



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:32 PM UTC

PDB ID : 5K02 / pdb\_00005k02  
Title : Structure of human SOD1 with T2D mutation  
Authors : Fay, J.M.; Zhu, C.; Cui, W.; Ke, H.; Dokholyan, N.V.  
Deposited on : 2016-05-17  
Resolution : 1.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

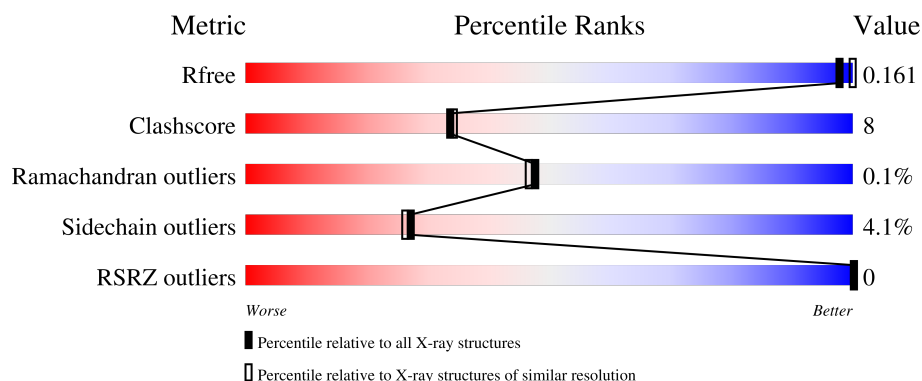
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 Å.

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



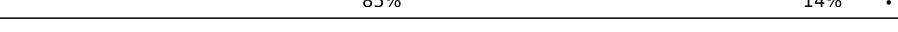
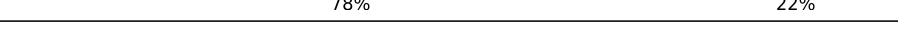
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 10052 (2.00-2.00)                                     |
| Clashscore            | 190562                      | 11152 (2.00-2.00)                                     |
| Ramachandran outliers | 187476                      | 11031 (2.00-2.00)                                     |
| Sidechain outliers    | 187428                      | 11029 (2.00-2.00)                                     |
| RSRZ outliers         | 180081                      | 10067 (2.00-2.00)                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 153    |                  |
| 1   | B     | 153    |                  |
| 1   | C     | 153    |                  |
| 1   | D     | 153    |                  |
| 1   | E     | 153    |                  |

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| Mol | Chain | Length | Quality of chain                                                                               |
|-----|-------|--------|------------------------------------------------------------------------------------------------|
| 1   | F     | 153    |  85% 14% .   |
| 1   | G     | 153    |  88% 12% .   |
| 1   | H     | 153    |  84% 16% .   |
| 1   | I     | 153    |  78% 21% .   |
| 1   | J     | 153    |  81% 18% .   |
| 1   | K     | 153    |  81% 17% .   |
| 1   | L     | 153    |  77% 22% .   |
| 1   | M     | 153    |  79% 20% .   |
| 1   | N     | 153    |  80% 18% .   |
| 1   | O     | 153    |  85% 14% .   |
| 1   | P     | 153    |  82% 17% .   |
| 1   | Q     | 153    |  81% 18% .   |
| 1   | R     | 153    |  86% 14% . |
| 1   | S     | 153    |  78% 20% . |
| 1   | T     | 153    |  79% 21% . |
| 1   | U     | 153    |  85% 14% . |
| 1   | V     | 153    |  78% 22% . |
| 1   | W     | 153    |  88% 12% . |
| 1   | X     | 153    |  84% 13% . |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27396 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Superoxide dismutase [Cu-Zn].

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | B     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | C     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | D     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | E     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | F     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | G     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | H     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | I     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | J     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | K     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | L     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | M     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | N     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | O     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | P     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | Q     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | R     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | S     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | T     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | U     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | V     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | W     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |
| 1   | X     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 679 | 203 | 225 | 4 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| B     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| C     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| D     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| E     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| F     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| G     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| H     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| I     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| J     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| K     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| L     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| M     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| N     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| O     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| P     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| Q     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| R     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| S     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| T     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| U     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| V     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |
| W     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| X     | 2       | ASP      | THR    | engineered mutation | UNP P00441 |

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | A     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | B     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | C     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | D     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | E     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | F     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | G     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | H     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | I     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | J     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | K     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | L     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | M     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | N     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | O     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | P     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | Q     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | R     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | S     | 1        | Total Cu<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | T     | 1        | Total<br>1 | Cu<br>1 | 0       | 0       |
| 2   | U     | 1        | Total<br>1 | Cu<br>1 | 0       | 0       |
| 2   | V     | 1        | Total<br>1 | Cu<br>1 | 0       | 0       |
| 2   | W     | 1        | Total<br>1 | Cu<br>1 | 0       | 0       |
| 2   | X     | 1        | Total<br>1 | Cu<br>1 | 0       | 0       |

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | A     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | B     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | C     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | D     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | E     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | F     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | G     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | H     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | I     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | J     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | K     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | L     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | M     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | N     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | O     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | P     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | Q     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | R     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | S     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | T     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | U     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | V     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | W     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | X     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | A     | 36       | Total<br>36 | O<br>36 | 0       | 0       |
| 4   | B     | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 4   | C     | 32       | Total<br>32 | O<br>32 | 0       | 0       |
| 4   | D     | 39       | Total<br>39 | O<br>39 | 0       | 0       |
| 4   | E     | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 4   | F     | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 4   | G     | 42       | Total<br>42 | O<br>42 | 0       | 0       |
| 4   | H     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 4   | I     | 27       | Total<br>27 | O<br>27 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | J     | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 4   | K     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 4   | L     | 30       | Total<br>30 | O<br>30 | 0       | 0       |
| 4   | M     | 34       | Total<br>34 | O<br>34 | 0       | 0       |
| 4   | N     | 35       | Total<br>35 | O<br>35 | 0       | 0       |
| 4   | O     | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 4   | P     | 31       | Total<br>31 | O<br>31 | 0       | 0       |
| 4   | Q     | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 4   | R     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 4   | S     | 31       | Total<br>31 | O<br>31 | 0       | 0       |
| 4   | T     | 29       | Total<br>29 | O<br>29 | 0       | 0       |
| 4   | U     | 29       | Total<br>29 | O<br>29 | 0       | 0       |
| 4   | V     | 31       | Total<br>31 | O<br>31 | 0       | 0       |
| 4   | W     | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 4   | X     | 19       | Total<br>19 | O<br>19 | 0       | 0       |

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

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

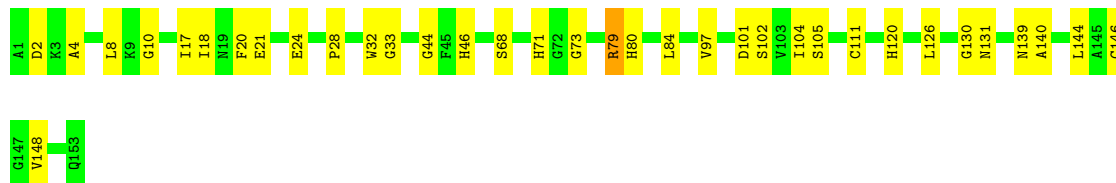
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  76% 23% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  77% 22% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain C:  80% 18% .



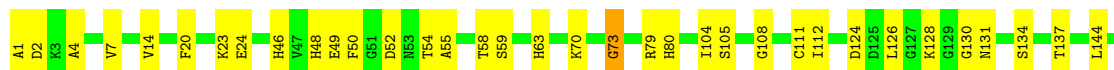
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain D:  86% 13% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain E:  77% 22% .



Q153

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain F:  85% 14%

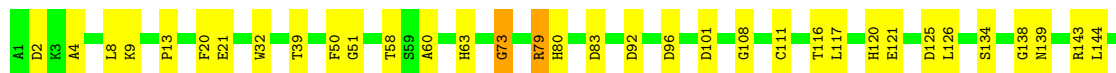

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain G:  88% 12%


- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain H:  84% 16%


- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain I:  78% 21%


Q153

- Molecule 1: Superoxide dismutase [Cu-Zn]

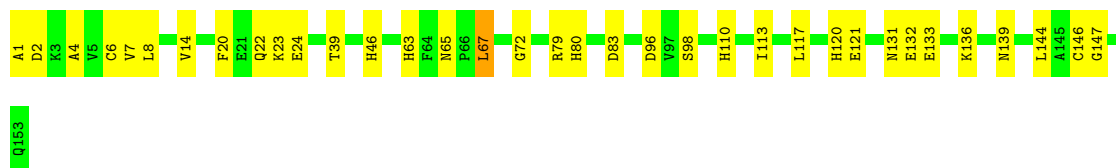
Chain J:  81% 18%


- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain K:  81% 17%

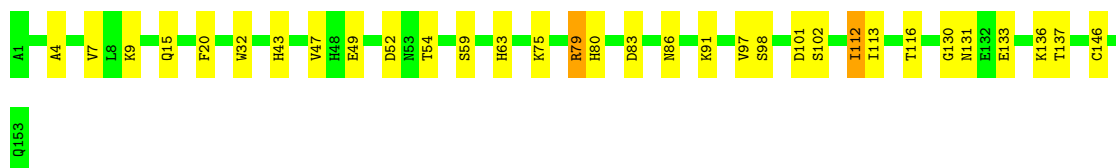

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain L:  77% 22% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain M:  79% 20% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain N:  80% 18% .



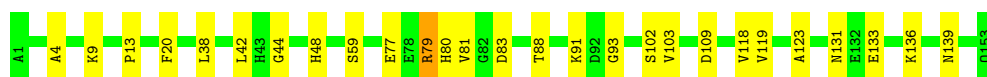
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain O:  85% 14% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain P:  82% 17% .



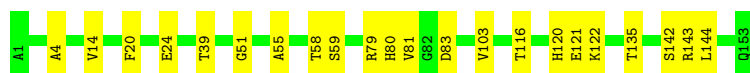
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain Q:  81% 18% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain R:  86% 14% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain S: 78% 20% .



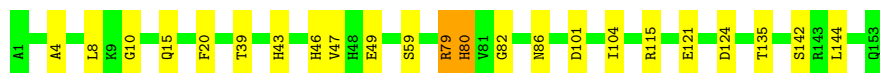
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain T: 79% 21% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain U: 85% 14% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain V: 78% 22% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain W: 88% 12% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain X: 84% 13% .



## 4 Data and refinement statistics

| Property                                                                | Value                                                                                                                                                                                                                                           | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                                                                                                                                                                                                             | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 111.98Å 111.96Å 149.88Å<br>89.86° 89.85° 60.13°                                                                                                                                                                                                 | Depositor        |
| Resolution (Å)                                                          | 149.92 – 1.99<br>149.88 – 2.00                                                                                                                                                                                                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 80.4 (149.92-1.99)<br>80.6 (149.88-2.00)                                                                                                                                                                                                        | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                                                                                                                                                                                                            | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                                                                                                                                                                                                 | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.25 (at 2.00Å)                                                                                                                                                                                                                                 | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0117                                                                                                                                                                                                                                 | Depositor        |
| R, $R_{free}$                                                           | 0.146 , 0.162<br>0.146 , 0.161                                                                                                                                                                                                                  | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 17442 reflections (4.06%)                                                                                                                                                                                                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 34.0                                                                                                                                                                                                                                            | Xtriage          |
| Anisotropy                                                              | 0.163                                                                                                                                                                                                                                           | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.37 , 17.1                                                                                                                                                                                                                                     | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$                                                                                                                                                                                     | Xtriage          |
| Estimated twinning fraction                                             | 0.427 for h-k,h,l<br>0.427 for k,-h+k,l<br>0.426 for -k,h-k,l<br>0.426 for -h+k,-h,l<br>0.427 for -h+k,k,-l<br>0.467 for h,h-k,-l<br>0.469 for -h,-k,l<br>0.428 for k,h,-l<br>0.430 for -k,-h,-l<br>0.427 for h-k,-k,-l<br>0.459 for -h,-h+k,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                                                                                                                                                                                                            | EDS              |
| Total number of atoms                                                   | 27396                                                                                                                                                                                                                                           | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 36.0                                                                                                                                                                                                                                            | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CU

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

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 1   | A     | 0.72         | 0/1129  | 0.89        | 1/1521 (0.1%)   |
| 1   | B     | 0.71         | 0/1129  | 0.86        | 0/1521          |
| 1   | C     | 0.73         | 0/1129  | 0.86        | 0/1521          |
| 1   | D     | 0.71         | 0/1129  | 0.80        | 0/1521          |
| 1   | E     | 0.70         | 0/1129  | 0.83        | 3/1521 (0.2%)   |
| 1   | F     | 0.70         | 0/1129  | 0.81        | 0/1521          |
| 1   | G     | 0.70         | 0/1129  | 0.80        | 0/1521          |
| 1   | H     | 0.70         | 0/1129  | 0.81        | 0/1521          |
| 1   | I     | 0.69         | 0/1129  | 0.84        | 2/1521 (0.1%)   |
| 1   | J     | 0.71         | 0/1129  | 0.79        | 0/1521          |
| 1   | K     | 0.72         | 0/1129  | 0.85        | 1/1521 (0.1%)   |
| 1   | L     | 0.74         | 0/1129  | 0.85        | 0/1521          |
| 1   | M     | 0.73         | 0/1129  | 0.84        | 1/1521 (0.1%)   |
| 1   | N     | 0.70         | 0/1129  | 0.86        | 3/1521 (0.2%)   |
| 1   | O     | 0.72         | 0/1129  | 0.83        | 0/1521          |
| 1   | P     | 0.72         | 0/1129  | 0.81        | 0/1521          |
| 1   | Q     | 0.70         | 0/1129  | 0.83        | 0/1521          |
| 1   | R     | 0.72         | 0/1129  | 0.81        | 0/1521          |
| 1   | S     | 0.72         | 0/1129  | 0.80        | 0/1521          |
| 1   | T     | 0.71         | 0/1129  | 0.82        | 3/1521 (0.2%)   |
| 1   | U     | 0.72         | 0/1129  | 0.83        | 0/1521          |
| 1   | V     | 0.72         | 0/1129  | 0.82        | 0/1521          |
| 1   | W     | 0.71         | 0/1129  | 0.82        | 0/1521          |
| 1   | X     | 0.72         | 0/1129  | 0.85        | 0/1521          |
| All | All   | 0.71         | 0/27096 | 0.83        | 14/36504 (0.0%) |

There are no bond length outliers.

All (14) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | N     | 27  | GLY  | CA-C-N | 7.05 | 128.65      | 119.84   |
| 1   | N     | 27  | GLY  | C-N-CA | 7.05 | 128.65      | 119.84   |
| 1   | E     | 49  | GLU  | N-CA-C | 6.43 | 117.95      | 111.07   |
| 1   | T     | 27  | GLY  | CA-C-N | 6.07 | 126.01      | 119.76   |
| 1   | T     | 27  | GLY  | C-N-CA | 6.07 | 126.01      | 119.76   |
| 1   | M     | 49  | GLU  | N-CA-C | 5.66 | 117.12      | 111.07   |
| 1   | E     | 73  | GLY  | CA-C-N | 5.40 | 125.74      | 119.47   |
| 1   | E     | 73  | GLY  | C-N-CA | 5.40 | 125.74      | 119.47   |
| 1   | K     | 49  | GLU  | N-CA-C | 5.32 | 117.07      | 111.28   |
| 1   | N     | 49  | GLU  | N-CA-C | 5.26 | 116.70      | 111.07   |
| 1   | I     | 73  | GLY  | CA-C-N | 5.25 | 126.40      | 119.84   |
| 1   | I     | 73  | GLY  | C-N-CA | 5.25 | 126.40      | 119.84   |
| 1   | A     | 23  | LYS  | N-CA-C | 5.21 | 117.04      | 111.36   |
| 1   | T     | 49  | GLU  | N-CA-C | 5.14 | 116.57      | 111.07   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1111  | 0        | 1074     | 25      | 0            |
| 1   | B     | 1111  | 0        | 1074     | 24      | 0            |
| 1   | C     | 1111  | 0        | 1073     | 20      | 0            |
| 1   | D     | 1111  | 0        | 1074     | 13      | 0            |
| 1   | E     | 1111  | 0        | 1074     | 20      | 0            |
| 1   | F     | 1111  | 0        | 1074     | 16      | 0            |
| 1   | G     | 1111  | 0        | 1074     | 14      | 0            |
| 1   | H     | 1111  | 0        | 1074     | 18      | 0            |
| 1   | I     | 1111  | 0        | 1074     | 21      | 0            |
| 1   | J     | 1111  | 0        | 1074     | 19      | 0            |
| 1   | K     | 1111  | 0        | 1074     | 17      | 0            |
| 1   | L     | 1111  | 0        | 1074     | 20      | 0            |
| 1   | M     | 1111  | 0        | 1074     | 22      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | N     | 1111  | 0        | 1074     | 21      | 0            |
| 1   | O     | 1111  | 0        | 1074     | 12      | 0            |
| 1   | P     | 1111  | 0        | 1074     | 17      | 0            |
| 1   | Q     | 1111  | 0        | 1074     | 18      | 0            |
| 1   | R     | 1111  | 0        | 1074     | 13      | 0            |
| 1   | S     | 1111  | 0        | 1074     | 21      | 0            |
| 1   | T     | 1111  | 0        | 1074     | 22      | 0            |
| 1   | U     | 1111  | 0        | 1074     | 13      | 0            |
| 1   | V     | 1111  | 0        | 1074     | 20      | 0            |
| 1   | W     | 1111  | 0        | 1074     | 13      | 0            |
| 1   | X     | 1111  | 0        | 1073     | 18      | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 2   | I     | 1     | 0        | 0        | 0       | 0            |
| 2   | J     | 1     | 0        | 0        | 0       | 0            |
| 2   | K     | 1     | 0        | 0        | 0       | 0            |
| 2   | L     | 1     | 0        | 0        | 0       | 0            |
| 2   | M     | 1     | 0        | 0        | 0       | 0            |
| 2   | N     | 1     | 0        | 0        | 0       | 0            |
| 2   | O     | 1     | 0        | 0        | 0       | 0            |
| 2   | P     | 1     | 0        | 0        | 0       | 0            |
| 2   | Q     | 1     | 0        | 0        | 0       | 0            |
| 2   | R     | 1     | 0        | 0        | 0       | 0            |
| 2   | S     | 1     | 0        | 0        | 0       | 0            |
| 2   | T     | 1     | 0        | 0        | 0       | 0            |
| 2   | U     | 1     | 0        | 0        | 0       | 0            |
| 2   | V     | 1     | 0        | 0        | 0       | 0            |
| 2   | W     | 1     | 0        | 0        | 0       | 0            |
| 2   | X     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| 3   | I     | 1     | 0        | 0        | 0       | 0            |
| 3   | J     | 1     | 0        | 0        | 0       | 0            |
| 3   | K     | 1     | 0        | 0        | 0       | 0            |
| 3   | L     | 1     | 0        | 0        | 0       | 0            |
| 3   | M     | 1     | 0        | 0        | 0       | 0            |
| 3   | N     | 1     | 0        | 0        | 0       | 0            |
| 3   | O     | 1     | 0        | 0        | 0       | 0            |
| 3   | P     | 1     | 0        | 0        | 0       | 0            |
| 3   | Q     | 1     | 0        | 0        | 0       | 0            |
| 3   | R     | 1     | 0        | 0        | 0       | 0            |
| 3   | S     | 1     | 0        | 0        | 0       | 0            |
| 3   | T     | 1     | 0        | 0        | 0       | 0            |
| 3   | U     | 1     | 0        | 0        | 0       | 0            |
| 3   | V     | 1     | 0        | 0        | 0       | 0            |
| 3   | W     | 1     | 0        | 0        | 0       | 0            |
| 3   | X     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 36    | 0        | 0        | 3       | 0            |
| 4   | B     | 26    | 0        | 0        | 3       | 0            |
| 4   | C     | 32    | 0        | 0        | 0       | 0            |
| 4   | D     | 39    | 0        | 0        | 0       | 0            |
| 4   | E     | 25    | 0        | 0        | 1       | 0            |
| 4   | F     | 26    | 0        | 0        | 1       | 0            |
| 4   | G     | 42    | 0        | 0        | 1       | 0            |
| 4   | H     | 20    | 0        | 0        | 1       | 0            |
| 4   | I     | 27    | 0        | 0        | 0       | 0            |
| 4   | J     | 26    | 0        | 0        | 1       | 0            |
| 4   | K     | 20    | 0        | 0        | 0       | 0            |
| 4   | L     | 30    | 0        | 0        | 3       | 0            |
| 4   | M     | 34    | 0        | 0        | 1       | 0            |
| 4   | N     | 35    | 0        | 0        | 4       | 0            |
| 4   | O     | 22    | 0        | 0        | 0       | 0            |
| 4   | P     | 31    | 0        | 0        | 2       | 0            |
| 4   | Q     | 26    | 0        | 0        | 1       | 0            |
| 4   | R     | 20    | 0        | 0        | 0       | 0            |
| 4   | S     | 31    | 0        | 0        | 0       | 0            |
| 4   | T     | 29    | 0        | 0        | 1       | 0            |
| 4   | U     | 29    | 0        | 0        | 0       | 0            |
| 4   | V     | 31    | 0        | 0        | 0       | 0            |
| 4   | W     | 28    | 0        | 0        | 0       | 0            |
| 4   | X     | 19    | 0        | 0        | 1       | 0            |
| All | All   | 27396 | 0        | 25774    | 404     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (404) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:8:LEU:HD21   | 1:X:117:LEU:HD23 | 1.37                     | 1.07              |
| 1:A:29:VAL:HG13  | 4:A:303:HOH:O    | 1.53                     | 1.07              |
| 1:X:131:ASN:HD21 | 1:X:139:ASN:HD21 | 1.09                     | 0.98              |
| 1:A:75:LYS:HG3   | 1:K:128:LYS:HA   | 1.48                     | 0.95              |
| 1:A:1:ALA:H1     | 1:A:23:LYS:HA    | 1.35                     | 0.89              |
| 1:B:111:CYS:HA   | 4:B:301:HOH:O    | 1.75                     | 0.86              |
| 1:P:88:THR:HA    | 4:P:301:HOH:O    | 1.74                     | 0.86              |
| 1:S:79:ARG:HD3   | 1:S:80:HIS:O     | 1.76                     | 0.85              |
| 1:V:79:ARG:HD2   | 1:V:80:HIS:O     | 1.78                     | 0.84              |
| 1:V:79:ARG:HD3   | 1:V:83:ASP:HB2   | 1.60                     | 0.83              |
| 1:S:38:LEU:O     | 1:S:93:GLY:HA2   | 1.79                     | 0.82              |
| 1:Q:14:VAL:HG21  | 1:Q:144:LEU:HD13 | 1.61                     | 0.82              |
| 1:A:1:ALA:N      | 1:A:23:LYS:HA    | 1.96                     | 0.80              |
| 1:A:4:ALA:HB3    | 1:A:20:PHE:HB2   | 1.64                     | 0.79              |
| 1:R:79:ARG:HD2   | 1:R:80:HIS:O     | 1.82                     | 0.79              |
| 1:P:42:LEU:HA    | 4:P:301:HOH:O    | 1.84                     | 0.77              |
| 1:T:4:ALA:HB3    | 1:T:20:PHE:HB2   | 1.67                     | 0.76              |
| 1:C:13:PRO:HG3   | 1:F:39:THR:HG22  | 1.68                     | 0.76              |
| 1:M:98:SER:O     | 1:W:131:ASN:HB2  | 1.85                     | 0.75              |
| 1:I:121:GLU:HA   | 1:I:144:LEU:HD11 | 1.70                     | 0.73              |
| 1:A:7:VAL:HG11   | 1:A:9:LYS:HE2    | 1.68                     | 0.73              |
| 1:U:49:GLU:O     | 1:U:115:ARG:NH1  | 2.22                     | 0.73              |
| 1:I:4:ALA:HB3    | 1:I:20:PHE:HB2   | 1.71                     | 0.73              |
| 1:C:79:ARG:HD3   | 1:C:80:HIS:O     | 1.90                     | 0.72              |
| 1:A:131:ASN:OD1  | 1:A:139:ASN:ND2  | 2.23                     | 0.71              |
| 1:A:81:VAL:HG12  | 4:A:328:HOH:O    | 1.89                     | 0.71              |
| 1:H:79:ARG:HD3   | 1:H:83:ASP:HB2   | 1.70                     | 0.70              |
| 1:M:63:HIS:CE1   | 1:M:137:THR:HA   | 2.27                     | 0.70              |
| 1:D:15:GLN:HE21  | 1:D:36:LYS:HE3   | 1.58                     | 0.69              |
| 1:K:79:ARG:NH2   | 1:K:101:ASP:OD1  | 2.25                     | 0.69              |
| 1:A:79:ARG:HD3   | 1:A:80:HIS:O     | 1.93                     | 0.68              |
| 1:R:121:GLU:HG3  | 1:R:122:LYS:HG3  | 1.76                     | 0.68              |
| 1:N:131:ASN:HB3  | 1:O:96:ASP:O     | 1.95                     | 0.67              |
| 1:N:46:HIS:CE1   | 1:N:120:HIS:CD2  | 2.84                     | 0.66              |
| 1:Q:71:HIS:HB2   | 1:Q:80:HIS:CE1   | 2.30                     | 0.66              |
| 1:W:79:ARG:HD3   | 1:W:80:HIS:O     | 1.94                     | 0.66              |
| 1:B:79:ARG:HD3   | 1:B:80:HIS:O     | 1.95                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:71:HIS:HB2   | 1:V:80:HIS:CE1   | 2.31                     | 0.65              |
| 1:H:79:ARG:HD2   | 1:H:80:HIS:O     | 1.96                     | 0.65              |
| 1:A:73:GLY:HA2   | 1:A:126:LEU:HD22 | 1.77                     | 0.65              |
| 1:N:132:GLU:O    | 1:N:136:LYS:HG3  | 1.97                     | 0.65              |
| 1:X:131:ASN:OD1  | 1:X:133:GLU:HB3  | 1.96                     | 0.65              |
| 1:L:8:LEU:HG     | 4:L:307:HOH:O    | 1.98                     | 0.64              |
| 1:E:128:LYS:HA   | 1:G:75:LYS:HG3   | 1.78                     | 0.64              |
| 1:G:5:VAL:HG23   | 1:G:19:ASN:ND2   | 2.11                     | 0.64              |
| 1:R:79:ARG:HD3   | 1:R:83:ASP:HB2   | 1.79                     | 0.64              |
| 1:M:63:HIS:HE1   | 1:M:137:THR:HA   | 1.62                     | 0.64              |
| 1:T:121:GLU:HG3  | 1:T:122:LYS:HG3  | 1.80                     | 0.64              |
| 1:X:131:ASN:HD21 | 1:X:139:ASN:ND2  | 1.90                     | 0.63              |
| 1:H:75:LYS:HG3   | 1:J:128:LYS:HE2  | 1.79                     | 0.63              |
| 1:G:31:VAL:HB    | 1:G:99:ILE:HB    | 1.81                     | 0.63              |
| 1:K:79:ARG:HD3   | 1:K:80:HIS:O     | 1.99                     | 0.63              |
| 1:H:4:ALA:HB3    | 1:H:20:PHE:HB2   | 1.80                     | 0.62              |
| 1:V:63:HIS:CE1   | 1:V:137:THR:HA   | 2.35                     | 0.62              |
| 1:B:4:ALA:HB3    | 1:B:20:PHE:HB2   | 1.81                     | 0.62              |
| 1:I:63:HIS:HB2   | 1:I:80:HIS:ND1   | 2.15                     | 0.62              |
| 1:I:108:GLY:O    | 1:I:111:CYS:HB2  | 2.00                     | 0.62              |
| 1:Q:128:LYS:HA   | 1:S:75:LYS:HG3   | 1.82                     | 0.62              |
| 1:Q:131:ASN:HB3  | 1:S:98:SER:O     | 2.00                     | 0.62              |
| 1:F:52:ASP:O     | 1:F:59:SER:HB2   | 2.00                     | 0.61              |
| 1:W:71:HIS:HB2   | 1:W:80:HIS:CE1   | 2.35                     | 0.61              |
| 1:S:65:ASN:CG    | 1:S:80:HIS:HD2   | 2.09                     | 0.60              |
| 1:I:125:ASP:OD2  | 1:I:139:ASN:ND2  | 2.34                     | 0.60              |
| 1:Q:4:ALA:HB3    | 1:Q:20:PHE:HB2   | 1.82                     | 0.60              |
| 1:U:121:GLU:HG2  | 1:U:142:SER:H    | 1.65                     | 0.60              |
| 1:H:44:GLY:HA3   | 1:H:120:HIS:HB2  | 1.83                     | 0.60              |
| 1:E:4:ALA:HB3    | 1:E:20:PHE:HB2   | 1.82                     | 0.60              |
| 1:J:81:VAL:HG22  | 1:J:103:VAL:HG12 | 1.84                     | 0.60              |
| 1:I:79:ARG:HB2   | 1:I:83:ASP:OD2   | 2.01                     | 0.59              |
| 1:W:98:SER:HB3   | 1:X:132:GLU:H    | 1.66                     | 0.59              |
| 1:T:73:GLY:N     | 1:T:76:ASP:OD2   | 2.30                     | 0.59              |
| 1:B:105:SER:HB3  | 4:B:301:HOH:O    | 2.02                     | 0.59              |
| 1:K:120:HIS:CE1  | 1:K:143:ARG:HG2  | 2.38                     | 0.59              |
| 1:V:4:ALA:HB3    | 1:V:20:PHE:HB2   | 1.85                     | 0.59              |
| 1:P:79:ARG:HD3   | 1:P:83:ASP:HB2   | 1.83                     | 0.58              |
| 1:G:4:ALA:HB3    | 1:G:20:PHE:HB2   | 1.84                     | 0.58              |
| 1:I:79:ARG:HD2   | 1:I:80:HIS:O     | 2.03                     | 0.58              |
| 1:L:14:VAL:HG21  | 1:L:144:LEU:HD13 | 1.86                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:79:ARG:HD3   | 1:P:80:HIS:O     | 2.04                     | 0.58              |
| 1:S:63:HIS:CE1   | 1:S:137:THR:HA   | 2.39                     | 0.58              |
| 1:U:79:ARG:NH2   | 1:U:101:ASP:OD1  | 2.27                     | 0.58              |
| 1:D:4:ALA:HB3    | 1:D:20:PHE:HB2   | 1.86                     | 0.57              |
| 1:U:10:GLY:HA3   | 1:U:144:LEU:O    | 2.05                     | 0.57              |
| 1:A:71:HIS:HB2   | 1:A:80:HIS:CE1   | 2.38                     | 0.57              |
| 1:B:46:HIS:CE1   | 1:B:120:HIS:CD2  | 2.91                     | 0.57              |
| 1:M:32:TRP:HA    | 1:M:97:VAL:O     | 2.04                     | 0.57              |
| 1:O:4:ALA:HB3    | 1:O:20:PHE:HB2   | 1.87                     | 0.57              |
| 1:H:108:GLY:O    | 1:H:111:CYS:HB2  | 2.04                     | 0.57              |
| 1:T:79:ARG:HH22  | 1:T:101:ASP:CG   | 2.12                     | 0.57              |
| 1:J:4:ALA:HB3    | 1:J:20:PHE:HB2   | 1.87                     | 0.57              |
| 1:X:79:ARG:HD3   | 1:X:80:HIS:O     | 2.05                     | 0.56              |
| 1:I:92:ASP:HA    | 1:K:91:LYS:HB2   | 1.86                     | 0.56              |
| 1:M:43:HIS:O     | 1:M:86:ASN:HA    | 2.06                     | 0.56              |
| 1:S:31:VAL:HB    | 1:S:99:ILE:HB    | 1.88                     | 0.56              |
| 1:V:79:ARG:CD    | 1:V:80:HIS:O     | 2.51                     | 0.56              |
| 1:B:130:GLY:HA3  | 1:C:87:VAL:HA    | 1.88                     | 0.56              |
| 1:D:46:HIS:CE1   | 1:D:120:HIS:CD2  | 2.94                     | 0.56              |
| 1:Q:121:GLU:HG2  | 1:Q:142:SER:H    | 1.71                     | 0.56              |
| 1:B:101:ASP:HB3  | 1:B:104:ILE:HG12 | 1.88                     | 0.55              |
| 1:Q:70:LYS:O     | 1:Q:79:ARG:HA    | 2.04                     | 0.55              |
| 1:U:39:THR:HG1   | 1:U:43:HIS:CE1   | 2.24                     | 0.55              |
| 1:J:71:HIS:HB2   | 1:J:80:HIS:CE1   | 2.41                     | 0.55              |
| 1:P:79:ARG:NH1   | 1:P:81:VAL:O     | 2.39                     | 0.55              |
| 1:T:121:GLU:HG2  | 1:T:142:SER:H    | 1.71                     | 0.55              |
| 1:P:13:PRO:HD3   | 1:S:15:GLN:NE2   | 2.22                     | 0.55              |
| 1:P:131:ASN:HD21 | 1:P:139:ASN:HD21 | 1.55                     | 0.54              |
| 1:A:132:GLU:N    | 1:L:98:SER:HB3   | 2.23                     | 0.54              |
| 1:F:101:ASP:HB3  | 1:F:104:ILE:HG12 | 1.89                     | 0.54              |
| 1:P:133:GLU:HA   | 1:P:136:LYS:HE2  | 1.90                     | 0.54              |
| 1:F:14:VAL:HG21  | 1:F:144:LEU:HB3  | 1.89                     | 0.54              |
| 1:M:79:ARG:HD3   | 1:M:83:ASP:HB2   | 1.89                     | 0.54              |
| 1:T:120:HIS:CE1  | 1:T:143:ARG:HG2  | 2.43                     | 0.54              |
| 1:N:113:ILE:HD13 | 1:N:151:ILE:HG12 | 1.89                     | 0.54              |
| 1:M:52:ASP:OD1   | 1:M:54:THR:OG1   | 2.24                     | 0.54              |
| 1:N:76:ASP:O     | 1:N:79:ARG:HG2   | 2.08                     | 0.54              |
| 1:M:47:VAL:HG11  | 1:M:112:ILE:HG22 | 1.88                     | 0.54              |
| 1:A:7:VAL:CG1    | 1:A:9:LYS:HE2    | 2.36                     | 0.54              |
| 1:H:14:VAL:HA    | 1:H:36:LYS:O     | 2.07                     | 0.54              |
| 1:M:54:THR:HG22  | 1:N:17:ILE:HG12  | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:23:LYS:NZ    | 1:N:30:LYS:HE3   | 2.22                     | 0.54              |
| 1:E:1:ALA:HA     | 1:E:23:LYS:HA    | 1.90                     | 0.54              |
| 1:J:46:HIS:CE1   | 1:J:120:HIS:CD2  | 2.95                     | 0.54              |
| 1:M:75:LYS:HG3   | 1:W:128:LYS:HA   | 1.90                     | 0.54              |
| 1:M:102:SER:HB2  | 4:M:328:HOH:O    | 2.07                     | 0.54              |
| 1:C:71:HIS:HB2   | 1:C:80:HIS:HE1   | 1.72                     | 0.53              |
| 1:F:136:LYS:HD2  | 4:F:322:HOH:O    | 2.08                     | 0.53              |
| 1:L:65:ASN:ND2   | 1:L:80:HIS:HD2   | 2.07                     | 0.53              |
| 1:T:50:PHE:C     | 1:T:52:ASP:H     | 2.16                     | 0.53              |
| 1:A:79:ARG:HD2   | 1:A:103:VAL:HG11 | 1.90                     | 0.53              |
| 1:E:108:GLY:O    | 1:E:111:CYS:HB2  | 2.08                     | 0.53              |
| 1:S:38:LEU:O     | 1:S:93:GLY:CA    | 2.55                     | 0.53              |
| 1:T:14:VAL:HG22  | 1:T:37:GLY:O     | 2.08                     | 0.53              |
| 1:G:49:GLU:HG2   | 1:G:50:PHE:CE1   | 2.44                     | 0.53              |
| 1:M:79:ARG:HD3   | 1:M:80:HIS:O     | 2.08                     | 0.53              |
| 1:K:120:HIS:HB3  | 1:K:140:ALA:O    | 2.09                     | 0.52              |
| 1:P:4:ALA:HB3    | 1:P:20:PHE:HB2   | 1.92                     | 0.52              |
| 1:A:112:ILE:HD12 | 1:A:149:ILE:HG21 | 1.90                     | 0.52              |
| 1:D:79:ARG:HD3   | 1:D:80:HIS:O     | 2.10                     | 0.52              |
| 1:W:98:SER:HB3   | 1:X:132:GLU:N    | 2.25                     | 0.52              |
| 1:A:101:ASP:OD2  | 1:A:104:ILE:HG12 | 2.10                     | 0.52              |
| 1:C:67:LEU:HD21  | 1:C:110:HIS:NE2  | 2.25                     | 0.52              |
| 1:G:5:VAL:HG23   | 1:G:19:ASN:HD22  | 1.74                     | 0.52              |
| 1:H:109:ASP:C    | 1:H:111:CYS:H    | 2.18                     | 0.52              |
| 1:M:4:ALA:HB3    | 1:M:20:PHE:HB2   | 1.91                     | 0.52              |
| 1:X:125:ASP:OD2  | 1:X:139:ASN:HB2  | 2.10                     | 0.52              |
| 1:E:79:ARG:HD2   | 1:E:80:HIS:O     | 2.10                     | 0.52              |
| 1:A:79:ARG:NH2   | 1:A:101:ASP:OD1  | 2.43                     | 0.52              |
| 1:E:63:HIS:HB2   | 1:E:80:HIS:ND1   | 2.25                     | 0.52              |
| 1:R:14:VAL:HG21  | 1:R:144:LEU:HD13 | 1.91                     | 0.52              |
| 1:A:81:VAL:HG11  | 1:A:110:HIS:HB3  | 1.93                     | 0.51              |
| 1:T:46:HIS:CE1   | 1:T:120:HIS:CD2  | 2.98                     | 0.51              |
| 1:Q:90:ASP:OD1   | 1:Q:94:VAL:N     | 2.43                     | 0.51              |
| 1:B:111:CYS:CA   | 4:B:301:HOH:O    | 2.47                     | 0.51              |
| 1:K:8:LEU:O      | 1:K:15:GLN:HA    | 2.10                     | 0.51              |
| 1:R:4:ALA:HB3    | 1:R:20:PHE:HB2   | 1.91                     | 0.51              |
| 1:E:104:ILE:HB   | 1:E:112:ILE:HD13 | 1.92                     | 0.51              |
| 1:O:10:GLY:HA3   | 1:O:144:LEU:O    | 2.10                     | 0.51              |
| 1:H:24:GLU:HB2   | 1:H:27:GLY:HA3   | 1.93                     | 0.51              |
| 1:C:130:GLY:HA3  | 1:D:86:ASN:O     | 2.11                     | 0.51              |
| 1:N:23:LYS:HZ1   | 1:N:30:LYS:HE3   | 1.76                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:7:VAL:HG23   | 4:E:316:HOH:O    | 2.11                     | 0.51              |
| 1:M:15:GLN:NE2   | 1:V:13:PRO:HD3   | 2.26                     | 0.51              |
| 1:T:101:ASP:HB3  | 1:T:104:ILE:HG12 | 1.91                     | 0.51              |
| 1:B:21:GLU:HB2   | 1:B:32:TRP:CZ3   | 2.46                     | 0.51              |
| 1:C:74:PRO:HG3   | 1:C:84:LEU:C     | 2.36                     | 0.51              |
| 1:F:98:SER:HB3   | 1:G:132:GLU:H    | 1.76                     | 0.50              |
| 1:T:53:ASN:HB3   | 4:T:328:HOH:O    | 2.10                     | 0.50              |
| 1:U:8:LEU:O      | 1:U:15:GLN:HA    | 2.11                     | 0.50              |
| 1:R:81:VAL:HG13  | 1:R:103:VAL:HG12 | 1.93                     | 0.50              |
| 1:G:79:ARG:NH2   | 1:G:101:ASP:OD1  | 2.44                     | 0.50              |
| 1:H:21:GLU:HB2   | 1:H:32:TRP:CZ3   | 2.47                     | 0.50              |
| 1:J:36:LYS:HB3   | 1:J:94:VAL:HG22  | 1.93                     | 0.50              |
| 1:O:118:VAL:HG11 | 1:O:143:ARG:HG2  | 1.92                     | 0.50              |
| 1:W:79:ARG:NH2   | 1:W:101:ASP:OD1  | 2.42                     | 0.50              |
| 1:E:70:LYS:O     | 1:E:79:ARG:HA    | 2.11                     | 0.50              |
| 1:M:133:GLU:HA   | 1:M:136:LYS:HE3  | 1.93                     | 0.50              |
| 1:O:79:ARG:HD3   | 1:O:80:HIS:O     | 2.11                     | 0.50              |
| 1:T:15:GLN:O     | 1:T:36:LYS:HG2   | 2.12                     | 0.50              |
| 1:D:15:GLN:NE2   | 1:D:36:LYS:HE3   | 2.25                     | 0.50              |
| 1:P:80:HIS:N     | 1:P:83:ASP:OD2   | 2.45                     | 0.50              |
| 1:X:80:HIS:HE1   | 1:X:136:LYS:O    | 1.95                     | 0.50              |
| 1:I:8:LEU:HD21   | 1:I:117:LEU:HD23 | 1.93                     | 0.50              |
| 1:L:4:ALA:HB3    | 1:L:20:PHE:HB2   | 1.93                     | 0.50              |
| 1:L:22:GLN:HG2   | 1:L:24:GLU:O     | 2.12                     | 0.50              |
| 1:L:133:GLU:HB3  | 1:L:139:ASN:OD1  | 2.11                     | 0.50              |
| 1:S:24:GLU:OE1   | 1:S:27:GLY:HA3   | 2.12                     | 0.49              |
| 1:T:46:HIS:CE1   | 1:T:120:HIS:HD2  | 2.30                     | 0.49              |
| 1:C:76:ASP:O     | 1:C:79:ARG:HG2   | 2.12                     | 0.49              |
| 1:Q:121:GLU:HG2  | 1:Q:142:SER:N    | 2.27                     | 0.49              |
| 1:L:7:VAL:O      | 1:L:147:GLY:HA3  | 2.13                     | 0.49              |
| 1:R:120:HIS:CE1  | 1:R:143:ARG:HG2  | 2.47                     | 0.49              |
| 1:C:71:HIS:HA    | 1:C:80:HIS:CE1   | 2.47                     | 0.49              |
| 1:R:121:GLU:HG2  | 1:R:142:SER:N    | 2.27                     | 0.49              |
| 1:E:14:VAL:HG21  | 1:E:144:LEU:HD13 | 1.95                     | 0.49              |
| 1:P:42:LEU:HB2   | 1:P:123:ALA:HB2  | 1.94                     | 0.49              |
| 1:P:81:VAL:HG13  | 1:P:103:VAL:HG12 | 1.94                     | 0.49              |
| 1:X:99:ILE:HG22  | 1:X:100:GLU:N    | 2.28                     | 0.49              |
| 1:H:21:GLU:HB2   | 1:H:32:TRP:HZ3   | 1.78                     | 0.49              |
| 1:V:44:GLY:HA3   | 1:V:120:HIS:HB2  | 1.95                     | 0.48              |
| 1:S:4:ALA:HB3    | 1:S:20:PHE:HB2   | 1.94                     | 0.48              |
| 1:U:47:VAL:HB    | 1:U:82:GLY:HA2   | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:71:HIS:HB2   | 1:C:80:HIS:CE1   | 2.47                     | 0.48              |
| 1:C:46:HIS:CE1   | 1:C:120:HIS:CD2  | 3.01                     | 0.48              |
| 1:V:38:LEU:O     | 1:V:93:GLY:HA2   | 2.14                     | 0.48              |
| 1:F:4:ALA:HB3    | 1:F:20:PHE:HB2   | 1.95                     | 0.48              |
| 1:R:55:ALA:HB3   | 1:R:59:SER:HB3   | 1.93                     | 0.48              |
| 1:S:6:CYS:HB2    | 1:S:149:ILE:HA   | 1.95                     | 0.48              |
| 1:U:39:THR:OG1   | 1:U:43:HIS:CE1   | 2.67                     | 0.48              |
| 1:E:128:LYS:HG2  | 1:G:75:LYS:HB2   | 1.95                     | 0.48              |
| 1:X:131:ASN:ND2  | 1:X:139:ASN:HD21 | 1.93                     | 0.48              |
| 1:N:113:ILE:HG21 | 1:N:151:ILE:HG13 | 1.95                     | 0.48              |
| 1:F:65:ASN:CG    | 1:F:80:HIS:HD2   | 2.21                     | 0.47              |
| 1:J:79:ARG:NH2   | 1:J:101:ASP:OD1  | 2.36                     | 0.47              |
| 1:S:65:ASN:CG    | 1:S:80:HIS:CD2   | 2.92                     | 0.47              |
| 1:V:121:GLU:HA   | 1:V:144:LEU:HD11 | 1.96                     | 0.47              |
| 1:C:5:VAL:HB     | 1:C:152:ALA:HB2  | 1.95                     | 0.47              |
| 1:H:46:HIS:CE1   | 1:H:120:HIS:CD2  | 3.02                     | 0.47              |
| 1:K:14:VAL:HG21  | 1:K:144:LEU:HB3  | 1.96                     | 0.47              |
| 1:A:133:GLU:HB3  | 1:A:139:ASN:ND2  | 2.29                     | 0.47              |
| 1:B:131:ASN:HD21 | 1:B:139:ASN:HD21 | 1.62                     | 0.47              |
| 1:F:64:PHE:O     | 1:F:80:HIS:HB3   | 2.14                     | 0.47              |
| 1:M:113:ILE:HG22 | 4:N:308:HOH:O    | 2.15                     | 0.47              |
| 1:T:79:ARG:NH2   | 1:T:101:ASP:OD1  | 2.47                     | 0.47              |
| 1:V:101:ASP:HB3  | 1:V:104:ILE:HG12 | 1.96                     | 0.47              |
| 1:U:46:HIS:NE2   | 1:U:124:ASP:OD2  | 2.46                     | 0.47              |
| 1:D:46:HIS:NE2   | 1:D:124:ASP:OD2  | 2.37                     | 0.47              |
| 1:O:79:ARG:NH2   | 1:O:101:ASP:OD1  | 2.46                     | 0.47              |
| 1:F:79:ARG:HH22  | 1:F:101:ASP:CG   | 2.23                     | 0.47              |
| 1:L:2:ASP:HB2    | 4:L:308:HOH:O    | 2.14                     | 0.47              |
| 1:S:131:ASN:OD1  | 1:S:139:ASN:ND2  | 2.48                     | 0.46              |
| 1:K:79:ARG:HH22  | 1:K:101:ASP:CG   | 2.22                     | 0.46              |
| 1:K:120:HIS:HE1  | 1:K:143:ARG:HG2  | 1.77                     | 0.46              |
| 1:T:125:ASP:OD1  | 1:T:125:ASP:C    | 2.58                     | 0.46              |
| 1:W:14:VAL:HG21  | 1:W:144:LEU:HB3  | 1.96                     | 0.46              |
| 1:L:8:LEU:HD22   | 1:L:146:CYS:HA   | 1.96                     | 0.46              |
| 1:L:63:HIS:H     | 1:L:63:HIS:CD2   | 2.33                     | 0.46              |
| 1:S:112:ILE:HD12 | 1:S:149:ILE:HD13 | 1.97                     | 0.46              |
| 1:V:81:VAL:HG13  | 1:V:103:VAL:HG12 | 1.96                     | 0.46              |
| 1:B:18:ILE:HD13  | 1:B:33:GLY:HA3   | 1.98                     | 0.46              |
| 1:F:8:LEU:HD21   | 1:F:117:LEU:HD23 | 1.97                     | 0.46              |
| 1:F:20:PHE:HA    | 1:F:30:LYS:O     | 2.16                     | 0.46              |
| 1:A:75:LYS:HG3   | 1:K:128:LYS:CA   | 2.35                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:81:VAL:HG23  | 4:H:309:HOH:O    | 2.15                     | 0.46              |
| 1:J:125:ASP:OD1  | 1:J:125:ASP:C    | 2.59                     | 0.46              |
| 1:N:65:ASN:CG    | 1:N:80:HIS:HD2   | 2.23                     | 0.46              |
| 1:B:79:ARG:NH2   | 1:B:101:ASP:OD1  | 2.49                     | 0.46              |
| 1:I:79:ARG:CD    | 1:I:80:HIS:O     | 2.63                     | 0.46              |
| 1:X:101:ASP:HB3  | 1:X:104:ILE:HG12 | 1.97                     | 0.46              |
| 1:B:32:TRP:HA    | 1:B:97:VAL:O     | 2.16                     | 0.46              |
| 1:C:79:ARG:NH2   | 1:C:101:ASP:OD1  | 2.49                     | 0.46              |
| 1:N:65:ASN:CG    | 1:N:80:HIS:CD2   | 2.94                     | 0.46              |
| 1:E:131:ASN:OD1  | 1:E:134:SER:N    | 2.49                     | 0.46              |
| 1:P:48:HIS:CD2   | 1:P:118:VAL:HB   | 2.51                     | 0.46              |
| 1:Q:121:GLU:HA   | 1:Q:144:LEU:HD11 | 1.97                     | 0.46              |
| 1:L:1:ALA:N      | 1:L:23:LYS:HA    | 2.30                     | 0.46              |
| 1:L:46:HIS:CE1   | 1:L:120:HIS:CD2  | 3.03                     | 0.45              |
| 1:V:53:ASN:ND2   | 1:V:56:GLY:O     | 2.48                     | 0.45              |
| 1:W:116:THR:CG2  | 1:W:146:CYS:HB2  | 2.46                     | 0.45              |
| 1:X:133:GLU:HA   | 1:X:136:LYS:HE2  | 1.98                     | 0.45              |
| 1:N:101:ASP:HB3  | 1:N:104:ILE:HG12 | 1.99                     | 0.45              |
| 1:P:38:LEU:O     | 1:P:93:GLY:HA2   | 2.16                     | 0.45              |
| 1:S:124:ASP:OD1  | 1:S:138:GLY:HA3  | 2.15                     | 0.45              |
| 1:B:71:HIS:HB2   | 1:B:80:HIS:CE1   | 2.51                     | 0.45              |
| 1:D:46:HIS:ND1   | 1:D:120:HIS:CD2  | 2.85                     | 0.45              |
| 1:J:79:ARG:HD2   | 1:J:80:HIS:O     | 2.15                     | 0.45              |
| 1:U:4:ALA:HB3    | 1:U:20:PHE:HB2   | 1.99                     | 0.45              |
| 1:N:109:ASP:C    | 1:N:111:CYS:H    | 2.25                     | 0.45              |
| 1:E:130:GLY:HA2  | 1:G:75:LYS:HE2   | 1.99                     | 0.45              |
| 1:I:73:GLY:HA2   | 1:I:126:LEU:HD22 | 1.98                     | 0.45              |
| 1:N:21:GLU:HB2   | 1:N:32:TRP:CZ3   | 2.52                     | 0.45              |
| 1:V:22:GLN:HG2   | 1:V:24:GLU:O     | 2.15                     | 0.45              |
| 1:K:96:ASP:O     | 1:L:131:ASN:HB3  | 2.16                     | 0.45              |
| 1:U:79:ARG:HD3   | 1:U:80:HIS:O     | 2.17                     | 0.45              |
| 1:F:71:HIS:HB2   | 1:F:80:HIS:CE1   | 2.51                     | 0.45              |
| 1:Q:79:ARG:HD2   | 1:Q:80:HIS:O     | 2.16                     | 0.45              |
| 1:S:7:VAL:O      | 1:S:147:GLY:HA3  | 2.17                     | 0.45              |
| 1:S:101:ASP:HB3  | 1:S:104:ILE:HG12 | 1.98                     | 0.45              |
| 1:O:38:LEU:O     | 1:O:93:GLY:HA2   | 2.17                     | 0.45              |
| 1:P:79:ARG:CD    | 1:P:80:HIS:O     | 2.64                     | 0.45              |
| 1:A:22:GLN:HG2   | 1:A:24:GLU:O     | 2.18                     | 0.44              |
| 1:N:13:PRO:HD3   | 1:Q:11:ASP:O     | 2.18                     | 0.44              |
| 1:N:65:ASN:OD1   | 1:N:80:HIS:HD2   | 1.99                     | 0.44              |
| 1:N:113:ILE:HG22 | 4:N:308:HOH:O    | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:44:GLY:O     | 1:P:119:VAL:HA   | 2.17                     | 0.44              |
| 1:T:81:VAL:HG11  | 1:T:110:HIS:HB3  | 1.99                     | 0.44              |
| 1:L:72:GLY:O     | 1:L:83:ASP:HB3   | 2.17                     | 0.44              |
| 1:C:118:VAL:HG11 | 1:C:143:ARG:HG2  | 1.99                     | 0.44              |
| 1:Q:71:HIS:HB2   | 1:Q:80:HIS:HE1   | 1.79                     | 0.44              |
| 1:T:79:ARG:HD2   | 1:T:80:HIS:O     | 2.17                     | 0.44              |
| 1:N:53:ASN:HB3   | 4:N:327:HOH:O    | 2.17                     | 0.44              |
| 1:T:5:VAL:HG23   | 1:T:19:ASN:HD22  | 1.82                     | 0.44              |
| 1:T:121:GLU:HG2  | 1:T:142:SER:N    | 2.32                     | 0.44              |
| 1:E:73:GLY:CA    | 1:E:126:LEU:HD22 | 2.48                     | 0.44              |
| 1:R:121:GLU:HG2  | 1:R:142:SER:H    | 1.83                     | 0.44              |
| 1:J:108:GLY:O    | 1:J:111:CYS:HB2  | 2.18                     | 0.44              |
| 1:T:79:ARG:HD3   | 1:T:83:ASP:HB2   | 2.00                     | 0.44              |
| 1:O:131:ASN:ND2  | 1:P:88:THR:HB    | 2.33                     | 0.44              |
| 1:S:73:GLY:HA2   | 1:S:126:LEU:HD22 | 2.00                     | 0.44              |
| 1:X:91:LYS:H     | 1:X:91:LYS:HG3   | 1.50                     | 0.44              |
| 1:J:125:ASP:OD2  | 1:J:134:SER:OG   | 2.25                     | 0.44              |
| 1:Q:74:PRO:HD3   | 1:Q:85:GLY:CA    | 2.48                     | 0.44              |
| 1:W:6:CYS:HB2    | 1:W:149:ILE:HA   | 2.00                     | 0.44              |
| 1:M:7:VAL:CG1    | 1:M:9:LYS:HE2    | 2.49                     | 0.43              |
| 1:Q:32:TRP:HA    | 1:Q:97:VAL:O     | 2.17                     | 0.43              |
| 1:E:55:ALA:HB3   | 1:E:59:SER:OG    | 2.17                     | 0.43              |
| 1:J:47:VAL:HB    | 1:J:82:GLY:HA2   | 2.00                     | 0.43              |
| 1:K:65:ASN:HB2   | 1:K:80:HIS:HB3   | 2.00                     | 0.43              |
| 1:C:122:LYS:HE3  | 1:C:141:GLY:HA3  | 1.99                     | 0.43              |
| 1:V:19:ASN:O     | 1:V:31:VAL:HA    | 2.18                     | 0.43              |
| 1:I:80:HIS:N     | 1:I:83:ASP:OD2   | 2.50                     | 0.43              |
| 1:J:20:PHE:N     | 1:J:20:PHE:CD1   | 2.86                     | 0.43              |
| 1:R:51:GLY:HA2   | 1:R:116:THR:OG1  | 2.19                     | 0.43              |
| 1:D:1:ALA:N      | 1:D:23:LYS:HA    | 2.33                     | 0.43              |
| 1:I:50:PHE:O     | 1:I:60:ALA:HA    | 2.18                     | 0.43              |
| 1:K:80:HIS:N     | 1:K:83:ASP:OD2   | 2.44                     | 0.43              |
| 1:Q:39:THR:O     | 1:Q:43:HIS:NE2   | 2.32                     | 0.43              |
| 1:F:98:SER:O     | 1:G:131:ASN:HA   | 2.19                     | 0.43              |
| 1:V:32:TRP:HA    | 1:V:97:VAL:O     | 2.19                     | 0.43              |
| 1:E:54:THR:HG22  | 1:J:17:ILE:HG12  | 2.01                     | 0.43              |
| 1:O:13:PRO:HG3   | 1:R:39:THR:HG22  | 2.01                     | 0.43              |
| 1:C:101:ASP:HB3  | 1:C:104:ILE:HG12 | 2.01                     | 0.43              |
| 1:D:116:THR:CG2  | 1:D:146:CYS:HB2  | 2.48                     | 0.43              |
| 1:V:20:PHE:HZ    | 1:V:117:LEU:HD22 | 1.84                     | 0.43              |
| 1:X:53:ASN:HB3   | 4:X:316:HOH:O    | 2.18                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:I:79:ARG:NH2  | 1:I:101:ASP:OD1  | 2.42                     | 0.42              |
| 1:O:63:HIS:CD2  | 1:O:63:HIS:H     | 2.37                     | 0.42              |
| 1:B:84:LEU:HD21 | 1:B:104:ILE:HD13 | 2.01                     | 0.42              |
| 1:I:21:GLU:HB2  | 1:I:32:TRP:HZ3   | 1.84                     | 0.42              |
| 1:V:44:GLY:CA   | 1:V:120:HIS:HB2  | 2.49                     | 0.42              |
| 1:G:2:ASP:O     | 1:G:21:GLU:HA    | 2.19                     | 0.42              |
| 1:M:79:ARG:NH2  | 1:M:101:ASP:OD1  | 2.51                     | 0.42              |
| 1:Q:22:GLN:HG3  | 1:Q:29:VAL:HG22  | 2.01                     | 0.42              |
| 1:V:38:LEU:HB3  | 1:V:43:HIS:NE2   | 2.34                     | 0.42              |
| 1:W:63:HIS:HE1  | 1:W:137:THR:O    | 2.02                     | 0.42              |
| 1:C:53:ASN:CG   | 1:C:53:ASN:O     | 2.62                     | 0.42              |
| 1:D:18:ILE:HD13 | 1:D:33:GLY:HA3   | 2.01                     | 0.42              |
| 1:G:125:ASP:OD1 | 1:G:134:SER:OG   | 2.37                     | 0.42              |
| 1:M:130:GLY:O   | 1:X:97:VAL:HA    | 2.20                     | 0.42              |
| 1:B:10:GLY:HA3  | 1:B:144:LEU:O    | 2.20                     | 0.42              |
| 1:B:73:GLY:HA3  | 1:B:126:LEU:HD13 | 2.01                     | 0.42              |
| 1:W:42:LEU:HB2  | 1:W:123:ALA:HB2  | 2.02                     | 0.42              |
| 1:I:8:LEU:O     | 1:I:9:LYS:HG3    | 2.20                     | 0.42              |
| 1:I:120:HIS:CE1 | 1:I:143:ARG:HG2  | 2.54                     | 0.42              |
| 1:O:22:GLN:HG2  | 1:O:24:GLU:O     | 2.20                     | 0.42              |
| 1:A:148:VAL:HB  | 1:B:148:VAL:HB   | 2.02                     | 0.42              |
| 1:B:8:LEU:HD22  | 1:B:146:CYS:HA   | 2.00                     | 0.42              |
| 1:B:120:HIS:CB  | 1:B:140:ALA:HB1  | 2.50                     | 0.42              |
| 1:I:51:GLY:HA2  | 1:I:116:THR:OG1  | 2.20                     | 0.42              |
| 1:V:55:ALA:HB3  | 1:V:59:SER:HB3   | 2.00                     | 0.42              |
| 1:B:28:PRO:HA   | 1:B:102:SER:HA   | 2.02                     | 0.42              |
| 1:H:42:LEU:HB2  | 1:H:123:ALA:HB2  | 2.02                     | 0.42              |
| 1:H:44:GLY:CA   | 1:H:120:HIS:HB2  | 2.48                     | 0.42              |
| 1:I:13:PRO:HG3  | 1:L:39:THR:CG2   | 2.50                     | 0.42              |
| 1:J:20:PHE:HZ   | 1:J:117:LEU:HD22 | 1.84                     | 0.42              |
| 1:K:4:ALA:HB3   | 1:K:20:PHE:HB2   | 2.02                     | 0.42              |
| 1:N:4:ALA:HB3   | 1:N:20:PHE:HB2   | 2.01                     | 0.42              |
| 1:U:101:ASP:HB3 | 1:U:104:ILE:HG12 | 2.01                     | 0.42              |
| 1:B:44:GLY:HA3  | 1:B:120:HIS:HB2  | 2.02                     | 0.41              |
| 1:A:81:VAL:HG23 | 4:A:301:HOH:O    | 2.18                     | 0.41              |
| 1:C:99:ILE:HG22 | 1:C:100:GLU:N    | 2.35                     | 0.41              |
| 1:I:134:SER:HA  | 1:I:138:GLY:HA2  | 2.03                     | 0.41              |
| 1:L:6:CYS:SG    | 1:L:117:LEU:HB3  | 2.60                     | 0.41              |
| 1:L:132:GLU:HG2 | 1:L:136:LYS:HE2  | 2.02                     | 0.41              |
| 1:N:91:LYS:HG3  | 4:N:330:HOH:O    | 2.19                     | 0.41              |
| 1:T:14:VAL:HG21 | 1:T:144:LEU:HB3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:79:ARG:NH2   | 1:D:101:ASP:OD1  | 2.51                     | 0.41              |
| 1:J:79:ARG:NH1   | 1:J:83:ASP:O     | 2.53                     | 0.41              |
| 1:S:32:TRP:HA    | 1:S:97:VAL:O     | 2.21                     | 0.41              |
| 1:I:63:HIS:CB    | 1:I:80:HIS:ND1   | 2.83                     | 0.41              |
| 1:K:72:GLY:HA3   | 1:K:78:GLU:O     | 2.20                     | 0.41              |
| 1:B:21:GLU:HB2   | 1:B:32:TRP:HZ3   | 1.84                     | 0.41              |
| 1:C:79:ARG:CD    | 1:C:80:HIS:O     | 2.65                     | 0.41              |
| 1:G:19:ASN:ND2   | 4:G:302:HOH:O    | 2.54                     | 0.41              |
| 1:H:20:PHE:CD2   | 1:H:31:VAL:HG22  | 2.56                     | 0.41              |
| 1:J:110:HIS:HB2  | 4:J:306:HOH:O    | 2.20                     | 0.41              |
| 1:K:35:ILE:HB    | 1:K:95:ALA:HB3   | 2.02                     | 0.41              |
| 1:L:96:ASP:HB3   | 4:L:324:HOH:O    | 2.21                     | 0.41              |
| 1:U:86:ASN:ND2   | 1:U:124:ASP:HB3  | 2.36                     | 0.41              |
| 1:X:120:HIS:HB3  | 1:X:140:ALA:O    | 2.21                     | 0.41              |
| 1:E:46:HIS:HB2   | 1:E:48:HIS:CD2   | 2.56                     | 0.41              |
| 1:E:63:HIS:CE1   | 1:E:137:THR:HA   | 2.56                     | 0.41              |
| 1:H:55:ALA:HB3   | 1:H:59:SER:OG    | 2.21                     | 0.41              |
| 1:J:125:ASP:OD1  | 1:J:127:GLY:N    | 2.51                     | 0.41              |
| 1:L:67:LEU:HD11  | 1:L:110:HIS:CE1  | 2.56                     | 0.41              |
| 1:M:47:VAL:HG11  | 1:M:112:ILE:CG2  | 2.50                     | 0.41              |
| 1:N:21:GLU:HB2   | 1:N:32:TRP:CH2   | 2.56                     | 0.41              |
| 1:E:124:ASP:C    | 1:E:126:LEU:H    | 2.29                     | 0.40              |
| 1:F:108:GLY:O    | 1:F:111:CYS:HB2  | 2.22                     | 0.40              |
| 1:A:54:THR:HG22  | 1:B:17:ILE:HG12  | 2.03                     | 0.40              |
| 1:J:79:ARG:HD3   | 1:J:83:ASP:HB2   | 2.03                     | 0.40              |
| 1:M:80:HIS:O     | 1:M:83:ASP:HB2   | 2.21                     | 0.40              |
| 1:S:120:HIS:ND1  | 1:S:141:GLY:O    | 2.52                     | 0.40              |
| 1:W:101:ASP:HB3  | 1:W:104:ILE:HG12 | 2.03                     | 0.40              |
| 1:X:71:HIS:HB2   | 1:X:80:HIS:CE1   | 2.56                     | 0.40              |
| 1:A:8:LEU:HA     | 1:A:146:CYS:O    | 2.21                     | 0.40              |
| 1:D:14:VAL:HG21  | 1:D:144:LEU:HB3  | 2.02                     | 0.40              |
| 1:E:50:PHE:C     | 1:E:52:ASP:H     | 2.29                     | 0.40              |
| 1:M:116:THR:CG2  | 1:M:146:CYS:HB2  | 2.51                     | 0.40              |
| 1:Q:135:THR:HG23 | 4:Q:308:HOH:O    | 2.20                     | 0.40              |
| 1:T:50:PHE:C     | 1:T:52:ASP:N     | 2.80                     | 0.40              |
| 1:C:13:PRO:CG    | 1:F:39:THR:HG22  | 2.46                     | 0.40              |
| 1:H:120:HIS:HB3  | 1:H:140:ALA:O    | 2.20                     | 0.40              |
| 1:O:76:ASP:O     | 1:O:79:ARG:HG2   | 2.21                     | 0.40              |
| 1:R:14:VAL:HG21  | 1:R:144:LEU:HB3  | 2.02                     | 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     | 151/153 (99%)   | 145 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 1   | B     | 151/153 (99%)   | 145 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 1   | C     | 151/153 (99%)   | 146 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 1   | D     | 151/153 (99%)   | 146 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 1   | E     | 151/153 (99%)   | 142 (94%)  | 9 (6%)   | 0        | 100         | 100 |
| 1   | F     | 151/153 (99%)   | 148 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 1   | G     | 151/153 (99%)   | 146 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 1   | H     | 151/153 (99%)   | 144 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 1   | I     | 151/153 (99%)   | 141 (93%)  | 10 (7%)  | 0        | 100         | 100 |
| 1   | J     | 151/153 (99%)   | 148 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 1   | K     | 151/153 (99%)   | 146 (97%)  | 4 (3%)   | 1 (1%)   | 18          | 14  |
| 1   | L     | 151/153 (99%)   | 146 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 1   | M     | 151/153 (99%)   | 146 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 1   | N     | 151/153 (99%)   | 144 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 1   | O     | 151/153 (99%)   | 145 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 1   | P     | 151/153 (99%)   | 149 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 1   | Q     | 151/153 (99%)   | 143 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 1   | R     | 151/153 (99%)   | 142 (94%)  | 9 (6%)   | 0        | 100         | 100 |
| 1   | S     | 151/153 (99%)   | 146 (97%)  | 4 (3%)   | 1 (1%)   | 18          | 14  |
| 1   | T     | 151/153 (99%)   | 142 (94%)  | 9 (6%)   | 0        | 100         | 100 |
| 1   | U     | 151/153 (99%)   | 143 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 1   | V     | 151/153 (99%)   | 145 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 1   | W     | 151/153 (99%)   | 145 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 1   | X     | 151/153 (99%)   | 146 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| All | All   | 3624/3672 (99%) | 3479 (96%) | 143 (4%) | 2 (0%)   | 48          | 46  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 140 | ALA  |
| 1   | S     | 149 | ILE  |

### 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     | 118/118 (100%) | 110 (93%) | 8 (7%)   | 14          | 11 |
| 1   | B     | 118/118 (100%) | 114 (97%) | 4 (3%)   | 32          | 33 |
| 1   | C     | 118/118 (100%) | 109 (92%) | 9 (8%)   | 12          | 9  |
| 1   | D     | 118/118 (100%) | 113 (96%) | 5 (4%)   | 26          | 25 |
| 1   | E     | 118/118 (100%) | 114 (97%) | 4 (3%)   | 32          | 33 |
| 1   | F     | 118/118 (100%) | 115 (98%) | 3 (2%)   | 42          | 45 |
| 1   | G     | 118/118 (100%) | 115 (98%) | 3 (2%)   | 42          | 45 |
| 1   | H     | 118/118 (100%) | 117 (99%) | 1 (1%)   | 73          | 80 |
| 1   | I     | 118/118 (100%) | 113 (96%) | 5 (4%)   | 26          | 25 |
| 1   | J     | 118/118 (100%) | 111 (94%) | 7 (6%)   | 18          | 14 |
| 1   | K     | 118/118 (100%) | 109 (92%) | 9 (8%)   | 12          | 9  |
| 1   | L     | 118/118 (100%) | 114 (97%) | 4 (3%)   | 32          | 33 |
| 1   | M     | 118/118 (100%) | 113 (96%) | 5 (4%)   | 26          | 25 |
| 1   | N     | 118/118 (100%) | 113 (96%) | 5 (4%)   | 26          | 25 |
| 1   | O     | 118/118 (100%) | 112 (95%) | 6 (5%)   | 21          | 19 |
| 1   | P     | 118/118 (100%) | 111 (94%) | 7 (6%)   | 18          | 14 |
| 1   | Q     | 118/118 (100%) | 112 (95%) | 6 (5%)   | 21          | 19 |
| 1   | R     | 118/118 (100%) | 115 (98%) | 3 (2%)   | 42          | 45 |
| 1   | S     | 118/118 (100%) | 114 (97%) | 4 (3%)   | 32          | 33 |
| 1   | T     | 118/118 (100%) | 116 (98%) | 2 (2%)   | 53          | 60 |
| 1   | U     | 118/118 (100%) | 114 (97%) | 4 (3%)   | 32          | 33 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | V     | 118/118 (100%)   | 116 (98%)  | 2 (2%)   | 53          | 60 |
| 1   | W     | 118/118 (100%)   | 116 (98%)  | 2 (2%)   | 53          | 60 |
| 1   | X     | 118/118 (100%)   | 110 (93%)  | 8 (7%)   | 14          | 11 |
| All | All   | 2832/2832 (100%) | 2716 (96%) | 116 (4%) | 27          | 26 |

All (116) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | ASP  |
| 1   | A     | 59  | SER  |
| 1   | A     | 79  | ARG  |
| 1   | A     | 98  | SER  |
| 1   | A     | 102 | SER  |
| 1   | A     | 113 | ILE  |
| 1   | A     | 134 | SER  |
| 1   | A     | 135 | THR  |
| 1   | B     | 2   | ASP  |
| 1   | B     | 24  | GLU  |
| 1   | B     | 68  | SER  |
| 1   | B     | 79  | ARG  |
| 1   | C     | 5   | VAL  |
| 1   | C     | 21  | GLU  |
| 1   | C     | 53  | ASN  |
| 1   | C     | 59  | SER  |
| 1   | C     | 77  | GLU  |
| 1   | C     | 79  | ARG  |
| 1   | C     | 92  | ASP  |
| 1   | C     | 109 | ASP  |
| 1   | C     | 113 | ILE  |
| 1   | D     | 36  | LYS  |
| 1   | D     | 59  | SER  |
| 1   | D     | 68  | SER  |
| 1   | D     | 79  | ARG  |
| 1   | D     | 135 | THR  |
| 1   | E     | 2   | ASP  |
| 1   | E     | 24  | GLU  |
| 1   | E     | 58  | THR  |
| 1   | E     | 105 | SER  |
| 1   | F     | 2   | ASP  |
| 1   | F     | 70  | LYS  |
| 1   | F     | 79  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 24  | GLU  |
| 1   | G     | 79  | ARG  |
| 1   | G     | 105 | SER  |
| 1   | H     | 46  | HIS  |
| 1   | I     | 2   | ASP  |
| 1   | I     | 39  | THR  |
| 1   | I     | 58  | THR  |
| 1   | I     | 79  | ARG  |
| 1   | I     | 96  | ASP  |
| 1   | J     | 20  | PHE  |
| 1   | J     | 77  | GLU  |
| 1   | J     | 79  | ARG  |
| 1   | J     | 87  | VAL  |
| 1   | J     | 105 | SER  |
| 1   | J     | 109 | ASP  |
| 1   | J     | 113 | ILE  |
| 1   | K     | 15  | GLN  |
| 1   | K     | 58  | THR  |
| 1   | K     | 59  | SER  |
| 1   | K     | 79  | ARG  |
| 1   | K     | 99  | ILE  |
| 1   | K     | 103 | VAL  |
| 1   | K     | 109 | ASP  |
| 1   | K     | 113 | ILE  |
| 1   | K     | 137 | THR  |
| 1   | L     | 67  | LEU  |
| 1   | L     | 79  | ARG  |
| 1   | L     | 113 | ILE  |
| 1   | L     | 121 | GLU  |
| 1   | M     | 59  | SER  |
| 1   | M     | 79  | ARG  |
| 1   | M     | 91  | LYS  |
| 1   | M     | 112 | ILE  |
| 1   | M     | 131 | ASN  |
| 1   | N     | 59  | SER  |
| 1   | N     | 77  | GLU  |
| 1   | N     | 79  | ARG  |
| 1   | N     | 91  | LYS  |
| 1   | N     | 122 | LYS  |
| 1   | O     | 11  | ASP  |
| 1   | O     | 39  | THR  |
| 1   | O     | 77  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 79  | ARG  |
| 1   | O     | 91  | LYS  |
| 1   | O     | 122 | LYS  |
| 1   | P     | 9   | LYS  |
| 1   | P     | 59  | SER  |
| 1   | P     | 77  | GLU  |
| 1   | P     | 79  | ARG  |
| 1   | P     | 91  | LYS  |
| 1   | P     | 102 | SER  |
| 1   | P     | 109 | ASP  |
| 1   | Q     | 26  | ASN  |
| 1   | Q     | 58  | THR  |
| 1   | Q     | 59  | SER  |
| 1   | Q     | 77  | GLU  |
| 1   | Q     | 109 | ASP  |
| 1   | Q     | 135 | THR  |
| 1   | R     | 24  | GLU  |
| 1   | R     | 58  | THR  |
| 1   | R     | 135 | THR  |
| 1   | S     | 24  | GLU  |
| 1   | S     | 46  | HIS  |
| 1   | S     | 79  | ARG  |
| 1   | S     | 131 | ASN  |
| 1   | T     | 58  | THR  |
| 1   | T     | 59  | SER  |
| 1   | U     | 59  | SER  |
| 1   | U     | 79  | ARG  |
| 1   | U     | 80  | HIS  |
| 1   | U     | 135 | THR  |
| 1   | V     | 2   | ASP  |
| 1   | V     | 26  | ASN  |
| 1   | W     | 77  | GLU  |
| 1   | W     | 79  | ARG  |
| 1   | X     | 7   | VAL  |
| 1   | X     | 8   | LEU  |
| 1   | X     | 39  | THR  |
| 1   | X     | 77  | GLU  |
| 1   | X     | 79  | ARG  |
| 1   | X     | 91  | LYS  |
| 1   | X     | 121 | GLU  |
| 1   | X     | 132 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | GLN  |
| 1   | A     | 19  | ASN  |
| 1   | A     | 131 | ASN  |
| 1   | A     | 139 | ASN  |
| 1   | B     | 19  | ASN  |
| 1   | B     | 53  | ASN  |
| 1   | B     | 139 | ASN  |
| 1   | C     | 19  | ASN  |
| 1   | C     | 80  | HIS  |
| 1   | D     | 15  | GLN  |
| 1   | D     | 80  | HIS  |
| 1   | D     | 139 | ASN  |
| 1   | E     | 19  | ASN  |
| 1   | G     | 19  | ASN  |
| 1   | H     | 53  | ASN  |
| 1   | J     | 53  | ASN  |
| 1   | K     | 139 | ASN  |
| 1   | L     | 15  | GLN  |
| 1   | L     | 53  | ASN  |
| 1   | L     | 80  | HIS  |
| 1   | M     | 131 | ASN  |
| 1   | M     | 139 | ASN  |
| 1   | N     | 110 | HIS  |
| 1   | O     | 19  | ASN  |
| 1   | P     | 19  | ASN  |
| 1   | P     | 139 | ASN  |
| 1   | Q     | 19  | ASN  |
| 1   | R     | 19  | ASN  |
| 1   | R     | 53  | ASN  |
| 1   | R     | 110 | HIS  |
| 1   | S     | 19  | ASN  |
| 1   | S     | 53  | ASN  |
| 1   | S     | 80  | HIS  |
| 1   | S     | 139 | ASN  |
| 1   | T     | 19  | ASN  |
| 1   | U     | 26  | ASN  |
| 1   | U     | 53  | ASN  |
| 1   | U     | 80  | HIS  |
| 1   | V     | 53  | ASN  |
| 1   | V     | 80  | HIS  |
| 1   | W     | 26  | ASN  |
| 1   | X     | 139 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 153/153 (100%) | -0.95  | 0 100 100 | 23, 32, 43, 46        | 0     |
| 1   | B     | 153/153 (100%) | -0.82  | 0 100 100 | 24, 36, 47, 52        | 0     |
| 1   | C     | 153/153 (100%) | -0.78  | 0 100 100 | 24, 36, 48, 58        | 0     |
| 1   | D     | 153/153 (100%) | -0.92  | 0 100 100 | 24, 33, 44, 49        | 0     |
| 1   | E     | 153/153 (100%) | -0.85  | 0 100 100 | 28, 37, 46, 55        | 0     |
| 1   | F     | 153/153 (100%) | -0.78  | 0 100 100 | 27, 37, 47, 56        | 0     |
| 1   | G     | 153/153 (100%) | -0.89  | 0 100 100 | 26, 36, 45, 52        | 0     |
| 1   | H     | 153/153 (100%) | -0.81  | 0 100 100 | 25, 36, 47, 54        | 0     |
| 1   | I     | 153/153 (100%) | -0.76  | 0 100 100 | 25, 37, 49, 54        | 0     |
| 1   | J     | 153/153 (100%) | -0.91  | 0 100 100 | 25, 34, 44, 58        | 0     |
| 1   | K     | 153/153 (100%) | -0.87  | 0 100 100 | 25, 36, 47, 53        | 0     |
| 1   | L     | 153/153 (100%) | -0.78  | 0 100 100 | 27, 36, 44, 48        | 0     |
| 1   | M     | 153/153 (100%) | -0.93  | 0 100 100 | 22, 32, 43, 49        | 0     |
| 1   | N     | 153/153 (100%) | -0.86  | 0 100 100 | 24, 35, 49, 58        | 0     |
| 1   | O     | 153/153 (100%) | -0.81  | 0 100 100 | 27, 36, 46, 54        | 0     |
| 1   | P     | 153/153 (100%) | -0.84  | 0 100 100 | 26, 35, 46, 53        | 0     |
| 1   | Q     | 153/153 (100%) | -0.87  | 0 100 100 | 26, 36, 43, 47        | 0     |
| 1   | R     | 153/153 (100%) | -0.78  | 0 100 100 | 25, 37, 46, 53        | 0     |
| 1   | S     | 153/153 (100%) | -0.92  | 0 100 100 | 24, 34, 43, 49        | 0     |
| 1   | T     | 153/153 (100%) | -0.88  | 0 100 100 | 26, 36, 50, 55        | 0     |
| 1   | U     | 153/153 (100%) | -0.77  | 0 100 100 | 25, 35, 47, 51        | 0     |
| 1   | V     | 153/153 (100%) | -0.93  | 0 100 100 | 24, 32, 42, 46        | 0     |
| 1   | W     | 153/153 (100%) | -0.84  | 0 100 100 | 28, 37, 49, 57        | 0     |
| 1   | X     | 153/153 (100%) | -0.77  | 0 100 100 | 26, 37, 47, 52        | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|-----------|-----------------------|-------|
| All | All   | 3672/3672 (100%) | -0.85  | 0 100 100 | 22, 35, 46, 58        | 0     |

There are no RSRZ outliers to report.

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | CU   | D     | 201 | 1/1   | 0.99 | 0.02 | 36,36,36,36                | 0     |
| 2   | CU   | J     | 201 | 1/1   | 0.99 | 0.03 | 36,36,36,36                | 0     |
| 2   | CU   | K     | 201 | 1/1   | 0.99 | 0.02 | 34,34,34,34                | 0     |
| 2   | CU   | P     | 201 | 1/1   | 0.99 | 0.03 | 33,33,33,33                | 0     |
| 2   | CU   | U     | 201 | 1/1   | 0.99 | 0.03 | 32,32,32,32                | 0     |
| 3   | ZN   | H     | 202 | 1/1   | 0.99 | 0.02 | 36,36,36,36                | 0     |
| 3   | ZN   | M     | 202 | 1/1   | 0.99 | 0.02 | 33,33,33,33                | 0     |
| 3   | ZN   | O     | 202 | 1/1   | 0.99 | 0.02 | 38,38,38,38                | 0     |
| 2   | CU   | I     | 201 | 1/1   | 1.00 | 0.02 | 44,44,44,44                | 0     |
| 2   | CU   | B     | 201 | 1/1   | 1.00 | 0.01 | 38,38,38,38                | 0     |
| 2   | CU   | C     | 201 | 1/1   | 1.00 | 0.01 | 35,35,35,35                | 0     |
| 2   | CU   | L     | 201 | 1/1   | 1.00 | 0.04 | 31,31,31,31                | 0     |
| 2   | CU   | M     | 201 | 1/1   | 1.00 | 0.01 | 34,34,34,34                | 0     |
| 2   | CU   | N     | 201 | 1/1   | 1.00 | 0.01 | 40,40,40,40                | 0     |
| 2   | CU   | O     | 201 | 1/1   | 1.00 | 0.02 | 35,35,35,35                | 0     |
| 2   | CU   | A     | 201 | 1/1   | 1.00 | 0.01 | 38,38,38,38                | 0     |
| 2   | CU   | Q     | 201 | 1/1   | 1.00 | 0.01 | 34,34,34,34                | 0     |
| 2   | CU   | R     | 201 | 1/1   | 1.00 | 0.02 | 37,37,37,37                | 0     |
| 2   | CU   | S     | 201 | 1/1   | 1.00 | 0.02 | 30,30,30,30                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | CU   | T     | 201 | 1/1   | 1.00 | 0.02 | 35,35,35,35                 | 0     |
| 2   | CU   | E     | 201 | 1/1   | 1.00 | 0.02 | 33,33,33,33                 | 0     |
| 2   | CU   | V     | 201 | 1/1   | 1.00 | 0.01 | 31,31,31,31                 | 0     |
| 2   | CU   | W     | 201 | 1/1   | 1.00 | 0.01 | 39,39,39,39                 | 0     |
| 2   | CU   | X     | 201 | 1/1   | 1.00 | 0.02 | 35,35,35,35                 | 0     |
| 3   | ZN   | A     | 202 | 1/1   | 1.00 | 0.01 | 30,30,30,30                 | 0     |
| 3   | ZN   | B     | 202 | 1/1   | 1.00 | 0.02 | 30,30,30,30                 | 0     |
| 3   | ZN   | C     | 202 | 1/1   | 1.00 | 0.01 | 26,26,26,26                 | 0     |
| 3   | ZN   | D     | 202 | 1/1   | 1.00 | 0.01 | 28,28,28,28                 | 0     |
| 3   | ZN   | E     | 202 | 1/1   | 1.00 | 0.02 | 33,33,33,33                 | 0     |
| 3   | ZN   | F     | 202 | 1/1   | 1.00 | 0.01 | 31,31,31,31                 | 0     |
| 3   | ZN   | G     | 202 | 1/1   | 1.00 | 0.01 | 32,32,32,32                 | 0     |
| 2   | CU   | F     | 201 | 1/1   | 1.00 | 0.04 | 35,35,35,35                 | 0     |
| 3   | ZN   | I     | 202 | 1/1   | 1.00 | 0.01 | 32,32,32,32                 | 0     |
| 3   | ZN   | J     | 202 | 1/1   | 1.00 | 0.02 | 32,32,32,32                 | 0     |
| 3   | ZN   | K     | 202 | 1/1   | 1.00 | 0.01 | 37,37,37,37                 | 0     |
| 3   | ZN   | L     | 202 | 1/1   | 1.00 | 0.01 | 32,32,32,32                 | 0     |
| 2   | CU   | G     | 201 | 1/1   | 1.00 | 0.02 | 37,37,37,37                 | 0     |
| 3   | ZN   | N     | 202 | 1/1   | 1.00 | 0.01 | 31,31,31,31                 | 0     |
| 2   | CU   | H     | 201 | 1/1   | 1.00 | 0.02 | 33,33,33,33                 | 0     |
| 3   | ZN   | P     | 202 | 1/1   | 1.00 | 0.01 | 31,31,31,31                 | 0     |
| 3   | ZN   | Q     | 202 | 1/1   | 1.00 | 0.01 | 33,33,33,33                 | 0     |
| 3   | ZN   | R     | 202 | 1/1   | 1.00 | 0.02 | 32,32,32,32                 | 0     |
| 3   | ZN   | S     | 202 | 1/1   | 1.00 | 0.01 | 31,31,31,31                 | 0     |
| 3   | ZN   | T     | 202 | 1/1   | 1.00 | 0.02 | 36,36,36,36                 | 0     |
| 3   | ZN   | U     | 202 | 1/1   | 1.00 | 0.01 | 31,31,31,31                 | 0     |
| 3   | ZN   | V     | 202 | 1/1   | 1.00 | 0.01 | 37,37,37,37                 | 0     |
| 3   | ZN   | W     | 202 | 1/1   | 1.00 | 0.01 | 37,37,37,37                 | 0     |
| 3   | ZN   | X     | 202 | 1/1   | 1.00 | 0.01 | 36,36,36,36                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.