



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:33 PM GMT

PDB ID : 2FHG  
Title : Crystal Structure of Mycobacterial Tuberculosis Proteasome  
Authors : Hu, G.; Lin, G.; Wang, M.; Dick, L.; Xu, R.M.; Nathan, C.; Li, H.  
Deposited on : 2005-12-23  
Resolution : 3.23 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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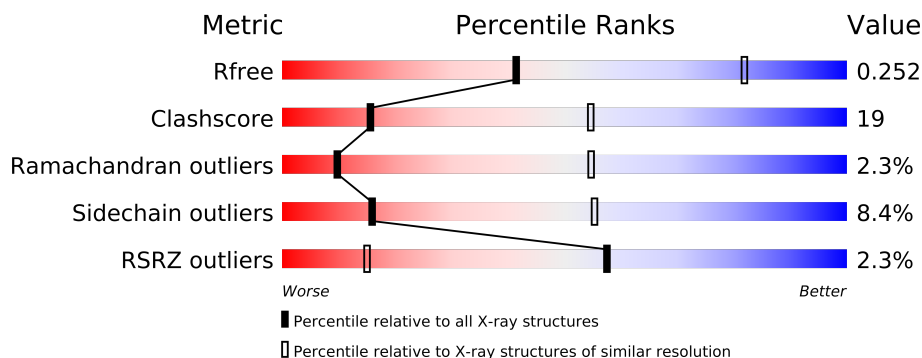
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.23 Å.

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









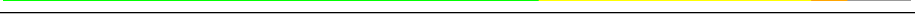


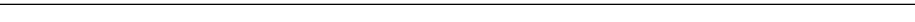



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1080 (3.30-3.18)                                      |
| Clashscore            | 79885                       | 1369 (3.30-3.18)                                      |
| Ramachandran outliers | 78287                       | 1342 (3.30-3.18)                                      |
| Sidechain outliers    | 78261                       | 1340 (3.30-3.18)                                      |
| RSRZ outliers         | 66119                       | 1081 (3.30-3.18)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1     | 250    |                  |
| 1   | A     | 250    |                  |
| 1   | B     | 250    |                  |
| 1   | D     | 250    |                  |
| 1   | F     | 250    |                  |
| 1   | I     | 250    |                  |
| 1   | K     | 250    |                  |
| 1   | M     | 250    |                  |
| 1   | O     | 250    |                  |
| 1   | Q     | 250    |                  |
| 1   | S     | 250    |                  |
| 1   | U     | 250    |                  |
| 1   | W     | 250    |                  |
| 1   | Y     | 250    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | 2     | 240    |  |
| 2   | C     | 240    |  |
| 2   | E     | 240    |  |
| 2   | G     | 240    |  |
| 2   | H     | 240    |  |
| 2   | J     | 240    |  |
| 2   | L     | 240    |  |
| 2   | N     | 240    |  |
| 2   | P     | 240    |  |
| 2   | R     | 240    |  |
| 2   | T     | 240    |  |
| 2   | V     | 240    |  |
| 2   | X     | 240    |  |
| 2   | Z     | 240    |  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46846 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called 20S proteasome, alpha and beta subunits.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | B     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | D     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | F     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | I     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | K     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | M     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | O     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | Q     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | S     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | U     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | W     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | Y     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |
| 1   | 1     | 220      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1692  | 1058 | 309 | 322 | 3 |         |         |       |

There are 42 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference   |
|-------|---------|----------|--------|-----------------------|-------------|
| A     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference   |
|-------|---------|----------|--------|-----------------------|-------------|
| A     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| A     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| B     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| B     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| B     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| D     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| D     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| D     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| F     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| F     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| F     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| I     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| I     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| I     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| K     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| K     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| K     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| M     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| M     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| M     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| O     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| O     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| O     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| Q     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| Q     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| Q     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| S     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| S     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| S     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| U     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| U     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| U     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| W     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| W     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| W     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| Y     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| Y     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| Y     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |
| 1     | -1      | MET      | -      | INITIATING METHIONINE | GB 13881852 |
| 1     | 0       | ASN      | -      | CLONING ARTIFACT      | GB 13881852 |
| 1     | 1       | SER      | -      | CLONING ARTIFACT      | GB 13881852 |

- Molecule 2 is a protein called proteasome, beta subunit.

| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 2   | H     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | C     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | E     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | G     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | J     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | L     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | N     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | P     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | R     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | T     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | V     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | X     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | Z     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |
| 2   | 2     | 222      | Total<br>1638 | C<br>1027 | N<br>282 | O<br>324 | S<br>5 | 0       | 0       | 0     |

There are 84 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference   |
|-------|---------|----------|--------|----------------|-------------|
| H     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| H     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| H     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| H     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| H     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| H     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| C     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| C     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| C     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| C     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| C     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| C     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference   |
|-------|---------|----------|--------|----------------|-------------|
| E     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| E     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| E     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| E     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| E     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| E     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| G     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| G     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| G     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| G     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| G     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| G     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| J     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| J     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| J     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| J     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| J     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| J     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| L     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| L     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| L     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| L     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| L     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| L     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| N     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| N     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| N     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| N     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| N     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| N     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| P     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| P     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| P     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| P     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| P     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| P     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| R     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| R     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| R     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| R     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| R     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| R     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference   |
|-------|---------|----------|--------|----------------|-------------|
| T     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| T     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| T     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| T     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| T     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| T     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| V     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| V     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| V     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| V     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| V     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| V     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| X     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| X     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| X     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| X     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| X     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| X     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| Z     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| Z     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| Z     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| Z     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| Z     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| Z     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| 2     | 535     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| 2     | 536     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| 2     | 537     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| 2     | 538     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| 2     | 539     | HIS      | -      | EXPRESSION TAG | GB 13881852 |
| 2     | 540     | HIS      | -      | EXPRESSION TAG | GB 13881852 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 3   | 1     | 13       | Total O<br>13 13 | 0       | 0       |
| 3   | 2     | 19       | Total O<br>19 19 | 0       | 0       |
| 3   | A     | 2        | Total O<br>2 2   | 0       | 0       |
| 3   | B     | 7        | Total O<br>7 7   | 0       | 0       |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 3   | C     | 6        | Total O<br>6 6   | 0       | 0       |
| 3   | D     | 11       | Total O<br>11 11 | 0       | 0       |
| 3   | E     | 9        | Total O<br>9 9   | 0       | 0       |
| 3   | F     | 10       | Total O<br>10 10 | 0       | 0       |
| 3   | G     | 9        | Total O<br>9 9   | 0       | 0       |
| 3   | H     | 1        | Total O<br>1 1   | 0       | 0       |
| 3   | I     | 7        | Total O<br>7 7   | 0       | 0       |
| 3   | J     | 5        | Total O<br>5 5   | 0       | 0       |
| 3   | K     | 15       | Total O<br>15 15 | 0       | 0       |
| 3   | L     | 4        | Total O<br>4 4   | 0       | 0       |
| 3   | M     | 11       | Total O<br>11 11 | 0       | 0       |
| 3   | N     | 7        | Total O<br>7 7   | 0       | 0       |
| 3   | O     | 8        | Total O<br>8 8   | 0       | 0       |
| 3   | P     | 4        | Total O<br>4 4   | 0       | 0       |
| 3   | Q     | 6        | Total O<br>6 6   | 0       | 0       |
| 3   | R     | 5        | Total O<br>5 5   | 0       | 0       |
| 3   | S     | 13       | Total O<br>13 13 | 0       | 0       |
| 3   | T     | 6        | Total O<br>6 6   | 0       | 0       |
| 3   | U     | 7        | Total O<br>7 7   | 0       | 0       |
| 3   | V     | 10       | Total O<br>10 10 | 0       | 0       |
| 3   | W     | 8        | Total O<br>8 8   | 0       | 0       |

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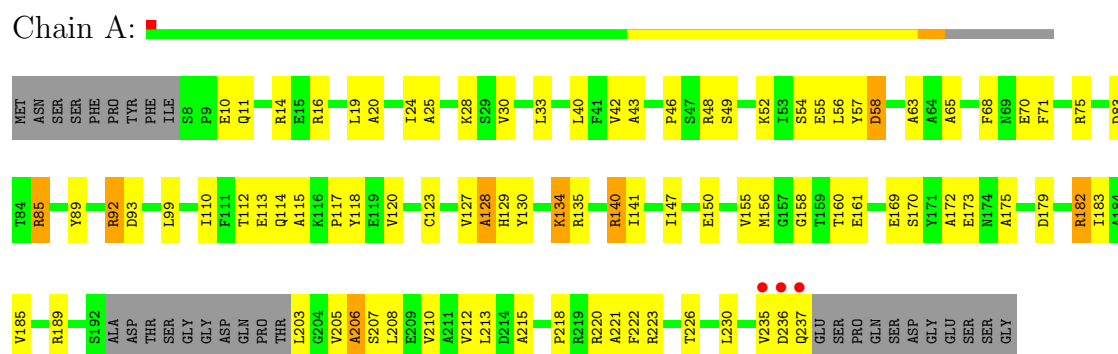
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | X     | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 3   | Y     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 3   | Z     | 7        | Total<br>7  | O<br>7  | 0       | 0       |

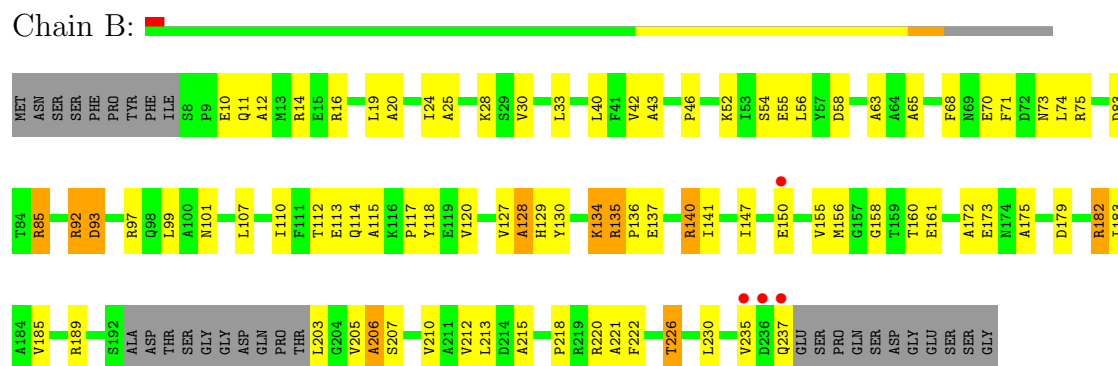
### 3 Residue-property plots

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

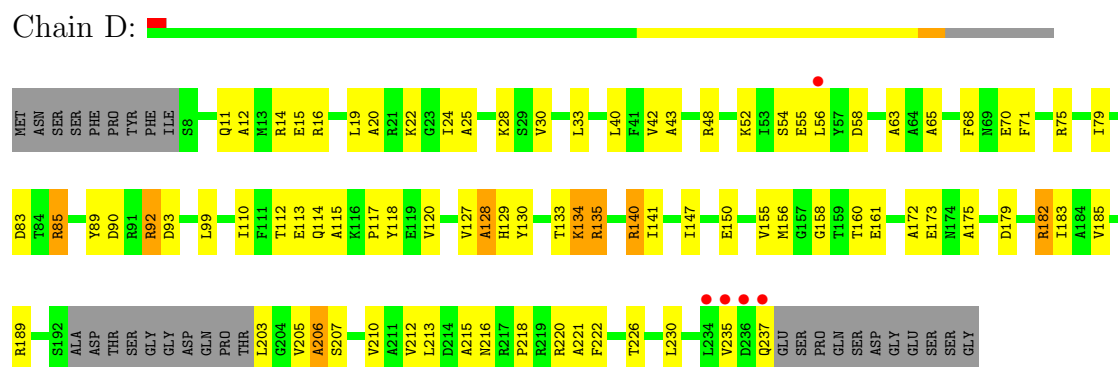
- Molecule 1: 20S proteasome, alpha and beta subunits



- Molecule 1: 20S proteasome, alpha and beta subunits

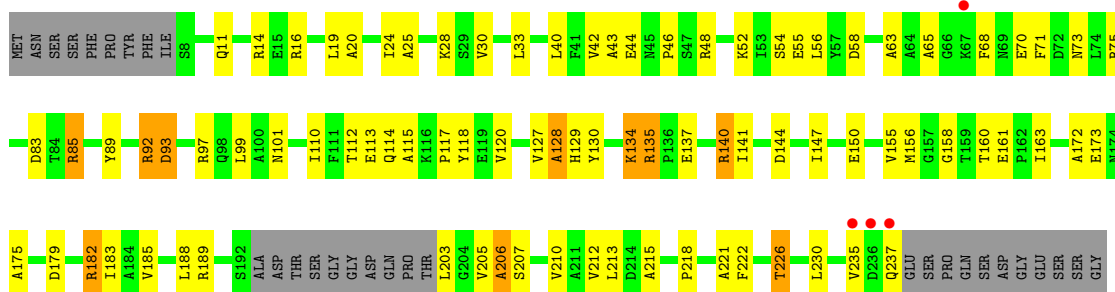


- Molecule 1: 20S proteasome, alpha and beta subunits



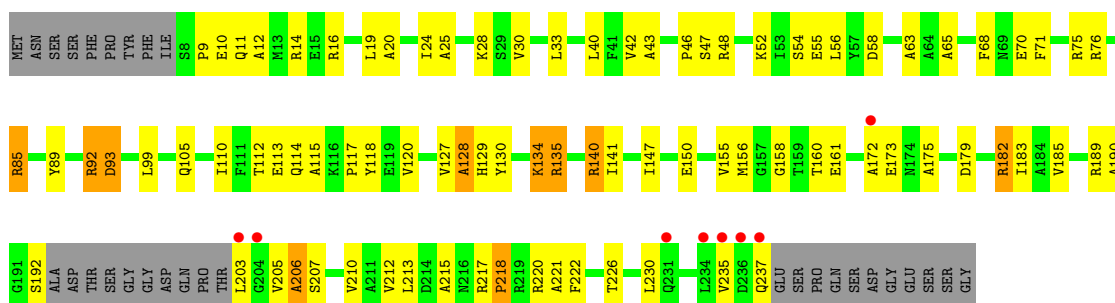
- Molecule 1: 20S proteasome, alpha and beta subunits

## Chain F:



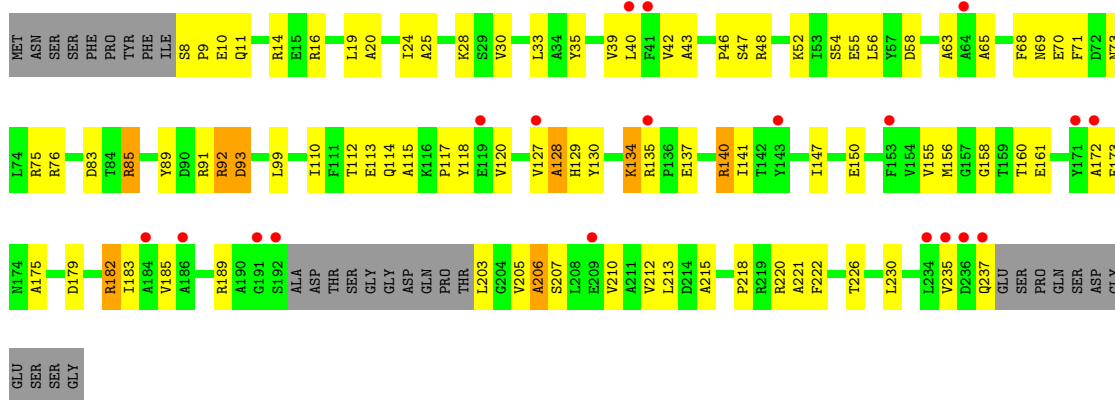
- Molecule 1: 20S proteasome, alpha and beta subunits

## Chain I:



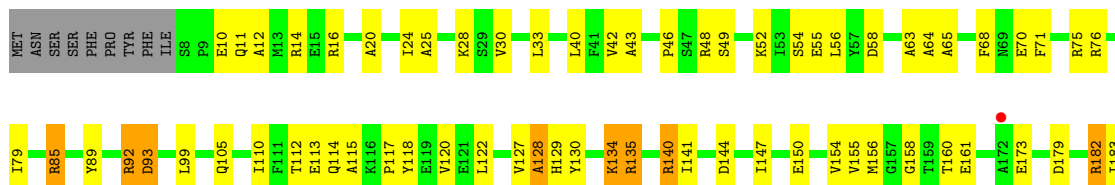
- Molecule 1: 20S proteasome, alpha and beta subunits

## Chain K:



- Molecule 1: 20S proteasome, alpha and beta subunits

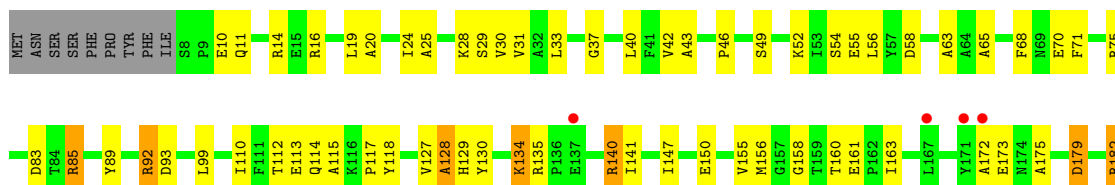
## Chain M:





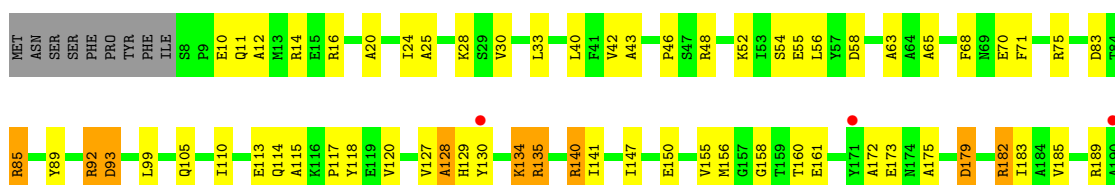
- Molecule 1: 20S proteasome, alpha and beta subunits

Chain O:



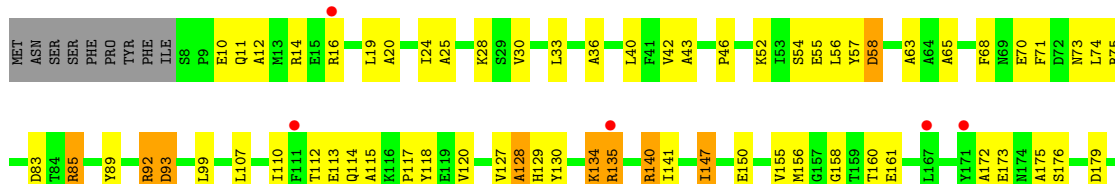
- Molecule 1: 20S proteasome, alpha and beta subunits

Chain Q:



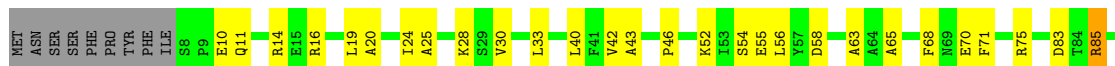
- Molecule 1: 20S proteasome, alpha and beta subunits

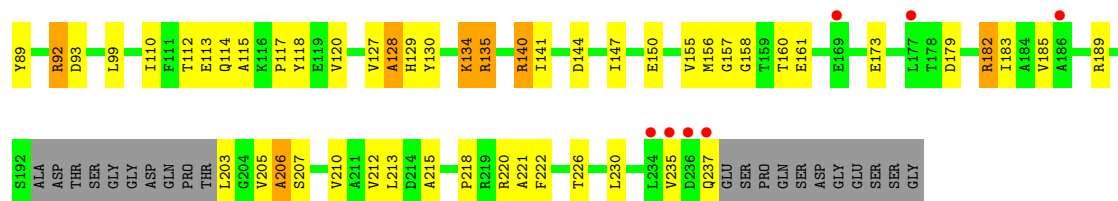
Chain S:



- Molecule 1: 20S proteasome, alpha and beta subunits

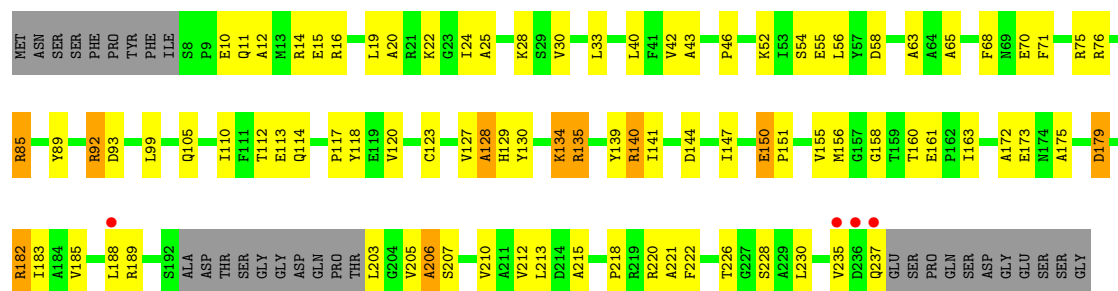
Chain U:





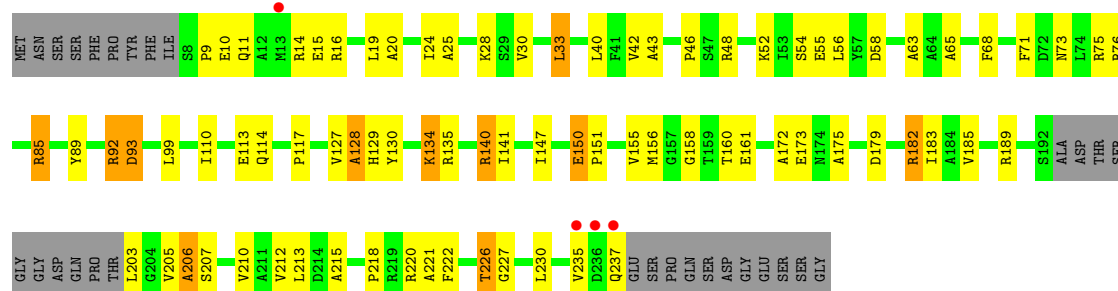
- Molecule 1: 20S proteasome, alpha and beta subunits

Chain W:



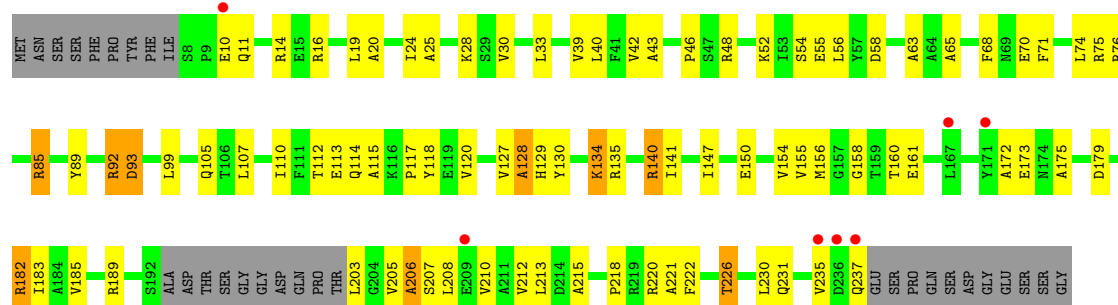
- Molecule 1: 20S proteasome, alpha and beta subunits

Chain Y:



- Molecule 1: 20S proteasome, alpha and beta subunits

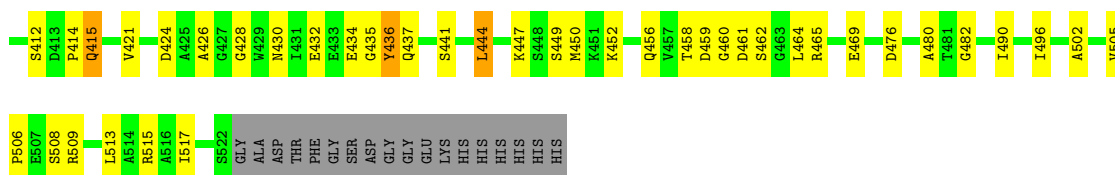
Chain 1:



- Molecule 2: proteasome, beta subunit

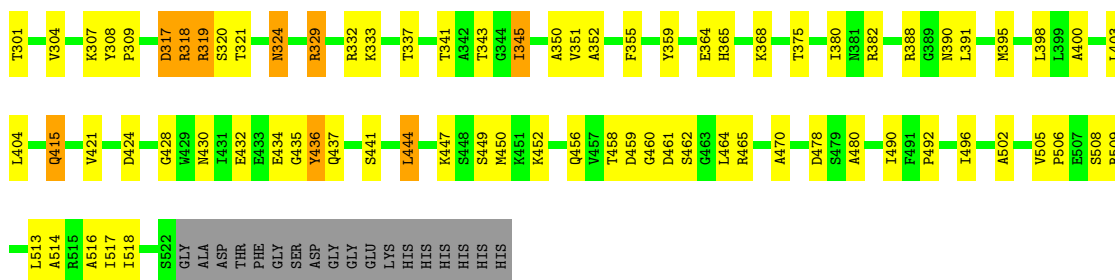
Chain H:





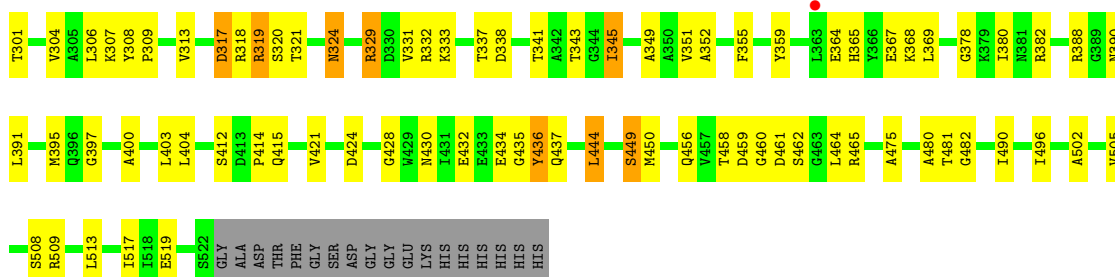
- Molecule 2: proteasome, beta subunit

Chain C:



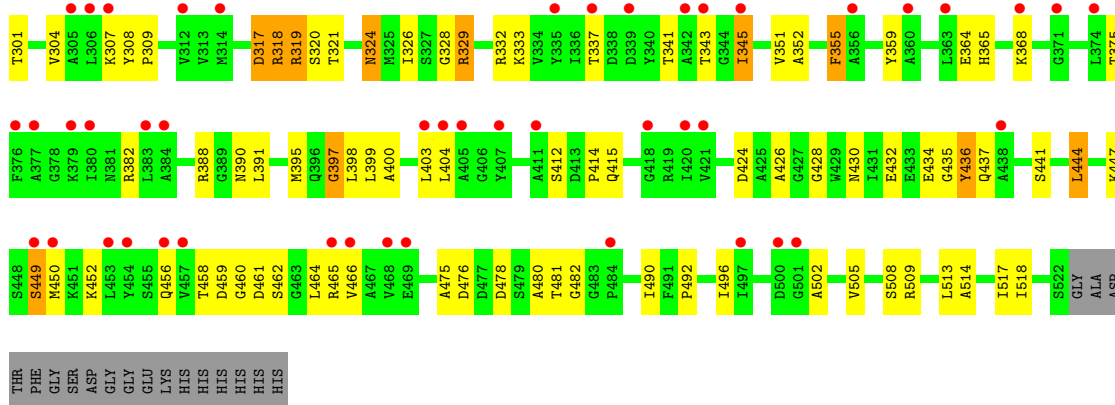
- Molecule 2: proteasome, beta subunit

Chain E:



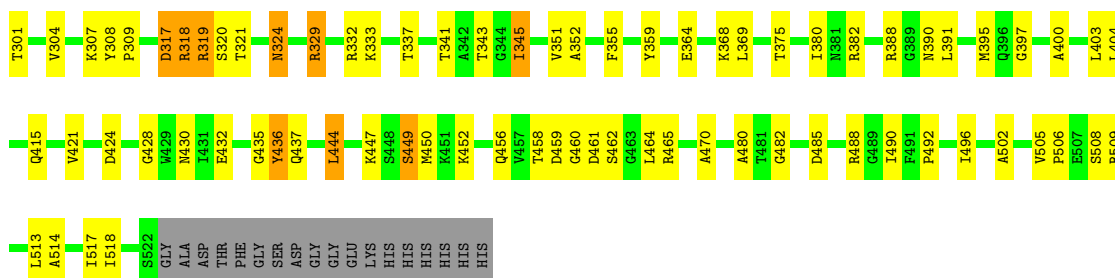
- Molecule 2: proteasome, beta subunit

Chain G:



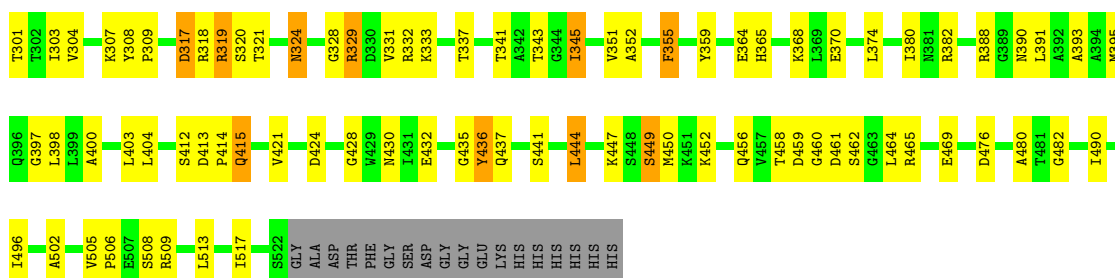
- Molecule 2: proteasome, beta subunit

Chain J:



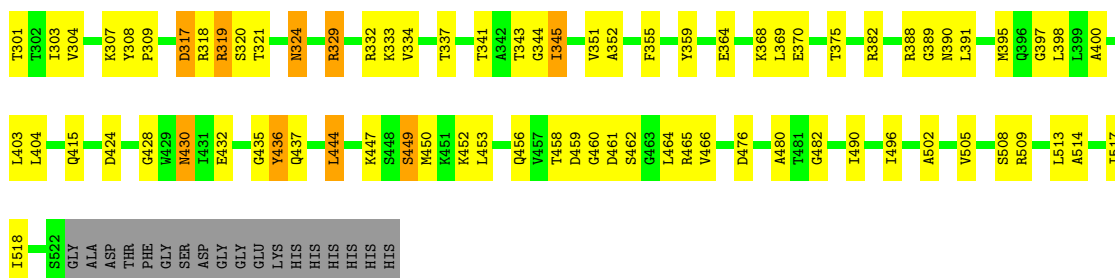
- Molecule 2: proteasome, beta subunit

Chain L:



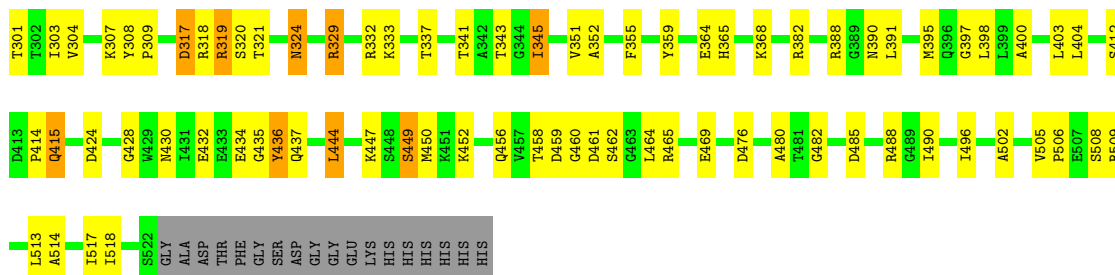
- Molecule 2: proteasome, beta subunit

Chain N:



- Molecule 2: proteasome, beta subunit

Chain P:

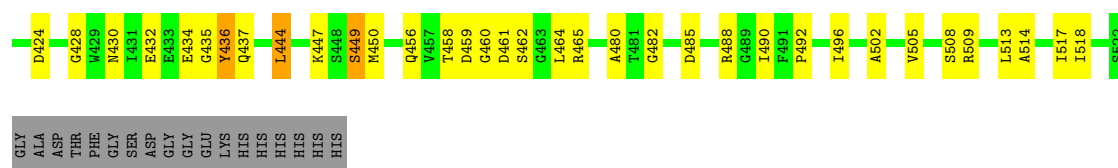


- Molecule 2: proteasome, beta subunit

Chain R:

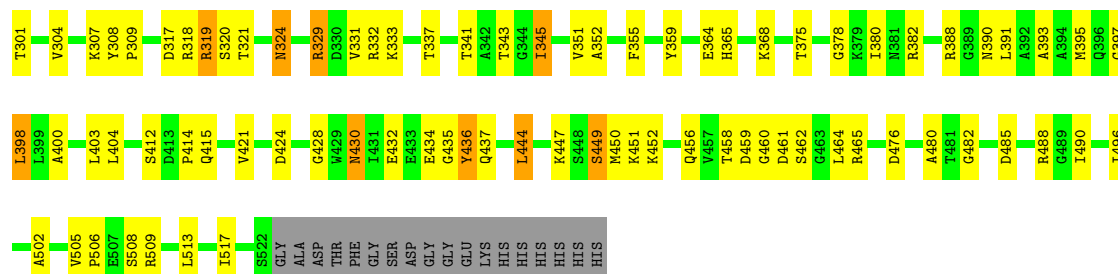






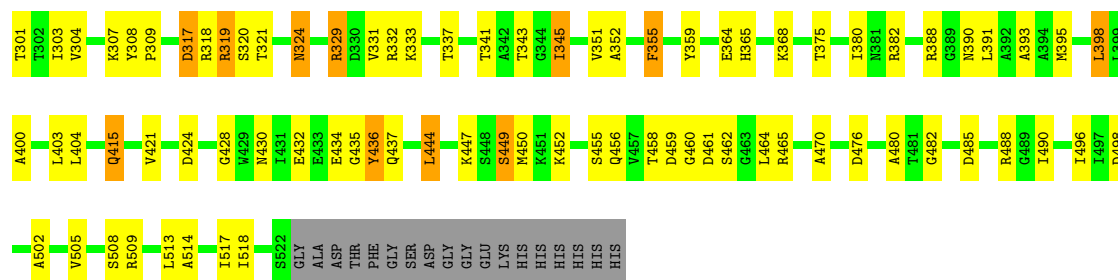
- Molecule 2: proteasome, beta subunit

Chain T:



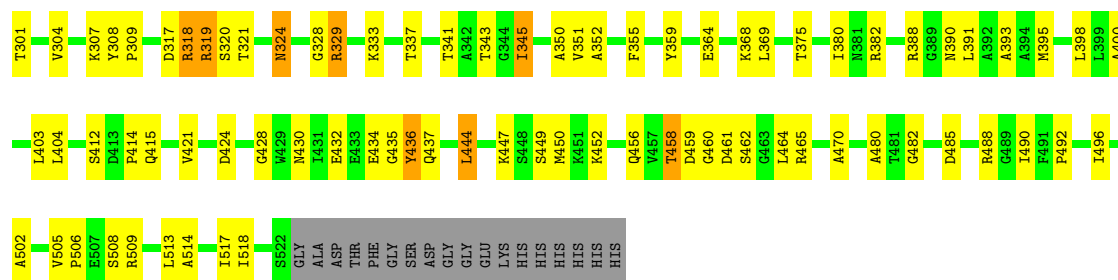
- Molecule 2: proteasome, beta subunit

Chain V:



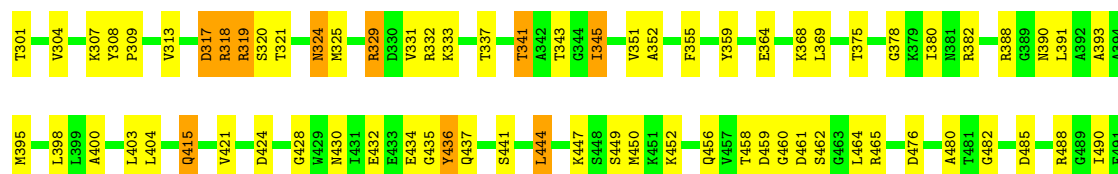
- Molecule 2: proteasome, beta subunit

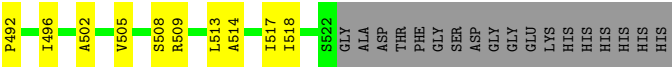
Chain X:



- Molecule 2: proteasome, beta subunit

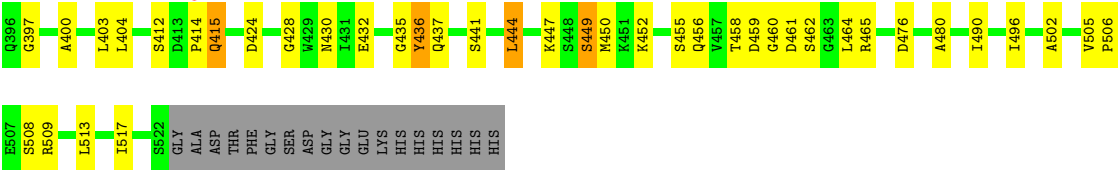
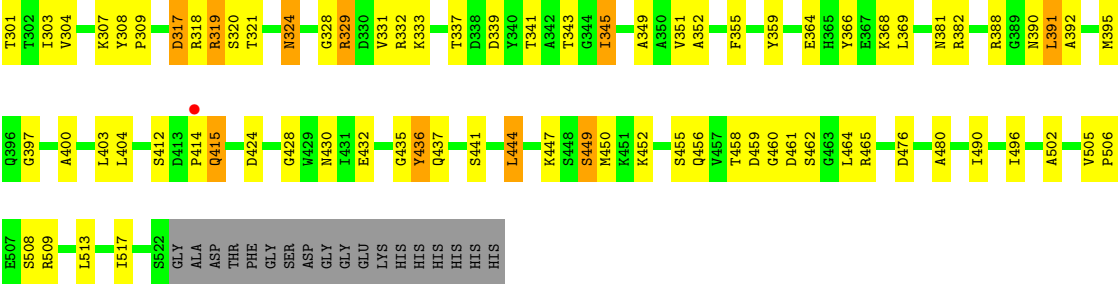
Chain Z:





● Molecule 2: proteasome, beta subunit

Chain 2:



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 173.33Å 113.80Å 200.13Å<br>90.00° 113.93° 90.00°            | Depositor        |
| Resolution (Å)  | 50.00 – 3.23<br>49.63 – 3.23                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 79.6 (50.00-3.23)<br>79.6 (49.63-3.23)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.06  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.49 (at 3.25Å)   | Xtriage          |
| Refinement program  | REFMAC 5.2.0005   | Depositor        |
| R, $R_{free}$   | 0.243 , 0.266<br>0.248 , 0.252                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2776 reflections (3.13%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 82.0  | Xtriage          |
| Anisotropy  | 0.332   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 100.0  | EDS              |
| Estimated twinning fraction   | 0.046 for h,-k,-h-l   | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Outliers  | 1 of 91405 reflections (0.001%)                             | Xtriage          |
| $F_o, F_c$ correlation  | 0.88  | EDS              |
| Total number of atoms   | 46846   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 99.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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   | 1     | 0.43         | 0/1717         | 0.59        | 0/2320      |
| 1   | A     | 0.54         | 1/1717 (0.1%)  | 0.63        | 0/2320      |
| 1   | B     | 0.49         | 0/1717         | 0.62        | 0/2320      |
| 1   | D     | 0.47         | 0/1717         | 0.61        | 0/2320      |
| 1   | F     | 0.45         | 0/1717         | 0.60        | 0/2320      |
| 1   | I     | 0.44         | 0/1717         | 0.60        | 0/2320      |
| 1   | K     | 0.43         | 0/1717         | 0.59        | 0/2320      |
| 1   | M     | 0.45         | 0/1717         | 0.60        | 0/2320      |
| 1   | O     | 0.45         | 0/1717         | 0.60        | 0/2320      |
| 1   | Q     | 0.44         | 0/1717         | 0.59        | 0/2320      |
| 1   | S     | 0.43         | 0/1717         | 0.59        | 0/2320      |
| 1   | U     | 0.43         | 0/1717         | 0.60        | 0/2320      |
| 1   | W     | 0.47         | 0/1717         | 0.61        | 0/2320      |
| 1   | Y     | 0.43         | 0/1717         | 0.59        | 0/2320      |
| 2   | 2     | 0.42         | 0/1662         | 0.61        | 0/2254      |
| 2   | C     | 0.52         | 0/1662         | 0.65        | 0/2254      |
| 2   | E     | 0.54         | 0/1662         | 0.66        | 0/2254      |
| 2   | G     | 0.48         | 0/1662         | 0.65        | 0/2254      |
| 2   | H     | 0.55         | 0/1662         | 0.66        | 0/2254      |
| 2   | J     | 0.49         | 0/1662         | 0.63        | 0/2254      |
| 2   | L     | 0.51         | 0/1662         | 0.65        | 0/2254      |
| 2   | N     | 0.49         | 0/1662         | 0.64        | 0/2254      |
| 2   | P     | 0.49         | 0/1662         | 0.64        | 0/2254      |
| 2   | R     | 0.50         | 0/1662         | 0.65        | 0/2254      |
| 2   | T     | 0.46         | 0/1662         | 0.63        | 0/2254      |
| 2   | V     | 0.47         | 0/1662         | 0.65        | 0/2254      |
| 2   | X     | 0.49         | 0/1662         | 0.64        | 0/2254      |
| 2   | Z     | 0.48         | 0/1662         | 0.64        | 0/2254      |
| All | All   | 0.47         | 1/47306 (0.0%) | 0.62        | 0/64036     |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 123 | CYS  | CB-SG | -5.45 | 1.73        | 1.81     |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 1692  | 0        | 1688     | 75      | 0            |
| 1   | A     | 1692  | 0        | 1688     | 77      | 4            |
| 1   | B     | 1692  | 0        | 1688     | 75      | 0            |
| 1   | D     | 1692  | 0        | 1688     | 72      | 4            |
| 1   | F     | 1692  | 0        | 1688     | 80      | 0            |
| 1   | I     | 1692  | 0        | 1688     | 72      | 2            |
| 1   | K     | 1692  | 0        | 1688     | 84      | 0            |
| 1   | M     | 1692  | 0        | 1688     | 88      | 0            |
| 1   | O     | 1692  | 0        | 1688     | 77      | 0            |
| 1   | Q     | 1692  | 0        | 1688     | 68      | 0            |
| 1   | S     | 1692  | 0        | 1688     | 77      | 0            |
| 1   | U     | 1692  | 0        | 1688     | 69      | 2            |
| 1   | W     | 1692  | 0        | 1688     | 77      | 1            |
| 1   | Y     | 1692  | 0        | 1688     | 72      | 0            |
| 2   | 2     | 1638  | 0        | 1630     | 67      | 1            |
| 2   | C     | 1638  | 0        | 1630     | 58      | 0            |
| 2   | E     | 1638  | 0        | 1630     | 60      | 1            |
| 2   | G     | 1638  | 0        | 1630     | 67      | 3            |
| 2   | H     | 1638  | 0        | 1630     | 62      | 0            |
| 2   | J     | 1638  | 0        | 1630     | 56      | 2            |
| 2   | L     | 1638  | 0        | 1630     | 68      | 0            |
| 2   | N     | 1638  | 0        | 1630     | 62      | 1            |
| 2   | P     | 1638  | 0        | 1630     | 61      | 1            |
| 2   | R     | 1638  | 0        | 1630     | 54      | 0            |
| 2   | T     | 1638  | 0        | 1630     | 60      | 0            |
| 2   | V     | 1638  | 0        | 1630     | 64      | 2            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | X     | 1638  | 0        | 1630     | 59      | 3            |
| 2   | Z     | 1638  | 0        | 1630     | 62      | 1            |
| 3   | 1     | 13    | 0        | 0        | 10      | 0            |
| 3   | 2     | 19    | 0        | 0        | 8       | 0            |
| 3   | A     | 2     | 0        | 0        | 2       | 0            |
| 3   | B     | 7     | 0        | 0        | 2       | 0            |
| 3   | C     | 6     | 0        | 0        | 0       | 0            |
| 3   | D     | 11    | 0        | 0        | 3       | 0            |
| 3   | E     | 9     | 0        | 0        | 3       | 0            |
| 3   | F     | 10    | 0        | 0        | 1       | 0            |
| 3   | G     | 9     | 0        | 0        | 3       | 0            |
| 3   | H     | 1     | 0        | 0        | 3       | 0            |
| 3   | I     | 7     | 0        | 0        | 3       | 0            |
| 3   | J     | 5     | 0        | 0        | 0       | 0            |
| 3   | K     | 15    | 0        | 0        | 8       | 0            |
| 3   | L     | 4     | 0        | 0        | 3       | 0            |
| 3   | M     | 11    | 0        | 0        | 5       | 0            |
| 3   | N     | 7     | 0        | 0        | 5       | 0            |
| 3   | O     | 8     | 0        | 0        | 8       | 0            |
| 3   | P     | 4     | 0        | 0        | 0       | 0            |
| 3   | Q     | 6     | 0        | 0        | 2       | 0            |
| 3   | R     | 5     | 0        | 0        | 2       | 0            |
| 3   | S     | 13    | 0        | 0        | 3       | 0            |
| 3   | T     | 6     | 0        | 0        | 4       | 0            |
| 3   | U     | 7     | 0        | 0        | 1       | 0            |
| 3   | V     | 10    | 0        | 0        | 4       | 0            |
| 3   | W     | 8     | 0        | 0        | 3       | 0            |
| 3   | X     | 4     | 0        | 0        | 1       | 0            |
| 3   | Y     | 12    | 0        | 0        | 8       | 0            |
| 3   | Z     | 7     | 0        | 0        | 4       | 0            |
| All | All   | 46846 | 0        | 46452    | 1730    | 14           |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (1730) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:J:444:LEU:HD12 | 2:Z:444:LEU:HD12 | 1.27        | 1.15     |
| 2:L:444:LEU:HD12 | 2:P:444:LEU:HD12 | 1.30        | 1.13     |
| 2:J:452:LYS:HG3  | 3:Z:190:HOH:O    | 1.47        | 1.12     |
| 1:K:14:ARG:HG2   | 3:K:260:HOH:O    | 1.56        | 1.06     |
| 2:N:444:LEU:HD12 | 2:V:444:LEU:HD12 | 1.35        | 1.04     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:C:444:LEU:HD12 | 2:R:444:LEU:HD12 | 1.38        | 1.04     |
| 1:O:49:SER:OG    | 3:O:255:HOH:O    | 1.78        | 1.02     |
| 1:Y:33:LEU:HD21  | 3:Y:254:HOH:O    | 1.59        | 1.02     |
| 1:D:15:GLU:OE1   | 1:K:9:PRO:HD2    | 1.59        | 1.00     |
| 2:L:382:ARG:HD3  | 1:M:89:TYR:HD1   | 1.26        | 0.99     |
| 2:N:461:ASP:HB2  | 3:N:140:HOH:O    | 1.61        | 0.99     |
| 1:W:14:ARG:HB3   | 1:W:14:ARG:HH11  | 1.29        | 0.98     |
| 2:T:430:ASN:HB2  | 3:T:45:HOH:O     | 1.62        | 0.98     |
| 2:N:345:ILE:HD13 | 2:N:352:ALA:HB1  | 1.46        | 0.97     |
| 1:Y:14:ARG:HB3   | 1:Y:14:ARG:HH11  | 1.29        | 0.97     |
| 2:Z:452:LYS:HB2  | 3:Z:190:HOH:O    | 1.64        | 0.97     |
| 1:S:14:ARG:HH11  | 1:S:14:ARG:HB3   | 1.30        | 0.97     |
| 1:U:14:ARG:HB3   | 1:U:14:ARG:HH11  | 1.26        | 0.97     |
| 1:I:14:ARG:HH11  | 1:I:14:ARG:HB3   | 1.25        | 0.96     |
| 1:K:14:ARG:HH11  | 1:K:14:ARG:HB3   | 1.30        | 0.96     |
| 1:I:14:ARG:HB3   | 1:I:14:ARG:HH11  | 1.30        | 0.96     |
| 1:B:93:ASP:O     | 3:B:252:HOH:O    | 1.83        | 0.96     |
| 2:L:382:ARG:HD3  | 1:M:89:TYR:CD1   | 2.01        | 0.95     |
| 2:H:444:LEU:HD12 | 2:E:444:LEU:HD12 | 1.47        | 0.95     |
| 1:Q:14:ARG:HH11  | 1:Q:14:ARG:HB3   | 1.32        | 0.95     |
| 1:O:14:ARG:HB3   | 1:O:14:ARG:HH11  | 1.27        | 0.95     |
| 1:M:14:ARG:HB3   | 1:M:14:ARG:HH11  | 1.29        | 0.94     |
| 1:B:14:ARG:HH11  | 1:B:14:ARG:HB3   | 1.30        | 0.94     |
| 2:G:444:LEU:HD12 | 2:2:444:LEU:HD12 | 1.48        | 0.94     |
| 1:A:48:ARG:HH22  | 1:B:135:ARG:HB3  | 1.28        | 0.93     |
| 1:F:14:ARG:HH11  | 1:F:14:ARG:HB3   | 1.31        | 0.93     |
| 2:X:375:THR:OG1  | 1:Y:93:ASP:OD1   | 1.86        | 0.92     |
| 1:A:14:ARG:HH11  | 1:A:14:ARG:HB3   | 1.32        | 0.92     |
| 2:J:444:LEU:HD12 | 2:Z:444:LEU:CD1  | 2.01        | 0.91     |
| 1:D:14:ARG:HB3   | 1:D:14:ARG:HH11  | 1.35        | 0.91     |
| 2:C:345:ILE:HD13 | 2:C:352:ALA:HB1  | 1.53        | 0.90     |
| 2:G:345:ILE:HD13 | 2:G:352:ALA:HB1  | 1.52        | 0.90     |
| 2:L:444:LEU:HD12 | 2:P:444:LEU:CD1  | 2.02        | 0.90     |
| 2:R:509:ARG:HG3  | 3:R:112:HOH:O    | 1.72        | 0.89     |
| 2:J:444:LEU:CD1  | 2:Z:444:LEU:HD12 | 2.02        | 0.89     |
| 2:P:345:ILE:HD13 | 2:P:352:ALA:HB1  | 1.54        | 0.89     |
| 2:X:345:ILE:HD13 | 2:X:352:ALA:HB1  | 1.54        | 0.89     |
| 2:J:345:ILE:HD13 | 2:J:352:ALA:HB1  | 1.56        | 0.88     |
| 2:L:444:LEU:CD1  | 2:P:444:LEU:HD12 | 2.02        | 0.88     |
| 1:K:115:ALA:HB3  | 1:M:112:THR:CG2  | 2.02        | 0.88     |
| 2:T:345:ILE:HD13 | 2:T:352:ALA:HB1  | 1.54        | 0.88     |
| 2:N:444:LEU:HD12 | 2:V:444:LEU:CD1  | 2.03        | 0.87     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:345:ILE:HD13 | 2:H:352:ALA:HB1  | 1.56        | 0.87     |
| 2:2:345:ILE:HD13 | 2:2:352:ALA:HB1  | 1.53        | 0.87     |
| 2:V:308:TYR:OH   | 3:V:32:HOH:O     | 1.94        | 0.86     |
| 1:A:11:GLN:HG2   | 1:A:14:ARG:HH12  | 1.40        | 0.86     |
| 2:N:444:LEU:CD1  | 2:V:444:LEU:HD12 | 2.05        | 0.86     |
| 2:V:345:ILE:HD13 | 2:V:352:ALA:HB1  | 1.56        | 0.86     |
| 2:L:345:ILE:HD13 | 2:L:352:ALA:HB1  | 1.56        | 0.86     |
| 2:T:444:LEU:HD12 | 2:X:444:LEU:HD12 | 1.57        | 0.86     |
| 1:D:83:ASP:OD2   | 2:E:365:HIS:HD2  | 1.59        | 0.86     |
| 1:D:11:GLN:HG2   | 1:D:14:ARG:NH1   | 1.89        | 0.85     |
| 1:A:11:GLN:HG2   | 1:A:14:ARG:NH1   | 1.90        | 0.85     |
| 1:D:92:ARG:HG3   | 1:D:129:HIS:HE1  | 1.41        | 0.85     |
| 1:O:92:ARG:HG3   | 1:O:129:HIS:HE1  | 1.42        | 0.85     |
| 2:R:345:ILE:HD13 | 2:R:352:ALA:HB1  | 1.56        | 0.84     |
| 1:U:92:ARG:HG3   | 1:U:129:HIS:HE1  | 1.42        | 0.84     |
| 1:D:11:GLN:HG2   | 1:D:14:ARG:HH12  | 1.42        | 0.84     |
| 2:E:345:ILE:HD13 | 2:E:352:ALA:HB1  | 1.60        | 0.84     |
| 2:Z:345:ILE:HD13 | 2:Z:352:ALA:HB1  | 1.59        | 0.83     |
| 2:V:303:ILE:HG13 | 3:V:155:HOH:O    | 1.76        | 0.83     |
| 1:U:11:GLN:HG2   | 1:U:14:ARG:HH12  | 1.44        | 0.83     |
| 1:W:11:GLN:HG2   | 1:W:14:ARG:NH1   | 1.94        | 0.82     |
| 1:S:11:GLN:HG2   | 1:S:14:ARG:NH1   | 1.94        | 0.82     |
| 1:Y:92:ARG:HG3   | 1:Y:129:HIS:HE1  | 1.43        | 0.82     |
| 1:S:92:ARG:HG3   | 1:S:129:HIS:HE1  | 1.43        | 0.82     |
| 1:K:92:ARG:HG3   | 1:K:129:HIS:HE1  | 1.43        | 0.82     |
| 2:P:304:VAL:HG21 | 2:P:450:MET:CE   | 2.09        | 0.82     |
| 1:U:11:GLN:HG2   | 1:U:14:ARG:NH1   | 1.95        | 0.82     |
| 1:I:92:ARG:HG3   | 1:I:129:HIS:HE1  | 1.43        | 0.82     |
| 1:B:92:ARG:HG3   | 1:B:129:HIS:HE1  | 1.43        | 0.82     |
| 1:S:11:GLN:HG2   | 1:S:14:ARG:HH12  | 1.46        | 0.81     |
| 1:K:115:ALA:HB3  | 1:M:112:THR:HG22 | 1.62        | 0.81     |
| 3:Q:254:HOH:O    | 2:Z:378:GLY:HA3  | 1.81        | 0.81     |
| 1:A:92:ARG:HG3   | 1:A:129:HIS:HE1  | 1.46        | 0.81     |
| 1:1:93:ASP:OD2   | 3:1:252:HOH:O    | 1.98        | 0.81     |
| 1:K:11:GLN:HG2   | 1:K:14:ARG:NH1   | 1.96        | 0.81     |
| 1:F:11:GLN:HG2   | 1:F:14:ARG:NH1   | 1.95        | 0.80     |
| 1:Q:92:ARG:HG3   | 1:Q:129:HIS:HE1  | 1.44        | 0.80     |
| 1:Q:11:GLN:HG2   | 1:Q:14:ARG:HH12  | 1.46        | 0.80     |
| 2:N:304:VAL:HG21 | 2:N:450:MET:CE   | 2.12        | 0.80     |
| 1:W:92:ARG:HG3   | 1:W:129:HIS:HE1  | 1.47        | 0.80     |
| 1:I:11:GLN:HG2   | 1:I:14:ARG:NH1   | 1.96        | 0.80     |
| 1:O:11:GLN:HG2   | 1:O:14:ARG:NH1   | 1.96        | 0.80     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:92:ARG:HG3   | 1:M:129:HIS:HE1  | 1.45        | 0.80     |
| 1:Q:11:GLN:HG2   | 1:Q:14:ARG:NH1   | 1.96        | 0.80     |
| 2:2:304:VAL:HG21 | 2:2:450:MET:CE   | 2.12        | 0.80     |
| 1:M:11:GLN:HG2   | 1:M:14:ARG:NH1   | 1.97        | 0.79     |
| 2:L:337:THR:OG1  | 2:L:343:THR:HG22 | 1.82        | 0.79     |
| 2:H:304:VAL:HG21 | 2:H:450:MET:CE   | 2.11        | 0.79     |
| 1:B:55:GLU:HB2   | 1:B:222:PHE:CD2  | 2.18        | 0.79     |
| 2:E:304:VAL:HG21 | 2:E:450:MET:CE   | 2.13        | 0.79     |
| 1:O:10:GLU:HA    | 1:U:19:LEU:HD12  | 1.65        | 0.79     |
| 1:1:92:ARG:HG3   | 1:1:129:HIS:HE1  | 1.48        | 0.79     |
| 1:B:11:GLN:HG2   | 1:B:14:ARG:NH1   | 1.97        | 0.78     |
| 1:F:11:GLN:HG2   | 1:F:14:ARG:HH12  | 1.47        | 0.78     |
| 1:F:135:ARG:HB3  | 1:M:48:ARG:HH22  | 1.48        | 0.78     |
| 1:O:29:SER:O     | 3:O:252:HOH:O    | 2.02        | 0.78     |
| 2:G:332:ARG:HD3  | 3:G:210:HOH:O    | 1.84        | 0.78     |
| 1:D:92:ARG:HG3   | 1:D:129:HIS:CE1  | 2.19        | 0.78     |
| 2:J:304:VAL:HG21 | 2:J:450:MET:CE   | 2.15        | 0.78     |
| 1:W:11:GLN:HG2   | 1:W:14:ARG:HH12  | 1.47        | 0.77     |
| 1:I:11:GLN:HG2   | 1:I:14:ARG:HH12  | 1.50        | 0.77     |
| 2:G:304:VAL:HG21 | 2:G:450:MET:CE   | 2.14        | 0.77     |
| 2:G:382:ARG:HD3  | 1:W:89:TYR:CD1   | 2.19        | 0.77     |
| 1:O:85:ARG:HH11  | 1:O:85:ARG:HG2   | 1.49        | 0.77     |
| 2:E:304:VAL:HG21 | 2:E:450:MET:HE3  | 1.65        | 0.77     |
| 1:B:11:GLN:HG2   | 1:B:14:ARG:HH12  | 1.50        | 0.77     |
| 1:1:55:GLU:HB2   | 1:1:222:PHE:CD2  | 2.20        | 0.77     |
| 1:U:89:TYR:CD1   | 2:2:382:ARG:HD3  | 2.19        | 0.77     |
| 1:K:11:GLN:HG2   | 1:K:14:ARG:HH12  | 1.47        | 0.77     |
| 1:Y:11:GLN:HG2   | 1:Y:14:ARG:NH1   | 1.98        | 0.77     |
| 1:1:11:GLN:HG2   | 1:1:14:ARG:NH1   | 1.99        | 0.77     |
| 2:P:304:VAL:HG21 | 2:P:450:MET:HE3  | 1.65        | 0.77     |
| 2:L:304:VAL:HG21 | 2:L:450:MET:CE   | 2.13        | 0.77     |
| 1:Y:85:ARG:HG2   | 1:Y:85:ARG:HH11  | 1.49        | 0.76     |
| 1:O:11:GLN:HG2   | 1:O:14:ARG:HH12  | 1.51        | 0.76     |
| 1:K:92:ARG:HG3   | 1:K:129:HIS:CE1  | 2.20        | 0.76     |
| 2:L:459:ASP:H    | 2:L:462:SER:HB3  | 1.50        | 0.76     |
| 1:I:92:ARG:HG3   | 1:I:129:HIS:CE1  | 2.21        | 0.76     |
| 1:F:85:ARG:HH11  | 1:F:85:ARG:HG2   | 1.51        | 0.76     |
| 2:V:304:VAL:HG21 | 2:V:450:MET:CE   | 2.16        | 0.76     |
| 2:H:459:ASP:H    | 2:H:462:SER:HB3  | 1.50        | 0.76     |
| 2:L:304:VAL:HG21 | 2:L:450:MET:HE3  | 1.67        | 0.76     |
| 1:A:48:ARG:HH22  | 1:B:135:ARG:CB   | 1.98        | 0.76     |
| 1:A:85:ARG:HH11  | 1:A:85:ARG:HG2   | 1.51        | 0.76     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:Q:92:ARG:HG3   | 1:Q:129:HIS:CE1  | 2.22        | 0.75     |
| 3:X:157:HOH:O    | 2:Z:325:MET:HE3  | 1.86        | 0.75     |
| 1:O:92:ARG:HG3   | 1:O:129:HIS:CE1  | 2.20        | 0.75     |
| 1:1:11:GLN:HG2   | 1:1:14:ARG:HH12  | 1.52        | 0.75     |
| 1:U:92:ARG:HG3   | 1:U:129:HIS:CE1  | 2.21        | 0.75     |
| 1:Q:93:ASP:OD2   | 3:Q:254:HOH:O    | 2.05        | 0.75     |
| 1:M:92:ARG:HG3   | 1:M:129:HIS:CE1  | 2.22        | 0.75     |
| 2:T:304:VAL:HG21 | 2:T:450:MET:CE   | 2.16        | 0.75     |
| 1:W:150:GLU:HG3  | 3:W:253:HOH:O    | 1.85        | 0.75     |
| 1:M:11:GLN:HG2   | 1:M:14:ARG:HH12  | 1.49        | 0.75     |
| 2:R:424:ASP:HB3  | 2:R:428:GLY:H    | 1.52        | 0.75     |
| 1:M:85:ARG:HH11  | 1:M:85:ARG:HG2   | 1.52        | 0.75     |
| 2:T:451:LYS:HB3  | 3:T:79:HOH:O     | 1.85        | 0.75     |
| 1:S:55:GLU:HB2   | 1:S:222:PHE:CD2  | 2.22        | 0.75     |
| 2:G:444:LEU:HD12 | 2:2:444:LEU:CD1  | 2.18        | 0.74     |
| 1:S:19:LEU:HD12  | 1:1:10:GLU:HA    | 1.68        | 0.74     |
| 1:A:55:GLU:HB2   | 1:A:222:PHE:CD2  | 2.22        | 0.74     |
| 2:X:304:VAL:HG21 | 2:X:450:MET:CE   | 2.18        | 0.74     |
| 2:2:459:ASP:H    | 2:2:462:SER:HB3  | 1.52        | 0.74     |
| 2:T:459:ASP:H    | 2:T:462:SER:HB3  | 1.53        | 0.74     |
| 1:A:208:LEU:HB3  | 3:A:250:HOH:O    | 1.87        | 0.74     |
| 2:R:459:ASP:H    | 2:R:462:SER:HB3  | 1.53        | 0.74     |
| 1:Y:11:GLN:HG2   | 1:Y:14:ARG:HH12  | 1.52        | 0.74     |
| 2:V:329:ARG:O    | 2:V:490:ILE:HG21 | 1.87        | 0.74     |
| 1:F:92:ARG:HG3   | 1:F:129:HIS:HE1  | 1.51        | 0.74     |
| 2:C:304:VAL:HG21 | 2:C:450:MET:CE   | 2.17        | 0.74     |
| 1:Y:92:ARG:HG3   | 1:Y:129:HIS:CE1  | 2.22        | 0.74     |
| 2:Z:424:ASP:HB3  | 2:Z:428:GLY:H    | 1.53        | 0.74     |
| 1:A:115:ALA:HB3  | 1:B:112:THR:HG22 | 1.70        | 0.74     |
| 2:G:444:LEU:CD1  | 2:2:444:LEU:HD12 | 2.18        | 0.74     |
| 1:B:92:ARG:HG3   | 1:B:129:HIS:CE1  | 2.21        | 0.74     |
| 1:Y:55:GLU:HB2   | 1:Y:222:PHE:CD2  | 2.23        | 0.74     |
| 1:S:85:ARG:HH11  | 1:S:85:ARG:HG2   | 1.53        | 0.73     |
| 1:S:92:ARG:HG3   | 1:S:129:HIS:CE1  | 2.22        | 0.73     |
| 1:U:112:THR:CG2  | 1:1:115:ALA:HB3  | 2.18        | 0.73     |
| 1:K:55:GLU:HB2   | 1:K:222:PHE:CD2  | 2.23        | 0.73     |
| 1:M:55:GLU:HB2   | 1:M:222:PHE:CD2  | 2.23        | 0.73     |
| 1:D:15:GLU:OE1   | 1:K:9:PRO:CD     | 2.36        | 0.73     |
| 1:1:206:ALA:HB1  | 3:1:258:HOH:O    | 1.88        | 0.73     |
| 2:C:459:ASP:H    | 2:C:462:SER:HB3  | 1.54        | 0.73     |
| 2:Z:304:VAL:HG21 | 2:Z:450:MET:CE   | 2.19        | 0.73     |
| 1:S:40:LEU:HA    | 1:S:212:VAL:HG12 | 1.69        | 0.73     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:112:THR:CG2  | 1:O:115:ALA:HB3  | 2.19        | 0.73     |
| 2:N:337:THR:OG1  | 2:N:343:THR:HG22 | 1.88        | 0.73     |
| 2:C:444:LEU:CD1  | 2:R:444:LEU:HD12 | 2.17        | 0.73     |
| 1:U:14:ARG:HB3   | 1:U:14:ARG:NH1   | 2.01        | 0.72     |
| 1:K:40:LEU:HA    | 1:K:212:VAL:HG12 | 1.70        | 0.72     |
| 1:A:92:ARG:HG3   | 1:A:129:HIS:CE1  | 2.24        | 0.72     |
| 1:W:92:ARG:HG3   | 1:W:129:HIS:CE1  | 2.25        | 0.72     |
| 2:T:319:ARG:HG3  | 2:T:320:SER:N    | 2.05        | 0.72     |
| 1:I:55:GLU:HB2   | 1:I:222:PHE:CD2  | 2.25        | 0.72     |
| 2:X:424:ASP:HB3  | 2:X:428:GLY:H    | 1.54        | 0.72     |
| 2:J:424:ASP:HB3  | 2:J:428:GLY:H    | 1.55        | 0.72     |
| 1:A:112:THR:HG22 | 1:O:115:ALA:HB3  | 1.72        | 0.72     |
| 2:R:304:VAL:HG21 | 2:R:450:MET:CE   | 2.20        | 0.72     |
| 1:I:40:LEU:HA    | 1:I:212:VAL:HG12 | 1.71        | 0.72     |
| 2:P:337:THR:OG1  | 2:P:343:THR:HG22 | 1.89        | 0.72     |
| 1:I:14:ARG:HB3   | 1:I:14:ARG:NH1   | 2.02        | 0.72     |
| 1:O:40:LEU:HA    | 1:O:212:VAL:HG12 | 1.72        | 0.72     |
| 1:D:40:LEU:HA    | 1:D:212:VAL:HG12 | 1.72        | 0.72     |
| 1:B:19:LEU:HD12  | 1:I:10:GLU:HA    | 1.72        | 0.72     |
| 1:F:55:GLU:HB2   | 1:F:222:PHE:CD2  | 2.24        | 0.72     |
| 1:W:85:ARG:HH11  | 1:W:85:ARG:HG2   | 1.55        | 0.72     |
| 2:C:337:THR:OG1  | 2:C:343:THR:HG22 | 1.89        | 0.72     |
| 2:J:382:ARG:HD3  | 1:S:89:TYR:CD1   | 2.25        | 0.71     |
| 1:F:19:LEU:HD12  | 1:W:10:GLU:HA    | 1.72        | 0.71     |
| 2:V:319:ARG:HG3  | 2:V:320:SER:N    | 2.04        | 0.71     |
| 1:F:112:THR:HG22 | 1:M:115:ALA:HB3  | 1.72        | 0.71     |
| 1:I:85:ARG:HH11  | 1:I:85:ARG:HG2   | 1.53        | 0.71     |
| 2:P:459:ASP:H    | 2:P:462:SER:HB3  | 1.55        | 0.71     |
| 1:B:14:ARG:HB3   | 1:B:14:ARG:NH1   | 2.06        | 0.71     |
| 1:I:92:ARG:HG3   | 1:I:129:HIS:CE1  | 2.25        | 0.71     |
| 1:O:55:GLU:HB2   | 1:O:222:PHE:CD2  | 2.25        | 0.71     |
| 2:G:459:ASP:H    | 2:G:462:SER:HB3  | 1.55        | 0.71     |
| 1:U:89:TYR:HD1   | 2:2:382:ARG:HD3  | 1.55        | 0.71     |
| 1:W:40:LEU:HA    | 1:W:212:VAL:HG12 | 1.73        | 0.71     |
| 1:A:40:LEU:HA    | 1:A:212:VAL:HG12 | 1.73        | 0.71     |
| 2:E:382:ARG:HD3  | 1:K:89:TYR:CD1   | 2.25        | 0.71     |
| 2:E:424:ASP:HB3  | 2:E:428:GLY:H    | 1.53        | 0.71     |
| 2:G:304:VAL:HG21 | 2:G:450:MET:HE3  | 1.72        | 0.71     |
| 1:U:55:GLU:HB2   | 1:U:222:PHE:CD2  | 2.24        | 0.71     |
| 1:D:55:GLU:HB2   | 1:D:222:PHE:CD2  | 2.25        | 0.71     |
| 1:F:40:LEU:HA    | 1:F:212:VAL:HG12 | 1.72        | 0.71     |
| 2:E:459:ASP:H    | 2:E:462:SER:HB3  | 1.55        | 0.71     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:T:382:ARG:HD3  | 1:I:89:TYR:CD1   | 2.25        | 0.71     |
| 2:G:329:ARG:O    | 2:G:490:ILE:HG21 | 1.90        | 0.71     |
| 1:Q:85:ARG:HH11  | 1:Q:85:ARG:HG2   | 1.55        | 0.71     |
| 2:G:462:SER:O    | 2:G:465:ARG:HG2  | 1.92        | 0.70     |
| 2:R:319:ARG:HG3  | 2:R:320:SER:N    | 2.06        | 0.70     |
| 2:X:459:ASP:H    | 2:X:462:SER:HB3  | 1.53        | 0.70     |
| 2:G:424:ASP:HB3  | 2:G:428:GLY:H    | 1.55        | 0.70     |
| 2:C:444:LEU:HD12 | 2:R:444:LEU:CD1  | 2.18        | 0.70     |
| 1:W:19:LEU:HD12  | 1:Y:10:GLU:HA    | 1.74        | 0.70     |
| 1:W:14:ARG:NH1   | 1:W:14:ARG:HB3   | 2.06        | 0.70     |
| 1:S:14:ARG:NH1   | 1:S:14:ARG:HB3   | 2.05        | 0.70     |
| 2:P:424:ASP:HB3  | 2:P:428:GLY:H    | 1.55        | 0.70     |
| 1:F:110:ILE:HG23 | 1:F:114:GLN:HG3  | 1.72        | 0.70     |
| 1:U:40:LEU:HA    | 1:U:212:VAL:HG12 | 1.73        | 0.70     |
| 1:U:85:ARG:HG2   | 1:U:85:ARG:HH11  | 1.56        | 0.70     |
| 2:T:329:ARG:O    | 2:T:490:ILE:HG21 | 1.91        | 0.70     |
| 2:J:329:ARG:O    | 2:J:490:ILE:HG21 | 1.91        | 0.70     |
| 1:F:189:ARG:NH1  | 3:F:254:HOH:O    | 2.22        | 0.70     |
| 2:P:329:ARG:O    | 2:P:490:ILE:HG21 | 1.92        | 0.69     |
| 2:V:337:THR:OG1  | 2:V:343:THR:HG22 | 1.92        | 0.69     |
| 1:Q:14:ARG:NH1   | 1:Q:14:ARG:HB3   | 2.07        | 0.69     |
| 1:Q:55:GLU:HB2   | 1:Q:222:PHE:CD2  | 2.28        | 0.69     |
| 1:I:28:LYS:HB2   | 1:I:52:LYS:NZ    | 2.07        | 0.69     |
| 1:D:83:ASP:OD2   | 2:E:365:HIS:CD2  | 2.43        | 0.69     |
| 2:2:304:VAL:HG21 | 2:2:450:MET:HE3  | 1.73        | 0.69     |
| 2:2:329:ARG:O    | 2:2:490:ILE:HG21 | 1.92        | 0.69     |
| 2:V:459:ASP:H    | 2:V:462:SER:HB3  | 1.57        | 0.69     |
| 2:G:337:THR:OG1  | 2:G:343:THR:HG22 | 1.92        | 0.69     |
| 1:K:14:ARG:HB3   | 1:K:14:ARG:NH1   | 2.05        | 0.69     |
| 2:V:498:ASP:HB3  | 3:V:32:HOH:O     | 1.93        | 0.69     |
| 1:M:76:ARG:NH2   | 2:N:370:GLU:OE2  | 2.21        | 0.69     |
| 2:E:337:THR:OG1  | 2:E:343:THR:HG22 | 1.93        | 0.69     |
| 2:Z:329:ARG:HG2  | 3:Z:131:HOH:O    | 1.91        | 0.69     |
| 2:V:424:ASP:HB3  | 2:V:428:GLY:H    | 1.58        | 0.69     |
| 2:N:459:ASP:H    | 2:N:462:SER:HB3  | 1.58        | 0.69     |
| 2:C:319:ARG:HG3  | 2:C:320:SER:N    | 2.07        | 0.69     |
| 2:T:424:ASP:HB3  | 2:T:428:GLY:H    | 1.57        | 0.69     |
| 2:H:424:ASP:HB3  | 2:H:428:GLY:H    | 1.55        | 0.69     |
| 1:Q:40:LEU:HA    | 1:Q:212:VAL:HG12 | 1.75        | 0.69     |
| 2:Z:459:ASP:H    | 2:Z:462:SER:HB3  | 1.58        | 0.69     |
| 1:Q:89:TYR:CD1   | 2:Z:382:ARG:HD3  | 2.28        | 0.69     |
| 2:J:459:ASP:H    | 2:J:462:SER:HB3  | 1.58        | 0.68     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:X:329:ARG:O    | 2:X:490:ILE:HG21 | 1.92        | 0.68     |
| 2:E:329:ARG:O    | 2:E:490:ILE:HG21 | 1.93        | 0.68     |
| 1:M:14:ARG:HB3   | 1:M:14:ARG:NH1   | 2.06        | 0.68     |
| 2:N:304:VAL:HG21 | 2:N:450:MET:HE3  | 1.75        | 0.68     |
| 1:F:14:ARG:HB3   | 1:F:14:ARG:NH1   | 2.05        | 0.68     |
| 2:R:304:VAL:HG21 | 2:R:450:MET:HE3  | 1.75        | 0.68     |
| 2:C:382:ARG:HD3  | 1:I:89:TYR:CD1   | 2.27        | 0.68     |
| 1:I:182:ARG:HD3  | 1:I:235:VAL:HB   | 1.75        | 0.68     |
| 2:G:308:TYR:HB2  | 2:G:309:PRO:HD2  | 1.75        | 0.68     |
| 1:Y:40:LEU:HA    | 1:Y:212:VAL:HG12 | 1.75        | 0.68     |
| 2:E:382:ARG:HD3  | 1:K:89:TYR:HD1   | 1.58        | 0.68     |
| 2:Z:329:ARG:O    | 2:Z:490:ILE:HG21 | 1.93        | 0.68     |
| 1:K:85:ARG:HG2   | 1:K:85:ARG:HH11  | 1.58        | 0.68     |
| 1:Q:110:ILE:HG23 | 1:Q:114:GLN:HG3  | 1.75        | 0.68     |
| 1:I:14:ARG:HB3   | 1:I:14:ARG:NH1   | 2.06        | 0.68     |
| 2:X:382:ARG:HD3  | 1:Y:89:TYR:CD1   | 2.29        | 0.68     |
| 1:B:115:ALA:HB3  | 1:I:112:THR:CG2  | 2.22        | 0.68     |
| 2:P:319:ARG:HG3  | 2:P:320:SER:N    | 2.08        | 0.68     |
| 1:D:85:ARG:HH11  | 1:D:85:ARG:HG2   | 1.59        | 0.68     |
| 1:I:40:LEU:HA    | 1:I:212:VAL:HG12 | 1.76        | 0.68     |
| 2:C:424:ASP:HB3  | 2:C:428:GLY:H    | 1.58        | 0.68     |
| 2:R:329:ARG:O    | 2:R:490:ILE:HG21 | 1.93        | 0.68     |
| 1:A:110:ILE:HG23 | 1:A:114:GLN:HG3  | 1.76        | 0.68     |
| 1:I:85:ARG:HH11  | 1:I:85:ARG:HG2   | 1.58        | 0.68     |
| 1:Y:14:ARG:HB3   | 1:Y:14:ARG:NH1   | 2.06        | 0.68     |
| 2:P:462:SER:O    | 2:P:465:ARG:HG2  | 1.94        | 0.68     |
| 2:N:424:ASP:HB3  | 2:N:428:GLY:H    | 1.58        | 0.68     |
| 1:W:55:GLU:HB2   | 1:W:222:PHE:CD2  | 2.28        | 0.68     |
| 1:F:93:ASP:OD1   | 2:N:375:THR:OG1  | 2.12        | 0.68     |
| 1:O:14:ARG:HB3   | 1:O:14:ARG:NH1   | 2.04        | 0.68     |
| 2:N:319:ARG:HG3  | 2:N:320:SER:N    | 2.09        | 0.67     |
| 2:H:337:THR:OG1  | 2:H:343:THR:HG22 | 1.94        | 0.67     |
| 2:E:319:ARG:HG3  | 2:E:320:SER:N    | 2.07        | 0.67     |
| 2:L:329:ARG:O    | 2:L:490:ILE:HG21 | 1.94        | 0.67     |
| 1:A:182:ARG:HD3  | 1:A:235:VAL:HB   | 1.75        | 0.67     |
| 2:N:329:ARG:O    | 2:N:490:ILE:HG21 | 1.94        | 0.67     |
| 2:G:319:ARG:HG3  | 2:G:320:SER:N    | 2.09        | 0.67     |
| 2:X:337:THR:OG1  | 2:X:343:THR:HG22 | 1.95        | 0.67     |
| 1:F:92:ARG:HG3   | 1:F:129:HIS:CE1  | 2.29        | 0.67     |
| 2:C:329:ARG:O    | 2:C:490:ILE:HG21 | 1.95        | 0.67     |
| 1:B:40:LEU:HA    | 1:B:212:VAL:HG12 | 1.75        | 0.67     |
| 2:J:337:THR:OG1  | 2:J:343:THR:HG22 | 1.94        | 0.67     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:110:ILE:HG23 | 1:D:114:GLN:HG3  | 1.77        | 0.67     |
| 1:A:189:ARG:CZ   | 1:A:237:GLN:HB3  | 2.24        | 0.67     |
| 2:H:319:ARG:HG3  | 2:H:320:SER:N    | 2.08        | 0.67     |
| 1:B:85:ARG:HH11  | 1:B:85:ARG:HG2   | 1.58        | 0.67     |
| 1:I:110:ILE:HG23 | 1:I:114:GLN:HG3  | 1.77        | 0.67     |
| 2:X:319:ARG:HG3  | 2:X:320:SER:N    | 2.11        | 0.66     |
| 2:Z:319:ARG:HG3  | 2:Z:320:SER:N    | 2.10        | 0.66     |
| 2:Z:436:TYR:H    | 2:Z:436:TYR:HD1  | 1.43        | 0.66     |
| 2:H:304:VAL:HG21 | 2:H:450:MET:HE3  | 1.76        | 0.66     |
| 1:A:14:ARG:NH1   | 1:A:14:ARG:HB3   | 2.09        | 0.66     |
| 1:D:14:ARG:HB3   | 1:D:14:ARG:NH1   | 2.08        | 0.66     |
| 1:M:40:LEU:HA    | 1:M:212:VAL:HG12 | 1.76        | 0.66     |
| 1:K:28:LYS:HB2   | 1:K:52:LYS:NZ    | 2.10        | 0.66     |
| 1:S:115:ALA:HB3  | 1:I:112:THR:HG22 | 1.76        | 0.66     |
| 2:J:319:ARG:HG3  | 2:J:320:SER:N    | 2.09        | 0.66     |
| 1:Y:227:GLY:O    | 3:Y:249:HOH:O    | 2.13        | 0.66     |
| 2:2:424:ASP:HB3  | 2:2:428:GLY:H    | 1.60        | 0.66     |
| 1:U:112:THR:HG22 | 1:I:115:ALA:HB3  | 1.78        | 0.66     |
| 2:L:449:SER:HB2  | 2:P:452:LYS:NZ   | 2.11        | 0.66     |
| 2:L:424:ASP:HB3  | 2:L:428:GLY:H    | 1.61        | 0.66     |
| 2:N:324:ASN:H    | 2:N:324:ASN:HD22 | 1.43        | 0.66     |
| 1:Y:15:GLU:HB2   | 3:Y:257:HOH:O    | 1.95        | 0.66     |
| 1:F:101:ASN:OD1  | 1:M:68:PHE:HE1   | 1.79        | 0.66     |
| 2:Z:304:VAL:HG21 | 2:Z:450:MET:HE3  | 1.78        | 0.66     |
| 2:T:304:VAL:HG21 | 2:T:450:MET:HE3  | 1.77        | 0.65     |
| 1:M:182:ARG:HD3  | 1:M:235:VAL:HB   | 1.78        | 0.65     |
| 2:H:329:ARG:O    | 2:H:490:ILE:HG21 | 1.96        | 0.65     |
| 1:M:30:VAL:O     | 3:M:256:HOH:O    | 2.13        | 0.65     |
| 2:J:436:TYR:H    | 2:J:436:TYR:HD1  | 1.44        | 0.65     |
| 1:K:115:ALA:HB3  | 1:M:112:THR:HG23 | 1.76        | 0.65     |
| 3:G:124:HOH:O    | 2:N:430:ASN:HB3  | 1.96        | 0.65     |
| 2:N:464:LEU:HD12 | 2:N:496:ILE:HD11 | 1.78        | 0.65     |
| 2:X:464:LEU:HD12 | 2:X:496:ILE:HD11 | 1.77        | 0.65     |
| 2:T:444:LEU:HD12 | 2:X:444:LEU:CD1  | 2.24        | 0.65     |
| 2:J:304:VAL:HG21 | 2:J:450:MET:HE3  | 1.78        | 0.65     |
| 1:F:115:ALA:HB3  | 1:W:112:THR:CG2  | 2.26        | 0.65     |
| 1:W:15:GLU:OE1   | 1:Y:9:PRO:HD2    | 1.96        | 0.65     |
| 2:T:444:LEU:CD1  | 2:X:444:LEU:HD12 | 2.25        | 0.65     |
| 1:F:182:ARG:HD3  | 1:F:235:VAL:HB   | 1.78        | 0.65     |
| 1:Y:182:ARG:HD3  | 1:Y:235:VAL:HB   | 1.79        | 0.65     |
| 2:L:308:TYR:HB2  | 2:L:309:PRO:HD2  | 1.79        | 0.65     |
| 2:X:308:TYR:HB2  | 2:X:309:PRO:HD2  | 1.79        | 0.65     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:U:16:ARG:HE    | 1:U:117:PRO:HD3  | 1.61        | 0.65     |
| 1:1:39:VAL:N     | 3:1:256:HOH:O    | 2.29        | 0.65     |
| 2:Z:337:THR:OG1  | 2:Z:343:THR:HG22 | 1.97        | 0.65     |
| 1:U:189:ARG:CZ   | 1:U:237:GLN:HB3  | 2.26        | 0.65     |
| 1:O:110:ILE:HG23 | 1:O:114:GLN:HG3  | 1.78        | 0.64     |
| 2:2:308:TYR:HB2  | 2:2:309:PRO:HD2  | 1.78        | 0.64     |
| 2:2:337:THR:OG1  | 2:2:343:THR:HG22 | 1.97        | 0.64     |
| 1:F:135:ARG:CB   | 1:M:48:ARG:HH22  | 2.09        | 0.64     |
| 1:W:189:ARG:CZ   | 1:W:237:GLN:HB3  | 2.28        | 0.64     |
| 2:X:304:VAL:HG21 | 2:X:450:MET:HE3  | 1.80        | 0.64     |
| 1:M:56:LEU:HD13  | 1:M:99:LEU:CD2   | 2.27        | 0.64     |
| 2:H:515:ARG:NE   | 3:H:114:HOH:O    | 2.30        | 0.64     |
| 2:E:308:TYR:HB2  | 2:E:309:PRO:HD2  | 1.78        | 0.64     |
| 2:V:462:SER:O    | 2:V:465:ARG:HG2  | 1.97        | 0.64     |
| 1:K:182:ARG:HD3  | 1:K:235:VAL:HB   | 1.78        | 0.64     |
| 1:1:208:LEU:HB3  | 3:1:253:HOH:O    | 1.97        | 0.64     |
| 2:2:319:ARG:HG3  | 2:2:320:SER:N    | 2.12        | 0.64     |
| 1:S:56:LEU:HD13  | 1:S:99:LEU:CD2   | 2.28        | 0.64     |
| 1:S:189:ARG:CZ   | 1:S:237:GLN:HB3  | 2.28        | 0.64     |
| 1:B:182:ARG:HD3  | 1:B:235:VAL:HB   | 1.78        | 0.64     |
| 1:M:156:MET:HG2  | 3:M:256:HOH:O    | 1.99        | 0.64     |
| 1:W:110:ILE:HG23 | 1:W:114:GLN:HG3  | 1.80        | 0.64     |
| 1:Q:56:LEU:HD13  | 1:Q:99:LEU:CD2   | 2.28        | 0.64     |
| 2:2:339:ASP:HA   | 3:2:95:HOH:O     | 1.97        | 0.64     |
| 2:C:464:LEU:HD12 | 2:C:496:ILE:HD11 | 1.80        | 0.63     |
| 2:N:303:ILE:HD12 | 3:N:120:HOH:O    | 1.96        | 0.63     |
| 2:2:462:SER:O    | 2:2:465:ARG:HG2  | 1.99        | 0.63     |
| 2:E:462:SER:O    | 2:E:465:ARG:HG2  | 1.99        | 0.63     |
| 2:T:382:ARG:HD3  | 1:1:89:TYR:HD1   | 1.63        | 0.63     |
| 2:2:464:LEU:HD12 | 2:2:496:ILE:HD11 | 1.79        | 0.63     |
| 1:B:110:ILE:HG23 | 1:B:114:GLN:HG3  | 1.79        | 0.63     |
| 2:G:382:ARG:HD3  | 1:W:89:TYR:HD1   | 1.62        | 0.63     |
| 1:A:115:ALA:HB3  | 1:B:112:THR:CG2  | 2.28        | 0.63     |
| 1:O:89:TYR:CD1   | 2:V:382:ARG:HD3  | 2.32        | 0.63     |
| 1:O:189:ARG:CZ   | 1:O:237:GLN:HB3  | 2.28        | 0.63     |
| 2:J:308:TYR:HB2  | 2:J:309:PRO:HD2  | 1.80        | 0.63     |
| 2:H:308:TYR:HB2  | 2:H:309:PRO:HD2  | 1.79        | 0.63     |
| 2:R:464:LEU:HD12 | 2:R:496:ILE:HD11 | 1.79        | 0.63     |
| 1:F:189:ARG:CZ   | 1:F:237:GLN:HB3  | 2.28        | 0.63     |
| 2:N:462:SER:O    | 2:N:465:ARG:HG2  | 1.99        | 0.63     |
| 1:1:189:ARG:CZ   | 1:1:237:GLN:HB3  | 2.29        | 0.63     |
| 2:V:351:VAL:HB   | 2:V:400:ALA:HB2  | 1.81        | 0.63     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:J:464:LEU:HD12 | 2:J:496:ILE:HD11 | 1.79        | 0.63     |
| 1:D:90:ASP:HB3   | 3:D:249:HOH:O    | 1.98        | 0.63     |
| 1:M:110:ILE:HG23 | 1:M:114:GLN:HG3  | 1.78        | 0.63     |
| 2:Z:462:SER:O    | 2:Z:465:ARG:HG2  | 1.97        | 0.63     |
| 1:F:73:ASN:HD22  | 1:W:105:GLN:CD   | 2.02        | 0.63     |
| 2:V:308:TYR:HB2  | 2:V:309:PRO:HD2  | 1.79        | 0.63     |
| 1:S:213:LEU:HA   | 1:S:221:ALA:O    | 1.99        | 0.63     |
| 2:R:462:SER:O    | 2:R:465:ARG:HG2  | 1.99        | 0.63     |
| 1:B:189:ARG:CZ   | 1:B:237:GLN:HB3  | 2.28        | 0.63     |
| 1:W:182:ARG:HD3  | 1:W:235:VAL:HB   | 1.79        | 0.63     |
| 2:X:462:SER:O    | 2:X:465:ARG:HG2  | 1.99        | 0.63     |
| 1:S:115:ALA:HB3  | 1:I:112:THR:CG2  | 2.28        | 0.63     |
| 1:Q:182:ARG:HD3  | 1:Q:235:VAL:HB   | 1.82        | 0.62     |
| 2:R:337:THR:OG1  | 2:R:343:THR:HG22 | 1.99        | 0.62     |
| 1:F:179:ASP:O    | 1:F:183:ILE:HG12 | 1.99        | 0.62     |
| 2:P:308:TYR:HB2  | 2:P:309:PRO:HD2  | 1.81        | 0.62     |
| 1:A:30:VAL:HG22  | 1:A:43:ALA:HB1   | 1.79        | 0.62     |
| 2:J:462:SER:O    | 2:J:465:ARG:HG2  | 1.99        | 0.62     |
| 2:T:308:TYR:HB2  | 2:T:309:PRO:HD2  | 1.81        | 0.62     |
| 1:S:182:ARG:HD3  | 1:S:235:VAL:HB   | 1.81        | 0.62     |
| 1:M:179:ASP:O    | 1:M:183:ILE:HG12 | 2.00        | 0.62     |
| 2:L:462:SER:O    | 2:L:465:ARG:HG2  | 1.99        | 0.62     |
| 2:C:308:TYR:HB2  | 2:C:309:PRO:HD2  | 1.80        | 0.62     |
| 2:G:449:SER:HB2  | 2:2:452:LYS:NZ   | 2.14        | 0.62     |
| 1:D:112:THR:CG2  | 1:Q:115:ALA:HB3  | 2.29        | 0.62     |
| 1:M:154:VAL:HG13 | 3:M:249:HOH:O    | 1.99        | 0.62     |
| 1:S:16:ARG:HE    | 1:S:117:PRO:HD3  | 1.64        | 0.62     |
| 1:Q:189:ARG:CZ   | 1:Q:237:GLN:HB3  | 2.30        | 0.62     |
| 2:T:462:SER:O    | 2:T:465:ARG:HG2  | 2.00        | 0.62     |
| 1:D:28:LYS:HB2   | 1:D:52:LYS:NZ    | 2.15        | 0.62     |
| 1:S:28:LYS:HB2   | 1:S:52:LYS:NZ    | 2.15        | 0.62     |
| 1:I:16:ARG:HE    | 1:I:117:PRO:HD3  | 1.64        | 0.62     |
| 1:Q:16:ARG:HE    | 1:Q:117:PRO:HD3  | 1.65        | 0.62     |
| 1:O:56:LEU:HD13  | 1:O:99:LEU:CD2   | 2.30        | 0.61     |
| 1:Y:16:ARG:HE    | 1:Y:117:PRO:HD3  | 1.65        | 0.61     |
| 1:U:182:ARG:HD3  | 1:U:235:VAL:HB   | 1.82        | 0.61     |
| 1:Q:10:GLU:HA    | 1:Y:19:LEU:HD12  | 1.82        | 0.61     |
| 1:M:79:ILE:HD13  | 2:N:368:LYS:HB3  | 1.80        | 0.61     |
| 2:R:436:TYR:HD1  | 2:R:436:TYR:H    | 1.49        | 0.61     |
| 2:L:319:ARG:HG3  | 2:L:320:SER:N    | 2.14        | 0.61     |
| 1:K:16:ARG:HE    | 1:K:117:PRO:HD3  | 1.66        | 0.61     |
| 2:E:461:ASP:OD1  | 2:E:509:ARG:HD2  | 2.01        | 0.61     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:452:LYS:NZ   | 2:E:449:SER:HB2  | 2.15        | 0.61     |
| 2:T:337:THR:OG1  | 2:T:343:THR:HG22 | 1.99        | 0.61     |
| 1:W:179:ASP:O    | 1:W:183:ILE:HG12 | 2.00        | 0.61     |
| 1:B:115:ALA:HB3  | 1:I:112:THR:HG22 | 1.82        | 0.61     |
| 2:C:351:VAL:HB   | 2:C:400:ALA:HB2  | 1.83        | 0.61     |
| 2:V:436:TYR:HD1  | 2:V:436:TYR:H    | 1.48        | 0.61     |
| 2:R:424:ASP:HB3  | 2:R:428:GLY:N    | 2.15        | 0.61     |
| 2:C:304:VAL:HG21 | 2:C:450:MET:HE3  | 1.82        | 0.61     |
| 2:N:344:GLY:HA3  | 3:N:120:HOH:O    | 2.00        | 0.61     |
| 1:O:68:PHE:HA    | 1:O:71:PHE:CE2   | 2.36        | 0.61     |
| 2:P:351:VAL:HB   | 2:P:400:ALA:HB2  | 1.83        | 0.61     |
| 1:D:179:ASP:O    | 1:D:183:ILE:HG12 | 2.01        | 0.61     |
| 1:K:189:ARG:CZ   | 1:K:237:GLN:HB3  | 2.30        | 0.61     |
| 1:K:110:ILE:HG23 | 1:K:114:GLN:HG3  | 1.83        | 0.61     |
| 2:G:464:LEU:HD12 | 2:G:496:ILE:HD11 | 1.80        | 0.61     |
| 1:1:182:ARG:HD3  | 1:1:235:VAL:HB   | 1.82        | 0.60     |
| 2:2:436:TYR:H    | 2:2:436:TYR:HD1  | 1.48        | 0.60     |
| 1:O:30:VAL:HA    | 3:O:250:HOH:O    | 2.01        | 0.60     |
| 2:C:462:SER:O    | 2:C:465:ARG:HG2  | 2.01        | 0.60     |
| 2:R:325:MET:HE3  | 3:Z:100:HOH:O    | 2.01        | 0.60     |
| 1:S:36:ALA:HB3   | 3:S:252:HOH:O    | 2.01        | 0.60     |
| 1:O:83:ASP:OD2   | 2:P:365:HIS:HD2  | 1.85        | 0.60     |
| 2:H:444:LEU:HD12 | 2:E:444:LEU:CD1  | 2.27        | 0.60     |
| 1:Y:189:ARG:CZ   | 1:Y:237:GLN:HB3  | 2.30        | 0.60     |
| 1:Y:206:ALA:HB1  | 3:Y:249:HOH:O    | 2.02        | 0.60     |
| 1:Q:68:PHE:HA    | 1:Q:71:PHE:CE2   | 2.37        | 0.60     |
| 2:L:436:TYR:H    | 2:L:436:TYR:HD1  | 1.50        | 0.60     |
| 2:T:436:TYR:H    | 2:T:436:TYR:HD1  | 1.49        | 0.60     |
| 2:R:324:ASN:H    | 2:R:324:ASN:HD22 | 1.49        | 0.60     |
| 2:J:449:SER:HB2  | 2:Z:452:LYS:NZ   | 2.17        | 0.60     |
| 1:O:213:LEU:HA   | 1:O:221:ALA:O    | 2.01        | 0.60     |
| 2:Z:308:TYR:HB2  | 2:Z:309:PRO:HD2  | 1.84        | 0.60     |
| 2:J:324:ASN:H    | 2:J:324:ASN:HD22 | 1.49        | 0.60     |
| 1:A:48:ARG:NH2   | 1:B:135:ARG:HB3  | 2.08        | 0.60     |
| 2:R:351:VAL:HB   | 2:R:400:ALA:HB2  | 1.82        | 0.60     |
| 1:I:48:ARG:HH22  | 1:S:135:ARG:HB3  | 1.67        | 0.60     |
| 1:1:213:LEU:HA   | 1:1:221:ALA:O    | 2.02        | 0.60     |
| 1:1:179:ASP:O    | 1:1:183:ILE:HG12 | 2.02        | 0.60     |
| 1:A:16:ARG:HE    | 1:A:117:PRO:HD3  | 1.66        | 0.60     |
| 2:T:452:LYS:NZ   | 3:T:79:HOH:O     | 2.34        | 0.60     |
| 1:I:179:ASP:O    | 1:I:183:ILE:HG12 | 2.02        | 0.60     |
| 1:A:213:LEU:HA   | 1:A:221:ALA:O    | 2.02        | 0.59     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:K:213:LEU:HA   | 1:K:221:ALA:O    | 2.02        | 0.59     |
| 1:I:189:ARG:CZ   | 1:I:237:GLN:HB3  | 2.32        | 0.59     |
| 1:F:16:ARG:HE    | 1:F:117:PRO:HD3  | 1.67        | 0.59     |
| 1:S:110:ILE:HG23 | 1:S:114:GLN:HG3  | 1.83        | 0.59     |
| 2:J:461:ASP:OD1  | 2:J:509:ARG:HD2  | 2.03        | 0.59     |
| 1:O:16:ARG:HE    | 1:O:117:PRO:HD3  | 1.67        | 0.59     |
| 2:C:375:THR:OG1  | 1:I:93:ASP:OD1   | 2.21        | 0.59     |
| 1:A:68:PHE:HE1   | 1:B:101:ASN:OD1  | 1.83        | 0.59     |
| 1:Y:205:VAL:C    | 1:Y:207:SER:H    | 2.05        | 0.59     |
| 1:U:68:PHE:HA    | 1:U:71:PHE:CE2   | 2.38        | 0.59     |
| 1:A:28:LYS:HB2   | 1:A:52:LYS:NZ    | 2.17        | 0.59     |
| 2:H:436:TYR:H    | 2:H:436:TYR:HD1  | 1.50        | 0.59     |
| 2:P:324:ASN:HD22 | 2:P:324:ASN:H    | 1.48        | 0.59     |
| 1:I:28:LYS:HB2   | 1:I:52:LYS:NZ    | 2.17        | 0.59     |
| 2:V:304:VAL:HG21 | 2:V:450:MET:HE3  | 1.83        | 0.59     |
| 1:M:16:ARG:HE    | 1:M:117:PRO:HD3  | 1.66        | 0.59     |
| 2:P:464:LEU:HD12 | 2:P:496:ILE:HD11 | 1.85        | 0.59     |
| 1:F:213:LEU:HA   | 1:F:221:ALA:O    | 2.03        | 0.59     |
| 2:N:436:TYR:H    | 2:N:436:TYR:HD1  | 1.49        | 0.59     |
| 2:H:444:LEU:CD1  | 2:E:444:LEU:HD12 | 2.26        | 0.59     |
| 1:B:213:LEU:HA   | 1:B:221:ALA:O    | 2.02        | 0.59     |
| 1:A:179:ASP:O    | 1:A:183:ILE:HG12 | 2.02        | 0.59     |
| 2:J:351:VAL:HB   | 2:J:400:ALA:HB2  | 1.85        | 0.59     |
| 1:I:56:LEU:HD13  | 1:I:99:LEU:CD2   | 2.32        | 0.59     |
| 1:U:213:LEU:HA   | 1:U:221:ALA:O    | 2.02        | 0.59     |
| 1:D:90:ASP:CB    | 3:D:249:HOH:O    | 2.50        | 0.59     |
| 1:O:182:ARG:HD3  | 1:O:235:VAL:HB   | 1.83        | 0.59     |
| 1:D:189:ARG:CZ   | 1:D:237:GLN:HB3  | 2.33        | 0.59     |
| 2:N:308:TYR:HB2  | 2:N:309:PRO:HD2  | 1.84        | 0.59     |
| 1:I:110:ILE:HG23 | 1:I:114:GLN:HG3  | 1.83        | 0.59     |
| 1:D:19:LEU:HD12  | 1:K:10:GLU:HA    | 1.83        | 0.59     |
| 2:H:324:ASN:HD22 | 2:H:324:ASN:H    | 1.50        | 0.59     |
| 2:G:436:TYR:HD1  | 2:G:436:TYR:H    | 1.51        | 0.59     |
| 2:H:329:ARG:NH2  | 2:L:476:ASP:O    | 2.34        | 0.59     |
| 1:I:213:LEU:HA   | 1:I:221:ALA:O    | 2.03        | 0.59     |
| 2:G:351:VAL:HB   | 2:G:400:ALA:HB2  | 1.85        | 0.59     |
| 2:L:413:ASP:HA   | 3:L:73:HOH:O     | 2.02        | 0.58     |
| 1:M:28:LYS:HB2   | 1:M:52:LYS:NZ    | 2.17        | 0.58     |
| 2:Z:351:VAL:HB   | 2:Z:400:ALA:HB2  | 1.85        | 0.58     |
| 2:R:308:TYR:HB2  | 2:R:309:PRO:HD2  | 1.85        | 0.58     |
| 1:F:112:THR:CG2  | 1:M:115:ALA:HB3  | 2.32        | 0.58     |
| 2:V:464:LEU:HD12 | 2:V:496:ILE:HD11 | 1.85        | 0.58     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:S:83:ASP:OD2   | 2:T:365:HIS:HD2  | 1.86        | 0.58     |
| 1:I:16:ARG:HE    | 1:I:117:PRO:HD3  | 1.67        | 0.58     |
| 2:H:462:SER:O    | 2:H:465:ARG:HG2  | 2.03        | 0.58     |
| 1:Y:213:LEU:HA   | 1:Y:221:ALA:O    | 2.04        | 0.58     |
| 2:N:449:SER:HB2  | 2:V:452:LYS:NZ   | 2.19        | 0.58     |
| 2:T:351:VAL:HB   | 2:T:400:ALA:HB2  | 1.85        | 0.58     |
| 1:O:205:VAL:C    | 1:O:207:SER:H    | 2.06        | 0.58     |
| 1:D:16:ARG:HE    | 1:D:117:PRO:HD3  | 1.68        | 0.58     |
| 1:O:93:ASP:OD1   | 2:V:375:THR:OG1  | 2.21        | 0.58     |
| 2:G:456:GLN:HE22 | 2:G:465:ARG:NH1  | 2.00        | 0.58     |
| 1:I:205:VAL:C    | 1:I:207:SER:H    | 2.07        | 0.58     |
| 1:B:16:ARG:HE    | 1:B:117:PRO:HD3  | 1.68        | 0.58     |
| 2:J:375:THR:OG1  | 1:S:93:ASP:OD1   | 2.20        | 0.58     |
| 1:K:69:ASN:ND2   | 3:K:258:HOH:O    | 2.36        | 0.58     |
| 2:T:464:LEU:HD12 | 2:T:496:ILE:HD11 | 1.84        | 0.58     |
| 1:S:56:LEU:HD13  | 1:S:99:LEU:HD22  | 1.86        | 0.58     |
| 2:G:375:THR:OG1  | 1:W:93:ASP:OD1   | 2.21        | 0.58     |
| 2:C:382:ARG:HD3  | 1:I:89:TYR:HD1   | 1.68        | 0.58     |
| 1:K:179:ASP:O    | 1:K:183:ILE:HG12 | 2.03        | 0.58     |
| 1:M:189:ARG:CZ   | 1:M:237:GLN:HB3  | 2.33        | 0.58     |
| 1:K:205:VAL:C    | 1:K:207:SER:H    | 2.07        | 0.58     |
| 1:U:28:LYS:HB2   | 1:U:52:LYS:NZ    | 2.18        | 0.58     |
| 1:B:28:LYS:HB2   | 1:B:52:LYS:NZ    | 2.19        | 0.58     |
| 1:I:14:ARG:HH11  | 1:I:14:ARG:CB    | 2.10        | 0.58     |
| 1:U:205:VAL:C    | 1:U:207:SER:H    | 2.05        | 0.58     |
| 1:W:16:ARG:HE    | 1:W:117:PRO:HD3  | 1.68        | 0.58     |
| 1:Y:179:ASP:O    | 1:Y:183:ILE:HG12 | 2.04        | 0.58     |
| 1:D:182:ARG:HD3  | 1:D:235:VAL:HB   | 1.84        | 0.58     |
| 1:Q:179:ASP:O    | 1:Q:183:ILE:HG12 | 2.03        | 0.58     |
| 1:Q:205:VAL:C    | 1:Q:207:SER:H    | 2.07        | 0.58     |
| 2:L:464:LEU:HD12 | 2:L:496:ILE:HD11 | 1.85        | 0.58     |
| 1:A:205:VAL:C    | 1:A:207:SER:H    | 2.07        | 0.58     |
| 1:W:205:VAL:C    | 1:W:207:SER:H    | 2.06        | 0.57     |
| 2:J:364:GLU:HG2  | 2:J:368:LYS:HE2  | 1.86        | 0.57     |
| 2:G:341:THR:CG2  | 2:G:404:LEU:HD11 | 2.34        | 0.57     |
| 1:F:28:LYS:HB2   | 1:F:52:LYS:NZ    | 2.19        | 0.57     |
| 2:E:424:ASP:HB3  | 2:E:428:GLY:N    | 2.17        | 0.57     |
| 1:B:68:PHE:HA    | 1:B:71:PHE:CE2   | 2.39        | 0.57     |
| 1:Q:30:VAL:HG22  | 1:Q:43:ALA:HB1   | 1.86        | 0.57     |
| 2:2:351:VAL:HB   | 2:2:400:ALA:HB2  | 1.86        | 0.57     |
| 2:C:461:ASP:OD1  | 2:C:509:ARG:HD2  | 2.04        | 0.57     |
| 1:M:127:VAL:CG2  | 1:M:215:ALA:HB2  | 2.35        | 0.57     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:Y:28:LYS:HB2   | 1:Y:52:LYS:NZ    | 2.19        | 0.57     |
| 1:Y:110:ILE:HG23 | 1:Y:114:GLN:HG3  | 1.85        | 0.57     |
| 1:A:30:VAL:HG22  | 1:A:43:ALA:CB    | 2.34        | 0.57     |
| 1:W:28:LYS:HB2   | 1:W:52:LYS:NZ    | 2.18        | 0.57     |
| 1:O:28:LYS:HB2   | 1:O:52:LYS:NZ    | 2.20        | 0.57     |
| 2:E:436:TYR:HD1  | 2:E:436:TYR:H    | 1.50        | 0.57     |
| 2:L:449:SER:HB2  | 2:P:452:LYS:HZ1  | 1.69        | 0.57     |
| 1:D:128:ALA:HB2  | 1:D:134:LYS:HB3  | 1.87        | 0.57     |
| 2:L:395:MET:HA   | 2:L:395:MET:CE   | 2.34        | 0.57     |
| 2:N:351:VAL:HB   | 2:N:400:ALA:HB2  | 1.85        | 0.57     |
| 2:T:341:THR:CG2  | 2:T:404:LEU:HD11 | 2.34        | 0.57     |
| 1:F:205:VAL:C    | 1:F:207:SER:H    | 2.08        | 0.57     |
| 1:B:179:ASP:O    | 1:B:183:ILE:HG12 | 2.04        | 0.57     |
| 1:F:89:TYR:CD1   | 2:N:382:ARG:HD3  | 2.39        | 0.57     |
| 1:D:205:VAL:C    | 1:D:207:SER:H    | 2.08        | 0.57     |
| 2:J:341:THR:CG2  | 2:J:404:LEU:HD11 | 2.34        | 0.57     |
| 2:E:351:VAL:HB   | 2:E:400:ALA:HB2  | 1.85        | 0.57     |
| 1:U:179:ASP:O    | 1:U:183:ILE:HG12 | 2.04        | 0.57     |
| 2:X:351:VAL:HB   | 2:X:400:ALA:HB2  | 1.87        | 0.57     |
| 2:G:424:ASP:HB3  | 2:G:428:GLY:N    | 2.19        | 0.57     |
| 1:Q:28:LYS:HB2   | 1:Q:52:LYS:NZ    | 2.20        | 0.57     |
| 1:S:179:ASP:O    | 1:S:183:ILE:HG12 | 2.04        | 0.57     |
| 1:I:68:PHE:HA    | 1:I:71:PHE:CE2   | 2.40        | 0.57     |
| 1:S:68:PHE:HA    | 1:S:71:PHE:CE2   | 2.40        | 0.57     |
| 2:C:436:TYR:H    | 2:C:436:TYR:HD1  | 1.51        | 0.57     |
| 2:G:341:THR:HG22 | 2:G:404:LEU:HD11 | 1.87        | 0.56     |
| 2:R:341:THR:CG2  | 2:R:404:LEU:HD11 | 2.35        | 0.56     |
| 1:S:205:VAL:C    | 1:S:207:SER:H    | 2.08        | 0.56     |
| 1:I:9:PRO:HD3    | 3:I:249:HOH:O    | 2.05        | 0.56     |
| 2:2:395:MET:HA   | 2:2:395:MET:CE   | 2.35        | 0.56     |
| 1:O:179:ASP:O    | 1:O:183:ILE:HG12 | 2.05        | 0.56     |
| 2:L:341:THR:CG2  | 2:L:404:LEU:HD11 | 2.35        | 0.56     |
| 2:T:452:LYS:HG2  | 3:T:79:HOH:O     | 2.04        | 0.56     |
| 1:1:205:VAL:C    | 1:1:207:SER:H    | 2.08        | 0.56     |
| 2:J:424:ASP:HB3  | 2:J:428:GLY:N    | 2.19        | 0.56     |
| 2:G:465:ARG:HG3  | 2:G:466:VAL:N    | 2.20        | 0.56     |
| 1:F:115:ALA:HB3  | 1:W:112:THR:HG22 | 1.86        | 0.56     |
| 2:N:364:GLU:HG2  | 2:N:368:LYS:HE2  | 1.88        | 0.56     |
| 2:Z:464:LEU:HD12 | 2:Z:496:ILE:HD11 | 1.86        | 0.56     |
| 1:D:56:LEU:HD13  | 1:D:99:LEU:CD2   | 2.35        | 0.56     |
| 1:K:56:LEU:HD13  | 1:K:99:LEU:CD2   | 2.34        | 0.56     |
| 1:U:30:VAL:HG22  | 1:U:43:ALA:HB1   | 1.87        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:L:324:ASN:HD22 | 2:L:324:ASN:H    | 1.53        | 0.56     |
| 2:H:366:TYR:OH   | 1:B:93:ASP:HB3   | 2.06        | 0.56     |
| 1:M:30:VAL:HG13  | 1:M:43:ALA:HB2   | 1.88        | 0.56     |
| 2:L:341:THR:HG22 | 2:L:404:LEU:HD11 | 1.86        | 0.56     |
| 1:M:213:LEU:HA   | 1:M:221:ALA:O    | 2.05        | 0.56     |
| 1:D:48:ARG:HD2   | 1:K:137:GLU:OE2  | 2.06        | 0.56     |
| 1:M:205:VAL:C    | 1:M:207:SER:H    | 2.08        | 0.56     |
| 1:K:73:ASN:HD22  | 1:M:105:GLN:CD   | 2.09        | 0.56     |
| 1:I:25:ALA:O     | 1:I:158:GLY:HA2  | 2.05        | 0.56     |
| 1:O:14:ARG:HH11  | 1:O:14:ARG:CB    | 2.12        | 0.56     |
| 2:H:424:ASP:HB3  | 2:H:428:GLY:N    | 2.21        | 0.56     |
| 2:L:464:LEU:HD11 | 2:L:505:VAL:HG11 | 1.87        | 0.56     |
| 1:A:128:ALA:HB2  | 1:A:134:LYS:HB3  | 1.88        | 0.56     |
| 2:H:351:VAL:HB   | 2:H:400:ALA:HB2  | 1.88        | 0.56     |
| 1:D:68:PHE:HA    | 1:D:71:PHE:CE2   | 2.40        | 0.56     |
| 1:B:205:VAL:C    | 1:B:207:SER:H    | 2.09        | 0.56     |
| 1:D:22:LYS:HD2   | 1:K:10:GLU:OE2   | 2.06        | 0.56     |
| 2:T:449:SER:HB2  | 2:X:452:LYS:NZ   | 2.20        | 0.56     |
| 2:H:461:ASP:OD1  | 2:H:509:ARG:HD2  | 2.05        | 0.56     |
| 2:V:324:ASN:H    | 2:V:324:ASN:HD22 | 1.52        | 0.56     |
| 2:L:456:GLN:HE22 | 2:L:465:ARG:NH1  | 2.04        | 0.56     |
| 1:I:30:VAL:HG13  | 1:I:43:ALA:HB2   | 1.88        | 0.56     |
| 2:P:395:MET:HA   | 2:P:395:MET:CE   | 2.35        | 0.56     |
| 2:T:424:ASP:HB3  | 2:T:428:GLY:N    | 2.20        | 0.56     |
| 1:M:68:PHE:HA    | 1:M:71:PHE:CE2   | 2.41        | 0.56     |
| 2:L:364:GLU:HG2  | 2:L:368:LYS:HE2  | 1.88        | 0.56     |
| 1:I:68:PHE:HA    | 1:I:71:PHE:CE2   | 2.40        | 0.56     |
| 2:H:464:LEU:HD12 | 2:H:496:ILE:HD11 | 1.88        | 0.56     |
| 2:2:324:ASN:HD22 | 2:2:324:ASN:H    | 1.54        | 0.56     |
| 2:P:436:TYR:H    | 2:P:436:TYR:HD1  | 1.52        | 0.56     |
| 2:Z:424:ASP:HB3  | 2:Z:428:GLY:N    | 2.18        | 0.55     |
| 2:P:424:ASP:HB3  | 2:P:428:GLY:N    | 2.19        | 0.55     |
| 2:H:337:THR:HG21 | 2:H:359:TYR:CD2  | 2.41        | 0.55     |
| 1:I:155:VAL:HG12 | 1:I:160:THR:HG22 | 1.87        | 0.55     |
| 2:X:456:GLN:HE22 | 2:X:465:ARG:NH1  | 2.04        | 0.55     |
| 2:V:424:ASP:HB3  | 2:V:428:GLY:N    | 2.20        | 0.55     |
| 2:Z:456:GLN:HE22 | 2:Z:465:ARG:NH1  | 2.04        | 0.55     |
| 1:Y:25:ALA:O     | 1:Y:158:GLY:HA2  | 2.06        | 0.55     |
| 2:2:341:THR:CG2  | 2:2:404:LEU:HD11 | 2.35        | 0.55     |
| 2:X:436:TYR:H    | 2:X:436:TYR:HD1  | 1.52        | 0.55     |
| 2:T:341:THR:HG22 | 2:T:404:LEU:HD11 | 1.88        | 0.55     |
| 2:R:341:THR:HG22 | 2:R:404:LEU:HD11 | 1.86        | 0.55     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:185:VAL:HB   | 1:A:235:VAL:HG11 | 1.88        | 0.55     |
| 1:U:110:ILE:HG23 | 1:U:114:GLN:HG3  | 1.89        | 0.55     |
| 1:O:42:VAL:HG22  | 1:O:210:VAL:HG22 | 1.88        | 0.55     |
| 1:O:25:ALA:O     | 1:O:158:GLY:HA2  | 2.06        | 0.55     |
| 1:S:30:VAL:HG22  | 1:S:43:ALA:HB1   | 1.88        | 0.55     |
| 2:Z:301:THR:HA   | 2:Z:333:LYS:NZ   | 2.21        | 0.55     |
| 1:Q:56:LEU:HD13  | 1:Q:99:LEU:HD22  | 1.88        | 0.55     |
| 1:A:56:LEU:HD13  | 1:A:99:LEU:CD2   | 2.37        | 0.55     |
| 2:2:392:ALA:HB3  | 3:2:136:HOH:O    | 2.07        | 0.55     |
| 1:U:56:LEU:HD13  | 1:U:99:LEU:CD2   | 2.37        | 0.55     |
| 1:Q:213:LEU:HA   | 1:Q:221:ALA:O    | 2.06        | 0.55     |
| 2:T:395:MET:CE   | 2:T:395:MET:HA   | 2.37        | 0.55     |
| 2:H:341:THR:CG2  | 2:H:404:LEU:HD11 | 2.36        | 0.55     |
| 2:L:351:VAL:HB   | 2:L:400:ALA:HB2  | 1.87        | 0.55     |
| 1:1:128:ALA:HB2  | 1:1:134:LYS:HB3  | 1.88        | 0.55     |
| 2:C:324:ASN:HD22 | 2:C:324:ASN:H    | 1.54        | 0.55     |
| 1:1:206:ALA:CB   | 3:1:258:HOH:O    | 2.51        | 0.55     |
| 1:A:19:LEU:HD12  | 1:B:10:GLU:HA    | 1.89        | 0.55     |
| 1:I:226:THR:O    | 1:I:230:LEU:HB2  | 2.06        | 0.55     |
| 1:K:83:ASP:OD2   | 2:L:365:HIS:HD2  | 1.90        | 0.55     |
| 2:J:513:LEU:O    | 2:J:517:ILE:HG12 | 2.07        | 0.55     |
| 1:A:68:PHE:HA    | 1:A:71:PHE:CE2   | 2.42        | 0.55     |
| 2:E:341:THR:HG22 | 2:E:404:LEU:HD11 | 1.88        | 0.55     |
| 2:H:456:GLN:HE22 | 2:H:465:ARG:NH1  | 2.05        | 0.55     |
| 1:W:213:LEU:HA   | 1:W:221:ALA:O    | 2.07        | 0.55     |
| 2:L:424:ASP:HB3  | 2:L:428:GLY:N    | 2.21        | 0.55     |
| 2:N:344:GLY:CA   | 3:N:120:HOH:O    | 2.52        | 0.55     |
| 2:E:317:ASP:OD1  | 2:E:333:LYS:NZ   | 2.39        | 0.55     |
| 2:N:395:MET:HA   | 2:N:395:MET:CE   | 2.37        | 0.55     |
| 1:S:25:ALA:O     | 1:S:158:GLY:HA2  | 2.07        | 0.54     |
| 1:F:56:LEU:HD13  | 1:F:99:LEU:CD2   | 2.37        | 0.54     |
| 2:G:364:GLU:HG2  | 2:G:368:LYS:HE2  | 1.87        | 0.54     |
| 2:Z:324:ASN:H    | 2:Z:324:ASN:HD22 | 1.55        | 0.54     |
| 1:Q:93:ASP:OD1   | 2:Z:375:THR:OG1  | 2.24        | 0.54     |
| 1:B:127:VAL:CG2  | 1:B:215:ALA:HB2  | 2.36        | 0.54     |
| 1:F:135:ARG:HB3  | 1:M:48:ARG:NH2   | 2.21        | 0.54     |
| 2:N:513:LEU:O    | 2:N:517:ILE:HG12 | 2.07        | 0.54     |
| 2:C:452:LYS:NZ   | 2:R:449:SER:HB2  | 2.21        | 0.54     |
| 2:E:456:GLN:HE22 | 2:E:465:ARG:NH1  | 2.05        | 0.54     |
| 1:F:25:ALA:O     | 1:F:158:GLY:HA2  | 2.07        | 0.54     |
| 1:B:56:LEU:HD13  | 1:B:99:LEU:CD2   | 2.37        | 0.54     |
| 1:K:128:ALA:HB2  | 1:K:134:LYS:HB3  | 1.90        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:R:513:LEU:O    | 2:R:517:ILE:HG12 | 2.07        | 0.54     |
| 1:F:42:VAL:HG22  | 1:F:210:VAL:HG22 | 1.90        | 0.54     |
| 2:C:395:MET:HA   | 2:C:395:MET:CE   | 2.38        | 0.54     |
| 2:X:395:MET:HA   | 2:X:395:MET:CE   | 2.38        | 0.54     |
| 1:W:56:LEU:HD13  | 1:W:99:LEU:CD2   | 2.36        | 0.54     |
| 2:X:301:THR:HA   | 2:X:333:LYS:NZ   | 2.21        | 0.54     |
| 1:U:42:VAL:HG22  | 1:U:210:VAL:HG22 | 1.90        | 0.54     |
| 1:I:14:ARG:HH11  | 1:I:14:ARG:CB    | 2.14        | 0.54     |
| 2:R:509:ARG:CG   | 3:R:112:HOH:O    | 2.43        | 0.54     |
| 1:1:127:VAL:CG2  | 1:1:215:ALA:HB2  | 2.38        | 0.54     |
| 2:J:341:THR:HG22 | 2:J:404:LEU:HD11 | 1.88        | 0.54     |
| 1:Y:155:VAL:HG12 | 1:Y:160:THR:HG22 | 1.89        | 0.54     |
| 2:H:513:LEU:O    | 2:H:517:ILE:HG12 | 2.07        | 0.54     |
| 1:F:48:ARG:HH22  | 1:W:135:ARG:HB3  | 1.73        | 0.54     |
| 1:F:68:PHE:HA    | 1:F:71:PHE:CE2   | 2.42        | 0.54     |
| 1:A:185:VAL:HB   | 1:A:235:VAL:CG1  | 2.38        | 0.54     |
| 1:I:76:ARG:NH1   | 2:J:369:LEU:HD22 | 2.22        | 0.54     |
| 1:W:68:PHE:HA    | 1:W:71:PHE:CE2   | 2.43        | 0.54     |
| 1:1:205:VAL:HG12 | 1:1:206:ALA:N    | 2.23        | 0.54     |
| 1:M:30:VAL:HG22  | 1:M:43:ALA:HB1   | 1.89        | 0.54     |
| 1:I:30:VAL:HG22  | 1:I:43:ALA:HB1   | 1.89        | 0.54     |
| 1:O:128:ALA:HB2  | 1:O:134:LYS:HB3  | 1.89        | 0.54     |
| 1:D:63:ALA:O     | 1:D:156:MET:HE1  | 2.07        | 0.54     |
| 1:1:56:LEU:HD13  | 1:1:99:LEU:CD2   | 2.38        | 0.54     |
| 1:I:20:ALA:O     | 1:I:24:ILE:HG12  | 2.08        | 0.54     |
| 1:M:128:ALA:HB2  | 1:M:134:LYS:HB3  | 1.88        | 0.54     |
| 2:N:476:ASP:O    | 2:P:329:ARG:NH2  | 2.41        | 0.54     |
| 1:M:76:ARG:HG2   | 2:N:369:LEU:HD22 | 1.90        | 0.54     |
| 1:D:185:VAL:HB   | 1:D:235:VAL:CG1  | 2.38        | 0.54     |
| 2:Z:464:LEU:HD11 | 2:Z:505:VAL:HG11 | 1.90        | 0.54     |
| 2:E:341:THR:CG2  | 2:E:404:LEU:HD11 | 2.37        | 0.54     |
| 1:F:30:VAL:HG22  | 1:F:43:ALA:HB1   | 1.89        | 0.54     |
| 1:K:76:ARG:NH2   | 2:L:370:GLU:OE2  | 2.36        | 0.54     |
| 2:N:424:ASP:HB3  | 2:N:428:GLY:N    | 2.22        | 0.54     |
| 1:K:127:VAL:CG2  | 1:K:215:ALA:HB2  | 2.38        | 0.54     |
| 1:M:205:VAL:HG12 | 1:M:206:ALA:N    | 2.23        | 0.54     |
| 2:2:381:ASN:HA   | 3:2:75:HOH:O     | 2.08        | 0.54     |
| 1:1:42:VAL:HG22  | 1:1:210:VAL:HG22 | 1.90        | 0.54     |
| 1:I:19:LEU:HD12  | 1:S:10:GLU:HA    | 1.90        | 0.54     |
| 2:V:395:MET:HA   | 2:V:395:MET:CE   | 2.38        | 0.54     |
| 2:G:395:MET:HA   | 2:G:395:MET:CE   | 2.37        | 0.54     |
| 1:Y:85:ARG:HG2   | 1:Y:85:ARG:NH1   | 2.22        | 0.53     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:X:424:ASP:HB3  | 2:X:428:GLY:N    | 2.21        | 0.53     |
| 1:U:127:VAL:CG2  | 1:U:215:ALA:HB2  | 2.38        | 0.53     |
| 1:D:30:VAL:HG22  | 1:D:43:ALA:HB1   | 1.89        | 0.53     |
| 1:W:140:ARG:HH11 | 1:W:140:ARG:HB3  | 1.73        | 0.53     |
| 2:E:324:ASN:H    | 2:E:324:ASN:HD22 | 1.55        | 0.53     |
| 1:D:213:LEU:HA   | 1:D:221:ALA:O    | 2.08        | 0.53     |
| 1:S:185:VAL:HB   | 1:S:235:VAL:CG1  | 2.38        | 0.53     |
| 2:H:364:GLU:HG2  | 2:H:368:LYS:HE2  | 1.90        | 0.53     |
| 1:F:128:ALA:HB2  | 1:F:134:LYS:HB3  | 1.89        | 0.53     |
| 1:I:48:ARG:HA    | 3:I:250:HOH:O    | 2.08        | 0.53     |
| 2:T:464:LEU:HD11 | 2:T:505:VAL:HG11 | 1.89        | 0.53     |
| 1:K:42:VAL:HG22  | 1:K:210:VAL:HG22 | 1.90        | 0.53     |
| 1:M:42:VAL:HG22  | 1:M:210:VAL:HG22 | 1.90        | 0.53     |
| 2:R:456:GLN:HE22 | 2:R:465:ARG:NH1  | 2.06        | 0.53     |
| 1:D:127:VAL:CG2  | 1:D:215:ALA:HB2  | 2.38        | 0.53     |
| 1:S:30:VAL:HG13  | 1:S:43:ALA:HB2   | 1.89        | 0.53     |
| 2:G:513:LEU:O    | 2:G:517:ILE:HG12 | 2.09        | 0.53     |
| 2:P:341:THR:CG2  | 2:P:404:LEU:HD11 | 2.38        | 0.53     |
| 1:U:25:ALA:O     | 1:U:158:GLY:HA2  | 2.09        | 0.53     |
| 1:W:230:LEU:HD13 | 3:W:250:HOH:O    | 2.07        | 0.53     |
| 1:M:226:THR:O    | 1:M:230:LEU:HB2  | 2.09        | 0.53     |
| 2:Z:395:MET:CE   | 2:Z:395:MET:HA   | 2.39        | 0.53     |
| 2:R:464:LEU:HD11 | 2:R:505:VAL:HG11 | 1.89        | 0.53     |
| 1:D:115:ALA:HB3  | 1:K:112:THR:HG22 | 1.90        | 0.53     |
| 1:A:83:ASP:OD2   | 2:H:365:HIS:HD2  | 1.91        | 0.53     |
| 1:W:25:ALA:O     | 1:W:158:GLY:HA2  | 2.09        | 0.53     |
| 2:E:395:MET:CE   | 2:E:395:MET:HA   | 2.39        | 0.53     |
| 1:F:185:VAL:HB   | 1:F:235:VAL:CG1  | 2.39        | 0.53     |
| 1:M:56:LEU:HD13  | 1:M:99:LEU:HD22  | 1.89        | 0.53     |
| 2:H:341:THR:HG22 | 2:H:404:LEU:HD11 | 1.90        | 0.53     |
| 1:I:128:ALA:HB2  | 1:I:134:LYS:HB3  | 1.90        | 0.53     |
| 2:L:513:LEU:O    | 2:L:517:ILE:HG12 | 2.08        | 0.53     |
| 2:V:301:THR:HA   | 2:V:333:LYS:NZ   | 2.24        | 0.53     |
| 1:O:20:ALA:O     | 1:O:24:ILE:HG12  | 2.08        | 0.53     |
| 1:Y:68:PHE:HA    | 1:Y:71:PHE:CE2   | 2.43        | 0.53     |
| 2:J:395:MET:HA   | 2:J:395:MET:CE   | 2.39        | 0.53     |
| 1:B:185:VAL:HB   | 1:B:235:VAL:CG1  | 2.39        | 0.53     |
| 1:W:30:VAL:HG22  | 1:W:43:ALA:HB1   | 1.90        | 0.53     |
| 1:B:25:ALA:O     | 1:B:158:GLY:HA2  | 2.09        | 0.53     |
| 1:K:68:PHE:HA    | 1:K:71:PHE:CE2   | 2.44        | 0.53     |
| 1:B:30:VAL:HG22  | 1:B:43:ALA:HB1   | 1.91        | 0.53     |
| 1:M:14:ARG:HH11  | 1:M:14:ARG:CB    | 2.13        | 0.53     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:T:456:GLN:HE22 | 2:T:465:ARG:NH1  | 2.06        | 0.53     |
| 2:P:513:LEU:O    | 2:P:517:ILE:HG12 | 2.09        | 0.53     |
| 2:T:301:THR:HA   | 2:T:333:LYS:HZ3  | 1.74        | 0.53     |
| 2:P:317:ASP:OD1  | 2:P:333:LYS:NZ   | 2.41        | 0.53     |
| 1:Q:89:TYR:HD1   | 2:Z:382:ARG:HD3  | 1.74        | 0.53     |
| 1:I:56:LEU:HD13  | 1:I:99:LEU:HD22  | 1.91        | 0.53     |
| 1:D:185:VAL:HB   | 1:D:235:VAL:HG11 | 1.91        | 0.53     |
| 2:X:461:ASP:OD1  | 2:X:509:ARG:HD2  | 2.09        | 0.53     |
| 1:Q:128:ALA:HB2  | 1:Q:134:LYS:HB3  | 1.91        | 0.53     |
| 2:T:461:ASP:OD1  | 2:T:509:ARG:HD2  | 2.09        | 0.53     |
| 2:R:461:ASP:OD1  | 2:R:509:ARG:HD2  | 2.09        | 0.53     |
| 1:I:127:VAL:CG2  | 1:I:215:ALA:HB2  | 2.39        | 0.53     |
| 1:M:127:VAL:HG21 | 1:M:215:ALA:HB2  | 1.91        | 0.53     |
| 2:T:449:SER:HB2  | 2:X:452:LYS:HZ1  | 1.74        | 0.53     |
| 1:B:42:VAL:HG22  | 1:B:210:VAL:HG22 | 1.91        | 0.53     |
| 1:F:63:ALA:O     | 1:F:156:MET:HE1  | 2.09        | 0.53     |
| 2:L:452:LYS:NZ   | 2:P:449:SER:HB2  | 2.24        | 0.53     |
| 2:2:424:ASP:HB3  | 2:2:428:GLY:N    | 2.24        | 0.52     |
| 2:N:324:ASN:H    | 2:N:324:ASN:ND2  | 2.06        | 0.52     |
| 1:I:48:ARG:HH22  | 1:S:135:ARG:CB   | 2.22        | 0.52     |
| 2:2:341:THR:HG22 | 2:2:404:LEU:HD11 | 1.90        | 0.52     |
| 1:B:30:VAL:HG13  | 1:B:43:ALA:HB2   | 1.91        | 0.52     |
| 2:Z:341:THR:HG22 | 2:Z:404:LEU:HD11 | 1.91        | 0.52     |
| 2:Z:364:GLU:HG2  | 2:Z:368:LYS:HE2  | 1.90        | 0.52     |
| 1:O:37:GLY:HA3   | 3:O:256:HOH:O    | 2.09        | 0.52     |
| 1:I:140:ARG:HB3  | 1:I:140:ARG:HH11 | 1.73        | 0.52     |
| 1:O:161:GLU:H    | 1:O:161:GLU:CD   | 2.13        | 0.52     |
| 1:O:30:VAL:HG22  | 1:O:43:ALA:HB1   | 1.92        | 0.52     |
| 1:F:226:THR:O    | 1:F:230:LEU:HB2  | 2.08        | 0.52     |
| 1:K:25:ALA:O     | 1:K:158:GLY:HA2  | 2.09        | 0.52     |
| 1:B:140:ARG:HB3  | 1:B:140:ARG:HH11 | 1.74        | 0.52     |
| 1:Y:14:ARG:HH11  | 1:Y:14:ARG:CB    | 2.13        | 0.52     |
| 1:U:14:ARG:CB    | 1:U:14:ARG:HH11  | 2.10        | 0.52     |
| 2:C:424:ASP:HB3  | 2:C:428:GLY:N    | 2.22        | 0.52     |
| 1:Q:185:VAL:HB   | 1:Q:235:VAL:CG1  | 2.39        | 0.52     |
| 2:V:364:GLU:HG2  | 2:V:368:LYS:HE2  | 1.92        | 0.52     |
| 1:F:20:ALA:O     | 1:F:24:ILE:HG12  | 2.09        | 0.52     |
| 2:G:452:LYS:NZ   | 2:2:449:SER:HB2  | 2.24        | 0.52     |
| 1:Q:155:VAL:HG12 | 1:Q:160:THR:HG22 | 1.91        | 0.52     |
| 1:D:141:ILE:N    | 1:D:141:ILE:HD12 | 2.24        | 0.52     |
| 1:O:85:ARG:NH1   | 1:O:85:ARG:HG2   | 2.22        | 0.52     |
| 2:2:364:GLU:HG2  | 2:2:368:LYS:HE2  | 1.91        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:X:513:LEU:O    | 2:X:517:ILE:HG12 | 2.10        | 0.52     |
| 1:U:205:VAL:HG12 | 1:U:206:ALA:N    | 2.25        | 0.52     |
| 2:X:341:THR:CG2  | 2:X:404:LEU:HD11 | 2.40        | 0.52     |
| 1:A:89:TYR:CD1   | 2:P:382:ARG:HD3  | 2.44        | 0.52     |
| 1:K:226:THR:O    | 1:K:230:LEU:HB2  | 2.09        | 0.52     |
| 1:M:54:SER:CB    | 1:M:75:ARG:HD2   | 2.40        | 0.52     |
| 2:V:341:THR:CG2  | 2:V:404:LEU:HD11 | 2.40        | 0.52     |
| 1:I:141:ILE:HD12 | 1:I:141:ILE:N    | 2.25        | 0.52     |
| 1:F:14:ARG:HH11  | 1:F:14:ARG:CB    | 2.14        | 0.52     |
| 1:W:22:LYS:HD2   | 1:Y:10:GLU:OE2   | 2.09        | 0.52     |
| 1:F:185:VAL:HB   | 1:F:235:VAL:HG11 | 1.91        | 0.52     |
| 1:S:185:VAL:HB   | 1:S:235:VAL:HG11 | 1.90        | 0.52     |
| 2:G:449:SER:HB2  | 2:2:452:LYS:HZ3  | 1.73        | 0.52     |
| 2:L:447:LYS:NZ   | 3:L:61:HOH:O     | 2.43        | 0.52     |
| 1:I:25:ALA:O     | 1:I:158:GLY:HA2  | 2.10        | 0.52     |
| 1:Q:14:ARG:HH11  | 1:Q:14:ARG:CB    | 2.15        | 0.52     |
| 1:1:231:GLN:HG2  | 3:1:258:HOH:O    | 2.10        | 0.52     |
| 1:O:56:LEU:HD13  | 1:O:99:LEU:HD22  | 1.90        | 0.52     |
| 1:Q:127:VAL:CG2  | 1:Q:215:ALA:HB2  | 2.40        | 0.52     |
| 2:Z:513:LEU:O    | 2:Z:517:ILE:HG12 | 2.10        | 0.52     |
| 2:E:464:LEU:HD12 | 2:E:496:ILE:HD11 | 1.92        | 0.52     |
| 1:Y:127:VAL:CG2  | 1:Y:215:ALA:HB2  | 2.40        | 0.52     |
| 2:2:464:LEU:HD11 | 2:2:505:VAL:HG11 | 1.92        | 0.52     |
| 2:V:464:LEU:HD11 | 2:V:505:VAL:HG11 | 1.92        | 0.52     |
| 1:A:205:VAL:HG12 | 1:A:206:ALA:H    | 1.75        | 0.52     |
| 1:A:205:VAL:HG12 | 1:A:206:ALA:N    | 2.24        | 0.52     |
| 2:2:455:SER:HB3  | 3:2:159:HOH:O    | 2.09        | 0.52     |
| 1:A:20:ALA:O     | 1:A:24:ILE:HG12  | 2.09        | 0.52     |
| 2:N:464:LEU:HD11 | 2:N:505:VAL:HG11 | 1.92        | 0.52     |
| 1:A:30:VAL:HG13  | 1:A:43:ALA:HB2   | 1.91        | 0.52     |
| 1:B:73:ASN:HD22  | 1:I:105:GLN:CD   | 2.13        | 0.52     |
| 1:1:30:VAL:HG22  | 1:1:43:ALA:HB1   | 1.92        | 0.52     |
| 1:U:155:VAL:HG12 | 1:U:160:THR:HG22 | 1.92        | 0.52     |
| 2:X:321:THR:HG21 | 2:X:480:ALA:HB1  | 1.92        | 0.52     |
| 2:R:337:THR:HG21 | 2:R:359:TYR:CD2  | 2.45        | 0.52     |
| 1:Q:205:VAL:HG12 | 1:Q:206:ALA:N    | 2.25        | 0.52     |
| 1:Q:42:VAL:HG22  | 1:Q:210:VAL:HG22 | 1.91        | 0.52     |
| 1:S:128:ALA:HB2  | 1:S:134:LYS:HB3  | 1.91        | 0.52     |
| 2:C:341:THR:HG22 | 2:C:404:LEU:HD11 | 1.91        | 0.52     |
| 1:U:20:ALA:O     | 1:U:24:ILE:HG12  | 2.10        | 0.52     |
| 1:Y:30:VAL:HG22  | 1:Y:43:ALA:HB1   | 1.90        | 0.52     |
| 2:T:324:ASN:HD22 | 2:T:324:ASN:H    | 1.57        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:30:VAL:HG13  | 1:O:43:ALA:HB2   | 1.92        | 0.51     |
| 2:P:324:ASN:N    | 2:P:324:ASN:HD22 | 2.06        | 0.51     |
| 2:T:513:LEU:O    | 2:T:517:ILE:HG12 | 2.09        | 0.51     |
| 1:A:25:ALA:O     | 1:A:158:GLY:HA2  | 2.10        | 0.51     |
| 1:Y:128:ALA:HB2  | 1:Y:134:LYS:HB3  | 1.90        | 0.51     |
| 2:2:307:LYS:N    | 3:2:14:HOH:O     | 2.21        | 0.51     |
| 2:H:324:ASN:N    | 2:H:324:ASN:HD22 | 2.07        | 0.51     |
| 1:I:42:VAL:HG22  | 1:I:210:VAL:HG22 | 1.92        | 0.51     |
| 1:A:42:VAL:HG22  | 1:A:210:VAL:HG22 | 1.92        | 0.51     |
| 1:1:185:VAL:HB   | 1:1:235:VAL:CG1  | 2.40        | 0.51     |
| 1:K:30:VAL:HG22  | 1:K:43:ALA:HB1   | 1.91        | 0.51     |
| 2:Z:461:ASP:OD1  | 2:Z:509:ARG:HD2  | 2.09        | 0.51     |
| 1:B:226:THR:O    | 1:B:230:LEU:HB2  | 2.09        | 0.51     |
| 2:C:301:THR:HA   | 2:C:333:LYS:NZ   | 2.25        | 0.51     |
| 2:J:301:THR:HA   | 2:J:333:LYS:NZ   | 2.25        | 0.51     |
| 2:R:307:LYS:HE2  | 2:R:435:GLY:HA2  | 1.92        | 0.51     |
| 1:A:141:ILE:N    | 1:A:141:ILE:HD12 | 2.25        | 0.51     |
| 1:U:140:ARG:HB3  | 1:U:140:ARG:HH11 | 1.75        | 0.51     |
| 1:1:161:GLU:CD   | 1:1:161:GLU:H    | 2.14        | 0.51     |
| 2:C:456:GLN:HE22 | 2:C:465:ARG:NH1  | 2.08        | 0.51     |
| 2:H:452:LYS:HZ1  | 2:E:449:SER:HB2  | 1.74        | 0.51     |
| 1:O:205:VAL:HG12 | 1:O:206:ALA:N    | 2.25        | 0.51     |
| 1:W:226:THR:O    | 1:W:230:LEU:HB2  | 2.10        | 0.51     |
| 2:L:461:ASP:OD1  | 2:L:509:ARG:HD2  | 2.10        | 0.51     |
| 2:H:301:THR:N    | 2:H:441:SER:HG   | 2.09        | 0.51     |
| 1:W:128:ALA:HB2  | 1:W:134:LYS:HB3  | 1.93        | 0.51     |
| 2:V:513:LEU:O    | 2:V:517:ILE:HG12 | 2.10        | 0.51     |
| 2:C:364:GLU:HG2  | 2:C:368:LYS:HE2  | 1.93        | 0.51     |
| 1:W:161:GLU:H    | 1:W:161:GLU:CD   | 2.13        | 0.51     |
| 1:B:30:VAL:CG2   | 1:B:65:ALA:HB2   | 2.41        | 0.51     |
| 1:1:226:THR:O    | 1:1:230:LEU:HB2  | 2.10        | 0.51     |
| 1:Q:226:THR:O    | 1:Q:230:LEU:HB2  | 2.10        | 0.51     |
| 1:1:141:ILE:HD12 | 1:1:141:ILE:N    | 2.26        | 0.51     |
| 2:G:464:LEU:HD11 | 2:G:505:VAL:HG11 | 1.93        | 0.51     |
| 1:K:91:ARG:HG3   | 3:K:257:HOH:O    | 2.10        | 0.51     |
| 1:Y:161:GLU:CD   | 1:Y:161:GLU:H    | 2.14        | 0.51     |
| 1:B:185:VAL:HB   | 1:B:235:VAL:HG11 | 1.92        | 0.51     |
| 2:C:452:LYS:HZ1  | 2:R:449:SER:HB2  | 1.75        | 0.51     |
| 1:O:112:THR:HG22 | 1:U:115:ALA:HB3  | 1.93        | 0.51     |
| 1:D:42:VAL:HG22  | 1:D:210:VAL:HG22 | 1.93        | 0.51     |
| 2:2:513:LEU:O    | 2:2:517:ILE:HG12 | 2.11        | 0.51     |
| 2:X:324:ASN:H    | 2:X:324:ASN:HD22 | 1.58        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:127:VAL:CG2  | 1:A:215:ALA:HB2  | 2.40        | 0.51     |
| 1:O:185:VAL:HB   | 1:O:235:VAL:CG1  | 2.41        | 0.51     |
| 2:N:341:THR:HG22 | 2:N:404:LEU:HD11 | 1.92        | 0.51     |
| 1:Y:56:LEU:HD13  | 1:Y:99:LEU:CD2   | 2.40        | 0.51     |
| 2:H:395:MET:HA   | 2:H:395:MET:CE   | 2.41        | 0.51     |
| 1:O:127:VAL:CG2  | 1:O:215:ALA:HB2  | 2.40        | 0.51     |
| 1:1:185:VAL:HB   | 1:1:235:VAL:HG11 | 1.93        | 0.51     |
| 2:R:324:ASN:HD22 | 2:R:324:ASN:N    | 2.08        | 0.51     |
| 1:B:155:VAL:HG12 | 1:B:160:THR:HG22 | 1.93        | 0.51     |
| 1:Q:25:ALA:O     | 1:Q:158:GLY:HA2  | 2.11        | 0.51     |
| 1:Q:140:ARG:HH11 | 1:Q:140:ARG:HB3  | 1.76        | 0.51     |
| 1:B:127:VAL:HG21 | 1:B:215:ALA:HB2  | 1.93        | 0.51     |
| 1:I:30:VAL:CG2   | 1:I:65:ALA:HB2   | 2.40        | 0.51     |
| 1:S:30:VAL:CG2   | 1:S:65:ALA:HB2   | 2.40        | 0.51     |
| 2:H:321:THR:HG21 | 2:H:480:ALA:HB1  | 1.93        | 0.51     |
| 1:M:20:ALA:O     | 1:M:24:ILE:HG12  | 2.11        | 0.51     |
| 2:C:513:LEU:O    | 2:C:517:ILE:HG12 | 2.11        | 0.51     |
| 1:S:226:THR:O    | 1:S:230:LEU:HB2  | 2.11        | 0.51     |
| 1:1:20:ALA:O     | 1:1:24:ILE:HG12  | 2.10        | 0.51     |
| 1:W:127:VAL:CG2  | 1:W:215:ALA:HB2  | 2.41        | 0.50     |
| 2:V:341:THR:HG22 | 2:V:404:LEU:HD11 | 1.92        | 0.50     |
| 2:V:456:GLN:HE22 | 2:V:465:ARG:NH1  | 2.09        | 0.50     |
| 1:Q:185:VAL:HB   | 1:Q:235:VAL:HG11 | 1.93        | 0.50     |
| 1:I:127:VAL:HG21 | 1:I:215:ALA:HB2  | 1.92        | 0.50     |
| 1:F:30:VAL:HG13  | 1:F:43:ALA:HB2   | 1.93        | 0.50     |
| 1:Q:63:ALA:O     | 1:Q:156:MET:HE1  | 2.12        | 0.50     |
| 2:2:317:ASP:OD1  | 2:2:333:LYS:NZ   | 2.38        | 0.50     |
| 2:R:301:THR:HA   | 2:R:333:LYS:NZ   | 2.26        | 0.50     |
| 1:W:185:VAL:HB   | 1:W:235:VAL:CG1  | 2.42        | 0.50     |
| 1:S:42:VAL:HG22  | 1:S:210:VAL:HG22 | 1.92        | 0.50     |
| 1:B:54:SER:CB    | 1:B:75:ARG:HD2   | 2.42        | 0.50     |
| 1:Y:226:THR:O    | 1:Y:230:LEU:HB2  | 2.10        | 0.50     |
| 2:C:464:LEU:HD11 | 2:C:505:VAL:HG11 | 1.94        | 0.50     |
| 1:W:205:VAL:HG12 | 1:W:206:ALA:N    | 2.26        | 0.50     |
| 1:B:128:ALA:HB2  | 1:B:134:LYS:HB3  | 1.92        | 0.50     |
| 2:G:461:ASP:OD1  | 2:G:509:ARG:HD2  | 2.11        | 0.50     |
| 1:O:155:VAL:HG12 | 1:O:160:THR:HG22 | 1.93        | 0.50     |
| 1:I:115:ALA:HB3  | 1:S:112:THR:CG2  | 2.42        | 0.50     |
| 2:E:517:ILE:HA   | 3:E:38:HOH:O     | 2.11        | 0.50     |
| 2:R:395:MET:CE   | 2:R:395:MET:HA   | 2.42        | 0.50     |
| 1:W:19:LEU:HD12  | 1:Y:10:GLU:CA    | 2.42        | 0.50     |
| 2:G:309:PRO:HG3  | 2:G:458:THR:O    | 2.12        | 0.50     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:182:ARG:HD3  | 1:A:235:VAL:CB   | 2.40        | 0.50     |
| 1:K:185:VAL:HB   | 1:K:235:VAL:CG1  | 2.41        | 0.50     |
| 2:E:464:LEU:HD11 | 2:E:505:VAL:HG11 | 1.94        | 0.50     |
| 1:K:30:VAL:HG13  | 1:K:43:ALA:HB2   | 1.93        | 0.50     |
| 2:G:301:THR:HA   | 2:G:333:LYS:NZ   | 2.26        | 0.50     |
| 1:M:25:ALA:O     | 1:M:158:GLY:HA2  | 2.12        | 0.50     |
| 1:S:161:GLU:CD   | 1:S:161:GLU:H    | 2.15        | 0.50     |
| 1:W:127:VAL:HG21 | 1:W:215:ALA:HB2  | 1.94        | 0.50     |
| 2:N:309:PRO:HG3  | 2:N:458:THR:O    | 2.12        | 0.50     |
| 1:U:128:ALA:HB2  | 1:U:134:LYS:HB3  | 1.93        | 0.50     |
| 1:U:85:ARG:NH1   | 1:U:85:ARG:HG2   | 2.26        | 0.50     |
| 2:J:309:PRO:HG3  | 2:J:458:THR:O    | 2.12        | 0.50     |
| 2:E:513:LEU:O    | 2:E:517:ILE:HG12 | 2.10        | 0.50     |
| 1:D:25:ALA:O     | 1:D:158:GLY:HA2  | 2.11        | 0.50     |
| 1:K:161:GLU:H    | 1:K:161:GLU:CD   | 2.15        | 0.50     |
| 1:W:141:ILE:HD12 | 1:W:141:ILE:N    | 2.26        | 0.50     |
| 2:H:309:PRO:HG3  | 2:H:458:THR:O    | 2.11        | 0.50     |
| 1:U:30:VAL:HG13  | 1:U:43:ALA:HB2   | 1.92        | 0.50     |
| 2:V:317:ASP:OD1  | 2:V:333:LYS:NZ   | 2.45        | 0.50     |
| 2:H:301:THR:HA   | 2:H:333:LYS:NZ   | 2.27        | 0.50     |
| 2:N:341:THR:CG2  | 2:N:404:LEU:HD11 | 2.42        | 0.50     |
| 1:K:48:ARG:HH22  | 1:M:135:ARG:CB   | 2.25        | 0.50     |
| 1:O:226:THR:O    | 1:O:230:LEU:HB2  | 2.11        | 0.50     |
| 1:B:14:ARG:CB    | 1:B:14:ARG:HH11  | 2.13        | 0.50     |
| 1:A:127:VAL:HG21 | 1:A:215:ALA:HB2  | 1.94        | 0.50     |
| 1:D:127:VAL:HG21 | 1:D:215:ALA:HB2  | 1.94        | 0.50     |
| 1:I:182:ARG:HB2  | 1:I:182:ARG:NH1  | 2.26        | 0.50     |
| 1:K:127:VAL:HG11 | 1:K:213:LEU:HB3  | 1.93        | 0.50     |
| 2:T:307:LYS:HE2  | 2:T:435:GLY:HA2  | 1.94        | 0.50     |
| 1:U:127:VAL:HG21 | 1:U:215:ALA:HB2  | 1.94        | 0.49     |
| 2:E:301:THR:HA   | 2:E:333:LYS:NZ   | 2.27        | 0.49     |
| 1:I:56:LEU:HD13  | 1:I:99:LEU:HD22  | 1.94        | 0.49     |
| 2:L:432:GLU:HG3  | 2:L:437:GLN:HB2  | 1.94        | 0.49     |
| 1:A:226:THR:O    | 1:A:230:LEU:HB2  | 2.12        | 0.49     |
| 1:M:155:VAL:HG12 | 1:M:160:THR:HG22 | 1.94        | 0.49     |
| 1:I:70:GLU:HB3   | 1:I:118:TYR:CD2  | 2.47        | 0.49     |
| 2:P:364:GLU:HG2  | 2:P:368:LYS:HE2  | 1.93        | 0.49     |
| 1:W:155:VAL:HG12 | 1:W:160:THR:HG22 | 1.94        | 0.49     |
| 1:Y:185:VAL:HB   | 1:Y:235:VAL:CG1  | 2.42        | 0.49     |
| 2:P:324:ASN:ND2  | 2:P:324:ASN:H    | 2.10        | 0.49     |
| 2:Z:341:THR:CG2  | 2:Z:404:LEU:HD11 | 2.42        | 0.49     |
| 1:K:30:VAL:CG2   | 1:K:65:ALA:HB2   | 2.42        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:R:437:GLN:OE1  | 2:R:447:LYS:HD3  | 2.12        | 0.49     |
| 1:A:63:ALA:O     | 1:A:156:MET:HE1  | 2.12        | 0.49     |
| 2:V:461:ASP:OD1  | 2:V:509:ARG:HD2  | 2.13        | 0.49     |
| 1:D:161:GLU:H    | 1:D:161:GLU:CD   | 2.15        | 0.49     |
| 1:F:85:ARG:NH1   | 1:F:85:ARG:HG2   | 2.24        | 0.49     |
| 2:P:341:THR:HG22 | 2:P:404:LEU:HD11 | 1.93        | 0.49     |
| 1:B:161:GLU:H    | 1:B:161:GLU:CD   | 2.15        | 0.49     |
| 2:C:380:ILE:HD11 | 2:C:421:VAL:HG21 | 1.94        | 0.49     |
| 2:C:309:PRO:HG3  | 2:C:458:THR:O    | 2.11        | 0.49     |
| 2:Z:309:PRO:HG3  | 2:Z:458:THR:O    | 2.12        | 0.49     |
| 1:1:127:VAL:HG21 | 1:1:215:ALA:HB2  | 1.94        | 0.49     |
| 2:X:301:THR:HA   | 2:X:333:LYS:HZ3  | 1.77        | 0.49     |
| 2:C:341:THR:CG2  | 2:C:404:LEU:HD11 | 2.41        | 0.49     |
| 1:Y:76:ARG:NH1   | 2:Z:369:LEU:HD22 | 2.27        | 0.49     |
| 1:S:140:ARG:HH11 | 1:S:140:ARG:HB3  | 1.76        | 0.49     |
| 1:M:161:GLU:CD   | 1:M:161:GLU:H    | 2.14        | 0.49     |
| 1:D:140:ARG:HH11 | 1:D:140:ARG:HB3  | 1.76        | 0.49     |
| 1:W:14:ARG:CB    | 1:W:14:ARG:HH11  | 2.14        | 0.49     |
| 2:P:309:PRO:HG3  | 2:P:458:THR:O    | 2.12        | 0.49     |
| 1:Q:30:VAL:HG13  | 1:Q:43:ALA:HB2   | 1.93        | 0.49     |
| 2:C:301:THR:HA   | 2:C:333:LYS:HZ3  | 1.77        | 0.49     |
| 1:S:147:ILE:HG22 | 3:S:251:HOH:O    | 2.12        | 0.49     |
| 1:U:226:THR:O    | 1:U:230:LEU:HB2  | 2.12        | 0.49     |
| 1:F:127:VAL:CG2  | 1:F:215:ALA:HB2  | 2.42        | 0.49     |
| 1:O:185:VAL:HB   | 1:O:235:VAL:HG11 | 1.93        | 0.49     |
| 1:D:56:LEU:HD13  | 1:D:99:LEU:HD22  | 1.95        | 0.49     |
| 1:W:56:LEU:HD13  | 1:W:99:LEU:HD22  | 1.94        | 0.49     |
| 1:B:20:ALA:O     | 1:B:24:ILE:HG12  | 2.12        | 0.49     |
| 1:I:54:SER:CB    | 1:I:75:ARG:HD2   | 2.42        | 0.49     |
| 1:S:14:ARG:HH11  | 1:S:14:ARG:CB    | 2.13        | 0.49     |
| 1:S:127:VAL:HG11 | 1:S:213:LEU:HB3  | 1.95        | 0.49     |
| 1:I:85:ARG:NH1   | 1:I:85:ARG:HG2   | 2.25        | 0.49     |
| 1:W:185:VAL:HB   | 1:W:235:VAL:HG11 | 1.93        | 0.49     |
| 1:U:185:VAL:HB   | 1:U:235:VAL:CG1  | 2.42        | 0.49     |
| 2:P:464:LEU:HD11 | 2:P:505:VAL:HG11 | 1.95        | 0.49     |
| 2:H:464:LEU:HD11 | 2:H:505:VAL:HG11 | 1.95        | 0.49     |
| 1:W:30:VAL:CG2   | 1:W:65:ALA:HB2   | 2.43        | 0.49     |
| 2:X:341:THR:HG22 | 2:X:404:LEU:HD11 | 1.94        | 0.49     |
| 1:Q:20:ALA:O     | 1:Q:24:ILE:HG12  | 2.13        | 0.49     |
| 1:I:161:GLU:H    | 1:I:161:GLU:CD   | 2.15        | 0.49     |
| 1:O:30:VAL:CG2   | 1:O:65:ALA:HB2   | 2.42        | 0.49     |
| 1:I:185:VAL:HB   | 1:I:235:VAL:CG1  | 2.41        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:71:PHE:HB3   | 1:M:120:VAL:HG11 | 1.94        | 0.49     |
| 2:E:364:GLU:HG2  | 2:E:368:LYS:HE2  | 1.95        | 0.49     |
| 1:S:20:ALA:O     | 1:S:24:ILE:HG12  | 2.13        | 0.49     |
| 2:L:307:LYS:HE2  | 2:L:435:GLY:HA2  | 1.95        | 0.49     |
| 1:S:85:ARG:NH1   | 1:S:85:ARG:HG2   | 2.25        | 0.49     |
| 1:K:71:PHE:HB3   | 1:K:120:VAL:HG11 | 1.94        | 0.49     |
| 1:D:155:VAL:HG12 | 1:D:160:THR:HG22 | 1.94        | 0.49     |
| 1:K:140:ARG:HH11 | 1:K:140:ARG:HB3  | 1.76        | 0.49     |
| 2:X:329:ARG:NH2  | 2:2:476:ASP:O    | 2.45        | 0.49     |
| 2:J:464:LEU:HD11 | 2:J:505:VAL:HG11 | 1.94        | 0.49     |
| 1:I:205:VAL:HG12 | 1:I:206:ALA:N    | 2.27        | 0.49     |
| 2:T:301:THR:HA   | 2:T:333:LYS:NZ   | 2.28        | 0.49     |
| 1:F:155:VAL:HG12 | 1:F:160:THR:HG22 | 1.94        | 0.49     |
| 1:S:155:VAL:HG12 | 1:S:160:THR:HG22 | 1.95        | 0.49     |
| 2:R:364:GLU:HG2  | 2:R:368:LYS:HE2  | 1.95        | 0.49     |
| 1:I:155:VAL:HG12 | 1:I:160:THR:HG22 | 1.93        | 0.49     |
| 2:L:393:ALA:HB2  | 3:L:166:HOH:O    | 2.13        | 0.49     |
| 1:F:85:ARG:HH11  | 1:F:85:ARG:CG    | 2.23        | 0.48     |
| 2:X:337:THR:HG21 | 2:X:359:TYR:CD2  | 2.48        | 0.48     |
| 2:R:324:ASN:H    | 2:R:324:ASN:ND2  | 2.11        | 0.48     |
| 2:N:449:SER:HB2  | 2:V:452:LYS:HZ1  | 1.77        | 0.48     |
| 1:D:205:VAL:HG12 | 1:D:206:ALA:N    | 2.27        | 0.48     |
| 2:P:301:THR:HA   | 2:P:333:LYS:NZ   | 2.28        | 0.48     |
| 2:X:432:GLU:HG3  | 2:X:437:GLN:HB2  | 1.95        | 0.48     |
| 1:K:155:VAL:HG12 | 1:K:160:THR:HG22 | 1.95        | 0.48     |
| 1:D:54:SER:CB    | 1:D:75:ARG:HD2   | 2.43        | 0.48     |
| 1:Y:42:VAL:HG22  | 1:Y:210:VAL:HG22 | 1.95        | 0.48     |
| 1:A:54:SER:CB    | 1:A:75:ARG:HD2   | 2.42        | 0.48     |
| 1:O:141:ILE:N    | 1:O:141:ILE:HD12 | 2.28        | 0.48     |
| 1:W:151:PRO:HD2  | 3:W:253:HOH:O    | 2.12        | 0.48     |
| 1:S:85:ARG:HH11  | 1:S:85:ARG:CG    | 2.25        | 0.48     |
| 2:P:456:GLN:HE22 | 2:P:465:ARG:NH1  | 2.10        | 0.48     |
| 1:B:56:LEU:HD13  | 1:B:99:LEU:HD22  | 1.96        | 0.48     |
| 2:X:437:GLN:OE1  | 2:X:447:LYS:HD3  | 2.13        | 0.48     |
| 2:V:485:ASP:OD2  | 2:V:488:ARG:HB2  | 2.13        | 0.48     |
| 1:A:172:ALA:HB3  | 1:A:175:ALA:HB2  | 1.95        | 0.48     |
| 2:G:324:ASN:H    | 2:G:324:ASN:HD22 | 1.59        | 0.48     |
| 2:N:461:ASP:OD1  | 2:N:509:ARG:HD2  | 2.13        | 0.48     |
| 1:I:185:VAL:HB   | 1:I:235:VAL:HG11 | 1.95        | 0.48     |
| 1:O:89:TYR:HD1   | 2:V:382:ARG:HD3  | 1.77        | 0.48     |
| 1:1:30:VAL:CG2   | 1:1:65:ALA:HB2   | 2.43        | 0.48     |
| 1:Y:54:SER:CB    | 1:Y:75:ARG:HD2   | 2.43        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:C:432:GLU:HG3  | 2:C:437:GLN:HB2  | 1.95        | 0.48     |
| 2:J:382:ARG:HD3  | 1:S:89:TYR:HD1   | 1.74        | 0.48     |
| 2:J:436:TYR:CD1  | 2:J:436:TYR:N    | 2.81        | 0.48     |
| 1:Q:127:VAL:HG21 | 1:Q:215:ALA:HB2  | 1.95        | 0.48     |
| 2:C:337:THR:HG21 | 2:C:359:TYR:CD2  | 2.49        | 0.48     |
| 2:X:464:LEU:HD11 | 2:X:505:VAL:HG11 | 1.95        | 0.48     |
| 2:2:337:THR:HG21 | 2:2:359:TYR:CD2  | 2.49        | 0.48     |
| 1:K:182:ARG:HD3  | 1:K:235:VAL:CB   | 2.43        | 0.48     |
| 1:U:185:VAL:HB   | 1:U:235:VAL:HG11 | 1.95        | 0.48     |
| 1:M:28:LYS:HB2   | 3:M:253:HOH:O    | 2.14        | 0.48     |
| 1:W:30:VAL:HG13  | 1:W:43:ALA:HB2   | 1.95        | 0.48     |
| 1:Y:30:VAL:CG2   | 1:Y:65:ALA:HB2   | 2.43        | 0.48     |
| 1:W:20:ALA:O     | 1:W:24:ILE:HG12  | 2.13        | 0.48     |
| 2:J:449:SER:HB2  | 2:Z:452:LYS:HZ1  | 1.77        | 0.48     |
| 2:Z:436:TYR:CD1  | 2:Z:436:TYR:N    | 2.81        | 0.48     |
| 1:M:185:VAL:HB   | 1:M:235:VAL:CG1  | 2.44        | 0.48     |
| 1:M:127:VAL:HG11 | 1:M:213:LEU:HB3  | 1.96        | 0.48     |
| 1:S:205:VAL:HG12 | 1:S:206:ALA:N    | 2.28        | 0.48     |
| 1:Y:140:ARG:HB3  | 1:Y:140:ARG:HH11 | 1.77        | 0.48     |
| 1:B:141:ILE:N    | 1:B:141:ILE:HD12 | 2.29        | 0.48     |
| 1:M:182:ARG:HD3  | 1:M:235:VAL:CB   | 2.44        | 0.48     |
| 2:J:324:ASN:N    | 2:J:324:ASN:HD22 | 2.09        | 0.48     |
| 1:F:30:VAL:CG2   | 1:F:65:ALA:HB2   | 2.43        | 0.48     |
| 2:2:307:LYS:HE2  | 2:2:435:GLY:HA2  | 1.95        | 0.48     |
| 1:O:140:ARG:HH11 | 1:O:140:ARG:HB3  | 1.78        | 0.48     |
| 1:B:182:ARG:HD3  | 1:B:235:VAL:CB   | 2.44        | 0.48     |
| 1:1:30:VAL:HG13  | 1:1:43:ALA:HB2   | 1.95        | 0.48     |
| 2:L:309:PRO:HG3  | 2:L:458:THR:O    | 2.14        | 0.48     |
| 2:C:317:ASP:OD1  | 2:C:333:LYS:NZ   | 2.46        | 0.48     |
| 1:K:141:ILE:HD12 | 1:K:141:ILE:N    | 2.28        | 0.48     |
| 1:Y:205:VAL:HG12 | 1:Y:206:ALA:N    | 2.29        | 0.48     |
| 1:B:205:VAL:HG12 | 1:B:206:ALA:N    | 2.29        | 0.48     |
| 2:N:301:THR:HA   | 2:N:333:LYS:NZ   | 2.29        | 0.48     |
| 1:K:54:SER:CB    | 1:K:75:ARG:HD2   | 2.43        | 0.48     |
| 2:Z:432:GLU:HG3  | 2:Z:437:GLN:HB2  | 1.96        | 0.48     |
| 2:T:364:GLU:HG2  | 2:T:368:LYS:HE2  | 1.96        | 0.48     |
| 1:Q:161:GLU:H    | 1:Q:161:GLU:CD   | 2.18        | 0.48     |
| 1:F:140:ARG:HB3  | 1:F:140:ARG:HH11 | 1.79        | 0.48     |
| 2:2:456:GLN:HE22 | 2:2:465:ARG:NH1  | 2.12        | 0.47     |
| 1:O:127:VAL:HG21 | 1:O:215:ALA:HB2  | 1.96        | 0.47     |
| 2:H:391:LEU:CD1  | 2:C:398:LEU:HD21 | 2.44        | 0.47     |
| 1:D:20:ALA:O     | 1:D:24:ILE:HG12  | 2.14        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:U:83:ASP:OD2   | 2:V:365:HIS:HD2  | 1.96        | 0.47     |
| 2:L:388:ARG:C    | 2:L:390:ASN:H    | 2.17        | 0.47     |
| 1:U:10:GLU:HA    | 1:1:19:LEU:HD12  | 1.95        | 0.47     |
| 2:L:301:THR:HA   | 2:L:333:LYS:NZ   | 2.29        | 0.47     |
| 1:Y:127:VAL:HG21 | 1:Y:215:ALA:HB2  | 1.95        | 0.47     |
| 2:X:309:PRO:HG3  | 2:X:458:THR:O    | 2.14        | 0.47     |
| 2:H:436:TYR:N    | 2:H:436:TYR:HD1  | 2.12        | 0.47     |
| 1:Q:30:VAL:HG22  | 1:Q:43:ALA:CB    | 2.44        | 0.47     |
| 1:D:127:VAL:HG11 | 1:D:213:LEU:HB3  | 1.96        | 0.47     |
| 1:Y:185:VAL:HB   | 1:Y:235:VAL:HG11 | 1.96        | 0.47     |
| 2:L:320:SER:HB3  | 2:L:328:GLY:HA3  | 1.96        | 0.47     |
| 1:U:30:VAL:CG2   | 1:U:65:ALA:HB2   | 2.44        | 0.47     |
| 1:Y:30:VAL:HG13  | 1:Y:43:ALA:HB2   | 1.95        | 0.47     |
| 1:S:73:ASN:HD22  | 1:1:105:GLN:CD   | 2.17        | 0.47     |
| 1:Y:20:ALA:O     | 1:Y:24:ILE:HG12  | 2.14        | 0.47     |
| 2:2:412:SER:HB2  | 3:2:97:HOH:O     | 2.14        | 0.47     |
| 2:T:321:THR:HG21 | 2:T:480:ALA:HB1  | 1.96        | 0.47     |
| 2:2:349:ALA:HB1  | 3:2:22:HOH:O     | 2.14        | 0.47     |
| 2:H:324:ASN:H    | 2:H:324:ASN:ND2  | 2.11        | 0.47     |
| 1:F:48:ARG:HH22  | 1:W:135:ARG:CB   | 2.27        | 0.47     |
| 1:B:172:ALA:HB3  | 1:B:175:ALA:HB2  | 1.95        | 0.47     |
| 2:Z:321:THR:HG21 | 2:Z:480:ALA:HB1  | 1.95        | 0.47     |
| 1:U:161:GLU:CD   | 1:U:161:GLU:H    | 2.17        | 0.47     |
| 2:C:450:MET:HE3  | 2:C:470:ALA:CB   | 2.44        | 0.47     |
| 1:B:182:ARG:HB2  | 1:B:182:ARG:NH1  | 2.30        | 0.47     |
| 2:2:324:ASN:N    | 2:2:324:ASN:HD22 | 2.12        | 0.47     |
| 2:P:301:THR:HA   | 2:P:333:LYS:HZ3  | 1.79        | 0.47     |
| 1:K:20:ALA:O     | 1:K:24:ILE:HG12  | 2.14        | 0.47     |
| 2:L:380:ILE:HD11 | 2:L:421:VAL:HG21 | 1.97        | 0.47     |
| 2:P:514:ALA:O    | 2:P:518:ILE:HG13 | 2.15        | 0.47     |
| 1:Q:105:GLN:CD   | 1:Y:73:ASN:HD22  | 2.18        | 0.47     |
| 1:M:140:ARG:HB3  | 1:M:140:ARG:HH11 | 1.79        | 0.47     |
| 1:A:140:ARG:HH11 | 1:A:140:ARG:HB3  | 1.80        | 0.47     |
| 1:A:85:ARG:NH1   | 1:A:85:ARG:HG2   | 2.23        | 0.47     |
| 1:1:205:VAL:HG12 | 1:1:206:ALA:H    | 1.78        | 0.47     |
| 1:A:99:LEU:HD12  | 1:A:99:LEU:H     | 1.80        | 0.47     |
| 1:F:172:ALA:HB3  | 1:F:175:ALA:HB2  | 1.95        | 0.47     |
| 2:X:364:GLU:HG2  | 2:X:368:LYS:HE2  | 1.96        | 0.47     |
| 1:O:85:ARG:HH11  | 1:O:85:ARG:CG    | 2.22        | 0.47     |
| 1:I:28:LYS:HB2   | 1:I:52:LYS:HZ2   | 1.79        | 0.47     |
| 1:F:182:ARG:NH1  | 1:F:182:ARG:HB2  | 2.29        | 0.47     |
| 1:Y:182:ARG:HD3  | 1:Y:235:VAL:CB   | 2.45        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:515:ARG:CD   | 3:H:114:HOH:O    | 2.63        | 0.47     |
| 1:K:185:VAL:HB   | 1:K:235:VAL:HG11 | 1.94        | 0.47     |
| 1:D:12:ALA:O     | 1:D:16:ARG:HG2   | 2.15        | 0.47     |
| 1:K:205:VAL:HG12 | 1:K:206:ALA:N    | 2.29        | 0.47     |
| 1:U:30:VAL:HG22  | 1:U:43:ALA:CB    | 2.45        | 0.47     |
| 2:C:324:ASN:N    | 2:C:324:ASN:HD22 | 2.12        | 0.47     |
| 2:G:301:THR:N    | 2:G:441:SER:HG   | 2.13        | 0.47     |
| 1:K:19:LEU:HD12  | 1:M:10:GLU:HA    | 1.97        | 0.47     |
| 1:W:63:ALA:O     | 1:W:156:MET:HE1  | 2.14        | 0.47     |
| 2:N:432:GLU:HG3  | 2:N:437:GLN:HB2  | 1.96        | 0.47     |
| 2:L:374:LEU:HD22 | 1:M:93:ASP:OD2   | 2.15        | 0.47     |
| 2:2:461:ASP:OD1  | 2:2:509:ARG:HD2  | 2.14        | 0.47     |
| 2:X:514:ALA:O    | 2:X:518:ILE:HG13 | 2.14        | 0.47     |
| 2:L:321:THR:HG21 | 2:L:480:ALA:HB1  | 1.97        | 0.47     |
| 1:A:161:GLU:H    | 1:A:161:GLU:CD   | 2.17        | 0.47     |
| 2:T:329:ARG:NH2  | 2:Z:476:ASP:O    | 2.46        | 0.47     |
| 2:L:324:ASN:HD22 | 2:L:324:ASN:N    | 2.12        | 0.47     |
| 1:D:172:ALA:HB3  | 1:D:175:ALA:HB2  | 1.97        | 0.47     |
| 2:V:432:GLU:HG3  | 2:V:437:GLN:HB2  | 1.95        | 0.47     |
| 1:S:63:ALA:O     | 1:S:156:MET:HE1  | 2.15        | 0.47     |
| 1:Y:85:ARG:HH11  | 1:Y:85:ARG:CG    | 2.21        | 0.47     |
| 2:E:337:THR:HG21 | 2:E:359:TYR:CD2  | 2.49        | 0.47     |
| 1:U:54:SER:CB    | 1:U:75:ARG:HD2   | 2.44        | 0.47     |
| 2:2:437:GLN:OE1  | 2:2:447:LYS:HD3  | 2.14        | 0.47     |
| 1:K:14:ARG:CB    | 1:K:14:ARG:HH11  | 2.13        | 0.47     |
| 1:O:205:VAL:HG12 | 1:O:206:ALA:H    | 1.80        | 0.47     |
| 1:F:56:LEU:HD13  | 1:F:99:LEU:HD22  | 1.96        | 0.47     |
| 1:W:42:VAL:HG22  | 1:W:210:VAL:HG22 | 1.96        | 0.47     |
| 1:1:63:ALA:O     | 1:1:156:MET:HE1  | 2.15        | 0.47     |
| 2:T:432:GLU:HG3  | 2:T:437:GLN:HB2  | 1.97        | 0.47     |
| 2:H:437:GLN:OE1  | 2:H:447:LYS:HD3  | 2.15        | 0.47     |
| 1:S:70:GLU:HB3   | 1:S:118:TYR:CD2  | 2.50        | 0.47     |
| 1:Y:129:HIS:HD2  | 3:Y:251:HOH:O    | 1.98        | 0.46     |
| 1:O:43:ALA:HA    | 3:O:250:HOH:O    | 2.15        | 0.46     |
| 2:N:337:THR:HG21 | 2:N:359:TYR:CD2  | 2.50        | 0.46     |
| 1:M:30:VAL:CG2   | 1:M:65:ALA:HB2   | 2.44        | 0.46     |
| 2:2:496:ILE:O    | 2:2:502:ALA:HA   | 2.14        | 0.46     |
| 1:K:127:VAL:HG21 | 1:K:215:ALA:HB2  | 1.96        | 0.46     |
| 2:H:436:TYR:CD1  | 2:H:436:TYR:N    | 2.82        | 0.46     |
| 1:F:127:VAL:HG21 | 1:F:215:ALA:HB2  | 1.96        | 0.46     |
| 1:S:30:VAL:HG22  | 1:S:43:ALA:CB    | 2.46        | 0.46     |
| 1:D:30:VAL:HG13  | 1:D:43:ALA:HB2   | 1.96        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:Y:56:LEU:HD13  | 1:Y:99:LEU:HD22  | 1.97        | 0.46     |
| 2:2:317:ASP:HB2  | 3:2:50:HOH:O     | 2.14        | 0.46     |
| 2:2:432:GLU:HG3  | 2:2:437:GLN:HB2  | 1.96        | 0.46     |
| 1:I:63:ALA:O     | 1:I:156:MET:HE1  | 2.16        | 0.46     |
| 1:F:182:ARG:HD3  | 1:F:235:VAL:CB   | 2.43        | 0.46     |
| 2:Z:337:THR:HG21 | 2:Z:359:TYR:CD2  | 2.51        | 0.46     |
| 1:O:63:ALA:O     | 1:O:156:MET:HE1  | 2.15        | 0.46     |
| 1:O:70:GLU:HB3   | 1:O:118:TYR:CD2  | 2.51        | 0.46     |
| 1:U:157:GLY:N    | 3:U:250:HOH:O    | 2.48        | 0.46     |
| 2:T:375:THR:N    | 3:1:252:HOH:O    | 2.45        | 0.46     |
| 1:U:55:GLU:OE2   | 1:U:220:ARG:CD   | 2.64        | 0.46     |
| 1:M:76:ARG:HG2   | 2:N:369:LEU:CD2  | 2.46        | 0.46     |
| 2:R:496:ILE:O    | 2:R:502:ALA:HA   | 2.15        | 0.46     |
| 1:F:205:VAL:HG12 | 1:F:206:ALA:N    | 2.30        | 0.46     |
| 2:V:324:ASN:H    | 2:V:324:ASN:ND2  | 2.13        | 0.46     |
| 1:Q:127:VAL:HG11 | 1:Q:213:LEU:HB3  | 1.97        | 0.46     |
| 2:V:485:ASP:OD2  | 2:V:488:ARG:CB   | 2.64        | 0.46     |
| 2:V:455:SER:HB3  | 3:V:51:HOH:O     | 2.14        | 0.46     |
| 2:J:388:ARG:C    | 2:J:390:ASN:H    | 2.19        | 0.46     |
| 1:K:47:SER:HA    | 3:K:256:HOH:O    | 2.16        | 0.46     |
| 1:D:226:THR:O    | 1:D:230:LEU:HB2  | 2.14        | 0.46     |
| 1:Y:141:ILE:N    | 1:Y:141:ILE:HD12 | 2.30        | 0.46     |
| 1:F:161:GLU:H    | 1:F:161:GLU:CD   | 2.18        | 0.46     |
| 1:A:55:GLU:OE2   | 1:A:220:ARG:CD   | 2.64        | 0.46     |
| 2:P:337:THR:HG21 | 2:P:359:TYR:CD2  | 2.51        | 0.46     |
| 1:I:28:LYS:HE2   | 1:I:46:PRO:HD3   | 1.97        | 0.46     |
| 1:B:85:ARG:HG2   | 1:B:85:ARG:NH1   | 2.29        | 0.46     |
| 2:J:324:ASN:ND2  | 2:J:324:ASN:H    | 2.11        | 0.46     |
| 1:1:160:THR:HG23 | 3:1:259:HOH:O    | 2.14        | 0.46     |
| 1:K:172:ALA:HB3  | 1:K:175:ALA:HB2  | 1.97        | 0.46     |
| 1:S:127:VAL:CG2  | 1:S:215:ALA:HB2  | 2.46        | 0.46     |
| 1:W:85:ARG:NH1   | 1:W:85:ARG:HG2   | 2.26        | 0.46     |
| 2:2:436:TYR:CD1  | 2:2:436:TYR:N    | 2.84        | 0.46     |
| 1:F:127:VAL:HG11 | 1:F:213:LEU:HB3  | 1.98        | 0.46     |
| 1:O:182:ARG:NH1  | 1:O:182:ARG:HB2  | 2.30        | 0.46     |
| 2:H:412:SER:O    | 2:H:414:PRO:HD3  | 2.16        | 0.46     |
| 2:G:432:GLU:HG3  | 2:G:437:GLN:HB2  | 1.97        | 0.46     |
| 2:R:514:ALA:O    | 2:R:518:ILE:HG13 | 2.16        | 0.46     |
| 1:M:55:GLU:OE2   | 1:M:220:ARG:CD   | 2.64        | 0.46     |
| 1:U:127:VAL:HG11 | 1:U:213:LEU:HB3  | 1.97        | 0.46     |
| 2:J:496:ILE:O    | 2:J:502:ALA:HA   | 2.16        | 0.46     |
| 1:Q:182:ARG:NH1  | 1:Q:182:ARG:HB2  | 2.31        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:M:205:VAL:HG12 | 1:M:206:ALA:H    | 1.80        | 0.46     |
| 2:Z:514:ALA:O    | 2:Z:518:ILE:HG13 | 2.15        | 0.46     |
| 2:N:514:ALA:O    | 2:N:518:ILE:HG13 | 2.15        | 0.46     |
| 2:G:317:ASP:HB2  | 3:G:109:HOH:O    | 2.16        | 0.46     |
| 1:A:48:ARG:HD2   | 1:B:137:GLU:CD   | 2.36        | 0.46     |
| 1:Q:85:ARG:NH1   | 1:Q:85:ARG:HG2   | 2.25        | 0.46     |
| 1:M:30:VAL:HG22  | 1:M:43:ALA:CB    | 2.46        | 0.46     |
| 1:W:28:LYS:HE2   | 1:W:46:PRO:HD3   | 1.97        | 0.46     |
| 1:I:140:ARG:HH11 | 1:I:140:ARG:HB3  | 1.80        | 0.46     |
| 1:A:48:ARG:HD2   | 1:B:137:GLU:OE2  | 2.15        | 0.46     |
| 1:B:55:GLU:OE2   | 1:B:220:ARG:CD   | 2.64        | 0.46     |
| 2:V:436:TYR:CD1  | 2:V:436:TYR:N    | 2.84        | 0.46     |
| 2:Z:301:THR:HA   | 2:Z:333:LYS:HZ3  | 1.81        | 0.46     |
| 2:L:301:THR:N    | 2:L:441:SER:HG   | 2.14        | 0.46     |
| 1:Y:172:ALA:HB3  | 1:Y:175:ALA:HB2  | 1.98        | 0.46     |
| 2:R:388:ARG:C    | 2:R:390:ASN:H    | 2.19        | 0.46     |
| 1:K:70:GLU:HB3   | 1:K:118:TYR:CD2  | 2.51        | 0.46     |
| 1:Q:83:ASP:OD2   | 2:R:365:HIS:HD2  | 1.98        | 0.46     |
| 1:F:137:GLU:CD   | 1:M:48:ARG:HD2   | 2.36        | 0.46     |
| 2:2:324:ASN:ND2  | 2:2:324:ASN:H    | 2.13        | 0.46     |
| 1:S:30:VAL:HG23  | 1:S:65:ALA:HB2   | 1.98        | 0.46     |
| 1:Y:30:VAL:HG22  | 1:Y:43:ALA:CB    | 2.46        | 0.46     |
| 2:L:317:ASP:OD1  | 2:L:333:LYS:NZ   | 2.47        | 0.46     |
| 1:S:172:ALA:HB3  | 1:S:175:ALA:HB2  | 1.97        | 0.46     |
| 2:X:388:ARG:C    | 2:X:390:ASN:H    | 2.20        | 0.46     |
| 1:S:141:ILE:HD12 | 1:S:141:ILE:N    | 2.31        | 0.46     |
| 1:K:55:GLU:OE2   | 1:K:220:ARG:CD   | 2.63        | 0.46     |
| 1:W:182:ARG:HD3  | 1:W:235:VAL:CB   | 2.46        | 0.46     |
| 1:U:182:ARG:HD3  | 1:U:235:VAL:CB   | 2.46        | 0.46     |
| 1:Q:30:VAL:CG2   | 1:Q:65:ALA:HB2   | 2.46        | 0.46     |
| 2:Z:496:ILE:O    | 2:Z:502:ALA:HA   | 2.16        | 0.46     |
| 1:K:56:LEU:HD13  | 1:K:99:LEU:HD22  | 1.98        | 0.46     |
| 2:G:301:THR:HA   | 2:G:333:LYS:HZ2  | 1.81        | 0.46     |
| 2:P:485:ASP:OD2  | 2:P:488:ARG:HB2  | 2.16        | 0.46     |
| 1:B:83:ASP:OD2   | 2:C:365:HIS:HD2  | 1.99        | 0.46     |
| 2:V:309:PRO:HG3  | 2:V:458:THR:O    | 2.16        | 0.45     |
| 1:F:137:GLU:OE2  | 1:M:48:ARG:HD2   | 2.16        | 0.45     |
| 2:L:496:ILE:O    | 2:L:502:ALA:HA   | 2.16        | 0.45     |
| 1:Y:28:LYS:HE2   | 1:Y:46:PRO:HD3   | 1.97        | 0.45     |
| 2:L:324:ASN:ND2  | 2:L:324:ASN:H    | 2.14        | 0.45     |
| 1:D:30:VAL:CG2   | 1:D:65:ALA:HB2   | 2.46        | 0.45     |
| 2:J:317:ASP:OD1  | 2:J:333:LYS:NZ   | 2.49        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:Q:70:GLU:HB3   | 1:Q:118:TYR:CD2  | 2.51        | 0.45     |
| 1:F:54:SER:CB    | 1:F:75:ARG:HD2   | 2.46        | 0.45     |
| 1:U:205:VAL:HG12 | 1:U:206:ALA:H    | 1.79        | 0.45     |
| 1:U:56:LEU:HD13  | 1:U:99:LEU:HD22  | 1.97        | 0.45     |
| 1:F:30:VAL:HG22  | 1:F:43:ALA:CB    | 2.46        | 0.45     |
| 2:V:307:LYS:HE2  | 2:V:435:GLY:HA2  | 1.98        | 0.45     |
| 2:E:388:ARG:C    | 2:E:390:ASN:H    | 2.20        | 0.45     |
| 1:D:135:ARG:CB   | 1:Q:48:ARG:HH22  | 2.29        | 0.45     |
| 2:J:432:GLU:HG3  | 2:J:437:GLN:HB2  | 1.97        | 0.45     |
| 1:F:141:ILE:N    | 1:F:141:ILE:HD12 | 2.30        | 0.45     |
| 2:V:309:PRO:O    | 2:V:415:GLN:HG2  | 2.16        | 0.45     |
| 1:B:127:VAL:HG11 | 1:B:213:LEU:HB3  | 1.97        | 0.45     |
| 1:O:127:VAL:HG11 | 1:O:213:LEU:HB3  | 1.97        | 0.45     |
| 2:C:496:ILE:O    | 2:C:502:ALA:HA   | 2.16        | 0.45     |
| 2:C:437:GLN:OE1  | 2:C:447:LYS:HD3  | 2.16        | 0.45     |
| 2:2:388:ARG:C    | 2:2:390:ASN:H    | 2.19        | 0.45     |
| 1:1:172:ALA:HB3  | 1:1:175:ALA:HB2  | 1.98        | 0.45     |
| 1:I:71:PHE:HB3   | 1:I:120:VAL:HG11 | 1.97        | 0.45     |
| 2:N:301:THR:HG23 | 2:N:333:LYS:HD3  | 1.98        | 0.45     |
| 1:U:135:ARG:CB   | 1:1:48:ARG:HH22  | 2.29        | 0.45     |
| 1:U:135:ARG:HB3  | 1:1:48:ARG:HH22  | 1.80        | 0.45     |
| 2:G:307:LYS:HE2  | 2:G:435:GLY:HA2  | 1.97        | 0.45     |
| 2:E:432:GLU:HG3  | 2:E:437:GLN:HB2  | 1.99        | 0.45     |
| 2:L:337:THR:OG1  | 2:L:343:THR:CG2  | 2.60        | 0.45     |
| 2:G:337:THR:HG21 | 2:G:359:TYR:CD2  | 2.51        | 0.45     |
| 1:I:182:ARG:HD3  | 1:I:235:VAL:CB   | 2.43        | 0.45     |
| 2:T:309:PRO:HG3  | 2:T:458:THR:O    | 2.17        | 0.45     |
| 2:2:301:THR:HA   | 2:2:333:LYS:HZ3  | 1.82        | 0.45     |
| 2:T:437:GLN:OE1  | 2:T:447:LYS:HD3  | 2.17        | 0.45     |
| 1:Y:63:ALA:O     | 1:Y:156:MET:HE1  | 2.17        | 0.45     |
| 1:A:85:ARG:CG    | 1:A:85:ARG:HH11  | 2.25        | 0.45     |
| 2:V:337:THR:HG21 | 2:V:359:TYR:CD2  | 2.52        | 0.45     |
| 1:W:127:VAL:HG11 | 1:W:213:LEU:HB3  | 1.99        | 0.45     |
| 1:S:182:ARG:HB2  | 1:S:182:ARG:NH1  | 2.32        | 0.45     |
| 1:I:30:VAL:HG22  | 1:I:43:ALA:CB    | 2.47        | 0.45     |
| 1:D:30:VAL:HG22  | 1:D:43:ALA:CB    | 2.46        | 0.45     |
| 2:R:436:TYR:N    | 2:R:436:TYR:CD1  | 2.83        | 0.45     |
| 1:F:115:ALA:HB3  | 1:W:112:THR:HG23 | 1.97        | 0.45     |
| 1:S:28:LYS:HE2   | 1:S:46:PRO:HD3   | 1.99        | 0.45     |
| 2:E:324:ASN:H    | 2:E:324:ASN:ND2  | 2.14        | 0.45     |
| 2:L:452:LYS:HZ3  | 2:P:449:SER:HB2  | 1.81        | 0.45     |
| 2:T:324:ASN:ND2  | 2:T:324:ASN:H    | 2.15        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:R:301:THR:HA   | 2:R:333:LYS:HZ2  | 1.81        | 0.45     |
| 1:A:223:ARG:NH1  | 3:A:249:HOH:O    | 2.50        | 0.45     |
| 1:S:54:SER:CB    | 1:S:75:ARG:HD2   | 2.47        | 0.45     |
| 2:X:318:ARG:HD2  | 2:X:492:PRO:HA   | 1.99        | 0.45     |
| 2:E:436:TYR:CD1  | 2:E:436:TYR:N    | 2.85        | 0.45     |
| 2:Z:317:ASP:OD1  | 2:Z:333:LYS:NZ   | 2.50        | 0.45     |
| 2:H:317:ASP:OD1  | 2:H:333:LYS:NZ   | 2.47        | 0.45     |
| 2:H:307:LYS:HE2  | 2:H:435:GLY:HA2  | 1.99        | 0.45     |
| 1:U:141:ILE:N    | 1:U:141:ILE:HD12 | 2.31        | 0.45     |
| 1:B:70:GLU:HB3   | 1:B:118:TYR:CD2  | 2.52        | 0.45     |
| 2:G:496:ILE:O    | 2:G:502:ALA:HA   | 2.17        | 0.45     |
| 1:1:182:ARG:NH1  | 1:1:182:ARG:HB2  | 2.31        | 0.45     |
| 1:S:176:SER:HA   | 3:S:252:HOH:O    | 2.15        | 0.45     |
| 2:Z:324:ASN:H    | 2:Z:324:ASN:ND2  | 2.15        | 0.45     |
| 2:N:437:GLN:OE1  | 2:N:447:LYS:HD3  | 2.17        | 0.45     |
| 1:M:141:ILE:N    | 1:M:141:ILE:HD12 | 2.32        | 0.45     |
| 2:G:320:SER:HB3  | 2:G:328:GLY:HA3  | 1.99        | 0.45     |
| 1:Y:182:ARG:NH1  | 1:Y:182:ARG:HB2  | 2.32        | 0.45     |
| 1:U:28:LYS:HE2   | 1:U:46:PRO:HD3   | 1.99        | 0.45     |
| 1:Q:205:VAL:HG12 | 1:Q:206:ALA:H    | 1.82        | 0.45     |
| 1:Q:54:SER:CB    | 1:Q:75:ARG:HD2   | 2.47        | 0.45     |
| 2:P:307:LYS:HE2  | 2:P:435:GLY:HA2  | 1.99        | 0.45     |
| 2:E:307:LYS:HE2  | 2:E:435:GLY:HA2  | 1.99        | 0.45     |
| 2:P:432:GLU:HG3  | 2:P:437:GLN:HB2  | 1.99        | 0.45     |
| 1:1:55:GLU:OE2   | 1:1:220:ARG:CD   | 2.66        | 0.44     |
| 1:M:185:VAL:HB   | 1:M:235:VAL:HG11 | 1.98        | 0.44     |
| 1:Q:182:ARG:HD3  | 1:Q:235:VAL:CB   | 2.46        | 0.44     |
| 1:U:182:ARG:HB2  | 1:U:182:ARG:NH1  | 2.32        | 0.44     |
| 1:1:127:VAL:HG11 | 1:1:213:LEU:HB3  | 2.00        | 0.44     |
| 1:W:205:VAL:HG12 | 1:W:206:ALA:H    | 1.83        | 0.44     |
| 2:V:324:ASN:N    | 2:V:324:ASN:HD22 | 2.12        | 0.44     |
| 2:C:324:ASN:H    | 2:C:324:ASN:ND2  | 2.14        | 0.44     |
| 1:F:71:PHE:HB3   | 1:F:120:VAL:HG11 | 1.99        | 0.44     |
| 2:L:469:GLU:HG3  | 2:L:517:ILE:HG21 | 1.98        | 0.44     |
| 1:F:97:ARG:HG3   | 1:M:49:SER:HB2   | 1.98        | 0.44     |
| 2:V:380:ILE:HD11 | 2:V:421:VAL:HG21 | 1.99        | 0.44     |
| 2:T:436:TYR:N    | 2:T:436:TYR:HD1  | 2.15        | 0.44     |
| 1:1:28:LYS:HE2   | 1:1:46:PRO:HD3   | 1.99        | 0.44     |
| 2:P:496:ILE:O    | 2:P:502:ALA:HA   | 2.17        | 0.44     |
| 1:M:28:LYS:HE2   | 1:M:46:PRO:HD3   | 2.00        | 0.44     |
| 2:V:496:ILE:O    | 2:V:502:ALA:HA   | 2.18        | 0.44     |
| 1:1:71:PHE:HB3   | 1:1:120:VAL:HG11 | 1.98        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:W:30:VAL:HG22  | 1:W:43:ALA:CB    | 2.47        | 0.44     |
| 1:B:134:LYS:NZ   | 3:B:254:HOH:O    | 2.51        | 0.44     |
| 2:R:432:GLU:HG3  | 2:R:437:GLN:HB2  | 1.99        | 0.44     |
| 2:V:437:GLN:OE1  | 2:V:447:LYS:HD3  | 2.16        | 0.44     |
| 2:X:485:ASP:OD2  | 2:X:488:ARG:HB2  | 2.17        | 0.44     |
| 1:A:182:ARG:HB2  | 1:A:182:ARG:NH1  | 2.32        | 0.44     |
| 1:A:56:LEU:HD13  | 1:A:99:LEU:HD22  | 1.99        | 0.44     |
| 2:N:307:LYS:HE2  | 2:N:435:GLY:HA2  | 1.99        | 0.44     |
| 1:O:172:ALA:HB3  | 1:O:175:ALA:HB2  | 1.99        | 0.44     |
| 1:M:182:ARG:HB2  | 1:M:182:ARG:NH1  | 2.33        | 0.44     |
| 1:M:63:ALA:O     | 1:M:156:MET:HE1  | 2.18        | 0.44     |
| 2:H:515:ARG:HD3  | 3:H:114:HOH:O    | 2.17        | 0.44     |
| 2:R:309:PRO:HG3  | 2:R:458:THR:O    | 2.17        | 0.44     |
| 1:1:30:VAL:HG22  | 1:1:43:ALA:CB    | 2.47        | 0.44     |
| 2:2:321:THR:HG21 | 2:2:480:ALA:HB1  | 1.98        | 0.44     |
| 2:2:320:SER:HB3  | 2:2:328:GLY:HA3  | 1.98        | 0.44     |
| 2:L:436:TYR:N    | 2:L:436:TYR:CD1  | 2.84        | 0.44     |
| 2:L:437:GLN:OE1  | 2:L:447:LYS:HD3  | 2.18        | 0.44     |
| 1:W:172:ALA:HB3  | 1:W:175:ALA:HB2  | 1.99        | 0.44     |
| 1:A:70:GLU:HB3   | 1:A:118:TYR:CD2  | 2.52        | 0.44     |
| 1:S:182:ARG:HD3  | 1:S:235:VAL:CB   | 2.46        | 0.44     |
| 2:C:436:TYR:CD1  | 2:C:436:TYR:N    | 2.85        | 0.44     |
| 2:E:496:ILE:O    | 2:E:502:ALA:HA   | 2.18        | 0.44     |
| 2:H:432:GLU:HG3  | 2:H:437:GLN:HB2  | 1.99        | 0.44     |
| 2:N:321:THR:HG21 | 2:N:480:ALA:HB1  | 1.99        | 0.44     |
| 1:D:79:ILE:HD12  | 2:E:369:LEU:HD23 | 1.99        | 0.44     |
| 1:Q:172:ALA:HB3  | 1:Q:175:ALA:HB2  | 2.00        | 0.44     |
| 1:W:85:ARG:HH11  | 1:W:85:ARG:CG    | 2.26        | 0.44     |
| 1:M:56:LEU:HD13  | 1:M:99:LEU:HD23  | 1.98        | 0.44     |
| 2:V:436:TYR:HD1  | 2:V:436:TYR:N    | 2.14        | 0.44     |
| 1:1:182:ARG:HD3  | 1:1:235:VAL:CB   | 2.46        | 0.44     |
| 2:T:496:ILE:O    | 2:T:502:ALA:HA   | 2.17        | 0.44     |
| 1:Y:28:LYS:HD3   | 3:Y:258:HOH:O    | 2.17        | 0.44     |
| 2:P:437:GLN:OE1  | 2:P:447:LYS:HD3  | 2.17        | 0.44     |
| 1:W:54:SER:CB    | 1:W:75:ARG:HD2   | 2.48        | 0.44     |
| 2:N:452:LYS:NZ   | 2:V:449:SER:HB2  | 2.33        | 0.44     |
| 1:A:57:TYR:O     | 1:A:58:ASP:C     | 2.56        | 0.44     |
| 1:M:70:GLU:HB3   | 1:M:118:TYR:CD2  | 2.52        | 0.44     |
| 2:Z:485:ASP:OD2  | 2:Z:488:ARG:HB2  | 2.18        | 0.44     |
| 2:T:485:ASP:OD2  | 2:T:488:ARG:HB2  | 2.18        | 0.44     |
| 2:T:320:SER:HB2  | 2:T:331:VAL:HG21 | 2.00        | 0.44     |
| 2:2:436:TYR:HD1  | 2:2:436:TYR:N    | 2.15        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:182:ARG:NH1  | 1:D:182:ARG:HB2  | 2.33        | 0.44     |
| 1:D:205:VAL:HG12 | 1:D:206:ALA:H    | 1.82        | 0.44     |
| 1:B:30:VAL:HG22  | 1:B:43:ALA:CB    | 2.48        | 0.44     |
| 2:P:388:ARG:C    | 2:P:390:ASN:H    | 2.20        | 0.44     |
| 2:H:380:ILE:HD11 | 2:H:421:VAL:HG21 | 1.99        | 0.44     |
| 1:S:83:ASP:OD2   | 2:T:365:HIS:CD2  | 2.68        | 0.44     |
| 1:B:30:VAL:HG23  | 1:B:65:ALA:HB2   | 2.00        | 0.44     |
| 2:G:412:SER:O    | 2:G:414:PRO:HD3  | 2.17        | 0.44     |
| 1:D:70:GLU:HB3   | 1:D:118:TYR:CD2  | 2.53        | 0.44     |
| 1:F:70:GLU:HB3   | 1:F:118:TYR:CD2  | 2.53        | 0.44     |
| 2:G:318:ARG:HD2  | 2:G:492:PRO:HA   | 2.00        | 0.44     |
| 1:O:31:VAL:N     | 3:O:250:HOH:O    | 2.50        | 0.43     |
| 2:N:436:TYR:CD1  | 2:N:436:TYR:N    | 2.85        | 0.43     |
| 1:O:182:ARG:HD3  | 1:O:235:VAL:CB   | 2.47        | 0.43     |
| 1:W:71:PHE:HB3   | 1:W:120:VAL:HG11 | 2.00        | 0.43     |
| 2:G:452:LYS:HZ1  | 2:2:449:SER:HB2  | 1.83        | 0.43     |
| 2:G:437:GLN:OE1  | 2:G:447:LYS:HD3  | 2.18        | 0.43     |
| 2:L:412:SER:O    | 2:L:414:PRO:HD3  | 2.17        | 0.43     |
| 1:F:83:ASP:OD2   | 2:G:365:HIS:HD2  | 2.01        | 0.43     |
| 2:V:450:MET:HE3  | 2:V:470:ALA:CB   | 2.47        | 0.43     |
| 2:G:476:ASP:O    | 2:V:329:ARG:NH2  | 2.50        | 0.43     |
| 2:X:496:ILE:HG13 | 2:X:505:VAL:CG2  | 2.48        | 0.43     |
| 2:E:309:PRO:HG3  | 2:E:458:THR:O    | 2.18        | 0.43     |
| 1:K:182:ARG:HB2  | 1:K:182:ARG:NH1  | 2.33        | 0.43     |
| 2:T:436:TYR:CD1  | 2:T:436:TYR:N    | 2.84        | 0.43     |
| 2:G:436:TYR:N    | 2:G:436:TYR:CD1  | 2.86        | 0.43     |
| 1:F:28:LYS:HE3   | 1:F:44:GLU:HG3   | 2.01        | 0.43     |
| 1:I:30:VAL:HG23  | 1:I:65:ALA:HB2   | 2.00        | 0.43     |
| 2:V:301:THR:HG23 | 2:V:333:LYS:HD3  | 2.00        | 0.43     |
| 2:G:324:ASN:N    | 2:G:324:ASN:HD22 | 2.16        | 0.43     |
| 2:P:461:ASP:OD1  | 2:P:509:ARG:HD2  | 2.17        | 0.43     |
| 1:Y:150:GLU:HG2  | 3:Y:253:HOH:O    | 2.18        | 0.43     |
| 1:K:35:TYR:HE2   | 3:K:249:HOH:O    | 2.01        | 0.43     |
| 1:K:93:ASP:OD2   | 3:K:254:HOH:O    | 2.21        | 0.43     |
| 2:N:324:ASN:ND2  | 2:N:324:ASN:N    | 2.66        | 0.43     |
| 2:G:449:SER:HB2  | 2:2:452:LYS:HZ1  | 1.83        | 0.43     |
| 1:I:127:VAL:HG11 | 1:I:213:LEU:HB3  | 1.99        | 0.43     |
| 1:O:28:LYS:HE2   | 1:O:46:PRO:HD3   | 2.00        | 0.43     |
| 1:S:71:PHE:HB3   | 1:S:120:VAL:HG11 | 2.00        | 0.43     |
| 2:2:391:LEU:O    | 2:2:395:MET:HG2  | 2.18        | 0.43     |
| 2:E:301:THR:HA   | 2:E:333:LYS:HZ3  | 1.83        | 0.43     |
| 2:E:324:ASN:N    | 2:E:324:ASN:HD22 | 2.12        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:X:324:ASN:H    | 2:X:324:ASN:ND2  | 2.16        | 0.43     |
| 1:U:70:GLU:HB3   | 1:U:118:TYR:CD2  | 2.53        | 0.43     |
| 2:V:388:ARG:C    | 2:V:390:ASN:H    | 2.22        | 0.43     |
| 2:G:514:ALA:O    | 2:G:518:ILE:HG13 | 2.17        | 0.43     |
| 2:G:426:ALA:HB3  | 2:X:350:ALA:CB   | 2.49        | 0.43     |
| 1:I:172:ALA:HB3  | 1:I:175:ALA:HB2  | 1.99        | 0.43     |
| 2:J:307:LYS:HE2  | 2:J:435:GLY:HA2  | 2.00        | 0.43     |
| 1:Y:85:ARG:NH1   | 1:Y:85:ARG:CG    | 2.78        | 0.43     |
| 1:D:220:ARG:HH22 | 2:E:367:GLU:CD   | 2.22        | 0.43     |
| 2:R:320:SER:HB3  | 2:R:328:GLY:HA3  | 2.01        | 0.43     |
| 1:D:85:ARG:NH1   | 1:D:85:ARG:HG2   | 2.29        | 0.43     |
| 2:H:476:ASP:O    | 2:L:329:ARG:NH2  | 2.52        | 0.43     |
| 1:A:28:LYS:HE2   | 1:A:46:PRO:HD3   | 2.00        | 0.43     |
| 2:P:301:THR:HG23 | 2:P:333:LYS:HD3  | 1.99        | 0.43     |
| 1:K:30:VAL:HG22  | 1:K:43:ALA:CB    | 2.48        | 0.43     |
| 1:F:97:ARG:NH1   | 1:M:49:SER:HB2   | 2.34        | 0.43     |
| 1:W:76:ARG:NH1   | 2:X:369:LEU:HD22 | 2.34        | 0.43     |
| 1:I:47:SER:HB2   | 3:I:254:HOH:O    | 2.18        | 0.43     |
| 2:L:337:THR:HG21 | 2:L:359:TYR:CD2  | 2.53        | 0.43     |
| 1:I:205:VAL:HG12 | 1:I:206:ALA:H    | 1.83        | 0.43     |
| 2:H:505:VAL:HA   | 2:H:506:PRO:HD3  | 1.89        | 0.43     |
| 1:1:30:VAL:HG23  | 1:1:65:ALA:HB2   | 2.00        | 0.43     |
| 1:Q:105:GLN:NE2  | 1:Y:73:ASN:HD22  | 2.16        | 0.43     |
| 2:J:485:ASP:OD2  | 2:J:488:ARG:HB2  | 2.18        | 0.43     |
| 1:Q:141:ILE:N    | 1:Q:141:ILE:HD12 | 2.33        | 0.43     |
| 2:N:496:ILE:O    | 2:N:502:ALA:HA   | 2.18        | 0.43     |
| 2:C:505:VAL:HA   | 2:C:506:PRO:HD3  | 1.89        | 0.43     |
| 1:W:12:ALA:O     | 1:W:16:ARG:HG2   | 2.18        | 0.43     |
| 1:D:71:PHE:HB3   | 1:D:120:VAL:HG11 | 2.01        | 0.43     |
| 2:V:301:THR:HA   | 2:V:333:LYS:HZ3  | 1.83        | 0.43     |
| 2:P:412:SER:O    | 2:P:414:PRO:HD3  | 2.18        | 0.43     |
| 2:E:338:ASP:HB2  | 3:E:189:HOH:O    | 2.18        | 0.43     |
| 2:N:324:ASN:HD22 | 2:N:324:ASN:N    | 2.05        | 0.43     |
| 2:C:436:TYR:HD1  | 2:C:436:TYR:N    | 2.15        | 0.43     |
| 2:T:324:ASN:HD22 | 2:T:324:ASN:N    | 2.13        | 0.43     |
| 2:L:303:ILE:HD11 | 2:L:333:LYS:HB3  | 2.01        | 0.43     |
| 2:C:388:ARG:C    | 2:C:390:ASN:H    | 2.21        | 0.43     |
| 2:G:321:THR:HG21 | 2:G:480:ALA:HB1  | 2.01        | 0.43     |
| 1:A:213:LEU:HD12 | 1:A:222:PHE:HD1  | 1.84        | 0.43     |
| 1:W:213:LEU:HD12 | 1:W:222:PHE:HD1  | 1.83        | 0.43     |
| 1:K:28:LYS:HE2   | 1:K:46:PRO:HD3   | 2.00        | 0.43     |
| 1:M:12:ALA:O     | 1:M:16:ARG:HG2   | 2.17        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:Z:437:GLN:OE1  | 2:Z:447:LYS:HD3  | 2.19        | 0.43     |
| 1:S:85:ARG:NH1   | 1:S:85:ARG:CG    | 2.82        | 0.43     |
| 1:S:205:VAL:HG12 | 1:S:206:ALA:H    | 1.84        | 0.43     |
| 1:1:76:ARG:NH1   | 2:2:369:LEU:HD22 | 2.33        | 0.43     |
| 1:W:70:GLU:HB3   | 1:W:118:TYR:CD2  | 2.53        | 0.43     |
| 1:D:89:TYR:CD1   | 2:R:382:ARG:HD3  | 2.54        | 0.43     |
| 2:Z:380:ILE:HD11 | 2:Z:421:VAL:HG21 | 2.01        | 0.43     |
| 2:R:355:PHE:HD1  | 2:R:355:PHE:HA   | 1.77        | 0.43     |
| 1:Y:213:LEU:HD12 | 1:Y:222:PHE:HD1  | 1.84        | 0.43     |
| 1:I:85:ARG:NH1   | 1:I:85:ARG:CG    | 2.82        | 0.43     |
| 2:C:309:PRO:O    | 2:C:415:GLN:HG2  | 2.19        | 0.43     |
| 1:O:83:ASP:OD2   | 2:P:365:HIS:CD2  | 2.69        | 0.43     |
| 2:E:436:TYR:HD1  | 2:E:436:TYR:N    | 2.15        | 0.43     |
| 1:M:234:LEU:O    | 3:M:252:HOH:O    | 2.21        | 0.43     |
| 1:1:54:SER:CB    | 1:1:75:ARG:HD2   | 2.49        | 0.43     |
| 2:P:321:THR:HG21 | 2:P:480:ALA:HB1  | 2.01        | 0.43     |
| 2:G:388:ARG:C    | 2:G:390:ASN:H    | 2.22        | 0.43     |
| 2:H:415:GLN:HE21 | 2:H:415:GLN:HB3  | 1.60        | 0.43     |
| 1:M:85:ARG:HG2   | 1:M:85:ARG:NH1   | 2.24        | 0.42     |
| 2:E:320:SER:HB2  | 2:E:331:VAL:HG21 | 2.01        | 0.42     |
| 2:L:320:SER:HB2  | 2:L:331:VAL:HG21 | 2.00        | 0.42     |
| 1:F:89:TYR:HD1   | 2:N:382:ARG:HD3  | 1.82        | 0.42     |
| 2:P:436:TYR:N    | 2:P:436:TYR:CD1  | 2.86        | 0.42     |
| 1:B:74:LEU:HD11  | 1:B:107:LEU:HD21 | 2.01        | 0.42     |
| 2:E:412:SER:O    | 2:E:414:PRO:HD3  | 2.19        | 0.42     |
| 2:H:388:ARG:C    | 2:H:390:ASN:H    | 2.22        | 0.42     |
| 1:S:127:VAL:HG21 | 1:S:215:ALA:HB2  | 2.00        | 0.42     |
| 1:A:127:VAL:HG11 | 1:A:213:LEU:HB3  | 2.01        | 0.42     |
| 1:Y:127:VAL:HG11 | 1:Y:213:LEU:HB3  | 2.00        | 0.42     |
| 1:Y:205:VAL:HG12 | 1:Y:206:ALA:H    | 1.84        | 0.42     |
| 2:2:309:PRO:HG3  | 2:2:458:THR:O    | 2.19        | 0.42     |
| 1:S:12:ALA:O     | 1:S:16:ARG:HG2   | 2.19        | 0.42     |
| 2:G:301:THR:HG23 | 2:G:333:LYS:HD3  | 2.00        | 0.42     |
| 2:T:388:ARG:C    | 2:T:390:ASN:H    | 2.22        | 0.42     |
| 2:L:415:GLN:HB3  | 2:L:415:GLN:HE21 | 1.61        | 0.42     |
| 2:J:337:THR:HG21 | 2:J:359:TYR:CD2  | 2.54        | 0.42     |
| 2:2:505:VAL:HA   | 2:2:506:PRO:HD3  | 1.92        | 0.42     |
| 1:D:112:THR:HG23 | 1:Q:115:ALA:HB3  | 2.01        | 0.42     |
| 2:J:301:THR:HG23 | 2:J:333:LYS:HD3  | 2.01        | 0.42     |
| 2:Z:307:LYS:HE2  | 2:Z:435:GLY:HA2  | 2.01        | 0.42     |
| 2:X:380:ILE:HD11 | 2:X:421:VAL:HG21 | 2.01        | 0.42     |
| 1:Q:135:ARG:HB3  | 1:Y:48:ARG:HH22  | 1.83        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:E:306:LEU:HB2  | 2:E:313:VAL:CG1  | 2.49        | 0.42     |
| 2:N:388:ARG:C    | 2:N:390:ASN:H    | 2.22        | 0.42     |
| 2:V:320:SER:HB2  | 2:V:331:VAL:HG21 | 2.01        | 0.42     |
| 1:D:55:GLU:OE2   | 1:D:220:ARG:CD   | 2.67        | 0.42     |
| 2:J:505:VAL:HA   | 2:J:506:PRO:HD3  | 1.87        | 0.42     |
| 1:I:12:ALA:O     | 1:I:16:ARG:HG2   | 2.18        | 0.42     |
| 1:O:205:VAL:C    | 1:O:207:SER:N    | 2.73        | 0.42     |
| 1:U:205:VAL:C    | 1:U:207:SER:N    | 2.72        | 0.42     |
| 2:H:496:ILE:O    | 2:H:502:ALA:HA   | 2.20        | 0.42     |
| 2:Z:324:ASN:N    | 2:Z:324:ASN:HD22 | 2.14        | 0.42     |
| 1:O:54:SER:CB    | 1:O:75:ARG:HD2   | 2.49        | 0.42     |
| 2:H:426:ALA:HB3  | 2:C:350:ALA:CB   | 2.49        | 0.42     |
| 2:T:380:ILE:HD11 | 2:T:421:VAL:HG21 | 2.02        | 0.42     |
| 1:S:74:LEU:HD11  | 1:S:107:LEU:HD21 | 2.01        | 0.42     |
| 1:O:213:LEU:HD12 | 1:O:222:PHE:HD1  | 1.84        | 0.42     |
| 1:U:213:LEU:HD12 | 1:U:222:PHE:HD1  | 1.84        | 0.42     |
| 1:K:85:ARG:HG2   | 1:K:85:ARG:NH1   | 2.28        | 0.42     |
| 2:Z:320:SER:HB2  | 2:Z:331:VAL:HG21 | 2.02        | 0.42     |
| 2:X:436:TYR:N    | 2:X:436:TYR:CD1  | 2.88        | 0.42     |
| 2:Z:301:THR:HG23 | 2:Z:333:LYS:HD3  | 2.01        | 0.42     |
| 2:P:469:GLU:HG3  | 2:P:517:ILE:HG21 | 2.02        | 0.42     |
| 2:2:303:ILE:HD11 | 2:2:333:LYS:HB3  | 2.01        | 0.42     |
| 2:P:485:ASP:OD2  | 2:P:488:ARG:CB   | 2.67        | 0.42     |
| 1:U:63:ALA:O     | 1:U:156:MET:HE1  | 2.19        | 0.42     |
| 2:C:307:LYS:HE2  | 2:C:435:GLY:HA2  | 2.00        | 0.42     |
| 1:B:63:ALA:O     | 1:B:156:MET:HE1  | 2.19        | 0.42     |
| 1:1:85:ARG:HG2   | 1:1:85:ARG:NH1   | 2.29        | 0.42     |
| 1:W:55:GLU:OE2   | 1:W:220:ARG:CD   | 2.68        | 0.42     |
| 1:S:56:LEU:HD13  | 1:S:99:LEU:HD23  | 2.02        | 0.42     |
| 1:O:56:LEU:HD13  | 1:O:99:LEU:HD23  | 2.01        | 0.42     |
| 2:P:505:VAL:HA   | 2:P:506:PRO:HD3  | 1.90        | 0.42     |
| 1:B:71:PHE:HB3   | 1:B:120:VAL:HG11 | 2.01        | 0.42     |
| 2:2:301:THR:HA   | 2:2:333:LYS:NZ   | 2.34        | 0.42     |
| 2:R:301:THR:HG23 | 2:R:333:LYS:HD3  | 2.02        | 0.42     |
| 2:R:485:ASP:OD2  | 2:R:488:ARG:HB2  | 2.19        | 0.42     |
| 2:Z:388:ARG:C    | 2:Z:390:ASN:H    | 2.22        | 0.42     |
| 2:2:415:GLN:HE21 | 2:2:415:GLN:HB3  | 1.60        | 0.42     |
| 2:L:505:VAL:HA   | 2:L:506:PRO:HD3  | 1.90        | 0.42     |
| 1:Q:28:LYS:HE2   | 1:Q:46:PRO:HD3   | 2.00        | 0.42     |
| 2:E:378:GLY:HA3  | 3:K:254:HOH:O    | 2.19        | 0.42     |
| 2:V:321:THR:HG21 | 2:V:480:ALA:HB1  | 2.02        | 0.42     |
| 2:X:393:ALA:HB1  | 2:X:398:LEU:HB2  | 2.00        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:L:355:PHE:HA   | 2:L:355:PHE:HD1  | 1.74        | 0.42     |
| 1:A:14:ARG:CB    | 1:A:14:ARG:HH11  | 2.17        | 0.42     |
| 2:H:304:VAL:HG21 | 2:H:450:MET:HE1  | 2.00        | 0.42     |
| 1:O:30:VAL:CA    | 3:O:250:HOH:O    | 2.65        | 0.42     |
| 2:X:450:MET:HE3  | 2:X:470:ALA:CB   | 2.50        | 0.42     |
| 1:D:213:LEU:HD12 | 1:D:222:PHE:HD1  | 1.85        | 0.42     |
| 2:E:456:GLN:NE2  | 2:E:465:ARG:NH1  | 2.68        | 0.42     |
| 1:U:85:ARG:HH11  | 1:U:85:ARG:CG    | 2.29        | 0.42     |
| 2:L:449:SER:HB2  | 2:P:452:LYS:HZ3  | 1.83        | 0.42     |
| 2:2:320:SER:HB2  | 2:2:331:VAL:HG21 | 2.01        | 0.42     |
| 1:U:182:ARG:HA   | 1:U:235:VAL:HB   | 2.02        | 0.42     |
| 1:1:182:ARG:HA   | 1:1:235:VAL:HB   | 2.02        | 0.42     |
| 2:P:303:ILE:HD11 | 2:P:333:LYS:HB3  | 2.02        | 0.42     |
| 2:N:317:ASP:OD1  | 2:N:333:LYS:NZ   | 2.52        | 0.42     |
| 1:Y:151:PRO:HD2  | 3:Y:250:HOH:O    | 2.18        | 0.42     |
| 2:G:326:ILE:HD12 | 2:G:326:ILE:H    | 1.84        | 0.42     |
| 1:O:30:VAL:HG22  | 1:O:43:ALA:CB    | 2.49        | 0.42     |
| 2:L:456:GLN:NE2  | 2:L:465:ARG:NH1  | 2.67        | 0.42     |
| 2:G:329:ARG:NH2  | 2:V:476:ASP:O    | 2.52        | 0.42     |
| 2:X:456:GLN:NE2  | 2:X:465:ARG:NH1  | 2.68        | 0.42     |
| 1:U:71:PHE:HB3   | 1:U:120:VAL:HG11 | 2.01        | 0.42     |
| 1:K:56:LEU:HD13  | 1:K:99:LEU:HD23  | 2.00        | 0.42     |
| 1:A:134:LYS:HE2  | 1:A:134:LYS:HA   | 2.01        | 0.42     |
| 2:X:307:LYS:HE2  | 2:X:435:GLY:HA2  | 2.01        | 0.42     |
| 2:R:436:TYR:CD2  | 2:R:450:MET:HG2  | 2.55        | 0.42     |
| 1:A:71:PHE:HB3   | 1:A:120:VAL:HG11 | 2.02        | 0.42     |
| 2:G:441:SER:HB2  | 2:G:478:ASP:OD2  | 2.20        | 0.42     |
| 2:E:306:LEU:HB2  | 2:E:313:VAL:HG13 | 2.01        | 0.42     |
| 1:I:70:GLU:HB3   | 1:I:118:TYR:CD2  | 2.54        | 0.42     |
| 2:E:349:ALA:N    | 3:E:69:HOH:O     | 2.52        | 0.42     |
| 2:P:415:GLN:HE21 | 2:P:415:GLN:HB3  | 1.60        | 0.42     |
| 2:N:334:VAL:HG22 | 3:N:120:HOH:O    | 2.20        | 0.41     |
| 2:T:505:VAL:HA   | 2:T:506:PRO:HD3  | 1.89        | 0.41     |
| 1:B:28:LYS:HE2   | 1:B:46:PRO:HD3   | 2.02        | 0.41     |
| 2:C:301:THR:HG23 | 2:C:333:LYS:HD3  | 2.02        | 0.41     |
| 2:J:301:THR:HA   | 2:J:333:LYS:HZ2  | 1.85        | 0.41     |
| 1:O:112:THR:CG2  | 1:U:115:ALA:HB3  | 2.49        | 0.41     |
| 2:G:324:ASN:ND2  | 2:G:324:ASN:H    | 2.18        | 0.41     |
| 1:W:123:CYS:HA   | 1:W:139:TYR:O    | 2.20        | 0.41     |
| 1:F:28:LYS:HE2   | 1:F:46:PRO:HD3   | 2.02        | 0.41     |
| 1:F:205:VAL:HG12 | 1:F:206:ALA:H    | 1.84        | 0.41     |
| 1:A:89:TYR:HD1   | 2:P:382:ARG:HD3  | 1.84        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:H:301:THR:HA   | 2:H:333:LYS:HZ3  | 1.84        | 0.41     |
| 1:S:217:ARG:HA   | 1:S:218:PRO:HD3  | 1.96        | 0.41     |
| 2:V:355:PHE:HD1  | 2:V:355:PHE:HA   | 1.76        | 0.41     |
| 2:T:378:GLY:HA3  | 3:1:252:HOH:O    | 2.20        | 0.41     |
| 1:B:213:LEU:HD12 | 1:B:222:PHE:HD1  | 1.86        | 0.41     |
| 1:M:85:ARG:NH1   | 1:M:85:ARG:CG    | 2.82        | 0.41     |
| 1:Q:56:LEU:HD13  | 1:Q:99:LEU:HD23  | 2.01        | 0.41     |
| 1:O:182:ARG:HA   | 1:O:235:VAL:HB   | 2.01        | 0.41     |
| 1:D:182:ARG:HA   | 1:D:235:VAL:HB   | 2.02        | 0.41     |
| 1:D:43:ALA:HA    | 3:D:251:HOH:O    | 2.20        | 0.41     |
| 1:K:30:VAL:HG23  | 1:K:65:ALA:HB2   | 2.03        | 0.41     |
| 1:F:97:ARG:HH11  | 1:M:49:SER:HB2   | 1.86        | 0.41     |
| 2:E:380:ILE:HD11 | 2:E:421:VAL:HG21 | 2.02        | 0.41     |
| 2:J:449:SER:HB2  | 2:Z:452:LYS:HZ3  | 1.85        | 0.41     |
| 2:N:456:GLN:HE22 | 2:N:465:ARG:NH1  | 2.18        | 0.41     |
| 1:B:205:VAL:HG12 | 1:B:206:ALA:H    | 1.84        | 0.41     |
| 1:F:56:LEU:O     | 2:G:368:LYS:HD2  | 2.20        | 0.41     |
| 2:C:513:LEU:O    | 2:C:516:ALA:HB3  | 2.19        | 0.41     |
| 2:2:301:THR:N    | 2:2:441:SER:HG   | 2.17        | 0.41     |
| 1:K:39:VAL:N     | 3:K:249:HOH:O    | 2.53        | 0.41     |
| 2:Z:318:ARG:HD2  | 2:Z:492:PRO:HA   | 2.01        | 0.41     |
| 1:1:74:LEU:HD11  | 1:1:107:LEU:HD21 | 2.02        | 0.41     |
| 1:S:57:TYR:O     | 1:S:58:ASP:C     | 2.59        | 0.41     |
| 2:C:441:SER:HB2  | 2:C:478:ASP:OD2  | 2.20        | 0.41     |
| 1:S:213:LEU:HD12 | 1:S:222:PHE:HD1  | 1.85        | 0.41     |
| 1:D:55:GLU:OE2   | 1:D:220:ARG:HD2  | 2.20        | 0.41     |
| 2:X:496:ILE:O    | 2:X:502:ALA:HA   | 2.19        | 0.41     |
| 2:J:496:ILE:HG13 | 2:J:505:VAL:CG2  | 2.50        | 0.41     |
| 1:W:182:ARG:HB2  | 1:W:182:ARG:NH1  | 2.35        | 0.41     |
| 2:T:337:THR:HG21 | 2:T:359:TYR:CD2  | 2.55        | 0.41     |
| 2:Z:313:VAL:HG23 | 2:Z:496:ILE:HG12 | 2.02        | 0.41     |
| 2:J:437:GLN:OE1  | 2:J:447:LYS:HD3  | 2.21        | 0.41     |
| 1:F:97:ARG:NH1   | 1:M:49:SER:O     | 2.53        | 0.41     |
| 2:V:514:ALA:O    | 2:V:518:ILE:HG13 | 2.19        | 0.41     |
| 2:G:475:ALA:HA   | 2:G:481:THR:HB   | 2.03        | 0.41     |
| 2:J:456:GLN:HE22 | 2:J:465:ARG:NH1  | 2.18        | 0.41     |
| 1:K:83:ASP:OD2   | 2:L:365:HIS:CD2  | 2.71        | 0.41     |
| 2:J:380:ILE:HD11 | 2:J:421:VAL:HG21 | 2.02        | 0.41     |
| 2:T:412:SER:O    | 2:T:414:PRO:HD3  | 2.20        | 0.41     |
| 1:I:217:ARG:HA   | 1:I:218:PRO:HD3  | 1.98        | 0.41     |
| 2:E:475:ALA:HB2  | 2:E:481:THR:HG22 | 2.01        | 0.41     |
| 2:J:514:ALA:O    | 2:J:518:ILE:HG13 | 2.20        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:P:355:PHE:HA   | 2:P:355:PHE:HD1  | 1.78        | 0.41     |
| 1:K:40:LEU:HD12  | 1:K:212:VAL:CG1  | 2.50        | 0.41     |
| 1:K:205:VAL:C    | 1:K:207:SER:N    | 2.74        | 0.41     |
| 1:D:205:VAL:C    | 1:D:207:SER:N    | 2.74        | 0.41     |
| 2:X:485:ASP:OD2  | 2:X:488:ARG:CB   | 2.69        | 0.41     |
| 1:A:10:GLU:HA    | 1:O:19:LEU:HD12  | 2.02        | 0.41     |
| 1:B:135:ARG:HA   | 1:B:136:PRO:HD2  | 1.96        | 0.41     |
| 1:O:30:VAL:HG23  | 1:O:65:ALA:HB2   | 2.02        | 0.41     |
| 1:Q:55:GLU:OE2   | 1:Q:220:ARG:CD   | 2.69        | 0.41     |
| 1:Q:182:ARG:HA   | 1:Q:235:VAL:HB   | 2.02        | 0.41     |
| 2:H:324:ASN:N    | 2:H:324:ASN:ND2  | 2.68        | 0.41     |
| 1:W:205:VAL:C    | 1:W:207:SER:N    | 2.72        | 0.41     |
| 2:C:318:ARG:HD2  | 2:C:492:PRO:HA   | 2.03        | 0.41     |
| 1:A:49:SER:HB2   | 1:B:97:ARG:HG3   | 2.03        | 0.41     |
| 2:E:321:THR:HG21 | 2:E:480:ALA:HB1  | 2.02        | 0.41     |
| 2:C:514:ALA:O    | 2:C:518:ILE:HG13 | 2.21        | 0.41     |
| 1:M:64:ALA:HB2   | 1:M:122:LEU:HG   | 2.02        | 0.41     |
| 1:I:154:VAL:HG13 | 3:I:249:HOH:O    | 2.20        | 0.41     |
| 2:R:321:THR:HG21 | 2:R:480:ALA:HB1  | 2.03        | 0.41     |
| 1:B:55:GLU:OE2   | 1:B:220:ARG:HD2  | 2.20        | 0.41     |
| 2:J:450:MET:HE3  | 2:J:470:ALA:CB   | 2.51        | 0.41     |
| 1:S:55:GLU:OE2   | 1:S:220:ARG:CD   | 2.69        | 0.41     |
| 1:Y:55:GLU:OE2   | 1:Y:220:ARG:CD   | 2.68        | 0.41     |
| 1:I:55:GLU:OE2   | 1:I:220:ARG:CD   | 2.69        | 0.41     |
| 1:A:189:ARG:NH2  | 1:A:237:GLN:HB3  | 2.35        | 0.41     |
| 2:X:320:SER:HB3  | 2:X:328:GLY:HA3  | 2.02        | 0.41     |
| 1:K:28:LYS:HB2   | 1:K:52:LYS:HZ2   | 1.83        | 0.41     |
| 1:S:182:ARG:HA   | 1:S:235:VAL:HB   | 2.01        | 0.41     |
| 1:B:12:ALA:O     | 1:B:16:ARG:HG2   | 2.20        | 0.41     |
| 2:X:324:ASN:HD22 | 2:X:324:ASN:N    | 2.16        | 0.41     |
| 2:L:301:THR:HA   | 2:L:333:LYS:HZ3  | 1.86        | 0.41     |
| 1:K:63:ALA:O     | 1:K:156:MET:HE1  | 2.21        | 0.41     |
| 2:X:412:SER:O    | 2:X:414:PRO:HD3  | 2.21        | 0.41     |
| 2:G:355:PHE:HD1  | 2:G:355:PHE:HA   | 1.77        | 0.41     |
| 2:Z:393:ALA:HB1  | 2:Z:398:LEU:HB2  | 2.03        | 0.41     |
| 2:R:415:GLN:HB3  | 2:R:415:GLN:HE21 | 1.60        | 0.41     |
| 1:O:43:ALA:HB1   | 3:O:252:HOH:O    | 2.21        | 0.41     |
| 1:K:55:GLU:OE2   | 1:K:220:ARG:HD2  | 2.21        | 0.41     |
| 2:T:476:ASP:O    | 2:Z:329:ARG:NH2  | 2.52        | 0.41     |
| 1:F:182:ARG:HA   | 1:F:235:VAL:HB   | 2.03        | 0.41     |
| 1:U:93:ASP:HB3   | 2:2:366:TYR:OH   | 2.21        | 0.41     |
| 1:A:155:VAL:HG12 | 1:A:160:THR:HG22 | 2.03        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:R:318:ARG:HD2  | 2:R:492:PRO:HA   | 2.02        | 0.41     |
| 2:G:456:GLN:NE2  | 2:G:465:ARG:NH1  | 2.66        | 0.40     |
| 1:A:30:VAL:CG2   | 1:A:65:ALA:HB2   | 2.51        | 0.40     |
| 1:Q:12:ALA:O     | 1:Q:16:ARG:HG2   | 2.20        | 0.40     |
| 1:K:205:VAL:HG12 | 1:K:206:ALA:H    | 1.85        | 0.40     |
| 1:A:205:VAL:C    | 1:A:207:SER:N    | 2.73        | 0.40     |
| 2:J:318:ARG:HD2  | 2:J:492:PRO:HA   | 2.03        | 0.40     |
| 1:O:163:ILE:HG23 | 1:O:188:LEU:HA   | 2.03        | 0.40     |
| 1:F:85:ARG:CG    | 1:F:85:ARG:NH1   | 2.80        | 0.40     |
| 1:W:40:LEU:HD12  | 1:W:212:VAL:CG1  | 2.51        | 0.40     |
| 1:Q:71:PHE:HB3   | 1:Q:120:VAL:HG11 | 2.04        | 0.40     |
| 1:I:134:LYS:HG3  | 1:I:135:ARG:N    | 2.36        | 0.40     |
| 1:W:30:VAL:HG23  | 1:W:65:ALA:HB2   | 2.02        | 0.40     |
| 1:K:48:ARG:HH22  | 1:M:135:ARG:HB3  | 1.86        | 0.40     |
| 2:V:393:ALA:HB1  | 2:V:398:LEU:HB2  | 2.03        | 0.40     |
| 2:G:397:GLY:O    | 2:G:399:LEU:N    | 2.54        | 0.40     |
| 1:W:163:ILE:HG23 | 1:W:188:LEU:HA   | 2.03        | 0.40     |
| 1:D:15:GLU:OE1   | 1:K:8:SER:HA     | 2.21        | 0.40     |
| 1:O:85:ARG:NH1   | 1:O:85:ARG:CG    | 2.79        | 0.40     |
| 2:X:505:VAL:HA   | 2:X:506:PRO:HD3  | 1.91        | 0.40     |
| 2:H:452:LYS:HZ3  | 2:E:449:SER:HB2  | 1.85        | 0.40     |
| 1:M:127:VAL:HG22 | 1:M:215:ALA:HB2  | 2.04        | 0.40     |
| 2:X:301:THR:HG23 | 2:X:333:LYS:HD3  | 2.02        | 0.40     |
| 2:H:393:ALA:HB1  | 2:H:398:LEU:HB2  | 2.04        | 0.40     |
| 1:F:163:ILE:HG23 | 1:F:188:LEU:HA   | 2.04        | 0.40     |
| 2:J:321:THR:HG21 | 2:J:480:ALA:HB1  | 2.02        | 0.40     |
| 1:O:40:LEU:HD12  | 1:O:212:VAL:CG1  | 2.52        | 0.40     |
| 1:D:40:LEU:HD12  | 1:D:212:VAL:CG1  | 2.51        | 0.40     |
| 1:U:55:GLU:OE2   | 1:U:220:ARG:HD2  | 2.22        | 0.40     |
| 1:U:40:LEU:HD12  | 1:U:212:VAL:CG1  | 2.51        | 0.40     |
| 2:N:329:ARG:NH2  | 2:P:476:ASP:O    | 2.54        | 0.40     |
| 2:2:496:ILE:HG13 | 2:2:505:VAL:CG2  | 2.52        | 0.40     |
| 2:Z:301:THR:N    | 2:Z:441:SER:HG   | 2.19        | 0.40     |
| 2:H:469:GLU:HG3  | 2:H:517:ILE:HG21 | 2.02        | 0.40     |
| 1:Q:134:LYS:HE2  | 1:Q:134:LYS:HA   | 2.03        | 0.40     |
| 2:C:321:THR:HG21 | 2:C:480:ALA:HB1  | 2.03        | 0.40     |
| 2:N:453:LEU:HB2  | 2:N:466:VAL:HG13 | 2.04        | 0.40     |
| 2:N:496:ILE:HG13 | 2:N:505:VAL:CG2  | 2.51        | 0.40     |
| 1:K:182:ARG:HA   | 1:K:235:VAL:HB   | 2.02        | 0.40     |
| 1:A:56:LEU:HD13  | 1:A:99:LEU:HD23  | 2.04        | 0.40     |
| 1:1:134:LYS:HA   | 1:1:134:LYS:HE2  | 2.02        | 0.40     |
| 1:M:134:LYS:HE2  | 1:M:134:LYS:HA   | 2.04        | 0.40     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:Q:135:ARG:CB  | 1:Y:48:ARG:HH22 | 2.35        | 0.40     |
| 1:M:217:ARG:HA  | 1:M:218:PRO:HD3 | 1.97        | 0.40     |
| 2:T:393:ALA:HB1 | 2:T:398:LEU:HB2 | 2.03        | 0.40     |

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Distance(Å) | Clash(Å) |
|-----------------|------------------------|-------------|----------|
| 2:G:465:ARG:NE  | 2:X:458:THR:CG2[2_554] | 1.40        | 0.80     |
| 1:A:236:ASP:O   | 1:D:133:THR:OG1[2_655] | 1.59        | 0.61     |
| 2:N:456:GLN:NE2 | 2:Z:415:GLN:OE1[1_565] | 1.83        | 0.37     |
| 1:W:228:SER:O   | 2:2:414:PRO:CB[2_544]  | 1.97        | 0.23     |
| 2:J:456:GLN:NE2 | 2:V:415:GLN:OE1[1_545] | 2.00        | 0.20     |
| 1:A:170:SER:CB  | 1:D:216:ASN:OD1[2_655] | 2.06        | 0.14     |
| 1:A:169:GLU:C   | 1:D:216:ASN:ND2[2_655] | 2.07        | 0.13     |
| 1:I:190:ALA:O   | 1:U:14:ARG:NE[2_545]   | 2.08        | 0.12     |
| 1:I:192:SER:N   | 1:U:14:ARG:NH2[2_545]  | 2.08        | 0.12     |
| 2:E:519:GLU:OE1 | 2:P:412:SER:O[2_645]   | 2.09        | 0.11     |
| 2:G:465:ARG:CD  | 2:X:458:THR:OG1[2_554] | 2.11        | 0.09     |
| 2:J:465:ARG:CD  | 2:V:415:GLN:NE2[1_545] | 2.15        | 0.05     |
| 2:G:465:ARG:CD  | 2:X:458:THR:CG2[2_554] | 2.16        | 0.04     |
| 1:A:169:GLU:O   | 1:D:216:ASN:ND2[2_655] | 2.19        | 0.01     |

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|----------|-------------|
| 1   | 1     | 216/250 (86%) | 188 (87%) | 22 (10%) | 6 (3%)   | 8 48        |
| 1   | A     | 216/250 (86%) | 192 (89%) | 19 (9%)  | 5 (2%)   | 10 55       |
| 1   | B     | 216/250 (86%) | 189 (88%) | 21 (10%) | 6 (3%)   | 8 48        |
| 1   | D     | 216/250 (86%) | 193 (89%) | 18 (8%)  | 5 (2%)   | 10 55       |
| 1   | F     | 216/250 (86%) | 190 (88%) | 20 (9%)  | 6 (3%)   | 8 48        |
| 1   | I     | 216/250 (86%) | 189 (88%) | 22 (10%) | 5 (2%)   | 10 55       |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | K     | 216/250 (86%)   | 191 (88%)  | 20 (9%)   | 5 (2%)   | 10          | 55 |
| 1   | M     | 216/250 (86%)   | 187 (87%)  | 24 (11%)  | 5 (2%)   | 10          | 55 |
| 1   | O     | 216/250 (86%)   | 188 (87%)  | 23 (11%)  | 5 (2%)   | 10          | 55 |
| 1   | Q     | 216/250 (86%)   | 188 (87%)  | 23 (11%)  | 5 (2%)   | 10          | 55 |
| 1   | S     | 216/250 (86%)   | 189 (88%)  | 22 (10%)  | 5 (2%)   | 10          | 55 |
| 1   | U     | 216/250 (86%)   | 189 (88%)  | 22 (10%)  | 5 (2%)   | 10          | 55 |
| 1   | W     | 216/250 (86%)   | 192 (89%)  | 19 (9%)   | 5 (2%)   | 10          | 55 |
| 1   | Y     | 216/250 (86%)   | 187 (87%)  | 23 (11%)  | 6 (3%)   | 8           | 48 |
| 2   | 2     | 220/240 (92%)   | 195 (89%)  | 22 (10%)  | 3 (1%)   | 16          | 68 |
| 2   | C     | 220/240 (92%)   | 195 (89%)  | 22 (10%)  | 3 (1%)   | 16          | 68 |
| 2   | E     | 220/240 (92%)   | 196 (89%)  | 19 (9%)   | 5 (2%)   | 10          | 55 |
| 2   | G     | 220/240 (92%)   | 196 (89%)  | 18 (8%)   | 6 (3%)   | 8           | 49 |
| 2   | H     | 220/240 (92%)   | 193 (88%)  | 22 (10%)  | 5 (2%)   | 10          | 55 |
| 2   | J     | 220/240 (92%)   | 194 (88%)  | 22 (10%)  | 4 (2%)   | 13          | 63 |
| 2   | L     | 220/240 (92%)   | 194 (88%)  | 21 (10%)  | 5 (2%)   | 10          | 55 |
| 2   | N     | 220/240 (92%)   | 198 (90%)  | 16 (7%)   | 6 (3%)   | 8           | 49 |
| 2   | P     | 220/240 (92%)   | 195 (89%)  | 19 (9%)   | 6 (3%)   | 8           | 49 |
| 2   | R     | 220/240 (92%)   | 193 (88%)  | 22 (10%)  | 5 (2%)   | 10          | 55 |
| 2   | T     | 220/240 (92%)   | 195 (89%)  | 19 (9%)   | 6 (3%)   | 8           | 49 |
| 2   | V     | 220/240 (92%)   | 194 (88%)  | 21 (10%)  | 5 (2%)   | 10          | 55 |
| 2   | X     | 220/240 (92%)   | 193 (88%)  | 23 (10%)  | 4 (2%)   | 13          | 63 |
| 2   | Z     | 220/240 (92%)   | 192 (87%)  | 24 (11%)  | 4 (2%)   | 13          | 63 |
| All | All   | 6104/6860 (89%) | 5375 (88%) | 588 (10%) | 141 (2%) | 10          | 55 |

All (141) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 128 | ALA  |
| 1   | B     | 128 | ALA  |
| 1   | D     | 128 | ALA  |
| 1   | F     | 128 | ALA  |
| 1   | I     | 128 | ALA  |
| 1   | K     | 128 | ALA  |
| 1   | M     | 128 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 128 | ALA  |
| 1   | Q     | 128 | ALA  |
| 1   | S     | 128 | ALA  |
| 1   | U     | 128 | ALA  |
| 1   | W     | 128 | ALA  |
| 1   | Y     | 128 | ALA  |
| 1   | 1     | 128 | ALA  |
| 1   | A     | 58  | ASP  |
| 1   | B     | 58  | ASP  |
| 1   | D     | 58  | ASP  |
| 1   | I     | 58  | ASP  |
| 1   | I     | 206 | ALA  |
| 1   | K     | 58  | ASP  |
| 1   | M     | 58  | ASP  |
| 1   | Q     | 58  | ASP  |
| 1   | S     | 58  | ASP  |
| 1   | S     | 206 | ALA  |
| 2   | T     | 317 | ASP  |
| 1   | U     | 58  | ASP  |
| 2   | V     | 317 | ASP  |
| 1   | W     | 58  | ASP  |
| 1   | Y     | 58  | ASP  |
| 1   | 1     | 58  | ASP  |
| 2   | 2     | 317 | ASP  |
| 2   | H     | 317 | ASP  |
| 1   | B     | 130 | TYR  |
| 1   | B     | 206 | ALA  |
| 2   | C     | 317 | ASP  |
| 1   | D     | 206 | ALA  |
| 2   | E     | 317 | ASP  |
| 1   | F     | 58  | ASP  |
| 1   | F     | 130 | TYR  |
| 1   | F     | 206 | ALA  |
| 2   | G     | 317 | ASP  |
| 2   | G     | 398 | LEU  |
| 1   | I     | 130 | TYR  |
| 2   | J     | 317 | ASP  |
| 1   | K     | 130 | TYR  |
| 1   | K     | 206 | ALA  |
| 2   | L     | 317 | ASP  |
| 1   | M     | 130 | TYR  |
| 1   | M     | 206 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 398 | LEU  |
| 1   | O     | 58  | ASP  |
| 1   | O     | 130 | TYR  |
| 1   | O     | 206 | ALA  |
| 2   | P     | 317 | ASP  |
| 1   | Q     | 130 | TYR  |
| 1   | Q     | 206 | ALA  |
| 2   | R     | 317 | ASP  |
| 1   | S     | 130 | TYR  |
| 2   | T     | 398 | LEU  |
| 1   | U     | 130 | TYR  |
| 1   | U     | 206 | ALA  |
| 1   | W     | 206 | ALA  |
| 2   | X     | 317 | ASP  |
| 1   | Y     | 130 | TYR  |
| 1   | Y     | 206 | ALA  |
| 2   | Z     | 317 | ASP  |
| 1   | 1     | 130 | TYR  |
| 1   | 1     | 206 | ALA  |
| 1   | A     | 130 | TYR  |
| 1   | A     | 206 | ALA  |
| 1   | A     | 218 | PRO  |
| 1   | B     | 218 | PRO  |
| 1   | B     | 226 | THR  |
| 2   | C     | 434 | GLU  |
| 1   | D     | 130 | TYR  |
| 1   | F     | 218 | PRO  |
| 1   | I     | 218 | PRO  |
| 1   | K     | 218 | PRO  |
| 1   | M     | 218 | PRO  |
| 1   | O     | 218 | PRO  |
| 1   | Q     | 218 | PRO  |
| 1   | S     | 218 | PRO  |
| 1   | U     | 218 | PRO  |
| 1   | W     | 130 | TYR  |
| 1   | W     | 218 | PRO  |
| 2   | X     | 460 | GLY  |
| 1   | Y     | 218 | PRO  |
| 2   | Z     | 460 | GLY  |
| 1   | 1     | 218 | PRO  |
| 2   | 2     | 460 | GLY  |
| 2   | H     | 460 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 218 | PRO  |
| 1   | F     | 226 | THR  |
| 2   | G     | 460 | GLY  |
| 2   | L     | 398 | LEU  |
| 2   | N     | 317 | ASP  |
| 2   | P     | 434 | GLU  |
| 2   | P     | 460 | GLY  |
| 2   | R     | 434 | GLU  |
| 2   | V     | 398 | LEU  |
| 2   | V     | 482 | GLY  |
| 1   | Y     | 226 | THR  |
| 2   | Z     | 434 | GLU  |
| 1   | 1     | 226 | THR  |
| 2   | H     | 434 | GLU  |
| 2   | E     | 434 | GLU  |
| 2   | G     | 434 | GLU  |
| 2   | G     | 482 | GLY  |
| 2   | P     | 398 | LEU  |
| 2   | T     | 434 | GLU  |
| 2   | T     | 460 | GLY  |
| 2   | T     | 482 | GLY  |
| 2   | V     | 434 | GLU  |
| 2   | X     | 434 | GLU  |
| 2   | C     | 460 | GLY  |
| 2   | R     | 460 | GLY  |
| 2   | R     | 482 | GLY  |
| 2   | V     | 460 | GLY  |
| 2   | J     | 482 | GLY  |
| 2   | L     | 397 | GLY  |
| 2   | N     | 460 | GLY  |
| 2   | H     | 397 | GLY  |
| 2   | H     | 482 | GLY  |
| 2   | E     | 397 | GLY  |
| 2   | E     | 460 | GLY  |
| 2   | J     | 460 | GLY  |
| 2   | L     | 460 | GLY  |
| 2   | L     | 482 | GLY  |
| 2   | N     | 482 | GLY  |
| 2   | P     | 397 | GLY  |
| 2   | R     | 397 | GLY  |
| 2   | X     | 482 | GLY  |
| 2   | E     | 482 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 397 | GLY  |
| 2   | J     | 397 | GLY  |
| 2   | P     | 482 | GLY  |
| 2   | T     | 397 | GLY  |
| 2   | Z     | 482 | GLY  |
| 2   | 2     | 397 | GLY  |
| 2   | N     | 389 | GLY  |
| 2   | N     | 397 | 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   | 1     | 169/194 (87%) | 156 (92%) | 13 (8%)  | 18          | 61 |
| 1   | A     | 169/194 (87%) | 156 (92%) | 13 (8%)  | 18          | 61 |
| 1   | B     | 169/194 (87%) | 156 (92%) | 13 (8%)  | 18          | 61 |
| 1   | D     | 169/194 (87%) | 156 (92%) | 13 (8%)  | 18          | 61 |
| 1   | F     | 169/194 (87%) | 155 (92%) | 14 (8%)  | 16          | 56 |
| 1   | I     | 169/194 (87%) | 156 (92%) | 13 (8%)  | 18          | 61 |
| 1   | K     | 169/194 (87%) | 156 (92%) | 13 (8%)  | 18          | 61 |
| 1   | M     | 169/194 (87%) | 155 (92%) | 14 (8%)  | 16          | 56 |
| 1   | O     | 169/194 (87%) | 156 (92%) | 13 (8%)  | 18          | 61 |
| 1   | Q     | 169/194 (87%) | 155 (92%) | 14 (8%)  | 16          | 56 |
| 1   | S     | 169/194 (87%) | 156 (92%) | 13 (8%)  | 18          | 61 |
| 1   | U     | 169/194 (87%) | 156 (92%) | 13 (8%)  | 18          | 61 |
| 1   | W     | 169/194 (87%) | 155 (92%) | 14 (8%)  | 16          | 56 |
| 1   | Y     | 169/194 (87%) | 156 (92%) | 13 (8%)  | 18          | 61 |
| 2   | 2     | 165/178 (93%) | 150 (91%) | 15 (9%)  | 14          | 49 |
| 2   | C     | 165/178 (93%) | 150 (91%) | 15 (9%)  | 14          | 49 |
| 2   | E     | 165/178 (93%) | 150 (91%) | 15 (9%)  | 14          | 49 |
| 2   | G     | 165/178 (93%) | 151 (92%) | 14 (8%)  | 15          | 54 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | H     | 165/178 (93%)   | 150 (91%)  | 15 (9%)  | 14          | 49 |
| 2   | J     | 165/178 (93%)   | 150 (91%)  | 15 (9%)  | 14          | 49 |
| 2   | L     | 165/178 (93%)   | 150 (91%)  | 15 (9%)  | 14          | 49 |
| 2   | N     | 165/178 (93%)   | 150 (91%)  | 15 (9%)  | 14          | 49 |
| 2   | P     | 165/178 (93%)   | 151 (92%)  | 14 (8%)  | 15          | 54 |
| 2   | R     | 165/178 (93%)   | 150 (91%)  | 15 (9%)  | 14          | 49 |
| 2   | T     | 165/178 (93%)   | 150 (91%)  | 15 (9%)  | 14          | 49 |
| 2   | V     | 165/178 (93%)   | 150 (91%)  | 15 (9%)  | 14          | 49 |
| 2   | X     | 165/178 (93%)   | 150 (91%)  | 15 (9%)  | 14          | 49 |
| 2   | Z     | 165/178 (93%)   | 149 (90%)  | 16 (10%) | 12          | 46 |
| All | All   | 4676/5208 (90%) | 4281 (92%) | 395 (8%) | 16          | 55 |

All (395) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | LEU  |
| 1   | A     | 85  | ARG  |
| 1   | A     | 92  | ARG  |
| 1   | A     | 93  | ASP  |
| 1   | A     | 113 | GLU  |
| 1   | A     | 134 | LYS  |
| 1   | A     | 135 | ARG  |
| 1   | A     | 140 | ARG  |
| 1   | A     | 147 | ILE  |
| 1   | A     | 150 | GLU  |
| 1   | A     | 173 | GLU  |
| 1   | A     | 182 | ARG  |
| 1   | A     | 203 | LEU  |
| 2   | H     | 318 | ARG  |
| 2   | H     | 319 | ARG  |
| 2   | H     | 324 | ASN  |
| 2   | H     | 329 | ARG  |
| 2   | H     | 332 | ARG  |
| 2   | H     | 345 | ILE  |
| 2   | H     | 355 | PHE  |
| 2   | H     | 391 | LEU  |
| 2   | H     | 403 | LEU  |
| 2   | H     | 415 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 430 | ASN  |
| 2   | H     | 436 | TYR  |
| 2   | H     | 444 | LEU  |
| 2   | H     | 449 | SER  |
| 2   | H     | 508 | SER  |
| 1   | B     | 33  | LEU  |
| 1   | B     | 85  | ARG  |
| 1   | B     | 92  | ARG  |
| 1   | B     | 93  | ASP  |
| 1   | B     | 113 | GLU  |
| 1   | B     | 134 | LYS  |
| 1   | B     | 135 | ARG  |
| 1   | B     | 140 | ARG  |
| 1   | B     | 147 | ILE  |
| 1   | B     | 150 | GLU  |
| 1   | B     | 173 | GLU  |
| 1   | B     | 182 | ARG  |
| 1   | B     | 203 | LEU  |
| 2   | C     | 318 | ARG  |
| 2   | C     | 319 | ARG  |
| 2   | C     | 324 | ASN  |
| 2   | C     | 329 | ARG  |
| 2   | C     | 332 | ARG  |
| 2   | C     | 345 | ILE  |
| 2   | C     | 355 | PHE  |
| 2   | C     | 391 | LEU  |
| 2   | C     | 403 | LEU  |
| 2   | C     | 415 | GLN  |
| 2   | C     | 430 | ASN  |
| 2   | C     | 436 | TYR  |
| 2   | C     | 444 | LEU  |
| 2   | C     | 449 | SER  |
| 2   | C     | 508 | SER  |
| 1   | D     | 33  | LEU  |
| 1   | D     | 85  | ARG  |
| 1   | D     | 92  | ARG  |
| 1   | D     | 93  | ASP  |
| 1   | D     | 113 | GLU  |
| 1   | D     | 134 | LYS  |
| 1   | D     | 135 | ARG  |
| 1   | D     | 140 | ARG  |
| 1   | D     | 147 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 150 | GLU  |
| 1   | D     | 173 | GLU  |
| 1   | D     | 182 | ARG  |
| 1   | D     | 203 | LEU  |
| 2   | E     | 318 | ARG  |
| 2   | E     | 319 | ARG  |
| 2   | E     | 324 | ASN  |
| 2   | E     | 329 | ARG  |
| 2   | E     | 332 | ARG  |
| 2   | E     | 345 | ILE  |
| 2   | E     | 355 | PHE  |
| 2   | E     | 391 | LEU  |
| 2   | E     | 403 | LEU  |
| 2   | E     | 415 | GLN  |
| 2   | E     | 430 | ASN  |
| 2   | E     | 436 | TYR  |
| 2   | E     | 444 | LEU  |
| 2   | E     | 449 | SER  |
| 2   | E     | 508 | SER  |
| 1   | F     | 33  | LEU  |
| 1   | F     | 85  | ARG  |
| 1   | F     | 92  | ARG  |
| 1   | F     | 93  | ASP  |
| 1   | F     | 113 | GLU  |
| 1   | F     | 134 | LYS  |
| 1   | F     | 135 | ARG  |
| 1   | F     | 140 | ARG  |
| 1   | F     | 144 | ASP  |
| 1   | F     | 147 | ILE  |
| 1   | F     | 150 | GLU  |
| 1   | F     | 173 | GLU  |
| 1   | F     | 182 | ARG  |
| 1   | F     | 203 | LEU  |
| 2   | G     | 318 | ARG  |
| 2   | G     | 319 | ARG  |
| 2   | G     | 324 | ASN  |
| 2   | G     | 329 | ARG  |
| 2   | G     | 345 | ILE  |
| 2   | G     | 355 | PHE  |
| 2   | G     | 391 | LEU  |
| 2   | G     | 403 | LEU  |
| 2   | G     | 415 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 430 | ASN  |
| 2   | G     | 436 | TYR  |
| 2   | G     | 444 | LEU  |
| 2   | G     | 449 | SER  |
| 2   | G     | 508 | SER  |
| 1   | I     | 33  | LEU  |
| 1   | I     | 85  | ARG  |
| 1   | I     | 92  | ARG  |
| 1   | I     | 93  | ASP  |
| 1   | I     | 113 | GLU  |
| 1   | I     | 134 | LYS  |
| 1   | I     | 135 | ARG  |
| 1   | I     | 140 | ARG  |
| 1   | I     | 147 | ILE  |
| 1   | I     | 150 | GLU  |
| 1   | I     | 173 | GLU  |
| 1   | I     | 182 | ARG  |
| 1   | I     | 203 | LEU  |
| 2   | J     | 318 | ARG  |
| 2   | J     | 319 | ARG  |
| 2   | J     | 324 | ASN  |
| 2   | J     | 329 | ARG  |
| 2   | J     | 332 | ARG  |
| 2   | J     | 345 | ILE  |
| 2   | J     | 355 | PHE  |
| 2   | J     | 391 | LEU  |
| 2   | J     | 403 | LEU  |
| 2   | J     | 415 | GLN  |
| 2   | J     | 430 | ASN  |
| 2   | J     | 436 | TYR  |
| 2   | J     | 444 | LEU  |
| 2   | J     | 449 | SER  |
| 2   | J     | 508 | SER  |
| 1   | K     | 33  | LEU  |
| 1   | K     | 85  | ARG  |
| 1   | K     | 92  | ARG  |
| 1   | K     | 93  | ASP  |
| 1   | K     | 113 | GLU  |
| 1   | K     | 134 | LYS  |
| 1   | K     | 135 | ARG  |
| 1   | K     | 140 | ARG  |
| 1   | K     | 147 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 150 | GLU  |
| 1   | K     | 173 | GLU  |
| 1   | K     | 182 | ARG  |
| 1   | K     | 203 | LEU  |
| 2   | L     | 318 | ARG  |
| 2   | L     | 319 | ARG  |
| 2   | L     | 324 | ASN  |
| 2   | L     | 329 | ARG  |
| 2   | L     | 332 | ARG  |
| 2   | L     | 345 | ILE  |
| 2   | L     | 355 | PHE  |
| 2   | L     | 391 | LEU  |
| 2   | L     | 403 | LEU  |
| 2   | L     | 415 | GLN  |
| 2   | L     | 430 | ASN  |
| 2   | L     | 436 | TYR  |
| 2   | L     | 444 | LEU  |
| 2   | L     | 449 | SER  |
| 2   | L     | 508 | SER  |
| 1   | M     | 33  | LEU  |
| 1   | M     | 85  | ARG  |
| 1   | M     | 92  | ARG  |
| 1   | M     | 93  | ASP  |
| 1   | M     | 113 | GLU  |
| 1   | M     | 134 | LYS  |
| 1   | M     | 135 | ARG  |
| 1   | M     | 140 | ARG  |
| 1   | M     | 144 | ASP  |
| 1   | M     | 147 | ILE  |
| 1   | M     | 150 | GLU  |
| 1   | M     | 173 | GLU  |
| 1   | M     | 182 | ARG  |
| 1   | M     | 203 | LEU  |
| 2   | N     | 318 | ARG  |
| 2   | N     | 319 | ARG  |
| 2   | N     | 324 | ASN  |
| 2   | N     | 329 | ARG  |
| 2   | N     | 332 | ARG  |
| 2   | N     | 345 | ILE  |
| 2   | N     | 355 | PHE  |
| 2   | N     | 391 | LEU  |
| 2   | N     | 403 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 415 | GLN  |
| 2   | N     | 430 | ASN  |
| 2   | N     | 436 | TYR  |
| 2   | N     | 444 | LEU  |
| 2   | N     | 449 | SER  |
| 2   | N     | 508 | SER  |
| 1   | O     | 33  | LEU  |
| 1   | O     | 85  | ARG  |
| 1   | O     | 92  | ARG  |
| 1   | O     | 113 | GLU  |
| 1   | O     | 134 | LYS  |
| 1   | O     | 135 | ARG  |
| 1   | O     | 140 | ARG  |
| 1   | O     | 147 | ILE  |
| 1   | O     | 150 | GLU  |
| 1   | O     | 173 | GLU  |
| 1   | O     | 179 | ASP  |
| 1   | O     | 182 | ARG  |
| 1   | O     | 203 | LEU  |
| 2   | P     | 318 | ARG  |
| 2   | P     | 319 | ARG  |
| 2   | P     | 324 | ASN  |
| 2   | P     | 329 | ARG  |
| 2   | P     | 332 | ARG  |
| 2   | P     | 345 | ILE  |
| 2   | P     | 391 | LEU  |
| 2   | P     | 403 | LEU  |
| 2   | P     | 415 | GLN  |
| 2   | P     | 430 | ASN  |
| 2   | P     | 436 | TYR  |
| 2   | P     | 444 | LEU  |
| 2   | P     | 449 | SER  |
| 2   | P     | 508 | SER  |
| 1   | Q     | 33  | LEU  |
| 1   | Q     | 85  | ARG  |
| 1   | Q     | 92  | ARG  |
| 1   | Q     | 93  | ASP  |
| 1   | Q     | 113 | GLU  |
| 1   | Q     | 134 | LYS  |
| 1   | Q     | 135 | ARG  |
| 1   | Q     | 140 | ARG  |
| 1   | Q     | 147 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 150 | GLU  |
| 1   | Q     | 173 | GLU  |
| 1   | Q     | 179 | ASP  |
| 1   | Q     | 182 | ARG  |
| 1   | Q     | 203 | LEU  |
| 2   | R     | 318 | ARG  |
| 2   | R     | 319 | ARG  |
| 2   | R     | 324 | ASN  |
| 2   | R     | 329 | ARG  |
| 2   | R     | 332 | ARG  |
| 2   | R     | 345 | ILE  |
| 2   | R     | 355 | PHE  |
| 2   | R     | 391 | LEU  |
| 2   | R     | 403 | LEU  |
| 2   | R     | 415 | GLN  |
| 2   | R     | 430 | ASN  |
| 2   | R     | 436 | TYR  |
| 2   | R     | 444 | LEU  |
| 2   | R     | 449 | SER  |
| 2   | R     | 508 | SER  |
| 1   | S     | 33  | LEU  |
| 1   | S     | 85  | ARG  |
| 1   | S     | 92  | ARG  |
| 1   | S     | 93  | ASP  |
| 1   | S     | 113 | GLU  |
| 1   | S     | 134 | LYS  |
| 1   | S     | 135 | ARG  |
| 1   | S     | 140 | ARG  |
| 1   | S     | 147 | ILE  |
| 1   | S     | 150 | GLU  |
| 1   | S     | 173 | GLU  |
| 1   | S     | 182 | ARG  |
| 1   | S     | 203 | LEU  |
| 2   | T     | 318 | ARG  |
| 2   | T     | 319 | ARG  |
| 2   | T     | 324 | ASN  |
| 2   | T     | 329 | ARG  |
| 2   | T     | 332 | ARG  |
| 2   | T     | 345 | ILE  |
| 2   | T     | 355 | PHE  |
| 2   | T     | 391 | LEU  |
| 2   | T     | 403 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | T     | 415 | GLN  |
| 2   | T     | 430 | ASN  |
| 2   | T     | 436 | TYR  |
| 2   | T     | 444 | LEU  |
| 2   | T     | 449 | SER  |
| 2   | T     | 508 | SER  |
| 1   | U     | 33  | LEU  |
| 1   | U     | 85  | ARG  |
| 1   | U     | 92  | ARG  |
| 1   | U     | 113 | GLU  |
| 1   | U     | 134 | LYS  |
| 1   | U     | 135 | ARG  |
| 1   | U     | 140 | ARG  |
| 1   | U     | 144 | ASP  |
| 1   | U     | 147 | ILE  |
| 1   | U     | 150 | GLU  |
| 1   | U     | 173 | GLU  |
| 1   | U     | 182 | ARG  |
| 1   | U     | 203 | LEU  |
| 2   | V     | 318 | ARG  |
| 2   | V     | 319 | ARG  |
| 2   | V     | 324 | ASN  |
| 2   | V     | 329 | ARG  |
| 2   | V     | 332 | ARG  |
| 2   | V     | 345 | ILE  |
| 2   | V     | 355 | PHE  |
| 2   | V     | 391 | LEU  |
| 2   | V     | 403 | LEU  |
| 2   | V     | 415 | GLN  |
| 2   | V     | 430 | ASN  |
| 2   | V     | 436 | TYR  |
| 2   | V     | 444 | LEU  |
| 2   | V     | 449 | SER  |
| 2   | V     | 508 | SER  |
| 1   | W     | 33  | LEU  |
| 1   | W     | 85  | ARG  |
| 1   | W     | 92  | ARG  |
| 1   | W     | 113 | GLU  |
| 1   | W     | 134 | LYS  |
| 1   | W     | 135 | ARG  |
| 1   | W     | 140 | ARG  |
| 1   | W     | 144 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | W     | 147 | ILE  |
| 1   | W     | 150 | GLU  |
| 1   | W     | 173 | GLU  |
| 1   | W     | 179 | ASP  |
| 1   | W     | 182 | ARG  |
| 1   | W     | 203 | LEU  |
| 2   | X     | 318 | ARG  |
| 2   | X     | 319 | ARG  |
| 2   | X     | 324 | ASN  |
| 2   | X     | 329 | ARG  |
| 2   | X     | 345 | ILE  |
| 2   | X     | 355 | PHE  |
| 2   | X     | 391 | LEU  |
| 2   | X     | 403 | LEU  |
| 2   | X     | 415 | GLN  |
| 2   | X     | 430 | ASN  |
| 2   | X     | 436 | TYR  |
| 2   | X     | 444 | LEU  |
| 2   | X     | 449 | SER  |
| 2   | X     | 458 | THR  |
| 2   | X     | 508 | SER  |
| 1   | Y     | 33  | LEU  |
| 1   | Y     | 85  | ARG  |
| 1   | Y     | 92  | ARG  |
| 1   | Y     | 93  | ASP  |
| 1   | Y     | 113 | GLU  |
| 1   | Y     | 134 | LYS  |
| 1   | Y     | 135 | ARG  |
| 1   | Y     | 140 | ARG  |
| 1   | Y     | 147 | ILE  |
| 1   | Y     | 150 | GLU  |
| 1   | Y     | 173 | GLU  |
| 1   | Y     | 182 | ARG  |
| 1   | Y     | 203 | LEU  |
| 2   | Z     | 318 | ARG  |
| 2   | Z     | 319 | ARG  |
| 2   | Z     | 324 | ASN  |
| 2   | Z     | 329 | ARG  |
| 2   | Z     | 332 | ARG  |
| 2   | Z     | 341 | THR  |
| 2   | Z     | 345 | ILE  |
| 2   | Z     | 355 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Z     | 391 | LEU  |
| 2   | Z     | 403 | LEU  |
| 2   | Z     | 415 | GLN  |
| 2   | Z     | 430 | ASN  |
| 2   | Z     | 436 | TYR  |
| 2   | Z     | 444 | LEU  |
| 2   | Z     | 449 | SER  |
| 2   | Z     | 508 | SER  |
| 1   | 1     | 33  | LEU  |
| 1   | 1     | 85  | ARG  |
| 1   | 1     | 92  | ARG  |
| 1   | 1     | 93  | ASP  |
| 1   | 1     | 113 | GLU  |
| 1   | 1     | 134 | LYS  |
| 1   | 1     | 135 | ARG  |
| 1   | 1     | 140 | ARG  |
| 1   | 1     | 147 | ILE  |
| 1   | 1     | 150 | GLU  |
| 1   | 1     | 173 | GLU  |
| 1   | 1     | 182 | ARG  |
| 1   | 1     | 203 | LEU  |
| 2   | 2     | 318 | ARG  |
| 2   | 2     | 319 | ARG  |
| 2   | 2     | 324 | ASN  |
| 2   | 2     | 329 | ARG  |
| 2   | 2     | 332 | ARG  |
| 2   | 2     | 345 | ILE  |
| 2   | 2     | 355 | PHE  |
| 2   | 2     | 391 | LEU  |
| 2   | 2     | 403 | LEU  |
| 2   | 2     | 415 | GLN  |
| 2   | 2     | 430 | ASN  |
| 2   | 2     | 436 | TYR  |
| 2   | 2     | 444 | LEU  |
| 2   | 2     | 449 | SER  |
| 2   | 2     | 508 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 51  | GLN  |
| 1   | A     | 73  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 98  | GLN  |
| 1   | A     | 105 | GLN  |
| 1   | A     | 129 | HIS  |
| 1   | A     | 165 | ASN  |
| 1   | A     | 231 | GLN  |
| 2   | H     | 324 | ASN  |
| 2   | H     | 365 | HIS  |
| 2   | H     | 415 | GLN  |
| 2   | H     | 456 | GLN  |
| 1   | B     | 51  | GLN  |
| 1   | B     | 73  | ASN  |
| 1   | B     | 80  | GLN  |
| 1   | B     | 98  | GLN  |
| 1   | B     | 129 | HIS  |
| 1   | B     | 165 | ASN  |
| 1   | B     | 231 | GLN  |
| 2   | C     | 324 | ASN  |
| 2   | C     | 365 | HIS  |
| 2   | C     | 415 | GLN  |
| 2   | C     | 456 | GLN  |
| 1   | D     | 51  | GLN  |
| 1   | D     | 73  | ASN  |
| 1   | D     | 98  | GLN  |
| 1   | D     | 129 | HIS  |
| 1   | D     | 165 | ASN  |
| 1   | D     | 231 | GLN  |
| 2   | E     | 324 | ASN  |
| 2   | E     | 365 | HIS  |
| 2   | E     | 415 | GLN  |
| 2   | E     | 456 | GLN  |
| 1   | F     | 51  | GLN  |
| 1   | F     | 73  | ASN  |
| 1   | F     | 80  | GLN  |
| 1   | F     | 98  | GLN  |
| 1   | F     | 105 | GLN  |
| 1   | F     | 129 | HIS  |
| 1   | F     | 165 | ASN  |
| 1   | F     | 231 | GLN  |
| 2   | G     | 324 | ASN  |
| 2   | G     | 365 | HIS  |
| 2   | G     | 415 | GLN  |
| 2   | G     | 456 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 51  | GLN  |
| 1   | I     | 73  | ASN  |
| 1   | I     | 80  | GLN  |
| 1   | I     | 98  | GLN  |
| 1   | I     | 105 | GLN  |
| 1   | I     | 129 | HIS  |
| 1   | I     | 165 | ASN  |
| 1   | I     | 231 | GLN  |
| 2   | J     | 324 | ASN  |
| 2   | J     | 365 | HIS  |
| 2   | J     | 415 | GLN  |
| 2   | J     | 456 | GLN  |
| 1   | K     | 51  | GLN  |
| 1   | K     | 73  | ASN  |
| 1   | K     | 80  | GLN  |
| 1   | K     | 98  | GLN  |
| 1   | K     | 129 | HIS  |
| 1   | K     | 165 | ASN  |
| 1   | K     | 231 | GLN  |
| 2   | L     | 324 | ASN  |
| 2   | L     | 365 | HIS  |
| 2   | L     | 415 | GLN  |
| 2   | L     | 456 | GLN  |
| 1   | M     | 51  | GLN  |
| 1   | M     | 80  | GLN  |
| 1   | M     | 98  | GLN  |
| 1   | M     | 129 | HIS  |
| 1   | M     | 165 | ASN  |
| 1   | M     | 231 | GLN  |
| 2   | N     | 324 | ASN  |
| 2   | N     | 365 | HIS  |
| 2   | N     | 415 | GLN  |
| 2   | N     | 456 | GLN  |
| 1   | O     | 51  | GLN  |
| 1   | O     | 73  | ASN  |
| 1   | O     | 98  | GLN  |
| 1   | O     | 105 | GLN  |
| 1   | O     | 129 | HIS  |
| 1   | O     | 165 | ASN  |
| 1   | O     | 231 | GLN  |
| 2   | P     | 324 | ASN  |
| 2   | P     | 365 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 415 | GLN  |
| 2   | P     | 456 | GLN  |
| 1   | Q     | 51  | GLN  |
| 1   | Q     | 98  | GLN  |
| 1   | Q     | 105 | GLN  |
| 1   | Q     | 129 | HIS  |
| 1   | Q     | 165 | ASN  |
| 1   | Q     | 231 | GLN  |
| 2   | R     | 324 | ASN  |
| 2   | R     | 365 | HIS  |
| 2   | R     | 415 | GLN  |
| 2   | R     | 456 | GLN  |
| 1   | S     | 51  | GLN  |
| 1   | S     | 73  | ASN  |
| 1   | S     | 98  | GLN  |
| 1   | S     | 105 | GLN  |
| 1   | S     | 129 | HIS  |
| 1   | S     | 165 | ASN  |
| 1   | S     | 231 | GLN  |
| 2   | T     | 324 | ASN  |
| 2   | T     | 365 | HIS  |
| 2   | T     | 415 | GLN  |
| 2   | T     | 456 | GLN  |
| 1   | U     | 51  | GLN  |
| 1   | U     | 73  | ASN  |
| 1   | U     | 80  | GLN  |
| 1   | U     | 98  | GLN  |
| 1   | U     | 105 | GLN  |
| 1   | U     | 129 | HIS  |
| 1   | U     | 165 | ASN  |
| 1   | U     | 231 | GLN  |
| 2   | V     | 324 | ASN  |
| 2   | V     | 365 | HIS  |
| 2   | V     | 415 | GLN  |
| 2   | V     | 456 | GLN  |
| 1   | W     | 51  | GLN  |
| 1   | W     | 73  | ASN  |
| 1   | W     | 80  | GLN  |
| 1   | W     | 98  | GLN  |
| 1   | W     | 129 | HIS  |
| 1   | W     | 165 | ASN  |
| 1   | W     | 231 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | X     | 324 | ASN  |
| 2   | X     | 365 | HIS  |
| 2   | X     | 415 | GLN  |
| 2   | X     | 456 | GLN  |
| 1   | Y     | 51  | GLN  |
| 1   | Y     | 73  | ASN  |
| 1   | Y     | 98  | GLN  |
| 1   | Y     | 129 | HIS  |
| 1   | Y     | 165 | ASN  |
| 1   | Y     | 231 | GLN  |
| 2   | Z     | 324 | ASN  |
| 2   | Z     | 365 | HIS  |
| 2   | Z     | 415 | GLN  |
| 2   | Z     | 456 | GLN  |
| 1   | 1     | 51  | GLN  |
| 1   | 1     | 73  | ASN  |
| 1   | 1     | 80  | GLN  |
| 1   | 1     | 98  | GLN  |
| 1   | 1     | 105 | GLN  |
| 1   | 1     | 129 | HIS  |
| 1   | 1     | 165 | ASN  |
| 1   | 1     | 231 | GLN  |
| 2   | 2     | 324 | ASN  |
| 2   | 2     | 365 | HIS  |
| 2   | 2     | 415 | GLN  |
| 2   | 2     | 456 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1   | 1     | 220/250 (88%) | 0.43   | 7 (3%) 45 10 | 100, 100, 100, 100    | 0     |
| 1   | A     | 220/250 (88%) | 0.38   | 3 (1%) 72 24 | 100, 100, 100, 100    | 0     |
| 1   | B     | 220/250 (88%) | 0.38   | 4 (1%) 65 20 | 100, 100, 100, 100    | 0     |
| 1   | D     | 220/250 (88%) | 0.50   | 5 (2%) 57 15 | 100, 100, 100, 100    | 0     |
| 1   | F     | 220/250 (88%) | 0.43   | 4 (1%) 65 20 | 100, 100, 100, 100    | 0     |
| 1   | I     | 220/250 (88%) | 0.51   | 8 (3%) 41 9  | 100, 100, 100, 100    | 0     |
| 1   | K     | 220/250 (88%) | 0.76   | 19 (8%) 11 3 | 100, 100, 100, 100    | 0     |
| 1   | M     | 220/250 (88%) | 0.45   | 4 (1%) 65 20 | 100, 100, 100, 100    | 0     |
| 1   | O     | 220/250 (88%) | 0.56   | 11 (5%) 28 6 | 100, 100, 100, 100    | 0     |
| 1   | Q     | 220/250 (88%) | 0.64   | 7 (3%) 45 10 | 100, 100, 100, 100    | 0     |
| 1   | S     | 220/250 (88%) | 0.54   | 10 (4%) 32 7 | 100, 100, 100, 100    | 0     |
| 1   | U     | 220/250 (88%) | 0.57   | 7 (3%) 45 10 | 100, 100, 100, 100    | 0     |
| 1   | W     | 220/250 (88%) | 0.42   | 4 (1%) 65 20 | 100, 100, 100, 100    | 0     |
| 1   | Y     | 220/250 (88%) | 0.54   | 4 (1%) 65 20 | 100, 100, 100, 100    | 0     |
| 2   | 2     | 222/240 (92%) | 0.35   | 1 (0%) 88 48 | 100, 100, 100, 100    | 0     |
| 2   | C     | 222/240 (92%) | 0.45   | 0 100 100    | 100, 100, 100, 100    | 0     |
| 2   | E     | 222/240 (92%) | 0.41   | 1 (0%) 88 48 | 100, 100, 100, 100    | 0     |
| 2   | G     | 222/240 (92%) | 1.49   | 46 (20%) 1 1 | 100, 100, 100, 100    | 0     |
| 2   | H     | 222/240 (92%) | 0.46   | 0 100 100    | 100, 100, 100, 100    | 0     |
| 2   | J     | 222/240 (92%) | 0.29   | 0 100 100    | 100, 100, 100, 100    | 0     |
| 2   | L     | 222/240 (92%) | 0.31   | 0 100 100    | 100, 100, 100, 100    | 0     |
| 2   | N     | 222/240 (92%) | 0.28   | 0 100 100    | 100, 100, 100, 100    | 0     |
| 2   | P     | 222/240 (92%) | 0.35   | 0 100 100    | 100, 100, 100, 100    | 0     |
| 2   | R     | 222/240 (92%) | 0.35   | 0 100 100    | 100, 100, 100, 100    | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|-----|-----|-----------------------|-------|
| 2   | T     | 222/240 (92%)   | 0.28   | 0        | 100 | 100 | 100, 100, 100, 100    | 0     |
| 2   | V     | 222/240 (92%)   | 0.32   | 0        | 100 | 100 | 100, 100, 100, 100    | 0     |
| 2   | X     | 222/240 (92%)   | 0.24   | 0        | 100 | 100 | 100, 100, 100, 100    | 0     |
| 2   | Z     | 222/240 (92%)   | 0.33   | 0        | 100 | 100 | 100, 100, 100, 100    | 0     |
| All | All   | 6188/6860 (90%) | 0.46   | 145 (2%) | 57  | 15  | 100, 100, 100, 100    | 0     |

All (145) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 235 | VAL  | 9.3  |
| 1   | U     | 237 | GLN  | 8.1  |
| 1   | S     | 236 | ASP  | 7.8  |
| 1   | S     | 235 | VAL  | 7.0  |
| 1   | A     | 235 | VAL  | 6.8  |
| 1   | I     | 235 | VAL  | 6.8  |
| 1   | Q     | 235 | VAL  | 5.9  |
| 1   | U     | 235 | VAL  | 5.8  |
| 1   | Q     | 237 | GLN  | 5.8  |
| 1   | U     | 236 | ASP  | 5.8  |
| 1   | M     | 235 | VAL  | 5.7  |
| 1   | Q     | 236 | ASP  | 5.7  |
| 1   | K     | 236 | ASP  | 5.3  |
| 1   | A     | 237 | GLN  | 5.2  |
| 1   | O     | 237 | GLN  | 5.2  |
| 1   | D     | 236 | ASP  | 5.2  |
| 1   | I     | 236 | ASP  | 5.2  |
| 1   | M     | 237 | GLN  | 5.1  |
| 1   | K     | 171 | TYR  | 5.0  |
| 1   | W     | 235 | VAL  | 4.9  |
| 1   | O     | 235 | VAL  | 4.6  |
| 1   | F     | 236 | ASP  | 4.5  |
| 1   | Y     | 236 | ASP  | 4.4  |
| 1   | D     | 237 | GLN  | 4.4  |
| 1   | D     | 235 | VAL  | 4.2  |
| 1   | O     | 236 | ASP  | 4.1  |
| 1   | Y     | 237 | GLN  | 4.0  |
| 1   | O     | 233 | LEU  | 4.0  |
| 1   | I     | 237 | GLN  | 3.9  |
| 1   | S     | 237 | GLN  | 3.8  |
| 1   | 1     | 236 | ASP  | 3.6  |
| 1   | K     | 172 | ALA  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 234 | LEU  | 3.5  |
| 2   | G     | 403 | LEU  | 3.5  |
| 1   | 1     | 235 | VAL  | 3.4  |
| 2   | G     | 345 | ILE  | 3.3  |
| 1   | A     | 236 | ASP  | 3.3  |
| 1   | K     | 237 | GLN  | 3.3  |
| 2   | G     | 420 | ILE  | 3.3  |
| 2   | G     | 497 | ILE  | 3.3  |
| 1   | 1     | 237 | GLN  | 3.2  |
| 2   | G     | 418 | GLY  | 3.2  |
| 1   | K     | 143 | TYR  | 3.2  |
| 2   | G     | 453 | LEU  | 3.2  |
| 1   | Q     | 234 | LEU  | 3.1  |
| 1   | I     | 203 | LEU  | 3.1  |
| 1   | B     | 236 | ASP  | 3.1  |
| 1   | M     | 236 | ASP  | 3.1  |
| 1   | O     | 225 | ILE  | 3.0  |
| 1   | K     | 186 | ALA  | 2.9  |
| 2   | 2     | 414 | PRO  | 2.9  |
| 1   | S     | 234 | LEU  | 2.9  |
| 2   | G     | 456 | GLN  | 2.9  |
| 1   | K     | 64  | ALA  | 2.9  |
| 2   | G     | 469 | GLU  | 2.9  |
| 1   | I     | 204 | GLY  | 2.9  |
| 1   | K     | 184 | ALA  | 2.9  |
| 1   | Q     | 190 | ALA  | 2.8  |
| 1   | K     | 119 | GLU  | 2.8  |
| 1   | O     | 137 | GLU  | 2.8  |
| 2   | G     | 404 | LEU  | 2.8  |
| 2   | G     | 465 | ARG  | 2.8  |
| 2   | G     | 306 | LEU  | 2.8  |
| 2   | G     | 356 | ALA  | 2.8  |
| 2   | G     | 307 | LYS  | 2.8  |
| 2   | G     | 342 | ALA  | 2.8  |
| 2   | G     | 337 | THR  | 2.7  |
| 2   | G     | 305 | ALA  | 2.7  |
| 2   | G     | 312 | VAL  | 2.7  |
| 1   | K     | 234 | LEU  | 2.7  |
| 1   | S     | 171 | TYR  | 2.7  |
| 1   | K     | 192 | SER  | 2.7  |
| 1   | K     | 40  | LEU  | 2.6  |
| 2   | G     | 466 | VAL  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 235 | VAL  | 2.6  |
| 1   | K     | 41  | PHE  | 2.6  |
| 2   | G     | 380 | ILE  | 2.6  |
| 1   | O     | 167 | LEU  | 2.6  |
| 1   | K     | 209 | GLU  | 2.6  |
| 1   | S     | 167 | LEU  | 2.6  |
| 2   | G     | 314 | MET  | 2.5  |
| 2   | G     | 363 | LEU  | 2.5  |
| 1   | W     | 236 | ASP  | 2.5  |
| 2   | E     | 363 | LEU  | 2.5  |
| 1   | Y     | 235 | VAL  | 2.5  |
| 1   | K     | 135 | ARG  | 2.5  |
| 2   | G     | 374 | LEU  | 2.5  |
| 1   | K     | 153 | PHE  | 2.5  |
| 1   | S     | 213 | LEU  | 2.4  |
| 1   | I     | 172 | ALA  | 2.4  |
| 1   | O     | 191 | GLY  | 2.4  |
| 2   | G     | 376 | PHE  | 2.4  |
| 2   | G     | 383 | LEU  | 2.4  |
| 1   | U     | 169 | GLU  | 2.4  |
| 2   | G     | 379 | LYS  | 2.4  |
| 2   | G     | 500 | ASP  | 2.4  |
| 1   | Q     | 130 | TYR  | 2.4  |
| 2   | G     | 368 | LYS  | 2.4  |
| 2   | G     | 438 | ALA  | 2.4  |
| 1   | O     | 171 | TYR  | 2.4  |
| 1   | Q     | 171 | TYR  | 2.4  |
| 2   | G     | 454 | TYR  | 2.4  |
| 1   | F     | 235 | VAL  | 2.4  |
| 2   | G     | 449 | SER  | 2.3  |
| 1   | B     | 237 | GLN  | 2.3  |
| 2   | G     | 405 | ALA  | 2.3  |
| 1   | U     | 177 | LEU  | 2.3  |
| 1   | B     | 150 | GLU  | 2.3  |
| 2   | G     | 421 | VAL  | 2.3  |
| 2   | G     | 360 | ALA  | 2.2  |
| 2   | G     | 450 | MET  | 2.2  |
| 1   | K     | 127 | VAL  | 2.2  |
| 2   | G     | 468 | VAL  | 2.2  |
| 2   | G     | 335 | TYR  | 2.2  |
| 1   | S     | 16  | ARG  | 2.2  |
| 2   | G     | 339 | ASP  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | G     | 457 | VAL  | 2.2  |
| 2   | G     | 411 | ALA  | 2.2  |
| 1   | O     | 203 | LEU  | 2.2  |
| 2   | G     | 484 | PRO  | 2.2  |
| 1   | S     | 135 | ARG  | 2.2  |
| 1   | M     | 172 | ALA  | 2.1  |
| 1   | Y     | 13  | MET  | 2.1  |
| 2   | G     | 377 | ALA  | 2.1  |
| 1   | K     | 191 | GLY  | 2.1  |
| 2   | G     | 501 | GLY  | 2.1  |
| 1   | S     | 111 | PHE  | 2.1  |
| 1   | 1     | 171 | TYR  | 2.1  |
| 1   | O     | 172 | ALA  | 2.1  |
| 2   | G     | 343 | THR  | 2.1  |
| 1   | 1     | 10  | GLU  | 2.1  |
| 1   | D     | 56  | LEU  | 2.1  |
| 1   | W     | 237 | GLN  | 2.1  |
| 1   | W     | 188 | LEU  | 2.1  |
| 1   | 1     | 209 | GLU  | 2.1  |
| 1   | F     | 237 | GLN  | 2.1  |
| 2   | G     | 384 | ALA  | 2.0  |
| 2   | G     | 371 | GLY  | 2.0  |
| 1   | U     | 234 | LEU  | 2.0  |
| 1   | F     | 67  | LYS  | 2.0  |
| 1   | U     | 186 | ALA  | 2.0  |
| 1   | 1     | 167 | LEU  | 2.0  |
| 2   | G     | 407 | TYR  | 2.0  |
| 1   | D     | 234 | LEU  | 2.0  |
| 1   | I     | 231 | GLN  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.