



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:31 PM EDT

PDB ID : 3WOF / pdb\_00003wof  
Title : Crystal structure of P23-45 gp39 (6-132) bound to Thermus thermophilus RNA polymerase beta-flap domain  
Authors : Tagami, S.; Sekine, S.; Minakhin, L.; Esyunina, D.; Akasaka, R.; Shirouzu, M.; Kulbachinskiy, A.; Severinov, K.; Yokoyama, S.  
Deposited on : 2013-12-26  
Resolution : 3.30 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                                                             |

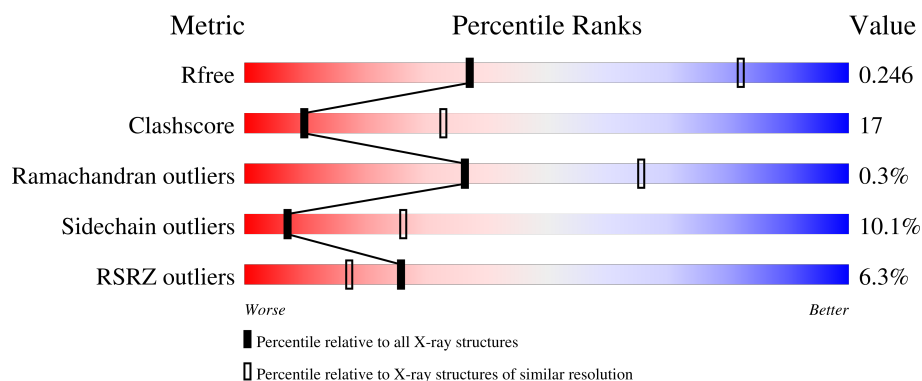
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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                      | 1169 (3.32-3.28)                                      |
| Clashscore            | 190562                      | 1209 (3.32-3.28)                                      |
| Ramachandran outliers | 187476                      | 1188 (3.32-3.28)                                      |
| Sidechain outliers    | 187428                      | 1187 (3.32-3.28)                                      |
| RSRZ outliers         | 180081                      | 1169 (3.32-3.28)                                      |

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     | 130    | <div> <div>6%</div> <div> <div></div> <div>57%</div> <div>31%</div> <div>12%</div> </div> </div> |
| 1   | C     | 130    | <div> <div>5%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>5%</div> </div> </div>  |
| 1   | E     | 130    | <div> <div>10%</div> <div> <div></div> <div>61%</div> <div>28%</div> <div>9%</div> </div> </div> |
| 1   | G     | 130    | <div> <div>7%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>6%</div> </div> </div>  |
| 1   | I     | 130    | <div> <div>13%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>5%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | K     | 130    |                  |
| 1   | M     | 130    |                  |
| 1   | O     | 130    |                  |
| 1   | Q     | 130    |                  |
| 1   | S     | 130    |                  |
| 1   | U     | 130    |                  |
| 1   | W     | 130    |                  |
| 2   | B     | 129    |                  |
| 2   | D     | 129    |                  |
| 2   | F     | 129    |                  |
| 2   | H     | 129    |                  |
| 2   | J     | 129    |                  |
| 2   | L     | 129    |                  |
| 2   | N     | 129    |                  |
| 2   | P     | 129    |                  |
| 2   | R     | 129    |                  |
| 2   | T     | 129    |                  |
| 2   | V     | 129    |                  |
| 2   | X     | 129    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22026 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-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 1   | A     | 129      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1009  | 627 | 191 | 191 |         |         |       |
| 1   | C     | 129      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1009  | 627 | 191 | 191 |         |         |       |
| 1   | E     | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 998   | 620 | 189 | 189 |         |         |       |
| 1   | G     | 129      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 631 | 192 | 191 |         |         |       |
| 1   | I     | 129      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 631 | 192 | 191 |         |         |       |
| 1   | K     | 128      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1005  | 625 | 190 | 190 |         |         |       |
| 1   | M     | 128      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1007  | 626 | 191 | 190 |         |         |       |
| 1   | O     | 129      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 631 | 192 | 191 |         |         |       |
| 1   | Q     | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 998   | 620 | 189 | 189 |         |         |       |
| 1   | S     | 129      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 631 | 192 | 191 |         |         |       |
| 1   | U     | 121      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 949   | 589 | 180 | 180 |         |         |       |
| 1   | W     | 129      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1014  | 631 | 192 | 191 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| A     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| C     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| C     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| E     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| G     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| G     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| I     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| I     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| K     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| K     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| M     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| M     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| O     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| O     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| Q     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| Q     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| S     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| S     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| U     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| U     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |
| W     | 701     | GLY      | -      | expression tag | UNP Q8RQE9 |
| W     | 702     | PRO      | -      | expression tag | UNP Q8RQE9 |

- Molecule 2 is a protein called Putative uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 830   | 544 | 141 | 144 | 1 |         |         |       |
| 2   | D     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 837   | 549 | 142 | 145 | 1 |         |         |       |
| 2   | F     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 837   | 549 | 142 | 145 | 1 |         |         |       |
| 2   | H     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 830   | 544 | 141 | 144 | 1 |         |         |       |
| 2   | J     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 830   | 544 | 141 | 144 | 1 |         |         |       |
| 2   | L     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 830   | 544 | 141 | 144 | 1 |         |         |       |
| 2   | N     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 837   | 549 | 142 | 145 | 1 |         |         |       |
| 2   | P     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 830   | 544 | 141 | 144 | 1 |         |         |       |
| 2   | R     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 830   | 544 | 141 | 144 | 1 |         |         |       |
| 2   | T     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 830   | 544 | 141 | 144 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | V     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 830   | 544 | 141 | 144 | 1 |         |         |       |
| 2   | X     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 830   | 544 | 141 | 144 | 1 |         |         |       |

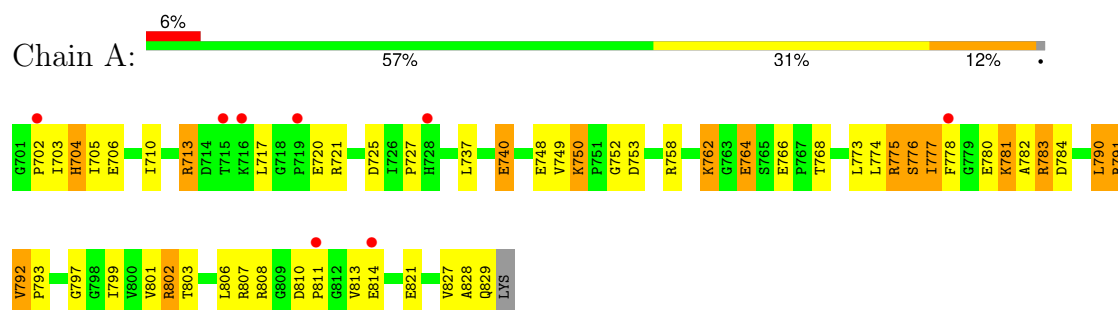
There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| B     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| D     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| D     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| F     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| F     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| H     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| H     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| J     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| J     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| L     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| L     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| N     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| N     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| P     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| P     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| R     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| R     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| T     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| T     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| V     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| V     | 5       | PRO      | -      | expression tag | UNP A7XX65 |
| X     | 4       | GLY      | -      | expression tag | UNP A7XX65 |
| X     | 5       | PRO      | -      | expression tag | UNP A7XX65 |

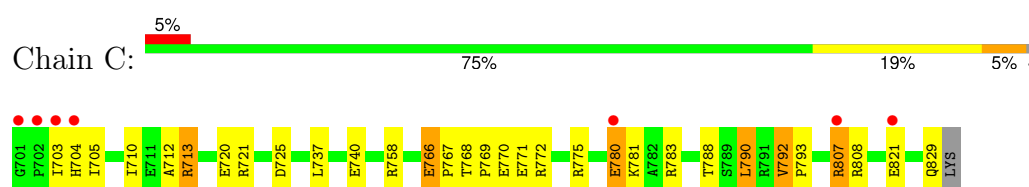
### 3 Residue-property plots [i](#)

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

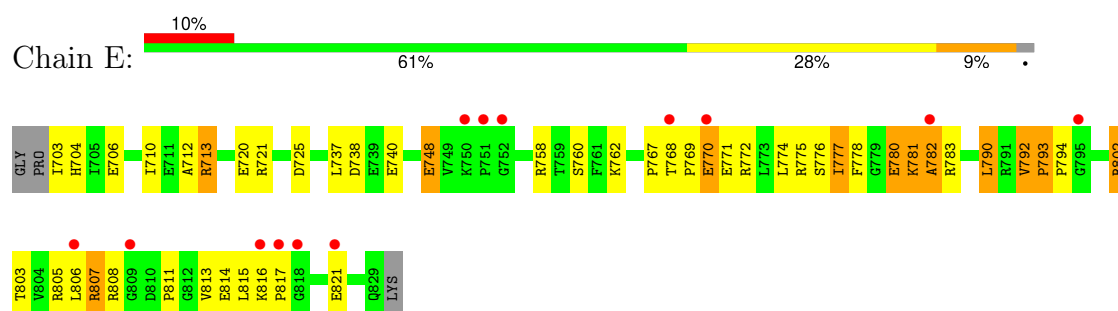
- Molecule 1: DNA-directed RNA polymerase subunit beta



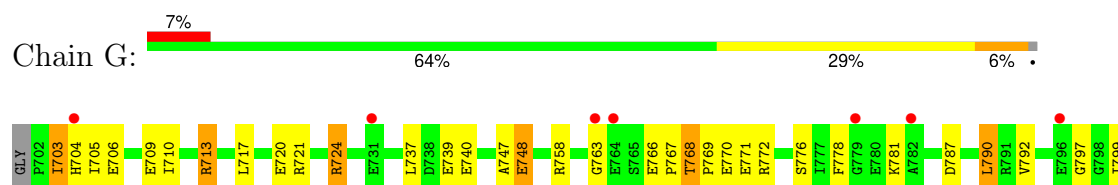
- Molecule 1: DNA-directed RNA polymerase subunit beta

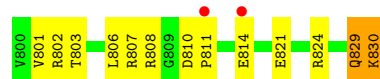


- Molecule 1: DNA-directed RNA polymerase subunit beta

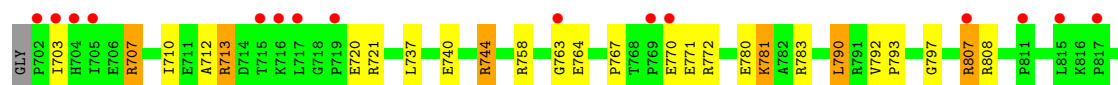
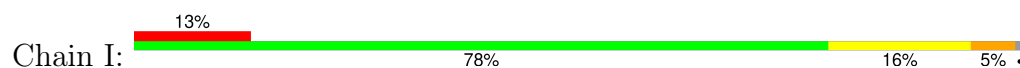


- Molecule 1: DNA-directed RNA polymerase subunit beta

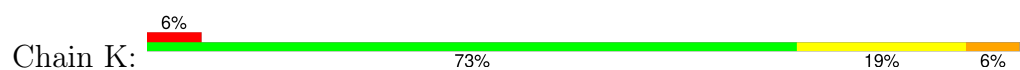




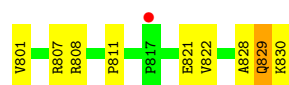
- Molecule 1: DNA-directed RNA polymerase subunit beta



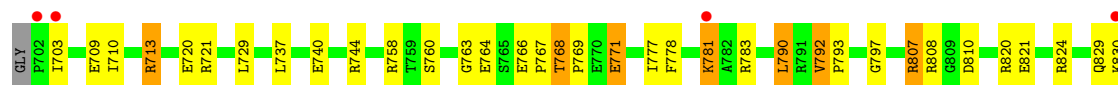
- Molecule 1: DNA-directed RNA polymerase subunit beta



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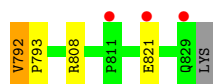


- Molecule 1: DNA-directed RNA polymerase subunit beta

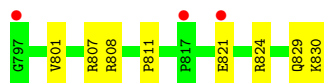


- Molecule 1: DNA-directed RNA polymerase subunit beta

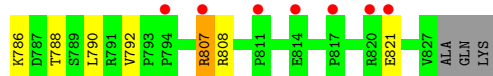




- Molecule 1: DNA-directed RNA polymerase subunit beta



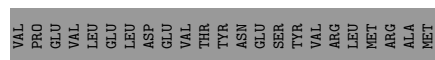
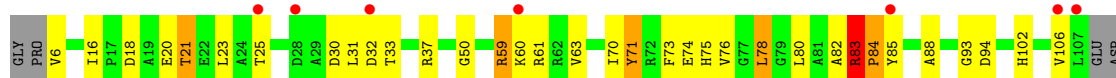
- Molecule 1: DNA-directed RNA polymerase subunit beta



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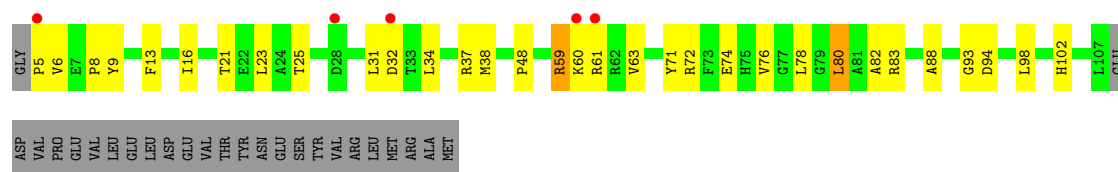


- Molecule 2: Putative uncharacterized protein

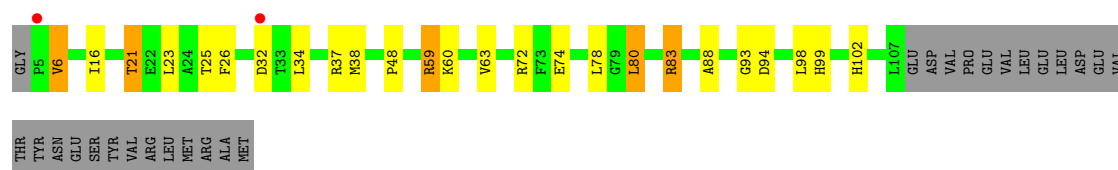


- Molecule 2: Putative uncharacterized protein





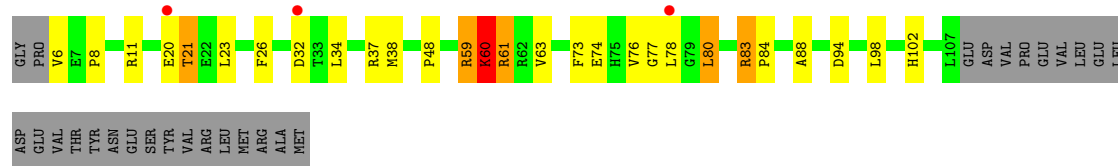
• Molecule 2: Putative uncharacterized protein



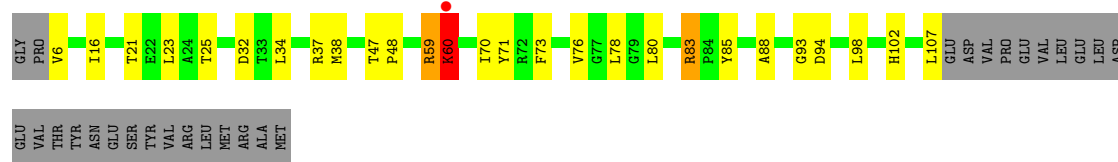
• Molecule 2: Putative uncharacterized protein



• Molecule 2: Putative uncharacterized protein

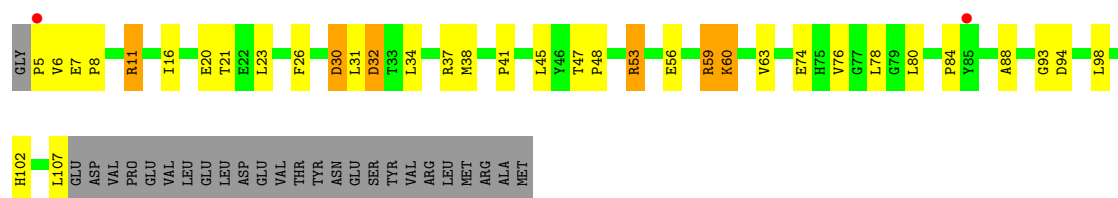


• Molecule 2: Putative uncharacterized protein

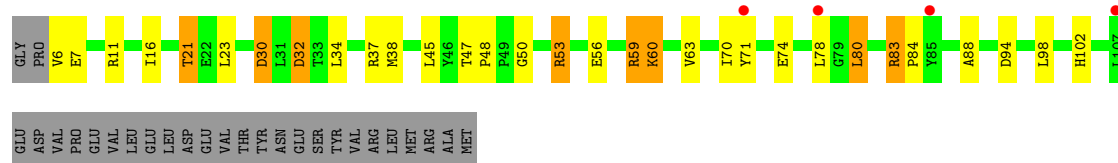


• Molecule 2: Putative uncharacterized protein

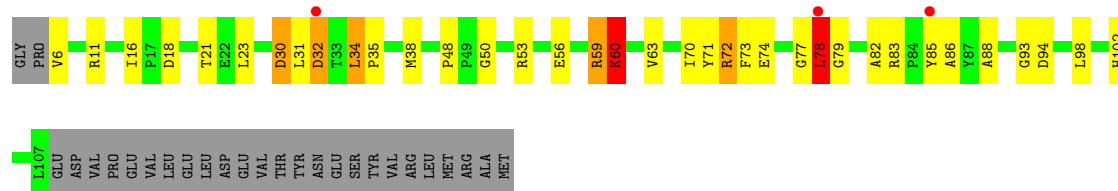




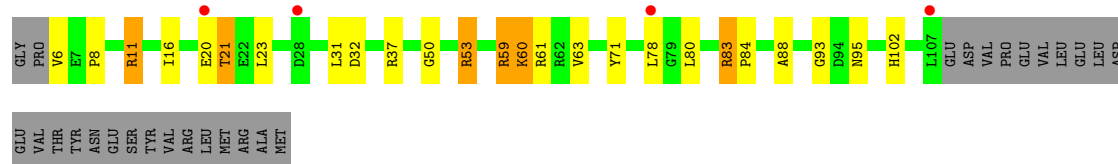
• Molecule 2: Putative uncharacterized protein



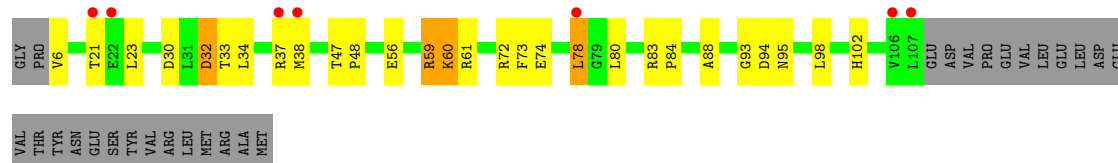
• Molecule 2: Putative uncharacterized protein



• Molecule 2: Putative uncharacterized protein

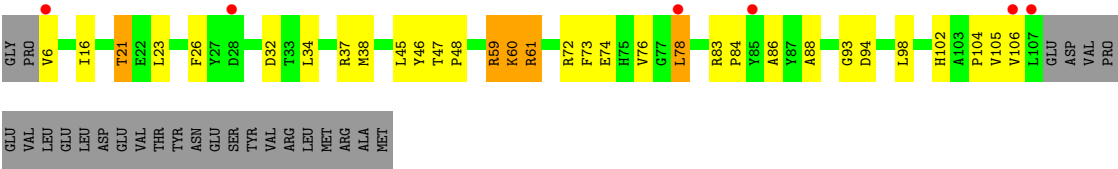


• Molecule 2: Putative uncharacterized protein



• Molecule 2: Putative uncharacterized protein





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 41 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 213.78Å 213.78Å 234.60Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 34.55 – 3.30<br>34.55 – 3.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (34.55-3.30)<br>99.8 (34.55-3.30)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.17                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 5.38 (at 3.32Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.8.4_1496)                          | Depositor        |
| R, $R_{free}$                                                           | 0.219 , 0.246<br>0.219 , 0.246                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4107 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 68.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.012                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 70.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 22026                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 81.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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     | 0.58         | 0/1024         | 1.10        | 6/1382 (0.4%)   |
| 1   | C     | 0.54         | 0/1024         | 0.95        | 2/1382 (0.1%)   |
| 1   | E     | 0.62         | 0/1012         | 1.04        | 5/1365 (0.4%)   |
| 1   | G     | 0.53         | 0/1029         | 0.91        | 2/1387 (0.1%)   |
| 1   | I     | 0.51         | 0/1029         | 0.94        | 4/1387 (0.3%)   |
| 1   | K     | 0.51         | 0/1020         | 0.93        | 2/1376 (0.1%)   |
| 1   | M     | 0.52         | 0/1021         | 0.97        | 2/1376 (0.1%)   |
| 1   | O     | 0.53         | 0/1029         | 0.96        | 2/1387 (0.1%)   |
| 1   | Q     | 0.55         | 0/1012         | 0.96        | 3/1365 (0.2%)   |
| 1   | S     | 0.55         | 0/1029         | 0.95        | 1/1387 (0.1%)   |
| 1   | U     | 0.53         | 0/962          | 0.97        | 3/1297 (0.2%)   |
| 1   | W     | 0.51         | 0/1029         | 0.92        | 3/1387 (0.2%)   |
| 2   | B     | 0.59         | 0/856          | 1.01        | 4/1169 (0.3%)   |
| 2   | D     | 0.53         | 0/864          | 0.89        | 0/1180          |
| 2   | F     | 0.55         | 0/864          | 0.95        | 3/1180 (0.3%)   |
| 2   | H     | 0.53         | 0/856          | 0.91        | 2/1169 (0.2%)   |
| 2   | J     | 0.52         | 0/856          | 0.99        | 3/1169 (0.3%)   |
| 2   | L     | 0.49         | 0/856          | 0.87        | 3/1169 (0.3%)   |
| 2   | N     | 0.62         | 1/864 (0.1%)   | 0.91        | 2/1180 (0.2%)   |
| 2   | P     | 0.58         | 0/856          | 0.94        | 4/1169 (0.3%)   |
| 2   | R     | 0.55         | 0/856          | 0.90        | 4/1169 (0.3%)   |
| 2   | T     | 0.55         | 0/856          | 0.91        | 3/1169 (0.3%)   |
| 2   | V     | 0.54         | 0/856          | 0.90        | 1/1169 (0.1%)   |
| 2   | X     | 0.52         | 0/856          | 0.96        | 2/1169 (0.2%)   |
| All | All   | 0.54         | 1/22516 (0.0%) | 0.95        | 66/30539 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | I     | 0                   | 1                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | N     | 11  | ARG  | C-O   | -6.16 | 1.17        | 1.24     |

All (66) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 777 | ILE  | N-CA-C | 13.81 | 123.51      | 110.53   |
| 2   | J     | 83  | ARG  | CA-C-N | 10.77 | 131.46      | 119.93   |
| 2   | J     | 83  | ARG  | C-N-CA | 10.77 | 131.46      | 119.93   |
| 2   | X     | 83  | ARG  | CA-C-N | 10.28 | 132.68      | 119.84   |
| 2   | X     | 83  | ARG  | C-N-CA | 10.28 | 132.68      | 119.84   |
| 1   | S     | 779 | GLY  | N-CA-C | 10.06 | 127.99      | 111.59   |
| 2   | B     | 83  | ARG  | CA-C-N | 9.32  | 129.40      | 119.89   |
| 2   | B     | 83  | ARG  | C-N-CA | 9.32  | 129.40      | 119.89   |
| 1   | E     | 770 | GLU  | N-CA-C | -7.41 | 102.90      | 112.23   |
| 1   | A     | 783 | ARG  | N-CA-C | 7.41  | 121.57      | 109.72   |
| 2   | B     | 84  | PRO  | N-CA-C | 7.09  | 122.38      | 111.11   |
| 1   | M     | 792 | VAL  | CA-C-N | 6.48  | 124.33      | 119.66   |
| 1   | M     | 792 | VAL  | C-N-CA | 6.48  | 124.33      | 119.66   |
| 1   | Q     | 792 | VAL  | CA-C-N | 6.47  | 124.32      | 119.66   |
| 1   | Q     | 792 | VAL  | C-N-CA | 6.47  | 124.32      | 119.66   |
| 1   | K     | 792 | VAL  | CA-C-N | 6.47  | 124.32      | 119.66   |
| 1   | K     | 792 | VAL  | C-N-CA | 6.47  | 124.32      | 119.66   |
| 2   | F     | 83  | ARG  | CA-C-N | 6.45  | 126.47      | 119.89   |
| 2   | F     | 83  | ARG  | C-N-CA | 6.45  | 126.47      | 119.89   |
| 1   | O     | 792 | VAL  | CA-C-N | 6.44  | 124.30      | 119.66   |
| 1   | O     | 792 | VAL  | C-N-CA | 6.44  | 124.30      | 119.66   |
| 1   | I     | 792 | VAL  | CA-C-N | 6.43  | 124.29      | 119.66   |
| 1   | I     | 792 | VAL  | C-N-CA | 6.43  | 124.29      | 119.66   |
| 1   | A     | 704 | HIS  | N-CA-C | -6.40 | 97.84       | 108.34   |
| 1   | G     | 792 | VAL  | CA-C-N | 6.37  | 124.25      | 119.66   |
| 1   | G     | 792 | VAL  | C-N-CA | 6.37  | 124.25      | 119.66   |
| 1   | A     | 792 | VAL  | CA-C-N | 6.37  | 124.24      | 119.66   |
| 1   | A     | 792 | VAL  | C-N-CA | 6.37  | 124.24      | 119.66   |
| 2   | F     | 6   | VAL  | N-CA-C | 6.36  | 117.14      | 110.72   |
| 1   | C     | 792 | VAL  | CA-C-N | 6.34  | 124.23      | 119.66   |
| 1   | C     | 792 | VAL  | C-N-CA | 6.34  | 124.23      | 119.66   |
| 1   | W     | 792 | VAL  | CA-C-N | 6.34  | 124.23      | 119.66   |
| 1   | W     | 792 | VAL  | C-N-CA | 6.34  | 124.23      | 119.66   |
| 1   | I     | 781 | LYS  | N-CA-C | 6.32  | 119.48      | 109.50   |
| 1   | U     | 792 | VAL  | CA-C-N | 6.31  | 124.20      | 119.66   |
| 1   | U     | 792 | VAL  | C-N-CA | 6.31  | 124.20      | 119.66   |
| 1   | E     | 792 | VAL  | CA-C-N | 6.28  | 124.18      | 119.66   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 792 | VAL  | C-N-CA | 6.28  | 124.18      | 119.66   |
| 2   | V     | 84  | PRO  | CA-C-O | -6.18 | 114.58      | 121.32   |
| 1   | A     | 727 | PRO  | N-CA-C | 5.93  | 120.30      | 111.41   |
| 2   | R     | 82  | ALA  | N-CA-C | 5.82  | 118.86      | 107.57   |
| 2   | B     | 71  | TYR  | N-CA-C | 5.51  | 118.68      | 110.14   |
| 2   | R     | 83  | ARG  | CA-C-N | 5.50  | 125.43      | 119.76   |
| 2   | R     | 83  | ARG  | C-N-CA | 5.50  | 125.43      | 119.76   |
| 2   | N     | 84  | PRO  | CA-C-O | -5.50 | 114.71      | 121.31   |
| 2   | L     | 83  | ARG  | CA-C-N | 5.40  | 126.59      | 119.84   |
| 2   | L     | 83  | ARG  | C-N-CA | 5.40  | 126.59      | 119.84   |
| 1   | E     | 808 | ARG  | N-CA-C | -5.32 | 102.17      | 110.10   |
| 2   | T     | 83  | ARG  | CA-C-N | 5.31  | 125.31      | 119.89   |
| 2   | T     | 83  | ARG  | C-N-CA | 5.31  | 125.31      | 119.89   |
| 2   | H     | 83  | ARG  | CA-C-N | 5.26  | 125.27      | 119.90   |
| 2   | H     | 83  | ARG  | C-N-CA | 5.26  | 125.27      | 119.90   |
| 2   | P     | 83  | ARG  | CA-C-N | 5.22  | 126.03      | 120.13   |
| 2   | P     | 83  | ARG  | C-N-CA | 5.22  | 126.03      | 120.13   |
| 1   | Q     | 721 | ARG  | N-CA-C | 5.22  | 117.41      | 108.90   |
| 1   | U     | 781 | LYS  | N-CA-C | 5.21  | 117.91      | 109.06   |
| 2   | N     | 60  | LYS  | N-CA-C | -5.17 | 101.68      | 109.85   |
| 2   | T     | 60  | LYS  | N-CA-C | -5.13 | 101.74      | 109.85   |
| 2   | P     | 60  | LYS  | N-CA-C | -5.10 | 101.66      | 109.41   |
| 2   | L     | 60  | LYS  | N-CA-C | -5.08 | 101.65      | 109.52   |
| 2   | P     | 84  | PRO  | N-CA-C | 5.08  | 118.82      | 110.55   |
| 1   | W     | 793 | PRO  | O-C-N  | 5.05  | 123.52      | 121.15   |
| 2   | R     | 60  | LYS  | N-CA-C | -5.04 | 101.71      | 109.52   |
| 1   | E     | 793 | PRO  | O-C-N  | 5.02  | 123.51      | 121.15   |
| 1   | I     | 793 | PRO  | O-C-N  | 5.02  | 123.51      | 121.15   |
| 2   | J     | 60  | LYS  | N-CA-C | -5.00 | 102.38      | 110.14   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | I     | 744 | ARG  | Sidechain |

## 5.2 Too-close contacts [i](#)

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     | 1009  | 0        | 1037     | 85      | 0            |
| 1   | C     | 1009  | 0        | 1037     | 28      | 0            |
| 1   | E     | 998   | 0        | 1027     | 48      | 2            |
| 1   | G     | 1014  | 0        | 1048     | 68      | 0            |
| 1   | I     | 1014  | 0        | 1048     | 20      | 5            |
| 1   | K     | 1005  | 0        | 1035     | 33      | 0            |
| 1   | M     | 1007  | 0        | 1040     | 47      | 0            |
| 1   | O     | 1014  | 0        | 1048     | 24      | 6            |
| 1   | Q     | 998   | 0        | 1027     | 34      | 2            |
| 1   | S     | 1014  | 0        | 1048     | 56      | 0            |
| 1   | U     | 949   | 0        | 979      | 24      | 0            |
| 1   | W     | 1014  | 0        | 1048     | 39      | 0            |
| 2   | B     | 830   | 0        | 829      | 58      | 0            |
| 2   | D     | 837   | 0        | 837      | 39      | 0            |
| 2   | F     | 837   | 0        | 837      | 33      | 0            |
| 2   | H     | 830   | 0        | 829      | 41      | 0            |
| 2   | J     | 830   | 0        | 829      | 40      | 2            |
| 2   | L     | 830   | 0        | 829      | 33      | 0            |
| 2   | N     | 837   | 0        | 837      | 71      | 0            |
| 2   | P     | 830   | 0        | 829      | 38      | 0            |
| 2   | R     | 830   | 0        | 829      | 47      | 1            |
| 2   | T     | 830   | 0        | 829      | 50      | 0            |
| 2   | V     | 830   | 0        | 829      | 36      | 0            |
| 2   | X     | 830   | 0        | 829      | 55      | 0            |
| All | All   | 22026 | 0        | 22394    | 777     | 9            |

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 17.

All (777) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:11:ARG:HB3   | 1:S:801:VAL:CG1  | 1.23                     | 1.59              |
| 2:N:11:ARG:CB    | 1:S:801:VAL:HG11 | 1.38                     | 1.51              |
| 2:R:34:LEU:CD2   | 2:R:35:PRO:HD2   | 1.53                     | 1.39              |
| 2:H:20:GLU:HA    | 2:H:61:ARG:NH1   | 1.39                     | 1.32              |
| 2:B:20:GLU:HA    | 2:B:61:ARG:NH1   | 1.43                     | 1.32              |
| 2:J:23:LEU:HD13  | 2:X:59:ARG:HD2   | 1.25                     | 1.19              |
| 2:H:23:LEU:CD1   | 2:T:59:ARG:HD2   | 1.73                     | 1.19              |
| 1:W:721:ARG:HH22 | 2:X:94:ASP:CG    | 1.52                     | 1.17              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:34:LEU:HD23  | 2:R:35:PRO:CD    | 1.75                     | 1.17              |
| 2:L:37:ARG:HH12  | 1:S:769:PRO:HG2  | 1.06                     | 1.16              |
| 2:J:59:ARG:HG3   | 2:X:23:LEU:HD12  | 1.29                     | 1.13              |
| 1:W:807:ARG:HH12 | 2:X:21:THR:HG22  | 1.13                     | 1.12              |
| 2:J:59:ARG:CD    | 2:X:23:LEU:HD13  | 1.78                     | 1.12              |
| 1:A:703:ILE:CD1  | 1:G:703:ILE:HD11 | 1.79                     | 1.11              |
| 1:A:752:GLY:O    | 1:A:791:ARG:HD3  | 1.49                     | 1.11              |
| 1:A:828:ALA:O    | 1:A:829:GLN:HG3  | 1.50                     | 1.11              |
| 2:T:53:ARG:HG2   | 2:T:53:ARG:HH11  | 1.08                     | 1.11              |
| 1:Q:721:ARG:HH22 | 2:R:94:ASP:CG    | 1.58                     | 1.10              |
| 1:A:791:ARG:HG3  | 1:A:791:ARG:HH11 | 1.08                     | 1.10              |
| 2:F:23:LEU:HD13  | 2:P:59:ARG:HD2   | 1.30                     | 1.09              |
| 2:H:23:LEU:HD13  | 2:T:59:ARG:HD2   | 1.20                     | 1.09              |
| 2:F:23:LEU:CD1   | 2:P:59:ARG:HD2   | 1.81                     | 1.08              |
| 2:J:59:ARG:HD3   | 2:X:23:LEU:HD13  | 1.28                     | 1.08              |
| 1:G:830:LYS:HD2  | 1:G:830:LYS:C    | 1.76                     | 1.07              |
| 2:B:23:LEU:HD13  | 2:N:59:ARG:HD2   | 1.30                     | 1.06              |
| 2:H:59:ARG:HD2   | 2:T:23:LEU:HD13  | 1.37                     | 1.04              |
| 1:A:810:ASP:O    | 1:A:813:VAL:HG22 | 1.57                     | 1.03              |
| 1:E:748:GLU:CD   | 1:E:748:GLU:H    | 1.64                     | 1.02              |
| 2:V:30:ASP:OD1   | 2:V:32:ASP:HB2   | 1.58                     | 1.01              |
| 2:B:32:ASP:OD1   | 2:B:33:THR:HG23  | 1.61                     | 1.01              |
| 2:R:30:ASP:OD1   | 2:R:32:ASP:N     | 1.94                     | 1.00              |
| 1:S:807:ARG:NH2  | 2:T:21:THR:CG2   | 2.25                     | 0.99              |
| 1:W:807:ARG:NH1  | 2:X:21:THR:HG22  | 1.76                     | 0.99              |
| 1:E:769:PRO:HB2  | 2:N:37:ARG:HH12  | 1.26                     | 0.99              |
| 2:P:30:ASP:OD1   | 2:P:32:ASP:N     | 1.93                     | 0.99              |
| 1:E:781:LYS:HB3  | 2:F:34:LEU:HD12  | 1.41                     | 0.99              |
| 1:K:775:ARG:HE   | 1:K:780:GLU:HG2  | 1.28                     | 0.98              |
| 1:S:807:ARG:NH2  | 2:T:21:THR:HG22  | 1.80                     | 0.97              |
| 1:A:799:ILE:HD12 | 1:A:801:VAL:HG13 | 1.43                     | 0.96              |
| 2:H:20:GLU:CA    | 2:H:61:ARG:NH1   | 2.27                     | 0.96              |
| 1:E:771:GLU:HG3  | 1:M:770:GLU:HG2  | 1.47                     | 0.95              |
| 1:G:830:LYS:HD2  | 1:G:830:LYS:O    | 1.65                     | 0.95              |
| 2:T:53:ARG:HG2   | 2:T:53:ARG:NH1   | 1.69                     | 0.95              |
| 2:H:59:ARG:HD2   | 2:T:23:LEU:CD1   | 1.95                     | 0.95              |
| 2:J:59:ARG:HD3   | 2:X:23:LEU:CD1   | 1.97                     | 0.95              |
| 2:D:5:PRO:O      | 2:D:8:PRO:HD2    | 1.67                     | 0.94              |
| 2:D:5:PRO:HB2    | 2:D:8:PRO:CG     | 1.96                     | 0.94              |
| 1:M:721:ARG:HH22 | 2:N:94:ASP:CG    | 1.76                     | 0.94              |
| 2:F:32:ASP:OD2   | 2:P:53:ARG:NH2   | 2.00                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:23:LEU:HD12  | 2:X:59:ARG:HG3   | 1.47                     | 0.94              |
| 1:M:703:ILE:HG21 | 2:T:8:PRO:HB2    | 1.46                     | 0.94              |
| 2:B:20:GLU:HA    | 2:B:61:ARG:HH12  | 1.31                     | 0.94              |
| 2:H:20:GLU:HA    | 2:H:61:ARG:HH12  | 1.29                     | 0.94              |
| 2:T:53:ARG:HH11  | 2:T:53:ARG:CG    | 1.80                     | 0.94              |
| 2:J:59:ARG:CD    | 2:X:23:LEU:CD1   | 2.45                     | 0.93              |
| 1:K:721:ARG:HH22 | 2:L:94:ASP:CG    | 1.77                     | 0.93              |
| 1:E:769:PRO:HB2  | 2:N:37:ARG:NH1   | 1.82                     | 0.93              |
| 2:B:20:GLU:CA    | 2:B:61:ARG:NH1   | 2.33                     | 0.92              |
| 1:G:709:GLU:OE2  | 1:G:824:ARG:NH2  | 2.01                     | 0.92              |
| 2:D:32:ASP:OD2   | 2:R:53:ARG:NH2   | 2.02                     | 0.92              |
| 1:K:707:ARG:HG3  | 1:K:826:TYR:CE2  | 2.04                     | 0.92              |
| 2:D:5:PRO:HB2    | 2:D:8:PRO:HG3    | 1.52                     | 0.91              |
| 1:A:799:ILE:HD11 | 1:G:705:ILE:HD11 | 1.53                     | 0.91              |
| 2:J:21:THR:H     | 2:J:61:ARG:NH1   | 1.68                     | 0.91              |
| 1:U:768:THR:HG23 | 1:U:771:GLU:HB2  | 1.51                     | 0.91              |
| 1:W:807:ARG:HH12 | 2:X:21:THR:CG2   | 1.84                     | 0.91              |
| 1:U:784:ASP:OD1  | 2:V:37:ARG:NH1   | 2.03                     | 0.91              |
| 2:J:23:LEU:HD13  | 2:X:59:ARG:CD    | 1.99                     | 0.90              |
| 2:L:37:ARG:NH1   | 1:S:769:PRO:HG2  | 1.84                     | 0.90              |
| 2:J:21:THR:O     | 2:J:61:ARG:NH1   | 2.05                     | 0.89              |
| 2:X:21:THR:H     | 2:X:61:ARG:NH1   | 1.70                     | 0.89              |
| 1:E:748:GLU:CD   | 1:E:748:GLU:N    | 2.30                     | 0.89              |
| 1:A:811:PRO:HB3  | 2:T:20:GLU:OE2   | 1.73                     | 0.88              |
| 2:F:23:LEU:CD1   | 2:P:59:ARG:CD    | 2.51                     | 0.88              |
| 1:A:828:ALA:O    | 1:A:829:GLN:CG   | 2.21                     | 0.88              |
| 2:D:23:LEU:CD1   | 2:R:59:ARG:HD2   | 2.03                     | 0.88              |
| 2:L:47:THR:HG21  | 1:S:772:ARG:HD2  | 1.53                     | 0.88              |
| 2:N:11:ARG:CB    | 1:S:801:VAL:CG1  | 2.19                     | 0.88              |
| 1:W:721:ARG:NH2  | 2:X:94:ASP:OD1   | 2.07                     | 0.87              |
| 2:J:59:ARG:CG    | 2:X:23:LEU:HD12  | 2.03                     | 0.87              |
| 2:B:59:ARG:HD2   | 2:N:23:LEU:HD13  | 1.57                     | 0.87              |
| 2:D:23:LEU:HD13  | 2:R:59:ARG:HD2   | 1.54                     | 0.87              |
| 1:O:797:GLY:O    | 1:O:829:GLN:HB3  | 1.73                     | 0.87              |
| 2:D:32:ASP:OD2   | 2:R:53:ARG:CZ    | 2.23                     | 0.86              |
| 2:J:26:PHE:CE2   | 2:J:59:ARG:NH2   | 2.43                     | 0.86              |
| 1:A:799:ILE:CD1  | 1:A:801:VAL:HG13 | 2.04                     | 0.86              |
| 2:N:30:ASP:OD1   | 2:N:32:ASP:N     | 2.08                     | 0.86              |
| 2:H:23:LEU:CD1   | 2:T:59:ARG:CD    | 2.54                     | 0.86              |
| 2:F:23:LEU:HD12  | 2:P:59:ARG:CD    | 2.06                     | 0.85              |
| 1:M:703:ILE:HG21 | 2:T:8:PRO:CB     | 2.04                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:791:ARG:HG3  | 1:A:791:ARG:NH1  | 1.81                     | 0.85              |
| 1:G:748:GLU:HG3  | 1:G:799:ILE:CD1  | 2.07                     | 0.85              |
| 2:L:23:LEU:CD1   | 2:V:59:ARG:HD2   | 2.05                     | 0.85              |
| 1:E:816:LYS:HB3  | 1:E:817:PRO:HD2  | 1.57                     | 0.85              |
| 1:A:799:ILE:CD1  | 1:A:801:VAL:CG1  | 2.54                     | 0.84              |
| 1:S:764:GLU:HB3  | 1:S:783:ARG:HE   | 1.41                     | 0.84              |
| 2:B:23:LEU:CD1   | 2:N:59:ARG:HD2   | 2.07                     | 0.84              |
| 1:Q:768:THR:HG23 | 1:Q:771:GLU:HB2  | 1.59                     | 0.84              |
| 1:S:708:TYR:OH   | 1:S:796:GLU:HG2  | 1.76                     | 0.83              |
| 1:O:709:GLU:OE2  | 1:O:824:ARG:NH2  | 2.11                     | 0.83              |
| 1:W:797:GLY:H    | 1:W:829:GLN:HE22 | 1.25                     | 0.83              |
| 2:N:30:ASP:OD1   | 2:N:31:LEU:N     | 2.11                     | 0.83              |
| 2:R:34:LEU:CD2   | 2:R:35:PRO:CD    | 2.43                     | 0.83              |
| 2:B:20:GLU:HA    | 2:B:61:ARG:HH11  | 1.40                     | 0.83              |
| 1:W:706:GLU:HG3  | 1:W:829:GLN:OE1  | 1.77                     | 0.83              |
| 1:G:797:GLY:O    | 1:G:829:GLN:HB3  | 1.77                     | 0.83              |
| 1:A:721:ARG:HH22 | 2:B:94:ASP:CG    | 1.87                     | 0.82              |
| 1:U:781:LYS:HB2  | 2:V:34:LEU:HD12  | 1.59                     | 0.82              |
| 2:B:23:LEU:HD13  | 2:N:59:ARG:CD    | 2.08                     | 0.82              |
| 1:C:721:ARG:HH22 | 2:D:94:ASP:CG    | 1.87                     | 0.82              |
| 2:H:20:GLU:HA    | 2:H:61:ARG:HH11  | 1.38                     | 0.82              |
| 1:M:704:HIS:NE2  | 1:M:706:GLU:OE1  | 2.13                     | 0.81              |
| 2:B:23:LEU:CD1   | 2:N:59:ARG:CD    | 2.59                     | 0.81              |
| 2:N:5:PRO:O      | 2:N:8:PRO:HD2    | 1.80                     | 0.81              |
| 1:S:740:GLU:OE1  | 1:S:807:ARG:NH2  | 2.14                     | 0.81              |
| 1:O:721:ARG:HH22 | 2:P:94:ASP:CG    | 1.88                     | 0.81              |
| 2:H:21:THR:H     | 2:H:61:ARG:HH11  | 1.25                     | 0.80              |
| 2:H:23:LEU:HD12  | 2:T:59:ARG:CD    | 2.11                     | 0.80              |
| 2:B:23:LEU:HD12  | 2:N:59:ARG:HG3   | 1.62                     | 0.80              |
| 2:N:11:ARG:HB3   | 1:S:801:VAL:HG13 | 1.61                     | 0.80              |
| 2:D:5:PRO:C      | 2:D:8:PRO:HD2    | 2.07                     | 0.80              |
| 1:A:703:ILE:HD11 | 1:G:703:ILE:HD11 | 1.64                     | 0.80              |
| 2:R:34:LEU:HD23  | 2:R:35:PRO:HD2   | 0.80                     | 0.80              |
| 2:D:5:PRO:O      | 2:D:8:PRO:CD     | 2.30                     | 0.80              |
| 2:T:53:ARG:HD3   | 2:T:71:TYR:CE2   | 2.17                     | 0.80              |
| 2:J:23:LEU:CD1   | 2:X:59:ARG:HD2   | 2.09                     | 0.79              |
| 2:J:73:PHE:HB2   | 1:U:777:ILE:HG12 | 1.64                     | 0.79              |
| 2:B:21:THR:H     | 2:B:61:ARG:HH11  | 1.29                     | 0.79              |
| 2:L:23:LEU:HD13  | 2:V:59:ARG:HD2   | 1.64                     | 0.79              |
| 1:Q:725:ASP:CG   | 2:R:93:GLY:HA3   | 2.08                     | 0.79              |
| 1:E:769:PRO:CB   | 2:N:37:ARG:HH12  | 1.94                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:752:GLY:O    | 1:A:791:ARG:CD   | 2.30                     | 0.78              |
| 2:J:23:LEU:CD1   | 2:X:59:ARG:CD    | 2.60                     | 0.78              |
| 2:H:23:LEU:HD12  | 2:T:59:ARG:HD2   | 1.63                     | 0.78              |
| 1:A:811:PRO:CB   | 2:T:20:GLU:OE2   | 2.31                     | 0.78              |
| 1:M:781:LYS:H    | 1:M:781:LYS:HD3  | 1.49                     | 0.78              |
| 2:B:30:ASP:HB3   | 2:B:32:ASP:OD1   | 1.83                     | 0.78              |
| 2:L:37:ARG:HH12  | 1:S:769:PRO:CG   | 1.93                     | 0.78              |
| 1:K:707:ARG:HD2  | 1:K:826:TYR:OH   | 1.83                     | 0.78              |
| 1:A:750:LYS:HG3  | 1:A:753:ASP:OD2  | 1.84                     | 0.77              |
| 1:G:769:PRO:HB3  | 2:X:45:LEU:HD21  | 1.65                     | 0.77              |
| 1:S:769:PRO:HG3  | 1:S:772:ARG:HH12 | 1.50                     | 0.77              |
| 2:P:30:ASP:OD1   | 2:P:32:ASP:HB2   | 1.85                     | 0.76              |
| 1:U:778:PHE:HB3  | 2:V:34:LEU:HD23  | 1.65                     | 0.76              |
| 1:A:828:ALA:C    | 1:A:829:GLN:HG3  | 2.11                     | 0.76              |
| 1:I:781:LYS:HB3  | 2:J:34:LEU:HD12  | 1.65                     | 0.76              |
| 1:A:799:ILE:HD12 | 1:A:801:VAL:CG1  | 2.16                     | 0.76              |
| 1:G:811:PRO:HB3  | 2:N:20:GLU:CD    | 2.11                     | 0.76              |
| 1:C:781:LYS:HD2  | 2:D:34:LEU:HD13  | 1.69                     | 0.75              |
| 2:B:78:LEU:H     | 2:B:78:LEU:HD12  | 1.51                     | 0.75              |
| 2:R:30:ASP:OD1   | 2:R:32:ASP:HB2   | 1.86                     | 0.75              |
| 1:A:703:ILE:CD1  | 1:G:703:ILE:CD1  | 2.64                     | 0.75              |
| 2:D:37:ARG:HH12  | 1:O:769:PRO:HG2  | 1.49                     | 0.75              |
| 2:B:74:GLU:OE2   | 2:B:83:ARG:NH1   | 2.20                     | 0.75              |
| 1:A:811:PRO:HB3  | 2:T:20:GLU:CD    | 2.12                     | 0.74              |
| 2:D:32:ASP:OD2   | 2:R:53:ARG:NH1   | 2.20                     | 0.74              |
| 1:C:772:ARG:HB3  | 2:P:47:THR:HG21  | 1.67                     | 0.74              |
| 1:W:750:LYS:HG3  | 1:W:753:ASP:OD2  | 1.87                     | 0.74              |
| 1:K:721:ARG:NH2  | 2:L:94:ASP:OD1   | 2.21                     | 0.74              |
| 2:N:8:PRO:HB3    | 1:S:705:ILE:HD11 | 1.69                     | 0.74              |
| 2:F:26:PHE:CE2   | 2:F:59:ARG:NH2   | 2.56                     | 0.74              |
| 2:B:59:ARG:HD2   | 2:N:23:LEU:CD1   | 2.17                     | 0.73              |
| 1:W:704:HIS:O    | 1:W:829:GLN:N    | 2.19                     | 0.73              |
| 1:S:740:GLU:O    | 1:S:740:GLU:HG3  | 1.87                     | 0.73              |
| 2:J:23:LEU:HD12  | 2:X:59:ARG:CG    | 2.17                     | 0.73              |
| 2:N:5:PRO:HB2    | 2:N:7:GLU:OE1    | 1.89                     | 0.73              |
| 1:I:797:GLY:O    | 1:I:829:GLN:HB3  | 1.88                     | 0.73              |
| 2:V:30:ASP:OD1   | 2:V:32:ASP:CB    | 2.36                     | 0.73              |
| 1:G:806:LEU:O    | 1:G:821:GLU:HG3  | 1.89                     | 0.73              |
| 1:W:775:ARG:NH2  | 1:W:780:GLU:OE1  | 2.19                     | 0.73              |
| 1:E:704:HIS:CE1  | 1:E:706:GLU:OE1  | 2.41                     | 0.73              |
| 1:W:721:ARG:NH2  | 2:X:94:ASP:CG    | 2.38                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:808:ARG:NH1  | 1:W:808:ARG:HG2  | 2.04                     | 0.72              |
| 1:W:808:ARG:HG2  | 1:W:808:ARG:HH11 | 1.54                     | 0.72              |
| 1:A:806:LEU:O    | 1:A:821:GLU:HG3  | 1.89                     | 0.72              |
| 2:H:21:THR:N     | 2:H:61:ARG:HH11  | 1.86                     | 0.72              |
| 2:J:59:ARG:CG    | 2:X:23:LEU:CD1   | 2.66                     | 0.72              |
| 1:G:771:GLU:OE1  | 1:G:781:LYS:NZ   | 2.22                     | 0.72              |
| 2:D:5:PRO:O      | 2:D:8:PRO:HG2    | 1.89                     | 0.72              |
| 2:X:61:ARG:HG2   | 2:X:61:ARG:HH11  | 1.53                     | 0.72              |
| 2:N:30:ASP:OD1   | 2:N:30:ASP:C     | 2.32                     | 0.71              |
| 1:W:778:PHE:HB3  | 2:X:34:LEU:HD23  | 1.71                     | 0.71              |
| 2:J:59:ARG:HD2   | 2:X:23:LEU:HD13  | 1.72                     | 0.71              |
| 1:U:721:ARG:HH22 | 2:V:94:ASP:CG    | 1.97                     | 0.71              |
| 1:A:797:GLY:O    | 1:A:829:GLN:HG2  | 1.89                     | 0.71              |
| 2:J:59:ARG:HG3   | 2:X:23:LEU:CD1   | 2.15                     | 0.71              |
| 1:A:778:PHE:HE2  | 1:Q:777:ILE:HD13 | 1.56                     | 0.71              |
| 2:D:60:LYS:HB2   | 2:D:63:VAL:HG23  | 1.71                     | 0.71              |
| 2:L:25:THR:HG23  | 2:V:56:GLU:OE1   | 1.91                     | 0.71              |
| 2:J:26:PHE:CD2   | 2:J:59:ARG:NH2   | 2.59                     | 0.71              |
| 1:K:777:ILE:HG22 | 1:K:778:PHE:CD2  | 2.26                     | 0.71              |
| 2:X:26:PHE:CE2   | 2:X:59:ARG:NH2   | 2.59                     | 0.71              |
| 2:H:20:GLU:CA    | 2:H:61:ARG:HH12  | 1.98                     | 0.70              |
| 1:Q:721:ARG:NH2  | 2:R:94:ASP:OD1   | 2.24                     | 0.70              |
| 1:I:771:GLU:HG2  | 1:U:770:GLU:HG2  | 1.71                     | 0.70              |
| 2:R:30:ASP:OD1   | 2:R:30:ASP:C     | 2.35                     | 0.70              |
| 1:E:721:ARG:HH22 | 2:F:94:ASP:CG    | 1.99                     | 0.70              |
| 2:J:26:PHE:HE2   | 2:J:59:ARG:NH2   | 1.86                     | 0.70              |
| 1:S:769:PRO:HG3  | 1:S:772:ARG:NH1  | 2.07                     | 0.69              |
| 1:M:703:ILE:CG2  | 2:T:8:PRO:CB     | 2.70                     | 0.69              |
| 2:N:53:ARG:HG2   | 2:N:53:ARG:HH11  | 1.57                     | 0.69              |
| 2:B:85:TYR:CE1   | 2:B:106:VAL:HG13 | 2.28                     | 0.69              |
| 1:A:799:ILE:HD11 | 1:A:801:VAL:CG1  | 2.22                     | 0.69              |
| 2:H:81:ALA:HB1   | 2:X:78:LEU:HD22  | 1.73                     | 0.69              |
| 2:F:38:MET:HE1   | 2:F:48:PRO:HB3   | 1.74                     | 0.68              |
| 2:B:23:LEU:HD12  | 2:N:59:ARG:CG    | 2.23                     | 0.68              |
| 1:M:731:GLU:CD   | 2:N:41:PRO:HB3   | 2.18                     | 0.68              |
| 2:F:23:LEU:HD13  | 2:P:59:ARG:CD    | 2.15                     | 0.68              |
| 1:C:775:ARG:HE   | 1:C:780:GLU:HG2  | 1.57                     | 0.68              |
| 1:G:814:GLU:HG2  | 1:M:811:PRO:HG3  | 1.76                     | 0.68              |
| 1:O:764:GLU:HB3  | 1:O:783:ARG:HE   | 1.59                     | 0.68              |
| 2:P:30:ASP:OD1   | 2:P:30:ASP:C     | 2.36                     | 0.68              |
| 2:R:38:MET:HE1   | 2:R:48:PRO:HB3   | 1.74                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:V:30:ASP:OD1   | 2:V:32:ASP:N     | 2.26                     | 0.68              |
| 1:Q:712:ALA:HB1  | 1:Q:720:GLU:O    | 1.93                     | 0.68              |
| 1:S:807:ARG:HH21 | 2:T:21:THR:CG2   | 2.07                     | 0.68              |
| 2:D:5:PRO:O      | 2:D:8:PRO:CG     | 2.42                     | 0.68              |
| 2:R:34:LEU:HD22  | 2:R:35:PRO:HD2   | 1.72                     | 0.67              |
| 1:U:766:GLU:HB2  | 1:U:767:PRO:HD2  | 1.75                     | 0.67              |
| 1:W:704:HIS:HB3  | 1:W:829:GLN:O    | 1.94                     | 0.67              |
| 1:M:778:PHE:HB2  | 2:N:34:LEU:HD23  | 1.75                     | 0.67              |
| 2:F:26:PHE:HE2   | 2:F:59:ARG:NH2   | 1.93                     | 0.67              |
| 1:M:740:GLU:O    | 1:M:740:GLU:HG3  | 1.95                     | 0.67              |
| 1:A:740:GLU:HG3  | 2:B:21:THR:HG21  | 1.76                     | 0.67              |
| 2:X:61:ARG:NH1   | 2:X:61:ARG:HG2   | 2.09                     | 0.67              |
| 1:A:797:GLY:H    | 1:A:829:GLN:NE2  | 1.93                     | 0.67              |
| 1:W:797:GLY:H    | 1:W:829:GLN:NE2  | 1.93                     | 0.67              |
| 1:C:769:PRO:HA   | 1:C:772:ARG:HB2  | 1.77                     | 0.66              |
| 2:J:83:ARG:HG2   | 2:J:84:PRO:HD2   | 1.77                     | 0.66              |
| 1:A:703:ILE:HD12 | 1:G:703:ILE:HD11 | 1.77                     | 0.66              |
| 1:A:799:ILE:CD1  | 1:G:705:ILE:HD11 | 2.26                     | 0.66              |
| 2:B:20:GLU:CA    | 2:B:61:ARG:HH12  | 2.03                     | 0.66              |
| 1:C:781:LYS:HA   | 2:D:34:LEU:HD12  | 1.77                     | 0.66              |
| 2:B:21:THR:N     | 2:B:61:ARG:HH11  | 1.93                     | 0.66              |
| 1:K:775:ARG:NE   | 1:K:780:GLU:HG2  | 2.09                     | 0.66              |
| 2:T:53:ARG:HD3   | 2:T:71:TYR:HE2   | 1.61                     | 0.66              |
| 1:A:814:GLU:HG2  | 1:S:811:PRO:HG2  | 1.76                     | 0.66              |
| 1:E:740:GLU:OE2  | 1:E:807:ARG:NH2  | 2.28                     | 0.66              |
| 1:G:724:ARG:O    | 1:G:724:ARG:HG2  | 1.96                     | 0.66              |
| 1:Q:762:LYS:HE2  | 1:Q:786:LYS:HD2  | 1.78                     | 0.66              |
| 1:C:769:PRO:HG2  | 2:P:37:ARG:NH1   | 2.10                     | 0.66              |
| 1:W:706:GLU:CG   | 1:W:829:GLN:OE1  | 2.43                     | 0.65              |
| 1:A:778:PHE:CE2  | 1:Q:777:ILE:HD13 | 2.32                     | 0.65              |
| 1:A:778:PHE:CE1  | 2:B:73:PHE:HE2   | 2.15                     | 0.65              |
| 1:K:707:ARG:HG3  | 1:K:826:TYR:CZ   | 2.32                     | 0.65              |
| 1:A:721:ARG:NH2  | 2:B:94:ASP:OD1   | 2.30                     | 0.65              |
| 2:L:23:LEU:HD12  | 2:V:59:ARG:CD    | 2.26                     | 0.65              |
| 1:S:793:PRO:HB2  | 1:S:796:GLU:OE1  | 1.97                     | 0.65              |
| 1:Q:721:ARG:NH2  | 2:R:94:ASP:CG    | 2.43                     | 0.65              |
| 1:W:775:ARG:HE   | 1:W:780:GLU:HG2  | 1.62                     | 0.64              |
| 2:D:59:ARG:HD2   | 2:R:23:LEU:CD1   | 2.27                     | 0.64              |
| 1:I:781:LYS:HB3  | 2:J:34:LEU:CD1   | 2.27                     | 0.64              |
| 2:X:26:PHE:HE2   | 2:X:59:ARG:CZ    | 2.11                     | 0.64              |
| 2:N:53:ARG:HG2   | 2:N:53:ARG:NH1   | 2.13                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:740:GLU:OE1  | 1:W:805:ARG:NH1  | 2.26                     | 0.64              |
| 1:G:830:LYS:O    | 1:G:830:LYS:CD   | 2.42                     | 0.63              |
| 1:U:781:LYS:HB2  | 2:V:34:LEU:CD1   | 2.26                     | 0.63              |
| 1:A:717:LEU:HD22 | 1:A:764:GLU:OE1  | 1.99                     | 0.63              |
| 2:B:60:LYS:HB2   | 2:B:63:VAL:HG23  | 1.79                     | 0.63              |
| 2:J:38:MET:HG2   | 2:J:98:LEU:HB2   | 1.81                     | 0.63              |
| 2:J:59:ARG:HG3   | 2:J:59:ARG:O     | 1.97                     | 0.63              |
| 1:A:799:ILE:CD1  | 1:G:705:ILE:CD1  | 2.77                     | 0.63              |
| 1:G:748:GLU:HG3  | 1:G:799:ILE:HD13 | 1.81                     | 0.63              |
| 2:L:23:LEU:HD12  | 2:V:59:ARG:HD2   | 1.80                     | 0.63              |
| 2:D:38:MET:HG2   | 2:D:98:LEU:HB2   | 1.81                     | 0.62              |
| 2:D:23:LEU:CD1   | 2:R:59:ARG:CD    | 2.77                     | 0.62              |
| 1:M:801:VAL:HB   | 2:T:11:ARG:HB3   | 1.80                     | 0.62              |
| 2:N:38:MET:HG2   | 2:N:98:LEU:HB2   | 1.81                     | 0.62              |
| 1:G:771:GLU:HG2  | 1:W:770:GLU:HG2  | 1.81                     | 0.62              |
| 2:D:23:LEU:HD12  | 2:R:59:ARG:CD    | 2.30                     | 0.62              |
| 2:H:21:THR:O     | 2:H:61:ARG:HD3   | 2.00                     | 0.62              |
| 1:A:703:ILE:HD11 | 1:G:703:ILE:CD1  | 2.25                     | 0.62              |
| 2:F:59:ARG:HD2   | 2:P:23:LEU:HD13  | 1.81                     | 0.62              |
| 1:W:762:LYS:HD3  | 1:W:786:LYS:HD3  | 1.82                     | 0.62              |
| 1:A:777:ILE:HG12 | 2:R:73:PHE:CD2   | 2.34                     | 0.62              |
| 2:F:37:ARG:HH12  | 1:M:769:PRO:HG2  | 1.65                     | 0.62              |
| 1:O:764:GLU:CD   | 1:O:783:ARG:HH21 | 2.07                     | 0.62              |
| 2:V:38:MET:HG2   | 2:V:98:LEU:HB2   | 1.81                     | 0.62              |
| 2:P:38:MET:HG2   | 2:P:98:LEU:HB2   | 1.81                     | 0.61              |
| 1:A:791:ARG:NH1  | 1:A:791:ARG:CG   | 2.59                     | 0.61              |
| 2:B:23:LEU:HD12  | 2:N:59:ARG:CD    | 2.29                     | 0.61              |
| 1:G:769:PRO:CB   | 2:X:37:ARG:HH12  | 2.13                     | 0.61              |
| 1:M:740:GLU:OE1  | 1:M:807:ARG:NH2  | 2.33                     | 0.61              |
| 2:J:23:LEU:CD1   | 2:X:59:ARG:CG    | 2.77                     | 0.61              |
| 2:L:59:ARG:HD2   | 2:V:23:LEU:CD1   | 2.30                     | 0.61              |
| 2:N:30:ASP:OD2   | 2:N:32:ASP:HB2   | 2.00                     | 0.61              |
| 2:N:26:PHE:HE2   | 2:N:59:ARG:CZ    | 2.13                     | 0.61              |
| 1:S:721:ARG:NH2  | 2:T:95:ASN:OD1   | 2.30                     | 0.60              |
| 1:A:799:ILE:HD11 | 1:G:705:ILE:CD1  | 2.29                     | 0.60              |
| 1:S:807:ARG:NH2  | 2:T:21:THR:HG23  | 2.13                     | 0.60              |
| 2:H:38:MET:HE1   | 2:H:48:PRO:HB3   | 1.82                     | 0.60              |
| 1:K:777:ILE:HG22 | 1:K:778:PHE:HD2  | 1.66                     | 0.60              |
| 2:L:38:MET:HE1   | 2:L:48:PRO:HB3   | 1.82                     | 0.60              |
| 1:A:778:PHE:CZ   | 2:B:73:PHE:CE2   | 2.90                     | 0.60              |
| 2:D:59:ARG:HD2   | 2:R:23:LEU:HD13  | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:47:THR:HG21  | 1:S:772:ARG:HH11 | 1.66                     | 0.60              |
| 1:M:736:ASP:O    | 1:M:744:ARG:HG2  | 2.01                     | 0.60              |
| 1:E:767:PRO:HG2  | 1:E:772:ARG:HH21 | 1.66                     | 0.60              |
| 1:G:811:PRO:HB3  | 2:N:20:GLU:OE2   | 2.02                     | 0.60              |
| 1:M:772:ARG:O    | 1:M:772:ARG:HD3  | 2.01                     | 0.60              |
| 1:S:736:ASP:O    | 1:S:744:ARG:HG2  | 2.02                     | 0.60              |
| 1:W:778:PHE:HB3  | 2:X:34:LEU:CD2   | 2.32                     | 0.60              |
| 2:P:70:ILE:C     | 2:P:71:TYR:HD2   | 2.10                     | 0.59              |
| 2:P:30:ASP:OD1   | 2:P:32:ASP:CB    | 2.50                     | 0.59              |
| 2:D:23:LEU:HD12  | 2:R:59:ARG:HD2   | 1.83                     | 0.59              |
| 2:R:30:ASP:OD1   | 2:R:32:ASP:CB    | 2.50                     | 0.59              |
| 2:X:38:MET:HE1   | 2:X:48:PRO:HB3   | 1.82                     | 0.59              |
| 1:E:772:ARG:HB3  | 2:N:47:THR:HG21  | 1.84                     | 0.59              |
| 1:W:808:ARG:HH11 | 1:W:808:ARG:CG   | 2.15                     | 0.59              |
| 1:G:769:PRO:HB2  | 2:X:37:ARG:HH12  | 1.68                     | 0.59              |
| 2:J:26:PHE:HE2   | 2:J:59:ARG:CZ    | 2.15                     | 0.59              |
| 1:Q:720:GLU:HG2  | 1:Q:760:SER:HA   | 1.84                     | 0.59              |
| 1:C:767:PRO:O    | 1:C:772:ARG:NH1  | 2.35                     | 0.59              |
| 1:E:721:ARG:NH2  | 2:F:94:ASP:OD1   | 2.31                     | 0.59              |
| 1:A:703:ILE:HD13 | 1:G:703:ILE:HD11 | 1.76                     | 0.59              |
| 1:G:703:ILE:HG22 | 1:G:703:ILE:O    | 2.03                     | 0.59              |
| 2:J:37:ARG:HH12  | 1:U:769:PRO:HG2  | 1.68                     | 0.59              |
| 1:A:802:ARG:HG3  | 1:A:803:THR:N    | 2.18                     | 0.58              |
| 1:E:767:PRO:HG2  | 1:E:772:ARG:NH2  | 2.18                     | 0.58              |
| 1:G:769:PRO:CG   | 2:X:37:ARG:HH12  | 2.16                     | 0.58              |
| 2:V:30:ASP:OD2   | 2:V:33:THR:HG23  | 2.03                     | 0.58              |
| 2:P:7:GLU:O      | 2:P:11:ARG:HG2   | 2.04                     | 0.58              |
| 1:E:704:HIS:HE1  | 1:E:706:GLU:OE1  | 1.86                     | 0.58              |
| 2:L:23:LEU:HD11  | 2:V:23:LEU:HD22  | 1.86                     | 0.58              |
| 1:A:799:ILE:HG13 | 1:A:828:ALA:HB3  | 1.85                     | 0.58              |
| 1:E:748:GLU:N    | 1:E:748:GLU:OE1  | 2.30                     | 0.58              |
| 1:A:801:VAL:HG12 | 1:G:705:ILE:CD1  | 2.34                     | 0.58              |
| 2:J:21:THR:N     | 2:J:61:ARG:NH1   | 2.48                     | 0.58              |
| 1:G:830:LYS:H    | 1:G:830:LYS:CE   | 2.17                     | 0.57              |
| 2:R:31:LEU:HD21  | 2:R:71:TYR:CE2   | 2.39                     | 0.57              |
| 1:S:764:GLU:HB3  | 1:S:783:ARG:NE   | 2.16                     | 0.57              |
| 1:G:724:ARG:NH1  | 2:H:91:TRP:CZ2   | 2.73                     | 0.57              |
| 1:A:811:PRO:CB   | 2:T:20:GLU:CD    | 2.78                     | 0.57              |
| 2:H:59:ARG:CD    | 2:T:23:LEU:CD1   | 2.77                     | 0.57              |
| 1:M:721:ARG:NH2  | 2:N:94:ASP:OD1   | 2.38                     | 0.57              |
| 1:Q:725:ASP:CG   | 2:R:93:GLY:CA    | 2.77                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:X:21:THR:H     | 2:X:61:ARG:HH12  | 1.48                     | 0.57              |
| 2:B:37:ARG:HH12  | 1:Q:769:PRO:HG2  | 1.70                     | 0.57              |
| 1:G:704:HIS:O    | 1:G:829:GLN:O    | 2.22                     | 0.57              |
| 1:O:767:PRO:HB3  | 1:O:781:LYS:HE3  | 1.86                     | 0.57              |
| 1:A:799:ILE:HD13 | 1:G:705:ILE:HD12 | 1.87                     | 0.56              |
| 1:C:769:PRO:HG3  | 2:P:45:LEU:HD21  | 1.86                     | 0.56              |
| 1:M:703:ILE:CG2  | 2:T:8:PRO:HB2    | 2.30                     | 0.56              |
| 1:G:767:PRO:O    | 1:G:772:ARG:NH2  | 2.37                     | 0.56              |
| 2:N:31:LEU:HG    | 2:N:53:ARG:HD2   | 1.87                     | 0.56              |
| 2:V:73:PHE:HB3   | 2:V:80:LEU:HD22  | 1.86                     | 0.56              |
| 2:L:25:THR:HG23  | 2:V:56:GLU:HG2   | 1.85                     | 0.56              |
| 1:Q:725:ASP:OD2  | 2:R:93:GLY:C     | 2.49                     | 0.56              |
| 2:X:21:THR:O     | 2:X:61:ARG:NH1   | 2.39                     | 0.56              |
| 1:G:748:GLU:OE1  | 1:G:748:GLU:N    | 2.38                     | 0.56              |
| 1:G:807:ARG:HB2  | 1:G:810:ASP:OD2  | 2.06                     | 0.56              |
| 2:L:23:LEU:CD1   | 2:V:59:ARG:CD    | 2.78                     | 0.56              |
| 1:C:725:ASP:CG   | 2:D:93:GLY:HA3   | 2.30                     | 0.56              |
| 2:L:70:ILE:O     | 2:L:85:TYR:HB3   | 2.06                     | 0.56              |
| 2:D:5:PRO:HB2    | 2:D:8:PRO:HG2    | 1.82                     | 0.56              |
| 2:V:78:LEU:HD13  | 2:V:78:LEU:H     | 1.70                     | 0.55              |
| 1:M:758:ARG:NE   | 1:M:788:THR:OG1  | 2.37                     | 0.55              |
| 2:X:38:MET:HG2   | 2:X:98:LEU:HB2   | 1.88                     | 0.55              |
| 1:A:801:VAL:HG12 | 1:G:705:ILE:HD13 | 1.87                     | 0.55              |
| 2:X:26:PHE:CD2   | 2:X:59:ARG:NH2   | 2.75                     | 0.55              |
| 1:K:764:GLU:CD   | 1:K:764:GLU:H    | 2.13                     | 0.55              |
| 1:M:704:HIS:CE1  | 1:M:706:GLU:OE1  | 2.60                     | 0.55              |
| 1:A:705:ILE:CD1  | 1:G:801:VAL:HG12 | 2.36                     | 0.55              |
| 1:Q:704:HIS:NE2  | 1:Q:706:GLU:OE1  | 2.32                     | 0.55              |
| 1:W:797:GLY:O    | 1:W:829:GLN:NE2  | 2.33                     | 0.55              |
| 1:A:717:LEU:HD22 | 1:A:764:GLU:CD   | 2.31                     | 0.55              |
| 1:K:761:PHE:CD1  | 1:K:783:ARG:HD3  | 2.42                     | 0.55              |
| 1:S:767:PRO:HB2  | 1:S:772:ARG:HE   | 1.72                     | 0.55              |
| 2:H:38:MET:HG2   | 2:H:98:LEU:HB2   | 1.88                     | 0.55              |
| 2:L:38:MET:HG2   | 2:L:98:LEU:HB2   | 1.88                     | 0.54              |
| 1:A:807:ARG:HH22 | 2:B:21:THR:CG2   | 2.20                     | 0.54              |
| 1:A:807:ARG:NH2  | 2:B:21:THR:HG22  | 2.22                     | 0.54              |
| 1:Q:762:LYS:CE   | 1:Q:786:LYS:HD2  | 2.37                     | 0.54              |
| 1:W:740:GLU:OE2  | 1:W:807:ARG:NH2  | 2.40                     | 0.54              |
| 2:B:32:ASP:CG    | 2:B:33:THR:HG23  | 2.32                     | 0.54              |
| 1:M:705:ILE:HD11 | 2:T:8:PRO:HB3    | 1.90                     | 0.54              |
| 2:L:59:ARG:HD2   | 2:V:23:LEU:HD13  | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:725:ASP:CB   | 2:R:93:GLY:HA3   | 2.37                     | 0.54              |
| 1:C:721:ARG:NH2  | 2:D:94:ASP:OD1   | 2.36                     | 0.54              |
| 2:F:59:ARG:HD2   | 2:P:23:LEU:CD1   | 2.38                     | 0.54              |
| 1:S:783:ARG:HG2  | 1:S:784:ASP:N    | 2.20                     | 0.54              |
| 1:I:721:ARG:HH22 | 2:J:94:ASP:CG    | 2.15                     | 0.54              |
| 2:P:50:GLY:HA3   | 2:P:71:TYR:O     | 2.08                     | 0.54              |
| 2:F:25:THR:HG23  | 2:P:56:GLU:HG2   | 1.89                     | 0.54              |
| 1:S:807:ARG:HH22 | 2:T:21:THR:HG23  | 1.71                     | 0.54              |
| 1:U:778:PHE:HB3  | 2:V:34:LEU:CD2   | 2.38                     | 0.54              |
| 1:G:797:GLY:O    | 1:G:829:GLN:CB   | 2.54                     | 0.54              |
| 2:B:50:GLY:HA3   | 2:B:71:TYR:O     | 2.08                     | 0.53              |
| 1:G:724:ARG:O    | 1:G:724:ARG:CG   | 2.56                     | 0.53              |
| 1:O:781:LYS:H    | 1:O:781:LYS:HD3  | 1.73                     | 0.53              |
| 1:Q:704:HIS:NE2  | 1:Q:706:GLU:HG2  | 2.23                     | 0.53              |
| 1:I:707:ARG:O    | 1:I:707:ARG:HG3  | 2.00                     | 0.53              |
| 1:A:764:GLU:HG2  | 1:A:783:ARG:NH2  | 2.23                     | 0.53              |
| 1:A:705:ILE:HD13 | 1:G:801:VAL:HG12 | 1.89                     | 0.53              |
| 2:D:31:LEU:HD13  | 2:D:82:ALA:HB3   | 1.90                     | 0.53              |
| 2:P:53:ARG:HH11  | 2:P:53:ARG:HG2   | 1.73                     | 0.53              |
| 1:E:781:LYS:NZ   | 1:E:782:ALA:HB3  | 2.23                     | 0.53              |
| 2:B:23:LEU:CD1   | 2:N:59:ARG:CG    | 2.87                     | 0.53              |
| 1:G:811:PRO:CB   | 2:N:20:GLU:OE2   | 2.57                     | 0.53              |
| 1:W:727:PRO:O    | 1:W:728:HIS:HB2  | 2.08                     | 0.53              |
| 2:H:16:ILE:HB    | 2:H:60:LYS:HE3   | 1.91                     | 0.53              |
| 2:D:38:MET:HE1   | 2:D:48:PRO:HB3   | 1.92                     | 0.52              |
| 1:W:806:LEU:O    | 1:W:821:GLU:HG3  | 2.09                     | 0.52              |
| 2:X:26:PHE:CE2   | 2:X:59:ARG:CZ    | 2.90                     | 0.52              |
| 1:K:707:ARG:CG   | 1:K:826:TYR:CE2  | 2.87                     | 0.52              |
| 2:N:38:MET:HE1   | 2:N:48:PRO:HB3   | 1.91                     | 0.52              |
| 2:P:53:ARG:HG2   | 2:P:53:ARG:NH1   | 2.22                     | 0.52              |
| 1:E:768:THR:OG1  | 1:E:771:GLU:HB2  | 2.09                     | 0.52              |
| 1:Q:725:ASP:HB2  | 2:R:93:GLY:HA3   | 1.90                     | 0.52              |
| 2:V:38:MET:HE1   | 2:V:48:PRO:HB3   | 1.91                     | 0.52              |
| 1:A:775:ARG:NE   | 1:A:781:LYS:HD2  | 2.25                     | 0.52              |
| 2:D:60:LYS:HB2   | 2:D:63:VAL:CG2   | 2.40                     | 0.52              |
| 2:R:72:ARG:HB3   | 2:R:85:TYR:HB2   | 1.91                     | 0.52              |
| 1:A:764:GLU:HG2  | 1:A:783:ARG:HH21 | 1.75                     | 0.52              |
| 2:D:74:GLU:O     | 2:D:80:LEU:HB3   | 2.10                     | 0.52              |
| 2:L:25:THR:CG2   | 2:V:56:GLU:HG2   | 2.40                     | 0.52              |
| 1:M:778:PHE:CB   | 2:N:34:LEU:HD23  | 2.40                     | 0.52              |
| 2:R:30:ASP:OD1   | 2:R:32:ASP:CA    | 2.57                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:38:MET:HE1   | 2:P:48:PRO:HB3   | 1.91                     | 0.51              |
| 2:V:59:ARG:O     | 2:V:59:ARG:HG3   | 2.10                     | 0.51              |
| 2:N:8:PRO:HB3    | 1:S:705:ILE:CD1  | 2.38                     | 0.51              |
| 2:P:30:ASP:OD1   | 2:P:32:ASP:CA    | 2.57                     | 0.51              |
| 1:U:783:ARG:HG2  | 1:U:784:ASP:N    | 2.26                     | 0.51              |
| 1:A:774:LEU:HG   | 1:Q:774:LEU:HD21 | 1.92                     | 0.51              |
| 1:G:717:LEU:HD22 | 1:G:763:GLY:HA3  | 1.93                     | 0.51              |
| 1:G:811:PRO:HB2  | 2:N:20:GLU:HG2   | 1.93                     | 0.51              |
| 2:R:31:LEU:HD21  | 2:R:71:TYR:CD2   | 2.46                     | 0.51              |
| 2:R:50:GLY:HA3   | 2:R:71:TYR:O     | 2.11                     | 0.51              |
| 1:C:781:LYS:HD2  | 2:D:34:LEU:CD1   | 2.39                     | 0.51              |
| 2:D:5:PRO:HG2    | 2:D:9:TYR:CE2    | 2.46                     | 0.51              |
| 1:O:781:LYS:H    | 1:O:781:LYS:CD   | 2.23                     | 0.51              |
| 2:T:53:ARG:NH1   | 2:T:53:ARG:CG    | 2.46                     | 0.51              |
| 1:U:762:LYS:HE2  | 1:U:786:LYS:HB3  | 1.93                     | 0.51              |
| 1:A:704:HIS:NE2  | 1:A:706:GLU:OE1  | 2.44                     | 0.51              |
| 2:H:20:GLU:CA    | 2:H:61:ARG:HH11  | 2.11                     | 0.51              |
| 1:E:740:GLU:CD   | 2:F:21:THR:HG21  | 2.36                     | 0.51              |
| 2:J:38:MET:HE1   | 2:J:48:PRO:HB3   | 1.91                     | 0.51              |
| 1:M:778:PHE:HB2  | 2:N:34:LEU:CD2   | 2.41                     | 0.51              |
| 2:B:74:GLU:CD    | 2:B:83:ARG:HH11  | 2.19                     | 0.51              |
| 1:Q:715:THR:HG22 | 1:Q:716:LYS:N    | 2.26                     | 0.51              |
| 1:S:807:ARG:HH21 | 2:T:21:THR:HG22  | 1.68                     | 0.51              |
| 1:W:725:ASP:CG   | 2:X:93:GLY:HA3   | 2.36                     | 0.51              |
| 2:H:26:PHE:CE2   | 2:H:59:ARG:NH2   | 2.79                     | 0.51              |
| 1:S:739:GLU:OE2  | 2:T:61:ARG:NH2   | 2.42                     | 0.51              |
| 1:U:740:GLU:OE2  | 1:U:807:ARG:NH2  | 2.38                     | 0.51              |
| 1:A:799:ILE:HD13 | 1:G:705:ILE:CD1  | 2.41                     | 0.50              |
| 1:C:775:ARG:HE   | 1:C:780:GLU:CG   | 2.24                     | 0.50              |
| 1:O:767:PRO:HB3  | 1:O:781:LYS:CE   | 2.42                     | 0.50              |
| 2:F:23:LEU:HD12  | 2:P:59:ARG:HD3   | 1.90                     | 0.50              |
| 1:I:772:ARG:HB3  | 2:V:47:THR:HG21  | 1.93                     | 0.50              |
| 2:N:16:ILE:HB    | 2:N:60:LYS:HE3   | 1.93                     | 0.50              |
| 1:O:721:ARG:NH2  | 2:P:94:ASP:OD1   | 2.43                     | 0.50              |
| 1:Q:721:ARG:CZ   | 1:Q:721:ARG:HB2  | 2.41                     | 0.50              |
| 2:N:26:PHE:CE2   | 2:N:59:ARG:CZ    | 2.93                     | 0.50              |
| 1:E:816:LYS:HB3  | 1:E:817:PRO:CD   | 2.37                     | 0.50              |
| 2:J:80:LEU:HD12  | 2:V:80:LEU:HB2   | 1.93                     | 0.50              |
| 1:M:788:THR:OG1  | 1:M:788:THR:O    | 2.28                     | 0.50              |
| 1:S:703:ILE:HG22 | 1:S:703:ILE:O    | 2.11                     | 0.50              |
| 1:A:778:PHE:CZ   | 2:B:73:PHE:HE2   | 2.27                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:781:LYS:CB   | 2:F:34:LEU:HD12  | 2.28                     | 0.50              |
| 1:K:770:GLU:HB3  | 1:S:774:LEU:HD13 | 1.93                     | 0.50              |
| 1:M:725:ASP:CG   | 2:N:93:GLY:HA3   | 2.37                     | 0.50              |
| 2:N:8:PRO:CB     | 1:S:705:ILE:HD11 | 2.40                     | 0.50              |
| 2:N:11:ARG:CG    | 1:S:801:VAL:HG11 | 2.29                     | 0.50              |
| 2:B:71:TYR:HD1   | 2:B:83:ARG:C     | 2.19                     | 0.50              |
| 1:E:781:LYS:HG3  | 1:E:782:ALA:N    | 2.25                     | 0.50              |
| 1:K:707:ARG:HD2  | 1:K:826:TYR:CZ   | 2.46                     | 0.50              |
| 2:L:25:THR:HG23  | 2:V:56:GLU:CG    | 2.42                     | 0.50              |
| 1:Q:727:PRO:O    | 1:Q:728:HIS:HB2  | 2.10                     | 0.50              |
| 1:S:739:GLU:OE1  | 2:T:60:LYS:HB3   | 2.11                     | 0.50              |
| 1:S:793:PRO:HG2  | 1:S:796:GLU:OE1  | 2.12                     | 0.50              |
| 1:M:731:GLU:OE2  | 2:N:41:PRO:HB3   | 2.12                     | 0.49              |
| 1:Q:712:ALA:HB3  | 1:Q:821:GLU:HG3  | 1.95                     | 0.49              |
| 1:S:712:ALA:HB3  | 1:S:821:GLU:HG3  | 1.95                     | 0.49              |
| 1:S:740:GLU:HG2  | 1:S:742:VAL:HG23 | 1.93                     | 0.49              |
| 1:I:712:ALA:HB3  | 1:I:821:GLU:HG3  | 1.95                     | 0.49              |
| 1:A:781:LYS:HG2  | 1:A:782:ALA:N    | 2.28                     | 0.49              |
| 1:A:797:GLY:H    | 1:A:829:GLN:HE21 | 1.59                     | 0.49              |
| 2:D:25:THR:HG23  | 2:R:56:GLU:OE1   | 2.13                     | 0.49              |
| 2:R:70:ILE:HD12  | 2:R:86:ALA:HB3   | 1.93                     | 0.49              |
| 2:T:16:ILE:HB    | 2:T:60:LYS:HE3   | 1.95                     | 0.49              |
| 2:T:50:GLY:HA3   | 2:T:71:TYR:O     | 2.13                     | 0.49              |
| 1:U:712:ALA:HB3  | 1:U:821:GLU:HG3  | 1.95                     | 0.49              |
| 1:K:725:ASP:CG   | 2:L:93:GLY:HA3   | 2.38                     | 0.49              |
| 1:G:811:PRO:CB   | 2:N:20:GLU:CD    | 2.85                     | 0.49              |
| 1:M:797:GLY:O    | 1:M:829:GLN:NE2  | 2.46                     | 0.48              |
| 2:N:26:PHE:CD2   | 2:N:59:ARG:NH2   | 2.81                     | 0.48              |
| 1:K:712:ALA:HB3  | 1:K:821:GLU:HG3  | 1.95                     | 0.48              |
| 1:M:703:ILE:HG22 | 2:T:8:PRO:HG3    | 1.95                     | 0.48              |
| 2:T:59:ARG:O     | 2:T:59:ARG:HG3   | 2.12                     | 0.48              |
| 2:F:16:ILE:HB    | 2:F:60:LYS:HE3   | 1.94                     | 0.48              |
| 1:Q:762:LYS:O    | 1:Q:764:GLU:N    | 2.46                     | 0.48              |
| 1:K:740:GLU:OE2  | 1:K:807:ARG:NH2  | 2.38                     | 0.48              |
| 1:A:801:VAL:CG1  | 1:G:705:ILE:CD1  | 2.91                     | 0.48              |
| 2:F:38:MET:HG2   | 2:F:98:LEU:HB2   | 1.95                     | 0.48              |
| 2:L:71:TYR:HD1   | 2:L:83:ARG:C     | 2.21                     | 0.48              |
| 2:N:30:ASP:CG    | 2:N:32:ASP:H     | 2.13                     | 0.48              |
| 1:C:704:HIS:HB3  | 1:C:829:GLN:HB2  | 1.95                     | 0.48              |
| 1:C:758:ARG:HH21 | 1:C:788:THR:HB   | 1.79                     | 0.48              |
| 2:H:71:TYR:HB3   | 2:H:82:ALA:HB1   | 1.94                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:R:34:LEU:HD22 | 2:R:35:PRO:CD    | 2.34                     | 0.48              |
| 2:B:16:ILE:O    | 2:B:60:LYS:HE3   | 2.14                     | 0.48              |
| 1:E:806:LEU:HB3 | 1:E:813:VAL:HG13 | 1.96                     | 0.48              |
| 1:G:740:GLU:CG  | 2:H:21:THR:HG21  | 2.44                     | 0.48              |
| 1:A:799:ILE:CD1 | 1:A:801:VAL:HG12 | 2.42                     | 0.48              |
| 1:C:712:ALA:HB3 | 1:C:821:GLU:HG3  | 1.95                     | 0.48              |
| 2:T:31:LEU:HD21 | 2:T:71:TYR:CD2   | 2.49                     | 0.48              |
| 1:M:774:LEU:HA  | 1:M:777:ILE:HD12 | 1.95                     | 0.48              |
| 2:P:16:ILE:HB   | 2:P:60:LYS:HE3   | 1.96                     | 0.48              |
| 2:J:60:LYS:HB2  | 2:J:63:VAL:HG23  | 1.96                     | 0.47              |
| 2:V:60:LYS:HG2  | 2:V:61:ARG:NH2   | 2.29                     | 0.47              |
| 2:H:60:LYS:HB2  | 2:H:63:VAL:HG23  | 1.96                     | 0.47              |
| 1:E:768:THR:HA  | 1:E:769:PRO:HD3  | 1.65                     | 0.47              |
| 1:E:725:ASP:HB2 | 2:F:93:GLY:HA3   | 1.96                     | 0.47              |
| 2:L:25:THR:HG23 | 2:V:56:GLU:CD    | 2.38                     | 0.47              |
| 1:M:775:ARG:HD2 | 1:M:781:LYS:HE3  | 1.96                     | 0.47              |
| 1:M:798:GLY:HA3 | 1:M:828:ALA:O    | 2.14                     | 0.47              |
| 2:B:25:THR:HG23 | 2:N:56:GLU:HG2   | 1.96                     | 0.47              |
| 2:B:32:ASP:OD2  | 2:N:53:ARG:NH2   | 2.47                     | 0.47              |
| 1:E:725:ASP:OD1 | 2:F:99:HIS:NE2   | 2.33                     | 0.47              |
| 2:F:80:LEU:HD12 | 2:N:80:LEU:HB2   | 1.96                     | 0.47              |
| 2:H:20:GLU:CB   | 2:H:61:ARG:HH12  | 2.28                     | 0.47              |
| 2:L:47:THR:CG2  | 1:S:772:ARG:HH11 | 2.28                     | 0.47              |
| 2:D:13:PHE:CZ   | 2:D:60:LYS:HG3   | 2.50                     | 0.47              |
| 1:E:712:ALA:HB3 | 1:E:821:GLU:HG3  | 1.95                     | 0.47              |
| 1:G:802:ARG:HG3 | 1:G:803:THR:N    | 2.28                     | 0.47              |
| 2:H:77:GLY:HA2  | 2:J:77:GLY:HA3   | 1.97                     | 0.47              |
| 2:X:86:ALA:HB1  | 2:X:105:VAL:O    | 2.14                     | 0.47              |
| 2:B:18:ASP:OD1  | 2:B:60:LYS:HD3   | 2.14                     | 0.47              |
| 1:G:747:ALA:C   | 1:G:748:GLU:OE1  | 2.57                     | 0.47              |
| 2:R:38:MET:HG2  | 2:R:98:LEU:HB2   | 1.95                     | 0.47              |
| 1:E:774:LEU:HA  | 1:E:777:ILE:HG23 | 1.95                     | 0.47              |
| 1:M:713:ARG:HG2 | 1:M:720:GLU:OE1  | 2.15                     | 0.47              |
| 2:N:26:PHE:CE2  | 2:N:59:ARG:NH2   | 2.83                     | 0.47              |
| 1:U:713:ARG:HG2 | 1:U:720:GLU:OE1  | 2.15                     | 0.47              |
| 1:C:713:ARG:HG2 | 1:C:720:GLU:OE1  | 2.15                     | 0.47              |
| 1:C:781:LYS:CA  | 2:D:34:LEU:HD12  | 2.44                     | 0.47              |
| 2:F:37:ARG:NH1  | 1:M:769:PRO:HG2  | 2.28                     | 0.47              |
| 1:S:771:GLU:OE2 | 1:S:781:LYS:HD3  | 2.15                     | 0.46              |
| 1:O:820:ARG:O   | 1:O:821:GLU:HG3  | 2.14                     | 0.46              |
| 1:A:725:ASP:CG  | 2:B:93:GLY:HA3   | 2.40                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:740:GLU:OE2  | 1:C:807:ARG:NH2  | 2.38                     | 0.46              |
| 1:I:713:ARG:HG2  | 1:I:720:GLU:OE1  | 2.15                     | 0.46              |
| 2:H:83:ARG:HG2   | 2:H:84:PRO:HD2   | 1.97                     | 0.46              |
| 1:K:713:ARG:HG2  | 1:K:720:GLU:OE1  | 2.15                     | 0.46              |
| 1:M:740:GLU:HG2  | 1:M:742:VAL:HG23 | 1.96                     | 0.46              |
| 1:A:807:ARG:HH22 | 2:B:21:THR:HG22  | 1.79                     | 0.46              |
| 2:D:16:ILE:HB    | 2:D:60:LYS:HE3   | 1.96                     | 0.46              |
| 1:A:713:ARG:HG2  | 1:A:720:GLU:OE1  | 2.15                     | 0.46              |
| 1:O:713:ARG:HG2  | 1:O:720:GLU:OE1  | 2.15                     | 0.46              |
| 1:Q:758:ARG:HH21 | 1:Q:788:THR:HB   | 1.81                     | 0.46              |
| 2:X:105:VAL:HG12 | 2:X:106:VAL:N    | 2.31                     | 0.46              |
| 1:W:707:ARG:HG2  | 1:W:707:ARG:O    | 2.10                     | 0.46              |
| 2:B:21:THR:N     | 2:B:61:ARG:NH1   | 2.63                     | 0.46              |
| 1:K:777:ILE:HG22 | 1:K:778:PHE:CE2  | 2.50                     | 0.46              |
| 1:W:713:ARG:HG2  | 1:W:720:GLU:OE1  | 2.15                     | 0.46              |
| 1:G:772:ARG:HB2  | 2:X:47:THR:HG21  | 1.97                     | 0.46              |
| 2:R:16:ILE:HB    | 2:R:60:LYS:HE3   | 1.98                     | 0.46              |
| 2:V:72:ARG:HG2   | 2:V:73:PHE:N     | 2.31                     | 0.46              |
| 1:W:778:PHE:CZ   | 2:X:73:PHE:HE2   | 2.34                     | 0.46              |
| 1:S:713:ARG:HG2  | 1:S:720:GLU:OE1  | 2.15                     | 0.45              |
| 1:E:713:ARG:HG2  | 1:E:720:GLU:OE1  | 2.15                     | 0.45              |
| 2:F:60:LYS:HB2   | 2:F:63:VAL:HG23  | 1.97                     | 0.45              |
| 1:O:807:ARG:HA   | 1:O:821:GLU:HG2  | 1.97                     | 0.45              |
| 1:S:740:GLU:O    | 1:S:740:GLU:CG   | 2.63                     | 0.45              |
| 1:W:767:PRO:HG2  | 1:W:772:ARG:HE   | 1.82                     | 0.45              |
| 1:C:713:ARG:HH21 | 1:C:758:ARG:HH12 | 1.65                     | 0.45              |
| 1:E:802:ARG:HG3  | 1:E:803:THR:N    | 2.32                     | 0.45              |
| 2:F:25:THR:HG23  | 2:P:56:GLU:CG    | 2.46                     | 0.45              |
| 2:R:77:GLY:C     | 2:R:79:GLY:H     | 2.23                     | 0.45              |
| 2:B:85:TYR:CE1   | 2:B:106:VAL:CG1  | 2.99                     | 0.45              |
| 2:F:25:THR:HG23  | 2:P:56:GLU:OE1   | 2.17                     | 0.45              |
| 1:I:713:ARG:HH21 | 1:I:758:ARG:HH12 | 1.65                     | 0.45              |
| 1:O:713:ARG:HH21 | 1:O:758:ARG:HH12 | 1.65                     | 0.45              |
| 2:P:53:ARG:HH11  | 2:P:53:ARG:CG    | 2.26                     | 0.45              |
| 2:X:21:THR:N     | 2:X:61:ARG:HH12  | 2.14                     | 0.45              |
| 1:A:773:LEU:O    | 1:A:777:ILE:HD12 | 2.17                     | 0.45              |
| 1:G:797:GLY:O    | 1:G:829:GLN:HG2  | 2.16                     | 0.45              |
| 1:O:768:THR:HG23 | 1:O:771:GLU:HB2  | 1.97                     | 0.45              |
| 1:A:799:ILE:C    | 1:A:827:VAL:HG13 | 2.42                     | 0.45              |
| 1:G:713:ARG:HG2  | 1:G:720:GLU:OE1  | 2.15                     | 0.45              |
| 1:A:807:ARG:NH1  | 2:B:21:THR:HG22  | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:814:GLU:O    | 1:E:815:LEU:HD23 | 2.16                     | 0.45              |
| 2:N:60:LYS:HB2   | 2:N:63:VAL:HG23  | 1.99                     | 0.45              |
| 1:S:713:ARG:HH21 | 1:S:758:ARG:HH12 | 1.65                     | 0.45              |
| 2:H:78:LEU:N     | 2:H:78:LEU:HD22  | 2.32                     | 0.45              |
| 2:L:16:ILE:HB    | 2:L:60:LYS:HE3   | 1.98                     | 0.45              |
| 1:U:713:ARG:HH21 | 1:U:758:ARG:HH12 | 1.65                     | 0.45              |
| 2:F:23:LEU:CD1   | 2:P:59:ARG:HD3   | 2.45                     | 0.45              |
| 1:Q:739:GLU:OE2  | 2:R:18:ASP:HA    | 2.17                     | 0.45              |
| 2:T:60:LYS:HB2   | 2:T:63:VAL:HG23  | 1.99                     | 0.45              |
| 1:O:778:PHE:CB   | 2:P:34:LEU:HD23  | 2.47                     | 0.44              |
| 2:R:72:ARG:CB    | 2:R:85:TYR:HB2   | 2.47                     | 0.44              |
| 1:S:740:GLU:OE1  | 2:T:21:THR:CG2   | 2.65                     | 0.44              |
| 1:E:775:ARG:HE   | 1:E:780:GLU:HB3  | 1.83                     | 0.44              |
| 1:C:703:ILE:HG23 | 1:C:705:ILE:HG13 | 1.99                     | 0.44              |
| 1:E:713:ARG:HH21 | 1:E:758:ARG:HH12 | 1.65                     | 0.44              |
| 1:E:738:ASP:OD2  | 1:E:805:ARG:NH2  | 2.41                     | 0.44              |
| 1:E:769:PRO:HB3  | 2:N:45:LEU:HD21  | 1.99                     | 0.44              |
| 2:N:5:PRO:HG2    | 2:N:8:PRO:HD3    | 1.99                     | 0.44              |
| 1:G:787:ASP:OD1  | 1:G:787:ASP:C    | 2.60                     | 0.44              |
| 1:U:713:ARG:HH21 | 1:U:758:ARG:NH1  | 2.16                     | 0.44              |
| 1:A:749:VAL:HB   | 1:A:792:VAL:HG21 | 1.98                     | 0.44              |
| 1:G:713:ARG:HH21 | 1:G:758:ARG:HH12 | 1.65                     | 0.44              |
| 2:L:85:TYR:O     | 2:L:107:LEU:HB2  | 2.17                     | 0.44              |
| 1:G:713:ARG:HH21 | 1:G:758:ARG:NH1  | 2.16                     | 0.44              |
| 2:H:59:ARG:O     | 2:H:59:ARG:HG3   | 2.17                     | 0.44              |
| 1:U:725:ASP:OD2  | 2:V:95:ASN:N     | 2.41                     | 0.44              |
| 1:E:740:GLU:CD   | 1:E:807:ARG:NH2  | 2.76                     | 0.44              |
| 1:M:740:GLU:O    | 1:M:740:GLU:CG   | 2.64                     | 0.44              |
| 1:O:713:ARG:HH21 | 1:O:758:ARG:NH1  | 2.16                     | 0.44              |
| 1:G:781:LYS:HA   | 2:H:34:LEU:HD12  | 2.00                     | 0.44              |
| 1:M:713:ARG:HH21 | 1:M:758:ARG:HH12 | 1.65                     | 0.44              |
| 1:Q:766:GLU:N    | 1:Q:766:GLU:OE1  | 2.50                     | 0.44              |
| 1:W:713:ARG:HH21 | 1:W:758:ARG:NH1  | 2.16                     | 0.44              |
| 1:A:775:ARG:O    | 1:A:775:ARG:HG3  | 2.17                     | 0.43              |
| 2:B:74:GLU:CD    | 2:B:83:ARG:HD2   | 2.43                     | 0.43              |
| 2:F:38:MET:HE2   | 2:F:48:PRO:HG3   | 2.00                     | 0.43              |
| 2:H:76:VAL:HG21  | 2:H:81:ALA:HB3   | 2.00                     | 0.43              |
| 1:K:713:ARG:HH21 | 1:K:758:ARG:NH1  | 2.16                     | 0.43              |
| 1:K:777:ILE:C    | 1:K:778:PHE:HD2  | 2.26                     | 0.43              |
| 2:N:11:ARG:HB3   | 1:S:801:VAL:HG11 | 0.49                     | 0.43              |
| 2:P:59:ARG:O     | 2:P:59:ARG:HG3   | 2.16                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:713:ARG:HH21 | 1:C:758:ARG:NH1  | 2.16                     | 0.43              |
| 2:N:31:LEU:CG    | 2:N:53:ARG:HD2   | 2.48                     | 0.43              |
| 1:Q:713:ARG:HH21 | 1:Q:758:ARG:NH1  | 2.16                     | 0.43              |
| 1:A:713:ARG:HH21 | 1:A:758:ARG:HH12 | 1.65                     | 0.43              |
| 1:A:807:ARG:CZ   | 2:B:21:THR:HG22  | 2.48                     | 0.43              |
| 1:M:781:LYS:HA   | 2:N:34:LEU:HD12  | 2.01                     | 0.43              |
| 1:G:769:PRO:HB2  | 2:X:37:ARG:NH1   | 2.33                     | 0.43              |
| 2:B:83:ARG:HG2   | 2:B:84:PRO:HD2   | 2.00                     | 0.43              |
| 1:M:703:ILE:HG21 | 2:T:8:PRO:HB3    | 1.97                     | 0.43              |
| 1:M:703:ILE:CG2  | 2:T:8:PRO:HB3    | 2.48                     | 0.43              |
| 2:N:5:PRO:C      | 2:N:8:PRO:HD2    | 2.42                     | 0.43              |
| 1:W:713:ARG:HH21 | 1:W:758:ARG:HH12 | 1.65                     | 0.43              |
| 1:G:769:PRO:HG2  | 1:G:770:GLU:OE1  | 2.18                     | 0.43              |
| 1:I:710:ILE:HB   | 1:I:790:LEU:HG   | 2.01                     | 0.43              |
| 1:S:793:PRO:CB   | 1:S:796:GLU:OE1  | 2.65                     | 0.43              |
| 1:U:720:GLU:HG2  | 1:U:760:SER:OG   | 2.18                     | 0.43              |
| 1:A:713:ARG:HH21 | 1:A:758:ARG:NH1  | 2.16                     | 0.43              |
| 1:C:710:ILE:HB   | 1:C:790:LEU:HG   | 2.01                     | 0.43              |
| 1:E:777:ILE:HG13 | 1:E:778:PHE:CD2  | 2.53                     | 0.43              |
| 1:A:764:GLU:CG   | 1:A:783:ARG:HH21 | 2.31                     | 0.43              |
| 1:I:740:GLU:CD   | 2:J:21:THR:HG21  | 2.44                     | 0.43              |
| 1:I:767:PRO:HB2  | 1:I:772:ARG:HG3  | 2.01                     | 0.43              |
| 1:K:713:ARG:HH21 | 1:K:758:ARG:HH12 | 1.65                     | 0.43              |
| 1:M:713:ARG:HH21 | 1:M:758:ARG:NH1  | 2.16                     | 0.43              |
| 2:N:5:PRO:O      | 2:N:8:PRO:CD     | 2.60                     | 0.43              |
| 1:Q:713:ARG:HH21 | 1:Q:758:ARG:HH12 | 1.65                     | 0.43              |
| 1:Q:808:ARG:HH11 | 1:Q:808:ARG:HG2  | 1.84                     | 0.43              |
| 1:S:713:ARG:HH21 | 1:S:758:ARG:NH1  | 2.16                     | 0.43              |
| 2:B:83:ARG:HG2   | 2:B:84:PRO:N     | 2.33                     | 0.43              |
| 1:G:721:ARG:HH22 | 2:H:94:ASP:CG    | 2.27                     | 0.43              |
| 1:G:769:PRO:HB3  | 2:X:45:LEU:CD2   | 2.42                     | 0.43              |
| 1:O:710:ILE:HB   | 1:O:790:LEU:HG   | 2.01                     | 0.43              |
| 2:P:60:LYS:HB2   | 2:P:63:VAL:HG23  | 2.00                     | 0.43              |
| 2:T:11:ARG:N     | 2:T:11:ARG:HD3   | 2.34                     | 0.43              |
| 1:U:808:ARG:HG2  | 1:U:808:ARG:HH11 | 1.84                     | 0.43              |
| 1:A:811:PRO:HB2  | 2:T:20:GLU:OE2   | 2.15                     | 0.43              |
| 1:C:808:ARG:HG2  | 1:C:808:ARG:HH11 | 1.84                     | 0.43              |
| 1:K:773:LEU:HD23 | 1:K:773:LEU:HA   | 1.68                     | 0.43              |
| 1:E:713:ARG:HH21 | 1:E:758:ARG:NH1  | 2.16                     | 0.42              |
| 1:E:777:ILE:HG13 | 1:E:778:PHE:N    | 2.32                     | 0.42              |
| 1:I:808:ARG:HG2  | 1:I:808:ARG:HH11 | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:781:LYS:HB3  | 2:L:34:LEU:CD1   | 2.49                     | 0.42              |
| 2:X:16:ILE:HB    | 2:X:60:LYS:HE3   | 2.00                     | 0.42              |
| 1:I:713:ARG:HH21 | 1:I:758:ARG:NH1  | 2.16                     | 0.42              |
| 1:K:808:ARG:HG2  | 1:K:808:ARG:HH11 | 1.84                     | 0.42              |
| 1:O:807:ARG:HG3  | 1:O:810:ASP:OD2  | 2.18                     | 0.42              |
| 1:O:808:ARG:HH11 | 1:O:808:ARG:HG2  | 1.84                     | 0.42              |
| 1:S:808:ARG:HG2  | 1:S:808:ARG:HH11 | 1.84                     | 0.42              |
| 1:E:710:ILE:HB   | 1:E:790:LEU:HG   | 2.01                     | 0.42              |
| 1:E:769:PRO:CB   | 2:N:37:ARG:NH1   | 2.63                     | 0.42              |
| 1:I:740:GLU:OE2  | 1:I:807:ARG:NH2  | 2.38                     | 0.42              |
| 1:K:720:GLU:HG2  | 1:K:760:SER:OG   | 2.19                     | 0.42              |
| 1:M:710:ILE:HB   | 1:M:790:LEU:HG   | 2.01                     | 0.42              |
| 2:R:38:MET:HE2   | 2:R:48:PRO:HG3   | 2.00                     | 0.42              |
| 2:T:83:ARG:HG3   | 2:T:84:PRO:HD2   | 2.01                     | 0.42              |
| 2:B:74:GLU:OE1   | 2:B:83:ARG:HD2   | 2.19                     | 0.42              |
| 1:C:792:VAL:HA   | 1:C:793:PRO:HD3  | 1.91                     | 0.42              |
| 1:Q:704:HIS:CD2  | 1:Q:704:HIS:C    | 2.97                     | 0.42              |
| 1:S:801:VAL:O    | 1:S:801:VAL:HG12 | 2.18                     | 0.42              |
| 1:G:710:ILE:HB   | 1:G:790:LEU:HG   | 2.01                     | 0.42              |
| 1:Q:710:ILE:HB   | 1:Q:790:LEU:HG   | 2.01                     | 0.42              |
| 1:S:793:PRO:CG   | 1:S:796:GLU:OE1  | 2.67                     | 0.42              |
| 1:K:778:PHE:HZ   | 2:L:73:PHE:CE2   | 2.37                     | 0.42              |
| 2:R:60:LYS:HB2   | 2:R:63:VAL:HG23  | 2.02                     | 0.42              |
| 2:B:32:ASP:OD1   | 2:B:33:THR:N     | 2.53                     | 0.42              |
| 1:E:806:LEU:HB3  | 1:E:813:VAL:CG1  | 2.50                     | 0.42              |
| 1:G:808:ARG:HG2  | 1:G:808:ARG:HH11 | 1.84                     | 0.42              |
| 1:Q:792:VAL:HA   | 1:Q:793:PRO:HD3  | 1.91                     | 0.42              |
| 1:A:710:ILE:HB   | 1:A:790:LEU:HG   | 2.01                     | 0.42              |
| 1:C:770:GLU:OE1  | 1:C:770:GLU:N    | 2.49                     | 0.42              |
| 1:E:720:GLU:HG2  | 1:E:760:SER:OG   | 2.20                     | 0.42              |
| 1:G:704:HIS:NE2  | 1:G:706:GLU:OE1  | 2.52                     | 0.42              |
| 1:I:740:GLU:CG   | 2:J:21:THR:HG21  | 2.49                     | 0.42              |
| 1:K:710:ILE:HB   | 1:K:790:LEU:HG   | 2.01                     | 0.42              |
| 2:B:31:LEU:CD1   | 2:R:78:LEU:HD23  | 2.50                     | 0.42              |
| 1:K:783:ARG:H    | 1:K:783:ARG:HG3  | 1.62                     | 0.42              |
| 1:W:710:ILE:HB   | 1:W:790:LEU:HG   | 2.01                     | 0.42              |
| 1:A:808:ARG:HG2  | 1:A:808:ARG:HH11 | 1.84                     | 0.41              |
| 1:C:768:THR:OG1  | 1:C:771:GLU:HG3  | 2.20                     | 0.41              |
| 2:F:59:ARG:O     | 2:F:59:ARG:HG3   | 2.16                     | 0.41              |
| 1:I:770:GLU:H    | 1:I:770:GLU:CD   | 2.27                     | 0.41              |
| 1:K:778:PHE:CZ   | 1:S:777:ILE:HD13 | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:781:LYS:HD3  | 1:M:781:LYS:N    | 2.25                     | 0.41              |
| 1:E:781:LYS:HZ2  | 1:E:782:ALA:HB3  | 1.84                     | 0.41              |
| 2:H:23:LEU:HD12  | 2:T:59:ARG:CG    | 2.49                     | 0.41              |
| 1:O:729:LEU:HD23 | 1:O:729:LEU:HA   | 1.88                     | 0.41              |
| 2:P:88:ALA:HA    | 2:P:102:HIS:CE1  | 2.56                     | 0.41              |
| 1:A:791:ARG:HH11 | 1:A:791:ARG:CG   | 1.95                     | 0.41              |
| 2:B:31:LEU:HD13  | 2:B:82:ALA:HB3   | 2.02                     | 0.41              |
| 2:F:88:ALA:HA    | 2:F:102:HIS:CE1  | 2.56                     | 0.41              |
| 2:J:59:ARG:HD2   | 2:X:23:LEU:HB3   | 2.02                     | 0.41              |
| 1:K:775:ARG:HA   | 1:K:779:GLY:O    | 2.20                     | 0.41              |
| 1:M:808:ARG:HG2  | 1:M:808:ARG:HH11 | 1.84                     | 0.41              |
| 1:W:828:ALA:C    | 1:W:829:GLN:HG2  | 2.45                     | 0.41              |
| 2:B:21:THR:H     | 2:B:61:ARG:NH1   | 2.06                     | 0.41              |
| 1:W:798:GLY:HA3  | 1:W:828:ALA:O    | 2.21                     | 0.41              |
| 1:A:807:ARG:NH2  | 2:B:21:THR:CG2   | 2.82                     | 0.41              |
| 2:D:80:LEU:HD12  | 2:P:80:LEU:HB2   | 2.03                     | 0.41              |
| 1:G:778:PHE:CZ   | 2:H:73:PHE:CE2   | 3.09                     | 0.41              |
| 2:N:59:ARG:HG3   | 2:N:59:ARG:O     | 2.15                     | 0.41              |
| 1:S:708:TYR:OH   | 1:S:796:GLU:CG   | 2.60                     | 0.41              |
| 1:U:721:ARG:NH2  | 2:V:94:ASP:OD1   | 2.52                     | 0.41              |
| 2:X:26:PHE:HE2   | 2:X:59:ARG:NH2   | 2.09                     | 0.41              |
| 2:D:71:TYR:HD1   | 2:D:83:ARG:C     | 2.29                     | 0.41              |
| 1:E:792:VAL:HA   | 1:E:793:PRO:HD3  | 1.91                     | 0.41              |
| 2:J:88:ALA:HA    | 2:J:102:HIS:CE1  | 2.56                     | 0.41              |
| 2:H:88:ALA:HA    | 2:H:102:HIS:CE1  | 2.56                     | 0.41              |
| 1:I:763:GLY:C    | 1:I:764:GLU:HG2  | 2.46                     | 0.41              |
| 1:K:769:PRO:HB2  | 2:T:37:ARG:HH12  | 1.84                     | 0.41              |
| 2:L:88:ALA:HA    | 2:L:102:HIS:CE1  | 2.55                     | 0.41              |
| 1:S:725:ASP:CG   | 2:T:93:GLY:HA3   | 2.46                     | 0.41              |
| 1:U:725:ASP:CG   | 2:V:93:GLY:HA3   | 2.46                     | 0.41              |
| 2:X:88:ALA:HA    | 2:X:102:HIS:CE1  | 2.56                     | 0.41              |
| 1:A:792:VAL:HA   | 1:A:793:PRO:HD3  | 1.91                     | 0.41              |
| 2:B:70:ILE:O     | 2:B:85:TYR:N     | 2.52                     | 0.41              |
| 2:D:88:ALA:HA    | 2:D:102:HIS:CE1  | 2.56                     | 0.41              |
| 2:X:72:ARG:HG2   | 2:X:73:PHE:O     | 2.21                     | 0.41              |
| 1:A:702:PRO:O    | 1:A:703:ILE:C    | 2.62                     | 0.41              |
| 1:A:774:LEU:O    | 1:A:776:SER:N    | 2.53                     | 0.41              |
| 2:B:88:ALA:HA    | 2:B:102:HIS:CE1  | 2.56                     | 0.41              |
| 1:E:769:PRO:CB   | 2:N:45:LEU:HD21  | 2.51                     | 0.41              |
| 1:E:780:GLU:H    | 1:E:780:GLU:HG3  | 1.56                     | 0.41              |
| 2:J:37:ARG:NH1   | 1:U:769:PRO:HG2  | 2.36                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:83:ARG:HA    | 2:L:83:ARG:HD2   | 1.89                     | 0.41              |
| 1:M:703:ILE:HG22 | 2:T:8:PRO:CG     | 2.51                     | 0.41              |
| 1:M:821:GLU:CG   | 1:M:822:VAL:N    | 2.83                     | 0.41              |
| 2:N:107:LEU:HD23 | 2:N:107:LEU:HA   | 1.87                     | 0.41              |
| 1:O:792:VAL:HA   | 1:O:793:PRO:HD3  | 1.91                     | 0.41              |
| 1:Q:715:THR:HG22 | 1:Q:716:LYS:H    | 1.86                     | 0.41              |
| 1:S:710:ILE:HB   | 1:S:790:LEU:HG   | 2.01                     | 0.41              |
| 2:V:88:ALA:HA    | 2:V:102:HIS:CE1  | 2.56                     | 0.41              |
| 1:W:781:LYS:HA   | 2:X:34:LEU:CD1   | 2.51                     | 0.41              |
| 2:H:21:THR:N     | 2:H:61:ARG:NH1   | 2.62                     | 0.41              |
| 2:N:5:PRO:HG2    | 2:N:8:PRO:CD     | 2.51                     | 0.41              |
| 2:R:88:ALA:HA    | 2:R:102:HIS:CE1  | 2.56                     | 0.41              |
| 2:T:88:ALA:HA    | 2:T:102:HIS:CE1  | 2.56                     | 0.41              |
| 1:A:762:LYS:HD3  | 1:A:784:ASP:HB3  | 2.03                     | 0.40              |
| 2:F:80:LEU:CD1   | 2:N:80:LEU:HB2   | 2.51                     | 0.40              |
| 1:M:722:ILE:HB   | 1:M:821:GLU:OE2  | 2.22                     | 0.40              |
| 1:M:773:LEU:HD23 | 1:M:773:LEU:HA   | 1.81                     | 0.40              |
| 1:O:740:GLU:CD   | 2:P:21:THR:HG21  | 2.46                     | 0.40              |
| 1:C:766:GLU:O    | 1:C:766:GLU:HG2  | 2.21                     | 0.40              |
| 2:H:37:ARG:HH12  | 1:W:769:PRO:HG2  | 1.85                     | 0.40              |
| 2:H:78:LEU:HD22  | 2:H:78:LEU:H     | 1.87                     | 0.40              |
| 1:K:766:GLU:HA   | 1:K:767:PRO:HD3  | 1.87                     | 0.40              |
| 2:N:88:ALA:HA    | 2:N:102:HIS:CE1  | 2.56                     | 0.40              |
| 1:A:778:PHE:O    | 2:B:32:ASP:O     | 2.40                     | 0.40              |
| 1:G:768:THR:HB   | 1:G:769:PRO:HD2  | 2.03                     | 0.40              |
| 2:N:8:PRO:HA     | 1:S:705:ILE:HD11 | 2.04                     | 0.40              |
| 2:R:59:ARG:O     | 2:R:59:ARG:HG3   | 2.16                     | 0.40              |
| 1:G:739:GLU:OE1  | 2:H:61:ARG:HB2   | 2.22                     | 0.40              |
| 1:I:780:GLU:H    | 1:I:780:GLU:HG3  | 1.56                     | 0.40              |
| 2:L:59:ARG:O     | 2:L:59:ARG:HG3   | 2.16                     | 0.40              |
| 2:X:46:TYR:CZ    | 2:X:104:PRO:HG2  | 2.57                     | 0.40              |

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:Q:751:PRO:CD  | 2:R:11:ARG:NH2[7_555]  | 1.80                     | 0.40              |
| 1:I:744:ARG:NH1 | 1:O:744:ARG:CZ[3_555]  | 1.83                     | 0.37              |
| 1:I:744:ARG:NH2 | 1:O:744:ARG:NH2[3_555] | 1.96                     | 0.24              |
| 1:E:794:PRO:CB  | 1:Q:720:GLU:OE2[5_455] | 2.00                     | 0.20              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:I:744:ARG:NH1 | 1:O:744:ARG:NE[3_555]  | 2.00                     | 0.20              |
| 1:I:744:ARG:CZ  | 1:O:744:ARG:NH2[3_555] | 2.02                     | 0.18              |
| 2:J:8:PRO:CB    | 1:O:703:ILE:CG2[3_555] | 2.09                     | 0.11              |
| 1:I:744:ARG:CZ  | 1:O:744:ARG:CZ[3_555]  | 2.11                     | 0.09              |
| 1:E:811:PRO:CB  | 2:J:20:GLU:OE2[4_454]  | 2.19                     | 0.01              |

## 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     | 127/130 (98%) | 123 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 1   | C     | 127/130 (98%) | 124 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | E     | 125/130 (96%) | 119 (95%)  | 5 (4%)  | 1 (1%)   | 16          | 45  |
| 1   | G     | 127/130 (98%) | 120 (94%)  | 7 (6%)  | 0        | 100         | 100 |
| 1   | I     | 127/130 (98%) | 124 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | K     | 126/130 (97%) | 123 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | M     | 126/130 (97%) | 123 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | O     | 127/130 (98%) | 120 (94%)  | 6 (5%)  | 1 (1%)   | 16          | 45  |
| 1   | Q     | 125/130 (96%) | 120 (96%)  | 4 (3%)  | 1 (1%)   | 16          | 45  |
| 1   | S     | 127/130 (98%) | 123 (97%)  | 3 (2%)  | 1 (1%)   | 16          | 45  |
| 1   | U     | 119/130 (92%) | 111 (93%)  | 8 (7%)  | 0        | 100         | 100 |
| 1   | W     | 127/130 (98%) | 124 (98%)  | 2 (2%)  | 1 (1%)   | 16          | 45  |
| 2   | B     | 100/129 (78%) | 99 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | D     | 101/129 (78%) | 100 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 2   | F     | 101/129 (78%) | 100 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 2   | H     | 100/129 (78%) | 99 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | J     | 100/129 (78%) | 100 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 2   | L     | 100/129 (78%)   | 98 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 2   | N     | 101/129 (78%)   | 98 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 2   | P     | 100/129 (78%)   | 98 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 2   | R     | 100/129 (78%)   | 96 (96%)   | 3 (3%)  | 1 (1%)   | 12          | 40  |
| 2   | T     | 100/129 (78%)   | 98 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 2   | V     | 100/129 (78%)   | 98 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 2   | X     | 100/129 (78%)   | 98 (98%)   | 1 (1%)  | 1 (1%)   | 12          | 40  |
| All | All   | 2713/3108 (87%) | 2636 (97%) | 70 (3%) | 7 (0%)   | 36          | 65  |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 782 | ALA  |
| 1   | Q     | 763 | GLY  |
| 1   | S     | 764 | GLU  |
| 2   | R     | 78  | LEU  |
| 2   | X     | 84  | PRO  |
| 1   | O     | 763 | GLY  |
| 1   | W     | 777 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 109/110 (99%)  | 93 (85%)  | 16 (15%) | 3           | 14 |
| 1   | C     | 109/110 (99%)  | 102 (94%) | 7 (6%)   | 16          | 44 |
| 1   | E     | 108/110 (98%)  | 94 (87%)  | 14 (13%) | 4           | 17 |
| 1   | G     | 110/110 (100%) | 99 (90%)  | 11 (10%) | 7           | 27 |
| 1   | I     | 110/110 (100%) | 102 (93%) | 8 (7%)   | 13          | 39 |
| 1   | K     | 109/110 (99%)  | 98 (90%)  | 11 (10%) | 7           | 26 |
| 1   | M     | 109/110 (99%)  | 96 (88%)  | 13 (12%) | 5           | 20 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | O     | 110/110 (100%)  | 99 (90%)   | 11 (10%)  | 7           | 27 |
| 1   | Q     | 108/110 (98%)   | 97 (90%)   | 11 (10%)  | 7           | 26 |
| 1   | S     | 110/110 (100%)  | 97 (88%)   | 13 (12%)  | 5           | 20 |
| 1   | U     | 103/110 (94%)   | 95 (92%)   | 8 (8%)    | 11          | 36 |
| 1   | W     | 110/110 (100%)  | 99 (90%)   | 11 (10%)  | 7           | 27 |
| 2   | B     | 86/111 (78%)    | 78 (91%)   | 8 (9%)    | 8           | 30 |
| 2   | D     | 87/111 (78%)    | 79 (91%)   | 8 (9%)    | 8           | 30 |
| 2   | F     | 87/111 (78%)    | 79 (91%)   | 8 (9%)    | 8           | 30 |
| 2   | H     | 86/111 (78%)    | 80 (93%)   | 6 (7%)    | 14          | 41 |
| 2   | J     | 86/111 (78%)    | 75 (87%)   | 11 (13%)  | 4           | 18 |
| 2   | L     | 86/111 (78%)    | 78 (91%)   | 8 (9%)    | 8           | 30 |
| 2   | N     | 87/111 (78%)    | 78 (90%)   | 9 (10%)   | 7           | 25 |
| 2   | P     | 86/111 (78%)    | 76 (88%)   | 10 (12%)  | 5           | 21 |
| 2   | R     | 86/111 (78%)    | 76 (88%)   | 10 (12%)  | 5           | 21 |
| 2   | T     | 86/111 (78%)    | 78 (91%)   | 8 (9%)    | 8           | 30 |
| 2   | V     | 86/111 (78%)    | 78 (91%)   | 8 (9%)    | 8           | 30 |
| 2   | X     | 86/111 (78%)    | 77 (90%)   | 9 (10%)   | 6           | 25 |
| All | All   | 2340/2652 (88%) | 2103 (90%) | 237 (10%) | 7           | 26 |

All (237) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 713 | ARG  |
| 1   | A     | 737 | LEU  |
| 1   | A     | 740 | GLU  |
| 1   | A     | 748 | GLU  |
| 1   | A     | 750 | LYS  |
| 1   | A     | 762 | LYS  |
| 1   | A     | 764 | GLU  |
| 1   | A     | 766 | GLU  |
| 1   | A     | 768 | THR  |
| 1   | A     | 775 | ARG  |
| 1   | A     | 776 | SER  |
| 1   | A     | 780 | GLU  |
| 1   | A     | 781 | LYS  |
| 1   | A     | 790 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 791 | ARG  |
| 1   | A     | 802 | ARG  |
| 2   | B     | 6   | VAL  |
| 2   | B     | 21  | THR  |
| 2   | B     | 59  | ARG  |
| 2   | B     | 75  | HIS  |
| 2   | B     | 76  | VAL  |
| 2   | B     | 78  | LEU  |
| 2   | B     | 80  | LEU  |
| 2   | B     | 83  | ARG  |
| 1   | C     | 713 | ARG  |
| 1   | C     | 737 | LEU  |
| 1   | C     | 766 | GLU  |
| 1   | C     | 780 | GLU  |
| 1   | C     | 783 | ARG  |
| 1   | C     | 790 | LEU  |
| 1   | C     | 807 | ARG  |
| 2   | D     | 6   | VAL  |
| 2   | D     | 21  | THR  |
| 2   | D     | 59  | ARG  |
| 2   | D     | 61  | ARG  |
| 2   | D     | 72  | ARG  |
| 2   | D     | 76  | VAL  |
| 2   | D     | 78  | LEU  |
| 2   | D     | 80  | LEU  |
| 1   | E     | 703 | ILE  |
| 1   | E     | 713 | ARG  |
| 1   | E     | 737 | LEU  |
| 1   | E     | 748 | GLU  |
| 1   | E     | 762 | LYS  |
| 1   | E     | 770 | GLU  |
| 1   | E     | 776 | SER  |
| 1   | E     | 777 | ILE  |
| 1   | E     | 780 | GLU  |
| 1   | E     | 781 | LYS  |
| 1   | E     | 783 | ARG  |
| 1   | E     | 790 | LEU  |
| 1   | E     | 802 | ARG  |
| 1   | E     | 807 | ARG  |
| 2   | F     | 6   | VAL  |
| 2   | F     | 21  | THR  |
| 2   | F     | 59  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 72  | ARG  |
| 2   | F     | 74  | GLU  |
| 2   | F     | 78  | LEU  |
| 2   | F     | 80  | LEU  |
| 2   | F     | 83  | ARG  |
| 1   | G     | 703 | ILE  |
| 1   | G     | 713 | ARG  |
| 1   | G     | 724 | ARG  |
| 1   | G     | 737 | LEU  |
| 1   | G     | 748 | GLU  |
| 1   | G     | 766 | GLU  |
| 1   | G     | 768 | THR  |
| 1   | G     | 776 | SER  |
| 1   | G     | 790 | LEU  |
| 1   | G     | 829 | GLN  |
| 1   | G     | 830 | LYS  |
| 2   | H     | 6   | VAL  |
| 2   | H     | 21  | THR  |
| 2   | H     | 32  | ASP  |
| 2   | H     | 59  | ARG  |
| 2   | H     | 78  | LEU  |
| 2   | H     | 80  | LEU  |
| 1   | I     | 703 | ILE  |
| 1   | I     | 707 | ARG  |
| 1   | I     | 713 | ARG  |
| 1   | I     | 737 | LEU  |
| 1   | I     | 783 | ARG  |
| 1   | I     | 790 | LEU  |
| 1   | I     | 807 | ARG  |
| 1   | I     | 829 | GLN  |
| 2   | J     | 6   | VAL  |
| 2   | J     | 11  | ARG  |
| 2   | J     | 21  | THR  |
| 2   | J     | 32  | ASP  |
| 2   | J     | 59  | ARG  |
| 2   | J     | 60  | LYS  |
| 2   | J     | 61  | ARG  |
| 2   | J     | 74  | GLU  |
| 2   | J     | 76  | VAL  |
| 2   | J     | 78  | LEU  |
| 2   | J     | 80  | LEU  |
| 1   | K     | 713 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 737 | LEU  |
| 1   | K     | 764 | GLU  |
| 1   | K     | 766 | GLU  |
| 1   | K     | 768 | THR  |
| 1   | K     | 770 | GLU  |
| 1   | K     | 781 | LYS  |
| 1   | K     | 783 | ARG  |
| 1   | K     | 790 | LEU  |
| 1   | K     | 802 | ARG  |
| 1   | K     | 807 | ARG  |
| 2   | L     | 6   | VAL  |
| 2   | L     | 21  | THR  |
| 2   | L     | 32  | ASP  |
| 2   | L     | 59  | ARG  |
| 2   | L     | 60  | LYS  |
| 2   | L     | 76  | VAL  |
| 2   | L     | 78  | LEU  |
| 2   | L     | 80  | LEU  |
| 1   | M     | 713 | ARG  |
| 1   | M     | 737 | LEU  |
| 1   | M     | 764 | GLU  |
| 1   | M     | 765 | SER  |
| 1   | M     | 766 | GLU  |
| 1   | M     | 771 | GLU  |
| 1   | M     | 772 | ARG  |
| 1   | M     | 781 | LYS  |
| 1   | M     | 783 | ARG  |
| 1   | M     | 788 | THR  |
| 1   | M     | 790 | LEU  |
| 1   | M     | 829 | GLN  |
| 1   | M     | 830 | LYS  |
| 2   | N     | 6   | VAL  |
| 2   | N     | 21  | THR  |
| 2   | N     | 30  | ASP  |
| 2   | N     | 32  | ASP  |
| 2   | N     | 53  | ARG  |
| 2   | N     | 59  | ARG  |
| 2   | N     | 74  | GLU  |
| 2   | N     | 76  | VAL  |
| 2   | N     | 78  | LEU  |
| 1   | O     | 713 | ARG  |
| 1   | O     | 737 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 760 | SER  |
| 1   | O     | 766 | GLU  |
| 1   | O     | 768 | THR  |
| 1   | O     | 771 | GLU  |
| 1   | O     | 777 | ILE  |
| 1   | O     | 781 | LYS  |
| 1   | O     | 790 | LEU  |
| 1   | O     | 807 | ARG  |
| 1   | O     | 830 | LYS  |
| 2   | P     | 6   | VAL  |
| 2   | P     | 21  | THR  |
| 2   | P     | 30  | ASP  |
| 2   | P     | 32  | ASP  |
| 2   | P     | 53  | ARG  |
| 2   | P     | 59  | ARG  |
| 2   | P     | 74  | GLU  |
| 2   | P     | 78  | LEU  |
| 2   | P     | 80  | LEU  |
| 2   | P     | 83  | ARG  |
| 1   | Q     | 713 | ARG  |
| 1   | Q     | 717 | LEU  |
| 1   | Q     | 721 | ARG  |
| 1   | Q     | 737 | LEU  |
| 1   | Q     | 764 | GLU  |
| 1   | Q     | 766 | GLU  |
| 1   | Q     | 768 | THR  |
| 1   | Q     | 771 | GLU  |
| 1   | Q     | 777 | ILE  |
| 1   | Q     | 783 | ARG  |
| 1   | Q     | 790 | LEU  |
| 2   | R     | 6   | VAL  |
| 2   | R     | 21  | THR  |
| 2   | R     | 30  | ASP  |
| 2   | R     | 32  | ASP  |
| 2   | R     | 34  | LEU  |
| 2   | R     | 59  | ARG  |
| 2   | R     | 60  | LYS  |
| 2   | R     | 72  | ARG  |
| 2   | R     | 74  | GLU  |
| 2   | R     | 78  | LEU  |
| 1   | S     | 703 | ILE  |
| 1   | S     | 713 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 737 | LEU  |
| 1   | S     | 740 | GLU  |
| 1   | S     | 768 | THR  |
| 1   | S     | 771 | GLU  |
| 1   | S     | 776 | SER  |
| 1   | S     | 781 | LYS  |
| 1   | S     | 790 | LEU  |
| 1   | S     | 796 | GLU  |
| 1   | S     | 824 | ARG  |
| 1   | S     | 829 | GLN  |
| 1   | S     | 830 | LYS  |
| 2   | T     | 6   | VAL  |
| 2   | T     | 11  | ARG  |
| 2   | T     | 21  | THR  |
| 2   | T     | 32  | ASP  |
| 2   | T     | 53  | ARG  |
| 2   | T     | 59  | ARG  |
| 2   | T     | 78  | LEU  |
| 2   | T     | 80  | LEU  |
| 1   | U     | 713 | ARG  |
| 1   | U     | 737 | LEU  |
| 1   | U     | 765 | SER  |
| 1   | U     | 766 | GLU  |
| 1   | U     | 768 | THR  |
| 1   | U     | 788 | THR  |
| 1   | U     | 790 | LEU  |
| 1   | U     | 807 | ARG  |
| 2   | V     | 6   | VAL  |
| 2   | V     | 21  | THR  |
| 2   | V     | 32  | ASP  |
| 2   | V     | 59  | ARG  |
| 2   | V     | 60  | LYS  |
| 2   | V     | 74  | GLU  |
| 2   | V     | 78  | LEU  |
| 2   | V     | 83  | ARG  |
| 1   | W     | 703 | ILE  |
| 1   | W     | 707 | ARG  |
| 1   | W     | 713 | ARG  |
| 1   | W     | 737 | LEU  |
| 1   | W     | 765 | SER  |
| 1   | W     | 766 | GLU  |
| 1   | W     | 781 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | W     | 790 | LEU  |
| 1   | W     | 807 | ARG  |
| 1   | W     | 808 | ARG  |
| 1   | W     | 829 | GLN  |
| 2   | X     | 6   | VAL  |
| 2   | X     | 21  | THR  |
| 2   | X     | 32  | ASP  |
| 2   | X     | 59  | ARG  |
| 2   | X     | 60  | LYS  |
| 2   | X     | 61  | ARG  |
| 2   | X     | 74  | GLU  |
| 2   | X     | 76  | VAL  |
| 2   | X     | 78  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 829 | GLN  |
| 1   | E     | 704 | HIS  |
| 1   | M     | 829 | GLN  |
| 1   | S     | 829 | GLN  |
| 2   | V     | 75  | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|----------------|-----------------------|-------|
| 1   | A     | 129/130 (99%) | 0.53   | 8 (6%) 26 18   | 34, 63, 131, 166      | 0     |
| 1   | C     | 129/130 (99%) | 0.43   | 7 (5%) 31 21   | 45, 81, 147, 170      | 0     |
| 1   | E     | 127/130 (97%) | 0.51   | 13 (10%) 12 10 | 52, 81, 143, 162      | 0     |
| 1   | G     | 129/130 (99%) | 0.49   | 9 (6%) 22 15   | 30, 70, 143, 176      | 0     |
| 1   | I     | 129/130 (99%) | 0.84   | 17 (13%) 7 6   | 58, 101, 156, 182     | 0     |
| 1   | K     | 128/130 (98%) | 0.70   | 8 (6%) 26 17   | 60, 97, 145, 163      | 0     |
| 1   | M     | 128/130 (98%) | 0.27   | 5 (3%) 43 29   | 34, 67, 116, 142      | 0     |
| 1   | O     | 129/130 (99%) | 0.44   | 4 (3%) 51 35   | 51, 90, 134, 156      | 0     |
| 1   | Q     | 127/130 (97%) | 0.85   | 12 (9%) 14 11  | 61, 104, 155, 170     | 0     |
| 1   | S     | 129/130 (99%) | 0.55   | 12 (9%) 14 11  | 22, 62, 128, 183      | 0     |
| 1   | U     | 121/130 (93%) | 1.32   | 22 (18%) 3 3   | 84, 163, 197, 208     | 0     |
| 1   | W     | 129/130 (99%) | 0.38   | 9 (6%) 22 15   | 41, 71, 121, 144      | 0     |
| 2   | B     | 102/129 (79%) | -0.01  | 7 (6%) 23 16   | 26, 47, 81, 113       | 0     |
| 2   | D     | 103/129 (79%) | 0.05   | 5 (4%) 35 23   | 36, 58, 93, 138       | 0     |
| 2   | F     | 103/129 (79%) | -0.10  | 2 (1%) 66 48   | 33, 56, 83, 123       | 0     |
| 2   | H     | 102/129 (79%) | 0.11   | 4 (3%) 43 29   | 35, 61, 93, 116       | 0     |
| 2   | J     | 102/129 (79%) | 0.11   | 3 (2%) 53 35   | 47, 74, 98, 122       | 0     |
| 2   | L     | 102/129 (79%) | 0.26   | 1 (0%) 79 63   | 51, 78, 106, 128      | 0     |
| 2   | N     | 103/129 (79%) | 0.01   | 2 (1%) 66 48   | 27, 44, 80, 117       | 0     |
| 2   | P     | 102/129 (79%) | 0.08   | 4 (3%) 43 29   | 38, 58, 82, 105       | 0     |
| 2   | R     | 102/129 (79%) | 0.03   | 3 (2%) 53 35   | 35, 58, 86, 115       | 0     |
| 2   | T     | 102/129 (79%) | 0.11   | 4 (3%) 43 29   | 31, 61, 97, 108       | 0     |
| 2   | V     | 102/129 (79%) | 0.64   | 7 (6%) 23 16   | 60, 101, 139, 180     | 0     |
| 2   | X     | 102/129 (79%) | 0.35   | 6 (5%) 28 19   | 51, 69, 106, 137      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|-------|
| All | All   | 2761/3108 (88%) | 0.40   | 174 (6%) | 26 | 17 | 22, 73, 148, 208      | 0     |

All (174) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Q     | 720 | GLU  | 6.2  |
| 1   | U     | 782 | ALA  | 5.5  |
| 2   | X     | 78  | LEU  | 5.2  |
| 1   | Q     | 715 | THR  | 5.0  |
| 1   | C     | 702 | PRO  | 4.9  |
| 2   | N     | 5   | PRO  | 4.6  |
| 1   | A     | 778 | PHE  | 4.5  |
| 2   | V     | 78  | LEU  | 4.5  |
| 2   | D     | 5   | PRO  | 4.5  |
| 2   | H     | 32  | ASP  | 4.4  |
| 2   | T     | 78  | LEU  | 4.4  |
| 1   | I     | 821 | GLU  | 4.2  |
| 2   | V     | 107 | LEU  | 4.2  |
| 2   | F     | 5   | PRO  | 4.1  |
| 1   | E     | 817 | PRO  | 4.0  |
| 1   | O     | 703 | ILE  | 4.0  |
| 1   | I     | 830 | LYS  | 3.9  |
| 1   | M     | 703 | ILE  | 3.9  |
| 2   | X     | 85  | TYR  | 3.9  |
| 2   | R     | 78  | LEU  | 3.9  |
| 1   | C     | 821 | GLU  | 3.8  |
| 1   | I     | 807 | ARG  | 3.8  |
| 1   | K     | 702 | PRO  | 3.7  |
| 1   | U     | 717 | LEU  | 3.7  |
| 1   | Q     | 717 | LEU  | 3.6  |
| 1   | W     | 830 | LYS  | 3.6  |
| 1   | U     | 719 | PRO  | 3.6  |
| 1   | K     | 782 | ALA  | 3.6  |
| 1   | S     | 821 | GLU  | 3.5  |
| 1   | C     | 807 | ARG  | 3.5  |
| 1   | E     | 795 | GLY  | 3.5  |
| 1   | K     | 781 | LYS  | 3.5  |
| 1   | Q     | 703 | ILE  | 3.5  |
| 1   | O     | 702 | PRO  | 3.4  |
| 1   | U     | 781 | LYS  | 3.4  |
| 2   | X     | 107 | LEU  | 3.4  |
| 2   | V     | 37  | ARG  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | J     | 20  | GLU  | 3.2  |
| 1   | I     | 703 | ILE  | 3.2  |
| 1   | O     | 781 | LYS  | 3.2  |
| 1   | W     | 704 | HIS  | 3.1  |
| 2   | N     | 85  | TYR  | 3.1  |
| 1   | C     | 704 | HIS  | 3.1  |
| 1   | Q     | 731 | GLU  | 3.1  |
| 1   | A     | 811 | PRO  | 3.1  |
| 1   | I     | 717 | LEU  | 3.1  |
| 2   | P     | 78  | LEU  | 3.0  |
| 1   | G     | 811 | PRO  | 2.9  |
| 2   | H     | 20  | GLU  | 2.9  |
| 2   | P     | 85  | TYR  | 2.9  |
| 1   | S     | 715 | THR  | 2.8  |
| 1   | E     | 816 | LYS  | 2.8  |
| 2   | P     | 71  | TYR  | 2.8  |
| 1   | I     | 719 | PRO  | 2.8  |
| 1   | I     | 769 | PRO  | 2.8  |
| 1   | I     | 811 | PRO  | 2.8  |
| 1   | A     | 715 | THR  | 2.8  |
| 2   | T     | 107 | LEU  | 2.8  |
| 2   | R     | 85  | TYR  | 2.8  |
| 1   | K     | 716 | LYS  | 2.8  |
| 2   | D     | 32  | ASP  | 2.8  |
| 1   | W     | 829 | GLN  | 2.8  |
| 1   | A     | 728 | HIS  | 2.7  |
| 1   | K     | 717 | LEU  | 2.7  |
| 2   | P     | 107 | LEU  | 2.7  |
| 1   | S     | 721 | ARG  | 2.7  |
| 2   | B     | 106 | VAL  | 2.7  |
| 1   | C     | 701 | GLY  | 2.7  |
| 1   | I     | 763 | GLY  | 2.7  |
| 2   | B     | 60  | LYS  | 2.7  |
| 1   | E     | 782 | ALA  | 2.7  |
| 1   | E     | 809 | GLY  | 2.7  |
| 1   | Q     | 763 | GLY  | 2.7  |
| 1   | I     | 817 | PRO  | 2.7  |
| 1   | S     | 817 | PRO  | 2.7  |
| 1   | G     | 704 | HIS  | 2.7  |
| 2   | B     | 32  | ASP  | 2.6  |
| 1   | G     | 764 | GLU  | 2.6  |
| 2   | X     | 6   | VAL  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 782 | ALA  | 2.6  |
| 1   | U     | 807 | ARG  | 2.6  |
| 1   | W     | 728 | HIS  | 2.6  |
| 1   | S     | 782 | ALA  | 2.6  |
| 2   | V     | 38  | MET  | 2.5  |
| 1   | M     | 704 | HIS  | 2.5  |
| 1   | E     | 821 | GLU  | 2.5  |
| 1   | O     | 830 | LYS  | 2.5  |
| 1   | C     | 703 | ILE  | 2.5  |
| 1   | W     | 703 | ILE  | 2.5  |
| 1   | A     | 702 | PRO  | 2.5  |
| 1   | K     | 811 | PRO  | 2.5  |
| 1   | U     | 712 | ALA  | 2.5  |
| 2   | D     | 60  | LYS  | 2.5  |
| 1   | I     | 704 | HIS  | 2.5  |
| 1   | Q     | 821 | GLU  | 2.4  |
| 1   | A     | 716 | LYS  | 2.4  |
| 1   | U     | 794 | PRO  | 2.4  |
| 1   | G     | 814 | GLU  | 2.4  |
| 1   | I     | 770 | GLU  | 2.4  |
| 1   | K     | 821 | GLU  | 2.4  |
| 2   | B     | 107 | LEU  | 2.4  |
| 2   | X     | 28  | ASP  | 2.4  |
| 1   | U     | 754 | ILE  | 2.4  |
| 1   | W     | 781 | LYS  | 2.4  |
| 1   | K     | 807 | ARG  | 2.4  |
| 1   | E     | 806 | LEU  | 2.4  |
| 1   | U     | 709 | GLU  | 2.4  |
| 1   | G     | 779 | GLY  | 2.3  |
| 2   | T     | 20  | GLU  | 2.3  |
| 1   | U     | 811 | PRO  | 2.3  |
| 1   | G     | 763 | GLY  | 2.3  |
| 1   | S     | 717 | LEU  | 2.3  |
| 1   | Q     | 829 | GLN  | 2.3  |
| 2   | X     | 106 | VAL  | 2.3  |
| 1   | E     | 751 | PRO  | 2.3  |
| 2   | L     | 60  | LYS  | 2.3  |
| 1   | U     | 817 | PRO  | 2.3  |
| 1   | U     | 763 | GLY  | 2.3  |
| 1   | Q     | 782 | ALA  | 2.3  |
| 1   | E     | 768 | THR  | 2.3  |
| 1   | S     | 797 | GLY  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 770 | GLU  | 2.2  |
| 1   | S     | 781 | LYS  | 2.2  |
| 1   | G     | 731 | GLU  | 2.2  |
| 1   | I     | 705 | ILE  | 2.2  |
| 1   | G     | 796 | GLU  | 2.2  |
| 2   | B     | 28  | ASP  | 2.2  |
| 1   | U     | 749 | VAL  | 2.2  |
| 2   | V     | 106 | VAL  | 2.2  |
| 1   | I     | 815 | LEU  | 2.2  |
| 1   | M     | 782 | ALA  | 2.2  |
| 1   | A     | 719 | PRO  | 2.2  |
| 1   | U     | 779 | GLY  | 2.2  |
| 1   | A     | 814 | GLU  | 2.1  |
| 1   | C     | 780 | GLU  | 2.1  |
| 1   | I     | 702 | PRO  | 2.1  |
| 2   | J     | 78  | LEU  | 2.1  |
| 1   | S     | 764 | GLU  | 2.1  |
| 1   | I     | 715 | THR  | 2.1  |
| 1   | U     | 745 | ILE  | 2.1  |
| 2   | B     | 25  | THR  | 2.1  |
| 1   | U     | 752 | GLY  | 2.1  |
| 1   | U     | 814 | GLU  | 2.1  |
| 1   | U     | 821 | GLU  | 2.1  |
| 1   | W     | 814 | GLU  | 2.1  |
| 1   | M     | 728 | HIS  | 2.1  |
| 2   | H     | 107 | LEU  | 2.1  |
| 2   | J     | 32  | ASP  | 2.1  |
| 1   | Q     | 721 | ARG  | 2.1  |
| 1   | U     | 783 | ARG  | 2.1  |
| 1   | E     | 752 | GLY  | 2.1  |
| 1   | Q     | 811 | PRO  | 2.1  |
| 1   | E     | 750 | LYS  | 2.1  |
| 2   | H     | 60  | LYS  | 2.1  |
| 2   | D     | 28  | ASP  | 2.1  |
| 2   | F     | 32  | ASP  | 2.1  |
| 2   | V     | 21  | THR  | 2.1  |
| 1   | U     | 731 | GLU  | 2.1  |
| 2   | V     | 22  | GLU  | 2.1  |
| 1   | W     | 715 | THR  | 2.0  |
| 2   | B     | 85  | TYR  | 2.0  |
| 1   | M     | 817 | PRO  | 2.0  |
| 1   | S     | 778 | PHE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | W     | 778 | PHE  | 2.0  |
| 1   | I     | 716 | LYS  | 2.0  |
| 1   | U     | 820 | ARG  | 2.0  |
| 2   | D     | 61  | ARG  | 2.0  |
| 2   | R     | 32  | ASP  | 2.0  |
| 2   | T     | 28  | ASP  | 2.0  |
| 1   | E     | 818 | GLY  | 2.0  |
| 1   | S     | 767 | PRO  | 2.0  |
| 1   | S     | 796 | GLU  | 2.0  |
| 1   | Q     | 783 | ARG  | 2.0  |
| 1   | U     | 726 | ILE  | 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.