



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:34 AM UTC

PDB ID : 5JK7 / pdb\_00005jk7  
Title : The X-ray structure of the DDB1-DCAF1-Vpr-UNG2 complex  
Authors : Calero, G.; Ahn, J.; Wu, Y.  
Deposited on : 2016-04-26  
Resolution : 3.49 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                                                             |

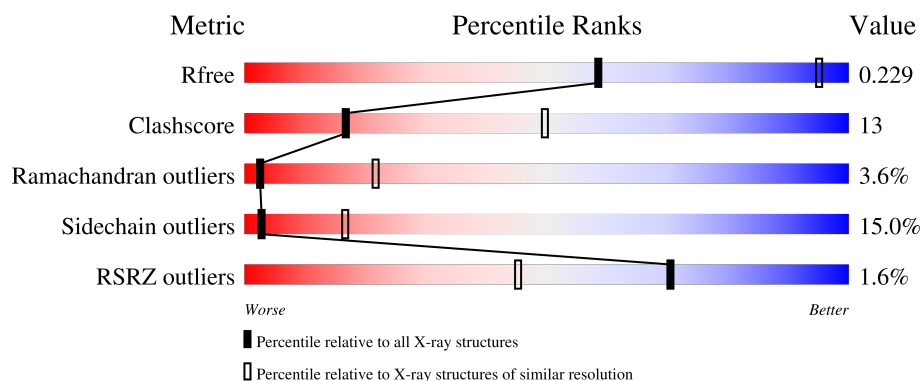
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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                      | 1085 (3.54-3.46)                                      |
| Clashscore            | 190562                      | 1140 (3.54-3.46)                                      |
| Ramachandran outliers | 187476                      | 1113 (3.54-3.46)                                      |
| Sidechain outliers    | 187428                      | 1114 (3.54-3.46)                                      |
| RSRZ outliers         | 180081                      | 1084 (3.54-3.46)                                      |

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     | 1140   | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 6%, yellow 31%, green 63%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>6%</span> <span>31%</span> <span>63%</span> </div> </div>           |
| 1   | B     | 1140   | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 6%, yellow 26%, green 68%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>6%</span> <span>26%</span> <span>68%</span> </div> </div>           |
| 2   | C     | 361    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 11%, yellow 35%, green 44%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>8%</span> <span>35%</span> <span>44%</span> </div> </div> |
| 2   | E     | 361    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 9%, yellow 32%, green 50%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>8%</span> <span>32%</span> <span>50%</span> </div> </div>  |
| 3   | D     | 222    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 27%, green 66%, orange 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>27%</span> <span>5%</span> <span>66%</span> </div> </div>                                   |

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| Mol | Chain | Length | Quality of chain                                                                                         |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------|
| 3   | G     | 222    | <div><div></div><div>64%</div><div>29%</div><div>7%</div></div>                                          |
| 4   | F     | 96     | <div>%<div><div></div><div>22%</div><div>21%</div><div>22%</div><div>12%</div><div>23%</div></div></div> |
| 4   | H     | 96     | <div><div></div><div>24%</div><div>31%</div><div>15%</div><div>7%</div><div>23%</div></div>              |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27684 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 DNA damage-binding protein 1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1133     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8865  | 5619 | 1486 | 1711 | 49 |         |         |       |
| 1   | B     | 1133     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8703  | 5541 | 1450 | 1663 | 49 |         |         |       |

- Molecule 2 is a protein called Protein VPRBP.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | C     | 331      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2635  | 1666 | 457 | 494 | 18 |         |         |       |
| 2   | E     | 331      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2635  | 1666 | 457 | 494 | 18 |         |         |       |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 1044    | ALA      | -      | expression tag | UNP Q9Y4B6 |
| C     | 1397    | LEU      | -      | expression tag | UNP Q9Y4B6 |
| C     | 1398    | GLU      | -      | expression tag | UNP Q9Y4B6 |
| C     | 1399    | HIS      | -      | expression tag | UNP Q9Y4B6 |
| C     | 1400    | HIS      | -      | expression tag | UNP Q9Y4B6 |
| C     | 1401    | HIS      | -      | expression tag | UNP Q9Y4B6 |
| C     | 1402    | HIS      | -      | expression tag | UNP Q9Y4B6 |
| C     | 1403    | HIS      | -      | expression tag | UNP Q9Y4B6 |
| C     | 1404    | HIS      | -      | expression tag | UNP Q9Y4B6 |
| E     | 1044    | ALA      | -      | expression tag | UNP Q9Y4B6 |
| E     | 1397    | LEU      | -      | expression tag | UNP Q9Y4B6 |
| E     | 1398    | GLU      | -      | expression tag | UNP Q9Y4B6 |
| E     | 1399    | HIS      | -      | expression tag | UNP Q9Y4B6 |
| E     | 1400    | HIS      | -      | expression tag | UNP Q9Y4B6 |
| E     | 1401    | HIS      | -      | expression tag | UNP Q9Y4B6 |
| E     | 1402    | HIS      | -      | expression tag | UNP Q9Y4B6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 1403    | HIS      | -      | expression tag | UNP Q9Y4B6 |
| E     | 1404    | HIS      | -      | expression tag | UNP Q9Y4B6 |

- Molecule 3 is a protein called Uracil-DNA glycosylase.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | D     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1791  | 1158 | 316 | 312 | 5 |         |         |       |
| 3   | G     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1791  | 1158 | 316 | 312 | 5 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | 83      | VAL      | -      | expression tag | UNP P13051 |
| D     | 84      | PHE      | -      | expression tag | UNP P13051 |
| G     | 83      | VAL      | -      | expression tag | UNP P13051 |
| G     | 84      | PHE      | -      | expression tag | UNP P13051 |

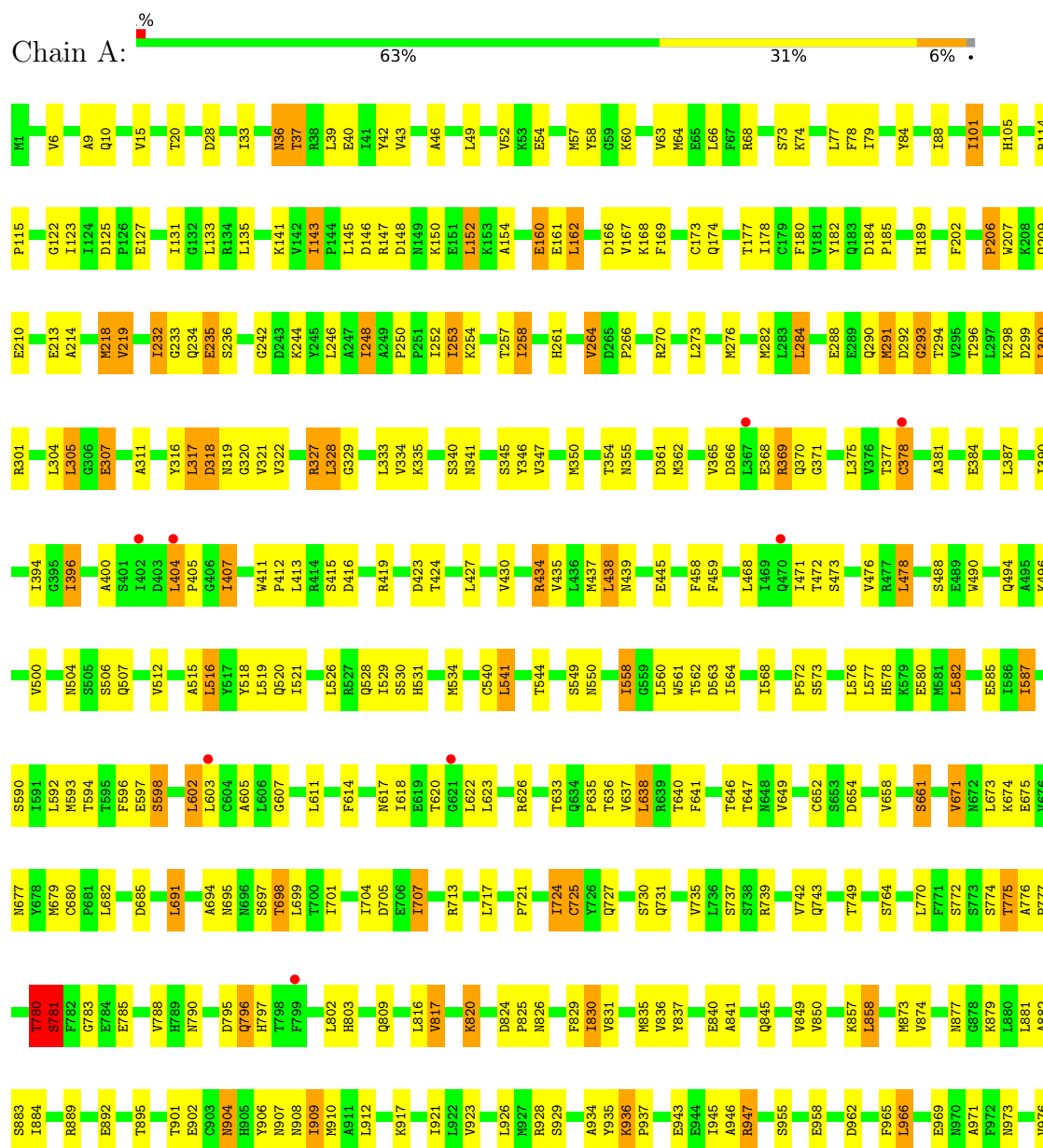
- Molecule 4 is a protein called Protein Vpr.

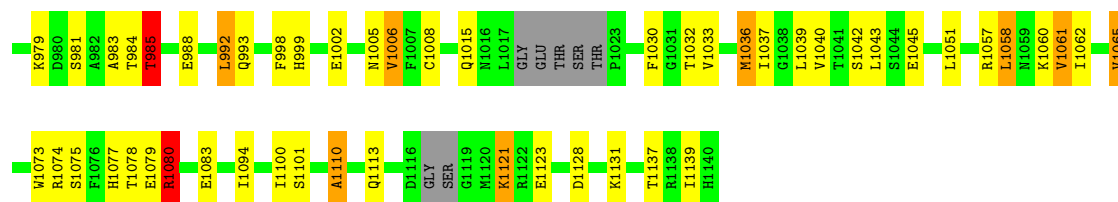
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | F     | 74       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 632   | 409 | 109 | 113 | 1 |         |         |       |
| 4   | H     | 74       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 632   | 409 | 109 | 113 | 1 |         |         |       |

### 3 Residue-property plots

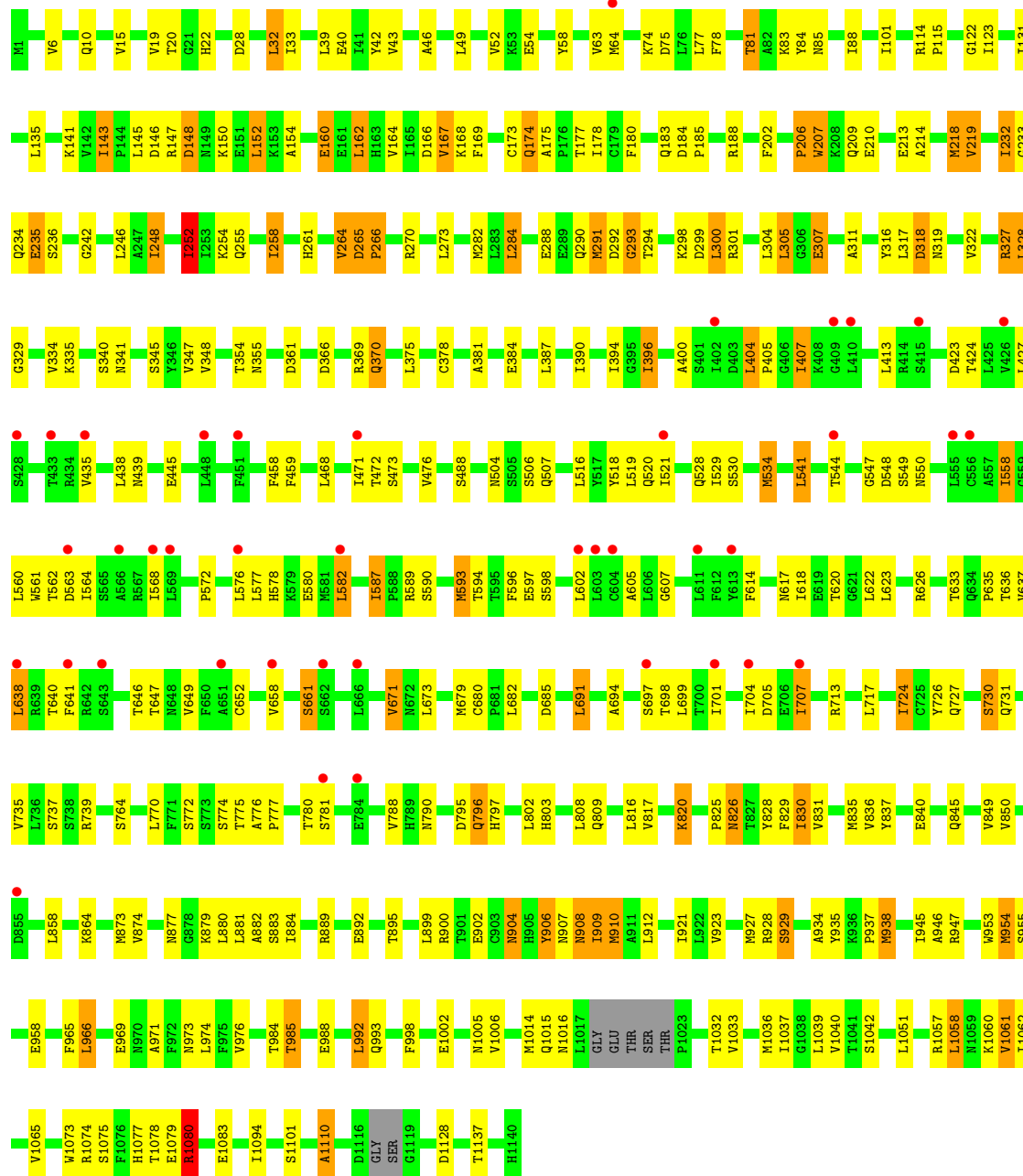
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: DNA damage-binding protein 1

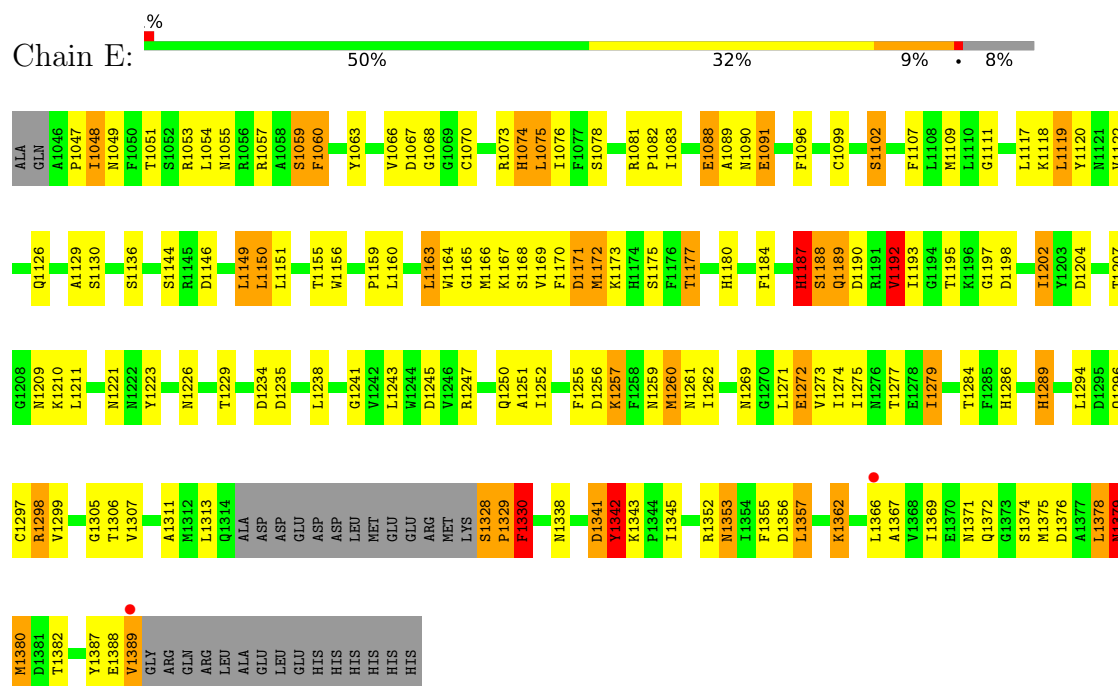




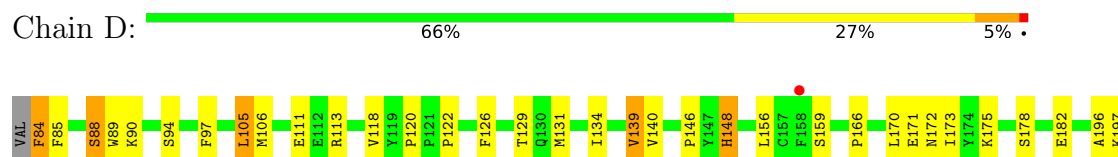
• Molecule 1: DNA damage-binding protein 1



• Molecule 2: Protein VPRBP



- Molecule 3: Uracil-DNA glycosylase







## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 119.90Å 128.20Å 129.20Å<br>75.11° 89.44° 65.37°             | Depositor        |
| Resolution (Å)                                                          | 40.30 – 3.49<br>40.30 – 3.49                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.6 (40.30-3.49)<br>90.5 (40.30-3.49)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.98 (at 3.48Å)                                             | Xtriage          |
| Refinement program                                                      | BUSTER 2.10.0                                               | Depositor        |
| R, $R_{free}$                                                           | 0.176 , 0.206<br>0.199 , 0.229                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2463 reflections (3.19%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 144.6                                                       | Xtriage          |
| Anisotropy                                                              | 0.404                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 156.3                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 27684                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 193.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

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     | 0.87         | 0/9028          | 1.37        | 59/12226 (0.5%)  |
| 1   | B     | 0.88         | 2/8864 (0.0%)   | 1.37        | 53/12030 (0.4%)  |
| 2   | C     | 0.97         | 2/2698 (0.1%)   | 1.52        | 34/3655 (0.9%)   |
| 2   | E     | 0.92         | 1/2698 (0.0%)   | 1.49        | 35/3655 (1.0%)   |
| 3   | D     | 0.87         | 3/1852 (0.2%)   | 1.48        | 12/2511 (0.5%)   |
| 3   | G     | 0.82         | 0/1852          | 1.44        | 11/2511 (0.4%)   |
| 4   | F     | 2.33         | 38/651 (5.8%)   | 2.10        | 27/885 (3.1%)    |
| 4   | H     | 2.38         | 36/651 (5.5%)   | 2.00        | 28/885 (3.2%)    |
| All | All   | 1.00         | 82/28294 (0.3%) | 1.45        | 259/38358 (0.7%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4   | F     | 0                   | 2                   |
| 4   | H     | 0                   | 3                   |
| All | All   | 0                   | 5                   |

All (82) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 4   | H     | 25  | GLU  | CA-C  | -14.43 | 1.34        | 1.52     |
| 4   | H     | 58  | GLU  | C-O   | -13.86 | 1.06        | 1.24     |
| 4   | H     | 25  | GLU  | C-O   | -13.43 | 1.03        | 1.23     |
| 4   | F     | 43  | GLY  | C-O   | -12.34 | 1.07        | 1.23     |
| 4   | F     | 22  | LEU  | C-O   | -11.37 | 1.09        | 1.24     |
| 4   | H     | 60  | ILE  | C-O   | -10.21 | 1.11        | 1.24     |
| 4   | F     | 11  | GLN  | CA-C  | -9.78  | 1.39        | 1.52     |
| 4   | H     | 59  | ALA  | CA-C  | -9.65  | 1.39        | 1.52     |
| 4   | H     | 59  | ALA  | C-O   | -9.60  | 1.11        | 1.24     |
| 4   | H     | 42  | LEU  | C-O   | -9.33  | 1.12        | 1.24     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4   | H     | 61   | ILE  | C-O   | -9.26 | 1.12        | 1.24     |
| 4   | H     | 12   | ARG  | CA-C  | -9.19 | 1.40        | 1.52     |
| 4   | F     | 19   | THR  | C-O   | -8.83 | 1.13        | 1.24     |
| 4   | F     | 9    | GLY  | C-O   | -8.79 | 1.12        | 1.24     |
| 4   | F     | 43   | GLY  | CA-C  | -8.46 | 1.40        | 1.51     |
| 4   | F     | 45   | HIS  | C-O   | -8.35 | 1.13        | 1.24     |
| 4   | H     | 60   | ILE  | CA-C  | -8.35 | 1.42        | 1.52     |
| 4   | F     | 58   | GLU  | CA-C  | -8.29 | 1.40        | 1.52     |
| 4   | F     | 23   | LEU  | C-O   | -8.24 | 1.13        | 1.24     |
| 4   | H     | 45   | HIS  | C-N   | -8.22 | 1.23        | 1.33     |
| 4   | F     | 18   | TRP  | CA-C  | -8.16 | 1.42        | 1.52     |
| 4   | F     | 23   | LEU  | CA-C  | -8.01 | 1.41        | 1.52     |
| 4   | H     | 59   | ALA  | CA-CB | -7.99 | 1.40        | 1.53     |
| 4   | F     | 20   | LEU  | CA-C  | -7.82 | 1.41        | 1.52     |
| 4   | H     | 45   | HIS  | C-O   | -7.81 | 1.14        | 1.24     |
| 4   | H     | 58   | GLU  | CA-C  | -7.64 | 1.42        | 1.52     |
| 4   | H     | 14   | PRO  | C-O   | -7.59 | 1.12        | 1.24     |
| 4   | F     | 16   | ASN  | C-O   | -7.52 | 1.14        | 1.24     |
| 4   | H     | 16   | ASN  | C-O   | -7.42 | 1.14        | 1.24     |
| 1   | B     | 534  | MET  | SD-CE | 7.35  | 1.98        | 1.79     |
| 4   | H     | 65   | GLN  | C-O   | -7.34 | 1.15        | 1.24     |
| 4   | F     | 56   | GLY  | C-O   | -7.32 | 1.14        | 1.23     |
| 4   | F     | 58   | GLU  | CA-CB | -7.15 | 1.40        | 1.53     |
| 4   | F     | 20   | LEU  | C-O   | -6.99 | 1.15        | 1.24     |
| 4   | H     | 41   | ASN  | C-O   | -6.99 | 1.15        | 1.24     |
| 4   | H     | 32   | ARG  | C-O   | -6.94 | 1.15        | 1.24     |
| 4   | F     | 10   | PRO  | CA-CB | -6.91 | 1.44        | 1.53     |
| 4   | H     | 16   | ASN  | CA-C  | -6.84 | 1.43        | 1.52     |
| 4   | H     | 58   | GLU  | CA-CB | -6.80 | 1.42        | 1.53     |
| 4   | F     | 46   | ILE  | C-O   | -6.77 | 1.15        | 1.24     |
| 3   | D     | 272  | LEU  | C-O   | -6.76 | 1.16        | 1.24     |
| 4   | H     | 44   | GLN  | C-O   | -6.65 | 1.16        | 1.24     |
| 4   | H     | 41   | ASN  | CA-C  | -6.63 | 1.43        | 1.52     |
| 1   | B     | 593  | MET  | SD-CE | 6.61  | 1.96        | 1.79     |
| 4   | H     | 57   | VAL  | CA-CB | -6.60 | 1.46        | 1.54     |
| 4   | F     | 16   | ASN  | CA-C  | -6.54 | 1.44        | 1.52     |
| 2   | C     | 1389 | VAL  | CA-C  | 6.53  | 1.66        | 1.52     |
| 4   | F     | 11   | GLN  | C-O   | -6.49 | 1.15        | 1.24     |
| 4   | F     | 18   | TRP  | C-O   | -6.47 | 1.16        | 1.24     |
| 4   | F     | 22   | LEU  | C-N   | -6.45 | 1.24        | 1.33     |
| 4   | F     | 39   | LEU  | C-O   | -6.34 | 1.15        | 1.24     |
| 4   | F     | 17   | GLU  | CA-C  | -6.22 | 1.44        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 273  | SER  | C-N     | -6.21 | 1.25        | 1.33     |
| 4   | H     | 12   | ARG  | C-O     | -6.17 | 1.16        | 1.24     |
| 4   | H     | 58   | GLU  | N-CA    | -6.13 | 1.38        | 1.46     |
| 4   | H     | 36   | ARG  | C-O     | -6.12 | 1.16        | 1.24     |
| 4   | F     | 13   | GLU  | C-N     | -6.08 | 1.28        | 1.33     |
| 4   | H     | 2    | GLU  | C-O     | -6.02 | 1.11        | 1.23     |
| 4   | F     | 11   | GLN  | N-CA    | -5.96 | 1.38        | 1.46     |
| 4   | F     | 58   | GLU  | C-O     | -5.82 | 1.16        | 1.24     |
| 3   | D     | 272  | LEU  | N-CA    | -5.78 | 1.39        | 1.46     |
| 4   | H     | 65   | GLN  | CD-NE2  | -5.75 | 1.21        | 1.33     |
| 4   | H     | 37   | ILE  | CA-C    | -5.70 | 1.45        | 1.52     |
| 4   | H     | 25   | GLU  | CA-CB   | -5.69 | 1.44        | 1.53     |
| 4   | F     | 65   | GLN  | N-CA    | -5.67 | 1.38        | 1.46     |
| 4   | F     | 40   | HIS  | CA-C    | -5.66 | 1.45        | 1.53     |
| 2   | E     | 1389 | VAL  | CA-C    | 5.61  | 1.64        | 1.52     |
| 4   | H     | 14   | PRO  | N-CD    | 5.54  | 1.55        | 1.47     |
| 4   | F     | 12   | ARG  | C-O     | -5.51 | 1.17        | 1.24     |
| 4   | F     | 16   | ASN  | N-CA    | -5.51 | 1.39        | 1.46     |
| 4   | F     | 41   | ASN  | N-CA    | -5.47 | 1.39        | 1.46     |
| 4   | H     | 37   | ILE  | C-O     | -5.45 | 1.17        | 1.23     |
| 4   | F     | 56   | GLY  | CA-C    | -5.43 | 1.44        | 1.51     |
| 4   | F     | 57   | VAL  | C-O     | -5.39 | 1.17        | 1.24     |
| 4   | F     | 32   | ARG  | C-O     | -5.33 | 1.16        | 1.24     |
| 4   | F     | 21   | GLU  | C-O     | -5.29 | 1.17        | 1.23     |
| 4   | F     | 31   | VAL  | C-O     | -5.20 | 1.17        | 1.24     |
| 4   | H     | 44   | GLN  | CA-C    | -5.15 | 1.46        | 1.52     |
| 4   | F     | 18   | TRP  | CE2-CZ2 | -5.12 | 1.29        | 1.39     |
| 2   | C     | 1388 | GLU  | CA-C    | 5.10  | 1.59        | 1.52     |
| 4   | H     | 45   | HIS  | CA-C    | -5.06 | 1.46        | 1.52     |
| 4   | H     | 44   | GLN  | CA-CB   | -5.04 | 1.45        | 1.53     |

All (259) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 4   | F     | 23   | LEU  | N-CA-C | -10.89 | 98.51       | 112.23   |
| 4   | F     | 10   | PRO  | N-CA-C | 10.25  | 133.59      | 112.47   |
| 2   | C     | 1059 | SER  | CA-C-N | 10.06  | 139.81      | 121.70   |
| 2   | C     | 1059 | SER  | C-N-CA | 10.06  | 139.81      | 121.70   |
| 2   | E     | 1059 | SER  | CA-C-N | 9.80   | 139.33      | 121.70   |
| 2   | E     | 1059 | SER  | C-N-CA | 9.80   | 139.33      | 121.70   |
| 2   | C     | 1148 | SER  | N-CA-C | -9.36  | 102.43      | 114.04   |
| 4   | H     | 3    | GLN  | N-CA-C | 9.28   | 123.69      | 110.23   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 4   | F     | 18   | TRP  | CA-C-N     | 9.13  | 133.48      | 120.79   |
| 4   | F     | 18   | TRP  | C-N-CA     | 9.13  | 133.48      | 120.79   |
| 4   | F     | 9    | GLY  | N-CA-C     | -9.00 | 93.98       | 112.34   |
| 4   | F     | 3    | GLN  | N-CA-C     | 8.95  | 122.64      | 110.55   |
| 1   | B     | 587  | ILE  | N-CA-C     | 8.92  | 117.32      | 109.02   |
| 1   | A     | 587  | ILE  | N-CA-C     | 8.88  | 117.28      | 109.02   |
| 4   | F     | 13   | GLU  | CA-C-N     | -8.64 | 110.86      | 120.45   |
| 4   | F     | 13   | GLU  | C-N-CA     | -8.64 | 110.86      | 120.45   |
| 4   | H     | 25   | GLU  | CB-CA-C    | -8.62 | 95.98       | 109.34   |
| 4   | F     | 18   | TRP  | N-CA-C     | -8.44 | 102.03      | 111.14   |
| 4   | F     | 10   | PRO  | CA-N-CD    | -8.34 | 100.32      | 112.00   |
| 2   | C     | 1274 | ILE  | N-CA-C     | 8.12  | 117.98      | 106.53   |
| 4   | H     | 12   | ARG  | N-CA-C     | 8.02  | 127.89      | 110.80   |
| 4   | F     | 65   | GLN  | CA-C-N     | 7.92  | 131.21      | 120.44   |
| 4   | F     | 65   | GLN  | C-N-CA     | 7.92  | 131.21      | 120.44   |
| 1   | A     | 293  | GLY  | CA-C-N     | 7.78  | 132.17      | 121.05   |
| 1   | A     | 293  | GLY  | C-N-CA     | 7.78  | 132.17      | 121.05   |
| 1   | B     | 293  | GLY  | CA-C-N     | 7.70  | 132.07      | 121.05   |
| 1   | B     | 293  | GLY  | C-N-CA     | 7.70  | 132.07      | 121.05   |
| 4   | H     | 61   | ILE  | CG1-CB-CG2 | -7.66 | 87.73       | 110.70   |
| 1   | B     | 724  | ILE  | N-CA-C     | 7.63  | 125.21      | 109.34   |
| 2   | E     | 1356 | ASP  | CA-CB-CG   | 7.62  | 120.22      | 112.60   |
| 4   | H     | 64   | LEU  | CA-C-N     | 7.59  | 131.46      | 120.38   |
| 4   | H     | 64   | LEU  | C-N-CA     | 7.59  | 131.46      | 120.38   |
| 4   | H     | 61   | ILE  | N-CA-C     | -7.43 | 101.80      | 111.09   |
| 4   | F     | 22   | LEU  | N-CA-C     | 7.39  | 126.55      | 110.80   |
| 4   | H     | 60   | ILE  | CA-C-O     | -7.34 | 111.61      | 120.78   |
| 4   | H     | 10   | PRO  | N-CA-C     | 7.29  | 127.48      | 112.47   |
| 4   | H     | 37   | ILE  | CB-CA-C    | -7.28 | 102.77      | 111.94   |
| 2   | C     | 1297 | CYS  | N-CA-C     | 7.23  | 121.02      | 109.24   |
| 2   | C     | 1155 | THR  | CB-CA-C    | 7.20  | 123.62      | 110.88   |
| 1   | A     | 327  | ARG  | N-CA-C     | -7.06 | 104.29      | 113.12   |
| 4   | H     | 65   | GLN  | CA-CB-CG   | 7.00  | 128.11      | 114.10   |
| 1   | A     | 161  | GLU  | N-CA-C     | 6.99  | 119.50      | 111.11   |
| 3   | D     | 271  | PRO  | N-CA-C     | 6.93  | 123.62      | 114.27   |
| 1   | A     | 143  | ILE  | N-CA-CB    | 6.92  | 119.47      | 111.31   |
| 1   | B     | 143  | ILE  | N-CA-CB    | 6.85  | 119.40      | 111.31   |
| 1   | B     | 826  | ASN  | CA-CB-CG   | 6.79  | 119.39      | 112.60   |
| 1   | B     | 900  | ARG  | CA-C-N     | -6.79 | 113.74      | 122.77   |
| 1   | B     | 900  | ARG  | C-N-CA     | -6.79 | 113.74      | 122.77   |
| 4   | F     | 14   | PRO  | CA-C-N     | 6.78  | 134.50      | 121.54   |
| 4   | F     | 14   | PRO  | C-N-CA     | 6.78  | 134.50      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | B     | 327  | ARG  | N-CA-C   | -6.78 | 104.65      | 113.12   |
| 2   | E     | 1171 | ASP  | CA-CB-CG | 6.74  | 119.34      | 112.60   |
| 4   | F     | 42   | LEU  | CB-CA-C  | -6.72 | 98.27       | 109.55   |
| 1   | A     | 826  | ASN  | CA-CB-CG | 6.66  | 119.26      | 112.60   |
| 1   | B     | 252  | ILE  | N-CA-C   | 6.61  | 116.71      | 110.30   |
| 4   | H     | 42   | LEU  | CB-CA-C  | -6.59 | 98.64       | 110.70   |
| 1   | A     | 777  | PRO  | CA-C-N   | 6.54  | 133.47      | 121.70   |
| 1   | A     | 777  | PRO  | C-N-CA   | 6.54  | 133.47      | 121.70   |
| 2   | C     | 1332 | SER  | N-CA-C   | -6.53 | 103.82      | 113.61   |
| 4   | H     | 25   | GLU  | CA-C-N   | 6.53  | 129.56      | 120.29   |
| 4   | H     | 25   | GLU  | C-N-CA   | 6.53  | 129.56      | 120.29   |
| 4   | H     | 37   | ILE  | CA-C-N   | 6.52  | 129.02      | 120.28   |
| 4   | H     | 37   | ILE  | C-N-CA   | 6.52  | 129.02      | 120.28   |
| 1   | B     | 341  | ASN  | CA-CB-CG | 6.51  | 119.11      | 112.60   |
| 2   | E     | 1374 | SER  | CA-C-N   | 6.50  | 133.96      | 121.54   |
| 2   | E     | 1374 | SER  | C-N-CA   | 6.50  | 133.96      | 121.54   |
| 1   | B     | 777  | PRO  | CA-C-N   | 6.46  | 133.34      | 121.70   |
| 1   | B     | 777  | PRO  | C-N-CA   | 6.46  | 133.34      | 121.70   |
| 2   | E     | 1378 | LEU  | CA-C-N   | 6.46  | 133.88      | 121.54   |
| 2   | E     | 1378 | LEU  | C-N-CA   | 6.46  | 133.88      | 121.54   |
| 1   | A     | 46   | ALA  | CA-C-N   | 6.46  | 128.93      | 120.28   |
| 1   | A     | 46   | ALA  | C-N-CA   | 6.46  | 128.93      | 120.28   |
| 2   | C     | 1102 | SER  | CA-CB-OG | 6.45  | 124.00      | 111.10   |
| 2   | C     | 1267 | HIS  | N-CA-C   | -6.44 | 100.84      | 110.24   |
| 1   | A     | 341  | ASN  | CA-CB-CG | 6.38  | 118.98      | 112.60   |
| 2   | C     | 1198 | ASP  | CA-CB-CG | 6.38  | 118.98      | 112.60   |
| 2   | C     | 1262 | ILE  | N-CA-C   | 6.33  | 117.19      | 108.84   |
| 2   | E     | 1066 | VAL  | CA-C-N   | 6.31  | 133.59      | 121.54   |
| 2   | E     | 1066 | VAL  | C-N-CA   | 6.31  | 133.59      | 121.54   |
| 2   | E     | 1330 | PHE  | CA-CB-CG | 6.29  | 120.08      | 113.80   |
| 4   | H     | 42   | LEU  | CA-CB-CG | 6.23  | 138.12      | 116.30   |
| 3   | D     | 219  | GLU  | CB-CG-CD | 6.21  | 123.15      | 112.60   |
| 1   | A     | 783  | GLY  | CA-C-N   | 6.14  | 130.58      | 120.94   |
| 1   | A     | 783  | GLY  | C-N-CA   | 6.14  | 130.58      | 120.94   |
| 1   | A     | 264  | VAL  | N-CA-C   | -6.09 | 105.20      | 110.74   |
| 2   | E     | 1078 | SER  | N-CA-C   | -6.08 | 105.15      | 113.30   |
| 1   | B     | 563  | ASP  | CA-CB-CG | 6.07  | 118.67      | 112.60   |
| 1   | B     | 1077 | HIS  | N-CA-C   | 6.03  | 119.09      | 107.44   |
| 2   | E     | 1305 | GLY  | CA-C-N   | 6.02  | 128.26      | 120.44   |
| 2   | E     | 1305 | GLY  | C-N-CA   | 6.02  | 128.26      | 120.44   |
| 1   | B     | 46   | ALA  | CA-C-N   | 6.01  | 128.33      | 120.28   |
| 1   | B     | 46   | ALA  | C-N-CA   | 6.01  | 128.33      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | B     | 633  | THR  | N-CA-C   | -6.00 | 106.50      | 113.88   |
| 1   | A     | 633  | THR  | N-CA-C   | -6.00 | 106.50      | 113.88   |
| 2   | C     | 1102 | SER  | N-CA-C   | -6.00 | 102.44      | 110.24   |
| 1   | A     | 563  | ASP  | CA-CB-CG | 5.99  | 118.59      | 112.60   |
| 1   | A     | 160  | GLU  | CA-C-N   | 5.97  | 128.60      | 120.54   |
| 1   | A     | 160  | GLU  | C-N-CA   | 5.97  | 128.60      | 120.54   |
| 2   | C     | 1078 | SER  | N-CA-C   | -5.97 | 105.30      | 113.30   |
| 1   | A     | 1077 | HIS  | N-CA-C   | 5.97  | 118.96      | 107.44   |
| 2   | E     | 1374 | SER  | N-CA-C   | 5.96  | 119.36      | 109.46   |
| 2   | E     | 1122 | VAL  | N-CA-CB  | 5.96  | 116.87      | 110.62   |
| 2   | E     | 1297 | CYS  | N-CA-C   | 5.95  | 118.94      | 109.24   |
| 3   | D     | 84   | PHE  | CA-CB-CG | 5.94  | 119.74      | 113.80   |
| 4   | H     | 65   | GLN  | CA-C-N   | 5.92  | 130.70      | 120.58   |
| 4   | H     | 65   | GLN  | C-N-CA   | 5.92  | 130.70      | 120.58   |
| 1   | A     | 929  | SER  | CB-CA-C  | -5.90 | 109.76      | 116.54   |
| 1   | A     | 572  | PRO  | CA-C-N   | 5.87  | 128.47      | 120.54   |
| 1   | A     | 572  | PRO  | C-N-CA   | 5.87  | 128.47      | 120.54   |
| 3   | G     | 273  | SER  | N-CA-C   | 5.87  | 123.30      | 110.80   |
| 1   | A     | 1061 | VAL  | N-CA-C   | 5.87  | 116.04      | 110.53   |
| 2   | C     | 1227 | CYS  | N-CA-C   | 5.86  | 117.93      | 107.80   |
| 2   | C     | 1070 | CYS  | N-CA-C   | -5.79 | 104.97      | 111.28   |
| 1   | A     | 549  | SER  | CA-C-N   | 5.79  | 128.84      | 120.38   |
| 1   | A     | 549  | SER  | C-N-CA   | 5.79  | 128.84      | 120.38   |
| 2   | E     | 1091 | GLU  | CB-CG-CD | 5.79  | 122.43      | 112.60   |
| 4   | H     | 25   | GLU  | N-CA-C   | -5.77 | 106.28      | 113.55   |
| 1   | A     | 1060 | LYS  | CA-C-N   | 5.75  | 127.93      | 120.56   |
| 1   | A     | 1060 | LYS  | C-N-CA   | 5.75  | 127.93      | 120.56   |
| 4   | F     | 43   | GLY  | N-CA-C   | -5.75 | 99.55       | 113.18   |
| 2   | E     | 1379 | ASN  | CA-C-N   | 5.74  | 132.51      | 121.54   |
| 2   | E     | 1379 | ASN  | C-N-CA   | 5.74  | 132.51      | 121.54   |
| 1   | B     | 28   | ASP  | CA-CB-CG | 5.74  | 118.34      | 112.60   |
| 3   | G     | 207  | LEU  | N-CA-C   | 5.71  | 120.40      | 113.38   |
| 2   | C     | 1257 | LYS  | N-CA-C   | 5.70  | 117.97      | 109.59   |
| 2   | C     | 1330 | PHE  | CA-CB-CG | 5.70  | 119.50      | 113.80   |
| 3   | G     | 173  | ILE  | N-CA-CB  | 5.69  | 118.28      | 110.54   |
| 4   | F     | 36   | ARG  | N-CA-C   | 5.69  | 122.92      | 110.80   |
| 3   | D     | 207  | LEU  | N-CA-C   | 5.69  | 120.37      | 113.38   |
| 2   | E     | 1257 | LYS  | N-CA-C   | 5.68  | 117.94      | 109.59   |
| 4   | F     | 25   | GLU  | CA-C-N   | 5.68  | 127.90      | 120.28   |
| 4   | F     | 25   | GLU  | C-N-CA   | 5.68  | 127.90      | 120.28   |
| 3   | G     | 219  | GLU  | CB-CG-CD | 5.68  | 122.25      | 112.60   |
| 4   | H     | 14   | PRO  | CA-N-CD  | -5.65 | 104.09      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | B     | 264  | VAL  | N-CA-C    | -5.65 | 105.60      | 110.74   |
| 1   | A     | 985  | THR  | N-CA-C    | 5.65  | 118.75      | 109.72   |
| 4   | F     | 39   | LEU  | CB-CG-CD1 | -5.65 | 93.76       | 110.70   |
| 1   | B     | 549  | SER  | CA-C-N    | 5.64  | 128.62      | 120.38   |
| 1   | B     | 549  | SER  | C-N-CA    | 5.64  | 128.62      | 120.38   |
| 4   | F     | 42   | LEU  | CB-CG-CD1 | -5.64 | 93.77       | 110.70   |
| 4   | H     | 43   | GLY  | O-C-N     | -5.62 | 115.39      | 122.70   |
| 2   | E     | 1298 | ARG  | N-CA-C    | -5.60 | 98.86       | 110.80   |
| 1   | B     | 236  | SER  | N-CA-C    | 5.60  | 118.59      | 109.24   |
| 1   | B     | 929  | SER  | CB-CA-C   | -5.60 | 110.10      | 116.54   |
| 1   | A     | 236  | SER  | N-CA-C    | 5.60  | 118.34      | 109.50   |
| 1   | B     | 954  | MET  | N-CA-C    | 5.59  | 117.96      | 110.35   |
| 2   | C     | 1088 | GLU  | CA-C-N    | 5.59  | 132.21      | 121.54   |
| 2   | C     | 1088 | GLU  | C-N-CA    | 5.59  | 132.21      | 121.54   |
| 1   | B     | 311  | ALA  | N-CA-C    | 5.58  | 117.31      | 108.67   |
| 1   | A     | 882  | ALA  | N-CA-C    | 5.57  | 118.30      | 109.50   |
| 2   | C     | 1122 | VAL  | N-CA-CB   | 5.56  | 116.46      | 110.62   |
| 1   | A     | 1100 | ILE  | CA-C-N    | 5.56  | 128.61      | 120.71   |
| 1   | A     | 1100 | ILE  | C-N-CA    | 5.56  | 128.61      | 120.71   |
| 1   | A     | 28   | ASP  | CA-CB-CG  | 5.56  | 118.16      | 112.60   |
| 2   | E     | 1187 | HIS  | CA-C-N    | 5.55  | 132.14      | 121.54   |
| 2   | E     | 1187 | HIS  | C-N-CA    | 5.55  | 132.14      | 121.54   |
| 2   | E     | 1048 | ILE  | N-CA-CB   | 5.54  | 117.03      | 110.55   |
| 3   | G     | 148  | HIS  | N-CA-C    | 5.54  | 119.74      | 113.15   |
| 1   | B     | 202  | PHE  | CA-CB-CG  | 5.53  | 119.33      | 113.80   |
| 1   | B     | 1061 | VAL  | N-CA-C    | 5.53  | 115.72      | 110.53   |
| 1   | A     | 550  | ASN  | N-CA-C    | 5.50  | 118.79      | 111.75   |
| 1   | B     | 909  | ILE  | N-CA-CB   | 5.50  | 116.86      | 110.65   |
| 3   | D     | 273  | SER  | CA-C-O    | 5.48  | 128.35      | 120.51   |
| 1   | A     | 573  | SER  | N-CA-C    | 5.47  | 117.67      | 111.11   |
| 1   | A     | 530  | SER  | N-CA-C    | 5.47  | 116.57      | 108.86   |
| 2   | C     | 1129 | ALA  | N-CA-C    | 5.47  | 117.40      | 108.76   |
| 2   | E     | 1341 | ASP  | N-CA-C    | -5.47 | 99.19       | 108.26   |
| 2   | E     | 1193 | ILE  | N-CA-C    | 5.46  | 115.19      | 106.88   |
| 4   | H     | 12   | ARG  | CB-CA-C   | -5.46 | 99.55       | 110.42   |
| 2   | C     | 1341 | ASP  | N-CA-C    | -5.46 | 99.19       | 108.26   |
| 1   | A     | 1121 | LYS  | N-CA-C    | 5.46  | 117.13      | 108.67   |
| 4   | F     | 36   | ARG  | CA-C-N    | 5.45  | 127.43      | 120.56   |
| 4   | F     | 36   | ARG  | C-N-CA    | 5.45  | 127.43      | 120.56   |
| 3   | G     | 235  | GLN  | N-CA-C    | 5.44  | 117.97      | 111.71   |
| 1   | A     | 638  | LEU  | N-CA-C    | 5.44  | 117.82      | 109.07   |
| 3   | D     | 271  | PRO  | CA-C-N    | 5.44  | 128.01      | 120.29   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | D     | 271  | PRO  | C-N-CA   | 5.44  | 128.01      | 120.29   |
| 1   | A     | 311  | ALA  | N-CA-C   | 5.41  | 117.12      | 108.41   |
| 1   | B     | 955  | SER  | N-CA-C   | -5.41 | 106.61      | 113.43   |
| 2   | C     | 1187 | HIS  | CA-C-N   | 5.40  | 131.85      | 121.54   |
| 2   | C     | 1187 | HIS  | C-N-CA   | 5.40  | 131.85      | 121.54   |
| 1   | B     | 1060 | LYS  | CA-C-N   | 5.37  | 127.44      | 120.56   |
| 1   | B     | 1060 | LYS  | C-N-CA   | 5.37  | 127.44      | 120.56   |
| 2   | C     | 1231 | ASN  | CA-CB-CG | 5.37  | 117.97      | 112.60   |
| 2   | E     | 1192 | VAL  | CB-CA-C  | 5.36  | 117.41      | 110.12   |
| 1   | A     | 904  | ASN  | CA-CB-CG | 5.36  | 117.95      | 112.60   |
| 4   | H     | 65   | GLN  | CB-CG-CD | 5.35  | 121.70      | 112.60   |
| 1   | B     | 550  | ASN  | N-CA-C   | 5.35  | 118.60      | 111.75   |
| 1   | B     | 160  | GLU  | CA-C-N   | 5.34  | 128.83      | 120.82   |
| 1   | B     | 160  | GLU  | C-N-CA   | 5.34  | 128.83      | 120.82   |
| 4   | F     | 57   | VAL  | N-CA-C   | -5.34 | 98.24       | 109.34   |
| 2   | C     | 1261 | ASN  | CA-C-N   | 5.34  | 129.19      | 121.18   |
| 2   | C     | 1261 | ASN  | C-N-CA   | 5.34  | 129.19      | 121.18   |
| 4   | H     | 1    | MET  | CA-C-N   | 5.33  | 131.29      | 121.70   |
| 4   | H     | 1    | MET  | C-N-CA   | 5.33  | 131.29      | 121.70   |
| 1   | B     | 882  | ALA  | N-CA-C   | 5.33  | 117.92      | 109.50   |
| 3   | G     | 285  | SER  | CA-C-N   | 5.31  | 127.66      | 120.38   |
| 3   | G     | 285  | SER  | C-N-CA   | 5.31  | 127.66      | 120.38   |
| 1   | A     | 368  | GLU  | CA-C-N   | 5.31  | 131.69      | 121.54   |
| 1   | A     | 368  | GLU  | C-N-CA   | 5.31  | 131.69      | 121.54   |
| 1   | B     | 638  | LEU  | N-CA-C   | 5.31  | 117.61      | 109.07   |
| 2   | E     | 1144 | SER  | N-CA-C   | -5.29 | 101.34      | 109.76   |
| 1   | B     | 726  | TYR  | N-CA-CB  | -5.29 | 101.92      | 110.81   |
| 1   | A     | 202  | PHE  | CA-CB-CG | 5.29  | 119.09      | 113.80   |
| 1   | B     | 530  | SER  | N-CA-C   | 5.28  | 116.31      | 108.86   |
| 1   | A     | 131  | ILE  | N-CA-CB  | 5.28  | 117.39      | 111.21   |
| 1   | A     | 983  | ALA  | N-CA-C   | 5.28  | 117.74      | 110.35   |
| 1   | B     | 904  | ASN  | CA-CB-CG | 5.27  | 117.87      | 112.60   |
| 1   | B     | 131  | ILE  | N-CA-CB  | 5.27  | 117.37      | 111.21   |
| 1   | A     | 841  | ALA  | N-CA-C   | 5.26  | 119.85      | 113.38   |
| 1   | A     | 145  | LEU  | N-CA-C   | 5.25  | 119.37      | 112.92   |
| 1   | A     | 909  | ILE  | N-CA-CB  | 5.25  | 116.58      | 110.65   |
| 1   | B     | 145  | LEU  | N-CA-C   | 5.22  | 119.34      | 112.92   |
| 3   | D     | 285  | SER  | CA-C-N   | 5.21  | 127.52      | 120.38   |
| 3   | D     | 285  | SER  | C-N-CA   | 5.21  | 127.52      | 120.38   |
| 1   | A     | 781  | SER  | CA-C-N   | 5.21  | 131.07      | 121.70   |
| 1   | A     | 781  | SER  | C-N-CA   | 5.21  | 131.07      | 121.70   |
| 2   | C     | 1282 | LEU  | N-CA-C   | 5.20  | 117.69      | 111.71   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 955  | SER  | N-CA-C    | -5.20 | 106.88      | 113.43   |
| 1   | A     | 906  | TYR  | N-CA-C    | 5.19  | 121.34      | 114.12   |
| 1   | B     | 341  | ASN  | CA-C-N    | 5.19  | 127.23      | 120.28   |
| 1   | B     | 341  | ASN  | C-N-CA    | 5.19  | 127.23      | 120.28   |
| 1   | B     | 166  | ASP  | CA-CB-CG  | 5.18  | 117.78      | 112.60   |
| 1   | B     | 906  | TYR  | N-CA-C    | 5.16  | 121.29      | 114.12   |
| 2   | E     | 1088 | GLU  | CA-C-N    | 5.16  | 131.39      | 121.54   |
| 2   | E     | 1088 | GLU  | C-N-CA    | 5.16  | 131.39      | 121.54   |
| 1   | A     | 166  | ASP  | CA-CB-CG  | 5.16  | 117.76      | 112.60   |
| 3   | G     | 162  | ARG  | N-CA-C    | -5.16 | 103.58      | 110.07   |
| 1   | A     | 774  | SER  | CA-C-N    | 5.15  | 130.97      | 121.70   |
| 1   | A     | 774  | SER  | C-N-CA    | 5.15  | 130.97      | 121.70   |
| 2   | E     | 1329 | PRO  | N-CA-C    | 5.14  | 123.06      | 112.47   |
| 2   | C     | 1255 | PHE  | CA-C-N    | 5.14  | 131.35      | 121.54   |
| 2   | C     | 1255 | PHE  | C-N-CA    | 5.14  | 131.35      | 121.54   |
| 1   | A     | 307  | GLU  | N-CA-C    | 5.12  | 117.74      | 109.40   |
| 4   | H     | 45   | HIS  | CA-C-O    | 5.11  | 127.81      | 120.51   |
| 1   | B     | 572  | PRO  | CA-C-N    | 5.10  | 128.47      | 120.82   |
| 1   | B     | 572  | PRO  | C-N-CA    | 5.10  | 128.47      | 120.82   |
| 3   | D     | 271  | PRO  | CB-CA-C   | -5.10 | 103.34      | 111.04   |
| 1   | B     | 307  | GLU  | N-CA-C    | 5.09  | 117.70      | 109.40   |
| 2   | E     | 1261 | ASN  | CA-C-N    | 5.09  | 128.73      | 122.37   |
| 2   | E     | 1261 | ASN  | C-N-CA    | 5.09  | 128.73      | 122.37   |
| 2   | C     | 1339 | ALA  | CA-C-N    | 5.08  | 127.34      | 120.38   |
| 2   | C     | 1339 | ALA  | C-N-CA    | 5.08  | 127.34      | 120.38   |
| 4   | H     | 32   | ARG  | NE-CZ-NH2 | 5.08  | 123.77      | 119.20   |
| 3   | D     | 235  | GLN  | N-CA-C    | 5.07  | 117.54      | 111.71   |
| 1   | B     | 774  | SER  | CA-C-N    | 5.05  | 130.79      | 121.70   |
| 1   | B     | 774  | SER  | C-N-CA    | 5.05  | 130.79      | 121.70   |
| 1   | B     | 781  | SER  | CA-C-N    | 5.04  | 130.78      | 121.70   |
| 1   | B     | 781  | SER  | C-N-CA    | 5.04  | 130.78      | 121.70   |
| 4   | F     | 21   | GLU  | N-CA-C    | 5.04  | 119.30      | 112.04   |
| 3   | G     | 134  | ILE  | CA-C-N    | 5.04  | 127.45      | 120.29   |
| 3   | G     | 134  | ILE  | C-N-CA    | 5.04  | 127.45      | 120.29   |
| 4   | F     | 42   | LEU  | CA-CB-CG  | 5.04  | 133.94      | 116.30   |
| 2   | C     | 1127 | GLU  | N-CA-C    | -5.04 | 100.86      | 108.67   |
| 2   | C     | 1275 | ILE  | CB-CA-C   | 5.03  | 117.13      | 111.80   |
| 1   | A     | 979  | LYS  | CA-C-N    | -5.01 | 115.34      | 122.41   |
| 1   | A     | 979  | LYS  | C-N-CA    | -5.01 | 115.34      | 122.41   |
| 3   | D     | 148  | HIS  | N-CA-C    | 5.01  | 119.12      | 113.15   |
| 2   | E     | 1129 | ALA  | N-CA-C    | 5.00  | 116.67      | 108.76   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 4   | F     | 11  | GLN  | Peptide   |
| 4   | F     | 21  | GLU  | Peptide   |
| 4   | H     | 1   | MET  | Peptide   |
| 4   | H     | 10  | PRO  | Mainchain |
| 4   | H     | 14  | PRO  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 8865  | 0        | 8824     | 180     | 0            |
| 1   | B     | 8703  | 0        | 8508     | 151     | 0            |
| 2   | C     | 2635  | 0        | 2533     | 101     | 0            |
| 2   | E     | 2635  | 0        | 2533     | 77      | 0            |
| 3   | D     | 1791  | 0        | 1747     | 49      | 0            |
| 3   | G     | 1791  | 0        | 1745     | 58      | 0            |
| 4   | F     | 632   | 0        | 609      | 58      | 0            |
| 4   | H     | 632   | 0        | 609      | 51      | 0            |
| All | All   | 27684 | 0        | 27108    | 699     | 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 13.

All (699) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 3:G:84:PHE:CE1   | 3:G:130:GLN:NE2   | 1.71                     | 1.55              |
| 3:G:84:PHE:CD1   | 3:G:130:GLN:NE2   | 1.84                     | 1.45              |
| 4:F:26:LEU:HD13  | 4:F:65:GLN:NE2    | 1.53                     | 1.23              |
| 2:E:1170:PHE:O   | 4:F:8:GLN:O       | 1.60                     | 1.17              |
| 4:H:1:MET:HB2    | 4:H:2:GLU:HG3     | 1.17                     | 1.11              |
| 4:F:20:LEU:HD13  | 4:F:54:TRP:CZ3    | 1.88                     | 1.08              |
| 2:E:1272:GLU:HB3 | 2:E:1279:ILE:HD11 | 1.34                     | 1.06              |
| 4:F:20:LEU:HD13  | 4:F:54:TRP:HZ3    | 1.24                     | 1.03              |
| 4:H:1:MET:CB     | 4:H:2:GLU:HG3     | 1.90                     | 1.02              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:G:84:PHE:O     | 3:G:130:GLN:HG3   | 1.60                     | 1.01              |
| 3:G:85:PHE:HE1   | 3:G:97:PHE:HZ     | 1.04                     | 0.97              |
| 3:G:85:PHE:CE1   | 3:G:97:PHE:HZ     | 1.83                     | 0.96              |
| 4:H:12:ARG:HH11  | 4:H:12:ARG:H      | 1.04                     | 0.96              |
| 4:F:20:LEU:CD1   | 4:F:54:TRP:HZ3    | 1.79                     | 0.96              |
| 2:C:1281:ASP:HB3 | 2:C:1284:THR:HG22 | 1.47                     | 0.94              |
| 3:D:172:ASN:ND2  | 3:D:271:PRO:HD3   | 1.82                     | 0.94              |
| 4:F:26:LEU:CD1   | 4:F:65:GLN:NE2    | 2.30                     | 0.94              |
| 3:G:84:PHE:HE1   | 3:G:130:GLN:NE2   | 1.46                     | 0.93              |
| 4:H:13:GLU:HB3   | 4:H:14:PRO:CD     | 1.99                     | 0.92              |
| 1:A:321:VAL:HG13 | 1:A:350:MET:HE1   | 1.51                     | 0.92              |
| 4:F:20:LEU:CD1   | 4:F:54:TRP:CZ3    | 2.53                     | 0.91              |
| 2:E:1204:ASP:HB3 | 2:E:1207:THR:HG22 | 1.51                     | 0.90              |
| 2:E:1073:ARG:HD3 | 2:E:1306:THR:CG2  | 2.02                     | 0.90              |
| 3:G:84:PHE:HD1   | 3:G:130:GLN:NE2   | 1.69                     | 0.88              |
| 3:G:85:PHE:HE1   | 3:G:97:PHE:CZ     | 1.92                     | 0.87              |
| 4:F:12:ARG:HD3   | 4:F:12:ARG:N      | 1.91                     | 0.86              |
| 1:A:10:GLN:HB3   | 1:A:1037:ILE:HB   | 1.57                     | 0.86              |
| 1:B:361:ASP:HB3  | 1:B:724:ILE:HG22  | 1.56                     | 0.85              |
| 1:B:724:ILE:HD13 | 1:B:735:VAL:HG22  | 1.58                     | 0.85              |
| 4:H:12:ARG:HH11  | 4:H:12:ARG:N      | 1.75                     | 0.84              |
| 4:F:26:LEU:HD13  | 4:F:65:GLN:HE22   | 1.39                     | 0.84              |
| 4:F:61:ILE:O     | 4:F:65:GLN:HB2    | 1.79                     | 0.83              |
| 2:C:1207:THR:HB  | 2:C:1209:ASN:HD22 | 1.45                     | 0.81              |
| 3:G:84:PHE:O     | 3:G:130:GLN:CG    | 2.28                     | 0.80              |
| 2:C:1281:ASP:HB3 | 2:C:1284:THR:CG2  | 2.11                     | 0.80              |
| 3:D:273:SER:O    | 3:D:275:TYR:N     | 2.15                     | 0.80              |
| 4:F:15:TYR:C     | 4:F:17:GLU:H      | 1.91                     | 0.79              |
| 2:E:1059:SER:HB3 | 2:E:1060:PHE:HB2  | 1.64                     | 0.79              |
| 2:E:1073:ARG:HE  | 2:E:1338:ASN:HD21 | 1.30                     | 0.79              |
| 4:H:1:MET:HB2    | 4:H:2:GLU:CG      | 2.08                     | 0.79              |
| 4:F:26:LEU:CD1   | 4:F:65:GLN:HE21   | 1.99                     | 0.76              |
| 4:F:32:ARG:HH11  | 4:F:32:ARG:HG2    | 1.49                     | 0.76              |
| 1:B:167:VAL:HG13 | 1:B:180:PHE:HB3   | 1.65                     | 0.76              |
| 1:A:413:LEU:HB2  | 1:A:424:THR:HB    | 1.69                     | 0.75              |
| 3:D:272:LEU:O    | 3:D:274:VAL:N     | 2.18                     | 0.75              |
| 1:A:39:LEU:HD13  | 1:A:64:MET:HE2    | 1.68                     | 0.75              |
| 1:B:177:THR:HG21 | 1:B:206:PRO:HG2   | 1.69                     | 0.75              |
| 2:C:1059:SER:HB3 | 2:C:1060:PHE:HB2  | 1.67                     | 0.75              |
| 4:F:20:LEU:HD13  | 4:F:54:TRP:CH2    | 2.22                     | 0.74              |
| 4:H:15:TYR:O     | 4:H:17:GLU:N      | 2.19                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1281:ASP:CB   | 2:C:1284:THR:HG22 | 2.16                     | 0.74              |
| 4:F:12:ARG:HD3    | 4:F:12:ARG:H      | 1.50                     | 0.74              |
| 4:H:15:TYR:O      | 4:H:18:TRP:N      | 2.19                     | 0.74              |
| 1:B:407:ILE:HD13  | 1:B:694:ALA:HB1   | 1.70                     | 0.74              |
| 4:F:15:TYR:O      | 4:F:17:GLU:N      | 2.21                     | 0.74              |
| 1:A:257:THR:OG1   | 1:A:276:MET:SD    | 2.46                     | 0.74              |
| 3:D:291:LEU:HD13  | 3:D:298:PRO:HA    | 1.69                     | 0.74              |
| 1:A:244:LYS:HD3   | 1:A:296:THR:HG23  | 1.69                     | 0.73              |
| 1:A:177:THR:HG21  | 1:A:206:PRO:HG2   | 1.69                     | 0.73              |
| 1:A:407:ILE:HD13  | 1:A:694:ALA:HB1   | 1.71                     | 0.73              |
| 3:D:131:MET:HG2   | 3:D:196:ALA:HB3   | 1.70                     | 0.73              |
| 3:D:139:VAL:HG13  | 3:D:241:VAL:HG13  | 1.71                     | 0.73              |
| 3:G:131:MET:HG2   | 3:G:196:ALA:HB3   | 1.70                     | 0.72              |
| 1:B:413:LEU:HB2   | 1:B:424:THR:HB    | 1.69                     | 0.72              |
| 2:C:1181:TYR:HE2  | 2:C:1183:GLU:HB2  | 1.54                     | 0.72              |
| 4:F:40:HIS:O      | 4:F:43:GLY:N      | 2.19                     | 0.72              |
| 2:C:1132:ASN:HB2  | 4:H:10:PRO:HB2    | 1.71                     | 0.72              |
| 4:F:15:TYR:C      | 4:F:17:GLU:N      | 2.42                     | 0.72              |
| 3:G:139:VAL:HG13  | 3:G:241:VAL:HG13  | 1.71                     | 0.72              |
| 2:C:1298:ARG:NH2  | 2:C:1330:PHE:HB3  | 2.04                     | 0.72              |
| 4:F:58:GLU:O      | 4:F:62:ARG:HG3    | 1.90                     | 0.71              |
| 1:A:1030:PHE:HE1  | 1:A:1036:MET:HE2  | 1.55                     | 0.71              |
| 3:G:291:LEU:HD13  | 3:G:298:PRO:HA    | 1.70                     | 0.71              |
| 3:G:97:PHE:H      | 3:G:97:PHE:HD1    | 1.38                     | 0.70              |
| 4:H:53:THR:HG23   | 4:H:56:GLY:H      | 1.57                     | 0.70              |
| 3:D:131:MET:HG2   | 3:D:196:ALA:CB    | 2.22                     | 0.70              |
| 1:A:603:LEU:HD23  | 1:A:611:LEU:HD21  | 1.72                     | 0.69              |
| 4:H:61:ILE:O      | 4:H:65:GLN:HB2    | 1.91                     | 0.69              |
| 1:B:835:MET:HB2   | 1:B:845:GLN:HG3   | 1.74                     | 0.69              |
| 3:D:273:SER:O     | 3:D:274:VAL:C     | 2.31                     | 0.69              |
| 4:H:10:PRO:O      | 4:H:11:GLN:O      | 2.09                     | 0.69              |
| 4:H:9:GLY:O       | 4:H:11:GLN:N      | 2.24                     | 0.68              |
| 3:D:172:ASN:HD21  | 3:D:271:PRO:HD3   | 1.56                     | 0.68              |
| 4:H:13:GLU:HB3    | 4:H:14:PRO:HD3    | 1.75                     | 0.68              |
| 3:G:131:MET:HG2   | 3:G:196:ALA:CB    | 2.23                     | 0.68              |
| 2:C:1279:ILE:HD11 | 2:C:1291:VAL:HG23 | 1.74                     | 0.68              |
| 2:C:1105:GLU:OE1  | 2:C:1361:THR:HG23 | 1.94                     | 0.67              |
| 4:H:1:MET:CA      | 4:H:2:GLU:HG3     | 2.25                     | 0.67              |
| 1:B:724:ILE:CD1   | 1:B:735:VAL:HG22  | 2.25                     | 0.67              |
| 2:E:1207:THR:HG23 | 2:E:1209:ASN:H    | 1.60                     | 0.67              |
| 1:B:168:LYS:HG3   | 1:B:219:VAL:O     | 1.93                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:9:GLY:O       | 4:H:11:GLN:HG2    | 1.95                     | 0.66              |
| 1:A:39:LEU:HD13   | 1:A:64:MET:CE     | 2.25                     | 0.66              |
| 2:C:1192:VAL:HG23 | 2:C:1205:ILE:HG22 | 1.77                     | 0.66              |
| 2:E:1357:LEU:HD12 | 2:E:1366:LEU:HD11 | 1.77                     | 0.66              |
| 1:A:57:MET:HE2    | 1:A:79:ILE:HG21   | 1.77                     | 0.66              |
| 4:H:10:PRO:C      | 4:H:11:GLN:O      | 2.37                     | 0.66              |
| 2:C:1087:ARG:HH12 | 2:C:1372:GLN:NE2  | 1.94                     | 0.66              |
| 2:E:1073:ARG:HD3  | 2:E:1306:THR:HG23 | 1.76                     | 0.66              |
| 2:C:1075:LEU:HD23 | 2:C:1076:ILE:HG13 | 1.77                     | 0.66              |
| 3:D:288:ASN:HA    | 3:D:291:LEU:HD12  | 1.78                     | 0.65              |
| 1:A:936:LYS:HG3   | 1:A:943:GLU:HG3   | 1.76                     | 0.65              |
| 1:A:658:VAL:HG11  | 1:A:707:ILE:HD12  | 1.78                     | 0.65              |
| 2:E:1272:GLU:CB   | 2:E:1279:ILE:HD11 | 2.20                     | 0.65              |
| 4:H:12:ARG:H      | 4:H:12:ARG:NH1    | 1.85                     | 0.65              |
| 2:E:1075:LEU:HD23 | 2:E:1076:ILE:HG13 | 1.77                     | 0.64              |
| 1:B:143:ILE:HG12  | 1:B:154:ALA:HB2   | 1.79                     | 0.64              |
| 4:F:44:GLN:O      | 4:F:47:TYR:N      | 2.30                     | 0.64              |
| 3:D:146:PRO:HD3   | 3:D:206:VAL:HG12  | 1.79                     | 0.64              |
| 1:A:329:GLY:HA3   | 1:A:384:GLU:HB3   | 1.80                     | 0.64              |
| 1:A:1030:PHE:CE1  | 1:A:1036:MET:HE2  | 2.31                     | 0.64              |
| 4:H:11:GLN:HB3    | 4:H:12:ARG:HH12   | 1.62                     | 0.64              |
| 1:B:582:LEU:HA    | 1:B:626:ARG:HH22  | 1.63                     | 0.64              |
| 2:E:1223:TYR:HE2  | 2:E:1241:GLY:HA3  | 1.63                     | 0.64              |
| 1:A:415:SER:H     | 1:A:423:ASP:CG    | 2.06                     | 0.63              |
| 3:G:288:ASN:HA    | 3:G:291:LEU:HD12  | 1.79                     | 0.63              |
| 1:B:329:GLY:HA3   | 1:B:384:GLU:HB3   | 1.80                     | 0.63              |
| 1:B:596:PHE:HB3   | 1:B:661:SER:HB2   | 1.80                     | 0.63              |
| 1:A:143:ILE:HG12  | 1:A:154:ALA:HB2   | 1.81                     | 0.63              |
| 1:A:596:PHE:HB3   | 1:A:661:SER:HB2   | 1.81                     | 0.63              |
| 4:F:31:VAL:HG12   | 4:F:31:VAL:O      | 1.97                     | 0.63              |
| 2:C:1279:ILE:CD1  | 2:C:1291:VAL:HG23 | 2.28                     | 0.63              |
| 4:F:22:LEU:HD12   | 4:F:22:LEU:O      | 1.99                     | 0.63              |
| 3:D:272:LEU:HD22  | 4:F:60:ILE:HG21   | 1.81                     | 0.63              |
| 3:D:242:PHE:HE2   | 3:D:256:ILE:HG12  | 1.63                     | 0.63              |
| 1:B:985:THR:HG22  | 1:B:988:GLU:HG3   | 1.81                     | 0.62              |
| 1:A:459:PHE:HB3   | 1:A:471:ILE:HD12  | 1.81                     | 0.62              |
| 3:D:273:SER:C     | 3:D:275:TYR:N     | 2.56                     | 0.62              |
| 1:B:459:PHE:HB3   | 1:B:471:ILE:HD12  | 1.81                     | 0.62              |
| 3:G:242:PHE:HE2   | 3:G:256:ILE:HG12  | 1.63                     | 0.62              |
| 1:A:235:GLU:HB2   | 1:A:254:LYS:HG2   | 1.80                     | 0.62              |
| 1:A:582:LEU:HA    | 1:A:626:ARG:HH22  | 1.64                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:282:MET:HB2   | 1:A:305:LEU:HD21  | 1.82                     | 0.62              |
| 2:E:1272:GLU:HB3  | 2:E:1279:ILE:CD1  | 2.22                     | 0.62              |
| 4:F:11:GLN:HG3    | 4:F:12:ARG:CD     | 2.29                     | 0.62              |
| 1:A:835:MET:HB2   | 1:A:845:GLN:HG3   | 1.82                     | 0.61              |
| 1:A:998:PHE:CE1   | 1:A:1074:ARG:HD3  | 2.35                     | 0.61              |
| 4:H:54:TRP:O      | 4:H:57:VAL:HB     | 1.99                     | 0.61              |
| 1:A:84:TYR:HE2    | 1:A:135:LEU:HB3   | 1.63                     | 0.61              |
| 3:D:172:ASN:HD22  | 3:D:271:PRO:HD3   | 1.62                     | 0.61              |
| 4:F:18:TRP:CZ3    | 4:F:22:LEU:HD23   | 2.34                     | 0.61              |
| 1:A:934:ALA:CB    | 1:A:945:ILE:HD11  | 2.30                     | 0.61              |
| 3:D:166:PRO:HB2   | 3:D:171:GLU:HG2   | 1.81                     | 0.61              |
| 1:A:36:ASN:HD22   | 1:A:37:THR:HG22   | 1.65                     | 0.61              |
| 1:A:1113:GLN:HB3  | 1:A:1121:LYS:HD2  | 1.82                     | 0.61              |
| 1:B:282:MET:HB2   | 1:B:305:LEU:HD21  | 1.82                     | 0.61              |
| 1:B:641:PHE:HB3   | 1:B:679:MET:HE1   | 1.82                     | 0.61              |
| 1:B:731:GLN:HA    | 1:B:796:GLN:HE21  | 1.66                     | 0.61              |
| 1:A:114:ARG:HD2   | 1:A:1079:GLU:OE2  | 2.01                     | 0.61              |
| 2:C:1073:ARG:NH1  | 2:C:1073:ARG:HB3  | 2.16                     | 0.61              |
| 2:C:1187:HIS:CG   | 2:C:1188:SER:N    | 2.68                     | 0.60              |
| 2:C:1294:LEU:HD11 | 2:C:1308:MET:HE1  | 1.82                     | 0.60              |
| 1:A:641:PHE:HB3   | 1:A:679:MET:HE1   | 1.83                     | 0.60              |
| 2:C:1201:HIS:CD2  | 2:C:1210:LYS:HD2  | 2.36                     | 0.60              |
| 1:B:864:LYS:HB2   | 1:B:899:LEU:HD12  | 1.83                     | 0.60              |
| 4:F:11:GLN:CG     | 4:F:12:ARG:HD3    | 2.32                     | 0.60              |
| 1:A:731:GLN:HA    | 1:A:796:GLN:HE21  | 1.66                     | 0.60              |
| 1:A:934:ALA:HB2   | 1:A:945:ILE:HD11  | 1.84                     | 0.60              |
| 3:D:258:ARG:HD3   | 3:D:263:VAL:HB    | 1.84                     | 0.60              |
| 1:A:423:ASP:HB2   | 1:A:437:MET:HE1   | 1.83                     | 0.60              |
| 1:B:32:LEU:HD23   | 1:B:39:LEU:HD11   | 1.84                     | 0.60              |
| 4:F:32:ARG:HH11   | 4:F:32:ARG:CG     | 2.13                     | 0.59              |
| 3:G:146:PRO:HD3   | 3:G:206:VAL:HG12  | 1.84                     | 0.59              |
| 2:C:1099:CYS:HB3  | 2:C:1369:ILE:HD11 | 1.83                     | 0.59              |
| 3:D:272:LEU:N     | 3:D:272:LEU:HD23  | 2.16                     | 0.59              |
| 1:B:934:ALA:CB    | 1:B:945:ILE:HD11  | 2.31                     | 0.59              |
| 2:C:1281:ASP:HB2  | 2:C:1288:LEU:HD11 | 1.82                     | 0.59              |
| 1:B:658:VAL:HG23  | 1:B:671:VAL:HG22  | 1.84                     | 0.59              |
| 1:A:327:ARG:HH12  | 2:C:1060:PHE:H    | 1.50                     | 0.59              |
| 1:B:207:TRP:HB3   | 1:B:242:GLY:HA2   | 1.84                     | 0.59              |
| 2:C:1267:HIS:ND1  | 2:C:1268:PRO:HD2  | 2.17                     | 0.59              |
| 2:E:1073:ARG:HD3  | 2:E:1306:THR:HG22 | 1.82                     | 0.59              |
| 3:G:250:GLN:HE21  | 3:G:265:GLN:HB2   | 1.68                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:724:ILE:HD13  | 1:B:735:VAL:CG2   | 2.31                     | 0.59              |
| 1:B:934:ALA:HB2   | 1:B:945:ILE:HD11  | 1.84                     | 0.59              |
| 2:C:1059:SER:CB   | 2:C:1060:PHE:HB2  | 2.32                     | 0.59              |
| 1:B:235:GLU:HB3   | 1:B:254:LYS:HD2   | 1.85                     | 0.59              |
| 2:C:1260:MET:O    | 2:C:1260:MET:HE2  | 2.02                     | 0.59              |
| 2:C:1152:THR:O    | 2:C:1161:SER:HA   | 2.02                     | 0.58              |
| 2:E:1059:SER:CB   | 2:E:1060:PHE:HB2  | 2.31                     | 0.58              |
| 2:E:1187:HIS:CG   | 2:E:1188:SER:N    | 2.71                     | 0.58              |
| 2:E:1136:SER:HB3  | 2:E:1155:THR:HB   | 1.84                     | 0.58              |
| 1:A:593:MET:HG2   | 1:A:602:LEU:HD12  | 1.84                     | 0.58              |
| 1:A:218:MET:HE3   | 1:A:261:HIS:HD2   | 1.68                     | 0.58              |
| 1:B:114:ARG:HD2   | 1:B:1079:GLU:OE2  | 2.03                     | 0.58              |
| 3:D:274:VAL:HG21  | 4:F:39:LEU:O      | 2.03                     | 0.58              |
| 3:G:258:ARG:HD3   | 3:G:263:VAL:HB    | 1.84                     | 0.58              |
| 1:A:658:VAL:HG23  | 1:A:671:VAL:HG22  | 1.84                     | 0.58              |
| 4:F:16:ASN:N      | 4:F:16:ASN:HD22   | 2.01                     | 0.58              |
| 2:C:1136:SER:HB3  | 2:C:1155:THR:HG22 | 1.86                     | 0.58              |
| 3:D:250:GLN:HE21  | 3:D:265:GLN:HB2   | 1.68                     | 0.58              |
| 1:B:143:ILE:HG21  | 1:B:152:LEU:HD23  | 1.86                     | 0.58              |
| 1:B:764:SER:HB2   | 1:B:803:HIS:NE2   | 2.18                     | 0.58              |
| 1:A:764:SER:HB2   | 1:A:803:HIS:NE2   | 2.17                     | 0.57              |
| 2:C:1131:TYR:OH   | 4:H:5:PRO:HG2     | 2.04                     | 0.57              |
| 4:H:11:GLN:HA     | 4:H:12:ARG:NH1    | 2.18                     | 0.57              |
| 1:A:40:GLU:HB3    | 1:A:42:TYR:HE1    | 1.70                     | 0.57              |
| 3:D:89:TRP:CD1    | 3:D:129:THR:HG1   | 2.23                     | 0.57              |
| 1:B:795:ASP:HB2   | 1:B:802:LEU:HD21  | 1.86                     | 0.57              |
| 2:C:1350:VAL:HG21 | 2:C:1354:ILE:CG2  | 2.34                     | 0.57              |
| 2:E:1378:LEU:HD11 | 4:F:46:ILE:HD13   | 1.86                     | 0.57              |
| 2:C:1352:ARG:HD3  | 2:C:1372:GLN:HA   | 1.87                     | 0.57              |
| 4:H:46:ILE:HD11   | 4:H:63:ILE:HD12   | 1.86                     | 0.57              |
| 1:A:1078:THR:HG23 | 1:A:1080:ARG:HG3  | 1.87                     | 0.57              |
| 1:B:10:GLN:HB3    | 1:B:1037:ILE:HB   | 1.87                     | 0.57              |
| 4:H:11:GLN:HB3    | 4:H:12:ARG:NH1    | 2.20                     | 0.57              |
| 1:A:795:ASP:HB2   | 1:A:802:LEU:HD21  | 1.87                     | 0.56              |
| 1:A:617:ASN:HB2   | 1:A:622:LEU:H     | 1.70                     | 0.56              |
| 3:D:213:GLN:HB3   | 3:D:216:SER:HB3   | 1.88                     | 0.56              |
| 1:B:218:MET:HE3   | 1:B:261:HIS:HD2   | 1.70                     | 0.56              |
| 3:G:213:GLN:HB3   | 3:G:216:SER:HB3   | 1.87                     | 0.56              |
| 3:G:113:ARG:HG3   | 3:G:118:VAL:HB    | 1.87                     | 0.56              |
| 2:C:1161:SER:HB2  | 2:C:1176:PHE:HB2  | 1.88                     | 0.56              |
| 2:C:1066:VAL:HG22 | 2:C:1067:ASP:H    | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1100:ALA:O    | 2:C:1109:MET:N    | 2.39                     | 0.56              |
| 4:H:13:GLU:HB3    | 4:H:14:PRO:HD2    | 1.86                     | 0.56              |
| 2:E:1355:PHE:CE1  | 2:E:1371:ASN:HB2  | 2.41                     | 0.55              |
| 2:C:1149:LEU:HD12 | 2:C:1205:ILE:HD12 | 1.88                     | 0.55              |
| 1:A:40:GLU:HB3    | 1:A:42:TYR:CE1    | 2.42                     | 0.55              |
| 1:A:917:LYS:NZ    | 1:A:962:ASP:OD2   | 2.36                     | 0.55              |
| 1:B:1078:THR:HG23 | 1:B:1080:ARG:HG3  | 1.89                     | 0.55              |
| 3:D:88:SER:HB2    | 3:D:134:ILE:HG22  | 1.87                     | 0.55              |
| 1:A:43:VAL:HG23   | 1:A:52:VAL:HG21   | 1.88                     | 0.55              |
| 2:C:1073:ARG:HB3  | 2:C:1073:ARG:CZ   | 2.35                     | 0.55              |
| 2:E:1260:MET:O    | 2:E:1260:MET:HE2  | 2.05                     | 0.55              |
| 1:A:248:ILE:HD13  | 1:A:300:LEU:HB2   | 1.89                     | 0.55              |
| 1:A:361:ASP:HA    | 1:A:1006:VAL:HG11 | 1.88                     | 0.55              |
| 1:A:879:LYS:HG2   | 1:A:892:GLU:HG3   | 1.89                     | 0.55              |
| 1:B:617:ASN:HB2   | 1:B:622:LEU:H     | 1.71                     | 0.55              |
| 1:A:607:GLY:HA2   | 1:A:635:PRO:HB3   | 1.89                     | 0.54              |
| 1:A:969:GLU:HG2   | 1:A:973:ASN:HB2   | 1.88                     | 0.54              |
| 2:C:1135:ASN:HB2  | 2:C:1157:SER:HB2  | 1.89                     | 0.54              |
| 4:F:15:TYR:O      | 4:F:18:TRP:N      | 2.40                     | 0.54              |
| 1:A:167:VAL:HG23  | 1:A:180:PHE:HB3   | 1.88                     | 0.54              |
| 1:A:458:PHE:HE1   | 1:A:473:SER:HA    | 1.72                     | 0.54              |
| 1:A:512:VAL:HB    | 1:A:515:ALA:HB3   | 1.87                     | 0.54              |
| 1:A:969:GLU:HG3   | 1:A:971:ALA:H     | 1.71                     | 0.54              |
| 1:B:284:LEU:HB2   | 1:B:301:ARG:HB2   | 1.90                     | 0.54              |
| 1:B:969:GLU:HG3   | 1:B:971:ALA:H     | 1.72                     | 0.54              |
| 2:C:1281:ASP:CG   | 2:C:1284:THR:HG22 | 2.32                     | 0.54              |
| 1:A:743:GLN:HG2   | 1:A:749:THR:HG22  | 1.88                     | 0.54              |
| 1:B:387:LEU:HG    | 1:B:717:LEU:HD11  | 1.89                     | 0.54              |
| 2:C:1279:ILE:HD11 | 2:C:1291:VAL:CG2  | 2.37                     | 0.54              |
| 1:B:928:ARG:HG3   | 1:B:928:ARG:HH11  | 1.73                     | 0.54              |
| 1:B:969:GLU:HG2   | 1:B:973:ASN:HB2   | 1.90                     | 0.54              |
| 2:C:1284:THR:HG23 | 2:C:1286:HIS:H    | 1.73                     | 0.54              |
| 4:F:16:ASN:ND2    | 4:F:16:ASN:H      | 2.05                     | 0.54              |
| 1:B:40:GLU:HB3    | 1:B:42:TYR:HE1    | 1.72                     | 0.54              |
| 2:C:1284:THR:HG23 | 2:C:1286:HIS:HB2  | 1.90                     | 0.54              |
| 3:D:273:SER:C     | 3:D:275:TYR:H     | 2.15                     | 0.54              |
| 2:E:1165:GLY:HA3  | 2:E:1173:LYS:HE2  | 1.89                     | 0.54              |
| 2:E:1357:LEU:HA   | 2:E:1367:ALA:O    | 2.08                     | 0.54              |
| 1:A:143:ILE:HG21  | 1:A:152:LEU:HD23  | 1.89                     | 0.54              |
| 1:B:81:THR:HG21   | 1:B:85:ASN:HD22   | 1.72                     | 0.54              |
| 1:B:427:LEU:HD21  | 1:B:699:LEU:HD22  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:369:ARG:HG3   | 1:B:370:GLN:H     | 1.72                     | 0.54              |
| 2:C:1221:ASN:HD21 | 2:C:1254:LYS:HG3  | 1.73                     | 0.54              |
| 4:F:11:GLN:CG     | 4:F:12:ARG:CD     | 2.86                     | 0.54              |
| 1:B:40:GLU:HB3    | 1:B:42:TYR:CE1    | 2.43                     | 0.53              |
| 1:B:607:GLY:HA2   | 1:B:635:PRO:HB3   | 1.89                     | 0.53              |
| 2:C:1180:HIS:HD1  | 2:C:1181:TYR:N    | 2.07                     | 0.53              |
| 2:E:1068:GLY:HA3  | 2:E:1070:CYS:H    | 1.72                     | 0.53              |
| 2:C:1046:ALA:HB2  | 2:C:1066:VAL:N    | 2.24                     | 0.53              |
| 2:E:1150:LEU:HD23 | 2:E:1164:TRP:HB2  | 1.90                     | 0.53              |
| 1:A:333:LEU:HB3   | 1:A:350:MET:HE3   | 1.91                     | 0.53              |
| 1:A:63:VAL:HG11   | 1:A:122:GLY:HA3   | 1.90                     | 0.53              |
| 1:A:250:PRO:HD2   | 1:A:253:ILE:HD11  | 1.90                     | 0.53              |
| 1:A:724:ILE:HG23  | 1:A:735:VAL:HG22  | 1.91                     | 0.53              |
| 1:A:387:LEU:HG    | 1:A:717:LEU:HD11  | 1.91                     | 0.53              |
| 1:A:58:TYR:HD1    | 1:A:1073:TRP:CD1  | 2.26                     | 0.53              |
| 1:B:63:VAL:HG11   | 1:B:122:GLY:HA3   | 1.89                     | 0.53              |
| 1:B:458:PHE:HE1   | 1:B:473:SER:HA    | 1.73                     | 0.53              |
| 1:A:928:ARG:HH11  | 1:A:928:ARG:HG3   | 1.74                     | 0.53              |
| 2:C:1113:CYS:O    | 2:C:1137:ALA:HA   | 2.08                     | 0.53              |
| 2:C:1200:ALA:HB3  | 2:C:1214:LEU:HB2  | 1.92                     | 0.52              |
| 3:D:85:PHE:CE1    | 3:D:97:PHE:HZ     | 2.27                     | 0.52              |
| 1:A:284:LEU:HB2   | 1:A:301:ARG:HB2   | 1.90                     | 0.52              |
| 2:C:1131:TYR:CZ   | 4:H:5:PRO:HG2     | 2.44                     | 0.52              |
| 3:G:273:SER:O     | 4:H:40:HIS:HD2    | 1.93                     | 0.52              |
| 1:A:427:LEU:HD21  | 1:A:699:LEU:HD22  | 1.90                     | 0.52              |
| 1:B:998:PHE:CZ    | 1:B:1074:ARG:HD3  | 2.44                     | 0.52              |
| 2:C:1167:LYS:HG3  | 2:C:1168:SER:H    | 1.73                     | 0.52              |
| 1:A:837:TYR:HB2   | 1:A:840:GLU:HG2   | 1.92                     | 0.52              |
| 1:B:43:VAL:HG23   | 1:B:52:VAL:HG21   | 1.91                     | 0.52              |
| 1:B:248:ILE:HD13  | 1:B:300:LEU:HB2   | 1.91                     | 0.52              |
| 1:A:9:ALA:HB3     | 1:A:1037:ILE:HG22 | 1.91                     | 0.52              |
| 1:A:985:THR:HG22  | 1:A:988:GLU:OE2   | 2.09                     | 0.52              |
| 1:B:378:CYS:SG    | 1:B:724:ILE:HB    | 2.49                     | 0.52              |
| 1:B:837:TYR:HB2   | 1:B:840:GLU:HG2   | 1.92                     | 0.52              |
| 2:E:1184:PHE:HB3  | 2:E:1189:GLN:HG2  | 1.91                     | 0.52              |
| 1:A:133:LEU:HD13  | 1:A:135:LEU:HD21  | 1.91                     | 0.51              |
| 2:E:1329:PRO:HD2  | 4:F:74:ILE:HD11   | 1.91                     | 0.51              |
| 3:G:275:TYR:HE2   | 4:H:40:HIS:ND1    | 2.08                     | 0.51              |
| 1:A:490:TRP:CD1   | 1:A:519:LEU:HD21  | 2.45                     | 0.51              |
| 1:B:929:SER:HA    | 1:B:954:MET:HE3   | 1.91                     | 0.51              |
| 2:C:1298:ARG:HB2  | 2:C:1311:ALA:HB3  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1181:TYR:CE2  | 2:C:1183:GLU:HB2  | 2.39                     | 0.51              |
| 3:D:241:VAL:HG11  | 3:D:287:THR:HG23  | 1.93                     | 0.51              |
| 2:E:1088:GLU:CD   | 4:F:62:ARG:HH22   | 2.19                     | 0.51              |
| 4:F:32:ARG:CG     | 4:F:32:ARG:NH1    | 2.73                     | 0.51              |
| 1:B:724:ILE:HG23  | 1:B:724:ILE:O     | 2.10                     | 0.51              |
| 2:C:1048:ILE:O    | 2:C:1053:ARG:NH1  | 2.43                     | 0.51              |
| 2:E:1274:ILE:HG13 | 2:E:1279:ILE:HD13 | 1.93                     | 0.51              |
| 2:E:1298:ARG:HB2  | 2:E:1311:ALA:HB3  | 1.92                     | 0.51              |
| 1:A:742:VAL:HG22  | 1:A:785:GLU:HG2   | 1.92                     | 0.51              |
| 1:B:335:LYS:HB3   | 1:B:348:VAL:HB    | 1.91                     | 0.51              |
| 2:C:1353:ASN:ND2  | 2:C:1375:MET:SD   | 2.84                     | 0.51              |
| 1:A:105:HIS:HA    | 1:A:152:LEU:HD12  | 1.93                     | 0.51              |
| 2:C:1350:VAL:HG21 | 2:C:1354:ILE:HG22 | 1.91                     | 0.51              |
| 4:F:32:ARG:HG2    | 4:F:32:ARG:NH1    | 2.24                     | 0.51              |
| 2:C:1149:LEU:HD13 | 2:C:1163:LEU:HD11 | 1.93                     | 0.51              |
| 3:G:275:TYR:CE2   | 4:H:40:HIS:ND1    | 2.79                     | 0.51              |
| 2:E:1328:SER:O    | 2:E:1353:ASN:ND2  | 2.44                     | 0.50              |
| 1:A:400:ALA:HB3   | 1:A:701:ILE:HB    | 1.93                     | 0.50              |
| 1:A:494:GLN:HE21  | 1:A:496:LYS:HD3   | 1.76                     | 0.50              |
| 3:G:241:VAL:HG11  | 3:G:287:THR:HG23  | 1.94                     | 0.50              |
| 1:A:378:CYS:SG    | 1:A:721:PRO:HB2   | 2.51                     | 0.50              |
| 2:E:1238:LEU:HD13 | 2:E:1273:VAL:HG21 | 1.94                     | 0.50              |
| 1:B:58:TYR:HD1    | 1:B:1073:TRP:CD1  | 2.29                     | 0.50              |
| 1:B:252:ILE:HD13  | 1:B:252:ILE:H     | 1.76                     | 0.50              |
| 4:H:12:ARG:HB2    | 4:H:13:GLU:CA     | 2.41                     | 0.50              |
| 1:A:594:THR:HG21  | 1:A:649:VAL:HG21  | 1.94                     | 0.50              |
| 1:B:400:ALA:HB3   | 1:B:701:ILE:HB    | 1.93                     | 0.50              |
| 2:C:1308:MET:O    | 2:C:1336:THR:HA   | 2.11                     | 0.50              |
| 3:D:113:ARG:NH1   | 3:D:120:PRO:O     | 2.44                     | 0.50              |
| 2:E:1245:ASP:HB2  | 2:E:1252:ILE:HD11 | 1.93                     | 0.50              |
| 3:G:166:PRO:HB2   | 3:G:171:GLU:HG2   | 1.94                     | 0.50              |
| 1:B:164:VAL:HG11  | 1:B:167:VAL:HG22  | 1.94                     | 0.50              |
| 1:B:270:ARG:HG2   | 1:B:284:LEU:HD23  | 1.94                     | 0.50              |
| 1:B:889:ARG:HG2   | 1:B:904:ASN:ND2   | 2.27                     | 0.50              |
| 2:C:1088:GLU:CD   | 4:H:62:ARG:HH22   | 2.20                     | 0.50              |
| 1:A:413:LEU:HD23  | 1:A:468:LEU:HD22  | 1.94                     | 0.49              |
| 1:A:999:HIS:O     | 1:A:1074:ARG:NH1  | 2.45                     | 0.49              |
| 1:B:966:LEU:HB2   | 1:B:976:VAL:HG22  | 1.93                     | 0.49              |
| 3:G:85:PHE:CD2    | 3:G:129:THR:HG21  | 2.47                     | 0.49              |
| 1:A:405:PRO:HA    | 1:A:697:SER:HA    | 1.93                     | 0.49              |
| 1:B:218:MET:HB2   | 1:B:232:ILE:HG22  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:594:THR:HG21  | 1:B:649:VAL:HG21  | 1.94                     | 0.49              |
| 1:B:879:LYS:HG2   | 1:B:892:GLU:HG3   | 1.94                     | 0.49              |
| 3:G:241:VAL:HG23  | 3:G:264:LEU:HD13  | 1.94                     | 0.49              |
| 1:A:998:PHE:CZ    | 1:A:1074:ARG:HD3  | 2.47                     | 0.49              |
| 3:D:241:VAL:HG23  | 3:D:264:LEU:HD13  | 1.94                     | 0.49              |
| 1:A:78:PHE:HD1    | 1:A:88:ILE:HD13   | 1.78                     | 0.49              |
| 1:B:84:TYR:HE2    | 1:B:135:LEU:HB3   | 1.77                     | 0.49              |
| 2:C:1047:PRO:HG2  | 2:C:1053:ARG:HA   | 1.94                     | 0.49              |
| 4:F:40:HIS:C      | 4:F:42:LEU:N      | 2.69                     | 0.49              |
| 1:A:288:GLU:HB2   | 1:A:298:LYS:HB2   | 1.94                     | 0.49              |
| 1:A:471:ILE:HG23  | 1:A:476:VAL:HG22  | 1.95                     | 0.49              |
| 3:G:242:PHE:CE2   | 3:G:256:ILE:HG12  | 2.47                     | 0.49              |
| 1:A:328:LEU:HD13  | 1:A:381:ALA:HB3   | 1.95                     | 0.49              |
| 1:A:1005:ASN:HD21 | 1:A:1033:VAL:HG22 | 1.78                     | 0.49              |
| 2:C:1233:THR:O    | 2:C:1234:ASP:HB2  | 2.12                     | 0.49              |
| 2:E:1155:THR:HG22 | 2:E:1156:TRP:HD1  | 1.77                     | 0.49              |
| 2:E:1250:GLN:HE21 | 2:E:1251:ALA:H    | 1.61                     | 0.49              |
| 3:D:166:PRO:HB3   | 3:D:170:LEU:HD23  | 1.94                     | 0.49              |
| 2:E:1109:MET:HB3  | 2:E:1119:LEU:CD2  | 2.43                     | 0.49              |
| 4:F:50:TYR:HB3    | 4:F:56:GLY:HA3    | 1.95                     | 0.49              |
| 2:C:1298:ARG:HH22 | 2:C:1330:PHE:HB3  | 1.76                     | 0.49              |
| 1:A:362:MET:HE2   | 1:A:1008:CYS:SG   | 2.52                     | 0.48              |
| 1:A:830:ILE:HG23  | 1:A:850:VAL:HG22  | 1.95                     | 0.48              |
| 3:G:97:PHE:N      | 3:G:97:PHE:CD1    | 2.77                     | 0.48              |
| 1:A:320:GLY:O     | 1:A:335:LYS:HA    | 2.12                     | 0.48              |
| 2:E:1202:ILE:HG22 | 2:E:1211:LEU:HB2  | 1.94                     | 0.48              |
| 3:G:88:SER:HB2    | 3:G:134:ILE:HG22  | 1.94                     | 0.48              |
| 1:A:958:GLU:HB3   | 1:A:966:LEU:HD23  | 1.95                     | 0.48              |
| 2:E:1102:SER:HA   | 2:E:1109:MET:HE3  | 1.96                     | 0.48              |
| 1:B:413:LEU:HD23  | 1:B:468:LEU:HD22  | 1.94                     | 0.48              |
| 1:B:946:ALA:HB3   | 1:B:992:LEU:HD13  | 1.94                     | 0.48              |
| 4:H:15:TYR:CE2    | 4:H:19:THR:OG1    | 2.65                     | 0.48              |
| 1:B:830:ILE:HG23  | 1:B:850:VAL:HG22  | 1.95                     | 0.48              |
| 1:B:1005:ASN:HD21 | 1:B:1033:VAL:HG22 | 1.78                     | 0.48              |
| 1:A:270:ARG:HG2   | 1:A:284:LEU:HD23  | 1.94                     | 0.48              |
| 1:A:946:ALA:HB3   | 1:A:992:LEU:HD13  | 1.95                     | 0.48              |
| 1:B:405:PRO:HA    | 1:B:697:SER:HA    | 1.95                     | 0.48              |
| 2:E:1198:ASP:HA   | 2:E:1226:ASN:HD22 | 1.79                     | 0.48              |
| 1:A:174:GLN:CD    | 1:A:174:GLN:H     | 2.22                     | 0.48              |
| 1:A:258:ILE:HG21  | 1:A:273:LEU:HB3   | 1.95                     | 0.48              |
| 1:B:873:MET:HE3   | 1:B:880:LEU:HD21  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:78:PHE:HD1    | 1:B:88:ILE:HD13   | 1.79                     | 0.48              |
| 1:B:394:ILE:HG23  | 1:B:705:ASP:HB2   | 1.95                     | 0.48              |
| 3:D:256:ILE:O     | 3:D:258:ARG:NH1   | 2.47                     | 0.48              |
| 4:F:46:ILE:CD1    | 4:F:63:ILE:HD13   | 2.44                     | 0.48              |
| 1:B:22:HIS:O      | 1:B:75:ASP:HB2    | 2.14                     | 0.48              |
| 2:E:1054:LEU:HD12 | 2:E:1057:ARG:HD2  | 1.95                     | 0.48              |
| 3:G:256:ILE:O     | 3:G:258:ARG:NH1   | 2.47                     | 0.48              |
| 1:B:258:ILE:HG21  | 1:B:273:LEU:HB3   | 1.96                     | 0.48              |
| 3:D:290:LEU:HD23  | 3:D:293:LYS:HD2   | 1.96                     | 0.48              |
| 1:A:516:LEU:O     | 1:A:531:HIS:HA    | 2.14                     | 0.47              |
| 1:A:775:THR:HA    | 1:A:776:ALA:HA    | 1.54                     | 0.47              |
| 1:A:966:LEU:HB2   | 1:A:976:VAL:HG22  | 1.95                     | 0.47              |
| 1:B:958:GLU:HB3   | 1:B:966:LEU:HD23  | 1.94                     | 0.47              |
| 2:E:1073:ARG:HE   | 2:E:1338:ASN:ND2  | 2.07                     | 0.47              |
| 1:B:288:GLU:HB2   | 1:B:298:LYS:HB2   | 1.95                     | 0.47              |
| 1:B:375:LEU:HD23  | 1:B:390:ILE:HD13  | 1.96                     | 0.47              |
| 1:B:1058:LEU:HD23 | 1:B:1062:ILE:HD11 | 1.96                     | 0.47              |
| 2:C:1074:HIS:HA   | 2:C:1345:ILE:HD13 | 1.96                     | 0.47              |
| 2:C:1204:ASP:HB3  | 2:C:1207:THR:OG1  | 2.14                     | 0.47              |
| 1:A:375:LEU:HD23  | 1:A:390:ILE:HD13  | 1.96                     | 0.47              |
| 1:A:1002:GLU:HB3  | 1:A:1032:THR:HG21 | 1.97                     | 0.47              |
| 2:C:1236:LEU:HD13 | 2:C:1243:LEU:HD11 | 1.95                     | 0.47              |
| 2:E:1049:ASN:OD1  | 2:E:1051:THR:HG22 | 2.15                     | 0.47              |
| 2:E:1096:PHE:HA   | 2:E:1111:GLY:O    | 2.14                     | 0.47              |
| 3:G:290:LEU:HD23  | 3:G:293:LYS:HD2   | 1.97                     | 0.47              |
| 4:H:34:PHE:HB2    | 4:H:39:LEU:HD11   | 1.96                     | 0.47              |
| 1:A:218:MET:HB2   | 1:A:232:ILE:HG22  | 1.95                     | 0.47              |
| 1:B:985:THR:HG22  | 1:B:988:GLU:CG    | 2.44                     | 0.47              |
| 2:C:1153:SER:HA   | 2:C:1160:LEU:O    | 2.15                     | 0.47              |
| 2:C:1273:VAL:HB   | 2:C:1282:LEU:HD13 | 1.97                     | 0.47              |
| 4:F:18:TRP:CZ3    | 4:F:22:LEU:CD2    | 2.97                     | 0.47              |
| 3:G:273:SER:C     | 3:G:275:TYR:H     | 2.21                     | 0.47              |
| 3:G:275:TYR:CE2   | 4:H:40:HIS:CG     | 3.02                     | 0.47              |
| 1:A:394:ILE:HG23  | 1:A:705:ASP:HB2   | 1.96                     | 0.47              |
| 3:D:208:THR:O     | 3:D:217:HIS:HB2   | 2.15                     | 0.47              |
| 1:A:910:MET:HB3   | 1:A:926:LEU:HB2   | 1.97                     | 0.47              |
| 3:G:85:PHE:CE1    | 3:G:97:PHE:CZ     | 2.76                     | 0.47              |
| 4:H:13:GLU:CB     | 4:H:14:PRO:CD     | 2.84                     | 0.47              |
| 1:A:691:LEU:HD21  | 1:A:704:ILE:HB    | 1.96                     | 0.47              |
| 1:A:889:ARG:HG2   | 1:A:904:ASN:ND2   | 2.30                     | 0.47              |
| 1:B:328:LEU:HD13  | 1:B:381:ALA:HB3   | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:637:VAL:HB    | 1:B:652:CYS:HB2   | 1.97                     | 0.47              |
| 2:E:1109:MET:HE1  | 2:E:1166:MET:HE2  | 1.97                     | 0.47              |
| 2:C:1137:ALA:O    | 2:C:1139:THR:HG23 | 2.16                     | 0.46              |
| 4:F:18:TRP:CH2    | 4:F:22:LEU:CD2    | 2.99                     | 0.46              |
| 3:G:85:PHE:HD2    | 3:G:86:GLY:H      | 1.63                     | 0.46              |
| 1:A:1058:LEU:HD23 | 1:A:1062:ILE:HD11 | 1.96                     | 0.46              |
| 1:B:830:ILE:HG12  | 1:B:850:VAL:HG13  | 1.97                     | 0.46              |
| 1:B:873:MET:HB3   | 1:B:880:LEU:HD11  | 1.96                     | 0.46              |
| 1:B:998:PHE:CE1   | 1:B:1074:ARG:HD3  | 2.50                     | 0.46              |
| 2:C:1054:LEU:HD12 | 2:C:1057:ARG:HD2  | 1.97                     | 0.46              |
| 2:C:1294:LEU:HD11 | 2:C:1308:MET:CE   | 2.45                     | 0.46              |
| 2:C:1298:ARG:HH22 | 2:C:1330:PHE:CB   | 2.28                     | 0.46              |
| 3:D:275:TYR:CD2   | 4:F:40:HIS:CE1    | 3.03                     | 0.46              |
| 1:A:362:MET:HB2   | 1:A:1006:VAL:HG21 | 1.96                     | 0.46              |
| 1:A:1057:ARG:HH12 | 1:A:1110:ALA:HB3  | 1.80                     | 0.46              |
| 2:C:1156:TRP:CG   | 4:H:29:GLU:HG2    | 2.50                     | 0.46              |
| 1:B:1057:ARG:HH12 | 1:B:1110:ALA:HB3  | 1.81                     | 0.46              |
| 3:D:242:PHE:CE2   | 3:D:256:ILE:HG12  | 2.47                     | 0.46              |
| 2:E:1187:HIS:HE1  | 2:E:1190:ASP:H    | 1.63                     | 0.46              |
| 4:F:18:TRP:CH2    | 4:F:22:LEU:HD22   | 2.50                     | 0.46              |
| 2:C:1187:HIS:HE1  | 2:C:1190:ASP:H    | 1.62                     | 0.46              |
| 2:C:1298:ARG:NH2  | 2:C:1330:PHE:CB   | 2.77                     | 0.46              |
| 3:D:85:PHE:CE1    | 3:D:97:PHE:CZ     | 3.04                     | 0.46              |
| 2:E:1172:MET:HE1  | 2:E:1175:SER:HB3  | 1.98                     | 0.46              |
| 1:A:316:TYR:CZ    | 1:A:318:ASP:HA    | 2.51                     | 0.46              |
| 1:B:547:GLY:HA2   | 1:B:548:ASP:HA    | 1.72                     | 0.46              |
| 2:C:1068:GLY:HA3  | 2:C:1069:GLY:HA3  | 1.42                     | 0.46              |
| 3:G:189:HIS:CD2   | 3:G:191:ASP:HB3   | 2.51                     | 0.46              |
| 1:B:316:TYR:CZ    | 1:B:318:ASP:HA    | 2.50                     | 0.46              |
| 1:B:836:VAL:HG22  | 2:E:1051:THR:HG21 | 1.96                     | 0.46              |
| 2:C:1049:ASN:OD1  | 2:C:1051:THR:HG22 | 2.15                     | 0.46              |
| 4:F:8:GLN:HE21    | 4:F:8:GLN:HB3     | 1.59                     | 0.46              |
| 1:A:478:LEU:HD23  | 1:A:526:LEU:HG    | 1.98                     | 0.46              |
| 1:B:361:ASP:H     | 1:B:378:CYS:HB2   | 1.81                     | 0.46              |
| 1:B:471:ILE:HG23  | 1:B:476:VAL:HG22  | 1.96                     | 0.46              |
| 2:E:1342:TYR:N    | 2:E:1342:TYR:CD1  | 2.84                     | 0.46              |
| 1:A:637:VAL:HB    | 1:A:652:CYS:HB2   | 1.98                     | 0.46              |
| 1:B:820:LYS:HD3   | 1:B:825:PRO:HA    | 1.98                     | 0.46              |
| 2:E:1279:ILE:HG22 | 2:E:1289:HIS:O    | 2.16                     | 0.46              |
| 4:H:46:ILE:CD1    | 4:H:60:ILE:HG13   | 2.46                     | 0.46              |
| 2:E:1149:LEU:HD13 | 2:E:1163:LEU:HD21 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:F:12:ARG:N      | 4:F:12:ARG:CD     | 2.72                     | 0.45              |
| 1:A:141:LYS:HE2   | 1:A:154:ALA:HB3   | 1.98                     | 0.45              |
| 1:A:820:LYS:HD3   | 1:A:825:PRO:HA    | 1.97                     | 0.45              |
| 2:C:1082:PRO:HA   | 2:C:1386:LEU:O    | 2.17                     | 0.45              |
| 2:C:1359:THR:HB   | 2:C:1366:LEU:HD12 | 1.98                     | 0.45              |
| 2:E:1073:ARG:CD   | 2:E:1306:THR:HG22 | 2.45                     | 0.45              |
| 2:E:1376:ASP:C    | 2:E:1378:LEU:H    | 2.25                     | 0.45              |
| 1:B:1002:GLU:HB3  | 1:B:1032:THR:HG21 | 1.96                     | 0.45              |
| 3:D:97:PHE:HD1    | 3:D:97:PHE:H      | 1.63                     | 0.45              |
| 3:D:148:HIS:ND1   | 3:D:212:HIS:HA    | 2.31                     | 0.45              |
| 2:E:1180:HIS:HD2  | 2:E:1197:GLY:H    | 1.63                     | 0.45              |
| 3:G:208:THR:O     | 3:G:217:HIS:HB2   | 2.17                     | 0.45              |
| 1:A:830:ILE:HG12  | 1:A:850:VAL:HG13  | 1.98                     | 0.45              |
| 1:A:291:MET:HE3   | 1:A:291:MET:HB3   | 1.74                     | 0.45              |
| 1:B:207:TRP:CD1   | 1:B:242:GLY:H     | 2.34                     | 0.45              |
| 3:G:126:PHE:HB3   | 3:G:129:THR:CG2   | 2.47                     | 0.45              |
| 4:H:44:GLN:O      | 4:H:47:TYR:N      | 2.49                     | 0.45              |
| 1:A:504:ASN:HD21  | 1:A:507:GLN:HB2   | 1.81                     | 0.45              |
| 1:A:857:LYS:HG2   | 1:A:858:LEU:H     | 1.82                     | 0.45              |
| 3:D:271:PRO:O     | 4:F:27:LYS:NZ     | 2.45                     | 0.45              |
| 1:A:416:ASP:HB3   | 1:A:419:ARG:HD3   | 1.99                     | 0.45              |
| 1:A:731:GLN:O     | 1:A:796:GLN:HB2   | 2.17                     | 0.45              |
| 1:B:691:LEU:HD21  | 1:B:704:ILE:HB    | 1.99                     | 0.45              |
| 2:C:1087:ARG:HH12 | 2:C:1372:GLN:HE21 | 1.64                     | 0.45              |
| 2:C:1342:TYR:HD1  | 2:C:1342:TYR:H    | 1.64                     | 0.45              |
| 1:B:64:MET:HG3    | 1:B:77:LEU:HD11   | 1.98                     | 0.45              |
| 2:C:1250:GLN:HE21 | 2:C:1251:ALA:H    | 1.64                     | 0.45              |
| 1:A:123:ILE:HD12  | 1:A:169:PHE:CD1   | 2.52                     | 0.45              |
| 1:B:84:TYR:OH     | 1:B:115:PRO:HB3   | 2.17                     | 0.45              |
| 1:B:775:THR:HA    | 1:B:776:ALA:HA    | 1.53                     | 0.45              |
| 2:C:1066:VAL:HG13 | 2:C:1067:ASP:N    | 2.31                     | 0.45              |
| 2:E:1102:SER:HB3  | 2:E:1107:PHE:O    | 2.17                     | 0.45              |
| 1:A:561:TRP:CD1   | 1:A:587:ILE:HD11  | 2.52                     | 0.45              |
| 2:C:1096:PHE:HA   | 2:C:1111:GLY:O    | 2.16                     | 0.45              |
| 2:E:1099:CYS:HB3  | 2:E:1369:ILE:HD11 | 1.98                     | 0.45              |
| 1:A:15:VAL:HG13   | 1:A:33:ILE:HG23   | 1.99                     | 0.44              |
| 1:B:123:ILE:HD12  | 1:B:169:PHE:CD1   | 2.53                     | 0.44              |
| 2:C:1379:ASN:ND2  | 2:C:1379:ASN:H    | 2.13                     | 0.44              |
| 1:A:36:ASN:HD21   | 1:A:60:LYS:HG2    | 1.81                     | 0.44              |
| 1:A:614:PHE:HB2   | 1:A:623:LEU:HD22  | 1.99                     | 0.44              |
| 3:G:206:VAL:HG22  | 3:G:222:TRP:HB2   | 2.00                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:H:12:ARG:N     | 4:H:12:ARG:HD3    | 2.32                     | 0.44              |
| 1:A:500:VAL:HG21 | 1:A:540:CYS:HA    | 1.99                     | 0.44              |
| 1:B:81:THR:HG23  | 1:B:83:LYS:H      | 1.82                     | 0.44              |
| 1:B:561:TRP:CD1  | 1:B:587:ILE:HD11  | 2.53                     | 0.44              |
| 3:G:273:SER:O    | 4:H:40:HIS:CD2    | 2.70                     | 0.44              |
| 2:E:1118:LYS:HE2 | 2:E:1130:SER:HB2  | 1.99                     | 0.44              |
| 3:G:246:GLY:HA3  | 3:G:268:HIS:HB2   | 1.99                     | 0.44              |
| 1:B:504:ASN:HD21 | 1:B:507:GLN:HB2   | 1.83                     | 0.44              |
| 2:E:1159:PRO:HA  | 2:E:1177:THR:HA   | 1.99                     | 0.44              |
| 3:G:204:ASN:O    | 3:G:226:THR:HG21  | 2.18                     | 0.44              |
| 4:H:11:GLN:CA    | 4:H:12:ARG:NH1    | 2.81                     | 0.44              |
| 1:B:81:THR:HG21  | 1:B:85:ASN:ND2    | 2.32                     | 0.44              |
| 3:D:85:PHE:CD1   | 3:D:97:PHE:HZ     | 2.35                     | 0.44              |
| 3:D:113:ARG:HG2  | 3:D:118:VAL:HB    | 1.98                     | 0.44              |
| 2:E:1221:ASN:HB3 | 2:E:1257:LYS:HD2  | 2.00                     | 0.44              |
| 4:F:42:LEU:O     | 4:F:46:ILE:HG12   | 2.17                     | 0.44              |
| 4:H:20:LEU:O     | 4:H:24:GLU:OE1    | 2.35                     | 0.44              |
| 1:B:15:VAL:HG13  | 1:B:33:ILE:HG23   | 1.98                     | 0.44              |
| 1:B:183:GLN:NE2  | 1:B:188:ARG:HE    | 2.14                     | 0.44              |
| 1:B:265:ASP:HA   | 1:B:266:PRO:HD2   | 1.81                     | 0.44              |
| 3:G:105:LEU:HD11 | 3:G:222:TRP:CE2   | 2.53                     | 0.44              |
| 1:A:105:HIS:CA   | 1:A:152:LEU:HD12  | 2.47                     | 0.44              |
| 2:C:1102:SER:HB3 | 2:C:1107:PHE:O    | 2.18                     | 0.44              |
| 3:G:84:PHE:CD1   | 3:G:84:PHE:O      | 2.71                     | 0.44              |
| 4:H:23:LEU:O     | 4:H:27:LYS:HG3    | 2.17                     | 0.44              |
| 3:D:204:ASN:O    | 3:D:226:THR:HG21  | 2.18                     | 0.44              |
| 3:G:173:ILE:HG22 | 3:G:278:PHE:CZ    | 2.53                     | 0.44              |
| 1:A:168:LYS:HG3  | 1:A:219:VAL:O     | 2.16                     | 0.43              |
| 1:B:6:VAL:HG22   | 1:B:1040:VAL:HG22 | 2.00                     | 0.43              |
| 1:B:174:GLN:HG3  | 1:B:175:ALA:H     | 1.82                     | 0.43              |
| 1:B:404:LEU:O    | 1:B:407:ILE:HD11  | 2.18                     | 0.43              |
| 2:C:1077:PHE:CD2 | 2:C:1307:VAL:HG21 | 2.53                     | 0.43              |
| 2:C:1337:PHE:HD1 | 2:C:1344:PRO:HA   | 1.83                     | 0.43              |
| 2:E:1059:SER:HG  | 2:E:1060:PHE:HD1  | 1.65                     | 0.43              |
| 4:H:46:ILE:HD13  | 4:H:60:ILE:HB     | 1.99                     | 0.43              |
| 1:A:936:LYS:HG3  | 1:A:943:GLU:CG    | 2.46                     | 0.43              |
| 1:A:437:MET:HE3  | 1:A:438:LEU:H     | 1.82                     | 0.43              |
| 1:B:334:VAL:HG13 | 1:B:347:VAL:HG23  | 2.00                     | 0.43              |
| 1:B:679:MET:HE2  | 1:B:691:LEU:HD13  | 2.00                     | 0.43              |
| 1:B:864:LYS:CB   | 1:B:899:LEU:HD12  | 2.48                     | 0.43              |
| 2:E:1118:LYS:HB3 | 2:E:1120:TYR:CE2  | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1149:LEU:HD13 | 2:E:1163:LEU:HD11 | 2.00                     | 0.43              |
| 3:G:148:HIS:ND1   | 3:G:212:HIS:HA    | 2.33                     | 0.43              |
| 3:G:279:PHE:HD1   | 3:G:279:PHE:HA    | 1.70                     | 0.43              |
| 1:A:935:TYR:O     | 1:A:937:PRO:HD3   | 2.18                     | 0.43              |
| 1:B:614:PHE:HB2   | 1:B:623:LEU:HD22  | 1.99                     | 0.43              |
| 2:C:1121:ASN:HB3  | 2:C:1124:SER:OG   | 2.18                     | 0.43              |
| 1:A:292:ASP:HA    | 1:A:293:GLY:HA2   | 1.72                     | 0.43              |
| 1:B:816:LEU:HB3   | 1:B:831:VAL:HG22  | 2.00                     | 0.43              |
| 3:D:105:LEU:HD11  | 3:D:222:TRP:CE2   | 2.53                     | 0.43              |
| 2:E:1342:TYR:N    | 2:E:1342:TYR:HD1  | 2.15                     | 0.43              |
| 1:A:780:THR:HA    | 1:A:781:SER:HA    | 1.95                     | 0.43              |
| 1:A:884:ILE:HD13  | 1:A:889:ARG:HD2   | 2.01                     | 0.43              |
| 2:C:1149:LEU:CD1  | 2:C:1205:ILE:HD12 | 2.47                     | 0.43              |
| 2:C:1355:PHE:CE1  | 2:C:1371:ASN:HB2  | 2.53                     | 0.43              |
| 1:A:64:MET:HG3    | 1:A:77:LEU:HD11   | 2.01                     | 0.43              |
| 1:A:541:LEU:HB3   | 1:A:558:ILE:HD12  | 2.00                     | 0.43              |
| 1:B:928:ARG:HD2   | 1:B:947:ARG:HH12  | 1.83                     | 0.43              |
| 1:A:58:TYR:CD1    | 1:A:1073:TRP:CD1  | 3.05                     | 0.43              |
| 1:A:334:VAL:HG13  | 1:A:347:VAL:HG23  | 2.01                     | 0.43              |
| 1:A:396:ILE:HD12  | 1:A:673:LEU:HD11  | 2.01                     | 0.43              |
| 1:A:578:HIS:HE1   | 1:A:580:GLU:HG2   | 1.83                     | 0.43              |
| 1:B:114:ARG:HA    | 1:B:115:PRO:HD3   | 1.88                     | 0.43              |
| 1:B:506:SER:HA    | 1:B:521:ILE:HB    | 2.01                     | 0.43              |
| 1:B:568:ILE:HD12  | 1:B:578:HIS:HB3   | 2.00                     | 0.43              |
| 2:E:1081:ARG:O    | 2:E:1388:GLU:N    | 2.48                     | 0.43              |
| 4:H:16:ASN:OD1    | 4:H:16:ASN:N      | 2.47                     | 0.43              |
| 1:A:1080:ARG:H    | 1:A:1080:ARG:HG2  | 1.48                     | 0.43              |
| 1:B:578:HIS:HE1   | 1:B:580:GLU:HG2   | 1.83                     | 0.43              |
| 2:C:1069:GLY:O    | 2:C:1073:ARG:HG2  | 2.18                     | 0.43              |
| 4:F:16:ASN:O      | 4:F:17:GLU:HG3    | 2.19                     | 0.43              |
| 1:A:404:LEU:HD11  | 1:A:434:ARG:HH12  | 1.83                     | 0.43              |
| 1:B:327:ARG:HH12  | 2:E:1060:PHE:H    | 1.66                     | 0.43              |
| 1:B:541:LEU:HB3   | 1:B:558:ILE:HD12  | 2.00                     | 0.43              |
| 4:F:16:ASN:HD22   | 4:F:16:ASN:H      | 1.60                     | 0.43              |
| 4:F:41:ASN:O      | 4:F:45:HIS:HD2    | 2.02                     | 0.43              |
| 1:A:84:TYR:OH     | 1:A:115:PRO:HB3   | 2.18                     | 0.42              |
| 2:C:1156:TRP:CD2  | 4:H:29:GLU:HG2    | 2.54                     | 0.42              |
| 2:C:1366:LEU:HB3  | 2:C:1387:TYR:HB2  | 2.01                     | 0.42              |
| 3:G:97:PHE:HD1    | 3:G:97:PHE:N      | 2.12                     | 0.42              |
| 3:G:139:VAL:HB    | 3:G:200:VAL:HG13  | 2.01                     | 0.42              |
| 1:A:816:LEU:HB3   | 1:A:831:VAL:HG22  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:881:LEU:HD21  | 1:A:921:ILE:HG21  | 2.02                     | 0.42              |
| 2:C:1342:TYR:N    | 2:C:1342:TYR:CD1  | 2.87                     | 0.42              |
| 1:A:362:MET:HG3   | 1:A:377:THR:HG22  | 2.01                     | 0.42              |
| 1:A:679:MET:HE2   | 1:A:691:LEU:HD13  | 2.01                     | 0.42              |
| 1:B:881:LEU:HD21  | 1:B:921:ILE:HG21  | 2.02                     | 0.42              |
| 1:B:974:LEU:HB2   | 1:B:998:PHE:HB3   | 2.02                     | 0.42              |
| 1:B:1080:ARG:H    | 1:B:1080:ARG:HG2  | 1.48                     | 0.42              |
| 1:A:506:SER:HA    | 1:A:521:ILE:HB    | 2.00                     | 0.42              |
| 1:A:578:HIS:CE1   | 1:A:580:GLU:HG2   | 2.55                     | 0.42              |
| 1:A:836:VAL:HG22  | 2:C:1051:THR:HG21 | 2.01                     | 0.42              |
| 1:B:58:TYR:CD1    | 1:B:1073:TRP:CD1  | 3.07                     | 0.42              |
| 1:B:605:ALA:HB1   | 1:B:636:THR:HB    | 2.01                     | 0.42              |
| 3:D:206:VAL:HG22  | 3:D:222:TRP:HB2   | 2.00                     | 0.42              |
| 3:G:156:LEU:HB2   | 3:G:159:SER:HB3   | 2.00                     | 0.42              |
| 1:A:739:ARG:HG3   | 1:A:788:VAL:HB    | 2.02                     | 0.42              |
| 1:B:578:HIS:CE1   | 1:B:580:GLU:HG2   | 2.55                     | 0.42              |
| 1:B:935:TYR:O     | 1:B:937:PRO:HD3   | 2.19                     | 0.42              |
| 1:B:937:PRO:HD2   | 1:B:938:MET:HE3   | 2.01                     | 0.42              |
| 1:A:605:ALA:HB1   | 1:A:636:THR:HB    | 2.00                     | 0.42              |
| 2:C:1059:SER:HG   | 2:C:1060:PHE:HD1  | 1.66                     | 0.42              |
| 2:C:1274:ILE:HD12 | 2:C:1279:ILE:HG12 | 2.02                     | 0.42              |
| 2:E:1259:ASN:CG   | 2:E:1260:MET:N    | 2.78                     | 0.42              |
| 1:A:407:ILE:HG21  | 1:A:427:LEU:HD23  | 2.02                     | 0.42              |
| 1:B:316:TYR:CE2   | 1:B:318:ASP:HA    | 2.54                     | 0.42              |
| 1:B:739:ARG:HG3   | 1:B:788:VAL:HB    | 2.02                     | 0.42              |
| 2:E:1082:PRO:HA   | 2:E:1387:TYR:HA   | 2.01                     | 0.42              |
| 2:E:1180:HIS:CD2  | 2:E:1197:GLY:H    | 2.38                     | 0.42              |
| 4:F:46:ILE:HD12   | 4:F:63:ILE:HD13   | 2.02                     | 0.42              |
| 1:A:404:LEU:O     | 1:A:407:ILE:HD11  | 2.19                     | 0.42              |
| 1:A:638:LEU:HD23  | 1:A:649:VAL:HG11  | 2.01                     | 0.42              |
| 1:B:927:MET:HG3   | 1:B:953:TRP:CE2   | 2.55                     | 0.42              |
| 3:D:126:PHE:HB3   | 3:D:129:THR:CG2   | 2.49                     | 0.42              |
| 2:E:1047:PRO:HG2  | 2:E:1053:ARG:HA   | 2.02                     | 0.42              |
| 1:B:518:TYR:CD1   | 1:B:529:ILE:HB    | 2.55                     | 0.42              |
| 1:B:724:ILE:CD1   | 1:B:735:VAL:CG2   | 2.93                     | 0.42              |
| 1:B:731:GLN:O     | 1:B:796:GLN:HB2   | 2.19                     | 0.42              |
| 2:E:1109:MET:HB2  | 2:E:1117:LEU:HD11 | 2.02                     | 0.42              |
| 3:G:158:PHE:O     | 3:G:170:LEU:HD13  | 2.20                     | 0.42              |
| 1:A:411:TRP:HA    | 1:A:412:PRO:HD3   | 1.96                     | 0.42              |
| 1:A:568:ILE:HD12  | 1:A:578:HIS:HB3   | 2.02                     | 0.42              |
| 1:A:1030:PHE:CE1  | 1:A:1036:MET:CE   | 3.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:141:LYS:HE2   | 1:B:154:ALA:HB3   | 2.01                     | 0.42              |
| 1:B:1014:MET:HE2  | 1:B:1016:ASN:HD21 | 1.85                     | 0.42              |
| 2:C:1223:TYR:HE2  | 2:C:1241:GLY:HA3  | 1.85                     | 0.42              |
| 2:E:1074:HIS:CD2  | 2:E:1345:ILE:HG12 | 2.55                     | 0.42              |
| 1:A:1131:LYS:HA   | 1:A:1131:LYS:HD2  | 1.94                     | 0.41              |
| 2:E:1380:MET:HE1  | 4:F:70:ILE:HD11   | 2.01                     | 0.41              |
| 3:G:131:MET:HG3   | 3:G:197:LYS:HG3   | 2.02                     | 0.41              |
| 3:G:140:VAL:HB    | 3:G:242:PHE:CE1   | 2.55                     | 0.41              |
| 1:A:518:TYR:CD1   | 1:A:529:ILE:HB    | 2.55                     | 0.41              |
| 3:D:140:VAL:HB    | 3:D:242:PHE:CE1   | 2.55                     | 0.41              |
| 3:G:275:TYR:CD2   | 4:H:40:HIS:CG     | 3.09                     | 0.41              |
| 4:H:15:TYR:HB3    | 4:H:16:ASN:H      | 1.71                     | 0.41              |
| 1:A:39:LEU:CD1    | 1:A:64:MET:CE     | 2.97                     | 0.41              |
| 1:A:476:VAL:HB    | 1:A:490:TRP:HB3   | 2.02                     | 0.41              |
| 2:E:1259:ASN:OD1  | 2:E:1262:ILE:N    | 2.49                     | 0.41              |
| 1:A:182:TYR:CE2   | 1:A:189:HIS:HB2   | 2.54                     | 0.41              |
| 1:A:317:LEU:HD12  | 1:A:321:VAL:HG12  | 2.01                     | 0.41              |
| 1:A:415:SER:N     | 1:A:423:ASP:OD1   | 2.43                     | 0.41              |
| 1:A:727:GLN:HB3   | 1:A:730:SER:HB2   | 2.02                     | 0.41              |
| 1:A:824:ASP:HA    | 1:A:825:PRO:HD3   | 1.90                     | 0.41              |
| 2:E:1243:LEU:HB2  | 2:E:1255:PHE:HE2  | 1.86                     | 0.41              |
| 4:F:23:LEU:HD11   | 4:F:60:ILE:HG23   | 2.01                     | 0.41              |
| 4:F:64:LEU:HA     | 4:F:67:LEU:HD12   | 2.02                     | 0.41              |
| 1:A:928:ARG:HD2   | 1:A:947:ARG:HH12  | 1.85                     | 0.41              |
| 1:B:19:VAL:HG12   | 1:B:64:MET:HE3    | 2.02                     | 0.41              |
| 3:D:139:VAL:HB    | 3:D:200:VAL:HG13  | 2.02                     | 0.41              |
| 2:E:1202:ILE:O    | 2:E:1210:LYS:HA   | 2.20                     | 0.41              |
| 4:F:59:ALA:O      | 4:F:63:ILE:HD12   | 2.21                     | 0.41              |
| 1:A:305:LEU:HA    | 1:A:346:TYR:HD2   | 1.85                     | 0.41              |
| 2:E:1330:PHE:CD1  | 2:E:1330:PHE:N    | 2.88                     | 0.41              |
| 1:A:125:ASP:OD2   | 1:A:127:GLU:HB2   | 2.21                     | 0.41              |
| 1:B:578:HIS:HD2   | 1:B:622:LEU:HD23  | 1.86                     | 0.41              |
| 1:B:884:ILE:HD13  | 1:B:889:ARG:HD2   | 2.03                     | 0.41              |
| 1:B:910:MET:O     | 1:B:912:LEU:HG    | 2.21                     | 0.41              |
| 4:H:12:ARG:NH1    | 4:H:12:ARG:HG2    | 2.36                     | 0.41              |
| 1:A:654:ASP:HA    | 1:A:675:GLU:HG3   | 2.03                     | 0.41              |
| 1:A:985:THR:HA    | 3:D:219:GLU:OE2   | 2.21                     | 0.41              |
| 1:B:369:ARG:HG3   | 1:B:370:GLN:N     | 2.35                     | 0.41              |
| 1:B:826:ASN:HB2   | 1:B:828:TYR:CZ    | 2.56                     | 0.41              |
| 2:E:1151:LEU:HD11 | 2:E:1192:VAL:HG22 | 2.02                     | 0.41              |
| 4:H:43:GLY:O      | 4:H:44:GLN:C      | 2.63                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:6:VAL:HG22   | 1:A:1040:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:910:MET:O    | 1:A:912:LEU:HG    | 2.21                     | 0.41              |
| 1:B:291:MET:HB3  | 1:B:291:MET:HE3   | 1.72                     | 0.41              |
| 3:D:131:MET:HG3  | 3:D:197:LYS:HG3   | 2.03                     | 0.41              |
| 3:D:156:LEU:HB2  | 3:D:159:SER:HB3   | 2.02                     | 0.41              |
| 2:E:1342:TYR:HD1 | 2:E:1342:TYR:H    | 1.69                     | 0.41              |
| 1:A:592:LEU:HD22 | 1:A:594:THR:HB    | 2.04                     | 0.40              |
| 1:B:906:TYR:C    | 1:B:908:ASN:H     | 2.29                     | 0.40              |
| 2:C:1088:GLU:HB3 | 2:C:1094:SER:HA   | 2.03                     | 0.40              |
| 2:C:1191:ARG:HA  | 2:C:1203:TYR:O    | 2.21                     | 0.40              |
| 4:F:22:LEU:O     | 4:F:22:LEU:CG     | 2.69                     | 0.40              |
| 3:G:170:LEU:HD12 | 3:G:173:ILE:CG1   | 2.50                     | 0.40              |
| 1:A:57:MET:SD    | 1:A:1065:VAL:HB   | 2.61                     | 0.40              |
| 1:B:396:ILE:HD12 | 1:B:673:LEU:HD11  | 2.03                     | 0.40              |
| 2:C:1267:HIS:ND1 | 2:C:1269:ASN:ND2  | 2.70                     | 0.40              |
| 2:C:1267:HIS:CE1 | 2:C:1268:PRO:HD2  | 2.55                     | 0.40              |
| 1:A:58:TYR:HB3   | 1:A:1073:TRP:HB2  | 2.02                     | 0.40              |
| 1:A:328:LEU:HD23 | 1:A:328:LEU:HA    | 1.76                     | 0.40              |
| 1:A:677:ASN:HB2  | 1:A:695:ASN:HA    | 2.02                     | 0.40              |
| 1:B:638:LEU:HD23 | 1:B:649:VAL:HG11  | 2.03                     | 0.40              |
| 1:B:727:GLN:HB3  | 1:B:730:SER:HB2   | 2.02                     | 0.40              |
| 2:C:1187:HIS:ND1 | 2:C:1188:SER:N    | 2.69                     | 0.40              |
| 2:C:1245:ASP:HB2 | 2:C:1252:ILE:HD11 | 2.03                     | 0.40              |
| 4:F:2:GLU:HB3    | 4:F:3:GLN:H       | 1.70                     | 0.40              |
| 1:A:101:ILE:H    | 1:A:101:ILE:HG13  | 1.64                     | 0.40              |
| 1:A:725:CYS:SG   | 1:A:817:VAL:HA    | 2.62                     | 0.40              |
| 1:B:292:ASP:HA   | 1:B:293:GLY:HA2   | 1.73                     | 0.40              |
| 2:C:1188:SER:O   | 2:C:1189:GLN:C    | 2.63                     | 0.40              |
| 3:G:140:VAL:HG21 | 3:G:233:LEU:HD13  | 2.03                     | 0.40              |
| 4:H:1:MET:HA     | 4:H:2:GLU:CG      | 2.51                     | 0.40              |
| 1:A:207:TRP:HB3  | 1:A:242:GLY:HA2   | 2.04                     | 0.40              |
| 1:B:407:ILE:HG21 | 1:B:427:LEU:HD23  | 2.03                     | 0.40              |
| 2:C:1089:ALA:HB2 | 2:C:1127:GLU:OE1  | 2.22                     | 0.40              |
| 2:E:1269:ASN:O   | 2:E:1271:LEU:HD13 | 2.21                     | 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     | 1127/1140 (99%) | 991 (88%)  | 106 (9%)  | 30 (3%)  | 4           | 27 |
| 1   | B     | 1127/1140 (99%) | 997 (88%)  | 104 (9%)  | 26 (2%)  | 5           | 30 |
| 2   | C     | 327/361 (91%)   | 278 (85%)  | 31 (10%)  | 18 (6%)  | 1           | 13 |
| 2   | E     | 327/361 (91%)   | 279 (85%)  | 35 (11%)  | 13 (4%)  | 2           | 19 |
| 3   | D     | 219/222 (99%)   | 191 (87%)  | 17 (8%)   | 11 (5%)  | 1           | 15 |
| 3   | G     | 219/222 (99%)   | 186 (85%)  | 22 (10%)  | 11 (5%)  | 1           | 15 |
| 4   | F     | 72/96 (75%)     | 50 (69%)   | 12 (17%)  | 10 (14%) | 0           | 3  |
| 4   | H     | 72/96 (75%)     | 57 (79%)   | 8 (11%)   | 7 (10%)  | 0           | 6  |
| All | All   | 3490/3638 (96%) | 3029 (87%) | 335 (10%) | 126 (4%) | 2           | 22 |

All (126) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 162  | LEU  |
| 1   | A     | 206  | PRO  |
| 1   | A     | 290  | GLN  |
| 1   | A     | 576  | LEU  |
| 1   | A     | 770  | LEU  |
| 1   | A     | 772  | SER  |
| 1   | A     | 1110 | ALA  |
| 1   | B     | 162  | LEU  |
| 1   | B     | 206  | PRO  |
| 1   | B     | 290  | GLN  |
| 1   | B     | 576  | LEU  |
| 1   | B     | 770  | LEU  |
| 1   | B     | 772  | SER  |
| 1   | B     | 1110 | ALA  |
| 2   | C     | 1060 | PHE  |
| 2   | C     | 1089 | ALA  |
| 2   | C     | 1188 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1329 | PRO  |
| 2   | C     | 1342 | TYR  |
| 2   | C     | 1378 | LEU  |
| 2   | C     | 1379 | ASN  |
| 3   | D     | 94   | SER  |
| 3   | D     | 214  | ALA  |
| 3   | D     | 216  | SER  |
| 3   | D     | 247  | SER  |
| 3   | D     | 273  | SER  |
| 3   | D     | 276  | ARG  |
| 2   | E     | 1060 | PHE  |
| 2   | E     | 1067 | ASP  |
| 2   | E     | 1089 | ALA  |
| 2   | E     | 1188 | SER  |
| 2   | E     | 1342 | TYR  |
| 2   | E     | 1375 | MET  |
| 2   | E     | 1379 | ASN  |
| 4   | F     | 6    | GLU  |
| 4   | F     | 7    | ASP  |
| 4   | F     | 10   | PRO  |
| 4   | F     | 16   | ASN  |
| 3   | G     | 94   | SER  |
| 3   | G     | 214  | ALA  |
| 3   | G     | 216  | SER  |
| 3   | G     | 247  | SER  |
| 4   | H     | 2    | GLU  |
| 4   | H     | 10   | PRO  |
| 4   | H     | 11   | GLN  |
| 4   | H     | 15   | TYR  |
| 4   | H     | 16   | ASN  |
| 1   | A     | 214  | ALA  |
| 1   | A     | 318  | ASP  |
| 1   | A     | 371  | GLY  |
| 1   | A     | 618  | ILE  |
| 1   | A     | 780  | THR  |
| 1   | A     | 907  | ASN  |
| 1   | B     | 214  | ALA  |
| 1   | B     | 318  | ASP  |
| 1   | B     | 618  | ILE  |
| 1   | B     | 707  | ILE  |
| 1   | B     | 780  | THR  |
| 1   | B     | 907  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1167 | LYS  |
| 2   | C     | 1187 | HIS  |
| 2   | C     | 1189 | GLN  |
| 2   | C     | 1256 | ASP  |
| 2   | C     | 1362 | LYS  |
| 2   | C     | 1374 | SER  |
| 3   | D     | 274  | VAL  |
| 2   | E     | 1167 | LYS  |
| 2   | E     | 1189 | GLN  |
| 2   | E     | 1256 | ASP  |
| 2   | E     | 1362 | LYS  |
| 4   | F     | 2    | GLU  |
| 4   | F     | 44   | GLN  |
| 4   | F     | 45   | HIS  |
| 4   | H     | 13   | GLU  |
| 1   | A     | 36   | ASN  |
| 1   | A     | 369  | ARG  |
| 1   | A     | 534  | MET  |
| 1   | A     | 1080 | ARG  |
| 1   | B     | 147  | ARG  |
| 1   | B     | 319  | ASN  |
| 1   | B     | 534  | MET  |
| 1   | B     | 598  | SER  |
| 1   | B     | 1080 | ARG  |
| 2   | C     | 1278 | GLU  |
| 3   | D     | 122  | PRO  |
| 2   | E     | 1187 | HIS  |
| 2   | E     | 1380 | MET  |
| 4   | F     | 15   | TYR  |
| 3   | G     | 122  | PRO  |
| 3   | G     | 219  | GLU  |
| 3   | G     | 273  | SER  |
| 1   | A     | 234  | GLN  |
| 1   | A     | 319  | ASN  |
| 1   | A     | 370  | GLN  |
| 1   | A     | 562  | THR  |
| 1   | A     | 598  | SER  |
| 1   | B     | 562  | THR  |
| 4   | F     | 41   | ASN  |
| 1   | A     | 147  | ARG  |
| 1   | B     | 234  | GLN  |
| 1   | B     | 266  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1375 | MET  |
| 3   | D     | 218  | LYS  |
| 3   | D     | 219  | GLU  |
| 4   | F     | 13   | GLU  |
| 3   | G     | 218  | LYS  |
| 3   | G     | 222  | TRP  |
| 3   | G     | 277  | GLY  |
| 1   | A     | 597  | GLU  |
| 1   | A     | 698  | THR  |
| 1   | A     | 707  | ILE  |
| 1   | B     | 148  | ASP  |
| 1   | B     | 597  | GLU  |
| 2   | C     | 1066 | VAL  |
| 2   | C     | 1137 | ALA  |
| 3   | D     | 222  | TRP  |
| 4   | H     | 58   | GLU  |
| 1   | A     | 233  | GLY  |
| 1   | A     | 185  | PRO  |
| 1   | A     | 266  | PRO  |
| 1   | B     | 185  | PRO  |
| 1   | B     | 233  | GLY  |
| 1   | A     | 564  | ILE  |
| 1   | B     | 564  | ILE  |
| 2   | C     | 1138 | ILE  |
| 3   | G     | 274  | VAL  |

### 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     | 994/999 (100%) | 851 (86%) | 143 (14%) | 3           | 18 |
| 1   | B     | 934/999 (94%)  | 802 (86%) | 132 (14%) | 3           | 18 |
| 2   | C     | 291/317 (92%)  | 235 (81%) | 56 (19%)  | 1           | 8  |
| 2   | E     | 291/317 (92%)  | 237 (81%) | 54 (19%)  | 1           | 9  |
| 3   | D     | 193/194 (100%) | 174 (90%) | 19 (10%)  | 7           | 30 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 3   | G     | 193/194 (100%)  | 175 (91%)  | 18 (9%)   | 8           | 31 |
| 4   | F     | 66/83 (80%)     | 48 (73%)   | 18 (27%)  | 0           | 3  |
| 4   | H     | 66/83 (80%)     | 51 (77%)   | 15 (23%)  | 1           | 5  |
| All | All   | 3028/3186 (95%) | 2573 (85%) | 455 (15%) | 3           | 17 |

All (455) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | THR  |
| 1   | A     | 37  | THR  |
| 1   | A     | 49  | LEU  |
| 1   | A     | 54  | GLU  |
| 1   | A     | 66  | LEU  |
| 1   | A     | 68  | ARG  |
| 1   | A     | 73  | SER  |
| 1   | A     | 74  | LYS  |
| 1   | A     | 101 | ILE  |
| 1   | A     | 146 | ASP  |
| 1   | A     | 148 | ASP  |
| 1   | A     | 150 | LYS  |
| 1   | A     | 152 | LEU  |
| 1   | A     | 160 | GLU  |
| 1   | A     | 162 | LEU  |
| 1   | A     | 173 | CYS  |
| 1   | A     | 178 | ILE  |
| 1   | A     | 184 | ASP  |
| 1   | A     | 209 | GLN  |
| 1   | A     | 210 | GLU  |
| 1   | A     | 213 | GLU  |
| 1   | A     | 218 | MET  |
| 1   | A     | 219 | VAL  |
| 1   | A     | 232 | ILE  |
| 1   | A     | 235 | GLU  |
| 1   | A     | 246 | LEU  |
| 1   | A     | 248 | ILE  |
| 1   | A     | 252 | ILE  |
| 1   | A     | 253 | ILE  |
| 1   | A     | 258 | ILE  |
| 1   | A     | 264 | VAL  |
| 1   | A     | 284 | LEU  |
| 1   | A     | 291 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 294 | THR  |
| 1   | A     | 299 | ASP  |
| 1   | A     | 300 | LEU  |
| 1   | A     | 304 | LEU  |
| 1   | A     | 305 | LEU  |
| 1   | A     | 307 | GLU  |
| 1   | A     | 317 | LEU  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 328 | LEU  |
| 1   | A     | 340 | SER  |
| 1   | A     | 345 | SER  |
| 1   | A     | 354 | THR  |
| 1   | A     | 355 | ASN  |
| 1   | A     | 365 | VAL  |
| 1   | A     | 366 | ASP  |
| 1   | A     | 369 | ARG  |
| 1   | A     | 378 | CYS  |
| 1   | A     | 396 | ILE  |
| 1   | A     | 404 | LEU  |
| 1   | A     | 407 | ILE  |
| 1   | A     | 430 | VAL  |
| 1   | A     | 434 | ARG  |
| 1   | A     | 435 | VAL  |
| 1   | A     | 438 | LEU  |
| 1   | A     | 439 | ASN  |
| 1   | A     | 445 | GLU  |
| 1   | A     | 472 | THR  |
| 1   | A     | 478 | LEU  |
| 1   | A     | 488 | SER  |
| 1   | A     | 516 | LEU  |
| 1   | A     | 520 | GLN  |
| 1   | A     | 528 | GLN  |
| 1   | A     | 541 | LEU  |
| 1   | A     | 544 | THR  |
| 1   | A     | 558 | ILE  |
| 1   | A     | 560 | LEU  |
| 1   | A     | 577 | LEU  |
| 1   | A     | 582 | LEU  |
| 1   | A     | 585 | GLU  |
| 1   | A     | 590 | SER  |
| 1   | A     | 598 | SER  |
| 1   | A     | 602 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 620 | THR  |
| 1   | A     | 640 | THR  |
| 1   | A     | 646 | THR  |
| 1   | A     | 647 | THR  |
| 1   | A     | 661 | SER  |
| 1   | A     | 671 | VAL  |
| 1   | A     | 674 | LYS  |
| 1   | A     | 680 | CYS  |
| 1   | A     | 682 | LEU  |
| 1   | A     | 685 | ASP  |
| 1   | A     | 691 | LEU  |
| 1   | A     | 698 | THR  |
| 1   | A     | 713 | ARG  |
| 1   | A     | 724 | ILE  |
| 1   | A     | 725 | CYS  |
| 1   | A     | 737 | SER  |
| 1   | A     | 775 | THR  |
| 1   | A     | 780 | THR  |
| 1   | A     | 781 | SER  |
| 1   | A     | 790 | ASN  |
| 1   | A     | 796 | GLN  |
| 1   | A     | 797 | HIS  |
| 1   | A     | 809 | GLN  |
| 1   | A     | 817 | VAL  |
| 1   | A     | 820 | LYS  |
| 1   | A     | 829 | PHE  |
| 1   | A     | 830 | ILE  |
| 1   | A     | 849 | VAL  |
| 1   | A     | 858 | LEU  |
| 1   | A     | 873 | MET  |
| 1   | A     | 874 | VAL  |
| 1   | A     | 877 | ASN  |
| 1   | A     | 883 | SER  |
| 1   | A     | 895 | THR  |
| 1   | A     | 901 | THR  |
| 1   | A     | 902 | GLU  |
| 1   | A     | 908 | ASN  |
| 1   | A     | 909 | ILE  |
| 1   | A     | 923 | VAL  |
| 1   | A     | 936 | LYS  |
| 1   | A     | 947 | ARG  |
| 1   | A     | 965 | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 966  | LEU  |
| 1   | A     | 981  | SER  |
| 1   | A     | 984  | THR  |
| 1   | A     | 985  | THR  |
| 1   | A     | 992  | LEU  |
| 1   | A     | 993  | GLN  |
| 1   | A     | 1006 | VAL  |
| 1   | A     | 1015 | GLN  |
| 1   | A     | 1036 | MET  |
| 1   | A     | 1039 | LEU  |
| 1   | A     | 1042 | SER  |
| 1   | A     | 1043 | LEU  |
| 1   | A     | 1045 | GLU  |
| 1   | A     | 1051 | LEU  |
| 1   | A     | 1058 | LEU  |
| 1   | A     | 1061 | VAL  |
| 1   | A     | 1065 | VAL  |
| 1   | A     | 1075 | SER  |
| 1   | A     | 1080 | ARG  |
| 1   | A     | 1083 | GLU  |
| 1   | A     | 1094 | ILE  |
| 1   | A     | 1101 | SER  |
| 1   | A     | 1123 | GLU  |
| 1   | A     | 1128 | ASP  |
| 1   | A     | 1137 | THR  |
| 1   | A     | 1139 | ILE  |
| 1   | B     | 20   | THR  |
| 1   | B     | 32   | LEU  |
| 1   | B     | 49   | LEU  |
| 1   | B     | 54   | GLU  |
| 1   | B     | 74   | LYS  |
| 1   | B     | 81   | THR  |
| 1   | B     | 101  | ILE  |
| 1   | B     | 146  | ASP  |
| 1   | B     | 148  | ASP  |
| 1   | B     | 150  | LYS  |
| 1   | B     | 152  | LEU  |
| 1   | B     | 160  | GLU  |
| 1   | B     | 162  | LEU  |
| 1   | B     | 167  | VAL  |
| 1   | B     | 173  | CYS  |
| 1   | B     | 174  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 178 | ILE  |
| 1   | B     | 184 | ASP  |
| 1   | B     | 207 | TRP  |
| 1   | B     | 209 | GLN  |
| 1   | B     | 210 | GLU  |
| 1   | B     | 213 | GLU  |
| 1   | B     | 218 | MET  |
| 1   | B     | 219 | VAL  |
| 1   | B     | 232 | ILE  |
| 1   | B     | 235 | GLU  |
| 1   | B     | 246 | LEU  |
| 1   | B     | 248 | ILE  |
| 1   | B     | 252 | ILE  |
| 1   | B     | 255 | GLN  |
| 1   | B     | 258 | ILE  |
| 1   | B     | 264 | VAL  |
| 1   | B     | 265 | ASP  |
| 1   | B     | 284 | LEU  |
| 1   | B     | 291 | MET  |
| 1   | B     | 294 | THR  |
| 1   | B     | 299 | ASP  |
| 1   | B     | 300 | LEU  |
| 1   | B     | 304 | LEU  |
| 1   | B     | 305 | LEU  |
| 1   | B     | 307 | GLU  |
| 1   | B     | 317 | LEU  |
| 1   | B     | 322 | VAL  |
| 1   | B     | 328 | LEU  |
| 1   | B     | 340 | SER  |
| 1   | B     | 345 | SER  |
| 1   | B     | 354 | THR  |
| 1   | B     | 355 | ASN  |
| 1   | B     | 366 | ASP  |
| 1   | B     | 370 | GLN  |
| 1   | B     | 396 | ILE  |
| 1   | B     | 404 | LEU  |
| 1   | B     | 407 | ILE  |
| 1   | B     | 423 | ASP  |
| 1   | B     | 435 | VAL  |
| 1   | B     | 438 | LEU  |
| 1   | B     | 439 | ASN  |
| 1   | B     | 445 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 472 | THR  |
| 1   | B     | 488 | SER  |
| 1   | B     | 516 | LEU  |
| 1   | B     | 519 | LEU  |
| 1   | B     | 520 | GLN  |
| 1   | B     | 528 | GLN  |
| 1   | B     | 541 | LEU  |
| 1   | B     | 544 | THR  |
| 1   | B     | 558 | ILE  |
| 1   | B     | 560 | LEU  |
| 1   | B     | 577 | LEU  |
| 1   | B     | 582 | LEU  |
| 1   | B     | 589 | ARG  |
| 1   | B     | 590 | SER  |
| 1   | B     | 593 | MET  |
| 1   | B     | 602 | LEU  |
| 1   | B     | 620 | THR  |
| 1   | B     | 640 | THR  |
| 1   | B     | 646 | THR  |
| 1   | B     | 647 | THR  |
| 1   | B     | 661 | SER  |
| 1   | B     | 671 | VAL  |
| 1   | B     | 680 | CYS  |
| 1   | B     | 682 | LEU  |
| 1   | B     | 685 | ASP  |
| 1   | B     | 691 | LEU  |
| 1   | B     | 698 | THR  |
| 1   | B     | 707 | ILE  |
| 1   | B     | 713 | ARG  |
| 1   | B     | 730 | SER  |
| 1   | B     | 737 | SER  |
| 1   | B     | 790 | ASN  |
| 1   | B     | 796 | GLN  |
| 1   | B     | 797 | HIS  |
| 1   | B     | 808 | LEU  |
| 1   | B     | 809 | GLN  |
| 1   | B     | 817 | VAL  |
| 1   | B     | 820 | LYS  |
| 1   | B     | 829 | PHE  |
| 1   | B     | 830 | ILE  |
| 1   | B     | 849 | VAL  |
| 1   | B     | 858 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 874  | VAL  |
| 1   | B     | 877  | ASN  |
| 1   | B     | 883  | SER  |
| 1   | B     | 895  | THR  |
| 1   | B     | 902  | GLU  |
| 1   | B     | 908  | ASN  |
| 1   | B     | 909  | ILE  |
| 1   | B     | 910  | MET  |
| 1   | B     | 923  | VAL  |
| 1   | B     | 938  | MET  |
| 1   | B     | 965  | PHE  |
| 1   | B     | 966  | LEU  |
| 1   | B     | 984  | THR  |
| 1   | B     | 985  | THR  |
| 1   | B     | 992  | LEU  |
| 1   | B     | 993  | GLN  |
| 1   | B     | 1006 | VAL  |
| 1   | B     | 1015 | GLN  |
| 1   | B     | 1036 | MET  |
| 1   | B     | 1039 | LEU  |
| 1   | B     | 1042 | SER  |
| 1   | B     | 1051 | LEU  |
| 1   | B     | 1058 | LEU  |
| 1   | B     | 1061 | VAL  |
| 1   | B     | 1065 | VAL  |
| 1   | B     | 1075 | SER  |
| 1   | B     | 1080 | ARG  |
| 1   | B     | 1083 | GLU  |
| 1   | B     | 1094 | ILE  |
| 1   | B     | 1101 | SER  |
| 1   | B     | 1128 | ASP  |
| 1   | B     | 1137 | THR  |
| 2   | C     | 1048 | ILE  |
| 2   | C     | 1055 | ASN  |
| 2   | C     | 1063 | TYR  |
| 2   | C     | 1066 | VAL  |
| 2   | C     | 1073 | ARG  |
| 2   | C     | 1074 | HIS  |
| 2   | C     | 1075 | LEU  |
| 2   | C     | 1079 | ARG  |
| 2   | C     | 1083 | ILE  |
| 2   | C     | 1090 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1102 | SER  |
| 2   | C     | 1108 | LEU  |
| 2   | C     | 1109 | MET  |
| 2   | C     | 1117 | LEU  |
| 2   | C     | 1119 | LEU  |
| 2   | C     | 1126 | GLN  |
| 2   | C     | 1146 | ASP  |
| 2   | C     | 1155 | THR  |
| 2   | C     | 1157 | SER  |
| 2   | C     | 1168 | SER  |
| 2   | C     | 1169 | VAL  |
| 2   | C     | 1172 | MET  |
| 2   | C     | 1190 | ASP  |
| 2   | C     | 1202 | ILE  |
| 2   | C     | 1207 | THR  |
| 2   | C     | 1212 | LEU  |
| 2   | C     | 1229 | THR  |
| 2   | C     | 1231 | ASN  |
| 2   | C     | 1234 | ASP  |
| 2   | C     | 1235 | ASP  |
| 2   | C     | 1259 | ASN  |
| 2   | C     | 1260 | MET  |
| 2   | C     | 1272 | GLU  |
| 2   | C     | 1275 | ILE  |
| 2   | C     | 1278 | GLU  |
| 2   | C     | 1286 | HIS  |
| 2   | C     | 1289 | HIS  |
| 2   | C     | 1294 | LEU  |
| 2   | C     | 1296 | GLN  |
| 2   | C     | 1299 | VAL  |
| 2   | C     | 1313 | LEU  |
| 2   | C     | 1330 | PHE  |
| 2   | C     | 1341 | ASP  |
| 2   | C     | 1342 | TYR  |
| 2   | C     | 1343 | LYS  |
| 2   | C     | 1345 | ILE  |
| 2   | C     | 1350 | VAL  |
| 2   | C     | 1352 | ARG  |
| 2   | C     | 1354 | ILE  |
| 2   | C     | 1357 | LEU  |
| 2   | C     | 1362 | LYS  |
| 2   | C     | 1374 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1378 | LEU  |
| 2   | C     | 1379 | ASN  |
| 2   | C     | 1386 | LEU  |
| 2   | C     | 1389 | VAL  |
| 3   | D     | 84   | PHE  |
| 3   | D     | 88   | SER  |
| 3   | D     | 90   | LYS  |
| 3   | D     | 105  | LEU  |
| 3   | D     | 106  | MET  |
| 3   | D     | 111  | GLU  |
| 3   | D     | 139  | VAL  |
| 3   | D     | 173  | ILE  |
| 3   | D     | 175  | LYS  |
| 3   | D     | 178  | SER  |
| 3   | D     | 182  | GLU  |
| 3   | D     | 198  | GLN  |
| 3   | D     | 206  | VAL  |
| 3   | D     | 212  | HIS  |
| 3   | D     | 237  | SER  |
| 3   | D     | 241  | VAL  |
| 3   | D     | 270  | SER  |
| 3   | D     | 272  | LEU  |
| 3   | D     | 279  | PHE  |
| 2   | E     | 1048 | ILE  |
| 2   | E     | 1055 | ASN  |
| 2   | E     | 1063 | TYR  |
| 2   | E     | 1074 | HIS  |
| 2   | E     | 1075 | LEU  |
| 2   | E     | 1083 | ILE  |
| 2   | E     | 1090 | ASN  |
| 2   | E     | 1091 | GLU  |
| 2   | E     | 1102 | SER  |
| 2   | E     | 1119 | LEU  |
| 2   | E     | 1126 | GLN  |
| 2   | E     | 1146 | ASP  |
| 2   | E     | 1149 | LEU  |
| 2   | E     | 1150 | LEU  |
| 2   | E     | 1160 | LEU  |
| 2   | E     | 1163 | LEU  |
| 2   | E     | 1168 | SER  |
| 2   | E     | 1169 | VAL  |
| 2   | E     | 1171 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 1172 | MET  |
| 2   | E     | 1177 | THR  |
| 2   | E     | 1192 | VAL  |
| 2   | E     | 1195 | THR  |
| 2   | E     | 1202 | ILE  |
| 2   | E     | 1229 | THR  |
| 2   | E     | 1234 | ASP  |
| 2   | E     | 1235 | ASP  |
| 2   | E     | 1247 | ARG  |
| 2   | E     | 1260 | MET  |
| 2   | E     | 1272 | GLU  |
| 2   | E     | 1275 | ILE  |
| 2   | E     | 1277 | THR  |
| 2   | E     | 1279 | ILE  |
| 2   | E     | 1284 | THR  |
| 2   | E     | 1286 | HIS  |
| 2   | E     | 1289 | HIS  |
| 2   | E     | 1294 | LEU  |
| 2   | E     | 1296 | GLN  |
| 2   | E     | 1299 | VAL  |
| 2   | E     | 1307 | VAL  |
| 2   | E     | 1313 | LEU  |
| 2   | E     | 1328 | SER  |
| 2   | E     | 1330 | PHE  |
| 2   | E     | 1341 | ASP  |
| 2   | E     | 1342 | TYR  |
| 2   | E     | 1343 | LYS  |
| 2   | E     | 1352 | ARG  |
| 2   | E     | 1353 | ASN  |
| 2   | E     | 1357 | LEU  |
| 2   | E     | 1362 | LYS  |
| 2   | E     | 1372 | GLN  |
| 2   | E     | 1379 | ASN  |
| 2   | E     | 1382 | THR  |
| 2   | E     | 1389 | VAL  |
| 4   | F     | 1    | MET  |
| 4   | F     | 6    | GLU  |
| 4   | F     | 8    | GLN  |
| 4   | F     | 10   | PRO  |
| 4   | F     | 11   | GLN  |
| 4   | F     | 12   | ARG  |
| 4   | F     | 20   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | F     | 21  | GLU  |
| 4   | F     | 23  | LEU  |
| 4   | F     | 26  | LEU  |
| 4   | F     | 46  | ILE  |
| 4   | F     | 48  | GLU  |
| 4   | F     | 57  | VAL  |
| 4   | F     | 58  | GLU  |
| 4   | F     | 61  | ILE  |
| 4   | F     | 63  | ILE  |
| 4   | F     | 65  | GLN  |
| 4   | F     | 73  | ARG  |
| 3   | G     | 88  | SER  |
| 3   | G     | 90  | LYS  |
| 3   | G     | 97  | PHE  |
| 3   | G     | 105 | LEU  |
| 3   | G     | 106 | MET  |
| 3   | G     | 113 | ARG  |
| 3   | G     | 139 | VAL  |
| 3   | G     | 160 | VAL  |
| 3   | G     | 172 | ASN  |
| 3   | G     | 175 | LYS  |
| 3   | G     | 178 | SER  |
| 3   | G     | 182 | GLU  |
| 3   | G     | 198 | GLN  |
| 3   | G     | 206 | VAL  |
| 3   | G     | 212 | HIS  |
| 3   | G     | 237 | SER  |
| 3   | G     | 241 | VAL  |
| 3   | G     | 279 | PHE  |
| 4   | H     | 3   | GLN  |
| 4   | H     | 10  | PRO  |
| 4   | H     | 14  | PRO  |
| 4   | H     | 16  | ASN  |
| 4   | H     | 24  | GLU  |
| 4   | H     | 28  | SER  |
| 4   | H     | 31  | VAL  |
| 4   | H     | 36  | ARG  |
| 4   | H     | 37  | ILE  |
| 4   | H     | 42  | LEU  |
| 4   | H     | 48  | GLU  |
| 4   | H     | 58  | GLU  |
| 4   | H     | 65  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 68  | LEU  |
| 4   | H     | 73  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 4    | ASN  |
| 1   | A     | 36   | ASN  |
| 1   | A     | 156  | ASN  |
| 1   | A     | 189  | HIS  |
| 1   | A     | 203  | ASN  |
| 1   | A     | 234  | GLN  |
| 1   | A     | 241  | ASN  |
| 1   | A     | 261  | HIS  |
| 1   | A     | 290  | GLN  |
| 1   | A     | 319  | ASN  |
| 1   | A     | 392  | ASN  |
| 1   | A     | 432  | GLN  |
| 1   | A     | 470  | GLN  |
| 1   | A     | 494  | GLN  |
| 1   | A     | 520  | GLN  |
| 1   | A     | 524  | GLN  |
| 1   | A     | 578  | HIS  |
| 1   | A     | 670  | ASN  |
| 1   | A     | 727  | GLN  |
| 1   | A     | 778  | HIS  |
| 1   | A     | 796  | GLN  |
| 1   | A     | 809  | GLN  |
| 1   | A     | 810  | ASN  |
| 1   | A     | 826  | ASN  |
| 1   | A     | 852  | GLN  |
| 1   | A     | 908  | ASN  |
| 1   | A     | 964  | ASN  |
| 1   | A     | 993  | GLN  |
| 1   | A     | 1005 | ASN  |
| 1   | A     | 1016 | ASN  |
| 1   | A     | 1049 | ASN  |
| 1   | B     | 4    | ASN  |
| 1   | B     | 85   | ASN  |
| 1   | B     | 107  | ASN  |
| 1   | B     | 156  | ASN  |
| 1   | B     | 183  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 189  | HIS  |
| 1   | B     | 203  | ASN  |
| 1   | B     | 234  | GLN  |
| 1   | B     | 241  | ASN  |
| 1   | B     | 261  | HIS  |
| 1   | B     | 290  | GLN  |
| 1   | B     | 370  | GLN  |
| 1   | B     | 392  | ASN  |
| 1   | B     | 432  | GLN  |
| 1   | B     | 456  | GLN  |
| 1   | B     | 470  | GLN  |
| 1   | B     | 520  | GLN  |
| 1   | B     | 578  | HIS  |
| 1   | B     | 670  | ASN  |
| 1   | B     | 727  | GLN  |
| 1   | B     | 796  | GLN  |
| 1   | B     | 826  | ASN  |
| 1   | B     | 852  | GLN  |
| 1   | B     | 904  | ASN  |
| 1   | B     | 908  | ASN  |
| 1   | B     | 941  | ASN  |
| 1   | B     | 964  | ASN  |
| 1   | B     | 993  | GLN  |
| 1   | B     | 1005 | ASN  |
| 1   | B     | 1016 | ASN  |
| 1   | B     | 1113 | GLN  |
| 2   | C     | 1132 | ASN  |
| 2   | C     | 1174 | HIS  |
| 2   | C     | 1201 | HIS  |
| 2   | C     | 1209 | ASN  |
| 2   | C     | 1222 | ASN  |
| 2   | C     | 1250 | GLN  |
| 2   | C     | 1303 | HIS  |
| 2   | C     | 1338 | ASN  |
| 2   | C     | 1372 | GLN  |
| 2   | C     | 1379 | ASN  |
| 3   | D     | 130  | GLN  |
| 3   | D     | 144  | GLN  |
| 3   | D     | 172  | ASN  |
| 3   | D     | 236  | ASN  |
| 3   | D     | 250  | GLN  |
| 2   | E     | 1090 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 1116 | GLN  |
| 2   | E     | 1140 | HIS  |
| 2   | E     | 1174 | HIS  |
| 2   | E     | 1180 | HIS  |
| 2   | E     | 1201 | HIS  |
| 2   | E     | 1209 | ASN  |
| 2   | E     | 1222 | ASN  |
| 2   | E     | 1239 | ASN  |
| 2   | E     | 1250 | GLN  |
| 2   | E     | 1338 | ASN  |
| 2   | E     | 1371 | ASN  |
| 4   | F     | 8    | GLN  |
| 4   | F     | 16   | ASN  |
| 4   | F     | 33   | HIS  |
| 4   | F     | 41   | ASN  |
| 4   | F     | 45   | HIS  |
| 4   | F     | 65   | GLN  |
| 3   | G     | 144  | GLN  |
| 3   | G     | 152  | GLN  |
| 3   | G     | 189  | HIS  |
| 3   | G     | 236  | ASN  |
| 3   | G     | 250  | GLN  |
| 4   | H     | 40   | HIS  |
| 4   | H     | 41   | ASN  |
| 4   | H     | 45   | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2     | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 1   | A     | 1133/1140 (99%) | -0.60  | 8 (0%) 84 63  | 110, 180, 236, 272    | 0       |
| 1   | B     | 1133/1140 (99%) | -0.26  | 41 (3%) 46 25 | 157, 230, 290, 296    | 0       |
| 2   | C     | 331/361 (91%)   | -0.54  | 3 (0%) 81 58  | 107, 149, 194, 240    | 0       |
| 2   | E     | 331/361 (91%)   | -0.62  | 2 (0%) 85 65  | 121, 174, 216, 242    | 0       |
| 3   | D     | 221/222 (99%)   | -0.64  | 1 (0%) 87 68  | 121, 178, 222, 248    | 0       |
| 3   | G     | 221/222 (99%)   | -0.64  | 0 100 100     | 129, 172, 221, 253    | 0       |
| 4   | F     | 74/96 (77%)     | -0.34  | 1 (1%) 73 48  | 125, 161, 196, 206    | 0       |
| 4   | H     | 74/96 (77%)     | -0.46  | 0 100 100     | 120, 149, 184, 200    | 0       |
| All | All   | 3518/3638 (96%) | -0.48  | 56 (1%) 70 45 | 107, 190, 284, 296    | 0       |

All (56) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 566 | ALA  | 5.3  |
| 1   | B     | 448 | LEU  | 4.6  |
| 1   | B     | 604 | CYS  | 4.3  |
| 1   | B     | 568 | ILE  | 3.6  |
| 1   | B     | 602 | LEU  | 3.6  |
| 1   | B     | 613 | TYR  | 3.6  |
| 1   | B     | 603 | LEU  | 3.5  |
| 1   | B     | 704 | ILE  | 3.4  |
| 1   | B     | 611 | LEU  | 3.3  |
| 1   | B     | 658 | VAL  | 3.3  |
| 1   | B     | 662 | SER  | 3.2  |
| 1   | B     | 435 | VAL  | 3.2  |
| 1   | B     | 555 | LEU  | 3.2  |
| 1   | B     | 666 | LEU  | 3.1  |
| 1   | B     | 569 | LEU  | 3.1  |
| 1   | A     | 470 | GLN  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | E     | 1389 | VAL  | 2.9  |
| 1   | B     | 64   | MET  | 2.9  |
| 1   | B     | 651  | ALA  | 2.7  |
| 1   | B     | 471  | ILE  | 2.7  |
| 1   | B     | 781  | SER  | 2.7  |
| 1   | B     | 544  | THR  | 2.6  |
| 1   | B     | 707  | ILE  | 2.6  |
| 1   | B     | 428  | SER  | 2.6  |
| 1   | B     | 415  | SER  | 2.5  |
| 1   | B     | 556  | CYS  | 2.4  |
| 1   | B     | 697  | SER  | 2.4  |
| 2   | C     | 1366 | LEU  | 2.4  |
| 1   | B     | 701  | ILE  | 2.4  |
| 1   | B     | 855  | ASP  | 2.4  |
| 1   | B     | 638  | LEU  | 2.3  |
| 1   | A     | 402  | ILE  | 2.3  |
| 2   | C     | 1389 | VAL  | 2.3  |
| 1   | B     | 643  | SER  | 2.3  |
| 1   | B     | 582  | LEU  | 2.3  |
| 1   | B     | 641  | PHE  | 2.3  |
| 3   | D     | 158  | PHE  | 2.3  |
| 1   | A     | 603  | LEU  | 2.2  |
| 1   | B     | 433  | THR  | 2.2  |
| 1   | A     | 367  | LEU  | 2.2  |
| 1   | B     | 521  | ILE  | 2.2  |
| 1   | A     | 404  | LEU  | 2.2  |
| 1   | A     | 621  | GLY  | 2.2  |
| 1   | B     | 409  | GLY  | 2.2  |
| 2   | C     | 1180 | HIS  | 2.2  |
| 1   | A     | 799  | PHE  | 2.2  |
| 1   | B     | 402  | ILE  | 2.1  |
| 1   | B     | 576  | LEU  | 2.1  |
| 1   | B     | 426  | VAL  | 2.1  |
| 4   | F     | 53   | THR  | 2.1  |
| 1   | B     | 563  | ASP  | 2.0  |
| 1   | B     | 451  | PHE  | 2.0  |
| 1   | B     | 784  | GLU  | 2.0  |
| 2   | E     | 1366 | LEU  | 2.0  |
| 1   | A     | 378  | CYS  | 2.0  |
| 1   | B     | 410  | LEU  | 2.0  |

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.