



# Full wwPDB X-ray Structure Validation Report

Oct 21, 2014 – 08:54 PM EDT

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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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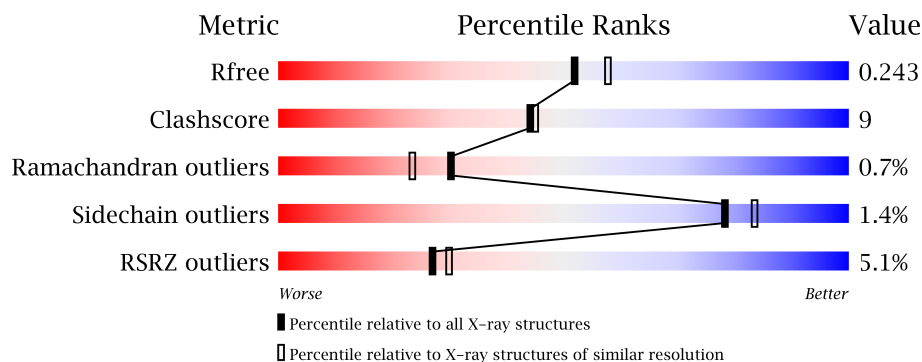
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 3012 (2.10-2.10)                                      |
| Clashscore            | 79885                       | 3649 (2.10-2.10)                                      |
| Ramachandran outliers | 78287                       | 3610 (2.10-2.10)                                      |
| Sidechain outliers    | 78261                       | 3611 (2.10-2.10)                                      |
| RSRZ outliers         | 66119                       | 3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 446    |                  |
| 1   | N     | 446    |                  |
| 2   | B     | 439    |                  |
| 2   | O     | 439    |                  |
| 3   | C     | 379    |                  |
| 3   | P     | 379    |                  |
| 4   | D     | 241    |                  |
| 4   | Q     | 241    |                  |
| 5   | E     | 196    |                  |
| 5   | R     | 196    |                  |
| 6   | F     | 110    |                  |
| 6   | S     | 110    |                  |
| 7   | G     | 81     |                  |
| 7   | T     | 81     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 11  | BHG  | C     | 2010 | -        | X                |
| 11  | BHG  | C     | 4002 | -        | X                |
| 11  | BHG  | D     | 4003 | -        | X                |
| 11  | BHG  | F     | 3011 | -        | X                |
| 11  | BHG  | F     | 4001 | -        | X                |
| 11  | BHG  | P     | 3010 | -        | X                |
| 11  | BHG  | R     | 4007 | -        | X                |
| 11  | BHG  | S     | 2011 | -        | X                |
| 12  | AZI  | A     | 4011 | X        | X                |
| 12  | AZI  | C     | 2005 | -        | X                |
| 12  | AZI  | G     | 4009 | -        | X                |
| 12  | AZI  | O     | 4010 | -        | X                |
| 13  | PO4  | C     | 4008 | -        | X                |
| 16  | FES  | E     | 501  | -        | X                |
| 16  | FES  | R     | 501  | -        | X                |
| 18  | CDL  | G     | 2004 | -        | X                |
| 18  | CDL  | T     | 3004 | -        | X                |
| 19  | PEE  | C     | 2007 | -        | X                |
| 19  | PEE  | D     | 2006 | -        | X                |
| 19  | PEE  | P     | 3007 | -        | X                |
| 19  | PEE  | Q     | 3006 | -        | X                |
| 21  | GOL  | B     | 2009 | -        | X                |
| 21  | GOL  | C     | 2008 | -        | X                |
| 21  | GOL  | C     | 4006 | -        | X                |
| 21  | GOL  | O     | 3009 | -        | X                |
| 21  | GOL  | P     | 3008 | -        | X                |
| 21  | GOL  | R     | 4005 | -        | X                |

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 33549 atoms, of which 0 are hydrogen and 0 are deuterium.

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 |         |         |       |

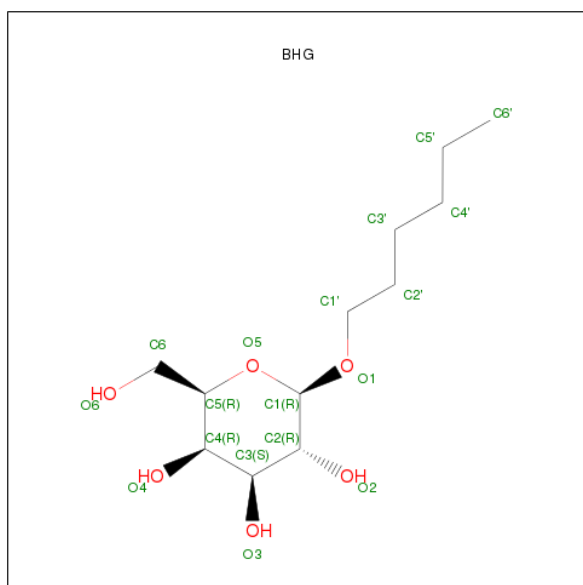
- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

| 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.

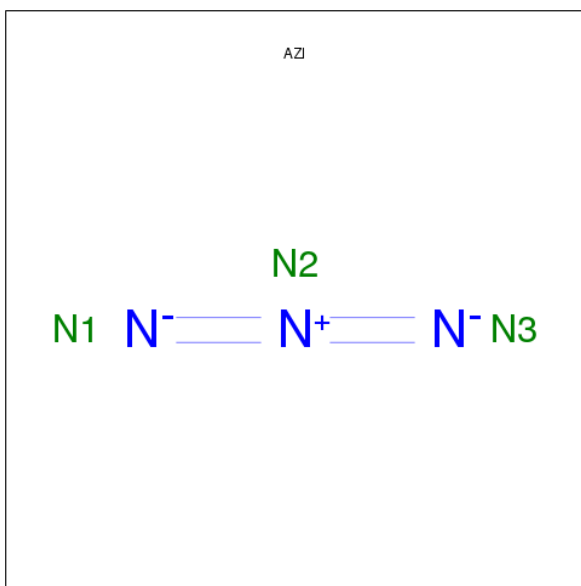
| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10  | J     | 33       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 284   | 185 | 50 | 49 |         |   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

- Molecule 11 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>6</sub>).



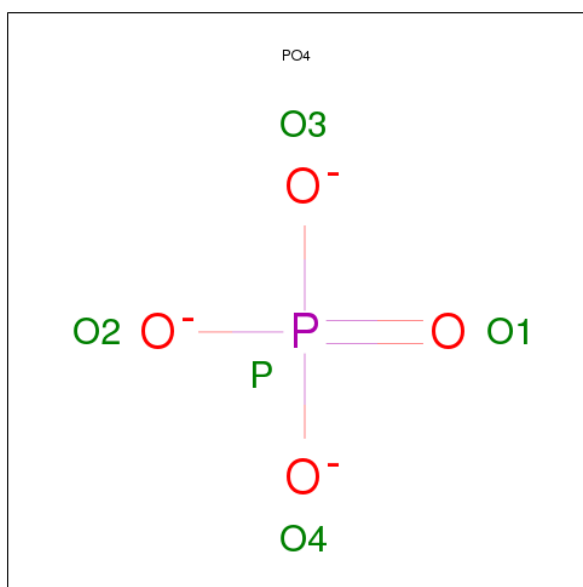
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 11  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 12 | 6 |         |         |
| 11  | S     | 1        | Total | C  | O | 0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

- Molecule 12 is AZIDE ION (three-letter code: AZI) (formula:  $N_3$ ).



| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 12  | C     | 1        | Total | N | 0       | 0       |
|     |       |          | 3     | 3 |         |         |
| 12  | P     | 1        | Total | N |         |         |
|     |       |          | 3     | 3 |         |         |
| 12  | G     | 1        | Total | N |         |         |
|     |       |          | 3     | 3 |         |         |
| 12  | O     | 1        | Total | N | 0       | 0       |
|     |       |          | 3     | 3 |         |         |
| 12  | A     | 1        | Total | N |         |         |
|     |       |          | 3     | 3 |         |         |
| 12  |       |          | Total | N |         |         |
|     |       |          | 3     | 3 |         |         |

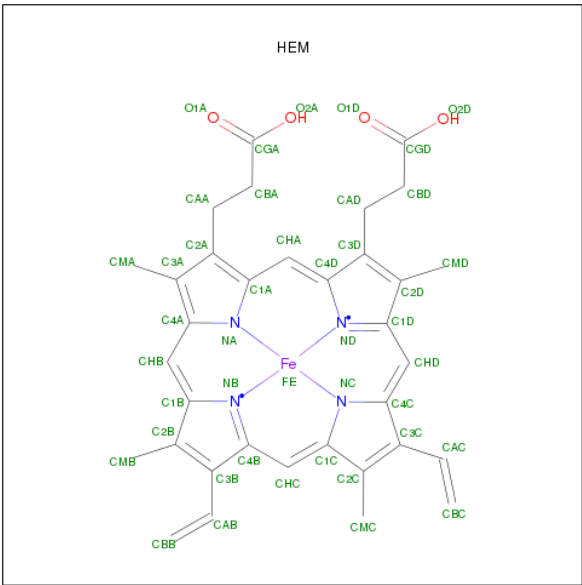
- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 13  | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 13  | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 13  | S     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 13  | P     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 13  | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

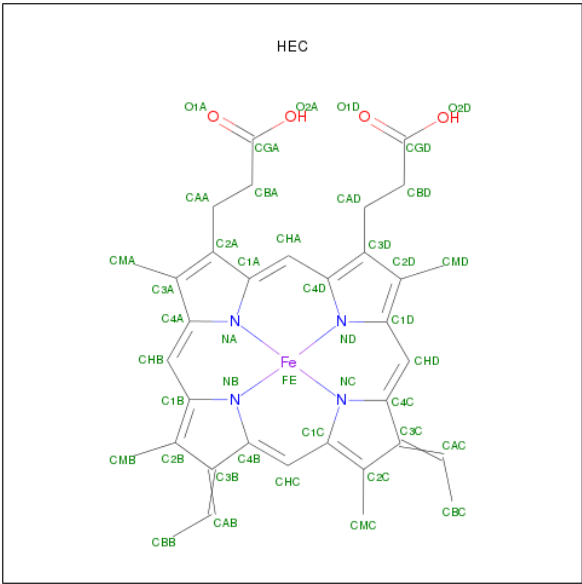
- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).





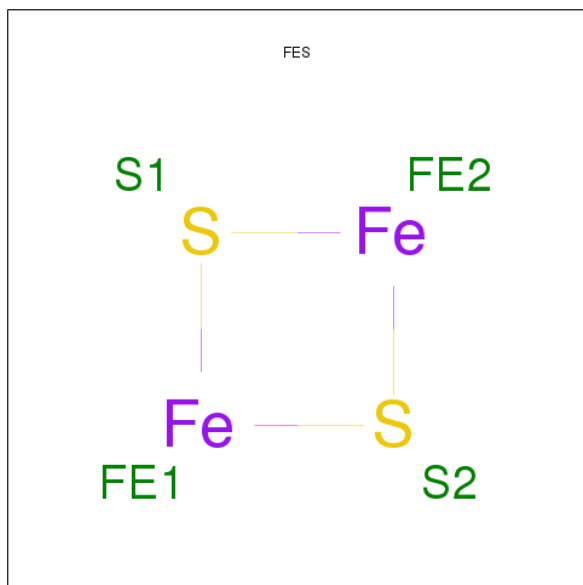
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 14  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 14  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 14  | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 14  | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 15 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



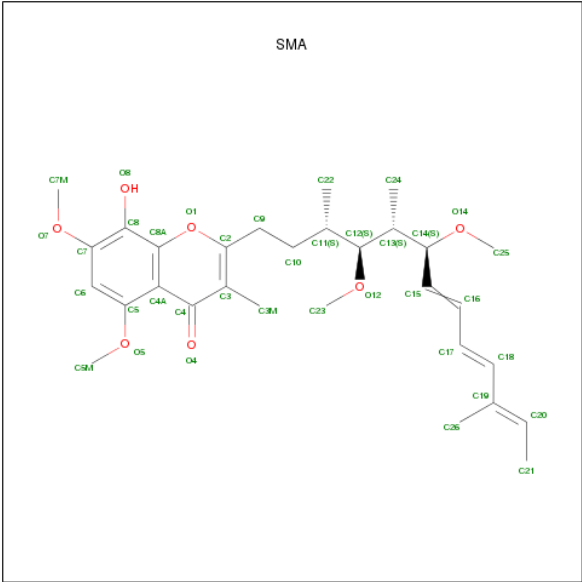
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 15  | D     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |
| 15  | Q     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



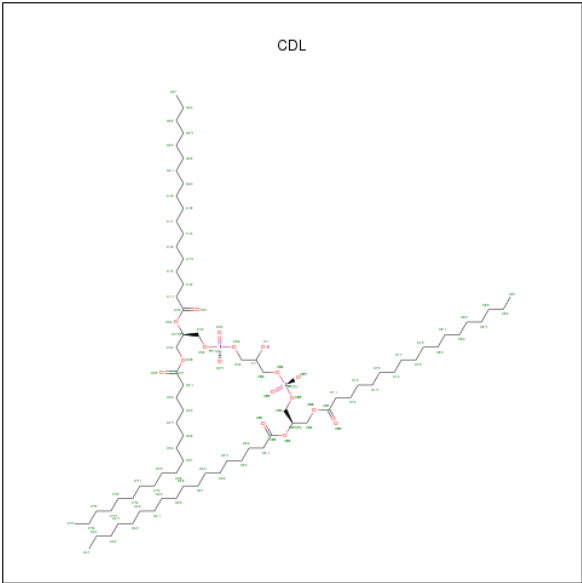
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 16  | E     | 1        | Total | Fe | S |         |         |
|     |       |          | 4     | 2  | 2 | 0       | 0       |
| 16  | R     | 1        | Total | Fe | S |         |         |
|     |       |          | 4     | 2  | 2 | 0       | 0       |

- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula:  $\text{C}_{30}\text{H}_{42}\text{O}_7$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 17  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 30 | 7 |         |         |
| 17  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 30 | 7 |         |         |

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).

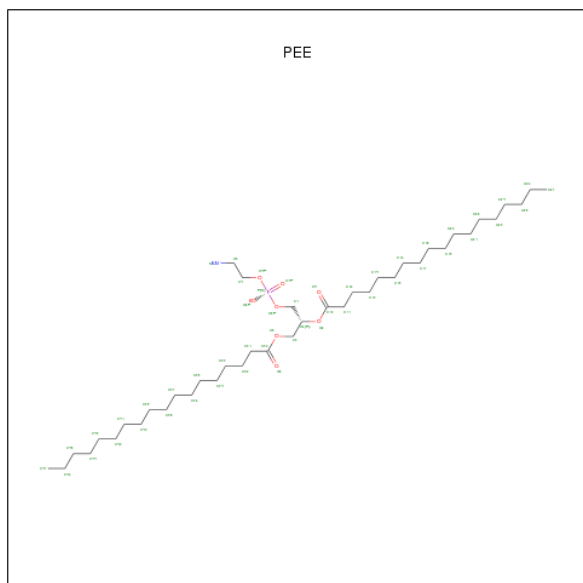


| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 18  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 24 | 13 | 2 |         |         |
| 18  | G     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 44    | 25 | 17 | 2 |         |         |

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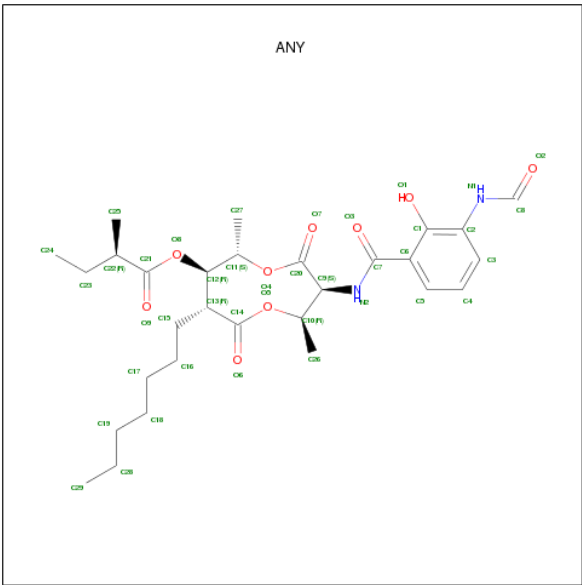
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 18  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 24 | 13 | 2 |         |         |
| 18  | T     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 30 | 17 | 2 |         |         |

- Molecule 19 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



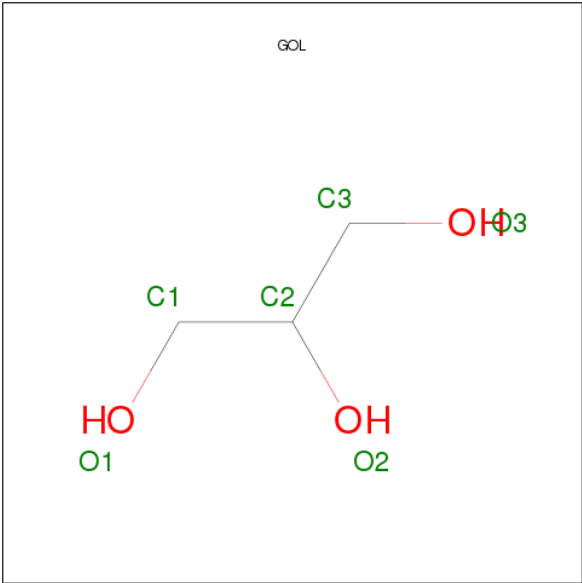
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 19  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |         |
| 19  | D     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 26    | 16 | 1 | 8 | 1 |         |         |
| 19  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |         |
| 19  | Q     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |

- Molecule 20 is 2-METHYL-BUTYRIC ACID 3-(3-FORMYLAMINO-2-HYDROXY-BENZOYLAMINO)-8-HEPTYL-2,6-DIMETHYL-4,9-DIOXO-[1,5]DIOXONAN-7-YLESTER (three-letter code: ANY) (formula:  $C_{29}H_{42}N_2O_9$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 20  | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 37    | 26 | 2 | 9 |         |         |
| 20  | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 37    | 26 | 2 | 9 |         |         |

- Molecule 21 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 21  | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 21  | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 21  | P     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 21  | O     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 21  | R     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 21  | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- 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  |         |         |

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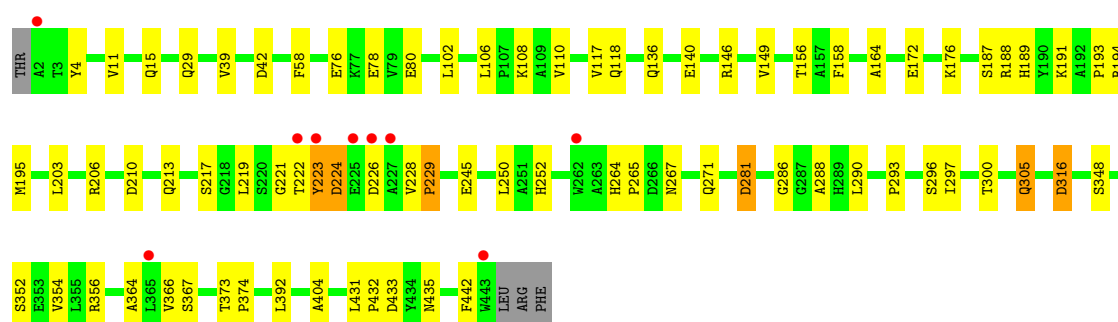
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 22  | S     | 63       | Total<br>63 | O<br>63 | 0       | 0       |
| 22  | T     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 22  | U     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 22  | V     | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 22  | W     | 9        | Total<br>9  | O<br>9  | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

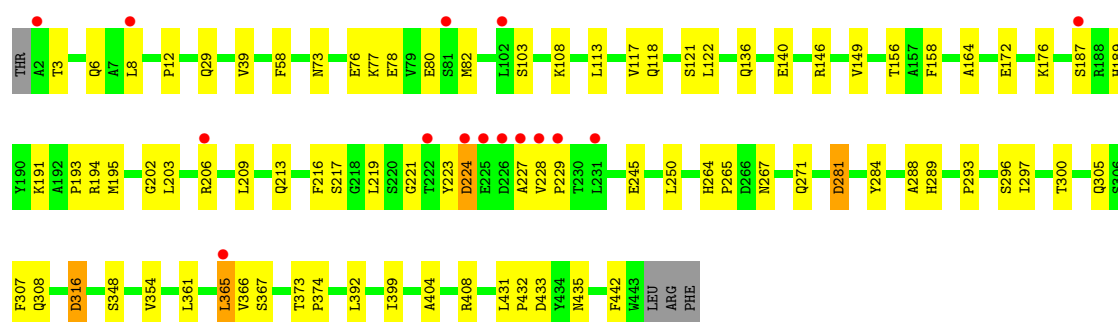
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain A: 



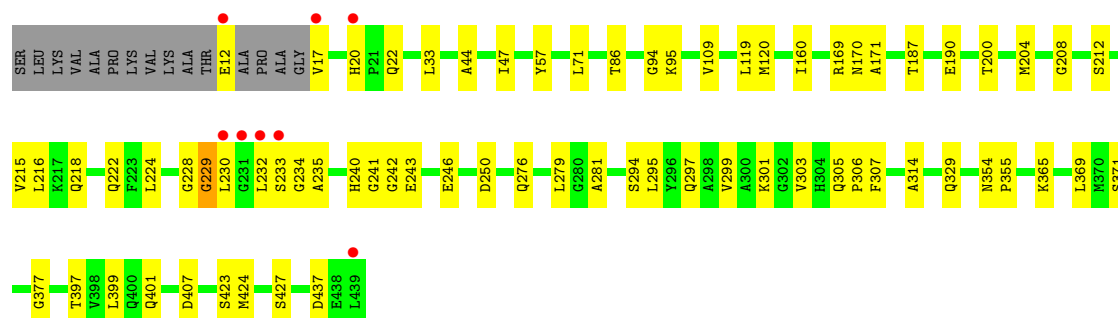
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain N: 



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

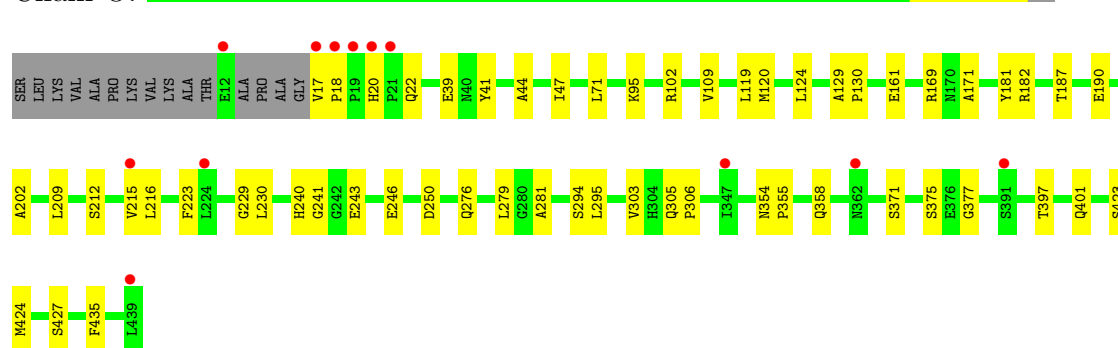
Chain B: 





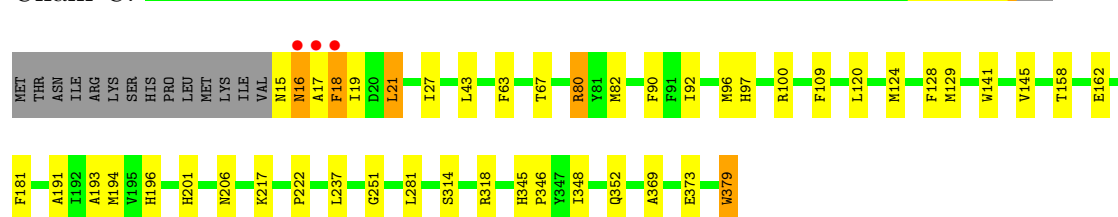
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

Chain O:



- Molecule 3: Cytochrome b

Chain C:



- Molecule 3: Cytochrome b

Chain P:



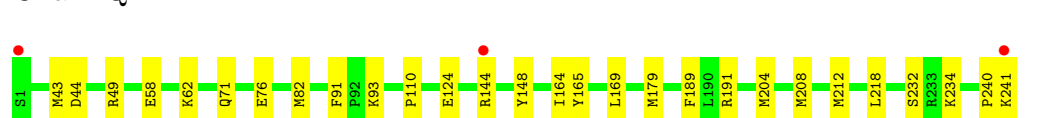
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



- Molecule 4: Cytochrome c1, heme protein, mitochondrial

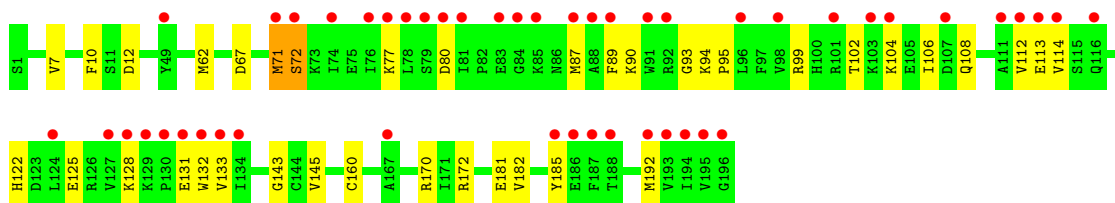
Chain Q:



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

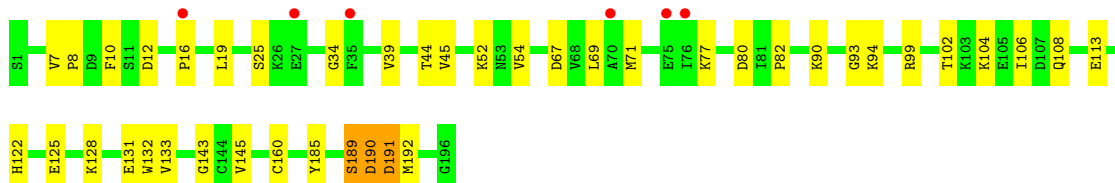
Chain E:





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

Chain R:



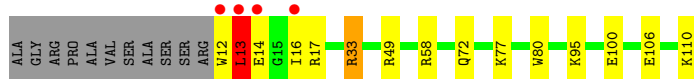
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



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

Chain S:



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

Chain G:



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

Chain T:



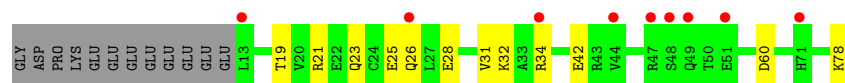
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:



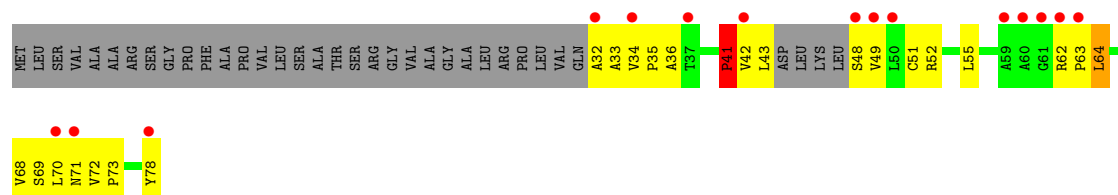
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain U:



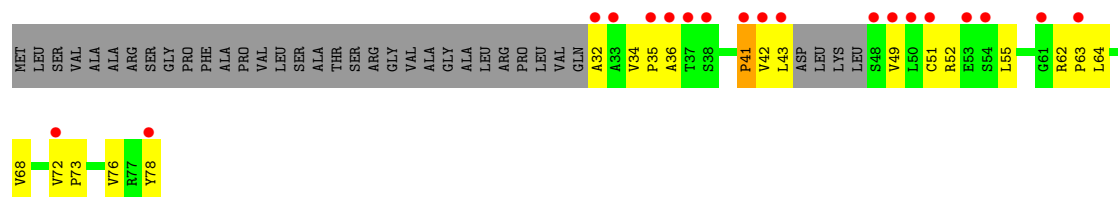
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain I:



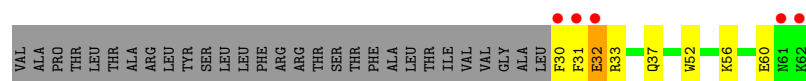
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain V:



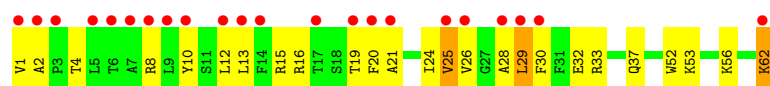
- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



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

Chain W:



## 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>0.226 , 0.243                              | Depositor<br>DCC |
| $R_{free}$ test set   | 14181 reflections (5.24%)                                   | DCC              |
| 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> ) | 0.40 , 65.3   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Outliers  | 0 of 285060 reflections                                     | 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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, CDL, PO4, BHG, 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| 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            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | F     | 36    | 0        | 48       | 3       | 0            |
| 11  | P     | 18    | 0        | 24       | 0       | 0            |
| 11  | R     | 18    | 0        | 24       | 1       | 0            |
| 11  | S     | 18    | 0        | 24       | 3       | 0            |
| 12  | A     | 3     | 0        | 0        | 0       | 0            |
| 12  | C     | 3     | 0        | 0        | 0       | 0            |
| 12  | G     | 3     | 0        | 0        | 0       | 0            |
| 12  | O     | 3     | 0        | 0        | 0       | 0            |
| 12  | P     | 3     | 0        | 0        | 0       | 0            |
| 13  | A     | 5     | 0        | 0        | 0       | 0            |
| 13  | C     | 5     | 0        | 0        | 0       | 0            |
| 13  | F     | 5     | 0        | 0        | 0       | 0            |
| 13  | P     | 5     | 0        | 0        | 0       | 0            |
| 13  | S     | 5     | 0        | 0        | 0       | 0            |
| 14  | C     | 86    | 0        | 60       | 3       | 0            |
| 14  | P     | 86    | 0        | 60       | 2       | 0            |
| 15  | D     | 43    | 0        | 30       | 3       | 0            |
| 15  | Q     | 43    | 0        | 30       | 1       | 0            |
| 16  | E     | 4     | 0        | 0        | 0       | 0            |
| 16  | R     | 4     | 0        | 0        | 0       | 0            |
| 17  | C     | 37    | 0        | 42       | 2       | 0            |
| 17  | P     | 37    | 0        | 42       | 2       | 0            |
| 18  | D     | 39    | 0        | 39       | 0       | 0            |
| 18  | G     | 44    | 0        | 32       | 0       | 0            |
| 18  | P     | 39    | 0        | 39       | 2       | 0            |
| 18  | T     | 49    | 0        | 42       | 2       | 0            |
| 19  | C     | 49    | 0        | 72       | 0       | 0            |
| 19  | D     | 26    | 0        | 26       | 3       | 0            |
| 19  | P     | 49    | 0        | 72       | 1       | 0            |
| 19  | Q     | 51    | 0        | 82       | 3       | 0            |
| 20  | C     | 37    | 0        | 28       | 1       | 0            |
| 20  | P     | 37    | 0        | 29       | 2       | 0            |
| 21  | B     | 6     | 0        | 8        | 0       | 0            |
| 21  | C     | 12    | 0        | 16       | 1       | 0            |
| 21  | O     | 6     | 0        | 8        | 0       | 0            |
| 21  | P     | 6     | 0        | 8        | 0       | 0            |
| 21  | R     | 6     | 0        | 8        | 1       | 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            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | F     | 63    | 0        | 0        | 0       | 0            |
| 22  | G     | 17    | 0        | 0        | 0       | 0            |
| 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            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (551) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2           | Distance(Å) | Clash(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:36:ALA:HB2   | 9:V:73:PRO:HD2   | 1.63        | 0.81     |
| 9:V:49:VAL:HG11  | 9:V:55:LEU:HD13  | 1.62        | 0.81     |
| 6:F:13:LEU:O     | 6:F:16:ILE:HG12  | 1.80        | 0.80     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(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  | 15: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     |
| 2:O:358:GLN:HB2  | 22:O:4120:HOH:O   | 1.95        | 0.66     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 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   | 15: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     |
| 14:P:501:HEM:HMC1 | 14: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     |
| 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     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:A:4157:HOH:O   | 9:I:41:PRO:HB3    | 2.00        | 0.60     |
| 14:C:501:HEM:HBC2 | 14: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:BHG:H2  | 1.87        | 0.57     |
| 3:C:251:GLY:HA2   | 21: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     |
| 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     |

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| Atom-1             | Atom-2           | Distance(Å) | Clash(Å) |
|--------------------|------------------|-------------|----------|
| 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     |
| 19:Q:3006:PEE:H132 | 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:BHG: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     |
| 1:N:281:ASP:OD2    | 9:V:73:PRO:HG3   | 2.07        | 0.55     |
| 2:O:202:ALA:HB1    | 2:O:230:LEU:HD23 | 1.89        | 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     |
| 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     |

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| Atom-1           | Atom-2             | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 5:E:95:PRO:HG2   | 5:E:145:VAL:HG22   | 1.90        | 0.53     |
| 4:Q:208:MET:HA   | 19:Q:3006:PEE:H312 | 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:BHG:H61  | 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  | 14:P:502:HEM:O2D   | 2.10        | 0.52     |
| 5:R:94:LYS:HE3   | 21: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:BHG: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     |
| 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     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 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    | 14: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   | 15: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     |
| 2:O:95:LYS:NZ      | 9:V:34:VAL:HG22    | 2.26        | 0.49     |
| 5:R:25:SER:HA      | 22:R:4016:HOH:O    | 2.12        | 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     |
| 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     |
| 18:P:3003:CDL:H721 | 18:P:3003:CDL:H511 | 1.95        | 0.49     |
| 5:E:102:THR:O      | 5:E:106:ILE:HG13   | 2.12        | 0.48     |

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| Atom-1           | Atom-2             | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 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   | 18: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:BHG:H62  | 1.94        | 0.47     |
| 3:C:27:ILE:HD12  | 20: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     |
| 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     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 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  | 17: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     |
| 17: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     |
| 3:C:97:HIS:CD2   | 14: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:BHG: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     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 4:D:207:LYS:HZ2   | 19:D:2006:PEE:H51 | 1.81        | 0.45     |
| 4:Q:204:MET:HE3   | 19: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     |
| 6:S:49:ARG:HH22   | 11:S:2011:BHG:H4  | 1.81        | 0.45     |
| 9:V:72:VAL:HG13   | 9:V:73:PRO:CD     | 2.46        | 0.45     |
| 5:R:52:LYS:HE3    | 10:W:32:GLU:OE2   | 2.17        | 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     |
| 2:B:240:HIS:CE1   | 2:O:435:PHE:CD1   | 3.05        | 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     |
| 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  | 17: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     |
| 15:D:501:HEC:HMB1 | 15: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     |
| 3:C:237:LEU:HD13  | 4:D:212:MET:HG3   | 1.99        | 0.44     |
| 4:D:124:GLU:OE2   | 4:D:191:ARG:CD    | 2.65        | 0.44     |
| 5:E:145:VAL:HG23  | 3:P:141:TRP:CH2   | 2.52        | 0.44     |
| 3:P:197:LEU:CD1   | 20: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  | 17:P:3001:SMA:H6  | 1.99        | 0.44     |

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| Atom-1           | Atom-2             | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 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:BHG:H6'3 | 1.83        | 0.43     |
| 2:B:279:LEU:HA   | 2:B:294:SER:HB3    | 2.00        | 0.43     |
| 1:N:213:GLN:O    | 1:N:217:SER:OG     | 2.29        | 0.43     |
| 1:N:82:MET:CE    | 1:N:108:LYS:HG2    | 2.48        | 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:BHG:O3   | 2.19        | 0.42     |
| 6:S:95:LYS:HB2   | 6:S:95:LYS:HZ3     | 1.82        | 0.42     |
| 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:175:THR:HG23 | 8:H:78:LYS:HE3     | 2.01        | 0.42     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 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:211:MET:HE1  | 10:J:31:PHE:CZ    | 2.54        | 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  | 19: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   | 19:D:2006:PEE:H51 | 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:BHG: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     |
| 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     |

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| Atom-1           | Atom-2             | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 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:BHG: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   | 18: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:43:MET:CE    | 4:Q:91:PHE:CE2     | 3.04        | 0.41     |
| 4:Q:58:GLU:O     | 4:Q:62:LYS:HG3     | 2.21        | 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     |
| 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:71:GLN:HG3   | 4:Q:82:MET:CE      | 2.51        | 0.41     |
| 4:Q:232:SER:O    | 5:R:10:PHE:HE1     | 2.04        | 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     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:P:159:ASN:ND2   | 22:P:3127:HOH:O   | 2.54        | 0.40     |
| 19:P:3007:PEE:H11 | 18: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   | 20:P:3002:ANY:H3  | 2.03        | 0.40     |
| 3:P:75:TYR:CE2    | 11:R:4007:BHG:H61 | 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%)   | 25          | 17  |
| 1   | N     | 440/446 (99%)   | 425 (97%)  | 11 (2%)  | 4 (1%)   | 25          | 17  |
| 2   | B     | 418/439 (95%)   | 405 (97%)  | 10 (2%)  | 3 (1%)   | 30          | 23  |
| 2   | O     | 419/439 (95%)   | 404 (96%)  | 13 (3%)  | 2 (0%)   | 38          | 33  |
| 3   | C     | 363/379 (96%)   | 352 (97%)  | 9 (2%)   | 2 (1%)   | 33          | 28  |
| 3   | P     | 363/379 (96%)   | 352 (97%)  | 10 (3%)  | 1 (0%)   | 50          | 49  |
| 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%)   | 15          | 8   |
| 5   | R     | 194/196 (99%)   | 183 (94%)  | 8 (4%)   | 3 (2%)   | 15          | 8   |
| 6   | F     | 97/110 (88%)    | 96 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 6   | S     | 97/110 (88%)    | 94 (97%)   | 1 (1%)   | 2 (2%)   | 11          | 4   |
| 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%)   | 8           | 2   |
| 9   | V     | 39/78 (50%)     | 36 (92%)   | 2 (5%)   | 1 (3%)   | 8           | 2   |
| 10  | J     | 30/62 (48%)     | 28 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 10  | W     | 59/62 (95%)     | 54 (92%)   | 4 (7%)   | 1 (2%)   | 14          | 6   |
| All | All   | 3945/4220 (94%) | 3803 (96%) | 115 (3%) | 27 (1%)  | 30          | 23  |

All (27) Ramachandran outliers are listed below:

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

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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%)   | 64          | 68  |
| 1   | N     | 363/370 (98%)  | 357 (98%)  | 6 (2%)   | 73          | 78  |
| 2   | B     | 332/343 (97%)  | 332 (100%) | 0        | 100         | 100 |
| 2   | O     | 328/343 (96%)  | 328 (100%) | 0        | 100         | 100 |
| 3   | C     | 312/327 (95%)  | 304 (97%)  | 8 (3%)   | 59          | 62  |
| 3   | P     | 311/327 (95%)  | 303 (97%)  | 8 (3%)   | 59          | 62  |
| 4   | D     | 206/206 (100%) | 206 (100%) | 0        | 100         | 100 |
| 4   | Q     | 206/206 (100%) | 204 (99%)  | 2 (1%)   | 85          | 90  |
| 5   | E     | 165/168 (98%)  | 164 (99%)  | 1 (1%)   | 92          | 95  |
| 5   | R     | 167/168 (99%)  | 164 (98%)  | 3 (2%)   | 71          | 75  |
| 6   | F     | 90/98 (92%)    | 90 (100%)  | 0        | 100         | 100 |
| 6   | S     | 90/98 (92%)    | 87 (97%)   | 3 (3%)   | 50          | 51  |
| 7   | G     | 66/71 (93%)    | 66 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 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%)   | 51          | 52  |
| 9   | I     | 27/60 (45%)     | 26 (96%)   | 1 (4%)   | 45          | 45  |
| 9   | V     | 27/60 (45%)     | 26 (96%)   | 1 (4%)   | 45          | 45  |
| 10  | J     | 27/52 (52%)     | 25 (93%)   | 2 (7%)   | 20          | 15  |
| 10  | W     | 51/52 (98%)     | 49 (96%)   | 2 (4%)   | 43          | 43  |
| All | All   | 3323/3538 (94%) | 3276 (99%) | 47 (1%)  | 78          | 83  |

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  |
| 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  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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  |
| 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  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 chains 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 carbohydrates 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$ |
| 13  | PO4  | A     | 2013 | -    | 4,4,4        | 0.65 | 0           | 6,6,6       | 0.30 | 0           |
| 11  | BHG  | A     | 4004 | -    | 18,18,18     | 1.53 | 3 (16%)     | 23,23,23    | 0.66 | 0           |
| 12  | AZI  | A     | 4011 | -    | 2,2,2        | 2.20 | 2 (100%)    | 0,1,1       | 0.00 | -           |
| 21  | GOL  | B     | 2009 | -    | 5,5,5        | 1.09 | 0           | 5,5,5       | 0.62 | 0           |
| 17  | SMA  | C     | 2001 | -    | 38,38,38     | 2.08 | 9 (23%)     | 50,52,52    | 1.58 | 7 (14%)     |
| 20  | ANY  | C     | 2002 | -    | 37,38,41     | 2.45 | 11 (29%)    | 50,52,55    | 1.53 | 8 (16%)     |
| 12  | AZI  | C     | 2005 | -    | 2,2,2        | 1.86 | 1 (50%)     | 0,1,1       | 0.00 | -           |
| 19  | PEE  | C     | 2007 | -    | 48,48,50     | 1.19 | 5 (10%)     | 53,53,55    | 0.92 | 5 (9%)      |
| 21  | GOL  | C     | 2008 | -    | 5,5,5        | 1.31 | 0           | 5,5,5       | 0.81 | 0           |
| 11  | BHG  | C     | 2010 | -    | 18,18,18     | 1.73 | 4 (22%)     | 23,23,23    | 0.71 | 0           |
| 11  | BHG  | C     | 4002 | -    | 18,18,18     | 1.79 | 4 (22%)     | 23,23,23    | 0.76 | 1 (4%)      |
| 21  | GOL  | C     | 4006 | -    | 5,5,5        | 1.19 | 0           | 5,5,5       | 0.67 | 0           |
| 13  | PO4  | C     | 4008 | -    | 4,4,4        | 0.69 | 0           | 6,6,6       | 0.30 | 0           |
| 14  | HEM  | C     | 501  | 3    | 42,50,50     | 2.75 | 11 (26%)    | 27,82,82    | 1.24 | 3 (11%)     |
| 14  | HEM  | C     | 502  | 3    | 42,50,50     | 2.97 | 13 (30%)    | 27,82,82    | 1.44 | 3 (11%)     |
| 18  | CDL  | D     | 2003 | -    | 38,38,99     | 1.15 | 2 (5%)      | 47,47,111   | 1.27 | 6 (12%)     |
| 19  | PEE  | D     | 2006 | -    | 25,25,50     | 1.51 | 6 (24%)     | 30,30,55    | 0.97 | 2 (6%)      |
| 11  | BHG  | D     | 4003 | -    | 18,18,18     | 1.76 | 4 (22%)     | 23,23,23    | 0.73 | 0           |
| 15  | HEC  | D     | 501  | 4    | 50,50,50     | 3.27 | 6 (12%)     | 56,82,82    | 1.95 | 7 (12%)     |
| 16  | FES  | E     | 501  | 5    | 0,4,4        | 0.00 | -           | 0,4,4       | 0.00 | -           |
| 13  | PO4  | F     | 2012 | -    | 4,4,4        | 0.60 | 0           | 6,6,6       | 0.30 | 0           |
| 11  | BHG  | F     | 3011 | -    | 18,18,18     | 1.73 | 4 (22%)     | 23,23,23    | 0.70 | 0           |
| 11  | BHG  | F     | 4001 | -    | 18,18,18     | 1.77 | 4 (22%)     | 23,23,23    | 0.74 | 0           |
| 18  | CDL  | G     | 2004 | -    | 41,43,99     | 1.16 | 3 (7%)      | 50,55,111   | 1.55 | 8 (16%)     |
| 12  | AZI  | G     | 4009 | -    | 2,2,2        | 1.72 | 0           | 0,1,1       | 0.00 | -           |
| 21  | GOL  | O     | 3009 | -    | 5,5,5        | 1.04 | 0           | 5,5,5       | 0.55 | 0           |
| 12  | AZI  | O     | 4010 | -    | 2,2,2        | 1.55 | 0           | 0,1,1       | 0.00 | -           |
| 17  | SMA  | P     | 3001 | -    | 38,38,38     | 2.07 | 9 (23%)     | 50,52,52    | 1.62 | 8 (16%)     |
| 20  | ANY  | P     | 3002 | -    | 37,38,41     | 2.43 | 12 (32%)    | 50,52,55    | 1.52 | 9 (18%)     |
| 18  | CDL  | P     | 3003 | -    | 38,38,99     | 1.14 | 2 (5%)      | 47,47,111   | 1.25 | 6 (12%)     |
| 12  | AZI  | P     | 3005 | -    | 2,2,2        | 1.77 | 0           | 0,1,1       | 0.00 | -           |
| 19  | PEE  | P     | 3007 | -    | 48,48,50     | 1.22 | 6 (12%)     | 53,53,55    | 0.91 | 5 (9%)      |
| 21  | GOL  | P     | 3008 | -    | 5,5,5        | 1.15 | 0           | 5,5,5       | 0.62 | 0           |
| 11  | BHG  | P     | 3010 | -    | 18,18,18     | 1.74 | 5 (27%)     | 23,23,23    | 0.71 | 0           |
| 13  | PO4  | P     | 3013 | -    | 4,4,4        | 0.67 | 0           | 6,6,6       | 0.30 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | HEM  | P     | 501  | 3    | 42,50,50     | 2.87 | 11 (26%) | 27,82,82    | 1.31 | 3 (11%)  |
| 14  | HEM  | P     | 502  | 3    | 42,50,50     | 2.77 | 13 (30%) | 27,82,82    | 1.38 | 3 (11%)  |
| 19  | PEE  | Q     | 3006 | -    | 50,50,50     | 1.19 | 6 (12%)  | 55,55,55    | 0.91 | 5 (9%)   |
| 15  | HEC  | Q     | 501  | 4    | 50,50,50     | 2.94 | 6 (12%)  | 56,82,82    | 1.95 | 10 (17%) |
| 21  | GOL  | R     | 4005 | -    | 5,5,5        | 1.17 | 0        | 5,5,5       | 0.63 | 0        |
| 11  | BHG  | R     | 4007 | -    | 18,18,18     | 1.77 | 4 (22%)  | 23,23,23    | 0.72 | 0        |
| 16  | FES  | R     | 501  | 5    | 0,4,4        | 0.00 | -        | 0,4,4       | 0.00 | -        |
| 11  | BHG  | S     | 2011 | -    | 18,18,18     | 1.71 | 3 (16%)  | 23,23,23    | 0.74 | 0        |
| 13  | PO4  | S     | 3012 | -    | 4,4,4        | 0.65 | 0        | 6,6,6       | 0.30 | 0        |
| 18  | CDL  | T     | 3004 | -    | 46,48,99     | 1.16 | 4 (8%)   | 56,60,111   | 1.43 | 6 (10%)  |

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   |
|-----|------|-------|------|------|---------|--------------|---------|
| 13  | PO4  | A     | 2013 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 11  | BHG  | A     | 4004 | -    | 1/1/5/5 | 0/9/29/29    | 0/1/1/1 |
| 12  | AZI  | A     | 4011 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 21  | GOL  | B     | 2009 | -    | -       | 0/4/4/4      | 0/0/0/0 |
| 17  | SMA  | C     | 2001 | -    | -       | 0/33/34/34   | 0/2/2/2 |
| 20  | ANY  | C     | 2002 | -    | -       | 0/50/52/56   | 0/2/2/2 |
| 12  | AZI  | C     | 2005 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 19  | PEE  | C     | 2007 | -    | -       | 0/52/52/54   | 0/0/0/0 |
| 21  | GOL  | C     | 2008 | -    | -       | 0/4/4/4      | 0/0/0/0 |
| 11  | BHG  | C     | 2010 | -    | 1/1/5/5 | 0/9/29/29    | 0/1/1/1 |
| 11  | BHG  | C     | 4002 | -    | 1/1/5/5 | 0/9/29/29    | 0/1/1/1 |
| 21  | GOL  | C     | 4006 | -    | -       | 0/4/4/4      | 0/0/0/0 |
| 13  | PO4  | C     | 4008 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 14  | HEM  | C     | 501  | 3    | -       | 0/14/114/114 | 0/0/8/8 |
| 14  | HEM  | C     | 502  | 3    | -       | 0/14/114/114 | 0/0/8/8 |
| 18  | CDL  | D     | 2003 | -    | -       | 0/43/43/110  | 0/0/0/0 |
| 19  | PEE  | D     | 2006 | -    | -       | 0/29/29/54   | 0/0/0/0 |
| 11  | BHG  | D     | 4003 | -    | 1/1/5/5 | 0/9/29/29    | 0/1/1/1 |
| 15  | HEC  | D     | 501  | 4    | -       | 0/10/54/54   | 0/0/8/8 |
| 16  | FES  | E     | 501  | 5    | -       | 0/0/4/4      | 0/1/1/1 |
| 13  | PO4  | F     | 2012 | -    | -       | 0/0/0/0      | 0/0/0/0 |
| 11  | BHG  | F     | 3011 | -    | 1/1/5/5 | 0/9/29/29    | 0/1/1/1 |
| 11  | BHG  | F     | 4001 | -    | 1/1/5/5 | 0/9/29/29    | 0/1/1/1 |
| 18  | CDL  | G     | 2004 | -    | 1/1/9/9 | 0/52/52/110  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 12  | AZI  | G     | 4009 | -    | -         | 0/0/0/0      | 0/0/0/0 |
| 21  | GOL  | O     | 3009 | -    | -         | 0/4/4/4      | 0/0/0/0 |
| 12  | AZI  | O     | 4010 | -    | -         | 0/0/0/0      | 0/0/0/0 |
| 17  | SMA  | P     | 3001 | -    | -         | 0/33/34/34   | 0/2/2/2 |
| 20  | ANY  | P     | 3002 | -    | 1/1/10/13 | 0/50/52/56   | 0/2/2/2 |
| 18  | CDL  | P     | 3003 | -    | -         | 0/43/43/110  | 0/0/0/0 |
| 12  | AZI  | P     | 3005 | -    | -         | 0/0/0/0      | 0/0/0/0 |
| 19  | PEE  | P     | 3007 | -    | -         | 0/52/52/54   | 0/0/0/0 |
| 21  | GOL  | P     | 3008 | -    | -         | 0/4/4/4      | 0/0/0/0 |
| 11  | BHG  | P     | 3010 | -    | 1/1/5/5   | 0/9/29/29    | 0/1/1/1 |
| 13  | PO4  | P     | 3013 | -    | -         | 0/0/0/0      | 0/0/0/0 |
| 14  | HEM  | P     | 501  | 3    | -         | 0/14/114/114 | 0/0/8/8 |
| 14  | HEM  | P     | 502  | 3    | -         | 0/14/114/114 | 0/0/8/8 |
| 19  | PEE  | Q     | 3006 | -    | -         | 0/54/54/54   | 0/0/0/0 |
| 15  | HEC  | Q     | 501  | 4    | -         | 0/10/54/54   | 0/0/8/8 |
| 21  | GOL  | R     | 4005 | -    | -         | 0/4/4/4      | 0/0/0/0 |
| 11  | BHG  | R     | 4007 | -    | 1/1/5/5   | 0/9/29/29    | 0/1/1/1 |
| 16  | FES  | R     | 501  | 5    | -         | 0/0/4/4      | 0/1/1/1 |
| 11  | BHG  | S     | 2011 | -    | 1/1/5/5   | 0/9/29/29    | 0/1/1/1 |
| 13  | PO4  | S     | 3012 | -    | -         | 0/0/0/0      | 0/0/0/0 |
| 18  | CDL  | T     | 3004 | -    | 1/1/9/9   | 0/57/57/110  | 0/0/0/0 |

All (173) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 15  | D     | 501  | HEC  | C3C-CAC | 14.59  | 1.54        | 1.34     |
| 15  | D     | 501  | HEC  | C3B-CAB | 14.14  | 1.53        | 1.34     |
| 15  | Q     | 501  | HEC  | C3C-CAC | 12.63  | 1.51        | 1.34     |
| 15  | Q     | 501  | HEC  | C3B-CAB | 12.16  | 1.51        | 1.34     |
| 14  | C     | 502  | HEM  | C3C-C2C | -10.92 | 1.36        | 1.45     |
| 14  | P     | 501  | HEM  | C3B-C2B | -10.19 | 1.35        | 1.45     |
| 14  | C     | 501  | HEM  | C3C-C2C | -9.80  | 1.37        | 1.45     |
| 20  | C     | 2002 | ANY  | C19-C18 | -9.43  | 1.51        | 1.55     |
| 20  | P     | 3002 | ANY  | C19-C18 | -9.15  | 1.51        | 1.55     |
| 14  | P     | 501  | HEM  | C3C-C2C | -8.90  | 1.38        | 1.45     |
| 14  | C     | 502  | HEM  | C3B-C2B | -8.84  | 1.37        | 1.45     |
| 14  | P     | 502  | HEM  | C3C-C2C | -8.35  | 1.38        | 1.45     |
| 14  | P     | 502  | HEM  | C3B-C2B | -8.01  | 1.37        | 1.45     |
| 14  | C     | 501  | HEM  | C3B-C2B | -7.61  | 1.38        | 1.45     |
| 15  | Q     | 501  | HEC  | C3C-C2C | -6.72  | 1.33        | 1.40     |
| 17  | P     | 3001 | SMA  | C4-C4A  | 6.70   | 1.50        | 1.41     |
| 17  | C     | 2001 | SMA  | C4-C4A  | 6.50   | 1.50        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | Q     | 501  | HEC  | C3B-C2B | -5.83 | 1.34        | 1.40     |
| 20  | P     | 3002 | ANY  | C8-N1   | 5.60  | 1.40        | 1.34     |
| 14  | C     | 502  | HEM  | CMB-C2B | 5.33  | 1.54        | 1.45     |
| 14  | C     | 502  | HEM  | CMD-C2D | 5.08  | 1.53        | 1.45     |
| 15  | D     | 501  | HEC  | C3C-C2C | -5.06 | 1.35        | 1.40     |
| 15  | D     | 501  | HEC  | C3B-C2B | -4.99 | 1.35        | 1.40     |
| 14  | P     | 502  | HEM  | CMB-C2B | 4.86  | 1.53        | 1.45     |
| 14  | P     | 502  | HEM  | CBB-CAB | 4.86  | 1.56        | 1.29     |
| 17  | P     | 3001 | SMA  | O1-C2   | 4.85  | 1.41        | 1.35     |
| 20  | C     | 2002 | ANY  | C8-N1   | 4.83  | 1.40        | 1.34     |
| 14  | P     | 501  | HEM  | CBB-CAB | 4.82  | 1.56        | 1.29     |
| 14  | C     | 501  | HEM  | CMB-C2B | 4.81  | 1.53        | 1.45     |
| 17  | C     | 2001 | SMA  | O1-C2   | 4.77  | 1.40        | 1.35     |
| 14  | P     | 502  | HEM  | CMC-C2C | 4.74  | 1.53        | 1.45     |
| 14  | C     | 501  | HEM  | CBC-CAC | 4.74  | 1.56        | 1.29     |
| 14  | P     | 501  | HEM  | CMC-C2C | 4.69  | 1.53        | 1.45     |
| 14  | P     | 501  | HEM  | CMB-C2B | 4.56  | 1.53        | 1.45     |
| 11  | C     | 4002 | BHG  | O1-C1   | 4.55  | 1.48        | 1.40     |
| 11  | S     | 2011 | BHG  | O1-C1   | 4.55  | 1.48        | 1.40     |
| 11  | D     | 4003 | BHG  | O1-C1   | 4.50  | 1.48        | 1.40     |
| 14  | P     | 501  | HEM  | CBC-CAC | 4.46  | 1.54        | 1.29     |
| 14  | C     | 502  | HEM  | CBC-CAC | 4.46  | 1.54        | 1.29     |
| 11  | F     | 4001 | BHG  | O1-C1   | 4.45  | 1.48        | 1.40     |
| 14  | P     | 502  | HEM  | CBC-CAC | 4.42  | 1.54        | 1.29     |
| 11  | C     | 2010 | BHG  | O1-C1   | 4.41  | 1.48        | 1.40     |
| 11  | R     | 4007 | BHG  | O1-C1   | 4.41  | 1.48        | 1.40     |
| 14  | C     | 501  | HEM  | CMD-C2D | 4.38  | 1.52        | 1.45     |
| 14  | C     | 501  | HEM  | CMC-C2C | 4.37  | 1.52        | 1.45     |
| 11  | P     | 3010 | BHG  | O1-C1   | 4.29  | 1.47        | 1.40     |
| 17  | C     | 2001 | SMA  | C20-C19 | 4.28  | 1.35        | 1.33     |
| 11  | F     | 3011 | BHG  | O1-C1   | 4.26  | 1.47        | 1.40     |
| 14  | P     | 502  | HEM  | CMD-C2D | 4.24  | 1.52        | 1.45     |
| 14  | C     | 502  | HEM  | CBB-CAB | 4.20  | 1.52        | 1.29     |
| 14  | C     | 501  | HEM  | CBB-CAB | 4.07  | 1.52        | 1.29     |
| 20  | C     | 2002 | ANY  | C2-C1   | 3.92  | 1.47        | 1.40     |
| 17  | P     | 3001 | SMA  | C20-C19 | 3.84  | 1.35        | 1.33     |
| 17  | C     | 2001 | SMA  | C4A-C8A | 3.75  | 1.46        | 1.41     |
| 20  | P     | 3002 | ANY  | C12-C11 | 3.75  | 1.60        | 1.52     |
| 20  | C     | 2002 | ANY  | C12-C11 | 3.74  | 1.60        | 1.52     |
| 14  | P     | 501  | HEM  | C3D-C2D | -3.67 | 1.34        | 1.43     |
| 20  | P     | 3002 | ANY  | C2-C1   | 3.66  | 1.46        | 1.40     |
| 14  | P     | 501  | HEM  | CMD-C2D | 3.64  | 1.51        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | P     | 3001 | SMA  | C8-C8A  | 3.60  | 1.43        | 1.41     |
| 20  | C     | 2002 | ANY  | C10-C9  | 3.45  | 1.60        | 1.54     |
| 14  | P     | 502  | HEM  | C1A-NA  | 3.42  | 1.42        | 1.36     |
| 11  | S     | 2011 | BHG  | O5-C1   | 3.41  | 1.50        | 1.41     |
| 11  | F     | 3011 | BHG  | O5-C1   | 3.40  | 1.50        | 1.41     |
| 17  | P     | 3001 | SMA  | C4-C3   | 3.40  | 1.51        | 1.41     |
| 20  | C     | 2002 | ANY  | C3-C2   | 3.36  | 1.45        | 1.39     |
| 11  | R     | 4007 | BHG  | O5-C1   | 3.34  | 1.50        | 1.41     |
| 11  | D     | 4003 | BHG  | O5-C1   | 3.32  | 1.50        | 1.41     |
| 20  | P     | 3002 | ANY  | C3-C2   | 3.29  | 1.45        | 1.39     |
| 11  | C     | 4002 | BHG  | O5-C1   | 3.26  | 1.50        | 1.41     |
| 11  | F     | 4001 | BHG  | O5-C1   | 3.26  | 1.50        | 1.41     |
| 17  | C     | 2001 | SMA  | C7-C8   | 3.24  | 1.44        | 1.40     |
| 11  | C     | 2010 | BHG  | O5-C1   | 3.22  | 1.50        | 1.41     |
| 14  | C     | 502  | HEM  | C1C-NC  | 3.19  | 1.41        | 1.33     |
| 17  | P     | 3001 | SMA  | C7-C8   | 3.15  | 1.44        | 1.40     |
| 11  | A     | 4004 | BHG  | O1-C1   | 3.15  | 1.45        | 1.40     |
| 18  | P     | 3003 | CDL  | PA1-OA5 | 3.12  | 1.57        | 1.51     |
| 11  | A     | 4004 | BHG  | O5-C1   | 3.09  | 1.49        | 1.41     |
| 11  | P     | 3010 | BHG  | O5-C1   | 3.09  | 1.49        | 1.41     |
| 17  | C     | 2001 | SMA  | C4-C3   | 3.07  | 1.50        | 1.41     |
| 19  | C     | 2007 | PEE  | O3-C30  | 3.04  | 1.42        | 1.33     |
| 14  | P     | 502  | HEM  | C3D-C2D | -3.00 | 1.35        | 1.43     |
| 18  | D     | 2003 | CDL  | PA1-OA5 | 2.98  | 1.56        | 1.51     |
| 17  | P     | 3001 | SMA  | C6-C7   | 2.94  | 1.44        | 1.38     |
| 17  | C     | 2001 | SMA  | C6-C7   | 2.94  | 1.44        | 1.38     |
| 14  | C     | 502  | HEM  | CMC-C2C | 2.92  | 1.50        | 1.45     |
| 14  | C     | 501  | HEM  | C3D-C2D | -2.92 | 1.36        | 1.43     |
| 19  | Q     | 3006 | PEE  | O3-C30  | 2.91  | 1.42        | 1.33     |
| 15  | D     | 501  | HEC  | C3C-C4C | 2.88  | 1.49        | 1.42     |
| 19  | P     | 3007 | PEE  | O3-C30  | 2.87  | 1.42        | 1.33     |
| 19  | Q     | 3006 | PEE  | C19-C18 | -2.85 | 1.34        | 1.51     |
| 15  | D     | 501  | HEC  | C1A-NA  | 2.83  | 1.40        | 1.36     |
| 14  | P     | 501  | HEM  | C4A-NA  | 2.83  | 1.41        | 1.36     |
| 14  | P     | 502  | HEM  | C1B-C2B | 2.83  | 1.47        | 1.45     |
| 19  | P     | 3007 | PEE  | C19-C18 | -2.81 | 1.34        | 1.51     |
| 17  | P     | 3001 | SMA  | C4A-C8A | 2.80  | 1.44        | 1.41     |
| 20  | P     | 3002 | ANY  | C13-C12 | 2.79  | 1.59        | 1.53     |
| 19  | Q     | 3006 | PEE  | C22-C21 | -2.78 | 1.34        | 1.51     |
| 14  | C     | 502  | HEM  | C1D-ND  | 2.77  | 1.40        | 1.33     |
| 19  | C     | 2007 | PEE  | C22-C21 | -2.76 | 1.34        | 1.51     |
| 19  | C     | 2007 | PEE  | C19-C18 | -2.75 | 1.35        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 19  | P     | 3007 | PEE  | C22-C21 | -2.74 | 1.35        | 1.51     |
| 19  | P     | 3007 | PEE  | O2-C10  | 2.73  | 1.42        | 1.34     |
| 19  | D     | 2006 | PEE  | O2-C10  | 2.72  | 1.42        | 1.34     |
| 19  | D     | 2006 | PEE  | P-O1P   | 2.72  | 1.61        | 1.51     |
| 19  | Q     | 3006 | PEE  | P-O1P   | 2.70  | 1.61        | 1.51     |
| 20  | P     | 3002 | ANY  | C7-N2   | 2.69  | 1.40        | 1.34     |
| 19  | P     | 3007 | PEE  | P-O1P   | 2.69  | 1.61        | 1.51     |
| 20  | C     | 2002 | ANY  | O8-C21  | 2.68  | 1.40        | 1.34     |
| 20  | C     | 2002 | ANY  | O5-C14  | 2.67  | 1.40        | 1.34     |
| 17  | C     | 2001 | SMA  | C8-C8A  | 2.65  | 1.43        | 1.41     |
| 19  | Q     | 3006 | PEE  | O2-C10  | 2.65  | 1.42        | 1.34     |
| 11  | A     | 4004 | BHG  | C4-C5   | 2.64  | 1.58        | 1.53     |
| 20  | P     | 3002 | ANY  | C10-C9  | 2.63  | 1.58        | 1.54     |
| 14  | P     | 502  | HEM  | C4C-NC  | 2.62  | 1.40        | 1.33     |
| 19  | D     | 2006 | PEE  | O3-C30  | 2.57  | 1.41        | 1.33     |
| 19  | C     | 2007 | PEE  | O2-C10  | 2.55  | 1.42        | 1.34     |
| 19  | D     | 2006 | PEE  | C3-C2   | 2.54  | 1.57        | 1.50     |
| 11  | C     | 4002 | BHG  | C4-C5   | 2.54  | 1.58        | 1.53     |
| 15  | Q     | 501  | HEC  | C3C-C4C | 2.54  | 1.48        | 1.42     |
| 11  | P     | 3010 | BHG  | C4-C5   | 2.51  | 1.58        | 1.53     |
| 19  | P     | 3007 | PEE  | C46-C45 | -2.50 | 1.54        | 1.55     |
| 14  | P     | 501  | HEM  | C1C-NC  | 2.48  | 1.40        | 1.33     |
| 11  | R     | 4007 | BHG  | C4-C5   | 2.48  | 1.58        | 1.53     |
| 20  | C     | 2002 | ANY  | C13-C12 | 2.47  | 1.58        | 1.53     |
| 14  | P     | 502  | HEM  | C1C-NC  | 2.42  | 1.39        | 1.33     |
| 17  | P     | 3001 | SMA  | O1-C8A  | 2.42  | 1.40        | 1.36     |
| 14  | C     | 501  | HEM  | C1D-ND  | 2.40  | 1.39        | 1.33     |
| 20  | P     | 3002 | ANY  | O5-C14  | 2.40  | 1.39        | 1.34     |
| 20  | P     | 3002 | ANY  | O8-C21  | 2.39  | 1.39        | 1.34     |
| 11  | F     | 4001 | BHG  | C4-C5   | 2.38  | 1.58        | 1.53     |
| 14  | C     | 502  | HEM  | C1A-NA  | 2.36  | 1.40        | 1.36     |
| 18  | T     | 3004 | CDL  | OB8-CB6 | -2.33 | 1.39        | 1.45     |
| 12  | A     | 4011 | AZI  | N1-N2   | -2.33 | 1.13        | 1.21     |
| 20  | C     | 2002 | ANY  | C5-C6   | 2.33  | 1.43        | 1.39     |
| 11  | F     | 3011 | BHG  | C4-C5   | 2.32  | 1.58        | 1.53     |
| 11  | D     | 4003 | BHG  | C4-C5   | 2.31  | 1.58        | 1.53     |
| 19  | D     | 2006 | PEE  | C1-C2   | 2.29  | 1.57        | 1.50     |
| 14  | P     | 502  | HEM  | C4D-ND  | 2.29  | 1.39        | 1.33     |
| 20  | P     | 3002 | ANY  | C5-C6   | 2.26  | 1.43        | 1.39     |
| 19  | C     | 2007 | PEE  | P-O1P   | 2.25  | 1.59        | 1.51     |
| 11  | C     | 4002 | BHG  | O5-C5   | 2.24  | 1.50        | 1.44     |
| 18  | T     | 3004 | CDL  | O1-C1   | 2.24  | 1.50        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | S     | 2011 | BHG  | O5-C5   | 2.24  | 1.50        | 1.44     |
| 14  | C     | 502  | HEM  | C1A-C2A | 2.23  | 1.47        | 1.43     |
| 11  | R     | 4007 | BHG  | O5-C5   | 2.23  | 1.49        | 1.44     |
| 20  | C     | 2002 | ANY  | C7-N2   | 2.22  | 1.39        | 1.34     |
| 14  | C     | 502  | HEM  | C4A-C3A | 2.22  | 1.47        | 1.43     |
| 14  | C     | 502  | HEM  | C3C-C4C | 2.22  | 1.47        | 1.45     |
| 18  | G     | 2004 | CDL  | O1-C1   | 2.21  | 1.50        | 1.43     |
| 18  | T     | 3004 | CDL  | CB3-CB4 | 2.21  | 1.56        | 1.50     |
| 11  | D     | 4003 | BHG  | O5-C5   | 2.20  | 1.49        | 1.44     |
| 14  | C     | 501  | HEM  | C4D-ND  | 2.20  | 1.39        | 1.33     |
| 18  | T     | 3004 | CDL  | OA8-CA6 | -2.17 | 1.40        | 1.45     |
| 17  | C     | 2001 | SMA  | O1-C8A  | 2.16  | 1.40        | 1.36     |
| 11  | F     | 4001 | BHG  | O5-C5   | 2.13  | 1.49        | 1.44     |
| 18  | D     | 2003 | CDL  | O1-C1   | 2.11  | 1.50        | 1.43     |
| 14  | C     | 501  | HEM  | C3C-C4C | 2.11  | 1.47        | 1.45     |
| 11  | C     | 2010 | BHG  | C4-C5   | 2.10  | 1.57        | 1.53     |
| 15  | Q     | 501  | HEC  | C4D-ND  | 2.09  | 1.39        | 1.36     |
| 18  | G     | 2004 | CDL  | OA8-CA6 | -2.07 | 1.40        | 1.45     |
| 19  | Q     | 3006 | PEE  | C3-C2   | 2.07  | 1.56        | 1.50     |
| 11  | F     | 3011 | BHG  | O5-C5   | 2.07  | 1.49        | 1.44     |
| 20  | P     | 3002 | ANY  | C6-C1   | 2.06  | 1.45        | 1.41     |
| 11  | C     | 2010 | BHG  | O5-C5   | 2.06  | 1.49        | 1.44     |
| 12  | A     | 4011 | AZI  | N3-N2   | -2.06 | 1.14        | 1.21     |
| 18  | G     | 2004 | CDL  | OB8-CB6 | -2.05 | 1.40        | 1.45     |
| 14  | P     | 501  | HEM  | C4C-NC  | 2.04  | 1.38        | 1.33     |
| 11  | P     | 3010 | BHG  | C1-C2   | 2.04  | 1.58        | 1.52     |
| 19  | D     | 2006 | PEE  | C31-C30 | 2.04  | 1.56        | 1.50     |
| 11  | P     | 3010 | BHG  | O5-C5   | 2.03  | 1.49        | 1.44     |
| 18  | P     | 3003 | CDL  | O1-C1   | 2.01  | 1.49        | 1.43     |
| 12  | C     | 2005 | AZI  | N1-N2   | -2.00 | 1.14        | 1.21     |

All (105) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | Q     | 501  | HEC  | CBB-CAB-C3B | -8.74 | 108.25      | 127.36   |
| 15  | D     | 501  | HEC  | CBC-CAC-C3C | -7.46 | 111.05      | 127.36   |
| 15  | D     | 501  | HEC  | CBB-CAB-C3B | -7.28 | 111.45      | 127.36   |
| 17  | P     | 3001 | SMA  | C9-C2-C3    | 6.51  | 128.27      | 120.42   |
| 15  | Q     | 501  | HEC  | CBC-CAC-C3C | -5.99 | 114.27      | 127.36   |
| 17  | C     | 2001 | SMA  | C9-C2-C3    | 5.89  | 127.53      | 120.42   |
| 15  | D     | 501  | HEC  | C2C-C1C-NC  | 5.40  | 113.11      | 109.50   |
| 17  | C     | 2001 | SMA  | C3-C4-C4A   | -4.88 | 114.79      | 121.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | P     | 3001 | SMA  | C3-C4-C4A   | -4.53 | 115.25      | 121.30   |
| 18  | G     | 2004 | CDL  | OB4-PB2-OB3 | -4.50 | 105.28      | 118.70   |
| 18  | T     | 3004 | CDL  | OB4-PB2-OB3 | -4.49 | 105.30      | 118.70   |
| 18  | T     | 3004 | CDL  | OA4-PA1-OA3 | -4.45 | 105.42      | 118.70   |
| 18  | G     | 2004 | CDL  | OA4-PA1-OA3 | -4.43 | 105.47      | 118.70   |
| 18  | D     | 2003 | CDL  | OB4-PB2-OB3 | -4.43 | 105.48      | 118.70   |
| 18  | P     | 3003 | CDL  | OB4-PB2-OB3 | -4.36 | 105.70      | 118.70   |
| 18  | T     | 3004 | CDL  | CB4-OB6-CB5 | -4.26 | 109.82      | 117.68   |
| 17  | P     | 3001 | SMA  | C9-C10-C11  | -4.14 | 108.65      | 114.60   |
| 14  | P     | 502  | HEM  | C4A-NA-C1A  | -4.12 | 102.80      | 107.93   |
| 14  | C     | 502  | HEM  | C3A-C4A-NA  | 4.06  | 112.21      | 109.50   |
| 14  | C     | 502  | HEM  | C4A-NA-C1A  | -3.99 | 102.96      | 107.93   |
| 20  | P     | 3002 | ANY  | O6-C14-C13  | 3.99  | 130.73      | 125.71   |
| 15  | Q     | 501  | HEC  | C2C-C1C-NC  | 3.90  | 112.10      | 109.50   |
| 20  | P     | 3002 | ANY  | O7-C20-C9   | 3.88  | 130.37      | 125.45   |
| 15  | D     | 501  | HEC  | CMB-C2B-C3B | -3.75 | 122.72      | 126.22   |
| 18  | G     | 2004 | CDL  | CB4-OB6-CB5 | -3.74 | 110.77      | 117.68   |
| 17  | C     | 2001 | SMA  | C9-C10-C11  | -3.73 | 109.23      | 114.60   |
| 20  | C     | 2002 | ANY  | O7-C20-C9   | 3.73  | 130.19      | 125.45   |
| 14  | P     | 502  | HEM  | C3A-C4A-NA  | 3.65  | 111.94      | 109.50   |
| 20  | C     | 2002 | ANY  | O2-C8-N1    | -3.51 | 121.82      | 125.85   |
| 20  | C     | 2002 | ANY  | O5-C14-O6   | -3.42 | 119.58      | 124.19   |
| 20  | C     | 2002 | ANY  | O6-C14-C13  | 3.41  | 130.00      | 125.71   |
| 14  | P     | 501  | HEM  | C4A-NA-C1A  | -3.40 | 103.70      | 107.93   |
| 20  | P     | 3002 | ANY  | O2-C8-N1    | -3.36 | 121.99      | 125.85   |
| 20  | C     | 2002 | ANY  | C25-C22-C21 | 3.36  | 119.39      | 111.99   |
| 20  | P     | 3002 | ANY  | O5-C14-O6   | -3.34 | 119.69      | 124.19   |
| 18  | D     | 2003 | CDL  | OA4-PA1-OA3 | -3.26 | 105.18      | 112.74   |
| 14  | P     | 501  | HEM  | C3A-C4A-NA  | 3.19  | 111.63      | 109.50   |
| 15  | Q     | 501  | HEC  | C1A-C2A-C3A | 3.18  | 109.26      | 106.70   |
| 18  | T     | 3004 | CDL  | CA4-OA6-CA5 | -3.17 | 110.42      | 117.86   |
| 18  | P     | 3003 | CDL  | OA4-PA1-OA3 | -3.14 | 105.47      | 112.74   |
| 15  | Q     | 501  | HEC  | C4D-ND-C1D  | -2.92 | 104.31      | 107.12   |
| 18  | G     | 2004 | CDL  | CA4-OA6-CA5 | -2.89 | 111.06      | 117.86   |
| 18  | T     | 3004 | CDL  | CB6-OB8-CB7 | -2.85 | 111.57      | 116.47   |
| 14  | C     | 502  | HEM  | CBD-CAD-C3D | -2.81 | 108.42      | 114.51   |
| 18  | G     | 2004 | CDL  | CA6-CA4-CA3 | -2.77 | 105.50      | 111.86   |
| 18  | G     | 2004 | CDL  | CB6-OB8-CB7 | -2.74 | 111.76      | 116.47   |
| 18  | D     | 2003 | CDL  | CB4-OB6-CB5 | -2.73 | 111.44      | 117.86   |
| 14  | P     | 502  | HEM  | CBD-CAD-C3D | -2.73 | 108.60      | 114.51   |
| 18  | P     | 3003 | CDL  | CB6-CB4-CB3 | -2.69 | 105.68      | 111.86   |
| 17  | C     | 2001 | SMA  | O1-C2-C3    | 2.68  | 123.44      | 120.32   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19  | C     | 2007 | PEE  | O4P-C4-C5   | 2.67  | 113.68      | 109.37   |
| 14  | C     | 501  | HEM  | C4A-NA-C1A  | -2.66 | 104.62      | 107.93   |
| 14  | C     | 501  | HEM  | C4A-C3A-C2A | -2.65 | 105.15      | 107.00   |
| 17  | P     | 3001 | SMA  | O1-C2-C9    | -2.65 | 108.35      | 112.08   |
| 15  | Q     | 501  | HEC  | C2B-C1B-NB  | 2.64  | 111.26      | 109.50   |
| 14  | C     | 501  | HEM  | C3A-C4A-NA  | 2.63  | 111.26      | 109.50   |
| 17  | P     | 3001 | SMA  | O1-C2-C3    | 2.63  | 123.37      | 120.32   |
| 19  | Q     | 3006 | PEE  | C20-C19-C18 | 2.62  | 128.49      | 114.56   |
| 14  | P     | 501  | HEM  | C4A-C3A-C2A | -2.60 | 105.19      | 107.00   |
| 18  | D     | 2003 | CDL  | CB6-CB4-CB3 | -2.60 | 105.89      | 111.86   |
| 18  | P     | 3003 | CDL  | CB4-OB6-CB5 | -2.54 | 111.90      | 117.86   |
| 19  | P     | 3007 | PEE  | C19-C18-C17 | 2.53  | 127.97      | 114.56   |
| 19  | P     | 3007 | PEE  | O4P-C4-C5   | 2.51  | 113.43      | 109.37   |
| 19  | C     | 2007 | PEE  | C19-C18-C17 | 2.50  | 127.86      | 114.56   |
| 15  | Q     | 501  | HEC  | C4A-C3A-C2A | -2.50 | 103.92      | 106.69   |
| 19  | C     | 2007 | PEE  | C20-C19-C18 | 2.49  | 127.78      | 114.56   |
| 15  | D     | 501  | HEC  | C4C-NC-C1C  | -2.49 | 103.21      | 106.77   |
| 19  | C     | 2007 | PEE  | C23-C22-C21 | 2.48  | 127.74      | 114.56   |
| 19  | P     | 3007 | PEE  | C20-C19-C18 | 2.48  | 127.72      | 114.56   |
| 15  | Q     | 501  | HEC  | C3A-C4A-NA  | 2.47  | 112.77      | 109.32   |
| 15  | D     | 501  | HEC  | C4D-ND-C1D  | -2.47 | 104.74      | 107.12   |
| 19  | P     | 3007 | PEE  | C23-C22-C21 | 2.47  | 127.67      | 114.56   |
| 17  | C     | 2001 | SMA  | C3M-C3-C4   | -2.45 | 116.94      | 121.04   |
| 17  | C     | 2001 | SMA  | C4-C3-C2    | 2.45  | 121.19      | 117.77   |
| 15  | D     | 501  | HEC  | C3A-C4A-NA  | 2.42  | 112.69      | 109.32   |
| 19  | D     | 2006 | PEE  | O4P-C4-C5   | 2.42  | 113.28      | 109.37   |
| 19  | Q     | 3006 | PEE  | C22-C21-C20 | 2.40  | 127.32      | 114.56   |
| 20  | P     | 3002 | ANY  | O5-C10-C9   | 2.36  | 112.59      | 106.17   |
| 19  | Q     | 3006 | PEE  | C19-C18-C17 | 2.36  | 127.07      | 114.56   |
| 18  | G     | 2004 | CDL  | OA6-CA5-C11 | 2.35  | 113.42      | 110.46   |
| 18  | G     | 2004 | CDL  | CB6-CB4-CB3 | -2.35 | 106.47      | 111.86   |
| 19  | Q     | 3006 | PEE  | O4P-C4-C5   | 2.33  | 113.13      | 109.37   |
| 20  | P     | 3002 | ANY  | C10-O5-C14  | 2.31  | 121.90      | 117.25   |
| 20  | P     | 3002 | ANY  | O4-C20-O7   | -2.30 | 121.09      | 124.19   |
| 18  | D     | 2003 | CDL  | OA4-PA1-OA2 | 2.28  | 112.81      | 105.91   |
| 20  | C     | 2002 | ANY  | C10-O5-C14  | 2.26  | 121.80      | 117.25   |
| 15  | Q     | 501  | HEC  | C2D-C1D-ND  | 2.25  | 111.00      | 109.50   |
| 19  | P     | 3007 | PEE  | C22-C21-C20 | 2.24  | 126.44      | 114.56   |
| 15  | Q     | 501  | HEC  | C4C-NC-C1C  | -2.23 | 103.58      | 106.77   |
| 19  | C     | 2007 | PEE  | C22-C21-C20 | 2.21  | 126.32      | 114.56   |
| 18  | P     | 3003 | CDL  | OA2-PA1-OA3 | 2.19  | 111.85      | 105.95   |
| 17  | C     | 2001 | SMA  | O1-C2-C9    | -2.18 | 109.01      | 112.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | P     | 3001 | SMA  | C3M-C3-C4   | -2.11 | 117.51      | 121.04   |
| 18  | P     | 3003 | CDL  | OA4-PA1-OA2 | 2.11  | 112.30      | 105.91   |
| 20  | C     | 2002 | ANY  | O5-C10-C9   | 2.11  | 111.93      | 106.17   |
| 17  | P     | 3001 | SMA  | C10-C9-C2   | 2.11  | 118.64      | 113.35   |
| 18  | D     | 2003 | CDL  | OA2-PA1-OA3 | 2.11  | 111.63      | 105.95   |
| 17  | P     | 3001 | SMA  | C4-C3-C2    | 2.10  | 120.71      | 117.77   |
| 19  | Q     | 3006 | PEE  | C23-C22-C21 | 2.10  | 125.74      | 114.56   |
| 20  | C     | 2002 | ANY  | O8-C21-O9   | -2.09 | 119.67      | 123.85   |
| 11  | C     | 4002 | BHG  | C1'-O1-C1   | 2.08  | 117.58      | 113.91   |
| 19  | D     | 2006 | PEE  | O3-C3-C2    | 2.06  | 114.22      | 108.80   |
| 20  | P     | 3002 | ANY  | O8-C21-O9   | -2.06 | 119.72      | 123.85   |
| 18  | T     | 3004 | CDL  | CA6-CA4-CA3 | -2.05 | 107.15      | 111.86   |
| 20  | P     | 3002 | ANY  | O9-C21-C22  | 2.01  | 129.93      | 124.14   |

All (12) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 11  | D     | 4003 | BHG  | C4   |
| 11  | P     | 3010 | BHG  | C4   |
| 18  | T     | 3004 | CDL  | CA4  |
| 11  | S     | 2011 | BHG  | C4   |
| 18  | G     | 2004 | CDL  | CA4  |
| 20  | P     | 3002 | ANY  | C22  |
| 11  | A     | 4004 | BHG  | C4   |
| 11  | F     | 3011 | BHG  | C4   |
| 11  | F     | 4001 | BHG  | C4   |
| 11  | C     | 4002 | BHG  | C4   |
| 11  | C     | 2010 | BHG  | C4   |
| 11  | R     | 4007 | BHG  | C4   |

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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%)   | 0.25   | 9 (2%) 62 67   | 25, 39, 60, 115       | 0      |
| 1   | N     | 441/446 (98%)   | 0.37   | 15 (3%) 43 47  | 33, 52, 76, 139       | 1 (0%) |
| 2   | B     | 424/439 (96%)   | 0.21   | 8 (1%) 64 68   | 29, 42, 66, 94        | 0      |
| 2   | O     | 424/439 (96%)   | 0.29   | 12 (2%) 50 55  | 30, 47, 70, 124       | 0      |
| 3   | C     | 365/379 (96%)   | 0.04   | 3 (0%) 83 87   | 23, 36, 53, 108       | 0      |
| 3   | P     | 365/379 (96%)   | 0.06   | 3 (0%) 83 87   | 29, 39, 53, 106       | 0      |
| 4   | D     | 241/241 (100%)  | 0.10   | 1 (0%) 90 92   | 31, 44, 64, 82        | 0      |
| 4   | Q     | 241/241 (100%)  | 0.14   | 3 (1%) 75 80   | 35, 48, 67, 89        | 0      |
| 5   | E     | 196/196 (100%)  | 1.20   | 48 (24%) 1 1   | 35, 62, 106, 111      | 0      |
| 5   | R     | 196/196 (100%)  | 0.33   | 6 (3%) 47 52   | 34, 51, 77, 95        | 0      |
| 6   | F     | 99/110 (90%)    | 0.10   | 2 (2%) 62 67   | 27, 40, 69, 79        | 0      |
| 6   | S     | 99/110 (90%)    | 0.26   | 4 (4%) 36 41   | 33, 42, 80, 102       | 0      |
| 7   | G     | 75/81 (92%)     | 0.49   | 5 (6%) 17 19   | 29, 53, 76, 89        | 0      |
| 7   | T     | 76/81 (93%)     | 0.83   | 12 (15%) 3 3   | 37, 63, 93, 95        | 0      |
| 8   | H     | 66/78 (84%)     | 0.30   | 2 (3%) 48 53   | 43, 59, 77, 81        | 0      |
| 8   | U     | 66/78 (84%)     | 0.92   | 9 (13%) 4 4    | 50, 66, 89, 104       | 0      |
| 9   | I     | 43/78 (55%)     | 1.63   | 15 (34%) 1 1   | 34, 65, 84, 89        | 0      |
| 9   | V     | 43/78 (55%)     | 2.41   | 19 (44%) 1 1   | 38, 72, 86, 91        | 0      |
| 10  | J     | 33/62 (53%)     | 1.05   | 5 (15%) 3 3    | 37, 54, 115, 130      | 0      |
| 10  | W     | 62/62 (100%)    | 1.99   | 22 (35%) 1 1   | 44, 74, 129, 144      | 0      |
| All | All   | 3997/4220 (94%) | 0.36   | 203 (5%) 27 30 | 23, 45, 81, 144       | 1 (0%) |

All (203) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 10  | J     | 62  | LYS  | 12.8 |
| 10  | W     | 2   | ALA  | 10.6 |
| 7   | G     | 75  | ALA  | 10.4 |
| 10  | W     | 12  | LEU  | 9.9  |
| 1   | N     | 227 | ALA  | 9.9  |
| 5   | E     | 76  | ILE  | 8.8  |
| 5   | E     | 195 | VAL  | 8.8  |
| 10  | W     | 1   | VAL  | 8.5  |
| 2   | B     | 232 | LEU  | 8.3  |
| 10  | W     | 25  | VAL  | 8.0  |
| 9   | V     | 41  | PRO  | 7.7  |
| 10  | W     | 5   | LEU  | 7.6  |
| 5   | E     | 187 | PHE  | 7.6  |
| 10  | W     | 9   | LEU  | 7.5  |
| 9   | V     | 50  | LEU  | 7.5  |
| 10  | J     | 31  | PHE  | 7.4  |
| 3   | C     | 17  | ALA  | 6.9  |
| 2   | O     | 12  | GLU  | 6.8  |
| 5   | E     | 194 | ILE  | 6.8  |
| 9   | V     | 36  | ALA  | 6.7  |
| 2   | B     | 233 | SER  | 6.3  |
| 2   | B     | 230 | LEU  | 6.3  |
| 10  | W     | 3   | PRO  | 6.2  |
| 1   | N     | 226 | ASP  | 6.2  |
| 9   | V     | 38  | SER  | 6.2  |
| 9   | I     | 49  | VAL  | 6.2  |
| 5   | E     | 127 | VAL  | 6.1  |
| 9   | I     | 50  | LEU  | 6.1  |
| 2   | O     | 17  | VAL  | 6.0  |
| 5   | E     | 78  | LEU  | 6.0  |
| 7   | T     | 76  | ALA  | 5.9  |
| 7   | T     | 1   | GLY  | 5.8  |
| 10  | W     | 13  | LEU  | 5.8  |
| 5   | E     | 132 | TRP  | 5.7  |
| 5   | E     | 71  | MET  | 5.5  |
| 1   | A     | 2   | ALA  | 5.4  |
| 9   | V     | 42  | VAL  | 5.4  |
| 5   | E     | 193 | VAL  | 5.3  |
| 9   | I     | 78  | TYR  | 5.2  |
| 3   | C     | 16  | ASN  | 5.2  |
| 10  | J     | 32  | GLU  | 5.0  |
| 9   | V     | 33  | ALA  | 4.9  |
| 7   | T     | 30  | PHE  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 10  | W     | 6   | THR  | 4.7  |
| 1   | N     | 229 | PRO  | 4.7  |
| 1   | A     | 226 | ASP  | 4.7  |
| 1   | N     | 222 | THR  | 4.7  |
| 10  | J     | 30  | PHE  | 4.6  |
| 5   | E     | 186 | GLU  | 4.4  |
| 5   | E     | 112 | VAL  | 4.4  |
| 2   | O     | 21  | PRO  | 4.4  |
| 1   | A     | 225 | GLU  | 4.4  |
| 10  | J     | 61  | ASN  | 4.3  |
| 5   | R     | 70  | ALA  | 4.3  |
| 1   | N     | 2   | ALA  | 4.2  |
| 1   | N     | 365 | LEU  | 4.2  |
| 6   | S     | 12  | TRP  | 4.2  |
| 10  | W     | 26  | VAL  | 4.2  |
| 5   | E     | 84  | GLY  | 4.1  |
| 9   | V     | 78  | TYR  | 4.1  |
| 5   | E     | 192 | MET  | 4.1  |
| 2   | B     | 439 | LEU  | 4.0  |
| 5   | E     | 196 | GLY  | 4.0  |
| 9   | V     | 37  | THR  | 4.0  |
| 10  | W     | 8   | ARG  | 4.0  |
| 9   | V     | 48  | SER  | 4.0  |
| 8   | U     | 51  | GLU  | 4.0  |
| 5   | E     | 134 | ILE  | 3.9  |
| 1   | A     | 227 | ALA  | 3.9  |
| 5   | E     | 83  | GLU  | 3.9  |
| 2   | B     | 12  | GLU  | 3.9  |
| 10  | W     | 21  | ALA  | 3.9  |
| 2   | O     | 19  | PRO  | 3.9  |
| 7   | T     | 29  | TYR  | 3.9  |
| 7   | G     | 30  | PHE  | 3.9  |
| 8   | U     | 49  | GLN  | 3.8  |
| 5   | E     | 81  | ILE  | 3.8  |
| 5   | R     | 27  | GLU  | 3.7  |
| 5   | E     | 89  | PHE  | 3.7  |
| 10  | W     | 14  | PHE  | 3.7  |
| 4   | Q     | 1   | SER  | 3.7  |
| 9   | V     | 49  | VAL  | 3.7  |
| 10  | W     | 62  | LYS  | 3.7  |
| 5   | E     | 167 | ALA  | 3.6  |
| 6   | S     | 16  | ILE  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | Q     | 241 | LYS  | 3.5  |
| 7   | T     | 31  | SER  | 3.5  |
| 9   | I     | 60  | ALA  | 3.5  |
| 9   | I     | 48  | SER  | 3.5  |
| 6   | S     | 14  | GLU  | 3.5  |
| 5   | E     | 128 | LYS  | 3.5  |
| 2   | B     | 231 | GLY  | 3.4  |
| 2   | O     | 224 | LEU  | 3.4  |
| 5   | E     | 104 | LYS  | 3.4  |
| 7   | G     | 29  | TYR  | 3.4  |
| 3   | C     | 18  | PHE  | 3.3  |
| 10  | W     | 29  | LEU  | 3.3  |
| 2   | O     | 20  | HIS  | 3.2  |
| 6   | F     | 13  | LEU  | 3.2  |
| 9   | I     | 63  | PRO  | 3.2  |
| 3   | P     | 168 | PHE  | 3.2  |
| 8   | U     | 47  | ARG  | 3.1  |
| 9   | V     | 51  | CYS  | 3.1  |
| 9   | V     | 35  | PRO  | 3.1  |
| 7   | T     | 38  | LEU  | 3.1  |
| 5   | E     | 98  | VAL  | 3.1  |
| 1   | N     | 102 | LEU  | 3.0  |
| 5   | E     | 111 | ALA  | 3.0  |
| 1   | N     | 225 | GLU  | 3.0  |
| 5   | E     | 77  | LYS  | 3.0  |
| 2   | B     | 20  | HIS  | 3.0  |
| 5   | E     | 87  | MET  | 3.0  |
| 9   | V     | 54  | SER  | 3.0  |
| 8   | U     | 48  | SER  | 3.0  |
| 9   | V     | 43  | LEU  | 3.0  |
| 5   | E     | 80  | ASP  | 2.9  |
| 5   | E     | 101 | ARG  | 2.9  |
| 10  | W     | 28  | ALA  | 2.9  |
| 5   | E     | 133 | VAL  | 2.9  |
| 10  | W     | 7   | ALA  | 2.9  |
| 5   | E     | 188 | THR  | 2.9  |
| 10  | W     | 19  | THR  | 2.8  |
| 9   | I     | 62  | ARG  | 2.8  |
| 5   | E     | 103 | LYS  | 2.8  |
| 9   | V     | 63  | PRO  | 2.8  |
| 5   | E     | 129 | LYS  | 2.8  |
| 9   | I     | 70  | LEU  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8   | U     | 34  | ARG  | 2.8  |
| 9   | V     | 61  | GLY  | 2.7  |
| 8   | U     | 13  | LEU  | 2.7  |
| 4   | Q     | 144 | ARG  | 2.7  |
| 2   | O     | 215 | VAL  | 2.7  |
| 10  | W     | 20  | PHE  | 2.7  |
| 5   | E     | 114 | VAL  | 2.7  |
| 9   | I     | 32  | ALA  | 2.7  |
| 9   | I     | 42  | VAL  | 2.7  |
| 5   | E     | 96  | LEU  | 2.7  |
| 1   | N     | 8   | LEU  | 2.6  |
| 7   | T     | 32  | LYS  | 2.6  |
| 7   | T     | 28  | HIS  | 2.6  |
| 7   | T     | 33  | GLY  | 2.6  |
| 5   | E     | 131 | GLU  | 2.6  |
| 6   | S     | 13  | LEU  | 2.6  |
| 5   | E     | 88  | ALA  | 2.6  |
| 7   | T     | 34  | ILE  | 2.5  |
| 10  | W     | 10  | TYR  | 2.5  |
| 1   | N     | 206 | ARG  | 2.5  |
| 5   | E     | 91  | TRP  | 2.5  |
| 5   | E     | 72  | SER  | 2.5  |
| 7   | G     | 64  | GLN  | 2.5  |
| 2   | O     | 18  | PRO  | 2.5  |
| 5   | E     | 185 | TYR  | 2.5  |
| 8   | U     | 44  | VAL  | 2.5  |
| 5   | E     | 49  | TYR  | 2.4  |
| 8   | U     | 26  | GLN  | 2.4  |
| 10  | W     | 17  | THR  | 2.4  |
| 2   | O     | 347 | ILE  | 2.4  |
| 5   | E     | 92  | ARG  | 2.4  |
| 9   | I     | 59  | ALA  | 2.4  |
| 5   | E     | 107 | ASP  | 2.4  |
| 5   | E     | 113 | GLU  | 2.3  |
| 5   | R     | 35  | PHE  | 2.3  |
| 1   | N     | 81  | SER  | 2.3  |
| 9   | V     | 72  | VAL  | 2.3  |
| 8   | H     | 61  | PHE  | 2.3  |
| 1   | A     | 262 | TRP  | 2.3  |
| 5   | E     | 74  | ILE  | 2.3  |
| 9   | I     | 71  | ASN  | 2.3  |
| 1   | A     | 223 | TYR  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7   | T     | 43  | ALA  | 2.3  |
| 5   | E     | 85  | LYS  | 2.3  |
| 6   | F     | 110 | LYS  | 2.3  |
| 5   | E     | 79  | SER  | 2.2  |
| 5   | E     | 116 | GLN  | 2.2  |
| 2   | B     | 17  | VAL  | 2.2  |
| 10  | W     | 30  | PHE  | 2.2  |
| 9   | I     | 34  | VAL  | 2.2  |
| 5   | R     | 75  | GLU  | 2.2  |
| 7   | T     | 73  | ASN  | 2.2  |
| 8   | H     | 34  | ARG  | 2.2  |
| 1   | A     | 365 | LEU  | 2.2  |
| 1   | A     | 222 | THR  | 2.2  |
| 5   | E     | 130 | PRO  | 2.2  |
| 8   | U     | 71  | HIS  | 2.2  |
| 9   | V     | 32  | ALA  | 2.1  |
| 1   | N     | 228 | VAL  | 2.1  |
| 7   | G     | 1   | GLY  | 2.1  |
| 9   | V     | 53  | GLU  | 2.1  |
| 2   | O     | 439 | LEU  | 2.1  |
| 5   | E     | 124 | LEU  | 2.1  |
| 2   | O     | 391 | SER  | 2.1  |
| 1   | N     | 187 | SER  | 2.1  |
| 9   | I     | 37  | THR  | 2.1  |
| 9   | I     | 61  | GLY  | 2.1  |
| 2   | O     | 362 | ASN  | 2.0  |
| 5   | R     | 16  | PRO  | 2.0  |
| 1   | A     | 443 | TRP  | 2.0  |
| 4   | D     | 1   | SER  | 2.0  |
| 3   | P     | 16  | ASN  | 2.0  |
| 3   | P     | 17  | ALA  | 2.0  |
| 1   | N     | 231 | LEU  | 2.0  |
| 1   | N     | 224 | ASP  | 2.0  |
| 5   | R     | 76  | ILE  | 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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  | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|--------|------|-------|----------------------------|-------|
| 21  | GOL  | C     | 4006 | 6/6    | 0.49 | 75.40 | 96,98,99,100               | 0     |
| 11  | BHG  | C     | 2010 | 18/18  | 0.44 | 40.18 | 94,103,108,108             | 0     |
| 11  | BHG  | F     | 3011 | 18/18  | 0.48 | 31.80 | 108,113,116,116            | 0     |
| 21  | GOL  | C     | 2008 | 6/6    | 0.29 | 21.00 | 61,65,68,75                | 0     |
| 11  | BHG  | S     | 2011 | 18/18  | 0.44 | 17.20 | 61,89,94,98                | 0     |
| 12  | AZI  | O     | 4010 | 3/3    | 0.49 | 16.70 | 102,102,104,104            | 0     |
| 11  | BHG  | F     | 4001 | 18/18  | 0.76 | 15.45 | 146,154,157,158            | 0     |
| 11  | BHG  | C     | 4002 | 18/18  | 0.69 | 13.17 | 114,122,125,125            | 0     |
| 11  | BHG  | P     | 3010 | 18/18  | 0.34 | 10.90 | 103,107,112,112            | 0     |
| 18  | CDL  | G     | 2004 | 44/100 | 0.21 | 9.52  | 73,87,99,102               | 0     |
| 11  | BHG  | R     | 4007 | 18/18  | 0.34 | 8.13  | 85,95,98,99                | 0     |
| 18  | CDL  | T     | 3004 | 49/100 | 0.31 | 7.80  | 74,89,107,107              | 0     |
| 19  | PEE  | Q     | 3006 | 51/51  | 0.41 | 7.57  | 65,75,98,100               | 0     |
| 11  | BHG  | D     | 4003 | 18/18  | 0.81 | 7.53  | 160,169,171,171            | 0     |
| 12  | AZI  | A     | 4011 | 3/3    | 0.43 | 6.83  | 61,61,66,69                | 0     |
| 21  | GOL  | B     | 2009 | 6/6    | 0.50 | 5.76  | 84,85,86,86                | 0     |
| 21  | GOL  | O     | 3009 | 6/6    | 0.49 | 5.75  | 82,84,85,85                | 0     |
| 19  | PEE  | D     | 2006 | 26/51  | 0.32 | 5.32  | 85,98,108,109              | 0     |
| 19  | PEE  | P     | 3007 | 49/51  | 0.27 | 4.52  | 41,57,81,81                | 0     |
| 12  | AZI  | G     | 4009 | 3/3    | 0.21 | 4.41  | 66,66,67,68                | 0     |
| 21  | GOL  | P     | 3008 | 6/6    | 0.16 | 3.72  | 67,69,71,71                | 0     |
| 19  | PEE  | C     | 2007 | 49/51  | 0.22 | 3.48  | 35,55,81,83                | 0     |
| 12  | AZI  | C     | 2005 | 3/3    | 0.18 | 3.45  | 54,54,56,58                | 0     |
| 16  | FES  | E     | 501  | 4/4    | 0.13 | 3.42  | 41,41,43,43                | 0     |
| 16  | FES  | R     | 501  | 4/4    | 0.15 | 3.03  | 35,35,37,37                | 0     |
| 21  | GOL  | R     | 4005 | 6/6    | 0.25 | 2.71  | 81,83,84,85                | 0     |
| 13  | PO4  | C     | 4008 | 5/5    | 0.16 | 2.07  | 153,153,153,153            | 0     |
| 13  | PO4  | S     | 3012 | 5/5    | 0.14 | 1.91  | 97,97,99,100               | 0     |
| 13  | PO4  | F     | 2012 | 5/5    | 0.13 | 1.67  | 81,82,83,84                | 0     |

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| Mol | Type | Chain | Res  | Atoms  | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|--------|------|-------|-----------------------------|-------|
| 17  | SMA  | P     | 3001 | 37/37  | 0.14 | 1.51  | 27,40,44,46                 | 0     |
| 18  | CDL  | P     | 3003 | 39/100 | 0.23 | 1.43  | 61,89,111,111               | 0     |
| 18  | CDL  | D     | 2003 | 39/100 | 0.18 | 1.36  | 53,78,93,94                 | 0     |
| 12  | AZI  | P     | 3005 | 3/3    | 0.13 | 1.32  | 51,51,54,56                 | 0     |
| 13  | PO4  | A     | 2013 | 5/5    | 0.16 | 1.00  | 119,120,121,122             | 0     |
| 20  | ANY  | P     | 3002 | 37/40  | 0.16 | 0.99  | 33,39,67,71                 | 0     |
| 14  | HEM  | C     | 502  | 43/43  | 0.13 | 0.90  | 22,28,34,37                 | 0     |
| 17  | SMA  | C     | 2001 | 37/37  | 0.14 | 0.87  | 31,39,44,48                 | 0     |
| 14  | HEM  | P     | 502  | 43/43  | 0.13 | 0.22  | 27,31,36,40                 | 0     |
| 14  | HEM  | C     | 501  | 43/43  | 0.12 | 0.10  | 20,31,38,47                 | 0     |
| 14  | HEM  | P     | 501  | 43/43  | 0.12 | 0.07  | 30,34,42,46                 | 0     |
| 15  | HEC  | Q     | 501  | 43/43  | 0.12 | 0.04  | 38,45,48,51                 | 0     |
| 20  | ANY  | C     | 2002 | 37/40  | 0.15 | 0.03  | 31,39,65,70                 | 0     |
| 11  | BHG  | A     | 4004 | 18/18  | 0.12 | 0.03  | 28,34,40,42                 | 0     |
| 15  | HEC  | D     | 501  | 43/43  | 0.12 | -0.17 | 35,41,44,45                 | 0     |
| 13  | PO4  | P     | 3013 | 5/5    | 0.10 | -0.46 | 104,105,106,106             | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.