



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:23 AM UTC

PDB ID : 4RO0 / pdb\_00004ro0  
Title : Crystal structure of MthK gating ring in a ligand-free form  
Authors : Dong, W.; Guo, R.; Chai, H.; Chen, Z.; Cui, H.; Ren, Z.; Li, Y.; Ye, S.  
Deposited on : 2014-10-27  
Resolution : 3.18 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                                                             |

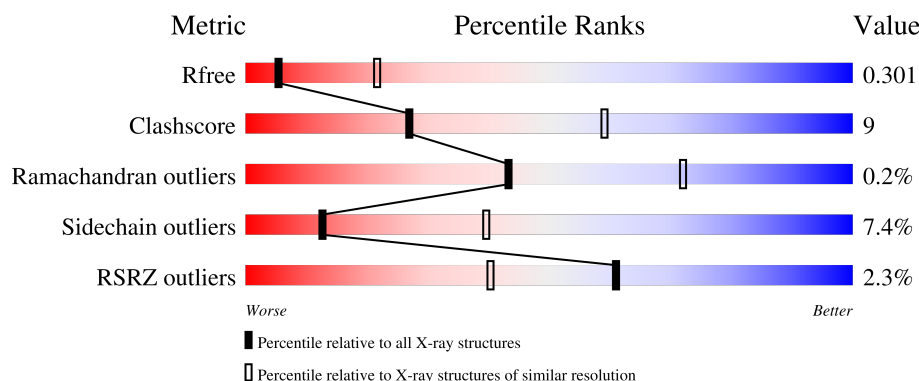
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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.



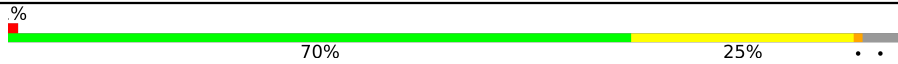
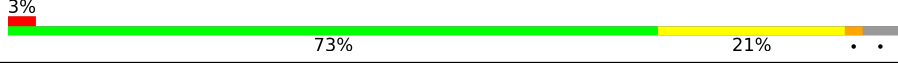
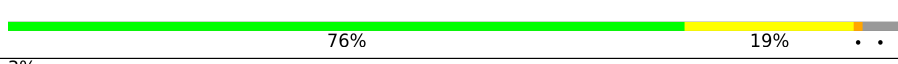
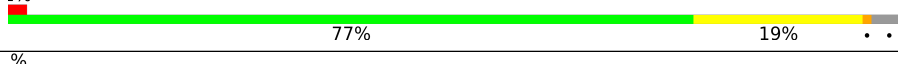
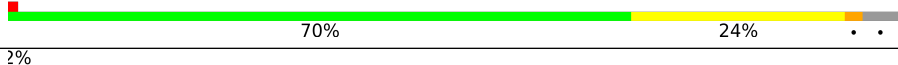
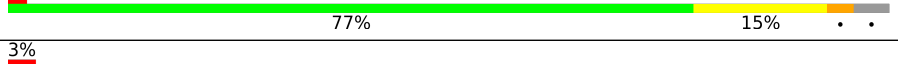
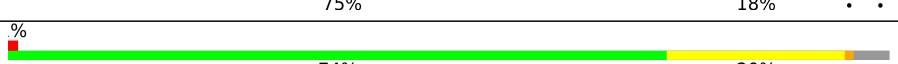
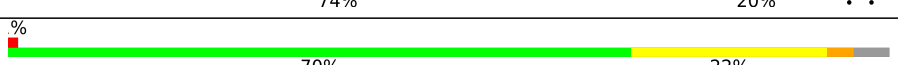
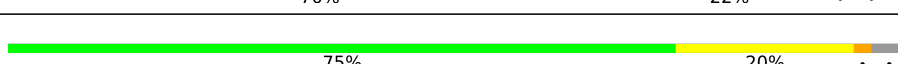
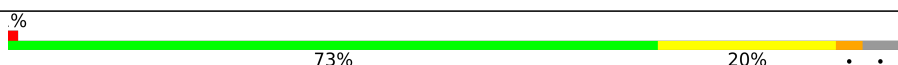
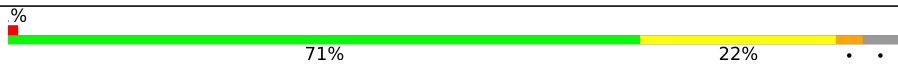
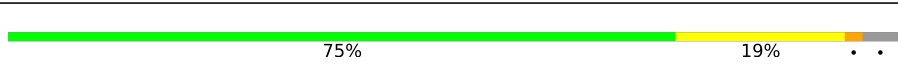
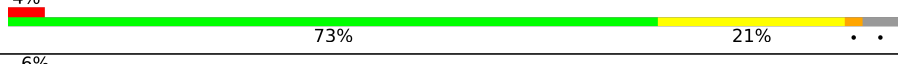
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2001 (3.20-3.16)                                      |
| Clashscore            | 190562                      | 2119 (3.20-3.16)                                      |
| Ramachandran outliers | 187476                      | 2070 (3.20-3.16)                                      |
| Sidechain outliers    | 187428                      | 2069 (3.20-3.16)                                      |
| RSRZ outliers         | 180081                      | 2001 (3.20-3.16)                                      |

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     | 230    |                  |
| 1   | B     | 230    |                  |
| 1   | C     | 230    |                  |
| 1   | D     | 230    |                  |
| 1   | E     | 230    |                  |

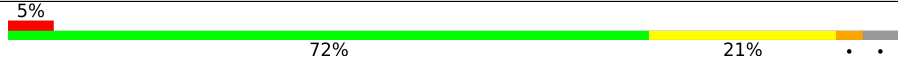
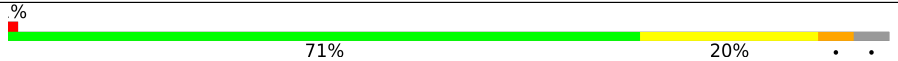
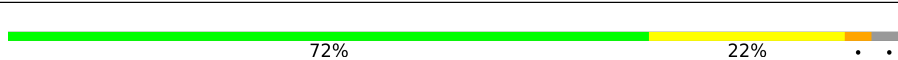
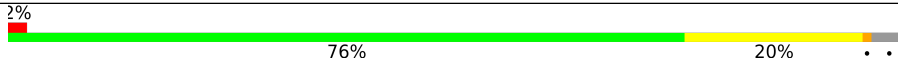
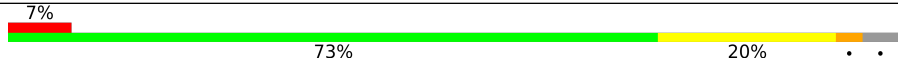
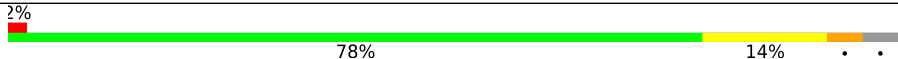
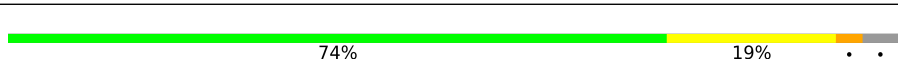
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | F     | 230    |    |
| 1   | G     | 230    |    |
| 1   | H     | 230    |    |
| 1   | I     | 230    |    |
| 1   | J     | 230    |    |
| 1   | K     | 230    |    |
| 1   | L     | 230    |    |
| 1   | M     | 230    |    |
| 1   | N     | 230    |    |
| 1   | O     | 230    |    |
| 1   | P     | 230    |    |
| 1   | Q     | 230    |   |
| 1   | R     | 230    |  |
| 1   | S     | 230    |  |
| 1   | T     | 230    |  |
| 1   | a     | 230    |  |
| 1   | b     | 230    |  |
| 1   | c     | 230    |  |
| 1   | d     | 230    |  |
| 1   | e     | 230    |  |
| 1   | f     | 230    |  |
| 1   | g     | 230    |  |
| 1   | h     | 230    |  |
| 1   | i     | 230    |  |
| 1   | j     | 230    |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | k     | 230    |  |
| 1   | l     | 230    |  |
| 1   | m     | 230    |  |
| 1   | n     | 230    |  |
| 1   | o     | 230    |  |
| 1   | p     | 230    |  |
| 1   | q     | 230    |  |
| 1   | r     | 230    |  |
| 1   | s     | 230    |  |
| 1   | t     | 230    |  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 68748 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 Calcium-gated potassium channel MthK.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | a     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | B     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | b     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | C     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | c     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | D     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | d     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | E     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | e     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | F     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | f     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | G     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | g     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | H     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | h     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | I     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | i     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | J     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | j     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | K     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | k     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | L     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | l     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | M     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | m     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | N     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1713  | 1066 | 302 | 338 | 7 |         |         |       |
| 1   | n     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | O     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | o     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | P     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | p     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | Q     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | q     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | R     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | r     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1713  | 1066 | 302 | 338 | 7 |         |         |       |
| 1   | S     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |

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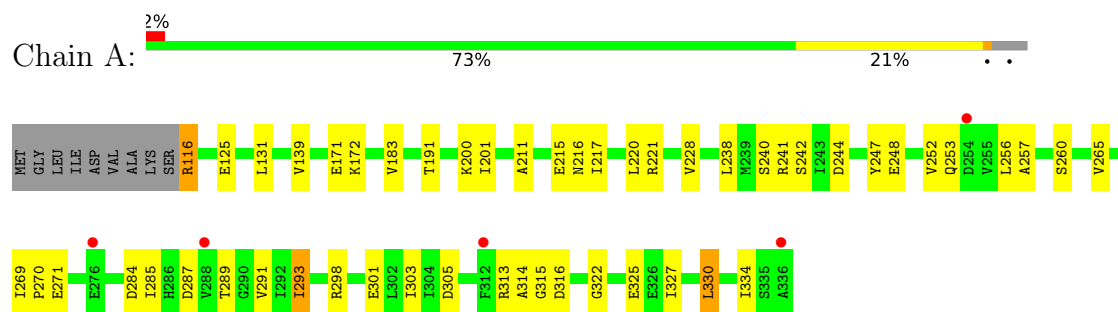
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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | s     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | T     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |
| 1   | t     | 221      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1069 | 305 | 338 | 7 |         |         |       |

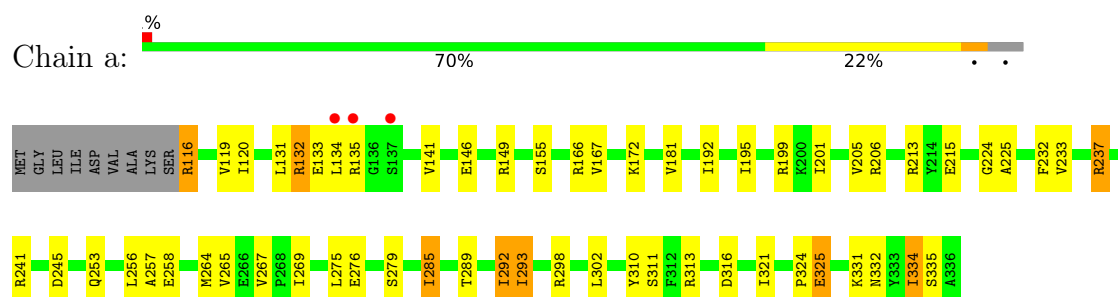
### 3 Residue-property plots

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

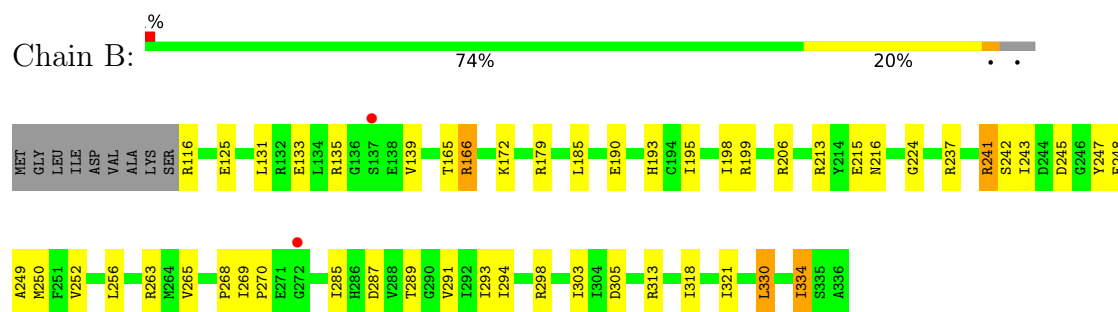
- Molecule 1: Calcium-gated potassium channel MthK



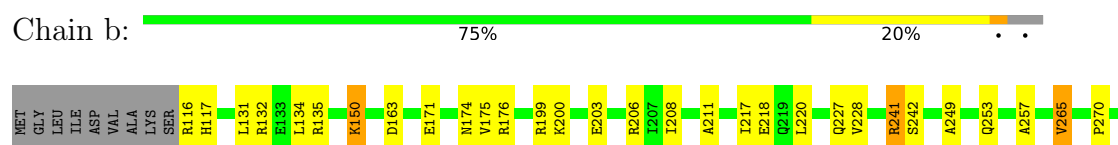
- Molecule 1: Calcium-gated potassium channel MthK



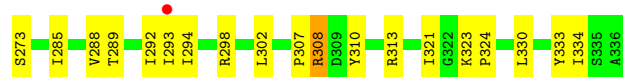
- Molecule 1: Calcium-gated potassium channel MthK



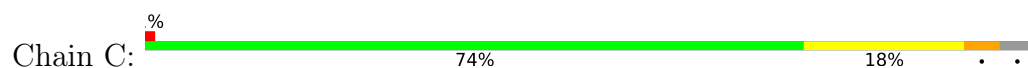
- Molecule 1: Calcium-gated potassium channel MthK







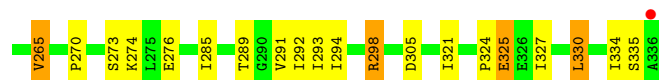
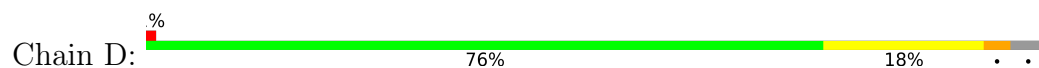
- Molecule 1: Calcium-gated potassium channel MthK



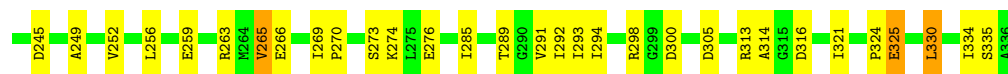
- Molecule 1: Calcium-gated potassium channel MthK



- Molecule 1: Calcium-gated potassium channel MthK

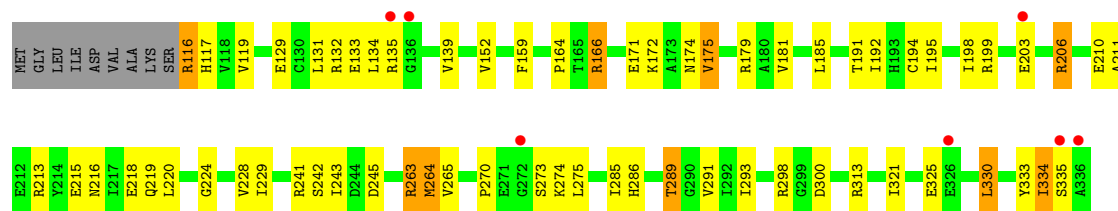


- Molecule 1: Calcium-gated potassium channel MthK



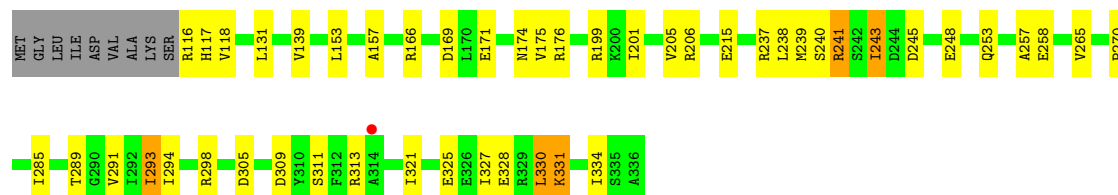
- Molecule 1: Calcium-gated potassium channel MthK





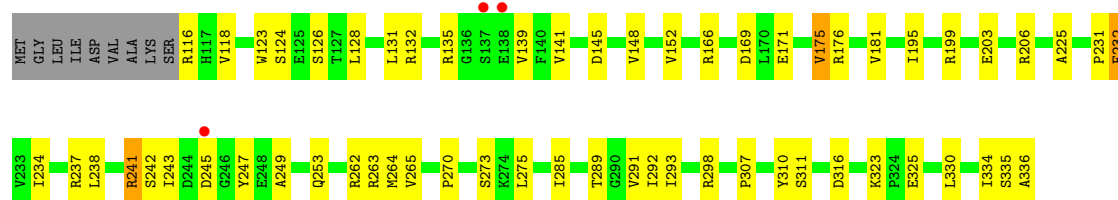
• Molecule 1: Calcium-gated potassium channel MthK

Chain e: 75% 19% . .



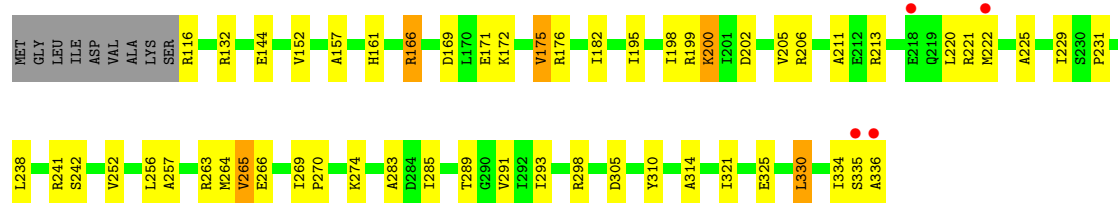
• Molecule 1: Calcium-gated potassium channel MthK

Chain F: 70% 25% . .



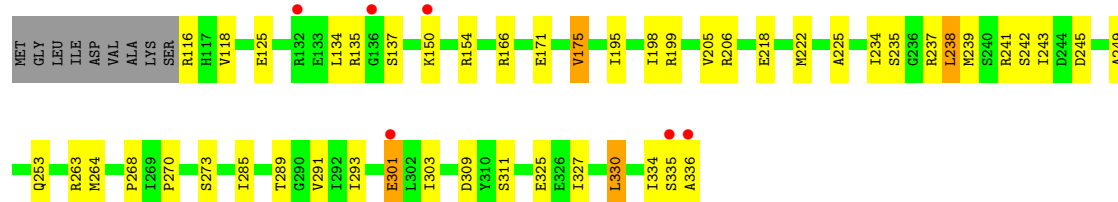
• Molecule 1: Calcium-gated potassium channel MthK

Chain f: 72% 22% . .

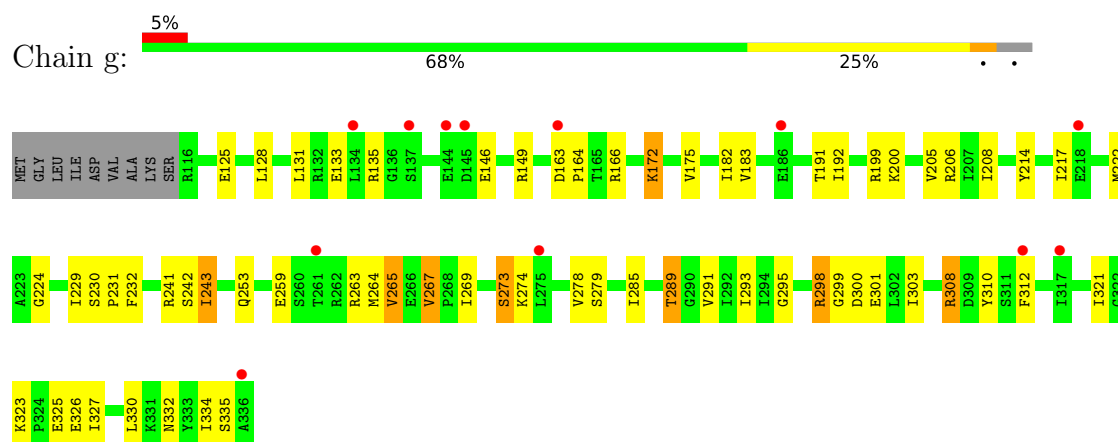


• Molecule 1: Calcium-gated potassium channel MthK

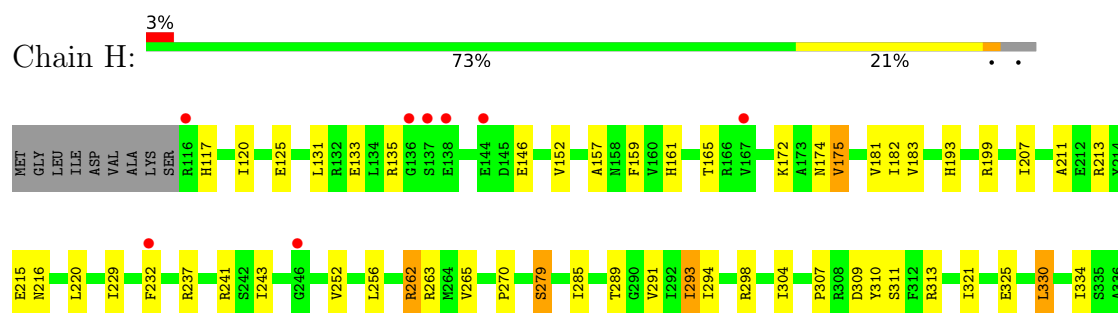
Chain G: 75% 20% . .



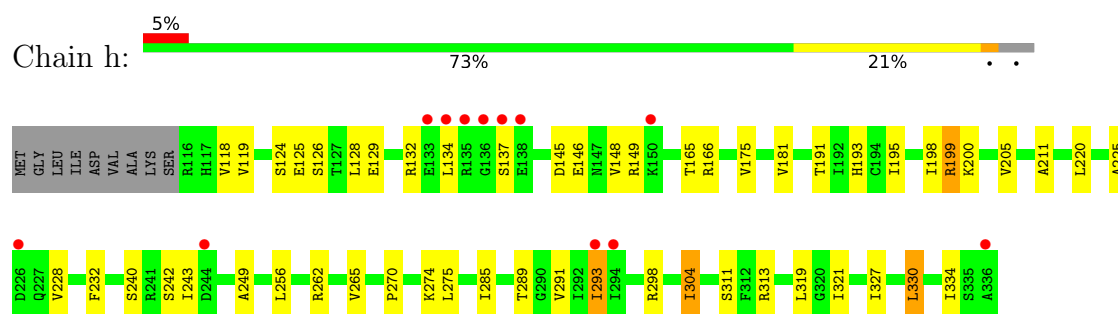
- Molecule 1: Calcium-gated potassium channel MthK



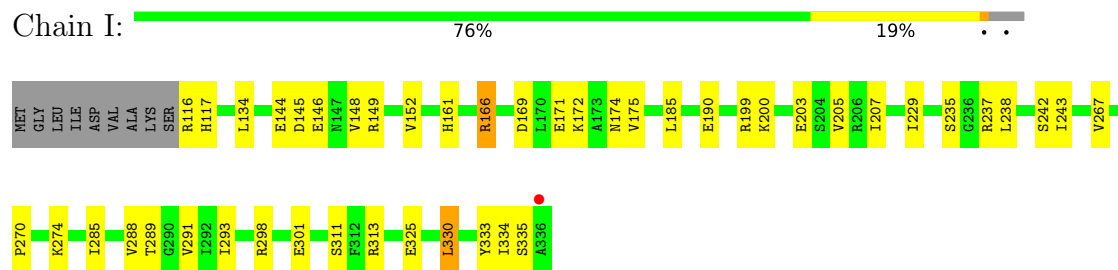
- Molecule 1: Calcium-gated potassium channel MthK



- Molecule 1: Calcium-gated potassium channel MthK

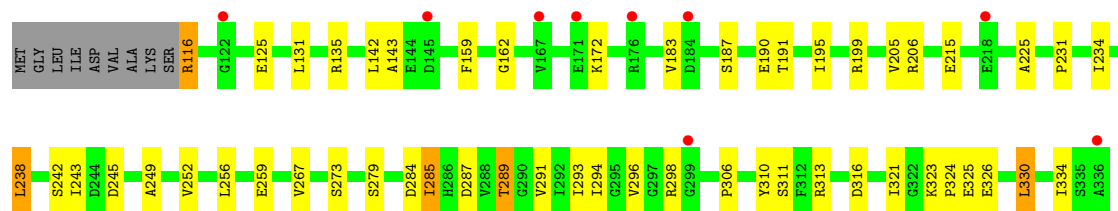


- Molecule 1: Calcium-gated potassium channel MthK

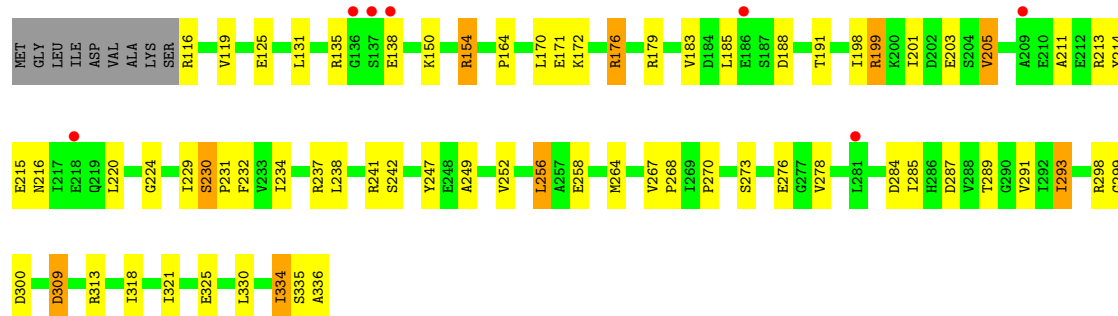


- Molecule 1: Calcium-gated potassium channel MthK

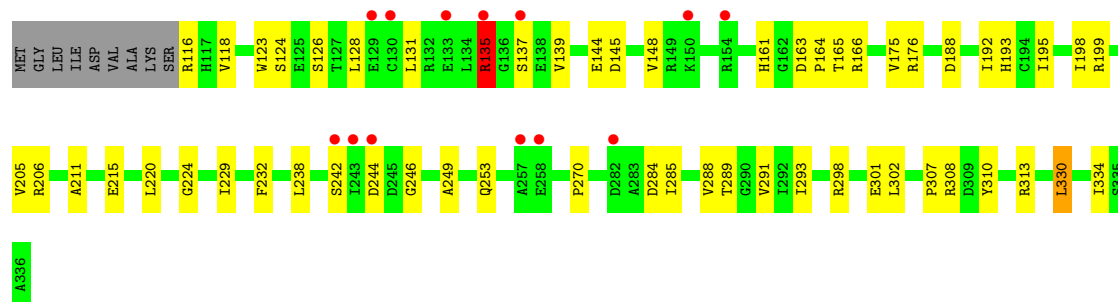
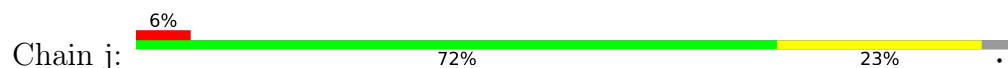




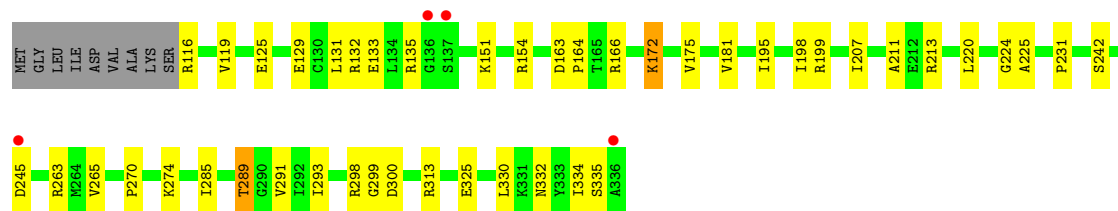
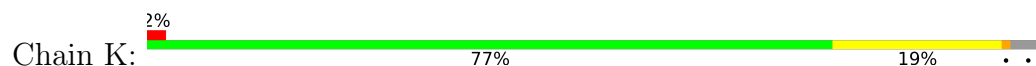
• Molecule 1: Calcium-gated potassium channel MthK



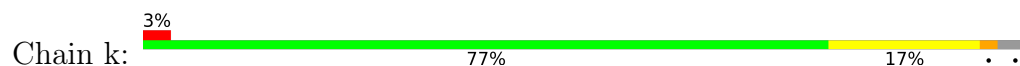
• Molecule 1: Calcium-gated potassium channel MthK

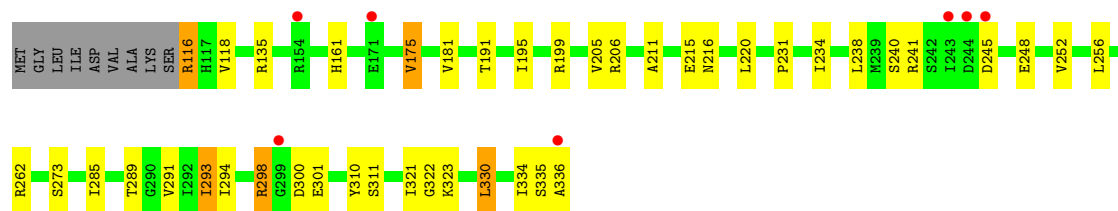


• Molecule 1: Calcium-gated potassium channel MthK

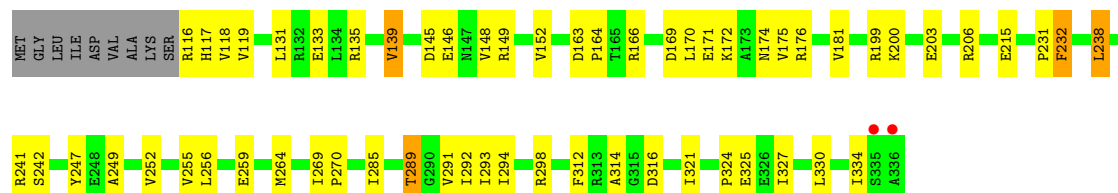


• Molecule 1: Calcium-gated potassium channel MthK

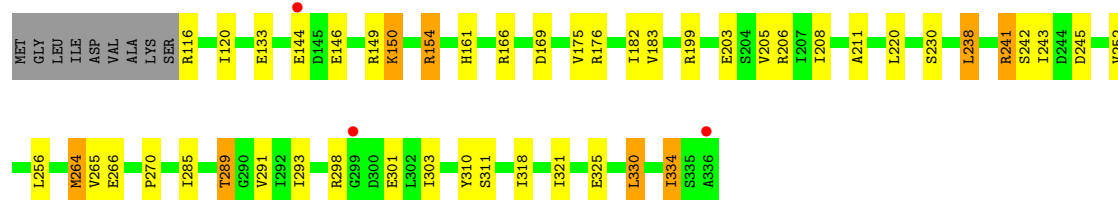
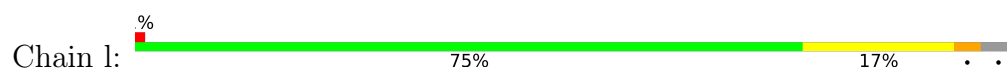




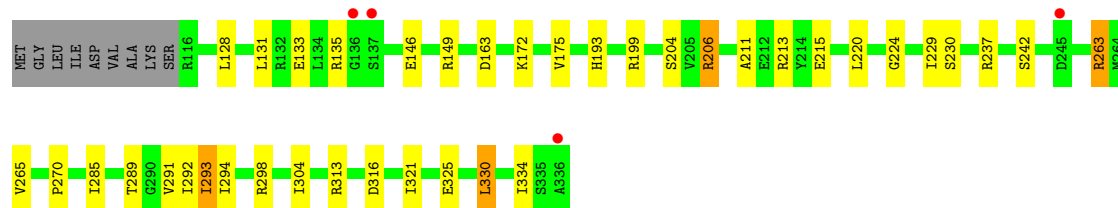
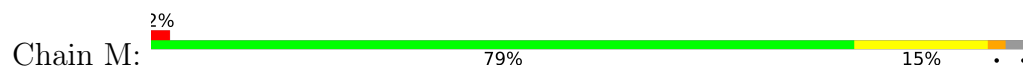
• Molecule 1: Calcium-gated potassium channel MthK



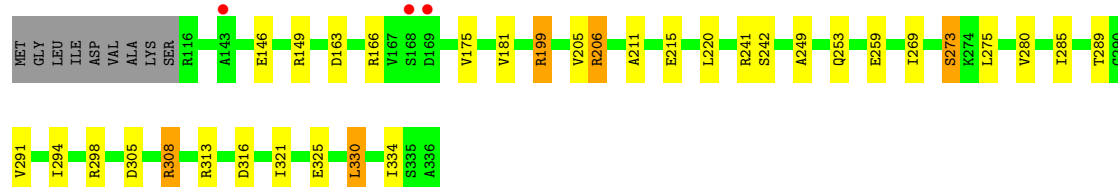
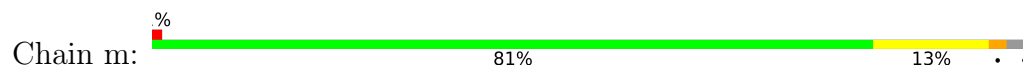
• Molecule 1: Calcium-gated potassium channel MthK



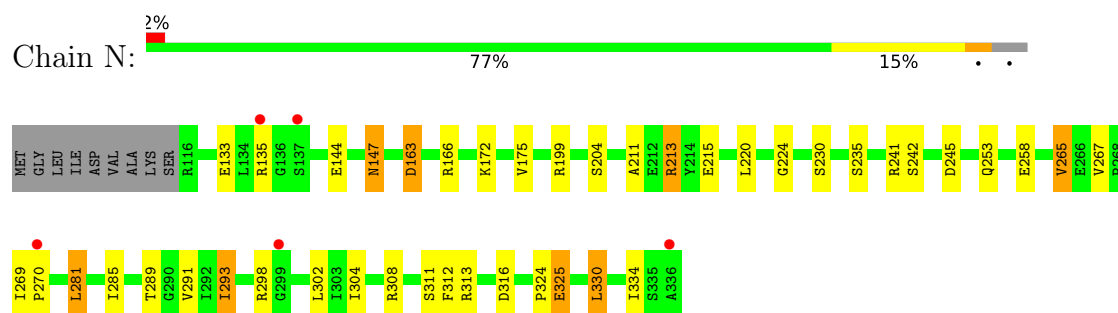
• Molecule 1: Calcium-gated potassium channel MthK



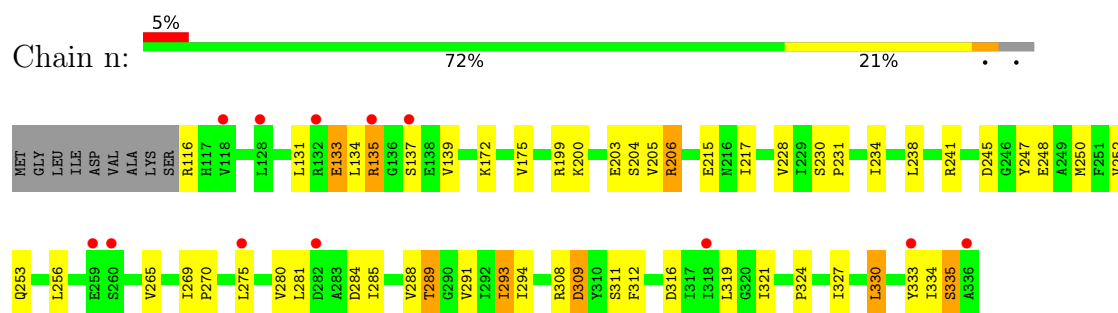
• Molecule 1: Calcium-gated potassium channel MthK



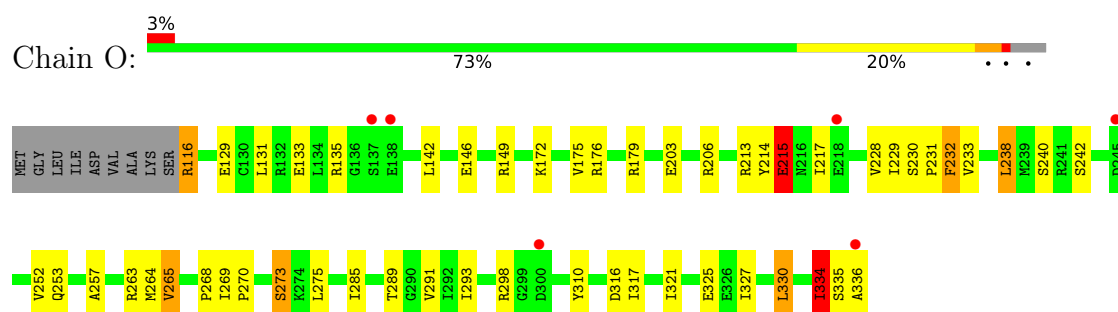
- Molecule 1: Calcium-gated potassium channel MthK



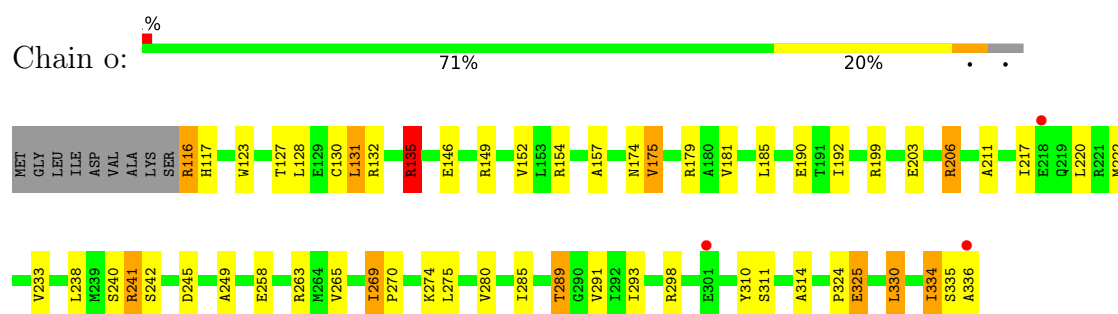
- Molecule 1: Calcium-gated potassium channel MthK



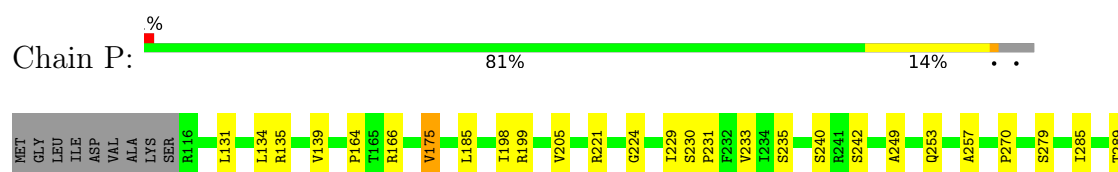
- Molecule 1: Calcium-gated potassium channel MthK



- Molecule 1: Calcium-gated potassium channel MthK



- Molecule 1: Calcium-gated potassium channel MthK





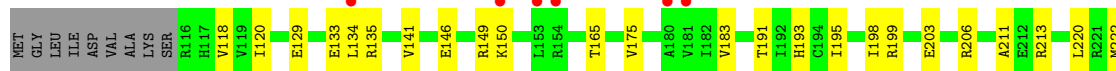
- Molecule 1: Calcium-gated potassium channel MthK

Chain p: 72% 22%



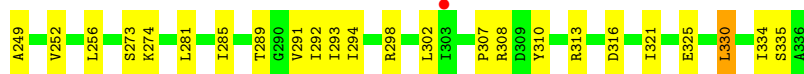
- Molecule 1: Calcium-gated potassium channel MthK

Chain Q: 3% 73% 22%



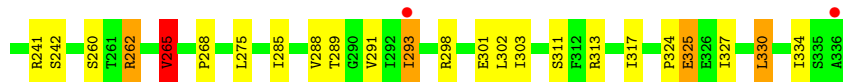
- Molecule 1: Calcium-gated potassium channel MthK

Chain q: 2% 76% 20%



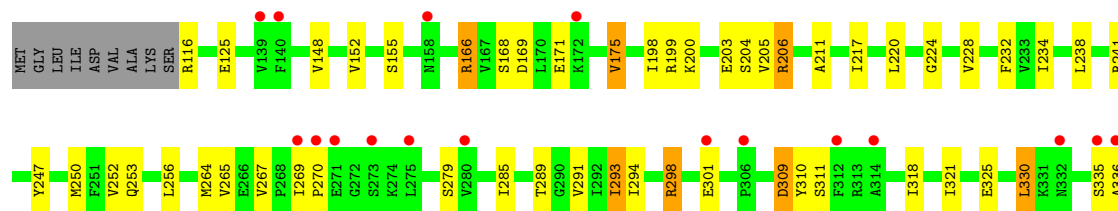
- Molecule 1: Calcium-gated potassium channel MthK

Chain R: 3% 75% 18%



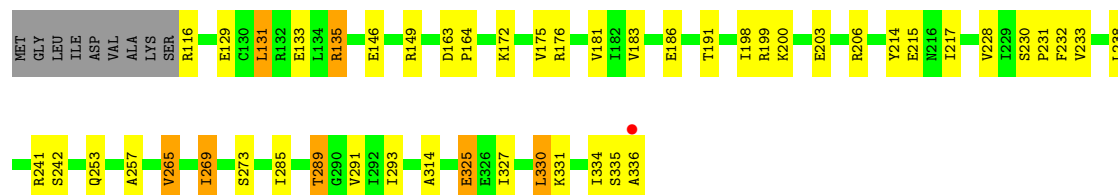
- Molecule 1: Calcium-gated potassium channel MthK

Chain r: 7% 73% 20%



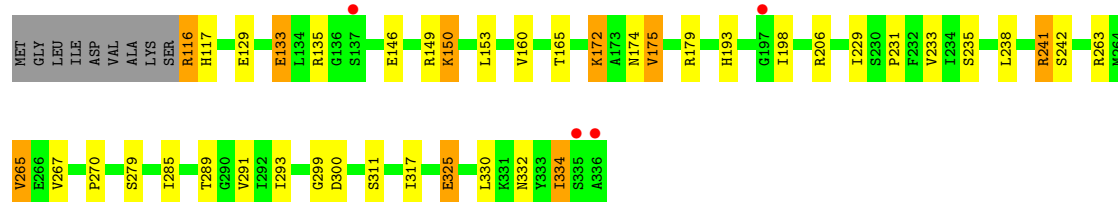
- Molecule 1: Calcium-gated potassium channel MthK

Chain S: 75% 18%



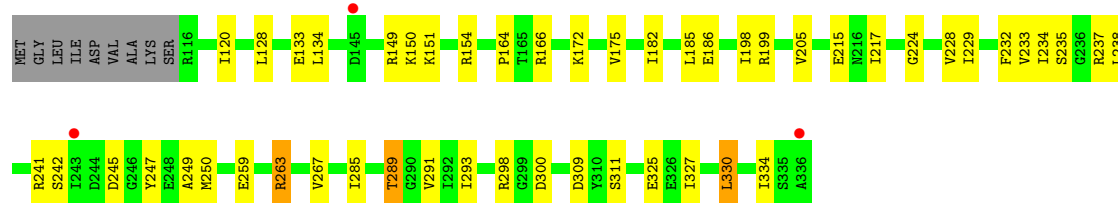
- Molecule 1: Calcium-gated potassium channel MthK

Chain s: 78% 14%



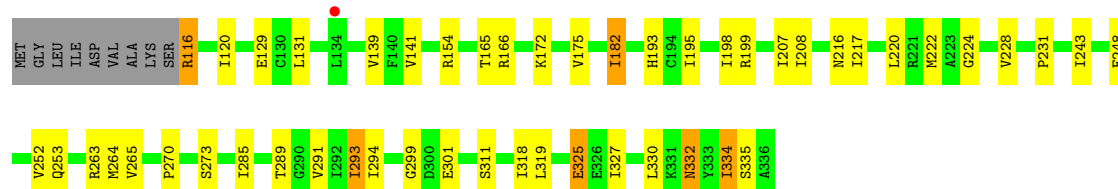
- Molecule 1: Calcium-gated potassium channel MthK

Chain T: 74% 20%



- Molecule 1: Calcium-gated potassium channel MthK

Chain t: 74% 19%





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 166.34Å 231.68Å 197.98Å<br>90.00° 94.58° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.26 – 3.18<br>49.26 – 3.19                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.2 (49.26-3.18)<br>92.2 (49.26-3.19)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.16                                                        | Depositor        |
| $R_{sym}$                                                               | 0.16                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.07 (at 3.19Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0049                                             | Depositor        |
| R, $R_{free}$                                                           | 0.263 , 0.301<br>0.263 , 0.301                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2303 reflections (1.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 68.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.444                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 45.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 68748                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 79.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4248e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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     | 0.49         | 0/1740  | 0.89        | 1/2347 (0.0%) |
| 1   | B     | 0.46         | 0/1740  | 0.86        | 1/2347 (0.0%) |
| 1   | C     | 0.48         | 0/1740  | 0.87        | 1/2347 (0.0%) |
| 1   | D     | 0.48         | 0/1740  | 0.88        | 0/2347        |
| 1   | E     | 0.54         | 0/1740  | 0.94        | 3/2347 (0.1%) |
| 1   | F     | 0.49         | 0/1740  | 0.85        | 0/2347        |
| 1   | G     | 0.49         | 0/1740  | 0.90        | 0/2347        |
| 1   | H     | 0.50         | 0/1740  | 0.88        | 0/2347        |
| 1   | I     | 0.45         | 0/1740  | 0.85        | 0/2347        |
| 1   | J     | 0.50         | 0/1740  | 0.92        | 0/2347        |
| 1   | K     | 0.48         | 0/1740  | 0.89        | 0/2347        |
| 1   | L     | 0.51         | 0/1740  | 0.89        | 0/2347        |
| 1   | M     | 0.46         | 0/1740  | 0.89        | 0/2347        |
| 1   | N     | 0.48         | 0/1734  | 0.90        | 1/2340 (0.0%) |
| 1   | O     | 0.54         | 0/1740  | 0.94        | 1/2347 (0.0%) |
| 1   | P     | 0.45         | 0/1740  | 0.87        | 0/2347        |
| 1   | Q     | 0.46         | 0/1740  | 0.88        | 0/2347        |
| 1   | R     | 0.51         | 0/1740  | 0.90        | 1/2347 (0.0%) |
| 1   | S     | 0.47         | 0/1740  | 0.86        | 0/2347        |
| 1   | T     | 0.47         | 0/1740  | 0.87        | 0/2347        |
| 1   | a     | 0.50         | 0/1740  | 0.89        | 2/2347 (0.1%) |
| 1   | b     | 0.45         | 0/1740  | 0.85        | 1/2347 (0.0%) |
| 1   | c     | 0.48         | 0/1740  | 0.89        | 1/2347 (0.0%) |
| 1   | d     | 0.53         | 0/1740  | 0.90        | 1/2347 (0.0%) |
| 1   | e     | 0.50         | 0/1740  | 0.91        | 0/2347        |
| 1   | f     | 0.50         | 0/1740  | 0.90        | 1/2347 (0.0%) |
| 1   | g     | 0.55         | 0/1740  | 0.92        | 4/2347 (0.2%) |
| 1   | h     | 0.48         | 0/1740  | 0.86        | 0/2347        |
| 1   | i     | 0.50         | 0/1740  | 0.89        | 0/2347        |
| 1   | j     | 0.47         | 0/1740  | 0.85        | 0/2347        |
| 1   | k     | 0.50         | 0/1740  | 0.93        | 1/2347 (0.0%) |
| 1   | l     | 0.50         | 0/1740  | 0.89        | 1/2347 (0.0%) |
| 1   | m     | 0.47         | 0/1740  | 0.87        | 2/2347 (0.1%) |
| 1   | n     | 0.49         | 0/1740  | 0.94        | 1/2347 (0.0%) |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 1   | o     | 0.54         | 0/1740  | 0.94        | 2/2347 (0.1%)   |
| 1   | p     | 0.46         | 0/1740  | 0.88        | 1/2347 (0.0%)   |
| 1   | q     | 0.46         | 0/1740  | 0.82        | 0/2347          |
| 1   | r     | 0.48         | 0/1734  | 0.88        | 1/2340 (0.0%)   |
| 1   | s     | 0.50         | 0/1740  | 0.89        | 1/2347 (0.0%)   |
| 1   | t     | 0.48         | 0/1740  | 0.87        | 1/2347 (0.0%)   |
| All | All   | 0.49         | 0/69588 | 0.89        | 30/93866 (0.0%) |

There are no bond length outliers.

All (30) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | g     | 334 | ILE  | N-CA-C | 6.84  | 118.88      | 111.77   |
| 1   | E     | 285 | ILE  | N-CA-C | 6.41  | 116.57      | 110.42   |
| 1   | o     | 334 | ILE  | N-CA-C | 6.31  | 117.24      | 111.81   |
| 1   | E     | 334 | ILE  | N-CA-C | 6.26  | 117.19      | 111.81   |
| 1   | n     | 335 | SER  | N-CA-C | 6.04  | 117.67      | 110.19   |
| 1   | f     | 265 | VAL  | N-CA-C | 5.99  | 117.10      | 108.48   |
| 1   | g     | 265 | VAL  | N-CA-C | 5.95  | 117.05      | 108.48   |
| 1   | m     | 163 | ASP  | CA-C-N | 5.86  | 125.54      | 119.56   |
| 1   | m     | 163 | ASP  | C-N-CA | 5.86  | 125.54      | 119.56   |
| 1   | A     | 322 | GLY  | N-CA-C | 5.80  | 119.55      | 110.91   |
| 1   | o     | 217 | ILE  | N-CA-C | -5.68 | 104.79      | 110.30   |
| 1   | a     | 335 | SER  | N-CA-C | 5.64  | 117.98      | 109.41   |
| 1   | a     | 265 | VAL  | N-CA-C | 5.59  | 117.98      | 108.86   |
| 1   | N     | 265 | VAL  | N-CA-C | 5.53  | 116.69      | 108.46   |
| 1   | C     | 335 | SER  | N-CA-C | 5.50  | 117.62      | 110.53   |
| 1   | O     | 334 | ILE  | N-CA-C | 5.46  | 116.51      | 111.81   |
| 1   | t     | 335 | SER  | N-CA-C | 5.39  | 118.06      | 110.14   |
| 1   | l     | 334 | ILE  | N-CA-C | 5.37  | 116.43      | 111.81   |
| 1   | E     | 335 | SER  | N-CA-C | 5.32  | 116.95      | 110.41   |
| 1   | g     | 335 | SER  | N-CA-C | 5.29  | 115.27      | 108.34   |
| 1   | B     | 334 | ILE  | N-CA-C | 5.20  | 116.11      | 111.90   |
| 1   | k     | 322 | GLY  | N-CA-C | 5.19  | 118.06      | 110.38   |
| 1   | p     | 335 | SER  | N-CA-C | 5.16  | 117.39      | 109.95   |
| 1   | g     | 295 | GLY  | N-CA-C | 5.14  | 119.10      | 110.56   |
| 1   | r     | 265 | VAL  | N-CA-C | 5.11  | 116.72      | 108.85   |
| 1   | b     | 265 | VAL  | N-CA-C | 5.10  | 115.82      | 108.48   |
| 1   | c     | 306 | PRO  | O-C-N  | 5.07  | 123.53      | 121.15   |
| 1   | R     | 265 | VAL  | N-CA-C | 5.07  | 116.01      | 108.46   |
| 1   | d     | 205 | VAL  | N-CA-C | 5.06  | 115.75      | 108.93   |
| 1   | s     | 334 | ILE  | N-CA-C | 5.02  | 115.88      | 111.56   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1719  | 0        | 1726     | 40      | 0            |
| 1   | B     | 1719  | 0        | 1726     | 33      | 0            |
| 1   | C     | 1719  | 0        | 1726     | 50      | 0            |
| 1   | D     | 1719  | 0        | 1726     | 38      | 0            |
| 1   | E     | 1719  | 0        | 1726     | 55      | 0            |
| 1   | F     | 1719  | 0        | 1726     | 34      | 0            |
| 1   | G     | 1719  | 0        | 1726     | 32      | 0            |
| 1   | H     | 1719  | 0        | 1726     | 45      | 0            |
| 1   | I     | 1719  | 0        | 1726     | 23      | 0            |
| 1   | J     | 1719  | 0        | 1726     | 58      | 0            |
| 1   | K     | 1719  | 0        | 1726     | 30      | 0            |
| 1   | L     | 1719  | 0        | 1726     | 41      | 0            |
| 1   | M     | 1719  | 0        | 1726     | 26      | 0            |
| 1   | N     | 1713  | 0        | 1715     | 32      | 0            |
| 1   | O     | 1719  | 0        | 1726     | 39      | 0            |
| 1   | P     | 1719  | 0        | 1726     | 29      | 0            |
| 1   | Q     | 1719  | 0        | 1726     | 36      | 0            |
| 1   | R     | 1719  | 0        | 1726     | 38      | 0            |
| 1   | S     | 1719  | 0        | 1726     | 29      | 0            |
| 1   | T     | 1719  | 0        | 1726     | 27      | 0            |
| 1   | a     | 1719  | 0        | 1726     | 59      | 0            |
| 1   | b     | 1719  | 0        | 1726     | 28      | 0            |
| 1   | c     | 1719  | 0        | 1726     | 37      | 0            |
| 1   | d     | 1719  | 0        | 1726     | 47      | 0            |
| 1   | e     | 1719  | 0        | 1726     | 33      | 0            |
| 1   | f     | 1719  | 0        | 1726     | 38      | 0            |
| 1   | g     | 1719  | 0        | 1726     | 38      | 0            |
| 1   | h     | 1719  | 0        | 1726     | 41      | 0            |
| 1   | i     | 1719  | 0        | 1726     | 34      | 0            |
| 1   | j     | 1719  | 0        | 1726     | 39      | 0            |
| 1   | k     | 1719  | 0        | 1726     | 24      | 0            |
| 1   | l     | 1719  | 0        | 1726     | 31      | 0            |
| 1   | m     | 1719  | 0        | 1726     | 34      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | n     | 1719  | 0        | 1726     | 41      | 0            |
| 1   | o     | 1719  | 0        | 1726     | 42      | 0            |
| 1   | p     | 1719  | 0        | 1726     | 34      | 0            |
| 1   | q     | 1719  | 0        | 1726     | 34      | 0            |
| 1   | r     | 1713  | 0        | 1715     | 34      | 0            |
| 1   | s     | 1719  | 0        | 1726     | 39      | 0            |
| 1   | t     | 1719  | 0        | 1726     | 31      | 0            |
| All | All   | 68748 | 0        | 69018    | 1263    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:324:PRO:HB2  | 1:S:325:GLU:HG2  | 1.13                     | 1.12              |
| 1:m:298:ARG:HH22 | 1:m:313:ARG:HB2  | 1.12                     | 1.12              |
| 1:a:116:ARG:HG2  | 1:a:116:ARG:HH21 | 1.13                     | 1.08              |
| 1:o:116:ARG:HH21 | 1:o:116:ARG:HG3  | 1.14                     | 1.07              |
| 1:J:298:ARG:HH22 | 1:J:313:ARG:HB2  | 1.15                     | 1.06              |
| 1:C:132:ARG:HG3  | 1:C:132:ARG:HH11 | 1.16                     | 1.06              |
| 1:D:116:ARG:HH21 | 1:D:116:ARG:HG3  | 1.20                     | 1.05              |
| 1:C:298:ARG:NH1  | 1:C:313:ARG:NH1  | 2.04                     | 1.05              |
| 1:m:308:ARG:HG2  | 1:m:308:ARG:HH11 | 1.21                     | 1.04              |
| 1:a:298:ARG:NH2  | 1:a:313:ARG:HB2  | 1.72                     | 1.04              |
| 1:d:325:GLU:HG2  | 1:R:324:PRO:HB2  | 1.09                     | 1.03              |
| 1:s:116:ARG:HH21 | 1:s:116:ARG:HG3  | 1.23                     | 1.03              |
| 1:a:298:ARG:HH22 | 1:a:313:ARG:HB2  | 0.88                     | 1.01              |
| 1:i:324:PRO:HB2  | 1:S:325:GLU:CG   | 1.90                     | 1.01              |
| 1:D:325:GLU:CG   | 1:N:324:PRO:HB2  | 1.91                     | 1.00              |
| 1:D:325:GLU:HG2  | 1:N:324:PRO:HB2  | 1.01                     | 1.00              |
| 1:a:132:ARG:HG3  | 1:a:132:ARG:HH11 | 1.26                     | 0.99              |
| 1:C:324:PRO:HB3  | 1:s:325:GLU:HG2  | 1.44                     | 0.99              |
| 1:d:116:ARG:HH21 | 1:d:116:ARG:HG3  | 1.28                     | 0.99              |
| 1:i:298:ARG:HH22 | 1:i:313:ARG:HB2  | 1.28                     | 0.99              |
| 1:J:176:ARG:HH21 | 1:J:176:ARG:HG3  | 1.28                     | 0.98              |
| 1:d:325:GLU:CG   | 1:R:324:PRO:HB2  | 1.93                     | 0.98              |
| 1:L:324:PRO:HB2  | 1:t:325:GLU:HG2  | 1.44                     | 0.98              |
| 1:D:325:GLU:HG2  | 1:N:324:PRO:CB   | 1.93                     | 0.97              |
| 1:a:298:ARG:HH22 | 1:a:313:ARG:CB   | 1.77                     | 0.96              |
| 1:A:298:ARG:HH12 | 1:A:313:ARG:HD2  | 1.29                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:324:PRO:CB   | 1:o:325:GLU:HG2  | 1.98                     | 0.94              |
| 1:J:188:ASP:HB3  | 1:J:216:ASN:HD22 | 1.33                     | 0.93              |
| 1:a:324:PRO:HB3  | 1:o:325:GLU:HG2  | 1.50                     | 0.92              |
| 1:O:298:ARG:NH2  | 1:O:316:ASP:OD2  | 2.01                     | 0.92              |
| 1:d:298:ARG:HH12 | 1:d:313:ARG:NE   | 1.68                     | 0.91              |
| 1:B:165:THR:HB   | 1:B:193:HIS:HD1  | 1.35                     | 0.91              |
| 1:d:324:PRO:HB2  | 1:R:325:GLU:HG2  | 1.53                     | 0.91              |
| 1:f:298:ARG:NH2  | 1:f:310:TYR:OH   | 2.03                     | 0.91              |
| 1:O:133:GLU:OE1  | 1:o:241:ARG:NH1  | 2.04                     | 0.90              |
| 1:E:298:ARG:CZ   | 1:E:313:ARG:HD2  | 2.01                     | 0.90              |
| 1:l:285:ILE:HB   | 1:l:293:ILE:HD11 | 1.54                     | 0.89              |
| 1:S:285:ILE:HB   | 1:S:293:ILE:HD11 | 1.55                     | 0.89              |
| 1:c:298:ARG:HH22 | 1:c:313:ARG:HB2  | 1.38                     | 0.88              |
| 1:I:242:SER:O    | 1:i:206:ARG:NH1  | 2.06                     | 0.88              |
| 1:d:325:GLU:HG2  | 1:R:324:PRO:CB   | 2.02                     | 0.88              |
| 1:H:285:ILE:O    | 1:H:289:THR:HG22 | 1.74                     | 0.87              |
| 1:d:298:ARG:HH12 | 1:d:313:ARG:CZ   | 1.88                     | 0.86              |
| 1:C:298:ARG:HH12 | 1:C:313:ARG:CZ   | 1.89                     | 0.86              |
| 1:R:262:ARG:HG3  | 1:R:262:ARG:HH11 | 1.41                     | 0.86              |
| 1:n:285:ILE:HB   | 1:n:293:ILE:HD11 | 1.58                     | 0.85              |
| 1:Q:206:ARG:NH1  | 1:q:242:SER:O    | 2.09                     | 0.85              |
| 1:b:285:ILE:O    | 1:b:289:THR:HG22 | 1.76                     | 0.85              |
| 1:s:285:ILE:O    | 1:s:289:THR:HG22 | 1.76                     | 0.85              |
| 1:P:298:ARG:HH22 | 1:P:313:ARG:HG3  | 1.41                     | 0.85              |
| 1:C:298:ARG:HH12 | 1:C:313:ARG:NH1  | 1.74                     | 0.85              |
| 1:J:285:ILE:O    | 1:J:289:THR:HG22 | 1.77                     | 0.84              |
| 1:d:285:ILE:O    | 1:d:289:THR:HG22 | 1.78                     | 0.83              |
| 1:F:285:ILE:O    | 1:F:289:THR:HG22 | 1.78                     | 0.83              |
| 1:A:285:ILE:O    | 1:A:289:THR:HG22 | 1.79                     | 0.82              |
| 1:k:116:ARG:HB2  | 1:k:116:ARG:HH21 | 1.43                     | 0.82              |
| 1:H:232:PHE:HD1  | 1:h:125:GLU:HB3  | 1.44                     | 0.81              |
| 1:R:133:GLU:OE1  | 1:r:241:ARG:NH1  | 2.14                     | 0.81              |
| 1:E:298:ARG:NH1  | 1:E:313:ARG:HD2  | 1.95                     | 0.80              |
| 1:F:242:SER:O    | 1:f:206:ARG:NH1  | 2.15                     | 0.80              |
| 1:L:131:LEU:HD21 | 1:L:139:VAL:HG11 | 1.63                     | 0.80              |
| 1:J:188:ASP:HB3  | 1:J:216:ASN:ND2  | 1.97                     | 0.80              |
| 1:A:116:ARG:HH21 | 1:A:116:ARG:HG3  | 1.46                     | 0.80              |
| 1:Q:213:ARG:HG2  | 1:t:166:ARG:NH2  | 1.95                     | 0.80              |
| 1:B:285:ILE:O    | 1:B:289:THR:HG22 | 1.81                     | 0.79              |
| 1:d:324:PRO:HB2  | 1:R:325:GLU:CG   | 2.11                     | 0.79              |
| 1:C:264:MET:HG2  | 1:c:248:GLU:HG3  | 1.65                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:285:ILE:HB   | 1:d:293:ILE:HD11 | 1.63                     | 0.78              |
| 1:R:217:ILE:HG23 | 1:R:228:VAL:HG11 | 1.65                     | 0.78              |
| 1:M:206:ARG:NH1  | 1:m:242:SER:O    | 2.17                     | 0.78              |
| 1:D:116:ARG:HG3  | 1:D:116:ARG:NH2  | 1.93                     | 0.78              |
| 1:E:116:ARG:NH2  | 1:E:179:ARG:HD2  | 1.98                     | 0.78              |
| 1:D:285:ILE:O    | 1:D:289:THR:HG22 | 1.85                     | 0.77              |
| 1:O:298:ARG:HH21 | 1:O:316:ASP:CG   | 1.92                     | 0.77              |
| 1:E:119:VAL:HB   | 1:E:181:VAL:HG13 | 1.67                     | 0.77              |
| 1:b:298:ARG:NH1  | 1:b:313:ARG:NH1  | 2.32                     | 0.77              |
| 1:m:308:ARG:HH11 | 1:m:308:ARG:CG   | 1.98                     | 0.77              |
| 1:O:275:LEU:HD12 | 1:O:334:ILE:HG23 | 1.67                     | 0.77              |
| 1:C:132:ARG:HG3  | 1:C:132:ARG:NH1  | 1.96                     | 0.77              |
| 1:J:237:ARG:NH1  | 1:J:241:ARG:HE   | 1.82                     | 0.77              |
| 1:J:176:ARG:HH21 | 1:J:176:ARG:CG   | 1.96                     | 0.76              |
| 1:N:281:LEU:HD12 | 1:N:308:ARG:HB3  | 1.66                     | 0.76              |
| 1:p:116:ARG:HG3  | 1:p:116:ARG:HH21 | 1.50                     | 0.76              |
| 1:J:298:ARG:NH2  | 1:J:313:ARG:HB2  | 1.98                     | 0.76              |
| 1:l:264:MET:HE2  | 1:l:321:ILE:HG12 | 1.66                     | 0.76              |
| 1:S:242:SER:O    | 1:s:206:ARG:NH1  | 2.19                     | 0.76              |
| 1:D:324:PRO:HB2  | 1:N:325:GLU:HG2  | 1.67                     | 0.76              |
| 1:m:285:ILE:O    | 1:m:289:THR:HG22 | 1.85                     | 0.76              |
| 1:q:298:ARG:NH2  | 1:q:313:ARG:HB2  | 2.00                     | 0.76              |
| 1:C:324:PRO:CB   | 1:s:325:GLU:HG2  | 2.16                     | 0.76              |
| 1:M:285:ILE:O    | 1:M:289:THR:HG22 | 1.86                     | 0.75              |
| 1:J:188:ASP:CB   | 1:J:216:ASN:HD22 | 1.98                     | 0.75              |
| 1:P:298:ARG:HH12 | 1:P:313:ARG:CD   | 2.00                     | 0.74              |
| 1:N:144:GLU:OE2  | 1:N:163:ASP:HB2  | 1.86                     | 0.74              |
| 1:O:116:ARG:HH21 | 1:O:116:ARG:HG3  | 1.51                     | 0.74              |
| 1:A:248:GLU:HG3  | 1:a:264:MET:HG2  | 1.69                     | 0.74              |
| 1:n:269:ILE:HD12 | 1:n:316:ASP:HB2  | 1.68                     | 0.74              |
| 1:t:285:ILE:O    | 1:t:289:THR:HG22 | 1.86                     | 0.74              |
| 1:L:324:PRO:HB2  | 1:t:325:GLU:CG   | 2.18                     | 0.74              |
| 1:G:270:PRO:HD2  | 1:G:334:ILE:HG22 | 1.70                     | 0.73              |
| 1:e:328:GLU:HA   | 1:e:331:LYS:HD3  | 1.70                     | 0.73              |
| 1:r:285:ILE:O    | 1:r:289:THR:HG22 | 1.88                     | 0.73              |
| 1:O:146:GLU:OE1  | 1:O:149:ARG:NH1  | 2.22                     | 0.73              |
| 1:a:116:ARG:HH21 | 1:a:116:ARG:CG   | 1.98                     | 0.73              |
| 1:t:116:ARG:HH21 | 1:t:116:ARG:HG3  | 1.52                     | 0.73              |
| 1:E:264:MET:HE2  | 1:E:321:ILE:HG12 | 1.71                     | 0.72              |
| 1:P:298:ARG:HH12 | 1:P:313:ARG:HD2  | 1.52                     | 0.72              |
| 1:S:133:GLU:OE1  | 1:s:241:ARG:NH1  | 2.23                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:324:PRO:HB2  | 1:o:325:GLU:CG   | 2.19                     | 0.72              |
| 1:c:116:ARG:HH21 | 1:c:116:ARG:HG3  | 1.54                     | 0.72              |
| 1:Q:134:LEU:HD11 | 1:q:243:ILE:HD11 | 1.69                     | 0.72              |
| 1:T:285:ILE:HB   | 1:T:293:ILE:HD11 | 1.71                     | 0.72              |
| 1:c:285:ILE:O    | 1:c:289:THR:HG22 | 1.90                     | 0.72              |
| 1:N:147:ASN:HD22 | 1:N:147:ASN:H    | 1.38                     | 0.72              |
| 1:H:298:ARG:HH12 | 1:H:313:ARG:HB2  | 1.54                     | 0.71              |
| 1:E:199:ARG:HE   | 1:E:203:GLU:HA   | 1.54                     | 0.71              |
| 1:p:171:GLU:HG3  | 1:p:201:ILE:HD13 | 1.71                     | 0.71              |
| 1:F:298:ARG:NH2  | 1:F:316:ASP:OD2  | 2.22                     | 0.71              |
| 1:f:285:ILE:O    | 1:f:289:THR:HG22 | 1.90                     | 0.71              |
| 1:e:285:ILE:O    | 1:e:289:THR:HG22 | 1.90                     | 0.71              |
| 1:M:285:ILE:HB   | 1:M:293:ILE:HD11 | 1.73                     | 0.71              |
| 1:i:285:ILE:O    | 1:i:289:THR:HG22 | 1.91                     | 0.71              |
| 1:m:298:ARG:NH2  | 1:m:313:ARG:HB2  | 1.98                     | 0.71              |
| 1:o:298:ARG:HG3  | 1:o:298:ARG:HH11 | 1.55                     | 0.71              |
| 1:T:237:ARG:HG2  | 1:T:241:ARG:HH12 | 1.53                     | 0.71              |
| 1:g:323:LYS:HB2  | 1:g:326:GLU:HG3  | 1.72                     | 0.71              |
| 1:N:289:THR:HG23 | 1:N:291:VAL:H    | 1.56                     | 0.71              |
| 1:E:298:ARG:HH12 | 1:E:313:ARG:NH1  | 1.88                     | 0.70              |
| 1:G:199:ARG:NH2  | 1:G:205:VAL:O    | 2.23                     | 0.70              |
| 1:h:285:ILE:O    | 1:h:289:THR:HG22 | 1.91                     | 0.70              |
| 1:E:263:ARG:NH1  | 1:E:265:VAL:HG12 | 2.07                     | 0.70              |
| 1:H:270:PRO:HD2  | 1:H:334:ILE:HG22 | 1.72                     | 0.70              |
| 1:q:199:ARG:NH1  | 1:q:224:GLY:O    | 2.25                     | 0.70              |
| 1:q:289:THR:HG21 | 1:q:330:LEU:HG   | 1.74                     | 0.70              |
| 1:O:285:ILE:O    | 1:O:289:THR:HG22 | 1.91                     | 0.70              |
| 1:o:116:ARG:HG3  | 1:o:116:ARG:NH2  | 1.91                     | 0.69              |
| 1:L:242:SER:O    | 1:l:206:ARG:NH1  | 2.25                     | 0.69              |
| 1:a:116:ARG:HG2  | 1:a:116:ARG:NH2  | 1.93                     | 0.69              |
| 1:Q:298:ARG:NH2  | 1:Q:316:ASP:OD2  | 2.22                     | 0.69              |
| 1:C:298:ARG:NH1  | 1:C:313:ARG:CZ   | 2.52                     | 0.69              |
| 1:C:298:ARG:NH1  | 1:C:313:ARG:HH11 | 1.91                     | 0.69              |
| 1:R:242:SER:O    | 1:r:206:ARG:NH1  | 2.25                     | 0.69              |
| 1:G:238:LEU:HD23 | 1:g:229:ILE:HG12 | 1.75                     | 0.68              |
| 1:q:166:ARG:HH21 | 1:R:213:ARG:HE   | 1.38                     | 0.68              |
| 1:k:216:ASN:O    | 1:k:220:LEU:HD12 | 1.92                     | 0.68              |
| 1:s:150:LYS:HA   | 1:s:150:LYS:HE2  | 1.75                     | 0.68              |
| 1:n:288:VAL:HG11 | 1:n:333:TYR:CE1  | 2.28                     | 0.68              |
| 1:s:270:PRO:HD2  | 1:s:334:ILE:HG22 | 1.75                     | 0.68              |
| 1:C:324:PRO:HB3  | 1:s:325:GLU:CG   | 2.21                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:298:ARG:NH1  | 1:A:313:ARG:HD2  | 2.05                     | 0.68              |
| 1:T:199:ARG:NH2  | 1:T:205:VAL:O    | 2.26                     | 0.68              |
| 1:c:298:ARG:NH2  | 1:c:316:ASP:OD2  | 2.26                     | 0.68              |
| 1:H:289:THR:HG23 | 1:H:291:VAL:H    | 1.60                     | 0.67              |
| 1:o:289:THR:HG23 | 1:o:291:VAL:H    | 1.59                     | 0.67              |
| 1:s:116:ARG:HG3  | 1:s:116:ARG:NH2  | 2.00                     | 0.67              |
| 1:R:289:THR:HG23 | 1:R:291:VAL:H    | 1.59                     | 0.67              |
| 1:p:116:ARG:HG3  | 1:p:116:ARG:NH2  | 2.09                     | 0.67              |
| 1:J:199:ARG:NH2  | 1:J:205:VAL:O    | 2.27                     | 0.67              |
| 1:j:211:ALA:HB2  | 1:j:220:LEU:HD22 | 1.77                     | 0.67              |
| 1:a:324:PRO:CB   | 1:o:325:GLU:CG   | 2.71                     | 0.67              |
| 1:C:183:VAL:HG12 | 1:C:191:THR:HG23 | 1.77                     | 0.66              |
| 1:D:242:SER:O    | 1:d:206:ARG:NH1  | 2.28                     | 0.66              |
| 1:E:242:SER:O    | 1:e:206:ARG:NH1  | 2.28                     | 0.66              |
| 1:L:270:PRO:HD2  | 1:L:334:ILE:HG22 | 1.77                     | 0.66              |
| 1:B:242:SER:O    | 1:b:206:ARG:NH1  | 2.28                     | 0.66              |
| 1:E:117:HIS:HE1  | 1:E:174:ASN:HB3  | 1.61                     | 0.66              |
| 1:e:298:ARG:HH22 | 1:e:313:ARG:NE   | 1.93                     | 0.66              |
| 1:L:298:ARG:NH2  | 1:L:316:ASP:OD2  | 2.29                     | 0.66              |
| 1:T:120:ILE:HG12 | 1:T:182:ILE:HB   | 1.77                     | 0.66              |
| 1:E:298:ARG:HH22 | 1:E:313:ARG:HH11 | 1.43                     | 0.66              |
| 1:e:298:ARG:HH22 | 1:e:313:ARG:CD   | 2.08                     | 0.66              |
| 1:o:146:GLU:OE1  | 1:o:149:ARG:NH1  | 2.29                     | 0.66              |
| 1:D:289:THR:HG23 | 1:D:291:VAL:H    | 1.61                     | 0.66              |
| 1:g:131:LEU:O    | 1:g:135:ARG:HB2  | 1.95                     | 0.66              |
| 1:d:298:ARG:NH1  | 1:d:313:ARG:CZ   | 2.57                     | 0.66              |
| 1:g:264:MET:HE2  | 1:g:321:ILE:HG12 | 1.78                     | 0.66              |
| 1:d:116:ARG:HG3  | 1:d:116:ARG:NH2  | 2.04                     | 0.66              |
| 1:J:176:ARG:HG3  | 1:J:176:ARG:NH2  | 2.02                     | 0.66              |
| 1:c:298:ARG:CZ   | 1:c:316:ASP:OD1  | 2.44                     | 0.65              |
| 1:l:330:LEU:HD22 | 1:l:334:ILE:HD11 | 1.77                     | 0.65              |
| 1:A:125:GLU:HB3  | 1:a:232:PHE:HD1  | 1.61                     | 0.65              |
| 1:L:289:THR:HG23 | 1:L:291:VAL:H    | 1.60                     | 0.65              |
| 1:J:237:ARG:HH11 | 1:J:241:ARG:HE   | 1.43                     | 0.65              |
| 1:a:131:LEU:O    | 1:a:135:ARG:HB2  | 1.95                     | 0.65              |
| 1:O:213:ARG:HB3  | 1:O:215:GLU:HG3  | 1.78                     | 0.65              |
| 1:s:289:THR:HG23 | 1:s:291:VAL:H    | 1.60                     | 0.65              |
| 1:I:270:PRO:HD2  | 1:I:334:ILE:HG22 | 1.78                     | 0.65              |
| 1:A:305:ASP:HB2  | 1:a:292:ILE:HD11 | 1.77                     | 0.65              |
| 1:K:133:GLU:OE1  | 1:k:241:ARG:NH1  | 2.30                     | 0.65              |
| 1:S:285:ILE:O    | 1:S:289:THR:HG22 | 1.97                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:146:GLU:OE1  | 1:s:149:ARG:NH1  | 2.29                     | 0.65              |
| 1:H:232:PHE:CD1  | 1:h:125:GLU:HB3  | 2.31                     | 0.65              |
| 1:E:286:HIS:HE1  | 1:e:305:ASP:OD1  | 1.79                     | 0.64              |
| 1:G:285:ILE:O    | 1:G:289:THR:HG22 | 1.97                     | 0.64              |
| 1:i:116:ARG:HH21 | 1:i:116:ARG:HG3  | 1.62                     | 0.64              |
| 1:q:285:ILE:O    | 1:q:289:THR:HG22 | 1.97                     | 0.64              |
| 1:D:324:PRO:HB2  | 1:N:325:GLU:CG   | 2.27                     | 0.64              |
| 1:m:298:ARG:HH22 | 1:m:313:ARG:CB   | 2.02                     | 0.64              |
| 1:B:294:ILE:HD11 | 1:B:321:ILE:HG13 | 1.79                     | 0.64              |
| 1:C:269:ILE:HD12 | 1:C:316:ASP:HB2  | 1.79                     | 0.64              |
| 1:E:117:HIS:CE1  | 1:E:174:ASN:HB3  | 2.32                     | 0.64              |
| 1:D:305:ASP:HB2  | 1:d:292:ILE:HD11 | 1.79                     | 0.64              |
| 1:H:165:THR:HB   | 1:H:193:HIS:ND1  | 2.13                     | 0.64              |
| 1:k:294:ILE:HD11 | 1:k:321:ILE:HD11 | 1.78                     | 0.64              |
| 1:d:270:PRO:HD2  | 1:d:273:SER:HB2  | 1.79                     | 0.64              |
| 1:K:131:LEU:O    | 1:K:135:ARG:HB2  | 1.98                     | 0.64              |
| 1:n:270:PRO:HD3  | 1:n:334:ILE:HG23 | 1.80                     | 0.64              |
| 1:p:199:ARG:NH1  | 1:p:224:GLY:O    | 2.30                     | 0.64              |
| 1:N:199:ARG:NH1  | 1:N:224:GLY:O    | 2.31                     | 0.64              |
| 1:f:298:ARG:NH2  | 1:f:310:TYR:CZ   | 2.65                     | 0.64              |
| 1:H:262:ARG:HH11 | 1:H:262:ARG:CG   | 2.11                     | 0.64              |
| 1:i:285:ILE:HB   | 1:i:293:ILE:HD11 | 1.79                     | 0.64              |
| 1:R:289:THR:HG21 | 1:R:330:LEU:HG   | 1.80                     | 0.64              |
| 1:a:298:ARG:CZ   | 1:a:316:ASP:OD1  | 2.46                     | 0.64              |
| 1:r:264:MET:HE2  | 1:r:321:ILE:HG12 | 1.79                     | 0.64              |
| 1:B:165:THR:HB   | 1:B:193:HIS:ND1  | 2.11                     | 0.63              |
| 1:R:285:ILE:O    | 1:R:289:THR:HG22 | 1.98                     | 0.63              |
| 1:i:324:PRO:CB   | 1:S:325:GLU:HG2  | 2.08                     | 0.63              |
| 1:k:234:ILE:O    | 1:k:238:LEU:HB2  | 1.99                     | 0.63              |
| 1:C:324:PRO:CB   | 1:s:325:GLU:CG   | 2.77                     | 0.63              |
| 1:f:274:LYS:HD3  | 1:f:335:SER:O    | 1.98                     | 0.63              |
| 1:L:294:ILE:HD11 | 1:L:321:ILE:HG13 | 1.81                     | 0.63              |
| 1:O:242:SER:O    | 1:o:206:ARG:NH1  | 2.31                     | 0.63              |
| 1:H:262:ARG:HH11 | 1:H:262:ARG:HG3  | 1.62                     | 0.63              |
| 1:C:132:ARG:HH11 | 1:C:132:ARG:CG   | 2.02                     | 0.63              |
| 1:f:330:LEU:HD22 | 1:f:334:ILE:HD11 | 1.81                     | 0.63              |
| 1:k:285:ILE:O    | 1:k:289:THR:HG22 | 1.99                     | 0.63              |
| 1:M:213:ARG:HG2  | 1:p:166:ARG:NH2  | 2.13                     | 0.63              |
| 1:B:133:GLU:OE1  | 1:b:241:ARG:NH1  | 2.32                     | 0.63              |
| 1:D:206:ARG:NH1  | 1:d:242:SER:O    | 2.29                     | 0.63              |
| 1:r:289:THR:HG23 | 1:r:291:VAL:H    | 1.64                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:131:LEU:HD21 | 1:F:139:VAL:HG11 | 1.82                     | 0.62              |
| 1:d:289:THR:HG23 | 1:d:291:VAL:H    | 1.65                     | 0.62              |
| 1:O:116:ARG:HG3  | 1:O:116:ARG:NH2  | 2.12                     | 0.62              |
| 1:g:285:ILE:HD12 | 1:g:293:ILE:HD11 | 1.82                     | 0.62              |
| 1:H:262:ARG:NH1  | 1:h:304:ILE:HB   | 2.13                     | 0.62              |
| 1:P:285:ILE:O    | 1:P:289:THR:HG22 | 2.00                     | 0.62              |
| 1:H:125:GLU:HB3  | 1:h:232:PHE:HD1  | 1.65                     | 0.62              |
| 1:I:199:ARG:HE   | 1:I:203:GLU:HA   | 1.64                     | 0.62              |
| 1:k:116:ARG:HB2  | 1:k:116:ARG:NH2  | 2.12                     | 0.62              |
| 1:k:161:HIS:O    | 1:l:154:ARG:NH1  | 2.33                     | 0.62              |
| 1:S:183:VAL:HG12 | 1:S:191:THR:HG23 | 1.80                     | 0.62              |
| 1:l:298:ARG:NH2  | 1:l:310:TYR:OH   | 2.33                     | 0.61              |
| 1:M:242:SER:O    | 1:m:206:ARG:NH1  | 2.33                     | 0.61              |
| 1:n:289:THR:HG21 | 1:n:330:LEU:HG   | 1.81                     | 0.61              |
| 1:L:298:ARG:HH21 | 1:L:316:ASP:CG   | 2.08                     | 0.61              |
| 1:N:298:ARG:NH1  | 1:N:313:ARG:NH1  | 2.48                     | 0.61              |
| 1:H:237:ARG:HH11 | 1:H:241:ARG:HH22 | 1.49                     | 0.61              |
| 1:D:211:ALA:HB2  | 1:D:220:LEU:HD22 | 1.83                     | 0.61              |
| 1:i:284:ASP:OD1  | 1:i:287:ASP:HB2  | 2.00                     | 0.61              |
| 1:J:211:ALA:HB2  | 1:J:220:LEU:HD22 | 1.83                     | 0.61              |
| 1:n:280:VAL:HG22 | 1:n:312:PHE:HE1  | 1.65                     | 0.61              |
| 1:Q:294:ILE:HD11 | 1:Q:321:ILE:HD11 | 1.82                     | 0.61              |
| 1:t:285:ILE:HB   | 1:t:293:ILE:HD11 | 1.81                     | 0.61              |
| 1:a:237:ARG:HH11 | 1:a:241:ARG:HD3  | 1.66                     | 0.61              |
| 1:G:270:PRO:HD2  | 1:G:334:ILE:CG2  | 2.30                     | 0.61              |
| 1:k:199:ARG:NH2  | 1:k:205:VAL:O    | 2.32                     | 0.61              |
| 1:h:270:PRO:HD2  | 1:h:334:ILE:HG22 | 1.83                     | 0.61              |
| 1:F:270:PRO:HD2  | 1:F:334:ILE:HG22 | 1.83                     | 0.60              |
| 1:k:289:THR:HG23 | 1:k:291:VAL:H    | 1.66                     | 0.60              |
| 1:P:289:THR:HG21 | 1:P:330:LEU:HG   | 1.82                     | 0.60              |
| 1:S:289:THR:HG23 | 1:S:291:VAL:H    | 1.66                     | 0.60              |
| 1:j:330:LEU:HD22 | 1:j:334:ILE:HD11 | 1.83                     | 0.60              |
| 1:m:308:ARG:HG2  | 1:m:308:ARG:NH1  | 2.02                     | 0.60              |
| 1:T:289:THR:HG21 | 1:T:330:LEU:HG   | 1.82                     | 0.60              |
| 1:c:298:ARG:NH2  | 1:c:316:ASP:OD1  | 2.35                     | 0.60              |
| 1:q:294:ILE:HD11 | 1:q:321:ILE:HG13 | 1.83                     | 0.60              |
| 1:J:289:THR:HG23 | 1:J:291:VAL:H    | 1.67                     | 0.60              |
| 1:N:241:ARG:NH1  | 1:n:133:GLU:OE1  | 2.35                     | 0.60              |
| 1:q:298:ARG:NE   | 1:q:316:ASP:OD1  | 2.30                     | 0.60              |
| 1:C:131:LEU:O    | 1:C:135:ARG:HB2  | 2.02                     | 0.60              |
| 1:n:294:ILE:HD11 | 1:n:321:ILE:HG13 | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:270:PRO:HD3  | 1:C:334:ILE:HG21 | 1.82                     | 0.60              |
| 1:o:116:ARG:HD2  | 1:o:179:ARG:HG2  | 1.83                     | 0.60              |
| 1:T:199:ARG:NH1  | 1:T:224:GLY:O    | 2.35                     | 0.60              |
| 1:a:298:ARG:CZ   | 1:a:313:ARG:HD2  | 2.31                     | 0.60              |
| 1:c:298:ARG:NH2  | 1:c:316:ASP:CG   | 2.60                     | 0.60              |
| 1:P:242:SER:O    | 1:p:206:ARG:NH1  | 2.35                     | 0.60              |
| 1:r:285:ILE:HG21 | 1:r:293:ILE:HD11 | 1.83                     | 0.60              |
| 1:C:264:MET:HE2  | 1:C:321:ILE:HG12 | 1.84                     | 0.60              |
| 1:e:171:GLU:OE2  | 1:e:176:ARG:NH2  | 2.35                     | 0.60              |
| 1:g:263:ARG:HH21 | 1:g:265:VAL:HG12 | 1.66                     | 0.60              |
| 1:I:199:ARG:NH1  | 1:I:207:ILE:HD12 | 2.16                     | 0.60              |
| 1:a:132:ARG:HG3  | 1:a:132:ARG:NH1  | 2.04                     | 0.60              |
| 1:B:287:ASP:OD1  | 1:b:308:ARG:NH2  | 2.35                     | 0.60              |
| 1:I:285:ILE:O    | 1:I:289:THR:HG22 | 2.01                     | 0.60              |
| 1:Q:285:ILE:O    | 1:Q:289:THR:HG22 | 2.02                     | 0.60              |
| 1:T:259:GLU:HG2  | 1:T:263:ARG:HB2  | 1.84                     | 0.60              |
| 1:I:134:LEU:HD11 | 1:i:243:ILE:HD11 | 1.84                     | 0.59              |
| 1:l:176:ARG:HD2  | 1:s:299:GLY:HA3  | 1.84                     | 0.59              |
| 1:H:131:LEU:O    | 1:H:135:ARG:HB2  | 2.01                     | 0.59              |
| 1:J:131:LEU:O    | 1:J:135:ARG:HB2  | 2.02                     | 0.59              |
| 1:K:289:THR:HG23 | 1:K:291:VAL:H    | 1.66                     | 0.59              |
| 1:R:145:ASP:HB3  | 1:R:148:VAL:HG23 | 1.85                     | 0.59              |
| 1:E:275:LEU:HD12 | 1:E:334:ILE:HG23 | 1.84                     | 0.59              |
| 1:o:285:ILE:O    | 1:o:289:THR:HG22 | 2.01                     | 0.59              |
| 1:H:330:LEU:HD22 | 1:H:334:ILE:HD11 | 1.85                     | 0.59              |
| 1:c:298:ARG:HH22 | 1:c:313:ARG:CB   | 2.12                     | 0.59              |
| 1:H:243:ILE:HD11 | 1:h:134:LEU:HD11 | 1.83                     | 0.59              |
| 1:P:270:PRO:HD2  | 1:P:334:ILE:HG22 | 1.84                     | 0.59              |
| 1:e:199:ARG:NH2  | 1:e:205:VAL:O    | 2.32                     | 0.59              |
| 1:r:335:SER:O    | 1:r:336:ALA:HB2  | 2.01                     | 0.59              |
| 1:j:285:ILE:O    | 1:j:289:THR:HG22 | 2.03                     | 0.59              |
| 1:l:270:PRO:HD2  | 1:l:334:ILE:HG22 | 1.85                     | 0.59              |
| 1:O:217:ILE:HG23 | 1:O:228:VAL:HG11 | 1.83                     | 0.59              |
| 1:E:263:ARG:HH11 | 1:E:265:VAL:HG12 | 1.66                     | 0.59              |
| 1:f:211:ALA:HB2  | 1:f:220:LEU:HD22 | 1.84                     | 0.59              |
| 1:R:262:ARG:HG3  | 1:R:262:ARG:NH1  | 2.12                     | 0.59              |
| 1:f:289:THR:HG23 | 1:f:291:VAL:H    | 1.67                     | 0.59              |
| 1:f:195:ILE:HA   | 1:f:198:ILE:HD12 | 1.84                     | 0.58              |
| 1:g:265:VAL:HG11 | 1:g:327:ILE:HG12 | 1.85                     | 0.58              |
| 1:Q:289:THR:HG21 | 1:Q:330:LEU:HG   | 1.83                     | 0.58              |
| 1:s:270:PRO:CD   | 1:s:334:ILE:HG22 | 2.33                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:211:ALA:HB2  | 1:b:220:LEU:HD22 | 1.85                     | 0.58              |
| 1:j:307:PRO:HG2  | 1:j:310:TYR:HB2  | 1.84                     | 0.58              |
| 1:N:242:SER:O    | 1:n:206:ARG:NH1  | 2.36                     | 0.58              |
| 1:q:219:GLN:HE21 | 1:R:200:LYS:HE2  | 1.66                     | 0.58              |
| 1:F:335:SER:O    | 1:F:336:ALA:HB2  | 2.04                     | 0.58              |
| 1:e:270:PRO:HD2  | 1:e:334:ILE:HG22 | 1.84                     | 0.58              |
| 1:J:234:ILE:HG22 | 1:J:238:LEU:HD13 | 1.86                     | 0.58              |
| 1:P:298:ARG:HH12 | 1:P:313:ARG:NE   | 2.00                     | 0.58              |
| 1:n:199:ARG:NH2  | 1:n:205:VAL:O    | 2.30                     | 0.58              |
| 1:G:134:LEU:O    | 1:G:137:SER:HB2  | 2.03                     | 0.58              |
| 1:j:242:SER:OG   | 1:j:249:ALA:HB2  | 2.04                     | 0.58              |
| 1:l:289:THR:HG23 | 1:l:291:VAL:H    | 1.68                     | 0.58              |
| 1:q:298:ARG:HH22 | 1:q:313:ARG:HD2  | 1.69                     | 0.58              |
| 1:D:247:TYR:H    | 1:d:266:GLU:CD   | 2.12                     | 0.58              |
| 1:D:270:PRO:HD2  | 1:D:273:SER:HB2  | 1.86                     | 0.58              |
| 1:H:252:VAL:HA   | 1:H:256:LEU:HD23 | 1.85                     | 0.58              |
| 1:I:298:ARG:HH12 | 1:I:313:ARG:HD2  | 1.69                     | 0.58              |
| 1:i:143:ALA:HB3  | 1:i:159:PHE:HE1  | 1.68                     | 0.58              |
| 1:p:298:ARG:HH12 | 1:p:313:ARG:CZ   | 2.17                     | 0.58              |
| 1:S:335:SER:O    | 1:S:336:ALA:CB   | 2.51                     | 0.58              |
| 1:g:199:ARG:NH2  | 1:g:205:VAL:O    | 2.37                     | 0.57              |
| 1:l:146:GLU:OE1  | 1:l:149:ARG:NH1  | 2.37                     | 0.57              |
| 1:E:298:ARG:NH2  | 1:E:313:ARG:HD2  | 2.19                     | 0.57              |
| 1:H:294:ILE:HD11 | 1:H:321:ILE:CD1  | 2.33                     | 0.57              |
| 1:L:285:ILE:O    | 1:L:289:THR:HG22 | 2.03                     | 0.57              |
| 1:m:298:ARG:NH2  | 1:m:313:ARG:HD2  | 2.19                     | 0.57              |
| 1:Q:298:ARG:NE   | 1:Q:316:ASP:OD1  | 2.37                     | 0.57              |
| 1:O:265:VAL:HG11 | 1:O:327:ILE:HG12 | 1.86                     | 0.57              |
| 1:G:289:THR:HG21 | 1:G:330:LEU:HG   | 1.86                     | 0.57              |
| 1:M:298:ARG:NH2  | 1:M:313:ARG:HB2  | 2.19                     | 0.57              |
| 1:N:147:ASN:HD22 | 1:N:147:ASN:N    | 2.02                     | 0.57              |
| 1:o:330:LEU:O    | 1:o:334:ILE:HG13 | 2.04                     | 0.57              |
| 1:f:199:ARG:NH2  | 1:f:205:VAL:O    | 2.34                     | 0.57              |
| 1:i:131:LEU:O    | 1:i:135:ARG:HB2  | 2.04                     | 0.57              |
| 1:K:285:ILE:O    | 1:K:289:THR:HG22 | 2.04                     | 0.57              |
| 1:O:206:ARG:NH1  | 1:o:242:SER:O    | 2.37                     | 0.57              |
| 1:T:164:PRO:HG3  | 1:T:185:LEU:HD21 | 1.85                     | 0.57              |
| 1:i:289:THR:HG23 | 1:i:291:VAL:H    | 1.69                     | 0.57              |
| 1:M:270:PRO:HD2  | 1:M:334:ILE:HG22 | 1.86                     | 0.57              |
| 1:r:279:SER:HA   | 1:r:310:TYR:O    | 2.05                     | 0.57              |
| 1:s:270:PRO:HD3  | 1:s:334:ILE:HG21 | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:253:GLN:O    | 1:a:257:ALA:HB3  | 2.05                     | 0.57              |
| 1:f:229:ILE:O    | 1:f:231:PRO:HD3  | 2.05                     | 0.57              |
| 1:I:166:ARG:HB3  | 1:I:169:ASP:HB2  | 1.85                     | 0.57              |
| 1:J:237:ARG:HH11 | 1:J:241:ARG:NE   | 2.03                     | 0.57              |
| 1:K:242:SER:O    | 1:k:206:ARG:NH1  | 2.38                     | 0.57              |
| 1:O:335:SER:O    | 1:O:336:ALA:CB   | 2.52                     | 0.57              |
| 1:f:171:GLU:OE2  | 1:f:176:ARG:NH2  | 2.38                     | 0.57              |
| 1:H:211:ALA:HB2  | 1:H:220:LEU:HD22 | 1.86                     | 0.57              |
| 1:Q:298:ARG:HE   | 1:Q:316:ASP:CG   | 2.12                     | 0.57              |
| 1:E:298:ARG:NH2  | 1:E:313:ARG:HB2  | 2.19                     | 0.57              |
| 1:N:302:LEU:HG   | 1:N:304:ILE:HG13 | 1.86                     | 0.57              |
| 1:b:298:ARG:HH12 | 1:b:313:ARG:CZ   | 2.19                     | 0.56              |
| 1:E:164:PRO:HG2  | 1:E:185:LEU:HD21 | 1.85                     | 0.56              |
| 1:I:199:ARG:NH2  | 1:I:205:VAL:O    | 2.37                     | 0.56              |
| 1:t:120:ILE:HB   | 1:t:141:VAL:HG22 | 1.88                     | 0.56              |
| 1:G:118:VAL:HG21 | 1:g:243:ILE:HD13 | 1.88                     | 0.56              |
| 1:F:298:ARG:NH2  | 1:F:310:TYR:OH   | 2.39                     | 0.56              |
| 1:O:289:THR:HG23 | 1:O:291:VAL:H    | 1.69                     | 0.56              |
| 1:h:242:SER:OG   | 1:h:249:ALA:HB2  | 2.05                     | 0.56              |
| 1:N:285:ILE:O    | 1:N:289:THR:HG22 | 2.05                     | 0.56              |
| 1:l:203:GLU:HG2  | 1:s:300:ASP:OD2  | 2.05                     | 0.56              |
| 1:s:285:ILE:HD12 | 1:s:293:ILE:HD11 | 1.87                     | 0.56              |
| 1:T:237:ARG:HG2  | 1:T:241:ARG:NH1  | 2.20                     | 0.56              |
| 1:n:270:PRO:HD3  | 1:n:334:ILE:CG2  | 2.36                     | 0.56              |
| 1:P:289:THR:HG23 | 1:P:291:VAL:H    | 1.71                     | 0.56              |
| 1:f:175:VAL:HG13 | 1:f:198:ILE:HG23 | 1.88                     | 0.56              |
| 1:I:289:THR:HG21 | 1:I:330:LEU:HG   | 1.86                     | 0.56              |
| 1:M:298:ARG:HH21 | 1:M:316:ASP:CG   | 2.13                     | 0.56              |
| 1:S:206:ARG:NH1  | 1:s:242:SER:O    | 2.39                     | 0.56              |
| 1:N:269:ILE:HD12 | 1:N:316:ASP:HB2  | 1.88                     | 0.56              |
| 1:n:131:LEU:O    | 1:n:135:ARG:HB2  | 2.06                     | 0.56              |
| 1:G:242:SER:OG   | 1:G:249:ALA:HB2  | 2.06                     | 0.55              |
| 1:F:289:THR:HG23 | 1:F:291:VAL:H    | 1.71                     | 0.55              |
| 1:l:206:ARG:NH1  | 1:l:208:ILE:HD11 | 2.21                     | 0.55              |
| 1:J:298:ARG:NH1  | 1:J:313:ARG:HD2  | 2.22                     | 0.55              |
| 1:K:298:ARG:NH2  | 1:K:313:ARG:HG3  | 2.21                     | 0.55              |
| 1:m:289:THR:HG21 | 1:m:330:LEU:HG   | 1.88                     | 0.55              |
| 1:n:284:ASP:O    | 1:n:288:VAL:HG23 | 2.05                     | 0.55              |
| 1:n:294:ILE:HD11 | 1:n:321:ILE:CD1  | 2.37                     | 0.55              |
| 1:o:131:LEU:O    | 1:o:135:ARG:HB2  | 2.07                     | 0.55              |
| 1:R:302:LEU:HD13 | 1:r:247:TYR:HB3  | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:131:LEU:O    | 1:j:135:ARG:HB2  | 2.05                     | 0.55              |
| 1:m:330:LEU:HD22 | 1:m:334:ILE:HD11 | 1.89                     | 0.55              |
| 1:C:298:ARG:HH11 | 1:C:313:ARG:NH1  | 1.95                     | 0.55              |
| 1:F:232:PHE:H    | 1:F:232:PHE:HD2  | 1.53                     | 0.55              |
| 1:l:285:ILE:O    | 1:l:289:THR:HG22 | 2.06                     | 0.55              |
| 1:q:281:LEU:HD13 | 1:q:308:ARG:HE   | 1.72                     | 0.55              |
| 1:T:285:ILE:O    | 1:T:289:THR:HG22 | 2.05                     | 0.55              |
| 1:f:200:LYS:HE3  | 1:G:218:GLU:HG2  | 1.88                     | 0.55              |
| 1:K:298:ARG:NH2  | 1:K:313:ARG:HB2  | 2.19                     | 0.55              |
| 1:B:330:LEU:O    | 1:B:334:ILE:HG13 | 2.06                     | 0.55              |
| 1:J:171:GLU:HG3  | 1:J:201:ILE:HD13 | 1.87                     | 0.55              |
| 1:M:292:ILE:HD11 | 1:m:305:ASP:HB2  | 1.88                     | 0.54              |
| 1:a:298:ARG:NH2  | 1:a:316:ASP:OD1  | 2.40                     | 0.54              |
| 1:K:199:ARG:NH1  | 1:K:224:GLY:O    | 2.39                     | 0.54              |
| 1:c:211:ALA:HB2  | 1:c:220:LEU:HD22 | 1.90                     | 0.54              |
| 1:d:199:ARG:HE   | 1:d:203:GLU:HA   | 1.72                     | 0.54              |
| 1:M:294:ILE:HD11 | 1:M:321:ILE:HD11 | 1.89                     | 0.54              |
| 1:E:264:MET:HG2  | 1:e:248:GLU:HG3  | 1.90                     | 0.54              |
| 1:J:318:ILE:HD12 | 1:J:334:ILE:HD11 | 1.88                     | 0.54              |
| 1:K:125:GLU:CD   | 1:L:166:ARG:HH22 | 2.15                     | 0.54              |
| 1:m:146:GLU:OE1  | 1:m:149:ARG:NH1  | 2.40                     | 0.54              |
| 1:O:330:LEU:HD22 | 1:O:334:ILE:HD11 | 1.89                     | 0.54              |
| 1:o:175:VAL:HG22 | 1:o:181:VAL:HG21 | 1.90                     | 0.54              |
| 1:o:192:ILE:HG13 | 1:o:220:LEU:HD12 | 1.90                     | 0.54              |
| 1:e:289:THR:HG23 | 1:e:291:VAL:H    | 1.73                     | 0.54              |
| 1:J:188:ASP:CB   | 1:J:216:ASN:ND2  | 2.64                     | 0.54              |
| 1:O:116:ARG:HD2  | 1:O:179:ARG:HG3  | 1.88                     | 0.54              |
| 1:F:335:SER:O    | 1:F:336:ALA:CB   | 2.56                     | 0.54              |
| 1:H:298:ARG:HH12 | 1:H:313:ARG:CB   | 2.21                     | 0.54              |
| 1:J:237:ARG:O    | 1:J:241:ARG:HD3  | 2.07                     | 0.54              |
| 1:K:211:ALA:HB2  | 1:K:220:LEU:HD22 | 1.88                     | 0.54              |
| 1:L:146:GLU:OE1  | 1:L:149:ARG:NH1  | 2.41                     | 0.54              |
| 1:l:199:ARG:HE   | 1:l:203:GLU:HA   | 1.72                     | 0.54              |
| 1:Q:298:ARG:CZ   | 1:Q:310:TYR:OH   | 2.56                     | 0.54              |
| 1:q:217:ILE:HG23 | 1:q:228:VAL:HG11 | 1.88                     | 0.54              |
| 1:L:145:ASP:HB3  | 1:L:148:VAL:HG23 | 1.89                     | 0.54              |
| 1:a:146:GLU:OE1  | 1:a:149:ARG:NH1  | 2.41                     | 0.54              |
| 1:m:298:ARG:CZ   | 1:m:316:ASP:OD1  | 2.56                     | 0.54              |
| 1:P:199:ARG:NH1  | 1:P:224:GLY:O    | 2.41                     | 0.54              |
| 1:R:330:LEU:O    | 1:R:334:ILE:HG13 | 2.07                     | 0.54              |
| 1:O:285:ILE:HG21 | 1:O:293:ILE:HD11 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:269:ILE:HD12 | 1:a:316:ASP:HB2  | 1.90                     | 0.53              |
| 1:c:171:GLU:HG3  | 1:c:201:ILE:HD13 | 1.90                     | 0.53              |
| 1:A:217:ILE:HG23 | 1:A:228:VAL:HG11 | 1.91                     | 0.53              |
| 1:a:324:PRO:HB2  | 1:o:325:GLU:HG3  | 1.88                     | 0.53              |
| 1:B:298:ARG:HH12 | 1:B:313:ARG:HD2  | 1.73                     | 0.53              |
| 1:E:213:ARG:HG2  | 1:h:166:ARG:NH2  | 2.23                     | 0.53              |
| 1:E:263:ARG:HG3  | 1:E:264:MET:N    | 2.24                     | 0.53              |
| 1:j:166:ARG:HH22 | 1:K:213:ARG:HG2  | 1.73                     | 0.53              |
| 1:s:270:PRO:CD   | 1:s:334:ILE:CG2  | 2.86                     | 0.53              |
| 1:B:268:PRO:O    | 1:B:270:PRO:HD3  | 2.07                     | 0.53              |
| 1:h:240:SER:HA   | 1:h:243:ILE:HD12 | 1.90                     | 0.53              |
| 1:j:242:SER:HA   | 1:j:246:GLY:HA3  | 1.90                     | 0.53              |
| 1:A:116:ARG:HG3  | 1:A:116:ARG:NH2  | 2.21                     | 0.53              |
| 1:e:237:ARG:HH11 | 1:e:241:ARG:NH2  | 2.06                     | 0.53              |
| 1:P:302:LEU:HD13 | 1:p:247:TYR:HB3  | 1.91                     | 0.53              |
| 1:D:294:ILE:HD11 | 1:D:321:ILE:HD11 | 1.90                     | 0.53              |
| 1:J:284:ASP:OD1  | 1:J:287:ASP:HB2  | 2.09                     | 0.53              |
| 1:m:289:THR:HG23 | 1:m:291:VAL:H    | 1.73                     | 0.53              |
| 1:F:118:VAL:HB   | 1:F:139:VAL:HG22 | 1.90                     | 0.53              |
| 1:M:289:THR:HG21 | 1:M:330:LEU:HG   | 1.90                     | 0.53              |
| 1:N:211:ALA:HB2  | 1:N:220:LEU:HD22 | 1.90                     | 0.53              |
| 1:P:270:PRO:HD2  | 1:P:334:ILE:CG2  | 2.37                     | 0.53              |
| 1:p:298:ARG:HH12 | 1:p:313:ARG:NE   | 2.06                     | 0.53              |
| 1:F:237:ARG:O    | 1:F:241:ARG:HB2  | 2.09                     | 0.53              |
| 1:G:270:PRO:O    | 1:G:273:SER:HB2  | 2.09                     | 0.53              |
| 1:L:166:ARG:HB3  | 1:L:169:ASP:HB2  | 1.91                     | 0.53              |
| 1:A:171:GLU:HG3  | 1:A:201:ILE:HD13 | 1.91                     | 0.53              |
| 1:f:285:ILE:HD12 | 1:f:293:ILE:HD11 | 1.90                     | 0.53              |
| 1:J:154:ARG:HE   | 1:K:172:LYS:NZ   | 2.06                     | 0.53              |
| 1:J:238:LEU:HD23 | 1:j:229:ILE:HG12 | 1.90                     | 0.53              |
| 1:L:199:ARG:HE   | 1:L:203:GLU:HA   | 1.73                     | 0.53              |
| 1:t:165:THR:HB   | 1:t:193:HIS:ND1  | 2.23                     | 0.53              |
| 1:A:298:ARG:NH1  | 1:A:313:ARG:HH11 | 2.06                     | 0.53              |
| 1:a:237:ARG:HD2  | 1:a:241:ARG:NH1  | 2.24                     | 0.53              |
| 1:a:298:ARG:NH2  | 1:a:313:ARG:HD2  | 2.24                     | 0.53              |
| 1:D:285:ILE:HB   | 1:D:293:ILE:HD11 | 1.90                     | 0.53              |
| 1:G:242:SER:O    | 1:g:206:ARG:NH1  | 2.42                     | 0.53              |
| 1:i:279:SER:HA   | 1:i:310:TYR:O    | 2.09                     | 0.53              |
| 1:j:199:ARG:NH2  | 1:j:205:VAL:O    | 2.42                     | 0.53              |
| 1:N:298:ARG:HH22 | 1:N:313:ARG:HB2  | 1.72                     | 0.53              |
| 1:R:298:ARG:HH22 | 1:R:313:ARG:HB2  | 1.74                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:131:LEU:HD21 | 1:E:139:VAL:HG11 | 1.91                     | 0.52              |
| 1:f:166:ARG:HB3  | 1:f:169:ASP:HB2  | 1.91                     | 0.52              |
| 1:h:211:ALA:HB2  | 1:h:220:LEU:HD22 | 1.90                     | 0.52              |
| 1:n:247:TYR:HA   | 1:n:250:MET:HG2  | 1.90                     | 0.52              |
| 1:e:253:GLN:O    | 1:e:257:ALA:HB3  | 2.09                     | 0.52              |
| 1:L:133:GLU:OE1  | 1:l:241:ARG:NH1  | 2.42                     | 0.52              |
| 1:o:152:VAL:HG13 | 1:o:157:ALA:HB3  | 1.91                     | 0.52              |
| 1:r:309:ASP:OD1  | 1:r:309:ASP:N    | 2.41                     | 0.52              |
| 1:o:335:SER:O    | 1:o:336:ALA:HB2  | 2.09                     | 0.52              |
| 1:P:131:LEU:O    | 1:P:135:ARG:HB2  | 2.09                     | 0.52              |
| 1:F:232:PHE:N    | 1:F:232:PHE:CD2  | 2.77                     | 0.52              |
| 1:D:146:GLU:OE1  | 1:D:149:ARG:NH1  | 2.42                     | 0.52              |
| 1:g:146:GLU:O    | 1:g:149:ARG:HB3  | 2.09                     | 0.52              |
| 1:H:307:PRO:HG2  | 1:H:310:TYR:HB2  | 1.91                     | 0.52              |
| 1:j:289:THR:HG23 | 1:j:291:VAL:H    | 1.75                     | 0.52              |
| 1:O:229:ILE:HG22 | 1:O:231:PRO:HD3  | 1.92                     | 0.52              |
| 1:o:117:HIS:CE1  | 1:o:174:ASN:HB3  | 2.44                     | 0.52              |
| 1:p:289:THR:HG23 | 1:p:291:VAL:H    | 1.74                     | 0.52              |
| 1:Q:289:THR:HG23 | 1:Q:291:VAL:H    | 1.74                     | 0.52              |
| 1:S:241:ARG:NH1  | 1:s:133:GLU:OE1  | 2.42                     | 0.52              |
| 1:b:298:ARG:HH12 | 1:b:313:ARG:NH1  | 2.05                     | 0.52              |
| 1:E:211:ALA:HB2  | 1:E:220:LEU:HD22 | 1.90                     | 0.52              |
| 1:H:237:ARG:NH1  | 1:H:241:ARG:HH12 | 2.07                     | 0.52              |
| 1:j:199:ARG:NH1  | 1:j:224:GLY:O    | 2.42                     | 0.52              |
| 1:A:241:ARG:NH1  | 1:a:133:GLU:OE1  | 2.43                     | 0.52              |
| 1:B:305:ASP:HB2  | 1:b:292:ILE:HD11 | 1.92                     | 0.52              |
| 1:p:285:ILE:O    | 1:p:289:THR:HG22 | 2.10                     | 0.52              |
| 1:A:211:ALA:HB2  | 1:A:220:LEU:HD22 | 1.92                     | 0.52              |
| 1:Q:248:GLU:O    | 1:Q:252:VAL:HG23 | 2.10                     | 0.52              |
| 1:D:183:VAL:HG12 | 1:D:191:THR:HG23 | 1.91                     | 0.52              |
| 1:K:270:PRO:HD3  | 1:K:334:ILE:HG21 | 1.92                     | 0.52              |
| 1:M:289:THR:HG23 | 1:M:291:VAL:H    | 1.74                     | 0.52              |
| 1:P:298:ARG:NH1  | 1:P:313:ARG:HD2  | 2.22                     | 0.52              |
| 1:d:298:ARG:HG3  | 1:d:316:ASP:OD1  | 2.10                     | 0.51              |
| 1:G:263:ARG:NH2  | 1:G:327:ILE:HD13 | 2.25                     | 0.51              |
| 1:H:199:ARG:NH1  | 1:H:207:ILE:HD12 | 2.25                     | 0.51              |
| 1:J:285:ILE:HB   | 1:J:293:ILE:HD11 | 1.91                     | 0.51              |
| 1:L:231:PRO:HG2  | 1:L:232:PHE:CD2  | 2.45                     | 0.51              |
| 1:B:116:ARG:HB3  | 1:B:179:ARG:HB2  | 1.93                     | 0.51              |
| 1:c:289:THR:HG23 | 1:c:291:VAL:H    | 1.74                     | 0.51              |
| 1:d:300:ASP:OD2  | 1:O:203:GLU:HG2  | 2.09                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:g:285:ILE:HD12 | 1:g:293:ILE:CD1  | 2.39                     | 0.51              |
| 1:I:146:GLU:OE1  | 1:I:149:ARG:NH1  | 2.43                     | 0.51              |
| 1:K:298:ARG:HH22 | 1:K:313:ARG:HG3  | 1.75                     | 0.51              |
| 1:P:131:LEU:HD21 | 1:P:139:VAL:HG11 | 1.92                     | 0.51              |
| 1:r:294:ILE:HD11 | 1:r:321:ILE:HD11 | 1.91                     | 0.51              |
| 1:T:175:VAL:HG11 | 1:T:198:ILE:HG23 | 1.92                     | 0.51              |
| 1:C:298:ARG:HH12 | 1:C:313:ARG:CD   | 2.22                     | 0.51              |
| 1:g:263:ARG:NH2  | 1:g:265:VAL:HG12 | 2.25                     | 0.51              |
| 1:Q:274:LYS:HD3  | 1:Q:335:SER:O    | 2.10                     | 0.51              |
| 1:E:330:LEU:O    | 1:E:334:ILE:HG13 | 2.11                     | 0.51              |
| 1:G:289:THR:HG23 | 1:G:291:VAL:H    | 1.76                     | 0.51              |
| 1:h:289:THR:HG23 | 1:h:291:VAL:H    | 1.75                     | 0.51              |
| 1:h:330:LEU:HD22 | 1:h:334:ILE:HD11 | 1.92                     | 0.51              |
| 1:J:214:TYR:C    | 1:J:216:ASN:H    | 2.18                     | 0.51              |
| 1:J:264:MET:HE2  | 1:J:321:ILE:HD11 | 1.91                     | 0.51              |
| 1:K:133:GLU:HG3  | 1:k:240:SER:OG   | 2.10                     | 0.51              |
| 1:K:195:ILE:HA   | 1:K:198:ILE:HD12 | 1.92                     | 0.51              |
| 1:E:131:LEU:O    | 1:E:135:ARG:HB2  | 2.11                     | 0.51              |
| 1:i:183:VAL:HG12 | 1:i:191:THR:HG23 | 1.92                     | 0.51              |
| 1:S:265:VAL:HG21 | 1:S:327:ILE:HG12 | 1.92                     | 0.51              |
| 1:h:199:ARG:NH2  | 1:h:205:VAL:O    | 2.41                     | 0.51              |
| 1:L:171:GLU:OE2  | 1:L:176:ARG:NH2  | 2.43                     | 0.51              |
| 1:R:232:PHE:HD1  | 1:r:125:GLU:HB3  | 1.75                     | 0.51              |
| 1:b:242:SER:OG   | 1:b:249:ALA:HB2  | 2.10                     | 0.51              |
| 1:c:171:GLU:OE2  | 1:c:176:ARG:NH2  | 2.44                     | 0.51              |
| 1:j:145:ASP:HB3  | 1:j:148:VAL:HG23 | 1.92                     | 0.51              |
| 1:j:298:ARG:NH1  | 1:j:313:ARG:HD2  | 2.25                     | 0.51              |
| 1:O:232:PHE:N    | 1:O:232:PHE:CD2  | 2.79                     | 0.51              |
| 1:q:146:GLU:OE1  | 1:q:149:ARG:NH1  | 2.43                     | 0.51              |
| 1:a:131:LEU:CD1  | 1:a:155:SER:HB3  | 2.41                     | 0.51              |
| 1:l:166:ARG:HB3  | 1:l:169:ASP:HB2  | 1.93                     | 0.51              |
| 1:l:270:PRO:HD2  | 1:l:334:ILE:CG2  | 2.40                     | 0.51              |
| 1:F:242:SER:OG   | 1:F:249:ALA:HB2  | 2.11                     | 0.51              |
| 1:f:270:PRO:HD2  | 1:f:334:ILE:HG22 | 1.92                     | 0.51              |
| 1:s:270:PRO:HD3  | 1:s:334:ILE:CG2  | 2.41                     | 0.51              |
| 1:A:221:ARG:NH2  | 1:a:258:GLU:OE2  | 2.44                     | 0.50              |
| 1:E:206:ARG:HG2  | 1:E:206:ARG:HH11 | 1.75                     | 0.50              |
| 1:I:235:SER:HB2  | 1:i:231:PRO:HB3  | 1.92                     | 0.50              |
| 1:A:270:PRO:HD2  | 1:A:334:ILE:HG22 | 1.93                     | 0.50              |
| 1:B:131:LEU:O    | 1:B:135:ARG:HB2  | 2.12                     | 0.50              |
| 1:b:199:ARG:HE   | 1:b:203:GLU:HA   | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:119:VAL:HB   | 1:d:181:VAL:HG22 | 1.93                     | 0.50              |
| 1:h:195:ILE:HA   | 1:h:198:ILE:HD12 | 1.93                     | 0.50              |
| 1:L:292:ILE:HD12 | 1:L:321:ILE:HB   | 1.93                     | 0.50              |
| 1:J:230:SER:H    | 1:j:253:GLN:HE22 | 1.58                     | 0.50              |
| 1:K:298:ARG:NH2  | 1:K:313:ARG:CG   | 2.74                     | 0.50              |
| 1:M:211:ALA:HB2  | 1:M:220:LEU:HD22 | 1.93                     | 0.50              |
| 1:R:268:PRO:HA   | 1:R:317:ILE:HD13 | 1.93                     | 0.50              |
| 1:C:298:ARG:HH12 | 1:C:313:ARG:NE   | 2.07                     | 0.50              |
| 1:c:119:VAL:HB   | 1:c:181:VAL:HG22 | 1.93                     | 0.50              |
| 1:D:125:GLU:HB3  | 1:d:232:PHE:HD1  | 1.77                     | 0.50              |
| 1:h:146:GLU:OE1  | 1:h:149:ARG:NH1  | 2.44                     | 0.50              |
| 1:J:116:ARG:HB2  | 1:J:179:ARG:HG3  | 1.93                     | 0.50              |
| 1:P:242:SER:OG   | 1:P:249:ALA:HB2  | 2.11                     | 0.50              |
| 1:T:175:VAL:CG1  | 1:T:198:ILE:HG23 | 2.41                     | 0.50              |
| 1:E:199:ARG:NH1  | 1:E:224:GLY:O    | 2.44                     | 0.50              |
| 1:h:265:VAL:HG11 | 1:h:327:ILE:CG2  | 2.42                     | 0.50              |
| 1:j:298:ARG:HH22 | 1:j:313:ARG:HB2  | 1.77                     | 0.50              |
| 1:L:232:PHE:H    | 1:L:232:PHE:HD2  | 1.60                     | 0.50              |
| 1:l:238:LEU:HD21 | 1:l:252:VAL:HG21 | 1.94                     | 0.50              |
| 1:a:275:LEU:HD12 | 1:a:334:ILE:HG13 | 1.92                     | 0.50              |
| 1:e:131:LEU:HD21 | 1:e:139:VAL:HG11 | 1.94                     | 0.50              |
| 1:m:308:ARG:CG   | 1:m:308:ARG:NH1  | 2.64                     | 0.50              |
| 1:S:199:ARG:HE   | 1:S:203:GLU:HA   | 1.77                     | 0.50              |
| 1:a:213:ARG:NE   | 1:B:166:ARG:HH12 | 2.09                     | 0.50              |
| 1:B:199:ARG:NH1  | 1:B:224:GLY:O    | 2.45                     | 0.50              |
| 1:M:131:LEU:O    | 1:M:135:ARG:HB2  | 2.12                     | 0.50              |
| 1:A:265:VAL:HG11 | 1:A:327:ILE:CG2  | 2.42                     | 0.49              |
| 1:A:269:ILE:HG22 | 1:A:314:ALA:HA   | 1.94                     | 0.49              |
| 1:d:242:SER:OG   | 1:d:249:ALA:HB2  | 2.11                     | 0.49              |
| 1:G:234:ILE:O    | 1:G:238:LEU:HB2  | 2.12                     | 0.49              |
| 1:N:230:SER:H    | 1:n:253:GLN:HE22 | 1.59                     | 0.49              |
| 1:D:242:SER:OG   | 1:D:249:ALA:HB2  | 2.11                     | 0.49              |
| 1:H:175:VAL:HG22 | 1:H:181:VAL:HG21 | 1.93                     | 0.49              |
| 1:d:229:ILE:HG22 | 1:d:231:PRO:HD3  | 1.93                     | 0.49              |
| 1:e:171:GLU:HG3  | 1:e:201:ILE:HD13 | 1.95                     | 0.49              |
| 1:f:213:ARG:HG2  | 1:G:166:ARG:HH22 | 1.76                     | 0.49              |
| 1:f:269:ILE:HG22 | 1:f:314:ALA:HA   | 1.93                     | 0.49              |
| 1:J:231:PRO:HG2  | 1:J:232:PHE:CD2  | 2.47                     | 0.49              |
| 1:P:229:ILE:HG22 | 1:P:231:PRO:HD3  | 1.94                     | 0.49              |
| 1:t:199:ARG:NH1  | 1:t:224:GLY:O    | 2.45                     | 0.49              |
| 1:f:175:VAL:CG1  | 1:f:198:ILE:HG23 | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:289:THR:HG21 | 1:k:330:LEU:HG   | 1.94                     | 0.49              |
| 1:l:206:ARG:HH11 | 1:l:208:ILE:HD11 | 1.78                     | 0.49              |
| 1:T:242:SER:OG   | 1:T:249:ALA:HB2  | 2.12                     | 0.49              |
| 1:a:131:LEU:HD12 | 1:a:155:SER:HB3  | 1.94                     | 0.49              |
| 1:d:294:ILE:HD11 | 1:d:321:ILE:HG13 | 1.94                     | 0.49              |
| 1:E:116:ARG:HH21 | 1:E:179:ARG:HD2  | 1.76                     | 0.49              |
| 1:F:195:ILE:HD13 | 1:F:225:ALA:HB2  | 1.94                     | 0.49              |
| 1:i:142:LEU:HD11 | 1:i:162:GLY:HA3  | 1.95                     | 0.49              |
| 1:j:123:TRP:HZ2  | 1:j:128:LEU:HD12 | 1.76                     | 0.49              |
| 1:g:183:VAL:HG12 | 1:g:191:THR:HG23 | 1.94                     | 0.49              |
| 1:n:252:VAL:HA   | 1:n:256:LEU:HD23 | 1.95                     | 0.49              |
| 1:O:129:GLU:HG3  | 1:o:233:VAL:HA   | 1.93                     | 0.49              |
| 1:p:131:LEU:HD21 | 1:p:139:VAL:HG11 | 1.95                     | 0.49              |
| 1:r:289:THR:HG21 | 1:r:330:LEU:HG   | 1.94                     | 0.49              |
| 1:S:217:ILE:HG23 | 1:S:228:VAL:HG11 | 1.94                     | 0.49              |
| 1:A:284:ASP:OD2  | 1:A:287:ASP:HB2  | 2.13                     | 0.49              |
| 1:O:253:GLN:O    | 1:O:257:ALA:HB3  | 2.12                     | 0.49              |
| 1:J:298:ARG:CZ   | 1:J:313:ARG:HD2  | 2.42                     | 0.49              |
| 1:l:144:GLU:O    | 1:l:161:HIS:NE2  | 2.46                     | 0.49              |
| 1:N:133:GLU:OE1  | 1:n:241:ARG:NH1  | 2.46                     | 0.49              |
| 1:O:270:PRO:HD2  | 1:O:273:SER:HB2  | 1.95                     | 0.49              |
| 1:o:285:ILE:HG13 | 1:o:293:ILE:HD11 | 1.93                     | 0.49              |
| 1:r:301:GLU:HA   | 1:r:301:GLU:OE1  | 2.13                     | 0.49              |
| 1:T:217:ILE:HG23 | 1:T:228:VAL:HG11 | 1.95                     | 0.49              |
| 1:C:199:ARG:NH1  | 1:C:224:GLY:O    | 2.46                     | 0.49              |
| 1:D:330:LEU:O    | 1:D:334:ILE:HG13 | 2.13                     | 0.49              |
| 1:j:298:ARG:HH12 | 1:j:313:ARG:HD2  | 1.77                     | 0.49              |
| 1:r:247:TYR:HA   | 1:r:250:MET:HG2  | 1.94                     | 0.49              |
| 1:A:216:ASN:O    | 1:A:220:LEU:HD13 | 2.13                     | 0.49              |
| 1:E:117:HIS:H    | 1:E:117:HIS:CD2  | 2.31                     | 0.49              |
| 1:j:165:THR:HB   | 1:j:193:HIS:ND1  | 2.28                     | 0.49              |
| 1:A:289:THR:HG23 | 1:A:291:VAL:H    | 1.78                     | 0.48              |
| 1:e:330:LEU:HD22 | 1:e:334:ILE:HD11 | 1.94                     | 0.48              |
| 1:F:175:VAL:HG22 | 1:F:181:VAL:HG21 | 1.95                     | 0.48              |
| 1:f:263:ARG:NH1  | 1:f:265:VAL:HG12 | 2.28                     | 0.48              |
| 1:J:252:VAL:HA   | 1:J:256:LEU:HD23 | 1.94                     | 0.48              |
| 1:n:134:LEU:O    | 1:n:137:SER:N    | 2.46                     | 0.48              |
| 1:Q:298:ARG:HG3  | 1:Q:316:ASP:OD1  | 2.13                     | 0.48              |
| 1:R:144:GLU:OE2  | 1:R:163:ASP:HB2  | 2.13                     | 0.48              |
| 1:r:291:VAL:HG21 | 1:r:330:LEU:HD12 | 1.95                     | 0.48              |
| 1:b:217:ILE:HG23 | 1:b:228:VAL:HG11 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:237:ARG:HD2  | 1:D:241:ARG:NH2  | 2.28                     | 0.48              |
| 1:S:233:VAL:HA   | 1:s:129:GLU:HG3  | 1.95                     | 0.48              |
| 1:A:200:LYS:HD2  | 1:d:219:GLN:HE21 | 1.78                     | 0.48              |
| 1:d:330:LEU:O    | 1:d:334:ILE:HG13 | 2.14                     | 0.48              |
| 1:h:145:ASP:HB3  | 1:h:148:VAL:HG23 | 1.94                     | 0.48              |
| 1:o:280:VAL:HG23 | 1:o:310:TYR:HB3  | 1.95                     | 0.48              |
| 1:A:248:GLU:CG   | 1:a:264:MET:HG2  | 2.43                     | 0.48              |
| 1:c:117:HIS:HE1  | 1:c:174:ASN:O    | 1.96                     | 0.48              |
| 1:e:117:HIS:HE1  | 1:e:174:ASN:O    | 1.96                     | 0.48              |
| 1:J:125:GLU:CD   | 1:K:166:ARG:HH22 | 2.22                     | 0.48              |
| 1:k:211:ALA:HB2  | 1:k:220:LEU:HD13 | 1.96                     | 0.48              |
| 1:l:293:ILE:HG23 | 1:l:318:ILE:HG23 | 1.94                     | 0.48              |
| 1:m:330:LEU:O    | 1:m:334:ILE:HG13 | 2.14                     | 0.48              |
| 1:h:129:GLU:O    | 1:h:132:ARG:HB2  | 2.13                     | 0.48              |
| 1:J:298:ARG:HH22 | 1:J:313:ARG:CB   | 2.05                     | 0.48              |
| 1:A:125:GLU:HB3  | 1:a:232:PHE:CD1  | 2.45                     | 0.48              |
| 1:a:331:LYS:O    | 1:a:334:ILE:HG22 | 2.13                     | 0.48              |
| 1:B:195:ILE:HA   | 1:B:198:ILE:HD12 | 1.96                     | 0.48              |
| 1:C:289:THR:HG23 | 1:C:291:VAL:H    | 1.79                     | 0.48              |
| 1:E:330:LEU:HD22 | 1:E:334:ILE:HD11 | 1.96                     | 0.48              |
| 1:e:294:ILE:HD11 | 1:e:321:ILE:HG13 | 1.95                     | 0.48              |
| 1:J:179:ARG:NH2  | 1:j:244:ASP:OD1  | 2.46                     | 0.48              |
| 1:K:270:PRO:HD3  | 1:K:334:ILE:CG2  | 2.44                     | 0.48              |
| 1:Q:134:LEU:HD11 | 1:q:243:ILE:CD1  | 2.39                     | 0.48              |
| 1:E:263:ARG:HG3  | 1:E:264:MET:O    | 2.14                     | 0.48              |
| 1:H:294:ILE:HD11 | 1:H:321:ILE:HG13 | 1.96                     | 0.48              |
| 1:s:165:THR:HB   | 1:s:193:HIS:ND1  | 2.28                     | 0.48              |
| 1:q:330:LEU:O    | 1:q:334:ILE:HG13 | 2.14                     | 0.48              |
| 1:E:195:ILE:HA   | 1:E:198:ILE:HD12 | 1.96                     | 0.48              |
| 1:F:263:ARG:NH1  | 1:F:265:VAL:HG12 | 2.28                     | 0.48              |
| 1:i:199:ARG:NH2  | 1:i:205:VAL:O    | 2.44                     | 0.48              |
| 1:r:199:ARG:HE   | 1:r:203:GLU:HA   | 1.78                     | 0.48              |
| 1:B:242:SER:OG   | 1:B:249:ALA:HB2  | 2.14                     | 0.48              |
| 1:b:270:PRO:HD2  | 1:b:334:ILE:HG22 | 1.96                     | 0.48              |
| 1:C:270:PRO:HD3  | 1:C:334:ILE:CG2  | 2.43                     | 0.48              |
| 1:h:293:ILE:H    | 1:h:293:ILE:HG13 | 1.41                     | 0.48              |
| 1:j:289:THR:HG21 | 1:j:330:LEU:HG   | 1.96                     | 0.48              |
| 1:N:144:GLU:OE2  | 1:N:163:ASP:CB   | 2.59                     | 0.48              |
| 1:p:116:ARG:HH21 | 1:p:116:ARG:CG   | 2.22                     | 0.48              |
| 1:Q:270:PRO:O    | 1:Q:273:SER:HB3  | 2.14                     | 0.48              |
| 1:t:116:ARG:HG3  | 1:t:116:ARG:NH2  | 2.24                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:269:ILE:HD12 | 1:A:316:ASP:HB2  | 1.95                     | 0.47              |
| 1:E:270:PRO:HD2  | 1:E:334:ILE:HG22 | 1.95                     | 0.47              |
| 1:f:152:VAL:HG13 | 1:f:157:ALA:HB3  | 1.95                     | 0.47              |
| 1:G:268:PRO:O    | 1:G:270:PRO:HD3  | 2.13                     | 0.47              |
| 1:I:274:LYS:HE2  | 1:I:335:SER:O    | 2.14                     | 0.47              |
| 1:Q:305:ASP:HB2  | 1:q:292:ILE:HD11 | 1.96                     | 0.47              |
| 1:F:206:ARG:NH1  | 1:f:242:SER:O    | 2.46                     | 0.47              |
| 1:I:288:VAL:HG11 | 1:I:333:TYR:CE1  | 2.49                     | 0.47              |
| 1:p:275:LEU:HD12 | 1:p:334:ILE:HG13 | 1.95                     | 0.47              |
| 1:Q:199:ARG:HE   | 1:Q:203:GLU:HA   | 1.78                     | 0.47              |
| 1:A:265:VAL:HG11 | 1:A:327:ILE:HG23 | 1.97                     | 0.47              |
| 1:A:270:PRO:HD2  | 1:A:334:ILE:CG2  | 2.44                     | 0.47              |
| 1:d:199:ARG:HH12 | 1:d:207:ILE:HG13 | 1.79                     | 0.47              |
| 1:f:335:SER:O    | 1:f:336:ALA:HB3  | 2.14                     | 0.47              |
| 1:m:269:ILE:HD12 | 1:m:316:ASP:HB2  | 1.96                     | 0.47              |
| 1:Q:330:LEU:O    | 1:Q:334:ILE:HG13 | 2.15                     | 0.47              |
| 1:q:274:LYS:HD3  | 1:q:335:SER:O    | 2.15                     | 0.47              |
| 1:T:233:VAL:HA   | 1:t:129:GLU:HG3  | 1.95                     | 0.47              |
| 1:K:274:LYS:HD3  | 1:K:335:SER:O    | 2.14                     | 0.47              |
| 1:m:298:ARG:NH2  | 1:m:316:ASP:OD1  | 2.48                     | 0.47              |
| 1:p:195:ILE:HD13 | 1:p:225:ALA:HB2  | 1.95                     | 0.47              |
| 1:g:166:ARG:HH22 | 1:H:213:ARG:HG2  | 1.80                     | 0.47              |
| 1:I:289:THR:HG23 | 1:I:291:VAL:H    | 1.78                     | 0.47              |
| 1:n:217:ILE:HG23 | 1:n:228:VAL:HG11 | 1.97                     | 0.47              |
| 1:q:213:ARG:HG2  | 1:R:166:ARG:NH2  | 2.29                     | 0.47              |
| 1:e:265:VAL:HG11 | 1:e:327:ILE:HG23 | 1.95                     | 0.47              |
| 1:f:285:ILE:CD1  | 1:f:293:ILE:HD11 | 2.45                     | 0.47              |
| 1:H:182:ILE:HD11 | 1:h:243:ILE:HD11 | 1.97                     | 0.47              |
| 1:h:199:ARG:HE   | 1:h:199:ARG:HA   | 1.80                     | 0.47              |
| 1:M:146:GLU:OE1  | 1:M:149:ARG:NH1  | 2.47                     | 0.47              |
| 1:M:263:ARG:CZ   | 1:M:265:VAL:HG12 | 2.45                     | 0.47              |
| 1:P:240:SER:OG   | 1:p:133:GLU:HG3  | 2.14                     | 0.47              |
| 1:s:270:PRO:HD2  | 1:s:334:ILE:CG2  | 2.43                     | 0.47              |
| 1:A:247:TYR:HB3  | 1:a:302:LEU:HD13 | 1.97                     | 0.47              |
| 1:a:167:VAL:HG13 | 1:a:201:ILE:HD11 | 1.96                     | 0.47              |
| 1:D:259:GLU:OE2  | 1:d:241:ARG:NH2  | 2.48                     | 0.47              |
| 1:D:274:LYS:HD2  | 1:D:335:SER:O    | 2.14                     | 0.47              |
| 1:e:298:ARG:HH12 | 1:e:313:ARG:HD2  | 1.79                     | 0.47              |
| 1:M:193:HIS:NE2  | 1:p:216:ASN:OD1  | 2.47                     | 0.47              |
| 1:n:234:ILE:O    | 1:n:238:LEU:HB2  | 2.13                     | 0.47              |
| 1:O:231:PRO:HG2  | 1:O:232:PHE:CD2  | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:289:THR:HG23 | 1:T:291:VAL:H    | 1.80                     | 0.47              |
| 1:a:199:ARG:NH2  | 1:a:205:VAL:O    | 2.44                     | 0.47              |
| 1:c:291:VAL:HG21 | 1:c:330:LEU:HD12 | 1.96                     | 0.47              |
| 1:E:213:ARG:HG2  | 1:h:166:ARG:HH22 | 1.80                     | 0.47              |
| 1:i:252:VAL:HA   | 1:i:256:LEU:HD23 | 1.97                     | 0.47              |
| 1:j:270:PRO:HD2  | 1:j:334:ILE:HG22 | 1.97                     | 0.47              |
| 1:l:176:ARG:HD2  | 1:s:299:GLY:CA   | 2.45                     | 0.47              |
| 1:O:330:LEU:O    | 1:O:334:ILE:HG13 | 2.15                     | 0.47              |
| 1:Q:213:ARG:HG2  | 1:t:166:ARG:HH21 | 1.75                     | 0.47              |
| 1:f:252:VAL:HG13 | 1:f:256:LEU:HD12 | 1.97                     | 0.47              |
| 1:k:298:ARG:NH2  | 1:k:310:TYR:OH   | 2.48                     | 0.47              |
| 1:d:175:VAL:HG22 | 1:d:181:VAL:HG21 | 1.97                     | 0.47              |
| 1:f:283:ALA:HB1  | 1:f:285:ILE:HG13 | 1.97                     | 0.47              |
| 1:i:125:GLU:CD   | 1:l:166:ARG:HH22 | 2.23                     | 0.47              |
| 1:J:199:ARG:NH1  | 1:J:224:GLY:O    | 2.48                     | 0.47              |
| 1:L:247:TYR:H    | 1:l:266:GLU:CD   | 2.23                     | 0.47              |
| 1:r:175:VAL:HG11 | 1:r:198:ILE:HG23 | 1.97                     | 0.47              |
| 1:T:309:ASP:OD1  | 1:T:309:ASP:N    | 2.48                     | 0.47              |
| 1:a:279:SER:HA   | 1:a:310:TYR:O    | 2.15                     | 0.46              |
| 1:F:275:LEU:HD12 | 1:F:334:ILE:HG12 | 1.97                     | 0.46              |
| 1:H:298:ARG:HH12 | 1:H:313:ARG:CG   | 2.27                     | 0.46              |
| 1:i:234:ILE:O    | 1:i:238:LEU:HB2  | 2.14                     | 0.46              |
| 1:M:237:ARG:HD2  | 1:m:259:GLU:OE2  | 2.13                     | 0.46              |
| 1:p:293:ILE:H    | 1:p:293:ILE:HG13 | 1.52                     | 0.46              |
| 1:t:131:LEU:HD21 | 1:t:139:VAL:HG11 | 1.97                     | 0.46              |
| 1:d:116:ARG:HH21 | 1:d:116:ARG:CG   | 2.14                     | 0.46              |
| 1:g:182:ILE:HA   | 1:g:208:ILE:O    | 2.16                     | 0.46              |
| 1:O:268:PRO:HA   | 1:O:317:ILE:HD13 | 1.97                     | 0.46              |
| 1:o:274:LYS:HD2  | 1:o:336:ALA:HB3  | 1.96                     | 0.46              |
| 1:Q:120:ILE:HB   | 1:Q:141:VAL:HG22 | 1.98                     | 0.46              |
| 1:S:231:PRO:HG2  | 1:S:232:PHE:CD2  | 2.49                     | 0.46              |
| 1:C:270:PRO:CD   | 1:C:334:ILE:CG2  | 2.92                     | 0.46              |
| 1:c:229:ILE:HG22 | 1:c:231:PRO:HD3  | 1.95                     | 0.46              |
| 1:n:324:PRO:HA   | 1:n:327:ILE:HD12 | 1.97                     | 0.46              |
| 1:r:148:VAL:HG12 | 1:r:152:VAL:HG23 | 1.98                     | 0.46              |
| 1:E:228:VAL:C    | 1:E:229:ILE:HG13 | 2.40                     | 0.46              |
| 1:L:117:HIS:H    | 1:L:117:HIS:CD2  | 2.33                     | 0.46              |
| 1:n:265:VAL:O    | 1:n:319:LEU:HA   | 2.15                     | 0.46              |
| 1:p:217:ILE:HG23 | 1:p:228:VAL:HG11 | 1.97                     | 0.46              |
| 1:p:234:ILE:O    | 1:p:238:LEU:HB2  | 2.14                     | 0.46              |
| 1:q:285:ILE:HG21 | 1:q:293:ILE:HD11 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:g:298:ARG:NE   | 1:g:310:TYR:OH   | 2.49                     | 0.46              |
| 1:H:330:LEU:O    | 1:H:334:ILE:HG13 | 2.15                     | 0.46              |
| 1:Q:296:VAL:HG23 | 1:Q:306:PRO:HG3  | 1.98                     | 0.46              |
| 1:R:293:ILE:H    | 1:R:293:ILE:HG13 | 1.49                     | 0.46              |
| 1:S:253:GLN:O    | 1:S:257:ALA:HB3  | 2.15                     | 0.46              |
| 1:t:182:ILE:HG13 | 1:t:208:ILE:HB   | 1.98                     | 0.46              |
| 1:b:131:LEU:O    | 1:b:135:ARG:HB2  | 2.16                     | 0.46              |
| 1:F:237:ARG:HG2  | 1:F:237:ARG:HH11 | 1.81                     | 0.46              |
| 1:k:285:ILE:HB   | 1:k:293:ILE:HD11 | 1.96                     | 0.46              |
| 1:L:232:PHE:CD2  | 1:L:232:PHE:N    | 2.83                     | 0.46              |
| 1:L:269:ILE:HG22 | 1:L:314:ALA:HA   | 1.98                     | 0.46              |
| 1:n:265:VAL:HG11 | 1:n:327:ILE:HG12 | 1.97                     | 0.46              |
| 1:n:294:ILE:HD11 | 1:n:321:ILE:CG1  | 2.46                     | 0.46              |
| 1:q:252:VAL:HA   | 1:q:256:LEU:HD13 | 1.96                     | 0.46              |
| 1:A:248:GLU:HG3  | 1:a:264:MET:CG   | 2.41                     | 0.46              |
| 1:d:165:THR:HB   | 1:d:193:HIS:ND1  | 2.31                     | 0.46              |
| 1:E:166:ARG:HH22 | 1:H:125:GLU:CD   | 2.24                     | 0.46              |
| 1:F:199:ARG:HE   | 1:F:203:GLU:HA   | 1.81                     | 0.46              |
| 1:g:253:GLN:HA   | 1:g:253:GLN:NE2  | 2.30                     | 0.46              |
| 1:I:145:ASP:HB3  | 1:I:148:VAL:HG23 | 1.98                     | 0.46              |
| 1:o:123:TRP:CZ2  | 1:o:128:LEU:HD12 | 2.50                     | 0.46              |
| 1:R:164:PRO:HG2  | 1:R:185:LEU:HD21 | 1.98                     | 0.46              |
| 1:R:330:LEU:HD22 | 1:R:334:ILE:HD11 | 1.96                     | 0.46              |
| 1:r:335:SER:O    | 1:r:336:ALA:CB   | 2.64                     | 0.46              |
| 1:t:270:PRO:HD2  | 1:t:273:SER:HB2  | 1.98                     | 0.46              |
| 1:e:309:ASP:OD1  | 1:e:309:ASP:N    | 2.46                     | 0.46              |
| 1:o:211:ALA:HB2  | 1:o:220:LEU:HD22 | 1.97                     | 0.46              |
| 1:Q:199:ARG:NH1  | 1:Q:224:GLY:O    | 2.49                     | 0.46              |
| 1:T:134:LEU:HD11 | 1:t:243:ILE:CD1  | 2.46                     | 0.46              |
| 1:a:119:VAL:HB   | 1:a:181:VAL:HG22 | 1.98                     | 0.46              |
| 1:B:185:LEU:HD13 | 1:B:190:GLU:HB3  | 1.97                     | 0.46              |
| 1:C:298:ARG:HG3  | 1:C:316:ASP:OD1  | 2.15                     | 0.46              |
| 1:E:133:GLU:HG3  | 1:e:240:SER:OG   | 2.16                     | 0.46              |
| 1:g:199:ARG:NH1  | 1:g:224:GLY:O    | 2.49                     | 0.46              |
| 1:n:285:ILE:O    | 1:n:289:THR:HG22 | 2.16                     | 0.46              |
| 1:p:248:GLU:O    | 1:p:252:VAL:HG23 | 2.16                     | 0.46              |
| 1:q:289:THR:HG23 | 1:q:291:VAL:H    | 1.81                     | 0.46              |
| 1:G:206:ARG:NH1  | 1:g:242:SER:O    | 2.48                     | 0.46              |
| 1:g:279:SER:HA   | 1:g:310:TYR:O    | 2.16                     | 0.46              |
| 1:I:134:LEU:HD11 | 1:i:243:ILE:CD1  | 2.45                     | 0.46              |
| 1:L:206:ARG:NH1  | 1:l:242:SER:O    | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:232:PHE:CD1  | 1:r:125:GLU:HB3  | 2.50                     | 0.46              |
| 1:B:247:TYR:HB3  | 1:b:302:LEU:HD13 | 1.97                     | 0.45              |
| 1:c:289:THR:HG21 | 1:c:330:LEU:HG   | 1.97                     | 0.45              |
| 1:e:237:ARG:NH1  | 1:e:241:ARG:NH2  | 2.65                     | 0.45              |
| 1:G:237:ARG:HG2  | 1:G:241:ARG:HH11 | 1.81                     | 0.45              |
| 1:j:195:ILE:HA   | 1:j:198:ILE:HD12 | 1.98                     | 0.45              |
| 1:p:298:ARG:HH12 | 1:p:313:ARG:NH2  | 2.13                     | 0.45              |
| 1:R:298:ARG:NH1  | 1:R:313:ARG:HD2  | 2.31                     | 0.45              |
| 1:b:307:PRO:HG2  | 1:b:310:TYR:HB2  | 1.98                     | 0.45              |
| 1:G:239:MET:HB3  | 1:g:182:ILE:HD13 | 1.98                     | 0.45              |
| 1:l:120:ILE:HG12 | 1:l:182:ILE:HB   | 1.97                     | 0.45              |
| 1:O:298:ARG:NH2  | 1:O:310:TYR:OH   | 2.50                     | 0.45              |
| 1:s:175:VAL:CG1  | 1:s:198:ILE:HG23 | 2.47                     | 0.45              |
| 1:T:232:PHE:H    | 1:T:232:PHE:HD2  | 1.64                     | 0.45              |
| 1:A:289:THR:HG21 | 1:A:330:LEU:HG   | 1.98                     | 0.45              |
| 1:C:237:ARG:HH21 | 1:C:241:ARG:NH1  | 2.14                     | 0.45              |
| 1:F:292:ILE:HD11 | 1:f:305:ASP:HB2  | 1.98                     | 0.45              |
| 1:I:237:ARG:HD2  | 1:i:259:GLU:OE1  | 2.16                     | 0.45              |
| 1:J:287:ASP:HA   | 1:j:308:ARG:NH2  | 2.31                     | 0.45              |
| 1:M:330:LEU:HD22 | 1:M:334:ILE:HD11 | 1.98                     | 0.45              |
| 1:O:232:PHE:N    | 1:O:232:PHE:HD2  | 2.14                     | 0.45              |
| 1:P:164:PRO:HG3  | 1:P:185:LEU:HD21 | 1.99                     | 0.45              |
| 1:P:199:ARG:NH2  | 1:P:205:VAL:O    | 2.42                     | 0.45              |
| 1:Q:146:GLU:OE1  | 1:Q:149:ARG:NH1  | 2.47                     | 0.45              |
| 1:C:206:ARG:NH1  | 1:c:242:SER:O    | 2.49                     | 0.45              |
| 1:f:264:MET:HE2  | 1:f:321:ILE:HG12 | 1.97                     | 0.45              |
| 1:G:335:SER:O    | 1:G:336:ALA:HB3  | 2.17                     | 0.45              |
| 1:h:298:ARG:HH22 | 1:h:313:ARG:HB2  | 1.82                     | 0.45              |
| 1:J:237:ARG:HH11 | 1:J:237:ARG:HG2  | 1.81                     | 0.45              |
| 1:j:166:ARG:NH2  | 1:K:213:ARG:HG2  | 2.32                     | 0.45              |
| 1:j:298:ARG:NH2  | 1:j:313:ARG:HD2  | 2.31                     | 0.45              |
| 1:K:270:PRO:CD   | 1:K:334:ILE:HG22 | 2.46                     | 0.45              |
| 1:s:172:LYS:HZ3  | 1:t:154:ARG:HD3  | 1.81                     | 0.45              |
| 1:A:221:ARG:HH22 | 1:a:258:GLU:CD   | 2.24                     | 0.45              |
| 1:B:131:LEU:HD21 | 1:B:139:VAL:HG11 | 1.99                     | 0.45              |
| 1:C:264:MET:CE   | 1:C:321:ILE:HG12 | 2.46                     | 0.45              |
| 1:H:213:ARG:HD2  | 1:H:216:ASN:ND2  | 2.31                     | 0.45              |
| 1:J:298:ARG:NH2  | 1:J:313:ARG:HD2  | 2.32                     | 0.45              |
| 1:n:309:ASP:OD1  | 1:n:309:ASP:N    | 2.45                     | 0.45              |
| 1:Q:183:VAL:HG12 | 1:Q:191:THR:HG23 | 1.98                     | 0.45              |
| 1:S:330:LEU:HD22 | 1:S:334:ILE:HD11 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:216:ASN:O    | 1:t:220:LEU:HD13 | 2.17                     | 0.45              |
| 1:c:273:SER:HB2  | 1:c:334:ILE:HG22 | 1.98                     | 0.45              |
| 1:J:125:GLU:HB3  | 1:j:232:PHE:HD1  | 1.82                     | 0.45              |
| 1:O:269:ILE:HA   | 1:O:270:PRO:HD3  | 1.80                     | 0.45              |
| 1:o:269:ILE:HG22 | 1:o:314:ALA:HA   | 1.99                     | 0.45              |
| 1:q:175:VAL:HG13 | 1:q:181:VAL:HG21 | 1.99                     | 0.45              |
| 1:R:199:ARG:HG3  | 1:R:224:GLY:HA3  | 1.98                     | 0.45              |
| 1:g:163:ASP:HA   | 1:g:164:PRO:HD3  | 1.88                     | 0.45              |
| 1:h:265:VAL:O    | 1:h:319:LEU:HA   | 2.17                     | 0.45              |
| 1:i:296:VAL:HG23 | 1:i:306:PRO:HG3  | 1.99                     | 0.45              |
| 1:J:214:TYR:C    | 1:J:216:ASN:N    | 2.75                     | 0.45              |
| 1:T:330:LEU:HD22 | 1:T:334:ILE:HD11 | 1.98                     | 0.45              |
| 1:D:237:ARG:O    | 1:D:241:ARG:HB2  | 2.17                     | 0.45              |
| 1:E:263:ARG:HG2  | 1:E:265:VAL:HG13 | 1.99                     | 0.45              |
| 1:e:166:ARG:HB3  | 1:e:169:ASP:HB2  | 1.99                     | 0.45              |
| 1:e:293:ILE:H    | 1:e:293:ILE:HG13 | 1.63                     | 0.45              |
| 1:F:124:SER:OG   | 1:F:126:SER:HB2  | 2.17                     | 0.45              |
| 1:H:252:VAL:O    | 1:H:256:LEU:HB2  | 2.16                     | 0.45              |
| 1:h:298:ARG:NH1  | 1:h:313:ARG:HD2  | 2.31                     | 0.45              |
| 1:K:129:GLU:OE1  | 1:K:132:ARG:HD2  | 2.17                     | 0.45              |
| 1:k:248:GLU:O    | 1:k:252:VAL:HG23 | 2.17                     | 0.45              |
| 1:Q:165:THR:HB   | 1:Q:193:HIS:ND1  | 2.32                     | 0.45              |
| 1:q:166:ARG:HH21 | 1:R:213:ARG:NE   | 2.12                     | 0.45              |
| 1:s:263:ARG:NH1  | 1:s:265:VAL:HG12 | 2.32                     | 0.45              |
| 1:A:252:VAL:HG13 | 1:A:256:LEU:HD12 | 1.99                     | 0.45              |
| 1:d:171:GLU:HG2  | 1:d:201:ILE:HD13 | 1.99                     | 0.45              |
| 1:e:289:THR:HG21 | 1:e:330:LEU:HG   | 1.98                     | 0.45              |
| 1:K:270:PRO:HD2  | 1:K:334:ILE:HG22 | 1.99                     | 0.45              |
| 1:P:134:LEU:HD21 | 1:p:243:ILE:HD13 | 1.99                     | 0.45              |
| 1:C:259:GLU:OE1  | 1:c:237:ARG:HD2  | 2.17                     | 0.45              |
| 1:f:270:PRO:HD2  | 1:f:334:ILE:CG2  | 2.47                     | 0.45              |
| 1:J:176:ARG:CG   | 1:J:176:ARG:NH2  | 2.66                     | 0.45              |
| 1:L:119:VAL:HB   | 1:L:181:VAL:HG22 | 1.99                     | 0.45              |
| 1:m:242:SER:OG   | 1:m:249:ALA:HB2  | 2.17                     | 0.45              |
| 1:m:298:ARG:CZ   | 1:m:313:ARG:HD2  | 2.47                     | 0.45              |
| 1:o:298:ARG:HH11 | 1:o:298:ARG:CG   | 2.28                     | 0.45              |
| 1:P:221:ARG:NH2  | 1:p:258:GLU:OE1  | 2.49                     | 0.45              |
| 1:Q:240:SER:HB2  | 1:q:133:GLU:HB2  | 1.98                     | 0.45              |
| 1:S:269:ILE:HG22 | 1:S:314:ALA:HA   | 1.99                     | 0.45              |
| 1:c:183:VAL:HG12 | 1:c:191:THR:HG23 | 1.98                     | 0.44              |
| 1:E:219:GLN:NE2  | 1:h:200:LYS:HD3  | 2.31                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:229:ILE:HA   | 1:m:253:GLN:NE2  | 2.32                     | 0.44              |
| 1:O:133:GLU:HG3  | 1:o:240:SER:OG   | 2.16                     | 0.44              |
| 1:o:242:SER:OG   | 1:o:249:ALA:HB2  | 2.17                     | 0.44              |
| 1:Q:285:ILE:HB   | 1:Q:293:ILE:HD11 | 1.99                     | 0.44              |
| 1:T:151:LYS:O    | 1:T:154:ARG:HB2  | 2.17                     | 0.44              |
| 1:B:125:GLU:CD   | 1:C:166:ARG:HH22 | 2.25                     | 0.44              |
| 1:k:175:VAL:HG22 | 1:k:181:VAL:HG21 | 1.98                     | 0.44              |
| 1:l:211:ALA:HB2  | 1:l:220:LEU:HD22 | 1.99                     | 0.44              |
| 1:m:308:ARG:H    | 1:m:308:ARG:HD2  | 1.82                     | 0.44              |
| 1:p:146:GLU:OE1  | 1:p:149:ARG:NH1  | 2.50                     | 0.44              |
| 1:R:275:LEU:HD12 | 1:R:334:ILE:HG23 | 1.98                     | 0.44              |
| 1:c:172:LYS:HE3  | 1:d:154:ARG:HH11 | 1.83                     | 0.44              |
| 1:E:152:VAL:HG11 | 1:E:159:PHE:HB2  | 1.98                     | 0.44              |
| 1:F:253:GLN:HG2  | 1:f:221:ARG:HH22 | 1.82                     | 0.44              |
| 1:f:195:ILE:HD13 | 1:f:225:ALA:HB2  | 2.00                     | 0.44              |
| 1:G:175:VAL:CG1  | 1:G:198:ILE:HG23 | 2.48                     | 0.44              |
| 1:H:285:ILE:HB   | 1:H:293:ILE:HD11 | 1.98                     | 0.44              |
| 1:h:232:PHE:N    | 1:h:232:PHE:CD2  | 2.86                     | 0.44              |
| 1:i:291:VAL:HG21 | 1:i:330:LEU:HD12 | 1.99                     | 0.44              |
| 1:O:238:LEU:HD21 | 1:O:252:VAL:HG21 | 1.98                     | 0.44              |
| 1:o:263:ARG:NH1  | 1:o:265:VAL:HG12 | 2.31                     | 0.44              |
| 1:C:193:HIS:HD2  | 1:C:193:HIS:O    | 1.99                     | 0.44              |
| 1:E:192:ILE:HD12 | 1:h:193:HIS:CD2  | 2.52                     | 0.44              |
| 1:G:235:SER:HB2  | 1:g:231:PRO:HB3  | 1.98                     | 0.44              |
| 1:k:330:LEU:O    | 1:k:334:ILE:HG13 | 2.17                     | 0.44              |
| 1:r:211:ALA:HB2  | 1:r:220:LEU:HD22 | 1.98                     | 0.44              |
| 1:T:263:ARG:HE   | 1:T:327:ILE:HD13 | 1.82                     | 0.44              |
| 1:a:293:ILE:H    | 1:a:293:ILE:HG13 | 1.59                     | 0.44              |
| 1:b:323:LYS:HB3  | 1:b:324:PRO:HD2  | 1.99                     | 0.44              |
| 1:d:116:ARG:HB2  | 1:d:179:ARG:HB2  | 2.00                     | 0.44              |
| 1:d:263:ARG:NH1  | 1:d:265:VAL:HG12 | 2.32                     | 0.44              |
| 1:E:116:ARG:HH22 | 1:E:179:ARG:HD2  | 1.77                     | 0.44              |
| 1:E:275:LEU:HD21 | 1:E:333:TYR:CE2  | 2.53                     | 0.44              |
| 1:H:120:ILE:HG12 | 1:H:182:ILE:HB   | 2.00                     | 0.44              |
| 1:h:195:ILE:HD13 | 1:h:225:ALA:HB2  | 2.00                     | 0.44              |
| 1:i:187:SER:OG   | 1:i:190:GLU:HG3  | 2.17                     | 0.44              |
| 1:J:231:PRO:HG2  | 1:J:232:PHE:HD2  | 1.83                     | 0.44              |
| 1:n:131:LEU:HD21 | 1:n:139:VAL:HG11 | 1.99                     | 0.44              |
| 1:n:280:VAL:HG22 | 1:n:312:PHE:CE1  | 2.49                     | 0.44              |
| 1:t:332:ASN:C    | 1:t:334:ILE:H    | 2.26                     | 0.44              |
| 1:A:330:LEU:O    | 1:A:334:ILE:HG13 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:116:ARG:CG   | 1:a:116:ARG:NH2  | 2.64                     | 0.44              |
| 1:c:237:ARG:NH2  | 1:c:248:GLU:OE2  | 2.50                     | 0.44              |
| 1:D:199:ARG:HE   | 1:D:203:GLU:HA   | 1.82                     | 0.44              |
| 1:D:298:ARG:HB2  | 1:S:176:ARG:NH1  | 2.33                     | 0.44              |
| 1:E:117:HIS:CD2  | 1:E:117:HIS:N    | 2.86                     | 0.44              |
| 1:H:279:SER:HA   | 1:H:310:TYR:O    | 2.17                     | 0.44              |
| 1:k:195:ILE:HD11 | 1:k:220:LEU:HD23 | 1.98                     | 0.44              |
| 1:L:324:PRO:HA   | 1:L:327:ILE:HD12 | 1.98                     | 0.44              |
| 1:M:298:ARG:NH2  | 1:M:316:ASP:OD2  | 2.49                     | 0.44              |
| 1:n:275:LEU:HD12 | 1:n:334:ILE:HG12 | 1.99                     | 0.44              |
| 1:R:218:GLU:OE2  | 1:R:222:MET:HE3  | 2.17                     | 0.44              |
| 1:S:335:SER:O    | 1:S:336:ALA:HB2  | 2.16                     | 0.44              |
| 1:C:217:ILE:HG23 | 1:C:228:VAL:HG11 | 1.98                     | 0.44              |
| 1:J:242:SER:OG   | 1:J:249:ALA:HB2  | 2.17                     | 0.44              |
| 1:q:298:ARG:NH2  | 1:q:313:ARG:HD2  | 2.32                     | 0.44              |
| 1:T:234:ILE:O    | 1:T:238:LEU:HB2  | 2.18                     | 0.44              |
| 1:F:231:PRO:HG2  | 1:F:232:PHE:CD2  | 2.53                     | 0.44              |
| 1:h:298:ARG:NH2  | 1:h:313:ARG:HD2  | 2.33                     | 0.44              |
| 1:J:270:PRO:CD   | 1:J:334:ILE:HG23 | 2.48                     | 0.44              |
| 1:m:166:ARG:NH2  | 1:N:213:ARG:HG2  | 2.33                     | 0.44              |
| 1:n:134:LEU:O    | 1:n:137:SER:HB2  | 2.17                     | 0.44              |
| 1:n:252:VAL:O    | 1:n:256:LEU:HB2  | 2.17                     | 0.44              |
| 1:P:233:VAL:HA   | 1:p:129:GLU:HG3  | 2.00                     | 0.44              |
| 1:a:199:ARG:NH1  | 1:a:224:GLY:O    | 2.51                     | 0.44              |
| 1:g:267:VAL:HG21 | 1:g:330:LEU:HD22 | 1.99                     | 0.44              |
| 1:I:229:ILE:HG12 | 1:i:238:LEU:HD23 | 2.00                     | 0.44              |
| 1:K:163:ASP:HA   | 1:K:164:PRO:HD3  | 1.92                     | 0.44              |
| 1:r:217:ILE:HG23 | 1:r:228:VAL:HG11 | 2.00                     | 0.44              |
| 1:r:298:ARG:O    | 1:r:298:ARG:HG3  | 2.17                     | 0.44              |
| 1:c:275:LEU:HD12 | 1:c:334:ILE:HG12 | 1.99                     | 0.43              |
| 1:G:301:GLU:OE1  | 1:G:303:ILE:HD11 | 2.18                     | 0.43              |
| 1:h:165:THR:HB   | 1:h:193:HIS:ND1  | 2.33                     | 0.43              |
| 1:J:309:ASP:OD1  | 1:J:309:ASP:N    | 2.45                     | 0.43              |
| 1:m:175:VAL:HG13 | 1:m:181:VAL:HG21 | 1.98                     | 0.43              |
| 1:N:293:ILE:H    | 1:N:293:ILE:HG13 | 1.56                     | 0.43              |
| 1:o:199:ARG:HE   | 1:o:203:GLU:HA   | 1.83                     | 0.43              |
| 1:o:275:LEU:HD12 | 1:o:334:ILE:HG23 | 2.00                     | 0.43              |
| 1:A:240:SER:OG   | 1:a:133:GLU:HG3  | 2.18                     | 0.43              |
| 1:D:292:ILE:HD11 | 1:d:305:ASP:HB2  | 2.00                     | 0.43              |
| 1:F:234:ILE:HG13 | 1:f:257:ALA:HB2  | 1.99                     | 0.43              |
| 1:g:308:ARG:H    | 1:g:308:ARG:HG2  | 1.63                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:262:ARG:CG   | 1:H:262:ARG:NH1  | 2.76                     | 0.43              |
| 1:K:119:VAL:HB   | 1:K:181:VAL:HG13 | 2.00                     | 0.43              |
| 1:k:262:ARG:NH2  | 1:k:323:LYS:HE3  | 2.34                     | 0.43              |
| 1:M:133:GLU:OE1  | 1:m:241:ARG:NH1  | 2.51                     | 0.43              |
| 1:N:147:ASN:N    | 1:N:147:ASN:ND2  | 2.65                     | 0.43              |
| 1:N:253:GLN:HG3  | 1:N:258:GLU:OE1  | 2.18                     | 0.43              |
| 1:D:231:PRO:HB2  | 1:d:231:PRO:HB2  | 1.99                     | 0.43              |
| 1:e:153:LEU:HD23 | 1:e:157:ALA:O    | 2.18                     | 0.43              |
| 1:h:262:ARG:HD3  | 1:h:321:ILE:CG2  | 2.48                     | 0.43              |
| 1:K:298:ARG:NH2  | 1:K:313:ARG:CB   | 2.80                     | 0.43              |
| 1:o:123:TRP:HZ2  | 1:o:128:LEU:HD12 | 1.83                     | 0.43              |
| 1:b:117:HIS:CE1  | 1:b:174:ASN:HB2  | 2.53                     | 0.43              |
| 1:C:150:LYS:HD3  | 1:D:161:HIS:CE1  | 2.53                     | 0.43              |
| 1:f:176:ARG:HB2  | 1:f:202:ASP:HB2  | 2.00                     | 0.43              |
| 1:H:262:ARG:HG3  | 1:h:304:ILE:HD13 | 2.00                     | 0.43              |
| 1:K:207:ILE:HB   | 1:K:225:ALA:HA   | 2.00                     | 0.43              |
| 1:o:335:SER:O    | 1:o:336:ALA:CB   | 2.67                     | 0.43              |
| 1:S:146:GLU:OE1  | 1:S:149:ARG:NH1  | 2.50                     | 0.43              |
| 1:t:217:ILE:HG23 | 1:t:228:VAL:HG11 | 2.00                     | 0.43              |
| 1:B:248:GLU:O    | 1:B:252:VAL:HG23 | 2.18                     | 0.43              |
| 1:F:247:TYR:H    | 1:f:266:GLU:CD   | 2.26                     | 0.43              |
| 1:h:220:LEU:HD23 | 1:h:228:VAL:HG13 | 2.01                     | 0.43              |
| 1:K:231:PRO:HB2  | 1:k:231:PRO:HB2  | 2.00                     | 0.43              |
| 1:L:118:VAL:HG21 | 1:l:243:ILE:HD13 | 2.01                     | 0.43              |
| 1:L:242:SER:OG   | 1:L:249:ALA:HB2  | 2.19                     | 0.43              |
| 1:O:335:SER:O    | 1:O:336:ALA:HB3  | 2.18                     | 0.43              |
| 1:r:234:ILE:O    | 1:r:238:LEU:HB2  | 2.18                     | 0.43              |
| 1:b:150:LYS:H    | 1:b:150:LYS:HG2  | 1.51                     | 0.43              |
| 1:c:199:ARG:NH2  | 1:c:205:VAL:O    | 2.43                     | 0.43              |
| 1:I:148:VAL:HG12 | 1:I:152:VAL:HG23 | 2.00                     | 0.43              |
| 1:J:164:PRO:HG2  | 1:J:185:LEU:HD21 | 2.00                     | 0.43              |
| 1:j:144:GLU:O    | 1:j:161:HIS:NE2  | 2.52                     | 0.43              |
| 1:j:188:ASP:O    | 1:j:192:ILE:HG13 | 2.19                     | 0.43              |
| 1:j:284:ASP:O    | 1:j:288:VAL:HG23 | 2.19                     | 0.43              |
| 1:T:232:PHE:CD2  | 1:T:232:PHE:N    | 2.87                     | 0.43              |
| 1:C:289:THR:CG2  | 1:C:291:VAL:H    | 2.32                     | 0.43              |
| 1:J:270:PRO:HD2  | 1:J:334:ILE:HG23 | 2.00                     | 0.43              |
| 1:L:270:PRO:HD2  | 1:L:334:ILE:CG2  | 2.47                     | 0.43              |
| 1:N:147:ASN:H    | 1:N:147:ASN:ND2  | 2.13                     | 0.43              |
| 1:b:288:VAL:HG11 | 1:b:333:TYR:CE1  | 2.52                     | 0.43              |
| 1:D:294:ILE:HD11 | 1:D:321:ILE:CD1  | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:152:VAL:HG13 | 1:H:157:ALA:HB3  | 2.00                     | 0.43              |
| 1:h:191:THR:HG22 | 1:h:220:LEU:HD11 | 2.00                     | 0.43              |
| 1:n:270:PRO:HG2  | 1:n:335:SER:HA   | 2.01                     | 0.43              |
| 1:o:185:LEU:HD13 | 1:o:190:GLU:HB3  | 2.00                     | 0.43              |
| 1:Q:211:ALA:HB2  | 1:Q:220:LEU:HD22 | 1.99                     | 0.43              |
| 1:R:298:ARG:HH12 | 1:R:313:ARG:HD2  | 1.81                     | 0.43              |
| 1:r:285:ILE:HD12 | 1:r:293:ILE:HD12 | 2.01                     | 0.43              |
| 1:b:253:GLN:O    | 1:b:257:ALA:HB3  | 2.18                     | 0.43              |
| 1:C:175:VAL:HG11 | 1:C:198:ILE:HG23 | 2.00                     | 0.43              |
| 1:D:119:VAL:HB   | 1:D:181:VAL:HG22 | 2.00                     | 0.43              |
| 1:f:166:ARG:HH22 | 1:g:125:GLU:CD   | 2.27                     | 0.43              |
| 1:G:330:LEU:O    | 1:G:334:ILE:HG13 | 2.19                     | 0.43              |
| 1:g:172:LYS:HE2  | 1:g:172:LYS:HB3  | 1.75                     | 0.43              |
| 1:g:278:VAL:O    | 1:g:312:PHE:HD1  | 2.02                     | 0.43              |
| 1:H:159:PHE:HE2  | 1:H:161:HIS:HB2  | 1.83                     | 0.43              |
| 1:L:163:ASP:HA   | 1:L:164:PRO:HD3  | 1.86                     | 0.43              |
| 1:o:298:ARG:HG3  | 1:o:298:ARG:NH1  | 2.29                     | 0.43              |
| 1:r:269:ILE:HA   | 1:r:270:PRO:HD3  | 1.90                     | 0.43              |
| 1:A:183:VAL:HG12 | 1:A:191:THR:HG23 | 2.00                     | 0.43              |
| 1:a:325:GLU:HG2  | 1:o:324:PRO:HB3  | 2.00                     | 0.43              |
| 1:B:243:ILE:HD13 | 1:b:134:LEU:HD21 | 2.00                     | 0.43              |
| 1:B:263:ARG:NH1  | 1:B:265:VAL:HG12 | 2.34                     | 0.43              |
| 1:L:170:LEU:HD23 | 1:L:170:LEU:HA   | 1.93                     | 0.43              |
| 1:p:148:VAL:HG12 | 1:p:152:VAL:HG23 | 2.00                     | 0.43              |
| 1:a:298:ARG:NH1  | 1:a:313:ARG:HD2  | 2.34                     | 0.42              |
| 1:B:285:ILE:H    | 1:B:285:ILE:HG13 | 1.62                     | 0.42              |
| 1:D:250:MET:O    | 1:D:254:ASP:OD2  | 2.36                     | 0.42              |
| 1:F:145:ASP:HB3  | 1:F:148:VAL:HG23 | 2.00                     | 0.42              |
| 1:F:166:ARG:HB3  | 1:F:169:ASP:HB2  | 2.01                     | 0.42              |
| 1:i:330:LEU:O    | 1:i:334:ILE:HG13 | 2.19                     | 0.42              |
| 1:L:294:ILE:HD11 | 1:L:321:ILE:CG1  | 2.48                     | 0.42              |
| 1:Q:252:VAL:HG13 | 1:Q:256:LEU:HD12 | 2.01                     | 0.42              |
| 1:Q:293:ILE:H    | 1:Q:293:ILE:HG13 | 1.68                     | 0.42              |
| 1:s:332:ASN:C    | 1:s:334:ILE:H    | 2.27                     | 0.42              |
| 1:a:192:ILE:HD12 | 1:B:193:HIS:CD2  | 2.54                     | 0.42              |
| 1:c:144:GLU:O    | 1:c:161:HIS:NE2  | 2.50                     | 0.42              |
| 1:E:213:ARG:HB2  | 1:E:216:ASN:HD22 | 1.84                     | 0.42              |
| 1:g:128:LEU:C    | 1:g:128:LEU:HD23 | 2.43                     | 0.42              |
| 1:s:117:HIS:CE1  | 1:s:174:ASN:HB3  | 2.55                     | 0.42              |
| 1:A:131:LEU:HD21 | 1:A:139:VAL:HG11 | 2.01                     | 0.42              |
| 1:B:213:ARG:HD2  | 1:B:216:ASN:ND2  | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:170:LEU:HD13 | 1:J:198:ILE:HG13 | 2.01                     | 0.42              |
| 1:K:263:ARG:NH2  | 1:K:265:VAL:HG12 | 2.33                     | 0.42              |
| 1:M:230:SER:H    | 1:m:253:GLN:HE22 | 1.67                     | 0.42              |
| 1:P:175:VAL:CG1  | 1:P:198:ILE:HG23 | 2.49                     | 0.42              |
| 1:p:265:VAL:O    | 1:p:319:LEU:HA   | 2.19                     | 0.42              |
| 1:t:263:ARG:HG2  | 1:t:264:MET:N    | 2.33                     | 0.42              |
| 1:c:298:ARG:NH2  | 1:c:313:ARG:HB2  | 2.20                     | 0.42              |
| 1:E:134:LEU:HD21 | 1:e:243:ILE:HD12 | 2.01                     | 0.42              |
| 1:G:125:GLU:HB3  | 1:g:232:PHE:HD1  | 1.84                     | 0.42              |
| 1:h:270:PRO:HD2  | 1:h:334:ILE:CG2  | 2.48                     | 0.42              |
| 1:m:273:SER:HB2  | 1:m:334:ILE:O    | 2.19                     | 0.42              |
| 1:R:213:ARG:HB2  | 1:R:216:ASN:HD22 | 1.85                     | 0.42              |
| 1:r:293:ILE:HD13 | 1:r:318:ILE:CG2  | 2.50                     | 0.42              |
| 1:s:175:VAL:HG11 | 1:s:198:ILE:HG23 | 2.01                     | 0.42              |
| 1:d:252:VAL:HA   | 1:d:256:LEU:HD23 | 2.01                     | 0.42              |
| 1:d:274:LYS:HD3  | 1:d:335:SER:O    | 2.20                     | 0.42              |
| 1:g:269:ILE:HG23 | 1:g:273:SER:CB   | 2.50                     | 0.42              |
| 1:g:274:LYS:HB3  | 1:g:274:LYS:HE2  | 1.85                     | 0.42              |
| 1:i:323:LYS:HB2  | 1:i:326:GLU:HG3  | 2.02                     | 0.42              |
| 1:j:118:VAL:HB   | 1:j:139:VAL:HG22 | 2.02                     | 0.42              |
| 1:m:199:ARG:NH2  | 1:m:205:VAL:O    | 2.52                     | 0.42              |
| 1:m:211:ALA:HB2  | 1:m:220:LEU:HD22 | 2.01                     | 0.42              |
| 1:o:269:ILE:HA   | 1:o:270:PRO:HD3  | 1.89                     | 0.42              |
| 1:P:175:VAL:HG11 | 1:P:198:ILE:HG23 | 2.02                     | 0.42              |
| 1:D:241:ARG:NH2  | 1:d:259:GLU:OE1  | 2.52                     | 0.42              |
| 1:e:298:ARG:HH12 | 1:e:313:ARG:CZ   | 2.33                     | 0.42              |
| 1:G:309:ASP:OD1  | 1:G:309:ASP:N    | 2.49                     | 0.42              |
| 1:g:289:THR:HG22 | 1:g:291:VAL:H    | 1.84                     | 0.42              |
| 1:J:183:VAL:HG12 | 1:J:191:THR:HG23 | 2.01                     | 0.42              |
| 1:m:294:ILE:HD11 | 1:m:321:ILE:HG13 | 2.02                     | 0.42              |
| 1:N:267:VAL:CG1  | 1:N:334:ILE:HD11 | 2.49                     | 0.42              |
| 1:O:214:TYR:HD1  | 1:O:233:VAL:HG11 | 1.84                     | 0.42              |
| 1:o:127:THR:O    | 1:o:130:CYS:HB3  | 2.19                     | 0.42              |
| 1:Q:247:TYR:HB3  | 1:q:302:LEU:HD13 | 2.01                     | 0.42              |
| 1:R:265:VAL:HG11 | 1:R:327:ILE:HG21 | 2.01                     | 0.42              |
| 1:S:131:LEU:O    | 1:S:135:ARG:HB2  | 2.20                     | 0.42              |
| 1:a:195:ILE:HD13 | 1:a:225:ALA:HB2  | 2.02                     | 0.42              |
| 1:C:232:PHE:CD1  | 1:c:125:GLU:HB3  | 2.54                     | 0.42              |
| 1:D:265:VAL:HG21 | 1:D:327:ILE:HG12 | 2.02                     | 0.42              |
| 1:h:119:VAL:HB   | 1:h:181:VAL:HG22 | 2.00                     | 0.42              |
| 1:J:267:VAL:HA   | 1:J:268:PRO:HD3  | 1.89                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:199:ARG:NH1  | 1:M:224:GLY:O    | 2.51                     | 0.42              |
| 1:Q:133:GLU:HB2  | 1:q:240:SER:HB2  | 2.01                     | 0.42              |
| 1:A:293:ILE:H    | 1:A:293:ILE:HG13 | 1.71                     | 0.42              |
| 1:a:233:VAL:O    | 1:a:237:ARG:HB2  | 2.19                     | 0.42              |
| 1:B:289:THR:HG23 | 1:B:291:VAL:H    | 1.84                     | 0.42              |
| 1:O:116:ARG:HH21 | 1:O:116:ARG:CG   | 2.26                     | 0.42              |
| 1:s:116:ARG:HD2  | 1:s:179:ARG:HG2  | 2.00                     | 0.42              |
| 1:E:298:ARG:HH12 | 1:E:313:ARG:CZ   | 2.31                     | 0.42              |
| 1:G:237:ARG:HD2  | 1:g:259:GLU:OE2  | 2.19                     | 0.42              |
| 1:N:235:SER:HB2  | 1:n:231:PRO:HG3  | 2.02                     | 0.42              |
| 1:n:275:LEU:HD21 | 1:n:333:TYR:CE2  | 2.55                     | 0.42              |
| 1:s:229:ILE:HG22 | 1:s:231:PRO:HD3  | 2.02                     | 0.42              |
| 1:a:285:ILE:H    | 1:a:285:ILE:HG13 | 1.63                     | 0.42              |
| 1:b:294:ILE:HD11 | 1:b:321:ILE:HG13 | 2.01                     | 0.42              |
| 1:E:289:THR:HG23 | 1:E:291:VAL:H    | 1.83                     | 0.42              |
| 1:G:335:SER:O    | 1:G:336:ALA:CB   | 2.68                     | 0.42              |
| 1:I:144:GLU:O    | 1:I:161:HIS:NE2  | 2.51                     | 0.42              |
| 1:j:298:ARG:HH22 | 1:j:313:ARG:HD2  | 1.85                     | 0.42              |
| 1:n:289:THR:HG23 | 1:n:291:VAL:H    | 1.85                     | 0.42              |
| 1:S:181:VAL:HG11 | 1:S:198:ILE:HD13 | 2.01                     | 0.42              |
| 1:t:289:THR:HG23 | 1:t:291:VAL:H    | 1.85                     | 0.42              |
| 1:A:242:SER:O    | 1:a:206:ARG:NH1  | 2.53                     | 0.41              |
| 1:C:232:PHE:HD1  | 1:c:125:GLU:HB3  | 1.85                     | 0.41              |
| 1:d:238:LEU:HD12 | 1:d:238:LEU:HA   | 1.91                     | 0.41              |
| 1:H:263:ARG:CZ   | 1:H:265:VAL:HG12 | 2.50                     | 0.41              |
| 1:P:330:LEU:O    | 1:P:334:ILE:HG13 | 2.20                     | 0.41              |
| 1:B:237:ARG:HH11 | 1:B:241:ARG:CZ   | 2.33                     | 0.41              |
| 1:F:307:PRO:HG2  | 1:F:310:TYR:HB2  | 2.02                     | 0.41              |
| 1:G:195:ILE:HD13 | 1:G:225:ALA:HB2  | 2.00                     | 0.41              |
| 1:J:335:SER:O    | 1:J:336:ALA:HB3  | 2.20                     | 0.41              |
| 1:k:191:THR:O    | 1:k:195:ILE:HG13 | 2.20                     | 0.41              |
| 1:l:150:LYS:H    | 1:l:150:LYS:HG2  | 1.58                     | 0.41              |
| 1:n:199:ARG:HE   | 1:n:203:GLU:HA   | 1.85                     | 0.41              |
| 1:n:269:ILE:HD11 | 1:n:312:PHE:HD2  | 1.83                     | 0.41              |
| 1:p:199:ARG:HE   | 1:p:203:GLU:HA   | 1.85                     | 0.41              |
| 1:Q:129:GLU:HG3  | 1:q:233:VAL:HA   | 2.01                     | 0.41              |
| 1:r:252:VAL:HG13 | 1:r:256:LEU:HD12 | 2.02                     | 0.41              |
| 1:C:324:PRO:HB2  | 1:s:325:GLU:HG3  | 2.01                     | 0.41              |
| 1:J:247:TYR:HB3  | 1:j:302:LEU:HD13 | 2.01                     | 0.41              |
| 1:L:148:VAL:HG12 | 1:L:152:VAL:HG23 | 2.02                     | 0.41              |
| 1:n:270:PRO:CD   | 1:n:334:ILE:HG23 | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:264:MET:HE2  | 1:O:321:ILE:HG12 | 2.01                     | 0.41              |
| 1:Q:195:ILE:HA   | 1:Q:198:ILE:HD12 | 2.01                     | 0.41              |
| 1:C:296:VAL:HG23 | 1:C:306:PRO:HG3  | 2.02                     | 0.41              |
| 1:D:237:ARG:HH11 | 1:D:241:ARG:HE   | 1.67                     | 0.41              |
| 1:E:243:ILE:HD13 | 1:e:118:VAL:HG21 | 2.00                     | 0.41              |
| 1:L:117:HIS:CE1  | 1:L:174:ASN:HB2  | 2.56                     | 0.41              |
| 1:m:275:LEU:HD12 | 1:m:334:ILE:HG23 | 2.02                     | 0.41              |
| 1:t:195:ILE:HG23 | 1:t:207:ILE:HD13 | 2.03                     | 0.41              |
| 1:t:265:VAL:O    | 1:t:319:LEU:HA   | 2.20                     | 0.41              |
| 1:B:250:MET:HB3  | 1:b:227:GLN:OE1  | 2.21                     | 0.41              |
| 1:B:330:LEU:HD22 | 1:B:334:ILE:HD11 | 2.02                     | 0.41              |
| 1:C:133:GLU:HB2  | 1:c:240:SER:HB2  | 2.02                     | 0.41              |
| 1:C:265:VAL:O    | 1:C:319:LEU:HA   | 2.20                     | 0.41              |
| 1:d:116:ARG:NH2  | 1:d:116:ARG:CG   | 2.78                     | 0.41              |
| 1:E:129:GLU:O    | 1:E:132:ARG:HB2  | 2.20                     | 0.41              |
| 1:k:335:SER:O    | 1:k:336:ALA:HB3  | 2.19                     | 0.41              |
| 1:M:163:ASP:OD2  | 1:p:213:ARG:NH2  | 2.53                     | 0.41              |
| 1:n:281:LEU:HB2  | 1:n:308:ARG:HB3  | 2.02                     | 0.41              |
| 1:q:242:SER:OG   | 1:q:249:ALA:HB2  | 2.20                     | 0.41              |
| 1:q:298:ARG:NH2  | 1:q:316:ASP:OD1  | 2.53                     | 0.41              |
| 1:T:247:TYR:HA   | 1:T:250:MET:HG2  | 2.02                     | 0.41              |
| 1:b:163:ASP:OD1  | 1:b:163:ASP:C    | 2.62                     | 0.41              |
| 1:E:210:GLU:HB2  | 1:e:239:MET:CE   | 2.50                     | 0.41              |
| 1:E:270:PRO:HD2  | 1:E:334:ILE:CG2  | 2.50                     | 0.41              |
| 1:i:195:ILE:HD13 | 1:i:225:ALA:HB2  | 2.03                     | 0.41              |
| 1:j:330:LEU:O    | 1:j:334:ILE:HG13 | 2.21                     | 0.41              |
| 1:O:263:ARG:CG   | 1:O:264:MET:N    | 2.84                     | 0.41              |
| 1:Q:231:PRO:HB3  | 1:q:235:SER:HB2  | 2.02                     | 0.41              |
| 1:R:163:ASP:OD1  | 1:R:163:ASP:C    | 2.63                     | 0.41              |
| 1:S:129:GLU:HG3  | 1:s:233:VAL:HA   | 2.03                     | 0.41              |
| 1:S:231:PRO:HB3  | 1:s:235:SER:HB2  | 2.02                     | 0.41              |
| 1:a:292:ILE:HD12 | 1:a:321:ILE:HB   | 2.03                     | 0.41              |
| 1:C:248:GLU:O    | 1:C:252:VAL:HG23 | 2.20                     | 0.41              |
| 1:F:141:VAL:HG11 | 1:F:152:VAL:HG21 | 2.03                     | 0.41              |
| 1:l:199:ARG:NH2  | 1:l:205:VAL:O    | 2.53                     | 0.41              |
| 1:O:238:LEU:HD12 | 1:O:238:LEU:HA   | 1.85                     | 0.41              |
| 1:T:229:ILE:HA   | 1:t:253:GLN:NE2  | 2.35                     | 0.41              |
| 1:a:253:GLN:NE2  | 1:a:253:GLN:HA   | 2.35                     | 0.41              |
| 1:C:199:ARG:HE   | 1:C:203:GLU:HA   | 1.84                     | 0.41              |
| 1:d:198:ILE:H    | 1:d:198:ILE:HG13 | 1.65                     | 0.41              |
| 1:E:194:CYS:SG   | 1:E:198:ILE:HD11 | 2.61                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:232:PHE:N    | 1:h:232:PHE:HD2  | 2.19                     | 0.41              |
| 1:L:238:LEU:HA   | 1:L:238:LEU:HD12 | 1.81                     | 0.41              |
| 1:L:259:GLU:OE2  | 1:l:241:ARG:NH2  | 2.54                     | 0.41              |
| 1:M:213:ARG:CG   | 1:p:166:ARG:NH2  | 2.81                     | 0.41              |
| 1:q:195:ILE:HD13 | 1:q:225:ALA:HB2  | 2.02                     | 0.41              |
| 1:R:230:SER:H    | 1:r:253:GLN:HE22 | 1.69                     | 0.41              |
| 1:A:240:SER:HB2  | 1:a:133:GLU:HB2  | 2.03                     | 0.41              |
| 1:A:253:GLN:O    | 1:A:257:ALA:HB3  | 2.21                     | 0.41              |
| 1:a:325:GLU:CD   | 1:a:325:GLU:H    | 2.29                     | 0.41              |
| 1:c:165:THR:HB   | 1:c:193:HIS:ND1  | 2.36                     | 0.41              |
| 1:c:285:ILE:HB   | 1:c:293:ILE:HD11 | 2.03                     | 0.41              |
| 1:F:243:ILE:HD11 | 1:f:182:ILE:HD11 | 2.03                     | 0.41              |
| 1:g:214:TYR:CD1  | 1:g:217:ILE:HD12 | 2.55                     | 0.41              |
| 1:H:159:PHE:CE2  | 1:H:161:HIS:HB2  | 2.56                     | 0.41              |
| 1:i:285:ILE:H    | 1:i:285:ILE:HG13 | 1.67                     | 0.41              |
| 1:i:298:ARG:CZ   | 1:i:316:ASP:OD1  | 2.68                     | 0.41              |
| 1:j:163:ASP:HA   | 1:j:164:PRO:HD2  | 1.87                     | 0.41              |
| 1:O:231:PRO:HG2  | 1:O:232:PHE:HD2  | 1.84                     | 0.41              |
| 1:p:183:VAL:HG12 | 1:p:191:THR:HG23 | 2.03                     | 0.41              |
| 1:R:165:THR:HB   | 1:R:193:HIS:CE1  | 2.56                     | 0.41              |
| 1:r:166:ARG:HB3  | 1:r:169:ASP:HB2  | 2.03                     | 0.41              |
| 1:r:199:ARG:NH1  | 1:r:224:GLY:O    | 2.54                     | 0.41              |
| 1:s:285:ILE:HB   | 1:s:293:ILE:HD11 | 2.03                     | 0.41              |
| 1:T:235:SER:HB2  | 1:t:231:PRO:HB3  | 2.03                     | 0.41              |
| 1:t:182:ILE:HA   | 1:t:208:ILE:O    | 2.21                     | 0.41              |
| 1:t:195:ILE:HA   | 1:t:198:ILE:HD12 | 2.02                     | 0.41              |
| 1:t:265:VAL:HG11 | 1:t:327:ILE:HG12 | 2.02                     | 0.41              |
| 1:b:203:GLU:H    | 1:b:203:GLU:HG2  | 1.77                     | 0.41              |
| 1:C:298:ARG:HH22 | 1:C:313:ARG:HG3  | 1.86                     | 0.41              |
| 1:H:232:PHE:N    | 1:H:232:PHE:CD2  | 2.88                     | 0.41              |
| 1:h:124:SER:OG   | 1:h:126:SER:HB2  | 2.21                     | 0.41              |
| 1:J:229:ILE:HG12 | 1:j:238:LEU:HD23 | 2.03                     | 0.41              |
| 1:j:124:SER:OG   | 1:j:126:SER:HB2  | 2.20                     | 0.41              |
| 1:L:252:VAL:HG13 | 1:L:256:LEU:HD12 | 2.02                     | 0.41              |
| 1:L:264:MET:HE2  | 1:L:321:ILE:HG12 | 2.03                     | 0.41              |
| 1:N:269:ILE:HA   | 1:N:270:PRO:HD3  | 1.90                     | 0.41              |
| 1:r:199:ARG:NH2  | 1:r:205:VAL:O    | 2.43                     | 0.41              |
| 1:B:269:ILE:HD11 | 1:B:318:ILE:HD11 | 2.01                     | 0.40              |
| 1:B:270:PRO:HD2  | 1:B:334:ILE:HG22 | 2.03                     | 0.40              |
| 1:g:192:ILE:HD12 | 1:H:193:HIS:CD2  | 2.56                     | 0.40              |
| 1:P:253:GLN:O    | 1:P:257:ALA:HB3  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:a:120:ILE:HB   | 1:a:141:VAL:HG22 | 2.02                     | 0.40              |
| 1:c:123:TRP:HZ2  | 1:c:128:LEU:HD12 | 1.85                     | 0.40              |
| 1:c:269:ILE:HD11 | 1:c:318:ILE:HD11 | 2.02                     | 0.40              |
| 1:F:123:TRP:HZ2  | 1:F:128:LEU:HD12 | 1.86                     | 0.40              |
| 1:F:262:ARG:HG3  | 1:F:323:LYS:HG3  | 2.02                     | 0.40              |
| 1:f:144:GLU:O    | 1:f:161:HIS:NE2  | 2.54                     | 0.40              |
| 1:G:253:GLN:HE22 | 1:g:230:SER:H    | 1.70                     | 0.40              |
| 1:H:133:GLU:HB2  | 1:h:240:SER:HB2  | 2.02                     | 0.40              |
| 1:J:203:GLU:H    | 1:J:203:GLU:HG2  | 1.75                     | 0.40              |
| 1:L:292:ILE:H    | 1:L:292:ILE:HG13 | 1.70                     | 0.40              |
| 1:P:325:GLU:CD   | 1:P:325:GLU:H    | 2.29                     | 0.40              |
| 1:t:248:GLU:O    | 1:t:252:VAL:HG23 | 2.21                     | 0.40              |
| 1:a:132:ARG:NH1  | 1:a:132:ARG:CG   | 2.75                     | 0.40              |
| 1:C:132:ARG:NH1  | 1:C:132:ARG:CG   | 2.71                     | 0.40              |
| 1:c:116:ARG:HH21 | 1:c:116:ARG:CG   | 2.28                     | 0.40              |
| 1:E:175:VAL:HG11 | 1:E:198:ILE:HG23 | 2.01                     | 0.40              |
| 1:e:298:ARG:HH22 | 1:e:313:ARG:CG   | 2.34                     | 0.40              |
| 1:e:298:ARG:HH12 | 1:e:313:ARG:NH1  | 2.19                     | 0.40              |
| 1:i:242:SER:OG   | 1:i:249:ALA:HB2  | 2.21                     | 0.40              |
| 1:i:294:ILE:HD11 | 1:i:321:ILE:CD1  | 2.51                     | 0.40              |
| 1:J:125:GLU:HB3  | 1:j:232:PHE:CD1  | 2.56                     | 0.40              |
| 1:L:285:ILE:HD11 | 1:L:312:PHE:CZ   | 2.56                     | 0.40              |
| 1:n:248:GLU:O    | 1:n:252:VAL:HG23 | 2.21                     | 0.40              |
| 1:P:235:SER:HB2  | 1:p:231:PRO:HB3  | 2.04                     | 0.40              |
| 1:r:232:PHE:CD2  | 1:r:232:PHE:N    | 2.89                     | 0.40              |
| 1:A:269:ILE:O    | 1:A:315:GLY:N    | 2.52                     | 0.40              |
| 1:b:218:GLU:HG2  | 1:C:200:LYS:NZ   | 2.36                     | 0.40              |
| 1:C:253:GLN:O    | 1:C:257:ALA:HB3  | 2.21                     | 0.40              |
| 1:C:324:PRO:HB2  | 1:s:325:GLU:CG   | 2.50                     | 0.40              |
| 1:d:269:ILE:HG22 | 1:d:314:ALA:HA   | 2.04                     | 0.40              |
| 1:d:269:ILE:HA   | 1:d:270:PRO:HD3  | 1.93                     | 0.40              |
| 1:E:191:THR:O    | 1:E:195:ILE:HG13 | 2.22                     | 0.40              |
| 1:H:263:ARG:NH2  | 1:H:265:VAL:HG12 | 2.36                     | 0.40              |
| 1:I:117:HIS:HE1  | 1:I:174:ASN:O    | 2.03                     | 0.40              |
| 1:I:185:LEU:HD13 | 1:I:190:GLU:HB3  | 2.04                     | 0.40              |
| 1:J:242:SER:O    | 1:j:206:ARG:NH1  | 2.55                     | 0.40              |
| 1:q:307:PRO:HG2  | 1:q:310:TYR:HB2  | 2.04                     | 0.40              |
| 1:S:214:TYR:HD1  | 1:S:233:VAL:HG11 | 1.86                     | 0.40              |
| 1:t:293:ILE:HG23 | 1:t:318:ILE:HG23 | 2.03                     | 0.40              |
| 1:b:171:GLU:OE2  | 1:b:176:ARG:NH2  | 2.55                     | 0.40              |
| 1:C:252:VAL:HG22 | 1:c:256:LEU:HD21 | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:285:ILE:HD12 | 1:D:293:ILE:HD11 | 2.03                     | 0.40              |
| 1:G:150:LYS:O    | 1:G:154:ARG:HB2  | 2.21                     | 0.40              |
| 1:H:117:HIS:HE1  | 1:H:174:ASN:O    | 2.05                     | 0.40              |
| 1:N:269:ILE:HD11 | 1:N:312:PHE:CD2  | 2.57                     | 0.40              |
| 1:N:330:LEU:O    | 1:N:334:ILE:HG12 | 2.22                     | 0.40              |
| 1:p:165:THR:HB   | 1:p:193:HIS:CE1  | 2.56                     | 0.40              |
| 1:S:163:ASP:HA   | 1:S:164:PRO:HD2  | 1.93                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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     | 219/230 (95%) | 209 (95%) | 9 (4%)  | 1 (0%)   | 24 57       |
| 1   | B     | 219/230 (95%) | 209 (95%) | 10 (5%) | 0        | 100 100     |
| 1   | C     | 219/230 (95%) | 210 (96%) | 8 (4%)  | 1 (0%)   | 24 57       |
| 1   | D     | 219/230 (95%) | 209 (95%) | 10 (5%) | 0        | 100 100     |
| 1   | E     | 219/230 (95%) | 208 (95%) | 11 (5%) | 0        | 100 100     |
| 1   | F     | 219/230 (95%) | 209 (95%) | 10 (5%) | 0        | 100 100     |
| 1   | G     | 219/230 (95%) | 206 (94%) | 13 (6%) | 0        | 100 100     |
| 1   | H     | 219/230 (95%) | 209 (95%) | 9 (4%)  | 1 (0%)   | 24 57       |
| 1   | I     | 219/230 (95%) | 212 (97%) | 7 (3%)  | 0        | 100 100     |
| 1   | J     | 219/230 (95%) | 208 (95%) | 9 (4%)  | 2 (1%)   | 14 45       |
| 1   | K     | 219/230 (95%) | 210 (96%) | 8 (4%)  | 1 (0%)   | 24 57       |
| 1   | L     | 219/230 (95%) | 208 (95%) | 11 (5%) | 0        | 100 100     |
| 1   | M     | 219/230 (95%) | 205 (94%) | 14 (6%) | 0        | 100 100     |
| 1   | N     | 219/230 (95%) | 208 (95%) | 10 (5%) | 1 (0%)   | 24 57       |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | O     | 219/230 (95%)   | 209 (95%)  | 9 (4%)   | 1 (0%)   | 24          | 57  |
| 1   | P     | 219/230 (95%)   | 212 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 1   | Q     | 219/230 (95%)   | 211 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 1   | R     | 219/230 (95%)   | 205 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 1   | S     | 219/230 (95%)   | 206 (94%)  | 12 (6%)  | 1 (0%)   | 24          | 57  |
| 1   | T     | 219/230 (95%)   | 211 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 1   | a     | 219/230 (95%)   | 211 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 1   | b     | 219/230 (95%)   | 210 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 1   | c     | 219/230 (95%)   | 207 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| 1   | d     | 219/230 (95%)   | 207 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| 1   | e     | 219/230 (95%)   | 207 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| 1   | f     | 219/230 (95%)   | 205 (94%)  | 13 (6%)  | 1 (0%)   | 24          | 57  |
| 1   | g     | 219/230 (95%)   | 209 (95%)  | 9 (4%)   | 1 (0%)   | 24          | 57  |
| 1   | h     | 219/230 (95%)   | 210 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 1   | i     | 219/230 (95%)   | 210 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 1   | j     | 219/230 (95%)   | 206 (94%)  | 12 (6%)  | 1 (0%)   | 24          | 57  |
| 1   | k     | 219/230 (95%)   | 208 (95%)  | 10 (5%)  | 1 (0%)   | 24          | 57  |
| 1   | l     | 219/230 (95%)   | 205 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 1   | m     | 219/230 (95%)   | 209 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 1   | n     | 219/230 (95%)   | 209 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 1   | o     | 219/230 (95%)   | 208 (95%)  | 10 (5%)  | 1 (0%)   | 24          | 57  |
| 1   | p     | 219/230 (95%)   | 208 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 1   | q     | 219/230 (95%)   | 210 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 1   | r     | 219/230 (95%)   | 207 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| 1   | s     | 219/230 (95%)   | 208 (95%)  | 10 (5%)  | 1 (0%)   | 24          | 57  |
| 1   | t     | 219/230 (95%)   | 209 (95%)  | 9 (4%)   | 1 (0%)   | 24          | 57  |
| All | All   | 8760/9200 (95%) | 8337 (95%) | 407 (5%) | 16 (0%)  | 43          | 72  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | k     | 135 | ARG  |
| 1   | o     | 135 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | s     | 135 | ARG  |
| 1   | O     | 215 | GLU  |
| 1   | A     | 244 | ASP  |
| 1   | H     | 215 | GLU  |
| 1   | J     | 215 | GLU  |
| 1   | N     | 135 | ARG  |
| 1   | C     | 135 | ARG  |
| 1   | f     | 172 | LYS  |
| 1   | j     | 135 | ARG  |
| 1   | S     | 135 | ARG  |
| 1   | t     | 299 | GLY  |
| 1   | J     | 299 | GLY  |
| 1   | g     | 299 | GLY  |
| 1   | K     | 299 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 189/196 (96%) | 178 (94%) | 11 (6%)  | 18          | 47 |
| 1   | B     | 189/196 (96%) | 179 (95%) | 10 (5%)  | 20          | 50 |
| 1   | C     | 189/196 (96%) | 172 (91%) | 17 (9%)  | 9           | 31 |
| 1   | D     | 189/196 (96%) | 178 (94%) | 11 (6%)  | 18          | 47 |
| 1   | E     | 189/196 (96%) | 170 (90%) | 19 (10%) | 7           | 27 |
| 1   | F     | 189/196 (96%) | 173 (92%) | 16 (8%)  | 10          | 34 |
| 1   | G     | 189/196 (96%) | 175 (93%) | 14 (7%)  | 13          | 39 |
| 1   | H     | 189/196 (96%) | 176 (93%) | 13 (7%)  | 14          | 42 |
| 1   | I     | 189/196 (96%) | 175 (93%) | 14 (7%)  | 13          | 39 |
| 1   | J     | 189/196 (96%) | 168 (89%) | 21 (11%) | 6           | 23 |
| 1   | K     | 189/196 (96%) | 177 (94%) | 12 (6%)  | 16          | 45 |
| 1   | L     | 189/196 (96%) | 174 (92%) | 15 (8%)  | 11          | 37 |
| 1   | M     | 189/196 (96%) | 178 (94%) | 11 (6%)  | 18          | 47 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | N     | 188/196 (96%)   | 173 (92%)  | 15 (8%)  | 11          | 37 |
| 1   | O     | 189/196 (96%)   | 172 (91%)  | 17 (9%)  | 9           | 31 |
| 1   | P     | 189/196 (96%)   | 182 (96%)  | 7 (4%)   | 30          | 59 |
| 1   | Q     | 189/196 (96%)   | 176 (93%)  | 13 (7%)  | 14          | 42 |
| 1   | R     | 189/196 (96%)   | 172 (91%)  | 17 (9%)  | 9           | 31 |
| 1   | S     | 189/196 (96%)   | 173 (92%)  | 16 (8%)  | 10          | 34 |
| 1   | T     | 189/196 (96%)   | 172 (91%)  | 17 (9%)  | 9           | 31 |
| 1   | a     | 189/196 (96%)   | 170 (90%)  | 19 (10%) | 7           | 27 |
| 1   | b     | 189/196 (96%)   | 177 (94%)  | 12 (6%)  | 16          | 45 |
| 1   | c     | 189/196 (96%)   | 174 (92%)  | 15 (8%)  | 11          | 37 |
| 1   | d     | 189/196 (96%)   | 176 (93%)  | 13 (7%)  | 14          | 42 |
| 1   | e     | 189/196 (96%)   | 176 (93%)  | 13 (7%)  | 14          | 42 |
| 1   | f     | 189/196 (96%)   | 179 (95%)  | 10 (5%)  | 20          | 50 |
| 1   | g     | 189/196 (96%)   | 172 (91%)  | 17 (9%)  | 9           | 31 |
| 1   | h     | 189/196 (96%)   | 177 (94%)  | 12 (6%)  | 16          | 45 |
| 1   | i     | 189/196 (96%)   | 177 (94%)  | 12 (6%)  | 16          | 45 |
| 1   | j     | 189/196 (96%)   | 180 (95%)  | 9 (5%)   | 23          | 53 |
| 1   | k     | 189/196 (96%)   | 176 (93%)  | 13 (7%)  | 14          | 42 |
| 1   | l     | 189/196 (96%)   | 170 (90%)  | 19 (10%) | 7           | 27 |
| 1   | m     | 189/196 (96%)   | 181 (96%)  | 8 (4%)   | 26          | 56 |
| 1   | n     | 189/196 (96%)   | 173 (92%)  | 16 (8%)  | 10          | 34 |
| 1   | o     | 189/196 (96%)   | 172 (91%)  | 17 (9%)  | 9           | 31 |
| 1   | p     | 189/196 (96%)   | 172 (91%)  | 17 (9%)  | 9           | 31 |
| 1   | q     | 189/196 (96%)   | 181 (96%)  | 8 (4%)   | 26          | 56 |
| 1   | r     | 188/196 (96%)   | 172 (92%)  | 16 (8%)  | 10          | 34 |
| 1   | s     | 189/196 (96%)   | 173 (92%)  | 16 (8%)  | 10          | 34 |
| 1   | t     | 189/196 (96%)   | 176 (93%)  | 13 (7%)  | 14          | 42 |
| All | All   | 7558/7840 (96%) | 6997 (93%) | 561 (7%) | 13          | 39 |

All (561) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 116 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 172 | LYS  |
| 1   | A     | 215 | GLU  |
| 1   | A     | 238 | LEU  |
| 1   | A     | 260 | SER  |
| 1   | A     | 271 | GLU  |
| 1   | A     | 293 | ILE  |
| 1   | A     | 301 | GLU  |
| 1   | A     | 303 | ILE  |
| 1   | A     | 325 | GLU  |
| 1   | A     | 330 | LEU  |
| 1   | a     | 116 | ARG  |
| 1   | a     | 132 | ARG  |
| 1   | a     | 134 | LEU  |
| 1   | a     | 166 | ARG  |
| 1   | a     | 172 | LYS  |
| 1   | a     | 215 | GLU  |
| 1   | a     | 237 | ARG  |
| 1   | a     | 245 | ASP  |
| 1   | a     | 256 | LEU  |
| 1   | a     | 267 | VAL  |
| 1   | a     | 276 | GLU  |
| 1   | a     | 285 | ILE  |
| 1   | a     | 289 | THR  |
| 1   | a     | 292 | ILE  |
| 1   | a     | 293 | ILE  |
| 1   | a     | 311 | SER  |
| 1   | a     | 325 | GLU  |
| 1   | a     | 332 | ASN  |
| 1   | a     | 334 | ILE  |
| 1   | B     | 166 | ARG  |
| 1   | B     | 172 | LYS  |
| 1   | B     | 206 | ARG  |
| 1   | B     | 215 | GLU  |
| 1   | B     | 241 | ARG  |
| 1   | B     | 245 | ASP  |
| 1   | B     | 256 | LEU  |
| 1   | B     | 293 | ILE  |
| 1   | B     | 303 | ILE  |
| 1   | B     | 330 | LEU  |
| 1   | b     | 116 | ARG  |
| 1   | b     | 132 | ARG  |
| 1   | b     | 150 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 175 | VAL  |
| 1   | b     | 200 | LYS  |
| 1   | b     | 208 | ILE  |
| 1   | b     | 241 | ARG  |
| 1   | b     | 265 | VAL  |
| 1   | b     | 273 | SER  |
| 1   | b     | 293 | ILE  |
| 1   | b     | 308 | ARG  |
| 1   | b     | 330 | LEU  |
| 1   | C     | 132 | ARG  |
| 1   | C     | 166 | ARG  |
| 1   | C     | 172 | LYS  |
| 1   | C     | 175 | VAL  |
| 1   | C     | 218 | GLU  |
| 1   | C     | 241 | ARG  |
| 1   | C     | 245 | ASP  |
| 1   | C     | 264 | MET  |
| 1   | C     | 265 | VAL  |
| 1   | C     | 273 | SER  |
| 1   | C     | 279 | SER  |
| 1   | C     | 289 | THR  |
| 1   | C     | 293 | ILE  |
| 1   | C     | 298 | ARG  |
| 1   | C     | 311 | SER  |
| 1   | C     | 325 | GLU  |
| 1   | C     | 330 | LEU  |
| 1   | c     | 116 | ARG  |
| 1   | c     | 133 | GLU  |
| 1   | c     | 134 | LEU  |
| 1   | c     | 172 | LYS  |
| 1   | c     | 200 | LYS  |
| 1   | c     | 215 | GLU  |
| 1   | c     | 241 | ARG  |
| 1   | c     | 255 | VAL  |
| 1   | c     | 256 | LEU  |
| 1   | c     | 273 | SER  |
| 1   | c     | 293 | ILE  |
| 1   | c     | 300 | ASP  |
| 1   | c     | 301 | GLU  |
| 1   | c     | 311 | SER  |
| 1   | c     | 330 | LEU  |
| 1   | D     | 116 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 175 | VAL  |
| 1   | D     | 176 | ARG  |
| 1   | D     | 238 | LEU  |
| 1   | D     | 241 | ARG  |
| 1   | D     | 245 | ASP  |
| 1   | D     | 265 | VAL  |
| 1   | D     | 276 | GLU  |
| 1   | D     | 298 | ARG  |
| 1   | D     | 325 | GLU  |
| 1   | D     | 330 | LEU  |
| 1   | d     | 116 | ARG  |
| 1   | d     | 132 | ARG  |
| 1   | d     | 150 | LYS  |
| 1   | d     | 175 | VAL  |
| 1   | d     | 176 | ARG  |
| 1   | d     | 237 | ARG  |
| 1   | d     | 238 | LEU  |
| 1   | d     | 241 | ARG  |
| 1   | d     | 245 | ASP  |
| 1   | d     | 265 | VAL  |
| 1   | d     | 276 | GLU  |
| 1   | d     | 325 | GLU  |
| 1   | d     | 330 | LEU  |
| 1   | E     | 116 | ARG  |
| 1   | E     | 166 | ARG  |
| 1   | E     | 171 | GLU  |
| 1   | E     | 172 | LYS  |
| 1   | E     | 175 | VAL  |
| 1   | E     | 206 | ARG  |
| 1   | E     | 215 | GLU  |
| 1   | E     | 218 | GLU  |
| 1   | E     | 241 | ARG  |
| 1   | E     | 245 | ASP  |
| 1   | E     | 263 | ARG  |
| 1   | E     | 264 | MET  |
| 1   | E     | 273 | SER  |
| 1   | E     | 274 | LYS  |
| 1   | E     | 289 | THR  |
| 1   | E     | 293 | ILE  |
| 1   | E     | 300 | ASP  |
| 1   | E     | 325 | GLU  |
| 1   | E     | 330 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | e     | 116 | ARG  |
| 1   | e     | 175 | VAL  |
| 1   | e     | 215 | GLU  |
| 1   | e     | 238 | LEU  |
| 1   | e     | 241 | ARG  |
| 1   | e     | 243 | ILE  |
| 1   | e     | 245 | ASP  |
| 1   | e     | 258 | GLU  |
| 1   | e     | 293 | ILE  |
| 1   | e     | 311 | SER  |
| 1   | e     | 325 | GLU  |
| 1   | e     | 330 | LEU  |
| 1   | e     | 331 | LYS  |
| 1   | F     | 116 | ARG  |
| 1   | F     | 132 | ARG  |
| 1   | F     | 135 | ARG  |
| 1   | F     | 171 | GLU  |
| 1   | F     | 175 | VAL  |
| 1   | F     | 176 | ARG  |
| 1   | F     | 232 | PHE  |
| 1   | F     | 238 | LEU  |
| 1   | F     | 241 | ARG  |
| 1   | F     | 245 | ASP  |
| 1   | F     | 264 | MET  |
| 1   | F     | 273 | SER  |
| 1   | F     | 293 | ILE  |
| 1   | F     | 311 | SER  |
| 1   | F     | 325 | GLU  |
| 1   | F     | 330 | LEU  |
| 1   | f     | 116 | ARG  |
| 1   | f     | 132 | ARG  |
| 1   | f     | 166 | ARG  |
| 1   | f     | 175 | VAL  |
| 1   | f     | 200 | LYS  |
| 1   | f     | 222 | MET  |
| 1   | f     | 238 | LEU  |
| 1   | f     | 241 | ARG  |
| 1   | f     | 325 | GLU  |
| 1   | f     | 330 | LEU  |
| 1   | G     | 116 | ARG  |
| 1   | G     | 135 | ARG  |
| 1   | G     | 171 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 175 | VAL  |
| 1   | G     | 222 | MET  |
| 1   | G     | 238 | LEU  |
| 1   | G     | 243 | ILE  |
| 1   | G     | 245 | ASP  |
| 1   | G     | 264 | MET  |
| 1   | G     | 293 | ILE  |
| 1   | G     | 301 | GLU  |
| 1   | G     | 311 | SER  |
| 1   | G     | 325 | GLU  |
| 1   | G     | 330 | LEU  |
| 1   | g     | 133 | GLU  |
| 1   | g     | 172 | LYS  |
| 1   | g     | 175 | VAL  |
| 1   | g     | 200 | LYS  |
| 1   | g     | 222 | MET  |
| 1   | g     | 241 | ARG  |
| 1   | g     | 243 | ILE  |
| 1   | g     | 267 | VAL  |
| 1   | g     | 273 | SER  |
| 1   | g     | 289 | THR  |
| 1   | g     | 298 | ARG  |
| 1   | g     | 300 | ASP  |
| 1   | g     | 301 | GLU  |
| 1   | g     | 303 | ILE  |
| 1   | g     | 308 | ARG  |
| 1   | g     | 325 | GLU  |
| 1   | g     | 332 | ASN  |
| 1   | H     | 146 | GLU  |
| 1   | H     | 172 | LYS  |
| 1   | H     | 175 | VAL  |
| 1   | H     | 183 | VAL  |
| 1   | H     | 229 | ILE  |
| 1   | H     | 262 | ARG  |
| 1   | H     | 279 | SER  |
| 1   | H     | 293 | ILE  |
| 1   | H     | 304 | ILE  |
| 1   | H     | 309 | ASP  |
| 1   | H     | 311 | SER  |
| 1   | H     | 325 | GLU  |
| 1   | H     | 330 | LEU  |
| 1   | h     | 118 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | h     | 128 | LEU  |
| 1   | h     | 137 | SER  |
| 1   | h     | 175 | VAL  |
| 1   | h     | 199 | ARG  |
| 1   | h     | 256 | LEU  |
| 1   | h     | 274 | LYS  |
| 1   | h     | 275 | LEU  |
| 1   | h     | 293 | ILE  |
| 1   | h     | 304 | ILE  |
| 1   | h     | 311 | SER  |
| 1   | h     | 330 | LEU  |
| 1   | I     | 116 | ARG  |
| 1   | I     | 166 | ARG  |
| 1   | I     | 171 | GLU  |
| 1   | I     | 172 | LYS  |
| 1   | I     | 175 | VAL  |
| 1   | I     | 200 | LYS  |
| 1   | I     | 238 | LEU  |
| 1   | I     | 243 | ILE  |
| 1   | I     | 267 | VAL  |
| 1   | I     | 293 | ILE  |
| 1   | I     | 301 | GLU  |
| 1   | I     | 311 | SER  |
| 1   | I     | 325 | GLU  |
| 1   | I     | 330 | LEU  |
| 1   | i     | 116 | ARG  |
| 1   | i     | 172 | LYS  |
| 1   | i     | 215 | GLU  |
| 1   | i     | 238 | LEU  |
| 1   | i     | 245 | ASP  |
| 1   | i     | 267 | VAL  |
| 1   | i     | 273 | SER  |
| 1   | i     | 285 | ILE  |
| 1   | i     | 289 | THR  |
| 1   | i     | 311 | SER  |
| 1   | i     | 325 | GLU  |
| 1   | i     | 330 | LEU  |
| 1   | J     | 119 | VAL  |
| 1   | J     | 138 | GLU  |
| 1   | J     | 150 | LYS  |
| 1   | J     | 154 | ARG  |
| 1   | J     | 172 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 176 | ARG  |
| 1   | J     | 199 | ARG  |
| 1   | J     | 205 | VAL  |
| 1   | J     | 213 | ARG  |
| 1   | J     | 230 | SER  |
| 1   | J     | 256 | LEU  |
| 1   | J     | 258 | GLU  |
| 1   | J     | 273 | SER  |
| 1   | J     | 276 | GLU  |
| 1   | J     | 278 | VAL  |
| 1   | J     | 293 | ILE  |
| 1   | J     | 300 | ASP  |
| 1   | J     | 309 | ASP  |
| 1   | J     | 325 | GLU  |
| 1   | J     | 330 | LEU  |
| 1   | J     | 334 | ILE  |
| 1   | j     | 116 | ARG  |
| 1   | j     | 135 | ARG  |
| 1   | j     | 137 | SER  |
| 1   | j     | 175 | VAL  |
| 1   | j     | 176 | ARG  |
| 1   | j     | 215 | GLU  |
| 1   | j     | 293 | ILE  |
| 1   | j     | 301 | GLU  |
| 1   | j     | 330 | LEU  |
| 1   | K     | 116 | ARG  |
| 1   | K     | 151 | LYS  |
| 1   | K     | 154 | ARG  |
| 1   | K     | 172 | LYS  |
| 1   | K     | 175 | VAL  |
| 1   | K     | 245 | ASP  |
| 1   | K     | 289 | THR  |
| 1   | K     | 293 | ILE  |
| 1   | K     | 300 | ASP  |
| 1   | K     | 325 | GLU  |
| 1   | K     | 330 | LEU  |
| 1   | K     | 332 | ASN  |
| 1   | k     | 116 | ARG  |
| 1   | k     | 118 | VAL  |
| 1   | k     | 175 | VAL  |
| 1   | k     | 215 | GLU  |
| 1   | k     | 245 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | k     | 256 | LEU  |
| 1   | k     | 273 | SER  |
| 1   | k     | 293 | ILE  |
| 1   | k     | 298 | ARG  |
| 1   | k     | 300 | ASP  |
| 1   | k     | 301 | GLU  |
| 1   | k     | 311 | SER  |
| 1   | k     | 330 | LEU  |
| 1   | L     | 116 | ARG  |
| 1   | L     | 135 | ARG  |
| 1   | L     | 139 | VAL  |
| 1   | L     | 172 | LYS  |
| 1   | L     | 175 | VAL  |
| 1   | L     | 200 | LYS  |
| 1   | L     | 215 | GLU  |
| 1   | L     | 232 | PHE  |
| 1   | L     | 238 | LEU  |
| 1   | L     | 241 | ARG  |
| 1   | L     | 255 | VAL  |
| 1   | L     | 289 | THR  |
| 1   | L     | 293 | ILE  |
| 1   | L     | 325 | GLU  |
| 1   | L     | 330 | LEU  |
| 1   | l     | 116 | ARG  |
| 1   | l     | 133 | GLU  |
| 1   | l     | 150 | LYS  |
| 1   | l     | 154 | ARG  |
| 1   | l     | 175 | VAL  |
| 1   | l     | 183 | VAL  |
| 1   | l     | 230 | SER  |
| 1   | l     | 238 | LEU  |
| 1   | l     | 241 | ARG  |
| 1   | l     | 245 | ASP  |
| 1   | l     | 256 | LEU  |
| 1   | l     | 264 | MET  |
| 1   | l     | 265 | VAL  |
| 1   | l     | 289 | THR  |
| 1   | l     | 301 | GLU  |
| 1   | l     | 303 | ILE  |
| 1   | l     | 311 | SER  |
| 1   | l     | 325 | GLU  |
| 1   | l     | 330 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 128 | LEU  |
| 1   | M     | 172 | LYS  |
| 1   | M     | 175 | VAL  |
| 1   | M     | 204 | SER  |
| 1   | M     | 206 | ARG  |
| 1   | M     | 215 | GLU  |
| 1   | M     | 263 | ARG  |
| 1   | M     | 293 | ILE  |
| 1   | M     | 304 | ILE  |
| 1   | M     | 325 | GLU  |
| 1   | M     | 330 | LEU  |
| 1   | m     | 199 | ARG  |
| 1   | m     | 206 | ARG  |
| 1   | m     | 215 | GLU  |
| 1   | m     | 273 | SER  |
| 1   | m     | 280 | VAL  |
| 1   | m     | 308 | ARG  |
| 1   | m     | 325 | GLU  |
| 1   | m     | 330 | LEU  |
| 1   | N     | 147 | ASN  |
| 1   | N     | 163 | ASP  |
| 1   | N     | 166 | ARG  |
| 1   | N     | 172 | LYS  |
| 1   | N     | 175 | VAL  |
| 1   | N     | 204 | SER  |
| 1   | N     | 213 | ARG  |
| 1   | N     | 215 | GLU  |
| 1   | N     | 245 | ASP  |
| 1   | N     | 265 | VAL  |
| 1   | N     | 281 | LEU  |
| 1   | N     | 293 | ILE  |
| 1   | N     | 311 | SER  |
| 1   | N     | 325 | GLU  |
| 1   | N     | 330 | LEU  |
| 1   | n     | 116 | ARG  |
| 1   | n     | 133 | GLU  |
| 1   | n     | 135 | ARG  |
| 1   | n     | 172 | LYS  |
| 1   | n     | 175 | VAL  |
| 1   | n     | 200 | LYS  |
| 1   | n     | 204 | SER  |
| 1   | n     | 206 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | n     | 215 | GLU  |
| 1   | n     | 230 | SER  |
| 1   | n     | 245 | ASP  |
| 1   | n     | 289 | THR  |
| 1   | n     | 293 | ILE  |
| 1   | n     | 309 | ASP  |
| 1   | n     | 311 | SER  |
| 1   | n     | 330 | LEU  |
| 1   | O     | 116 | ARG  |
| 1   | O     | 131 | LEU  |
| 1   | O     | 135 | ARG  |
| 1   | O     | 142 | LEU  |
| 1   | O     | 172 | LYS  |
| 1   | O     | 175 | VAL  |
| 1   | O     | 176 | ARG  |
| 1   | O     | 215 | GLU  |
| 1   | O     | 230 | SER  |
| 1   | O     | 232 | PHE  |
| 1   | O     | 238 | LEU  |
| 1   | O     | 240 | SER  |
| 1   | O     | 265 | VAL  |
| 1   | O     | 273 | SER  |
| 1   | O     | 325 | GLU  |
| 1   | O     | 330 | LEU  |
| 1   | O     | 334 | ILE  |
| 1   | o     | 116 | ARG  |
| 1   | o     | 131 | LEU  |
| 1   | o     | 132 | ARG  |
| 1   | o     | 135 | ARG  |
| 1   | o     | 154 | ARG  |
| 1   | o     | 175 | VAL  |
| 1   | o     | 206 | ARG  |
| 1   | o     | 222 | MET  |
| 1   | o     | 238 | LEU  |
| 1   | o     | 241 | ARG  |
| 1   | o     | 245 | ASP  |
| 1   | o     | 258 | GLU  |
| 1   | o     | 269 | ILE  |
| 1   | o     | 289 | THR  |
| 1   | o     | 311 | SER  |
| 1   | o     | 325 | GLU  |
| 1   | o     | 330 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 166 | ARG  |
| 1   | P     | 175 | VAL  |
| 1   | P     | 230 | SER  |
| 1   | P     | 279 | SER  |
| 1   | P     | 311 | SER  |
| 1   | P     | 325 | GLU  |
| 1   | P     | 330 | LEU  |
| 1   | p     | 116 | ARG  |
| 1   | p     | 132 | ARG  |
| 1   | p     | 172 | LYS  |
| 1   | p     | 175 | VAL  |
| 1   | p     | 215 | GLU  |
| 1   | p     | 238 | LEU  |
| 1   | p     | 245 | ASP  |
| 1   | p     | 265 | VAL  |
| 1   | p     | 267 | VAL  |
| 1   | p     | 279 | SER  |
| 1   | p     | 289 | THR  |
| 1   | p     | 293 | ILE  |
| 1   | p     | 294 | ILE  |
| 1   | p     | 325 | GLU  |
| 1   | p     | 330 | LEU  |
| 1   | p     | 332 | ASN  |
| 1   | p     | 334 | ILE  |
| 1   | Q     | 118 | VAL  |
| 1   | Q     | 135 | ARG  |
| 1   | Q     | 150 | LYS  |
| 1   | Q     | 175 | VAL  |
| 1   | Q     | 222 | MET  |
| 1   | Q     | 245 | ASP  |
| 1   | Q     | 273 | SER  |
| 1   | Q     | 279 | SER  |
| 1   | Q     | 293 | ILE  |
| 1   | Q     | 301 | GLU  |
| 1   | Q     | 325 | GLU  |
| 1   | Q     | 329 | ARG  |
| 1   | Q     | 330 | LEU  |
| 1   | q     | 131 | LEU  |
| 1   | q     | 135 | ARG  |
| 1   | q     | 172 | LYS  |
| 1   | q     | 199 | ARG  |
| 1   | q     | 215 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | q     | 273 | SER  |
| 1   | q     | 325 | GLU  |
| 1   | q     | 330 | LEU  |
| 1   | R     | 163 | ASP  |
| 1   | R     | 172 | LYS  |
| 1   | R     | 201 | ILE  |
| 1   | R     | 220 | LEU  |
| 1   | R     | 230 | SER  |
| 1   | R     | 238 | LEU  |
| 1   | R     | 241 | ARG  |
| 1   | R     | 260 | SER  |
| 1   | R     | 262 | ARG  |
| 1   | R     | 265 | VAL  |
| 1   | R     | 288 | VAL  |
| 1   | R     | 293 | ILE  |
| 1   | R     | 301 | GLU  |
| 1   | R     | 303 | ILE  |
| 1   | R     | 311 | SER  |
| 1   | R     | 325 | GLU  |
| 1   | R     | 330 | LEU  |
| 1   | r     | 116 | ARG  |
| 1   | r     | 155 | SER  |
| 1   | r     | 166 | ARG  |
| 1   | r     | 168 | SER  |
| 1   | r     | 171 | GLU  |
| 1   | r     | 175 | VAL  |
| 1   | r     | 200 | LYS  |
| 1   | r     | 204 | SER  |
| 1   | r     | 206 | ARG  |
| 1   | r     | 267 | VAL  |
| 1   | r     | 293 | ILE  |
| 1   | r     | 298 | ARG  |
| 1   | r     | 309 | ASP  |
| 1   | r     | 311 | SER  |
| 1   | r     | 325 | GLU  |
| 1   | r     | 330 | LEU  |
| 1   | S     | 116 | ARG  |
| 1   | S     | 131 | LEU  |
| 1   | S     | 172 | LYS  |
| 1   | S     | 175 | VAL  |
| 1   | S     | 186 | GLU  |
| 1   | S     | 200 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 215 | GLU  |
| 1   | S     | 230 | SER  |
| 1   | S     | 238 | LEU  |
| 1   | S     | 265 | VAL  |
| 1   | S     | 269 | ILE  |
| 1   | S     | 273 | SER  |
| 1   | S     | 289 | THR  |
| 1   | S     | 325 | GLU  |
| 1   | S     | 330 | LEU  |
| 1   | S     | 331 | LYS  |
| 1   | s     | 116 | ARG  |
| 1   | s     | 133 | GLU  |
| 1   | s     | 150 | LYS  |
| 1   | s     | 153 | LEU  |
| 1   | s     | 160 | VAL  |
| 1   | s     | 172 | LYS  |
| 1   | s     | 175 | VAL  |
| 1   | s     | 238 | LEU  |
| 1   | s     | 241 | ARG  |
| 1   | s     | 265 | VAL  |
| 1   | s     | 267 | VAL  |
| 1   | s     | 279 | SER  |
| 1   | s     | 311 | SER  |
| 1   | s     | 317 | ILE  |
| 1   | s     | 325 | GLU  |
| 1   | s     | 330 | LEU  |
| 1   | T     | 128 | LEU  |
| 1   | T     | 133 | GLU  |
| 1   | T     | 149 | ARG  |
| 1   | T     | 150 | LYS  |
| 1   | T     | 166 | ARG  |
| 1   | T     | 172 | LYS  |
| 1   | T     | 186 | GLU  |
| 1   | T     | 215 | GLU  |
| 1   | T     | 245 | ASP  |
| 1   | T     | 263 | ARG  |
| 1   | T     | 267 | VAL  |
| 1   | T     | 289 | THR  |
| 1   | T     | 298 | ARG  |
| 1   | T     | 300 | ASP  |
| 1   | T     | 311 | SER  |
| 1   | T     | 325 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 330 | LEU  |
| 1   | t     | 116 | ARG  |
| 1   | t     | 172 | LYS  |
| 1   | t     | 175 | VAL  |
| 1   | t     | 182 | ILE  |
| 1   | t     | 222 | MET  |
| 1   | t     | 293 | ILE  |
| 1   | t     | 294 | ILE  |
| 1   | t     | 301 | GLU  |
| 1   | t     | 311 | SER  |
| 1   | t     | 325 | GLU  |
| 1   | t     | 330 | LEU  |
| 1   | t     | 332 | ASN  |
| 1   | t     | 334 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 147 | ASN  |
| 1   | A     | 253 | GLN  |
| 1   | A     | 286 | HIS  |
| 1   | a     | 253 | GLN  |
| 1   | B     | 117 | HIS  |
| 1   | B     | 253 | GLN  |
| 1   | b     | 117 | HIS  |
| 1   | b     | 253 | GLN  |
| 1   | C     | 219 | GLN  |
| 1   | C     | 253 | GLN  |
| 1   | c     | 117 | HIS  |
| 1   | c     | 253 | GLN  |
| 1   | c     | 286 | HIS  |
| 1   | D     | 253 | GLN  |
| 1   | d     | 219 | GLN  |
| 1   | E     | 117 | HIS  |
| 1   | E     | 147 | ASN  |
| 1   | E     | 253 | GLN  |
| 1   | E     | 286 | HIS  |
| 1   | e     | 117 | HIS  |
| 1   | e     | 147 | ASN  |
| 1   | e     | 253 | GLN  |
| 1   | F     | 147 | ASN  |
| 1   | F     | 253 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | f     | 117 | HIS  |
| 1   | f     | 219 | GLN  |
| 1   | G     | 253 | GLN  |
| 1   | G     | 286 | HIS  |
| 1   | g     | 147 | ASN  |
| 1   | g     | 253 | GLN  |
| 1   | g     | 332 | ASN  |
| 1   | H     | 117 | HIS  |
| 1   | H     | 253 | GLN  |
| 1   | h     | 253 | GLN  |
| 1   | I     | 117 | HIS  |
| 1   | I     | 147 | ASN  |
| 1   | I     | 219 | GLN  |
| 1   | I     | 253 | GLN  |
| 1   | i     | 161 | HIS  |
| 1   | i     | 286 | HIS  |
| 1   | i     | 332 | ASN  |
| 1   | J     | 117 | HIS  |
| 1   | J     | 216 | ASN  |
| 1   | J     | 253 | GLN  |
| 1   | J     | 286 | HIS  |
| 1   | j     | 219 | GLN  |
| 1   | j     | 253 | GLN  |
| 1   | K     | 286 | HIS  |
| 1   | k     | 117 | HIS  |
| 1   | k     | 147 | ASN  |
| 1   | L     | 117 | HIS  |
| 1   | L     | 253 | GLN  |
| 1   | l     | 117 | HIS  |
| 1   | l     | 147 | ASN  |
| 1   | M     | 253 | GLN  |
| 1   | M     | 286 | HIS  |
| 1   | m     | 174 | ASN  |
| 1   | m     | 253 | GLN  |
| 1   | N     | 147 | ASN  |
| 1   | N     | 253 | GLN  |
| 1   | N     | 286 | HIS  |
| 1   | n     | 253 | GLN  |
| 1   | n     | 286 | HIS  |
| 1   | O     | 147 | ASN  |
| 1   | P     | 117 | HIS  |
| 1   | P     | 253 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | p     | 147 | ASN  |
| 1   | p     | 253 | GLN  |
| 1   | p     | 286 | HIS  |
| 1   | Q     | 147 | ASN  |
| 1   | Q     | 219 | GLN  |
| 1   | Q     | 253 | GLN  |
| 1   | q     | 117 | HIS  |
| 1   | q     | 147 | ASN  |
| 1   | q     | 219 | GLN  |
| 1   | q     | 253 | GLN  |
| 1   | r     | 117 | HIS  |
| 1   | r     | 147 | ASN  |
| 1   | r     | 253 | GLN  |
| 1   | r     | 286 | HIS  |
| 1   | S     | 117 | HIS  |
| 1   | S     | 147 | ASN  |
| 1   | s     | 253 | GLN  |
| 1   | t     | 286 | 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 ⓘ

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     | 221/230 (96%) | 0.20   | 5 (2%) 61 40 | 36, 70, 112, 146      | 0     |
| 1   | B     | 221/230 (96%) | 0.08   | 2 (0%) 81 64 | 53, 90, 142, 153      | 0     |
| 1   | C     | 221/230 (96%) | -0.15  | 2 (0%) 81 64 | 49, 71, 105, 156      | 0     |
| 1   | D     | 221/230 (96%) | -0.29  | 2 (0%) 81 64 | 36, 61, 89, 111       | 0     |
| 1   | E     | 221/230 (96%) | 0.21   | 7 (3%) 50 30 | 38, 68, 110, 128      | 0     |
| 1   | F     | 221/230 (96%) | -0.22  | 3 (1%) 73 53 | 34, 61, 93, 125       | 0     |
| 1   | G     | 221/230 (96%) | 0.23   | 6 (2%) 56 35 | 42, 76, 120, 151      | 0     |
| 1   | H     | 221/230 (96%) | 0.40   | 8 (3%) 46 27 | 48, 79, 114, 152      | 0     |
| 1   | I     | 221/230 (96%) | -0.05  | 1 (0%) 87 75 | 44, 76, 122, 144      | 0     |
| 1   | J     | 221/230 (96%) | 0.45   | 7 (3%) 50 30 | 51, 79, 118, 138      | 0     |
| 1   | K     | 221/230 (96%) | 0.01   | 4 (1%) 67 47 | 43, 71, 113, 133      | 0     |
| 1   | L     | 221/230 (96%) | -0.05  | 2 (0%) 81 64 | 33, 62, 90, 121       | 0     |
| 1   | M     | 221/230 (96%) | 0.10   | 4 (1%) 67 47 | 63, 92, 126, 149      | 0     |
| 1   | N     | 221/230 (96%) | 0.12   | 5 (2%) 61 40 | 53, 76, 113, 138      | 0     |
| 1   | O     | 221/230 (96%) | -0.12  | 6 (2%) 56 35 | 39, 59, 89, 133       | 0     |
| 1   | P     | 221/230 (96%) | -0.10  | 2 (0%) 81 64 | 46, 81, 130, 161      | 0     |
| 1   | Q     | 221/230 (96%) | 0.49   | 7 (3%) 50 30 | 78, 115, 147, 161     | 0     |
| 1   | R     | 221/230 (96%) | 0.44   | 8 (3%) 46 27 | 64, 87, 118, 146      | 0     |
| 1   | S     | 221/230 (96%) | -0.25  | 1 (0%) 87 75 | 45, 65, 98, 137       | 0     |
| 1   | T     | 221/230 (96%) | 0.18   | 3 (1%) 73 53 | 50, 87, 133, 172      | 0     |
| 1   | a     | 221/230 (96%) | -0.01  | 3 (1%) 73 53 | 47, 70, 106, 138      | 0     |
| 1   | b     | 221/230 (96%) | 0.04   | 1 (0%) 87 75 | 56, 92, 127, 147      | 0     |
| 1   | c     | 221/230 (96%) | -0.04  | 3 (1%) 73 53 | 36, 72, 114, 130      | 0     |
| 1   | d     | 221/230 (96%) | -0.09  | 3 (1%) 73 53 | 33, 57, 85, 113       | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|---------|-----------------------|-------|
| 1   | e     | 221/230 (96%)   | -0.01  | 1 (0%)   | 87 75   | 38, 71, 118, 139      | 0     |
| 1   | f     | 221/230 (96%)   | -0.12  | 4 (1%)   | 67 47   | 35, 59, 90, 114       | 0     |
| 1   | g     | 221/230 (96%)   | 0.49   | 12 (5%)  | 31 18   | 47, 71, 102, 138      | 0     |
| 1   | h     | 221/230 (96%)   | 0.44   | 12 (5%)  | 31 18   | 48, 84, 115, 145      | 0     |
| 1   | i     | 221/230 (96%)   | 0.28   | 9 (4%)   | 41 24   | 50, 76, 114, 140      | 0     |
| 1   | j     | 221/230 (96%)   | 0.34   | 13 (5%)  | 28 16   | 48, 85, 118, 147      | 0     |
| 1   | k     | 221/230 (96%)   | 0.15   | 7 (3%)   | 50 30   | 39, 72, 118, 148      | 0     |
| 1   | l     | 221/230 (96%)   | -0.16  | 3 (1%)   | 73 53   | 37, 61, 89, 113       | 0     |
| 1   | m     | 221/230 (96%)   | 0.16   | 3 (1%)   | 73 53   | 63, 99, 129, 150      | 0     |
| 1   | n     | 221/230 (96%)   | 0.41   | 12 (5%)  | 31 18   | 42, 77, 120, 136      | 0     |
| 1   | o     | 221/230 (96%)   | -0.06  | 3 (1%)   | 73 53   | 40, 58, 84, 105       | 0     |
| 1   | p     | 221/230 (96%)   | -0.05  | 0        | 100 100 | 57, 84, 114, 144      | 0     |
| 1   | q     | 221/230 (96%)   | 0.51   | 4 (1%)   | 67 47   | 71, 117, 152, 170     | 0     |
| 1   | r     | 221/230 (96%)   | 0.57   | 17 (7%)  | 19 11   | 51, 82, 120, 149      | 0     |
| 1   | s     | 221/230 (96%)   | -0.07  | 4 (1%)   | 67 47   | 46, 62, 92, 109       | 0     |
| 1   | t     | 221/230 (96%)   | 0.22   | 1 (0%)   | 87 75   | 62, 88, 119, 138      | 0     |
| All | All   | 8840/9200 (96%) | 0.12   | 200 (2%) | 61 40   | 33, 76, 124, 172      | 0     |

All (200) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 136 | GLY  | 6.4  |
| 1   | g     | 144 | GLU  | 5.3  |
| 1   | g     | 312 | PHE  | 5.0  |
| 1   | n     | 336 | ALA  | 4.7  |
| 1   | g     | 275 | LEU  | 4.4  |
| 1   | J     | 136 | GLY  | 4.4  |
| 1   | n     | 333 | TYR  | 4.3  |
| 1   | f     | 336 | ALA  | 4.0  |
| 1   | h     | 226 | ASP  | 4.0  |
| 1   | c     | 144 | GLU  | 4.0  |
| 1   | h     | 137 | SER  | 3.9  |
| 1   | k     | 171 | GLU  | 3.8  |
| 1   | H     | 246 | GLY  | 3.8  |
| 1   | T     | 243 | ILE  | 3.7  |
| 1   | P     | 301 | GLU  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 336 | ALA  | 3.7  |
| 1   | H     | 144 | GLU  | 3.6  |
| 1   | r     | 275 | LEU  | 3.6  |
| 1   | H     | 137 | SER  | 3.6  |
| 1   | g     | 218 | GLU  | 3.5  |
| 1   | B     | 272 | GLY  | 3.5  |
| 1   | k     | 244 | ASP  | 3.4  |
| 1   | h     | 136 | GLY  | 3.4  |
| 1   | O     | 336 | ALA  | 3.3  |
| 1   | r     | 301 | GLU  | 3.3  |
| 1   | i     | 184 | ASP  | 3.2  |
| 1   | j     | 257 | ALA  | 3.2  |
| 1   | i     | 171 | GLU  | 3.2  |
| 1   | Q     | 153 | LEU  | 3.2  |
| 1   | c     | 336 | ALA  | 3.2  |
| 1   | r     | 158 | ASN  | 3.2  |
| 1   | g     | 336 | ALA  | 3.2  |
| 1   | j     | 130 | CYS  | 3.2  |
| 1   | E     | 136 | GLY  | 3.1  |
| 1   | g     | 186 | GLU  | 3.1  |
| 1   | f     | 222 | MET  | 3.1  |
| 1   | M     | 136 | GLY  | 3.1  |
| 1   | n     | 275 | LEU  | 3.0  |
| 1   | q     | 200 | LYS  | 3.0  |
| 1   | s     | 336 | ALA  | 3.0  |
| 1   | n     | 135 | ARG  | 3.0  |
| 1   | Q     | 180 | ALA  | 3.0  |
| 1   | G     | 336 | ALA  | 3.0  |
| 1   | J     | 137 | SER  | 3.0  |
| 1   | r     | 269 | ILE  | 3.0  |
| 1   | h     | 293 | ILE  | 2.9  |
| 1   | N     | 336 | ALA  | 2.9  |
| 1   | n     | 259 | GLU  | 2.9  |
| 1   | R     | 122 | GLY  | 2.9  |
| 1   | k     | 245 | ASP  | 2.9  |
| 1   | h     | 138 | GLU  | 2.9  |
| 1   | i     | 218 | GLU  | 2.9  |
| 1   | k     | 243 | ILE  | 2.9  |
| 1   | n     | 318 | ILE  | 2.8  |
| 1   | l     | 336 | ALA  | 2.8  |
| 1   | j     | 150 | LYS  | 2.8  |
| 1   | j     | 243 | ILE  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 137 | SER  | 2.8  |
| 1   | K     | 137 | SER  | 2.8  |
| 1   | r     | 335 | SER  | 2.8  |
| 1   | f     | 218 | GLU  | 2.8  |
| 1   | r     | 172 | LYS  | 2.7  |
| 1   | J     | 138 | GLU  | 2.7  |
| 1   | r     | 336 | ALA  | 2.7  |
| 1   | E     | 203 | GLU  | 2.7  |
| 1   | h     | 244 | ASP  | 2.7  |
| 1   | j     | 282 | ASP  | 2.7  |
| 1   | T     | 145 | ASP  | 2.7  |
| 1   | L     | 336 | ALA  | 2.7  |
| 1   | t     | 134 | LEU  | 2.7  |
| 1   | A     | 276 | GLU  | 2.7  |
| 1   | i     | 299 | GLY  | 2.7  |
| 1   | E     | 335 | SER  | 2.7  |
| 1   | q     | 153 | LEU  | 2.7  |
| 1   | r     | 312 | PHE  | 2.7  |
| 1   | F     | 138 | GLU  | 2.7  |
| 1   | l     | 144 | GLU  | 2.7  |
| 1   | k     | 336 | ALA  | 2.7  |
| 1   | d     | 137 | SER  | 2.6  |
| 1   | s     | 335 | SER  | 2.6  |
| 1   | A     | 312 | PHE  | 2.6  |
| 1   | G     | 136 | GLY  | 2.6  |
| 1   | k     | 299 | GLY  | 2.6  |
| 1   | j     | 258 | GLU  | 2.6  |
| 1   | h     | 134 | LEU  | 2.6  |
| 1   | j     | 242 | SER  | 2.6  |
| 1   | g     | 317 | ILE  | 2.6  |
| 1   | i     | 336 | ALA  | 2.6  |
| 1   | r     | 306 | PRO  | 2.6  |
| 1   | i     | 145 | ASP  | 2.6  |
| 1   | b     | 293 | ILE  | 2.5  |
| 1   | m     | 168 | SER  | 2.5  |
| 1   | n     | 260 | SER  | 2.5  |
| 1   | N     | 299 | GLY  | 2.5  |
| 1   | Q     | 150 | LYS  | 2.5  |
| 1   | e     | 314 | ALA  | 2.5  |
| 1   | Q     | 134 | LEU  | 2.5  |
| 1   | h     | 135 | ARG  | 2.5  |
| 1   | G     | 301 | GLU  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | R     | 220 | LEU  | 2.5  |
| 1   | E     | 272 | GLY  | 2.5  |
| 1   | D     | 336 | ALA  | 2.5  |
| 1   | N     | 137 | SER  | 2.5  |
| 1   | E     | 326 | GLU  | 2.5  |
| 1   | G     | 132 | ARG  | 2.5  |
| 1   | i     | 167 | VAL  | 2.4  |
| 1   | I     | 336 | ALA  | 2.4  |
| 1   | R     | 225 | ALA  | 2.4  |
| 1   | C     | 137 | SER  | 2.4  |
| 1   | F     | 137 | SER  | 2.4  |
| 1   | o     | 218 | GLU  | 2.4  |
| 1   | g     | 145 | ASP  | 2.4  |
| 1   | s     | 197 | GLY  | 2.4  |
| 1   | h     | 150 | LYS  | 2.4  |
| 1   | g     | 134 | LEU  | 2.4  |
| 1   | h     | 294 | ILE  | 2.4  |
| 1   | Q     | 154 | ARG  | 2.4  |
| 1   | O     | 218 | GLU  | 2.4  |
| 1   | g     | 137 | SER  | 2.4  |
| 1   | T     | 336 | ALA  | 2.4  |
| 1   | j     | 154 | ARG  | 2.4  |
| 1   | i     | 122 | GLY  | 2.3  |
| 1   | g     | 163 | ASP  | 2.3  |
| 1   | O     | 245 | ASP  | 2.3  |
| 1   | L     | 335 | SER  | 2.3  |
| 1   | h     | 336 | ALA  | 2.3  |
| 1   | J     | 209 | ALA  | 2.3  |
| 1   | h     | 133 | GLU  | 2.3  |
| 1   | A     | 288 | VAL  | 2.3  |
| 1   | m     | 143 | ALA  | 2.3  |
| 1   | D     | 137 | SER  | 2.3  |
| 1   | k     | 154 | ARG  | 2.3  |
| 1   | R     | 293 | ILE  | 2.3  |
| 1   | a     | 137 | SER  | 2.3  |
| 1   | J     | 186 | GLU  | 2.2  |
| 1   | G     | 150 | LYS  | 2.2  |
| 1   | A     | 336 | ALA  | 2.2  |
| 1   | J     | 281 | LEU  | 2.2  |
| 1   | n     | 128 | LEU  | 2.2  |
| 1   | P     | 336 | ALA  | 2.2  |
| 1   | r     | 314 | ALA  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 116 | ARG  | 2.2  |
| 1   | G     | 335 | SER  | 2.2  |
| 1   | s     | 137 | SER  | 2.2  |
| 1   | H     | 167 | VAL  | 2.2  |
| 1   | K     | 245 | ASP  | 2.2  |
| 1   | O     | 300 | ASP  | 2.2  |
| 1   | r     | 270 | PRO  | 2.2  |
| 1   | K     | 136 | GLY  | 2.2  |
| 1   | d     | 135 | ARG  | 2.2  |
| 1   | H     | 232 | PHE  | 2.2  |
| 1   | r     | 280 | VAL  | 2.2  |
| 1   | B     | 137 | SER  | 2.2  |
| 1   | q     | 303 | ILE  | 2.2  |
| 1   | r     | 273 | SER  | 2.2  |
| 1   | S     | 336 | ALA  | 2.2  |
| 1   | c     | 272 | GLY  | 2.2  |
| 1   | i     | 176 | ARG  | 2.2  |
| 1   | j     | 244 | ASP  | 2.2  |
| 1   | Q     | 261 | THR  | 2.1  |
| 1   | a     | 134 | LEU  | 2.1  |
| 1   | o     | 336 | ALA  | 2.1  |
| 1   | Q     | 181 | VAL  | 2.1  |
| 1   | g     | 261 | THR  | 2.1  |
| 1   | j     | 135 | ARG  | 2.1  |
| 1   | R     | 336 | ALA  | 2.1  |
| 1   | J     | 218 | GLU  | 2.1  |
| 1   | O     | 138 | GLU  | 2.1  |
| 1   | r     | 271 | GLU  | 2.1  |
| 1   | r     | 139 | VAL  | 2.1  |
| 1   | a     | 135 | ARG  | 2.1  |
| 1   | d     | 138 | GLU  | 2.1  |
| 1   | R     | 215 | GLU  | 2.1  |
| 1   | E     | 135 | ARG  | 2.1  |
| 1   | K     | 336 | ALA  | 2.1  |
| 1   | j     | 129 | GLU  | 2.1  |
| 1   | j     | 133 | GLU  | 2.1  |
| 1   | r     | 140 | PHE  | 2.1  |
| 1   | j     | 137 | SER  | 2.1  |
| 1   | M     | 137 | SER  | 2.1  |
| 1   | A     | 254 | ASP  | 2.1  |
| 1   | F     | 245 | ASP  | 2.1  |
| 1   | n     | 282 | ASP  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 270 | PRO  | 2.1  |
| 1   | n     | 137 | SER  | 2.0  |
| 1   | n     | 132 | ARG  | 2.0  |
| 1   | R     | 207 | ILE  | 2.0  |
| 1   | M     | 245 | ASP  | 2.0  |
| 1   | M     | 336 | ALA  | 2.0  |
| 1   | o     | 301 | GLU  | 2.0  |
| 1   | n     | 118 | VAL  | 2.0  |
| 1   | N     | 135 | ARG  | 2.0  |
| 1   | R     | 135 | ARG  | 2.0  |
| 1   | f     | 335 | SER  | 2.0  |
| 1   | r     | 332 | ASN  | 2.0  |
| 1   | C     | 336 | ALA  | 2.0  |
| 1   | m     | 169 | ASP  | 2.0  |
| 1   | l     | 299 | GLY  | 2.0  |
| 1   | q     | 140 | PHE  | 2.0  |
| 1   | H     | 138 | GLU  | 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.