIS  | 2.6  |
| 9   | I     | 32  | ALA  | 2.6  |
| 10  | W     | 28  | ALA  | 2.6  |
| 9   | V     | 61  | GLY  | 2.6  |
| 1   | N     | 224 | ASP  | 2.5  |
| 1   | N     | 230 | THR  | 2.5  |
| 10  | W     | 8   | ARG  | 2.5  |
| 3   | P     | 17  | ALA  | 2.5  |
| 5   | E     | 133 | VAL  | 2.5  |
| 10  | W     | 7   | ALA  | 2.5  |
| 5   | E     | 49  | TYR  | 2.5  |
| 9   | V     | 57  | GLY  | 2.5  |
| 4   | D     | 3   | LEU  | 2.4  |
| 7   | T     | 33  | GLY  | 2.4  |
| 6   | S     | 14  | GLU  | 2.4  |
| 5   | E     | 106 | ILE  | 2.4  |
| 5   | E     | 116 | GLN  | 2.4  |
| 2   | B     | 17  | VAL  | 2.4  |
| 3   | P     | 330 | ALA  | 2.4  |
| 7   | G     | 43  | ALA  | 2.4  |
| 1   | N     | 213 | GLN  | 2.4  |
| 7   | G     | 1   | GLY  | 2.4  |
| 1   | N     | 219 | LEU  | 2.3  |
| 7   | T     | 73  | ASN  | 2.3  |
| 9   | V     | 62  | ARG  | 2.3  |
| 5   | R     | 75  | GLU  | 2.3  |
| 7   | T     | 28  | HIS  | 2.3  |
| 8   | U     | 67  | HIS  | 2.3  |
| 9   | V     | 51  | CYS  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 66  | GLY  | 2.3  |
| 1   | A     | 262 | TRP  | 2.3  |
| 5   | R     | 33  | LYS  | 2.2  |
| 8   | H     | 51  | GLU  | 2.2  |
| 9   | I     | 48  | SER  | 2.2  |
| 5   | E     | 191 | ASP  | 2.2  |
| 5   | E     | 38  | LEU  | 2.2  |
| 6   | F     | 13  | LEU  | 2.2  |
| 10  | W     | 10  | TYR  | 2.2  |
| 5   | E     | 124 | LEU  | 2.2  |
| 5   | R     | 23  | LYS  | 2.2  |
| 9   | I     | 71  | ASN  | 2.2  |
| 1   | N     | 231 | LEU  | 2.1  |
| 6   | S     | 13  | LEU  | 2.1  |
| 1   | N     | 193 | PRO  | 2.1  |
| 1   | N     | 209 | LEU  | 2.1  |
| 2   | O     | 232 | LEU  | 2.1  |
| 10  | W     | 26  | VAL  | 2.1  |
| 1   | N     | 187 | SER  | 2.1  |
| 1   | N     | 81  | SER  | 2.1  |
| 10  | W     | 15  | ARG  | 2.1  |
| 7   | T     | 38  | LEU  | 2.1  |
| 2   | B     | 391 | SER  | 2.1  |
| 1   | A     | 229 | PRO  | 2.1  |
| 2   | O     | 267 | ALA  | 2.1  |
| 9   | I     | 61  | GLY  | 2.1  |
| 1   | N     | 102 | LEU  | 2.0  |
| 2   | O     | 347 | ILE  | 2.0  |
| 8   | U     | 13  | LEU  | 2.0  |
| 9   | I     | 34  | VAL  | 2.0  |
| 7   | T     | 74  | PRO  | 2.0  |
| 5   | E     | 134 | ILE  | 2.0  |
| 9   | V     | 34  | VAL  | 2.0  |
| 2   | O     | 249 | GLY  | 2.0  |
| 5   | R     | 35  | PHE  | 2.0  |
| 1   | N     | 15  | GLN  | 2.0  |
| 9   | I     | 73  | PRO  | 2.0  |
| 8   | H     | 34  | ARG  | 2.0  |
| 5   | E     | 154 | GLY  | 2.0  |
| 5   | E     | 155 | GLY  | 2.0  |

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms  | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|--------|------|------|-----------------------------|-------|
| 11  | JZR  | F     | 4001 | 18/18  | 0.14 | 0.72 | 146,154,157,158             | 0     |
| 13  | AZI  | A     | 4011 | 3/3    | 0.20 | 0.46 | 61,61,66,69                 | 0     |
| 11  | JZR  | D     | 4003 | 18/18  | 0.28 | 0.70 | 160,169,171,171             | 0     |
| 14  | GOL  | B     | 2009 | 6/6    | 0.36 | 0.59 | 84,85,86,86                 | 0     |
| 11  | JZR  | S     | 2011 | 18/18  | 0.42 | 0.46 | 61,89,94,98                 | 0     |
| 11  | JZR  | C     | 4002 | 18/18  | 0.55 | 0.51 | 114,122,125,125             | 0     |
| 14  | GOL  | O     | 3009 | 6/6    | 0.56 | 0.65 | 82,84,85,85                 | 0     |
| 11  | JZR  | F     | 3011 | 18/18  | 0.58 | 0.42 | 108,113,116,116             | 0     |
| 13  | AZI  | O     | 4010 | 3/3    | 0.60 | 0.65 | 102,102,104,104             | 0     |
| 14  | GOL  | C     | 4006 | 6/6    | 0.62 | 0.52 | 96,98,99,100                | 0     |
| 11  | JZR  | P     | 3010 | 18/18  | 0.63 | 0.37 | 103,107,112,112             | 0     |
| 11  | JZR  | C     | 2010 | 18/18  | 0.63 | 0.38 | 94,103,108,108              | 0     |
| 11  | JZR  | R     | 4007 | 18/18  | 0.65 | 0.34 | 85,95,98,99                 | 0     |
| 17  | PEE  | D     | 2006 | 26/51  | 0.67 | 0.30 | 85,98,108,109               | 0     |
| 13  | AZI  | C     | 2005 | 3/3    | 0.67 | 0.20 | 54,54,56,58                 | 0     |
| 13  | AZI  | G     | 4009 | 3/3    | 0.69 | 0.22 | 66,66,67,68                 | 0     |
| 12  | PO4  | A     | 2013 | 5/5    | 0.71 | 0.16 | 119,120,121,122             | 0     |
| 12  | PO4  | C     | 4008 | 5/5    | 0.76 | 0.17 | 153,153,153,153             | 0     |
| 13  | AZI  | P     | 3005 | 3/3    | 0.78 | 0.12 | 51,51,54,56                 | 0     |
| 20  | CDL  | D     | 2003 | 39/100 | 0.79 | 0.18 | 53,78,93,94                 | 0     |
| 14  | GOL  | R     | 4005 | 6/6    | 0.81 | 0.20 | 81,83,84,85                 | 0     |
| 14  | GOL  | P     | 3008 | 6/6    | 0.82 | 0.15 | 67,69,71,71                 | 0     |
| 20  | CDL  | P     | 3003 | 39/100 | 0.84 | 0.19 | 61,89,111,111               | 0     |
| 17  | PEE  | Q     | 3006 | 51/51  | 0.86 | 0.29 | 65,75,98,100                | 0     |
| 20  | CDL  | G     | 2004 | 44/100 | 0.88 | 0.21 | 73,87,99,102                | 0     |
| 14  | GOL  | C     | 2008 | 6/6    | 0.89 | 0.31 | 61,65,68,75                 | 0     |
| 12  | PO4  | P     | 3013 | 5/5    | 0.91 | 0.10 | 104,105,106,106             | 0     |

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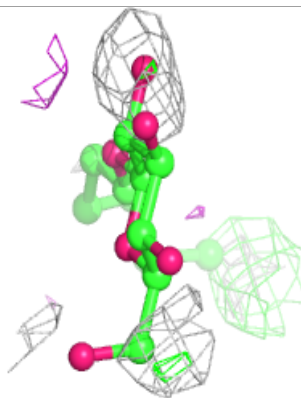
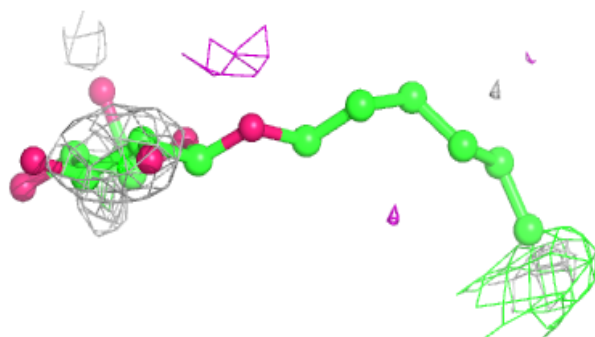
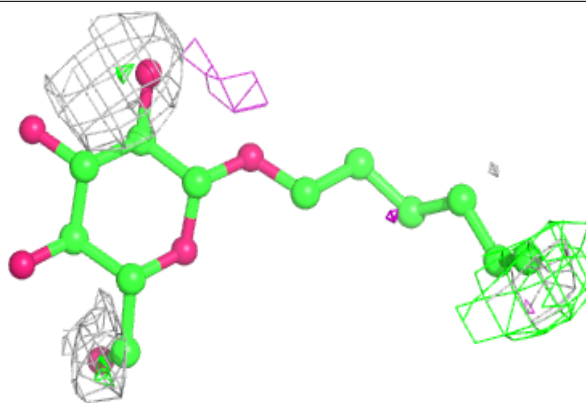
| Mol | Type | Chain | Res  | Atoms  | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|--------|------|------|-----------------------------|-------|
| 20  | CDL  | T     | 3004 | 49/100 | 0.91 | 0.23 | 74,89,107,107               | 0     |
| 12  | PO4  | S     | 3012 | 5/5    | 0.93 | 0.15 | 97,97,99,100                | 0     |
| 17  | PEE  | P     | 3007 | 49/51  | 0.94 | 0.20 | 41,57,81,81                 | 0     |
| 12  | PO4  | F     | 2012 | 5/5    | 0.95 | 0.12 | 81,82,83,84                 | 0     |
| 18  | ANY  | C     | 2002 | 37/40  | 0.95 | 0.14 | 31,39,65,70                 | 0     |
| 16  | SMA  | P     | 3001 | 37/37  | 0.95 | 0.13 | 27,40,44,46                 | 0     |
| 18  | ANY  | P     | 3002 | 37/40  | 0.95 | 0.16 | 33,39,67,71                 | 0     |
| 17  | PEE  | C     | 2007 | 49/51  | 0.95 | 0.18 | 35,55,81,83                 | 0     |
| 16  | SMA  | C     | 2001 | 37/37  | 0.96 | 0.13 | 31,39,44,48                 | 0     |
| 11  | JZR  | A     | 4004 | 18/18  | 0.96 | 0.13 | 28,34,40,42                 | 0     |
| 21  | FES  | E     | 501  | 4/4    | 0.97 | 0.10 | 41,41,43,43                 | 0     |
| 15  | HEM  | P     | 502  | 43/43  | 0.97 | 0.13 | 27,31,36,40                 | 0     |
| 15  | HEM  | C     | 501  | 43/43  | 0.97 | 0.12 | 20,31,38,47                 | 0     |
| 19  | HEC  | Q     | 501  | 43/43  | 0.97 | 0.12 | 38,45,48,51                 | 0     |
| 15  | HEM  | C     | 502  | 43/43  | 0.98 | 0.13 | 22,28,34,37                 | 0     |
| 21  | FES  | R     | 501  | 4/4    | 0.98 | 0.14 | 35,35,37,37                 | 0     |
| 15  | HEM  | P     | 501  | 43/43  | 0.98 | 0.12 | 30,34,42,46                 | 0     |
| 19  | HEC  | D     | 501  | 43/43  | 0.98 | 0.12 | 35,41,44,45                 | 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.

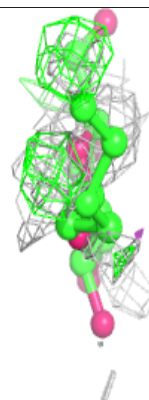
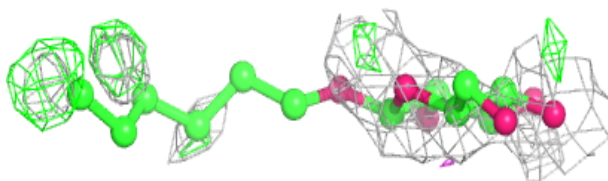
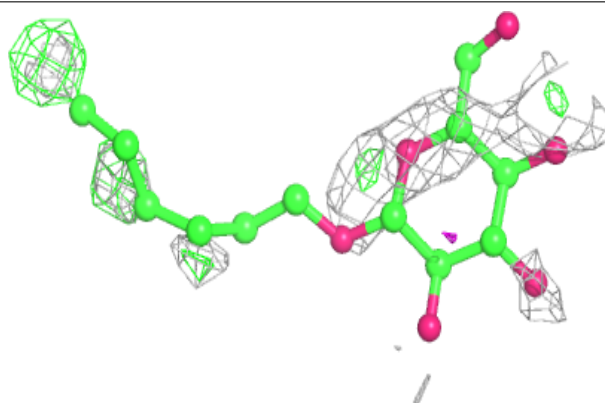


**Electron density around JZR F 4001:**

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

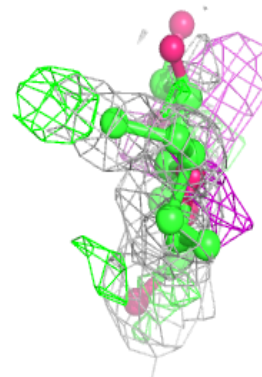
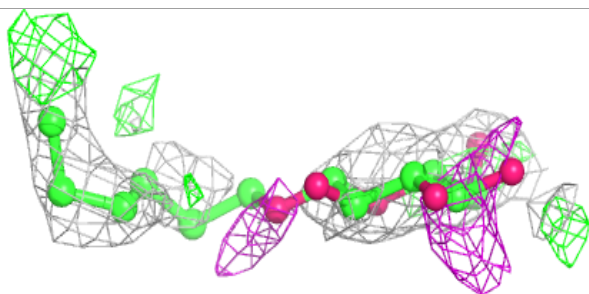
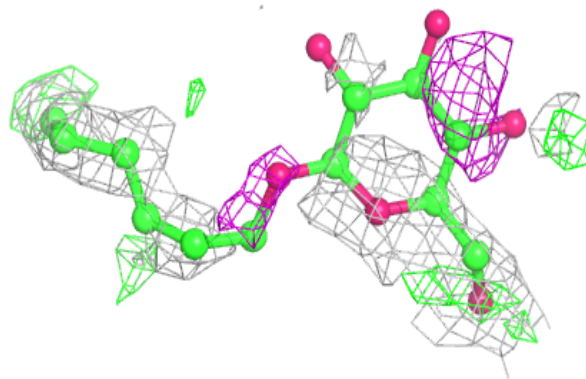
**Electron density around JZR D 4003:**

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

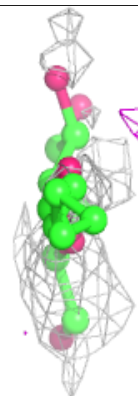
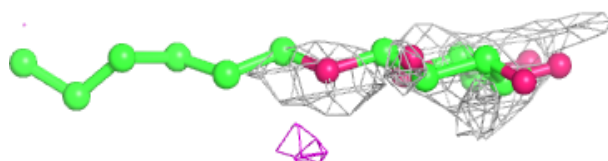
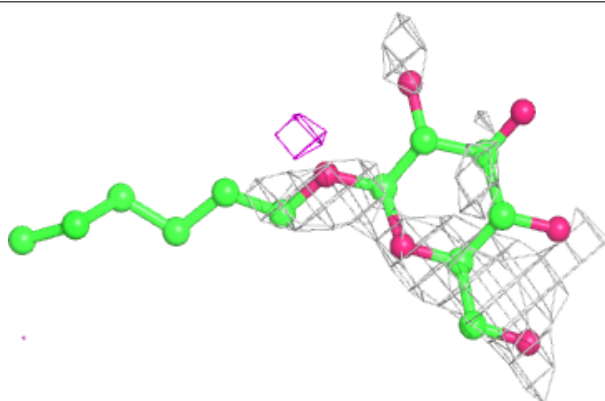


**Electron density around JZR S 2011:**

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

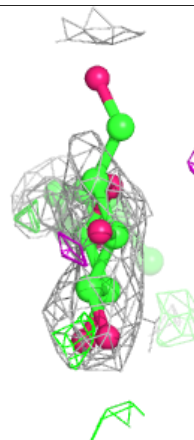
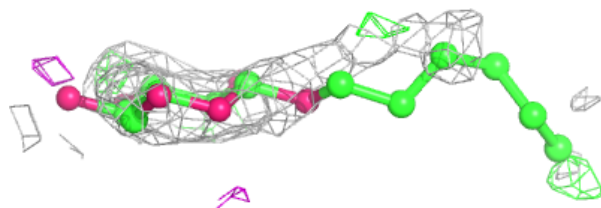
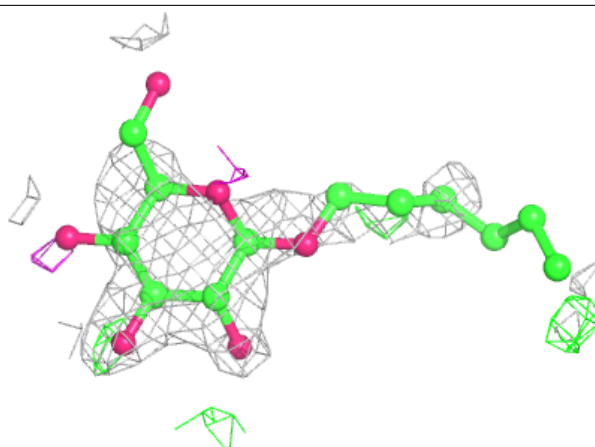
**Electron density around JZR C 4002:**

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

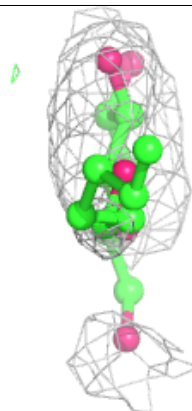
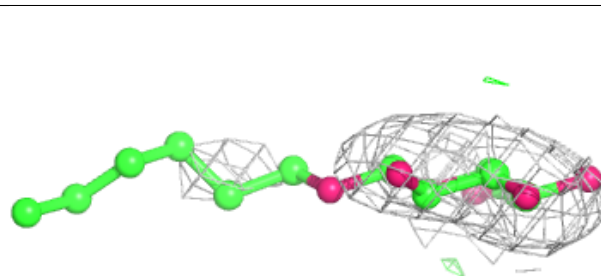
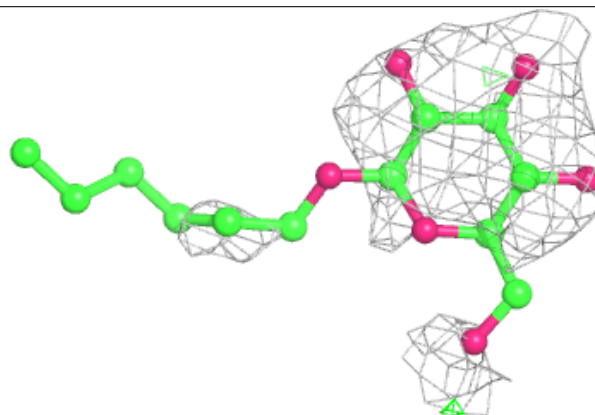


**Electron density around JZR F 3011:**

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

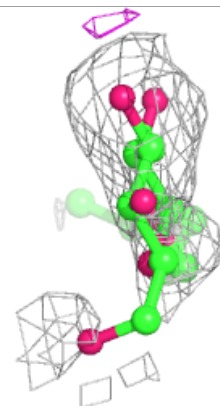
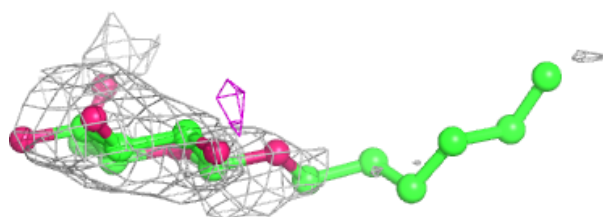
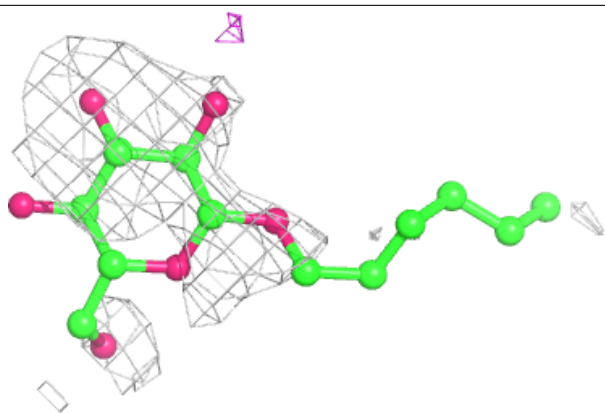
**Electron density around JZR P 3010:**

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

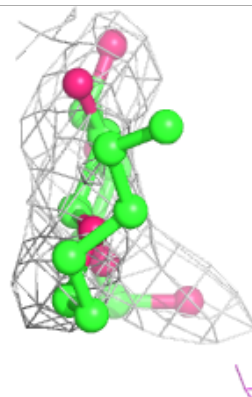
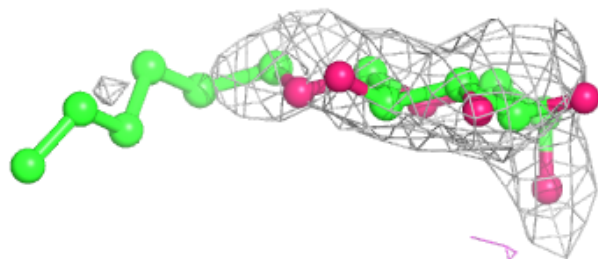
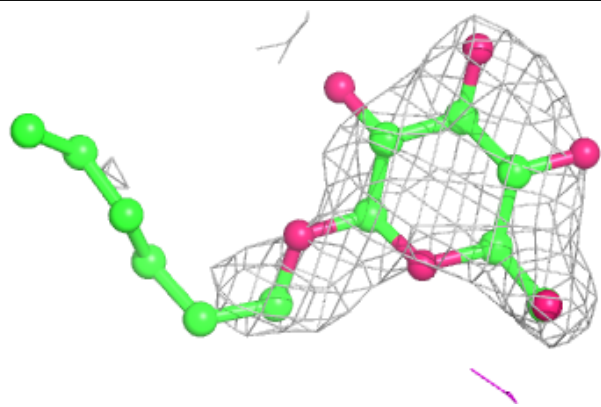


**Electron density around JZR C 2010:**

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

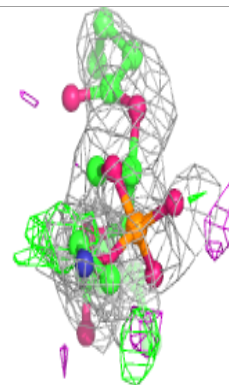
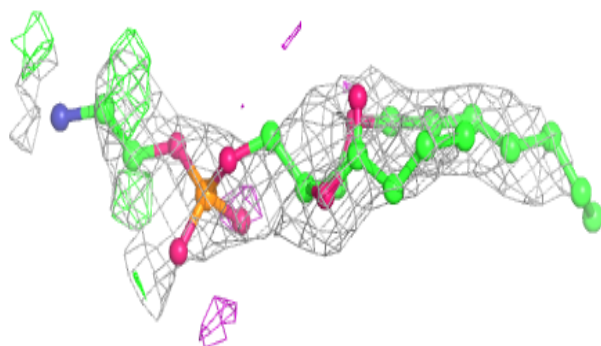
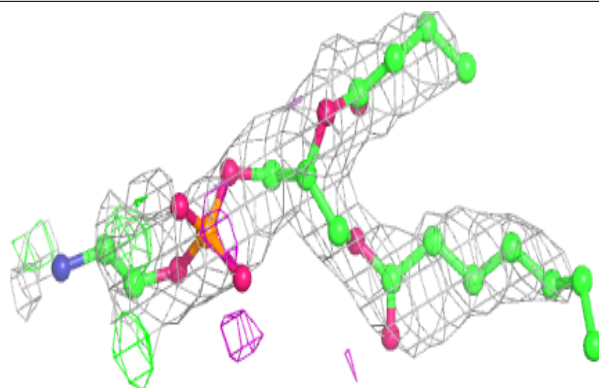
**Electron density around JZR R 4007:**

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

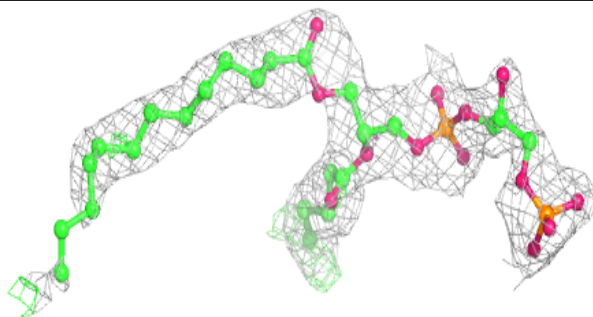
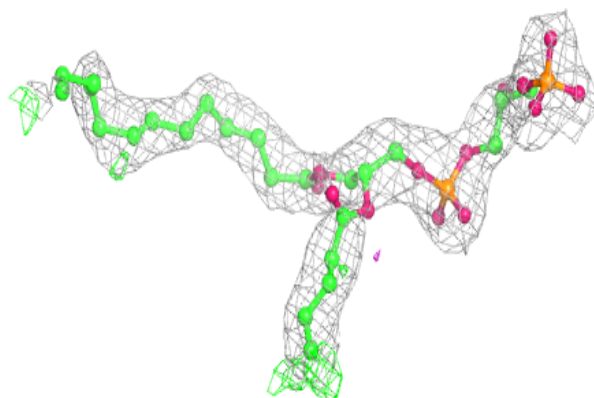


**Electron density around PEE D 2006:**

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

**Electron density around CDL D 2003:**

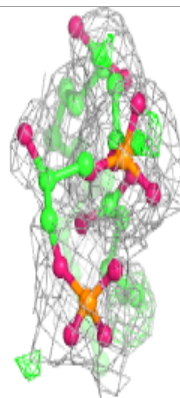
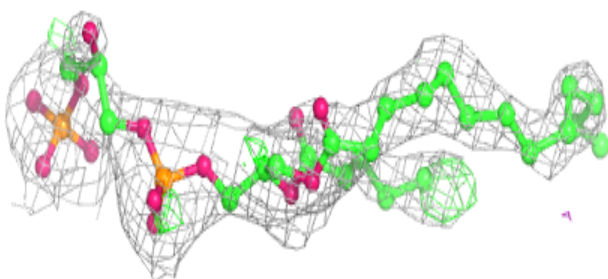
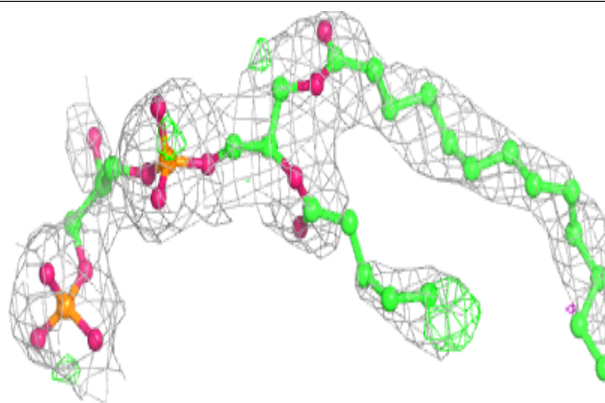
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



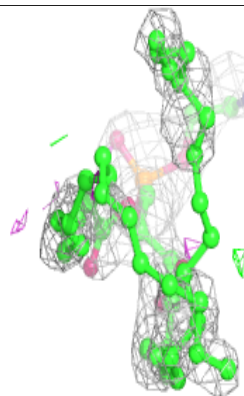
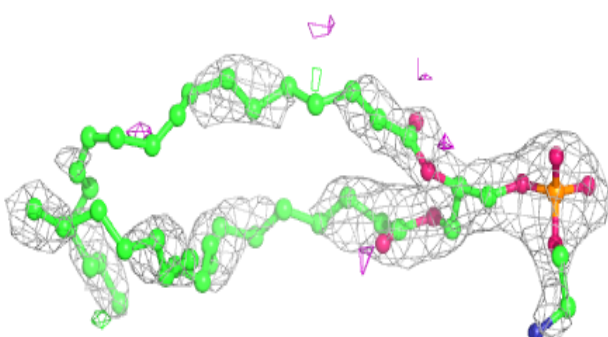
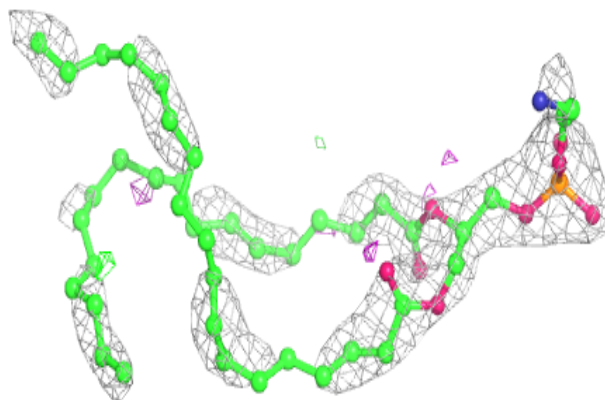


**Electron density around CDL P 3003:**

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

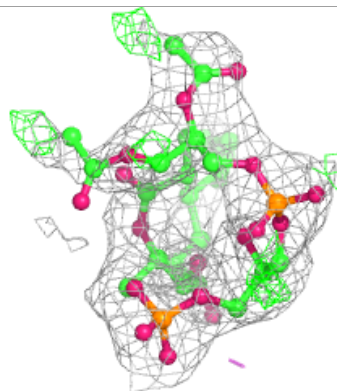
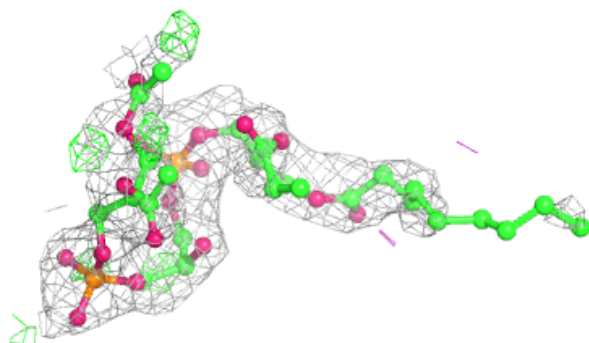
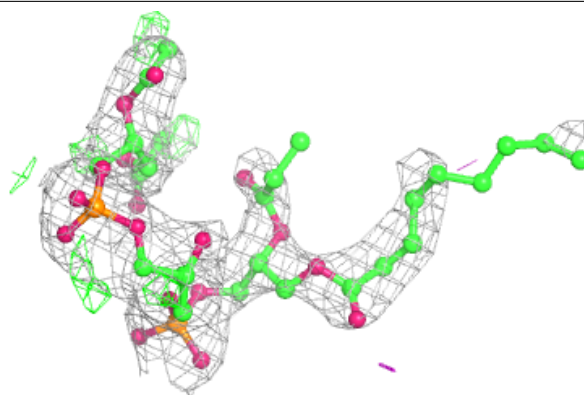
**Electron density around PEE Q 3006:**

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

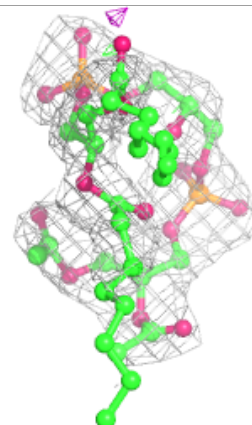
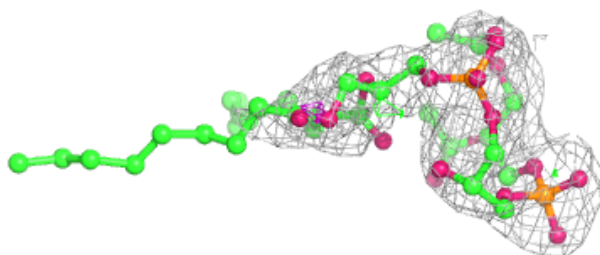
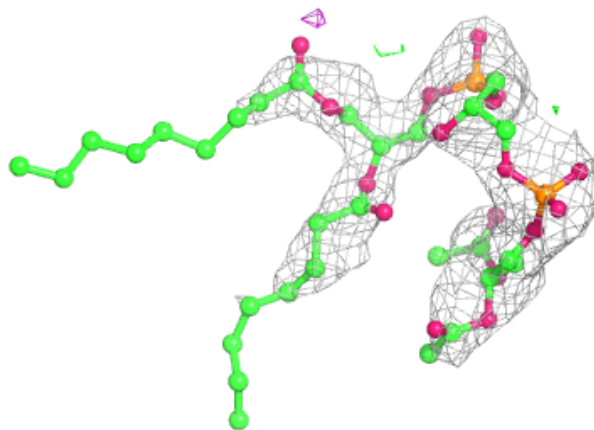


**Electron density around CDL G 2004:**

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

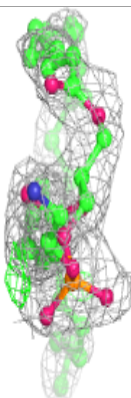
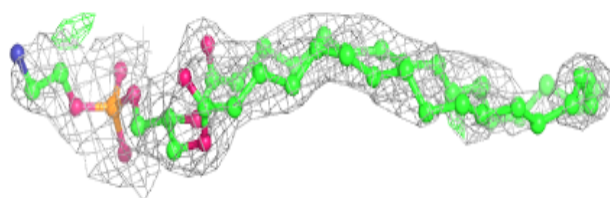
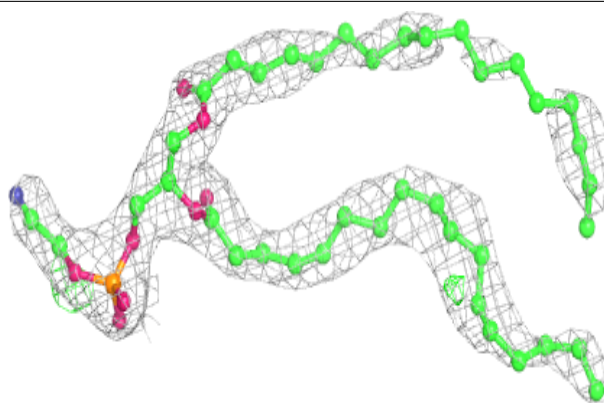
**Electron density around CDL T 3004:**

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

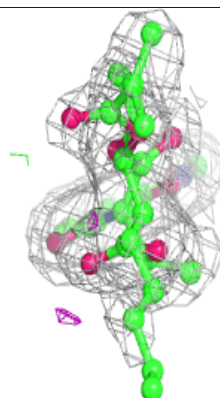
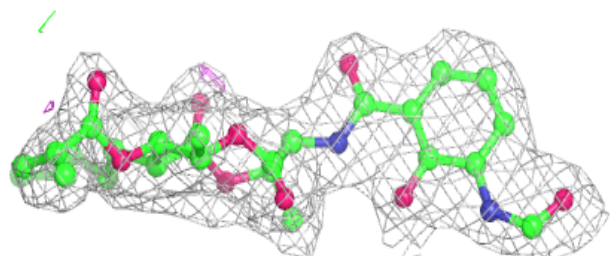
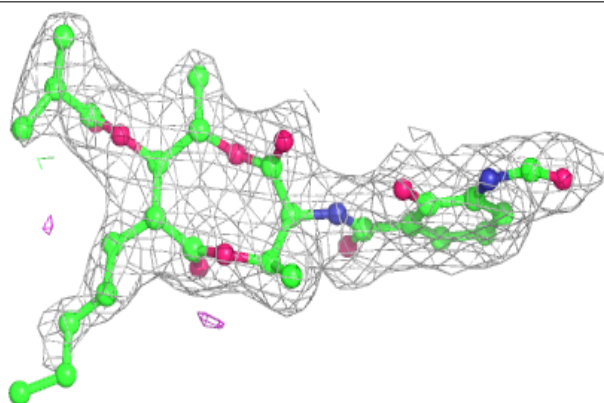


**Electron density around PEE P 3007:**

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

**Electron density around ANY C 2002:**

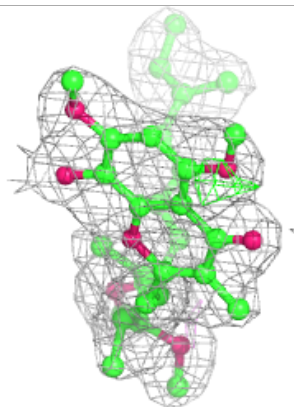
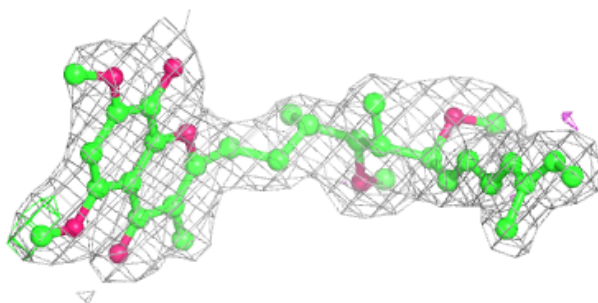
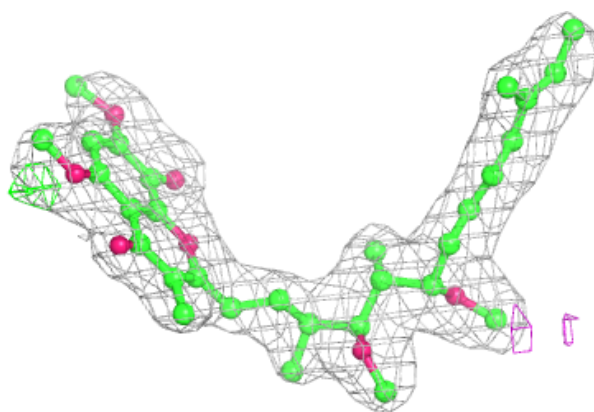
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





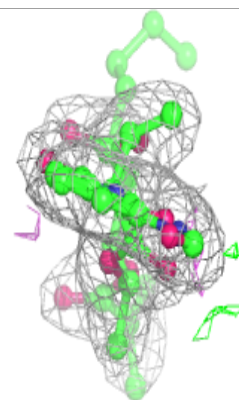
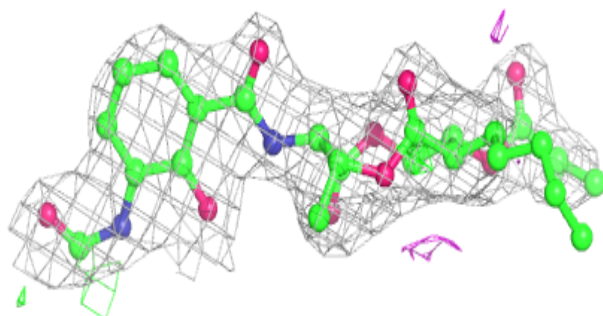
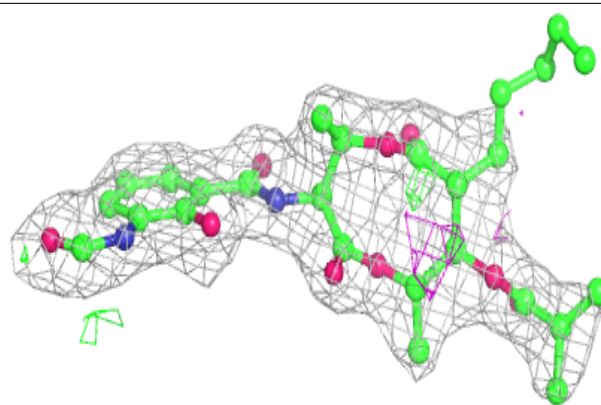
**Electron density around SMA P 3001:**

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

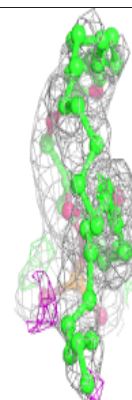
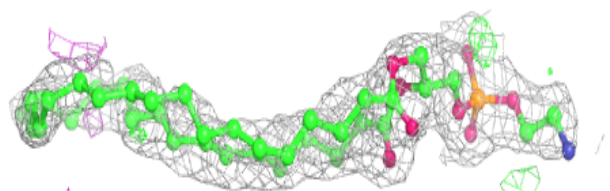
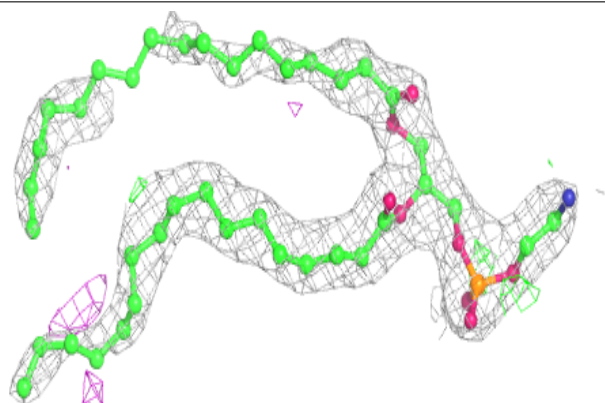


**Electron density around ANY P 3002:**

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

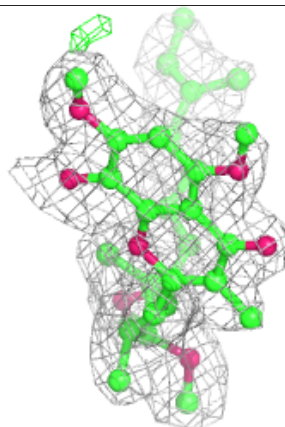
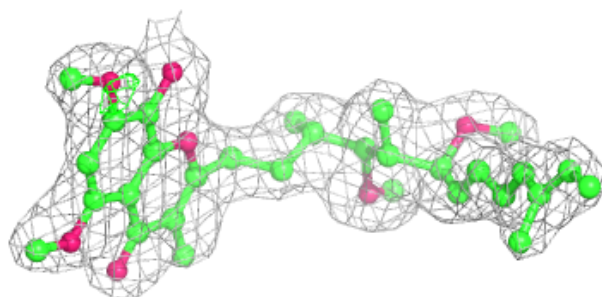
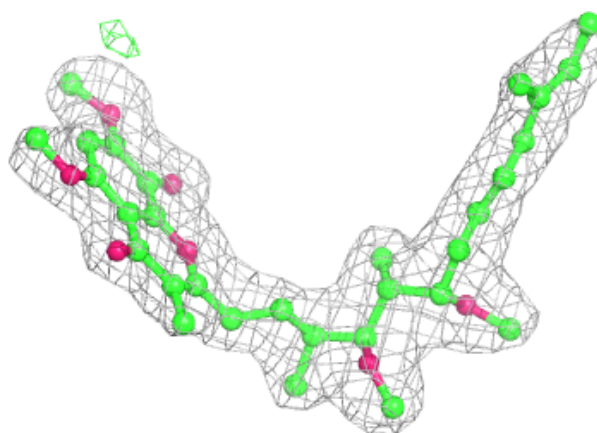
**Electron density around PEE C 2007:**

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

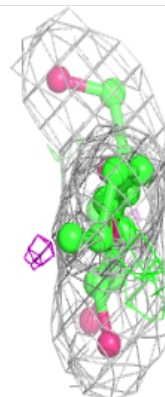
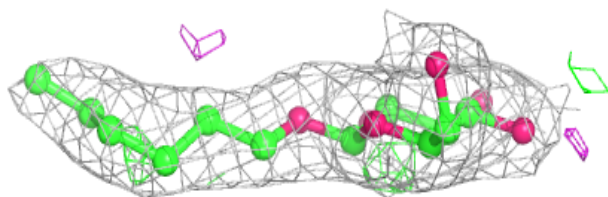
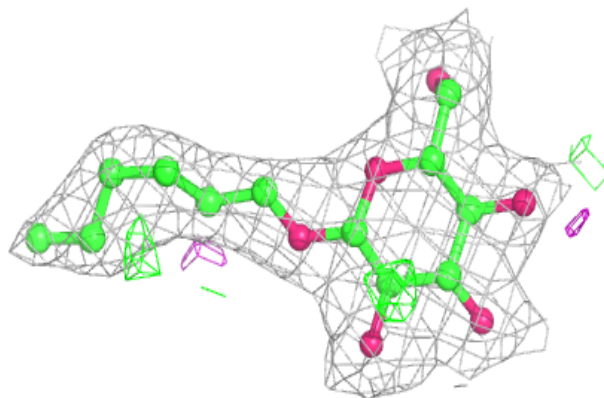


**Electron density around SMA C 2001:**

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

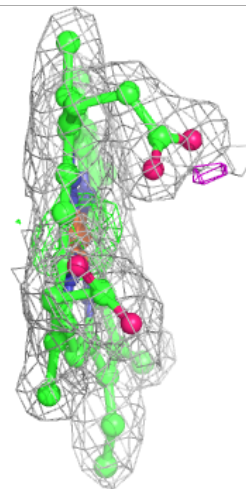
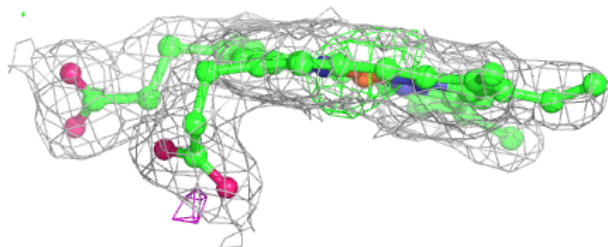
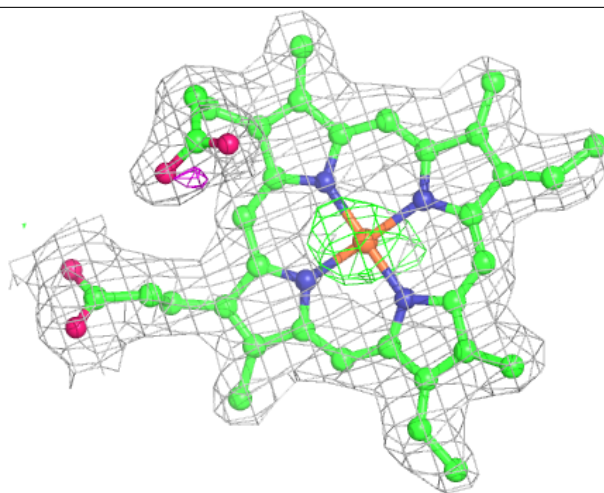
**Electron density around JZR A 4004:**

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



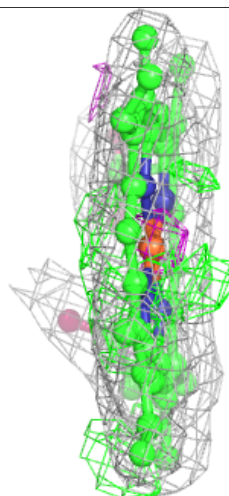
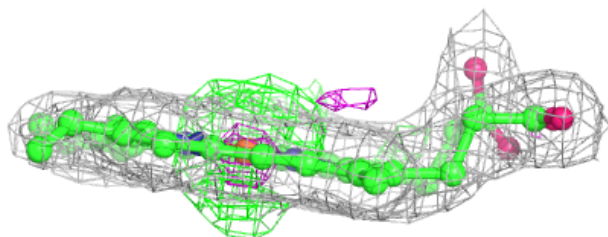
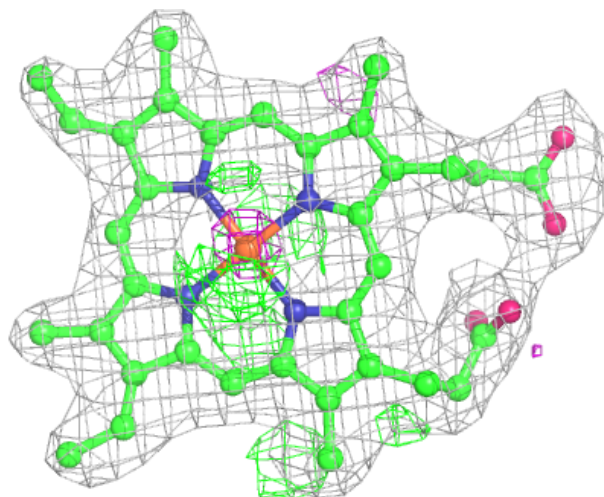
**Electron density around HEM P 502:**

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



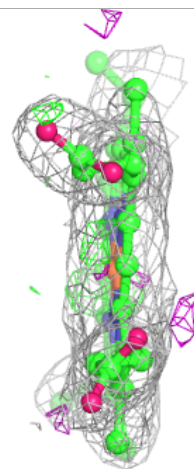
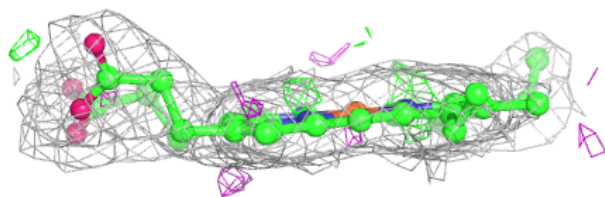
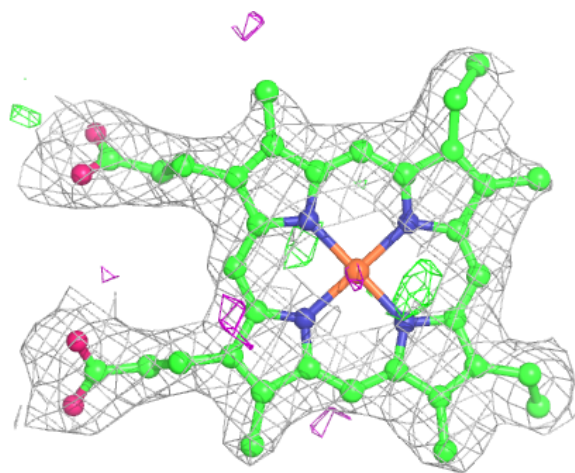
**Electron density around HEM C 501:**

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



**Electron density around HEC Q 501:**

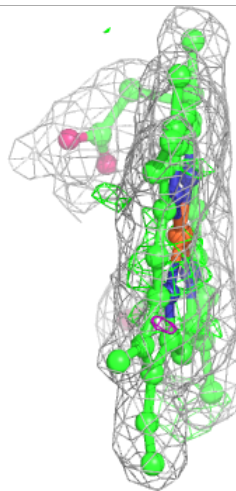
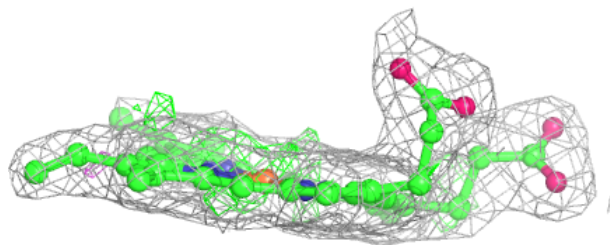
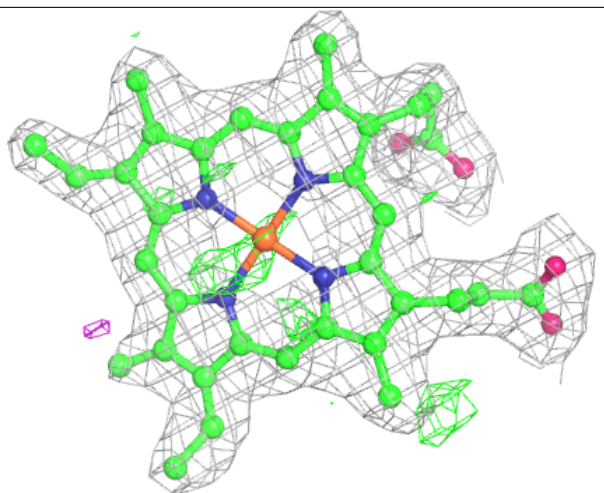
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





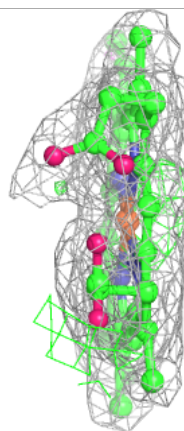
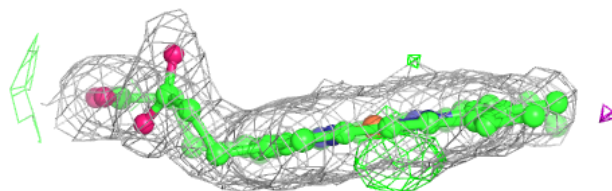
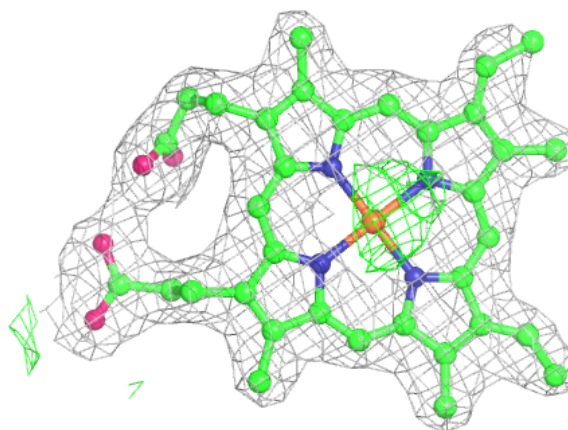
**Electron density around HEM C 502:**

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

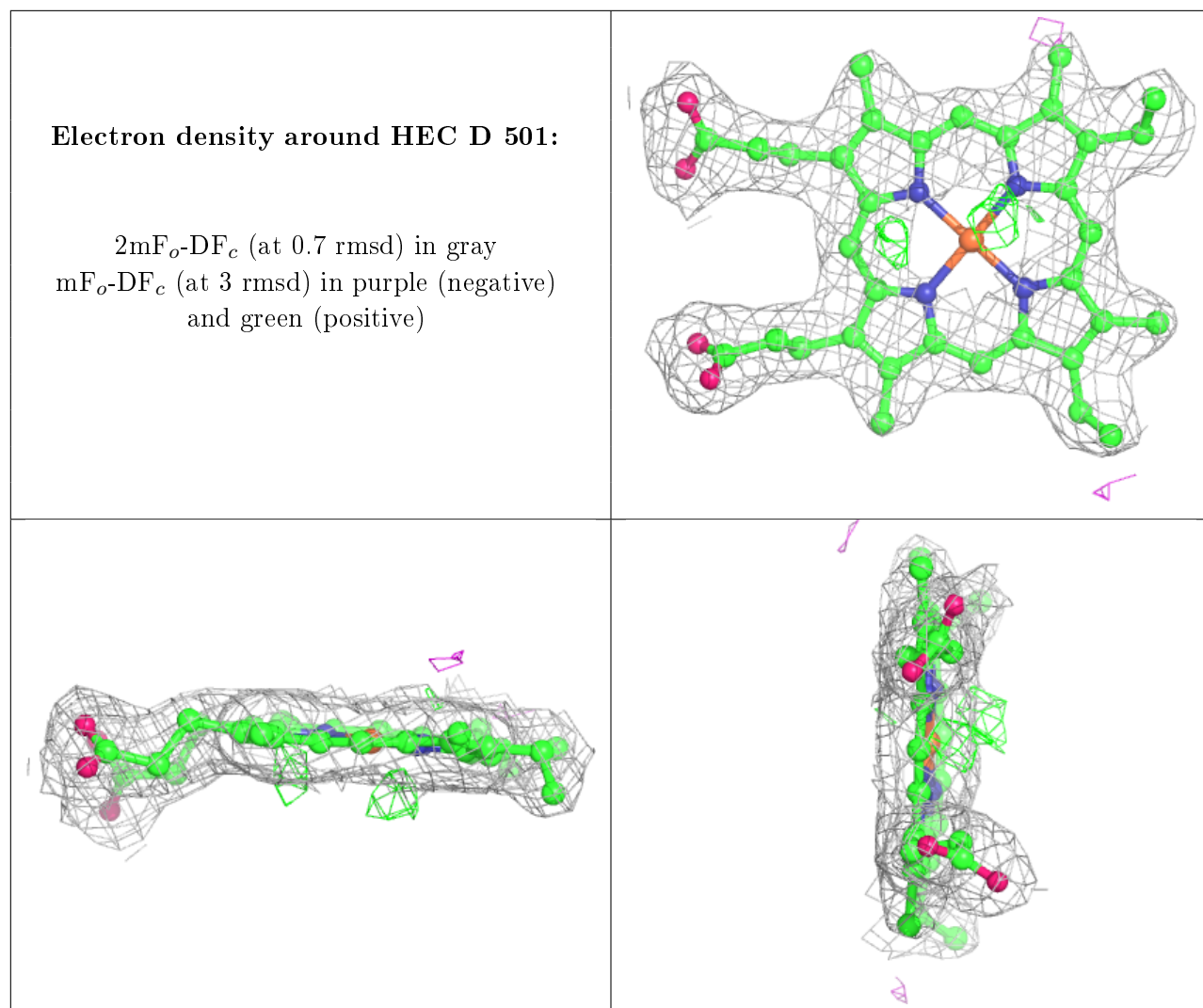


**Electron density around HEM P 501:**

$2mF_o-DF_c$  (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.