



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:16 PM UTC

PDB ID : 3C91 / pdb\_00003c91  
EMDB ID : EMD-1733  
Title : Thermoplasma acidophilum 20S proteasome with an open gate  
Authors : Rabl, J.; Smith, D.M.; Yu, Y.; Chang, S.C.; Goldberg, A.L.; Cheng, Y.  
Deposited on : 2008-02-14  
Resolution : 6.80 Å(reported)  
Based on initial model : 1PMA

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

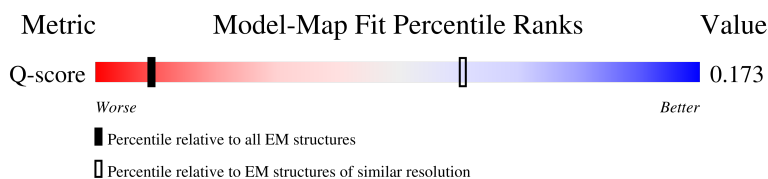
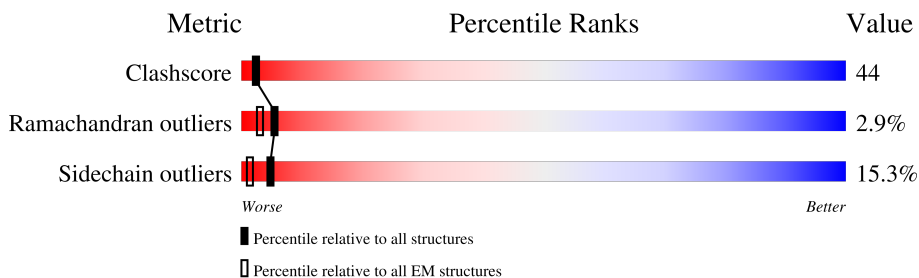
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.80 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 503 ( 6.30 - 7.30 )                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 233    |                  |
| 1   | B     | 233    |                  |
| 1   | C     | 233    |                  |
| 1   | D     | 233    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 233    |                  |
| 1   | F     | 233    |                  |
| 1   | G     | 233    |                  |
| 1   | O     | 233    |                  |
| 1   | P     | 233    |                  |
| 1   | Q     | 233    |                  |
| 1   | R     | 233    |                  |
| 1   | S     | 233    |                  |
| 1   | T     | 233    |                  |
| 1   | U     | 233    |                  |
| 2   | 1     | 203    |                  |
| 2   | 2     | 203    |                  |
| 2   | H     | 203    |                  |
| 2   | I     | 203    |                  |
| 2   | J     | 203    |                  |
| 2   | K     | 203    |                  |
| 2   | L     | 203    |                  |
| 2   | M     | 203    |                  |
| 2   | N     | 203    |                  |
| 2   | V     | 203    |                  |
| 2   | W     | 203    |                  |
| 2   | X     | 203    |                  |
| 2   | Y     | 203    |                  |
| 2   | Z     | 203    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46578 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Proteasome subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | B     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | C     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | D     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | E     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | F     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | G     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | O     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | P     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | Q     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | R     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | S     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | T     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |
| 1   | U     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1123 | 299 | 344 | 3 |         |       |

- Molecule 2 is a protein called Proteasome subunit beta.

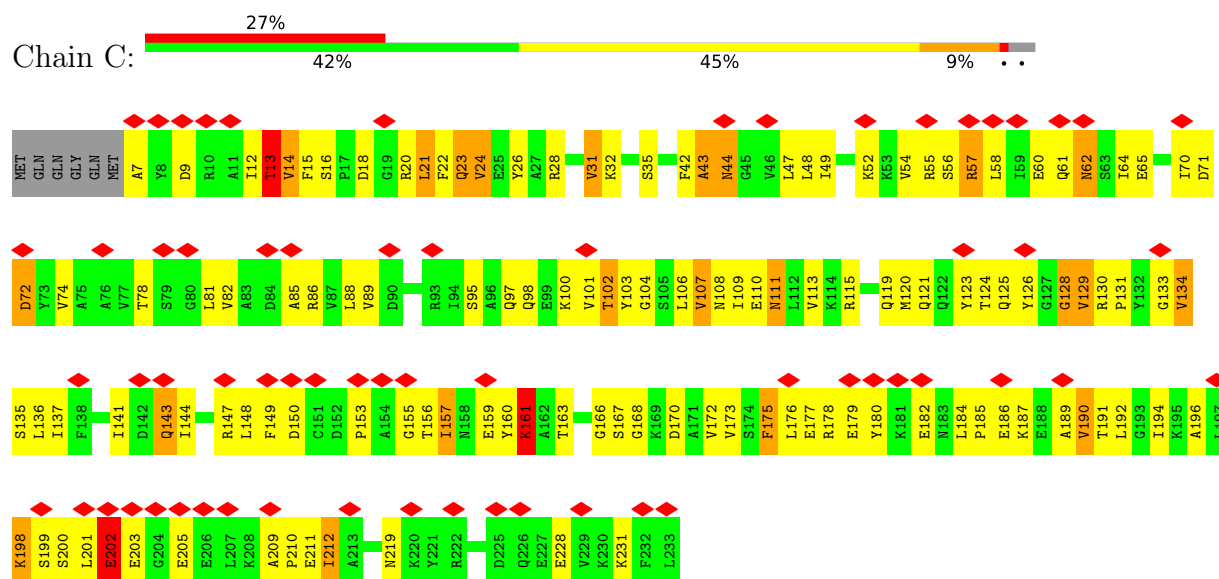
| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | H     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |

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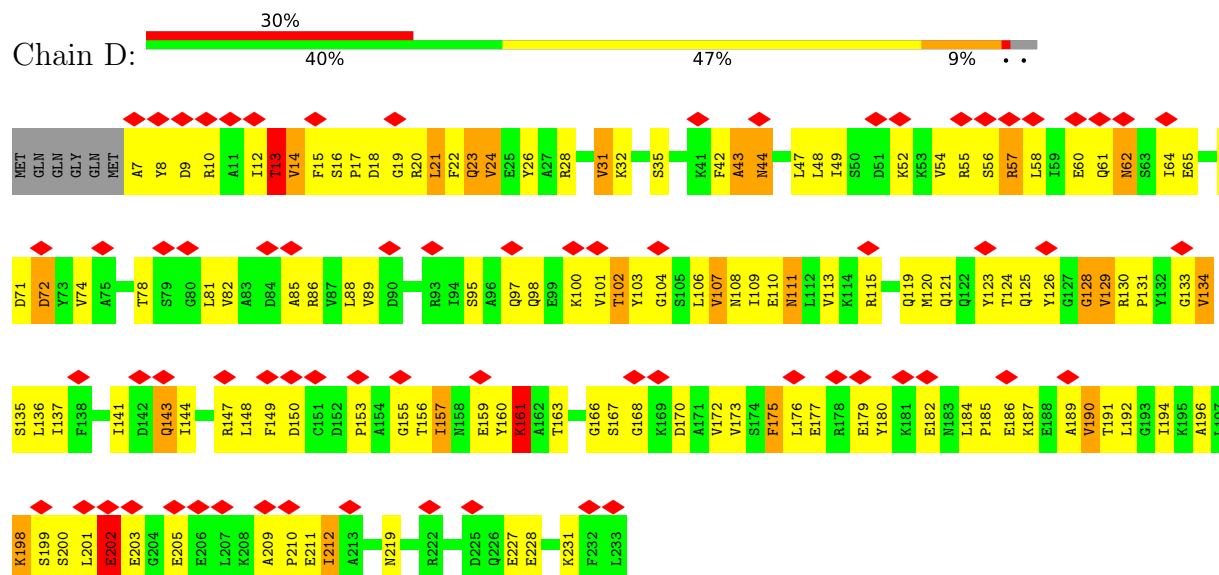
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| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | I     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | J     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | K     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | L     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | M     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | N     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | V     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | W     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | X     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | Y     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | Z     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | 1     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |
| 2   | 2     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1558  | 985 | 264 | 298 | 11 |         |       |

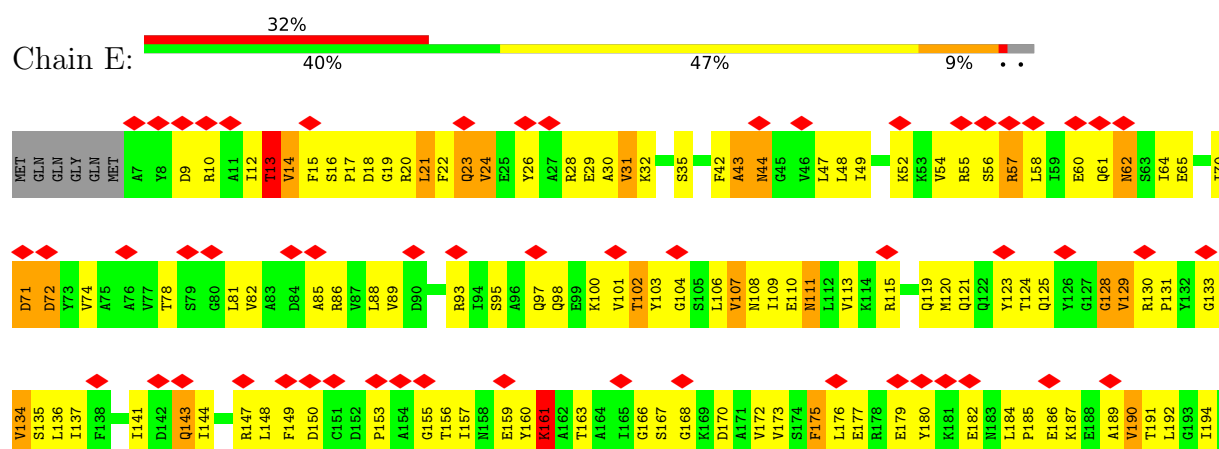


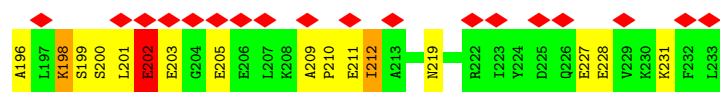


• Molecule 1: Proteasome subunit alpha

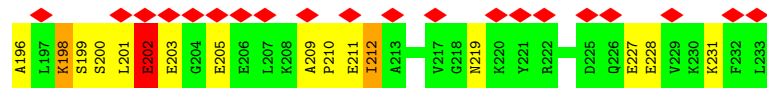
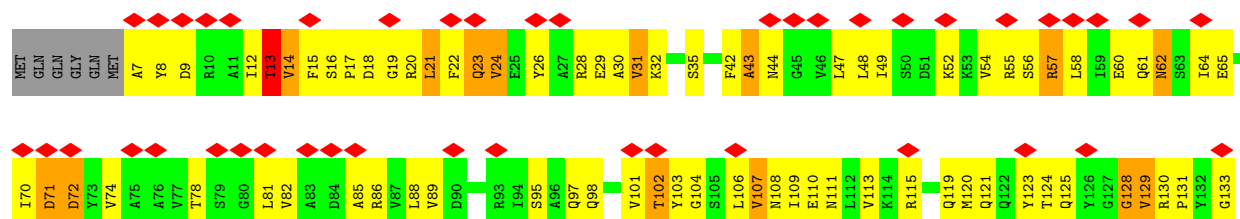


• Molecule 1: Proteasome subunit alpha

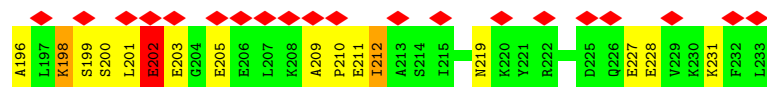
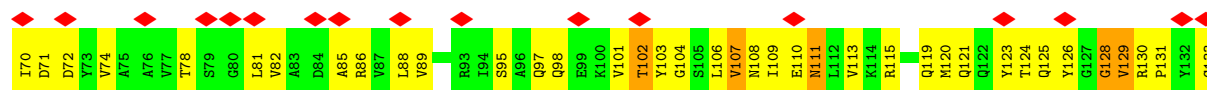
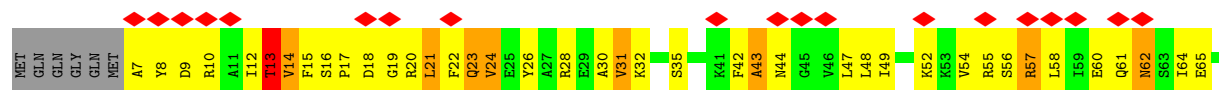
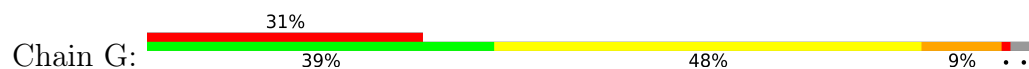




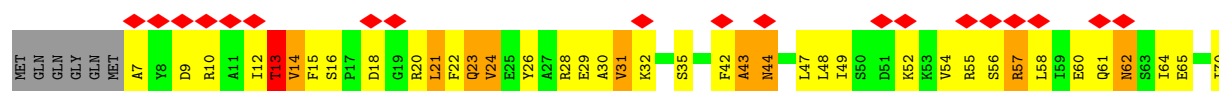
• Molecule 1: Proteasome subunit alpha

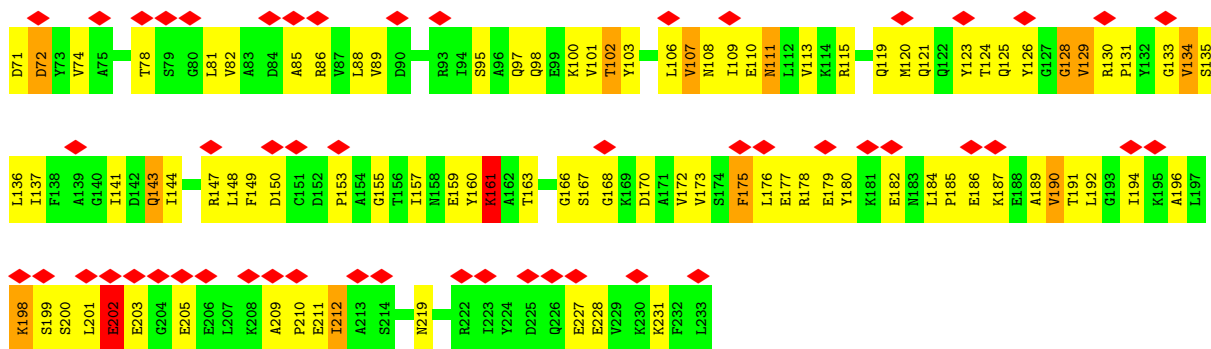


• Molecule 1: Proteasome subunit alpha

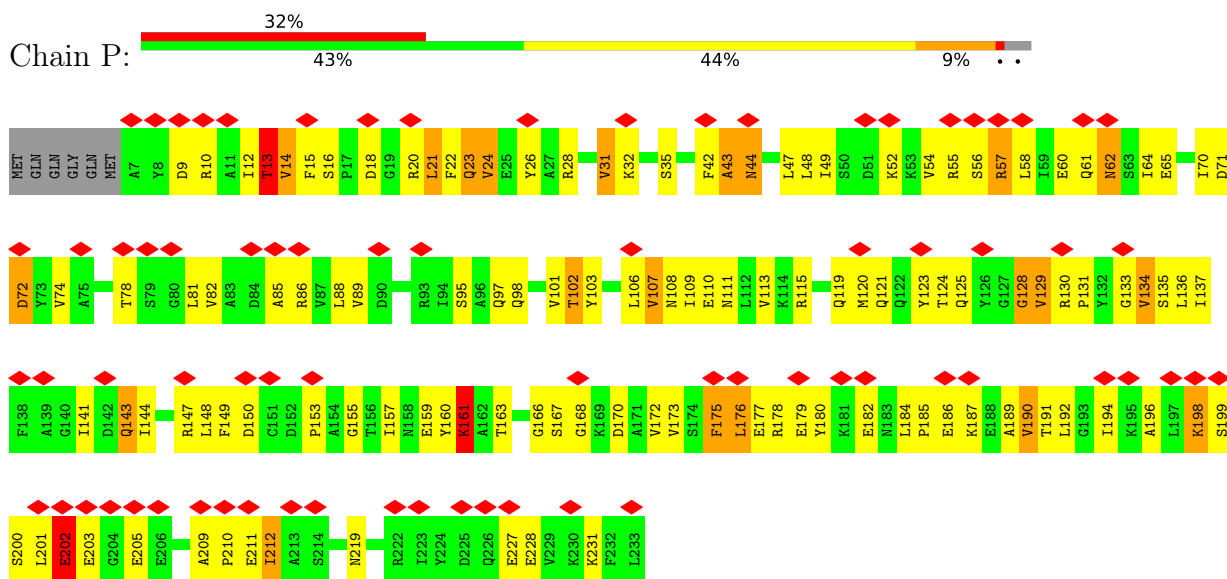


• Molecule 1: Proteasome subunit alpha

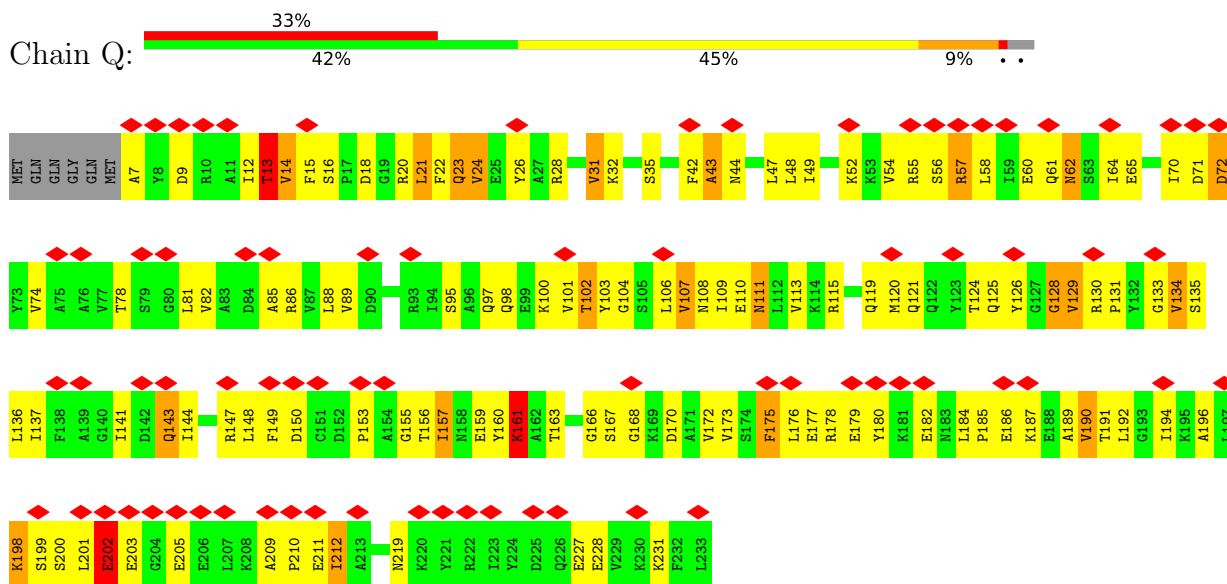




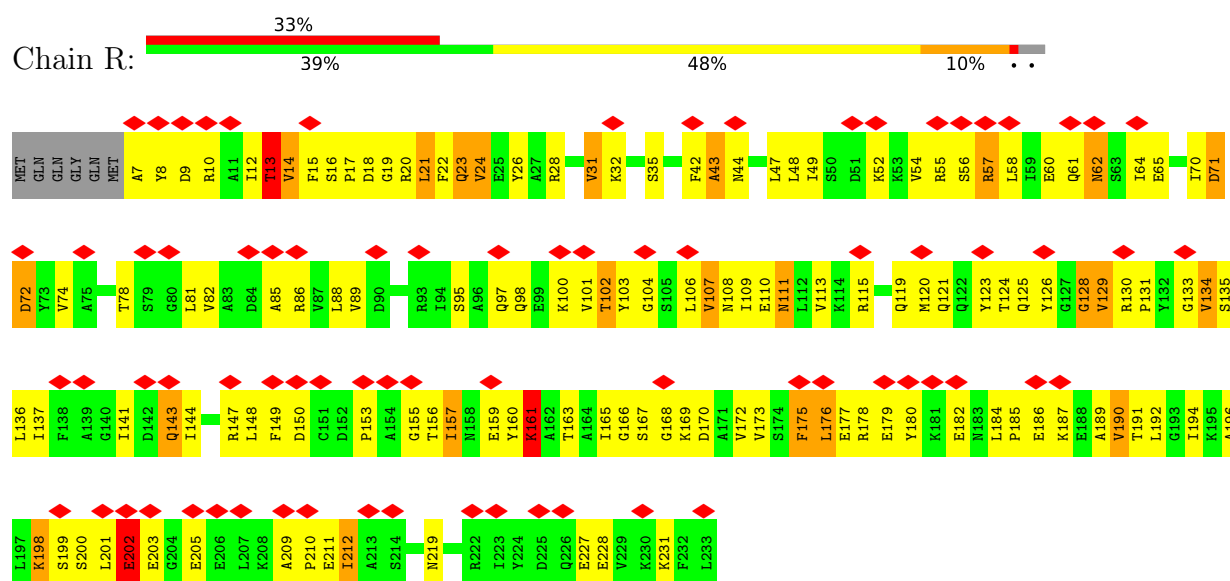
• Molecule 1: Proteasome subunit alpha



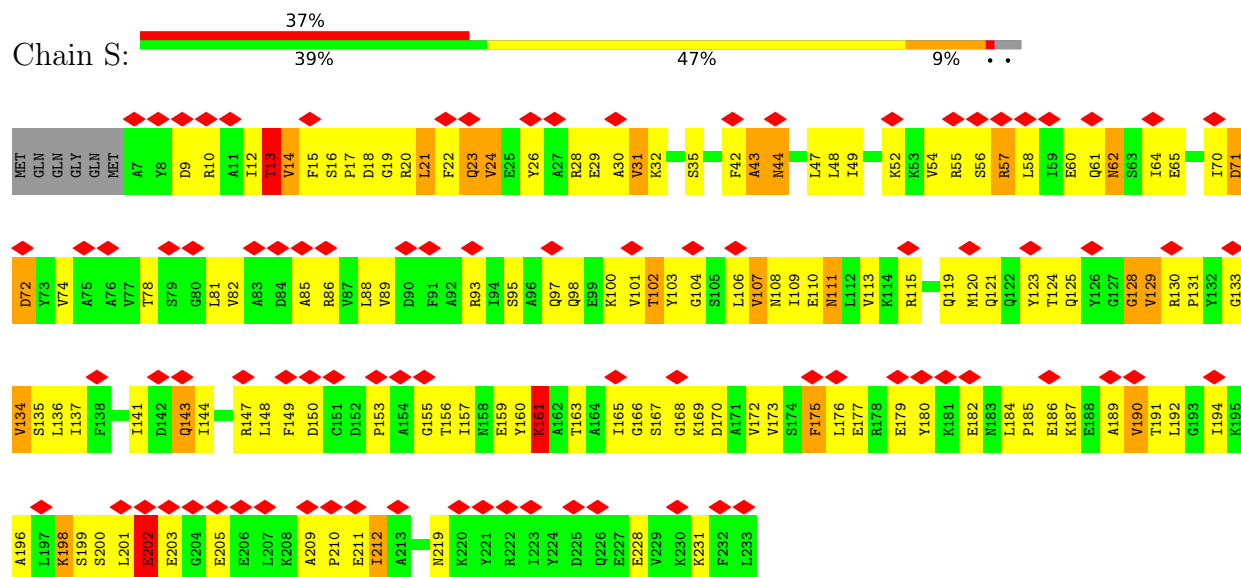
• Molecule 1: Proteasome subunit alpha



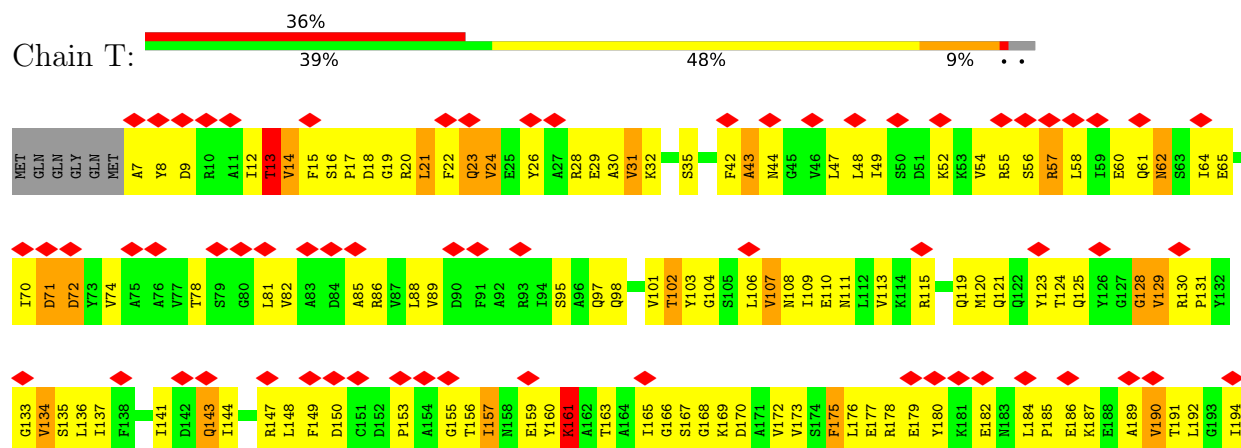
• Molecule 1: Proteasome subunit alpha

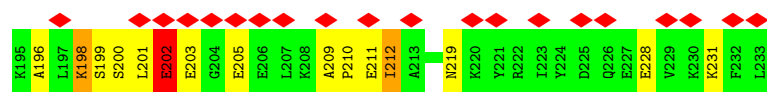


• Molecule 1: Proteasome subunit alpha

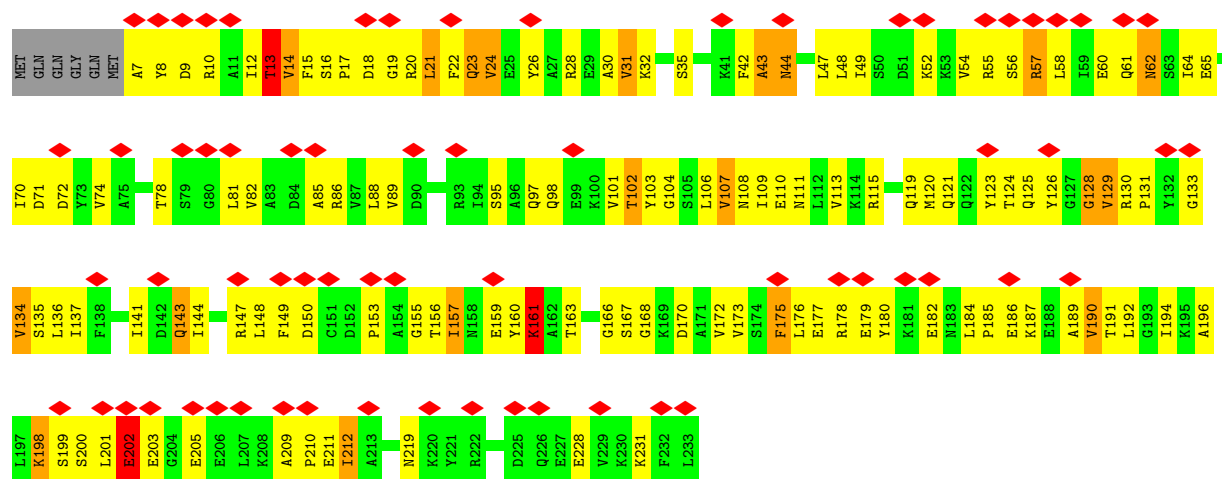
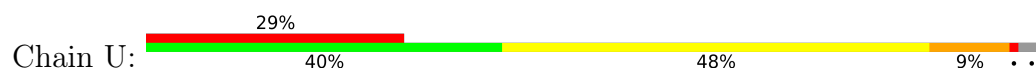


• Molecule 1: Proteasome subunit alpha

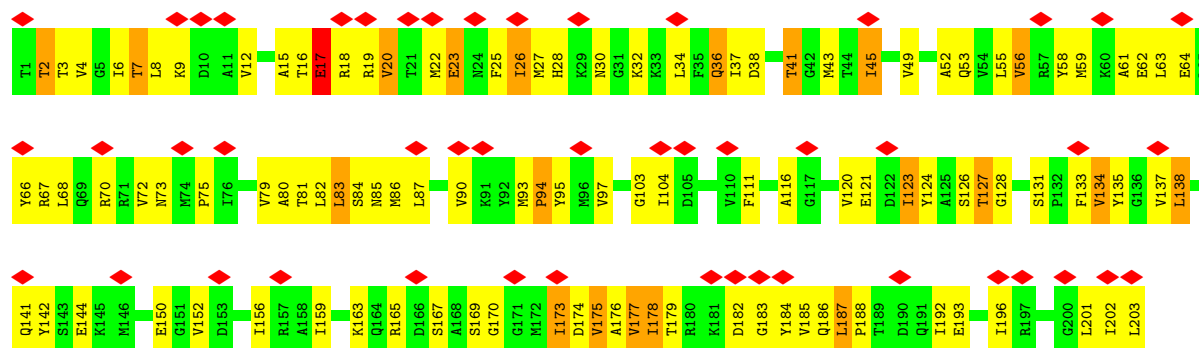




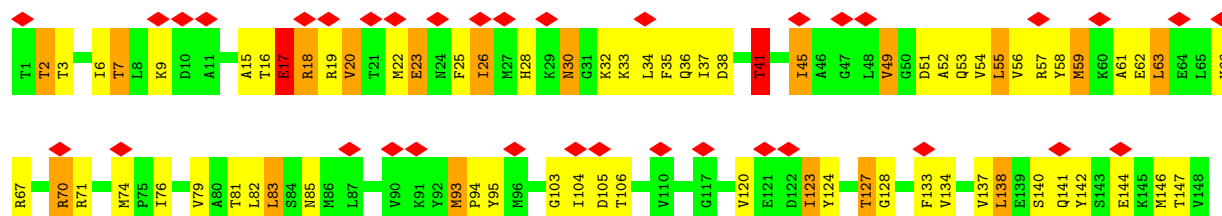
• Molecule 1: Proteasome subunit alpha

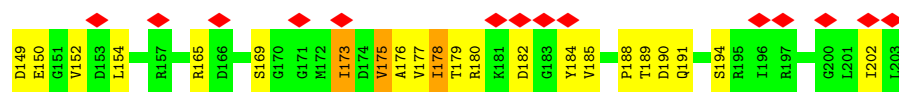


• Molecule 2: Proteasome subunit beta

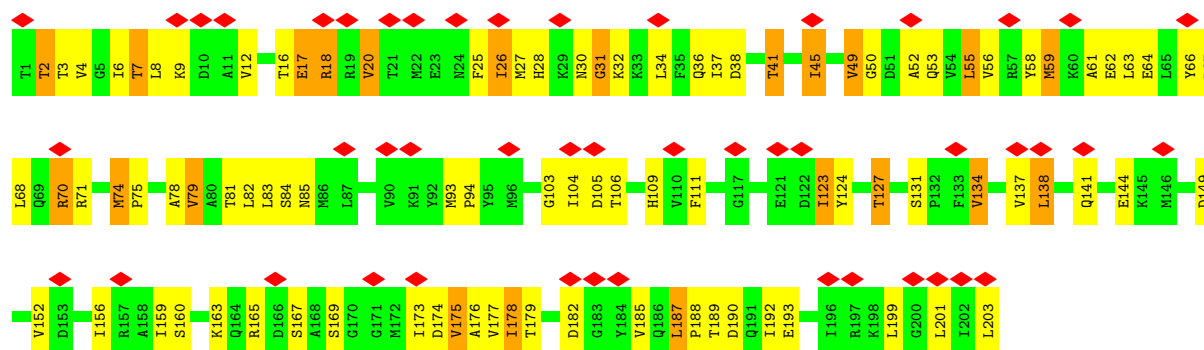


• Molecule 2: Proteasome subunit beta

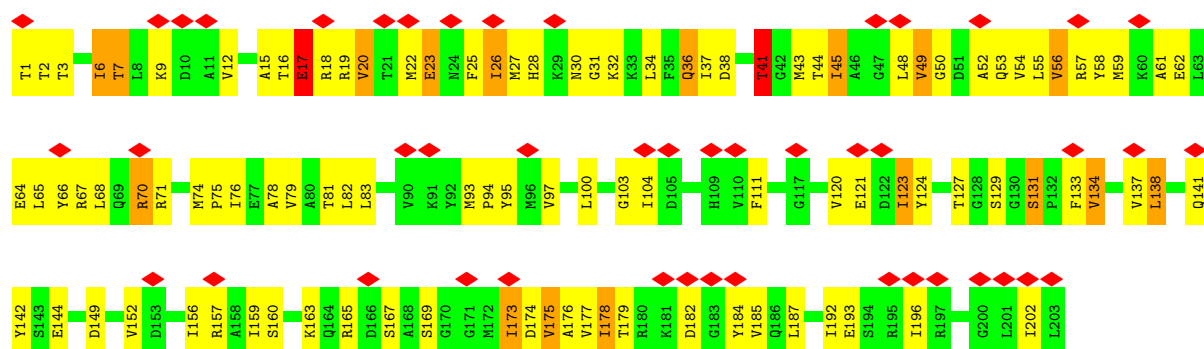




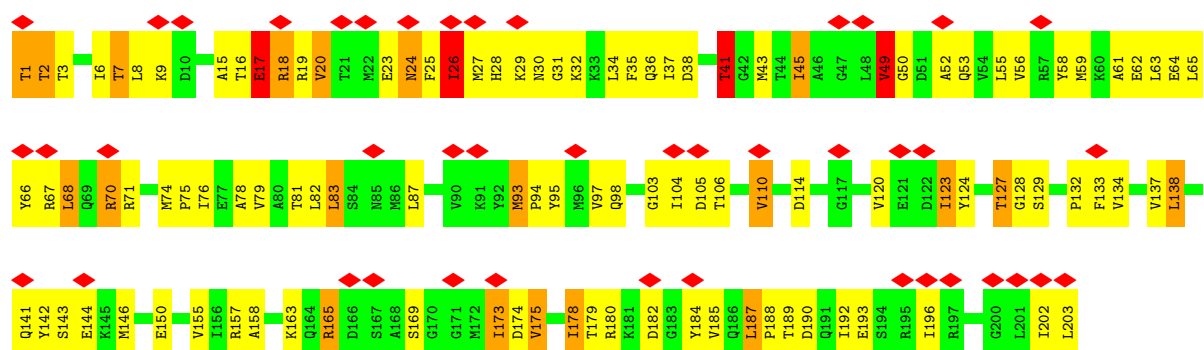
• Molecule 2: Proteasome subunit beta



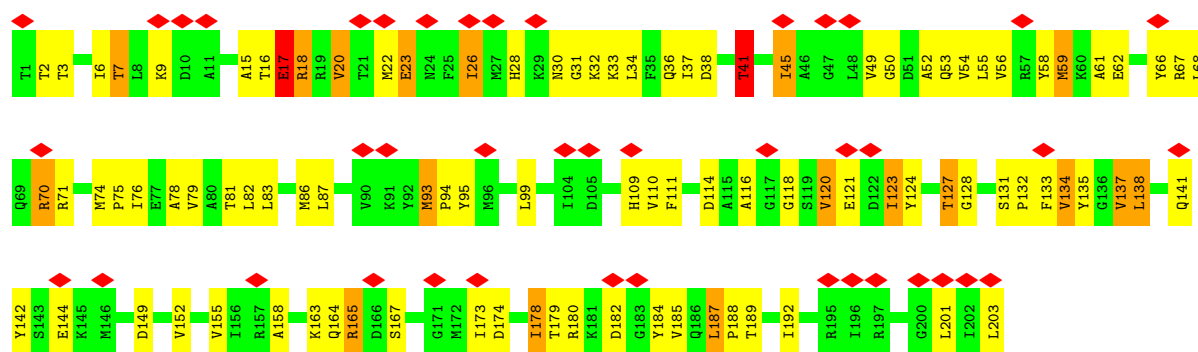
• Molecule 2: Proteasome subunit beta



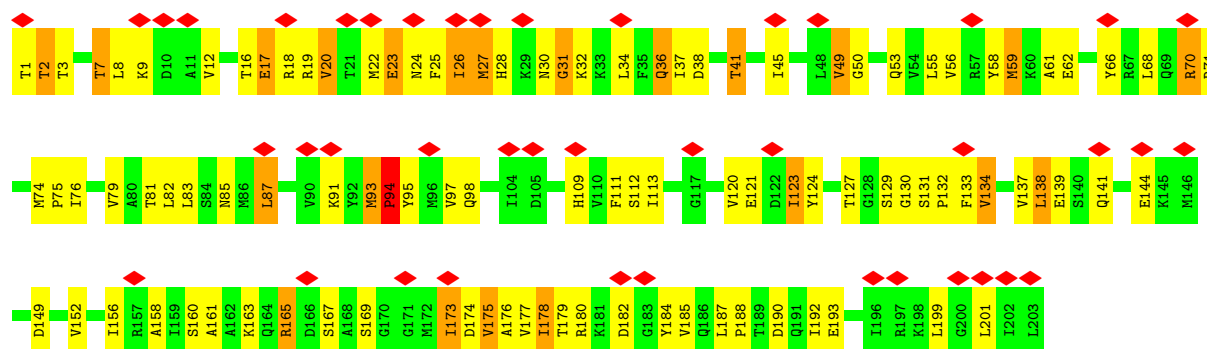
• Molecule 2: Proteasome subunit beta



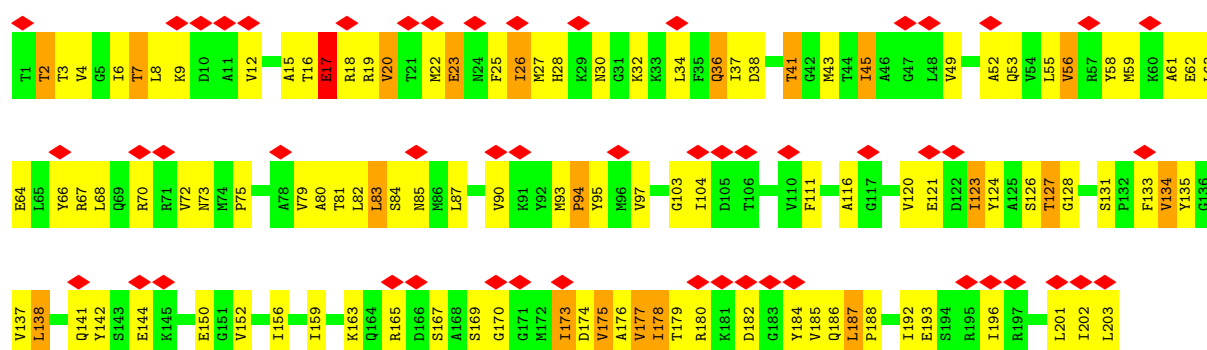
• Molecule 2: Proteasome subunit beta



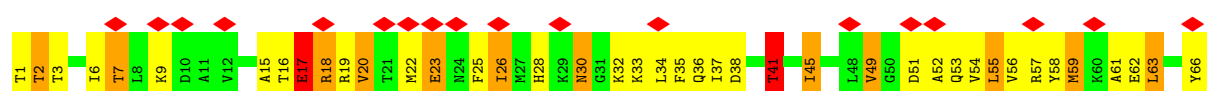
• Molecule 2: Proteasome subunit beta

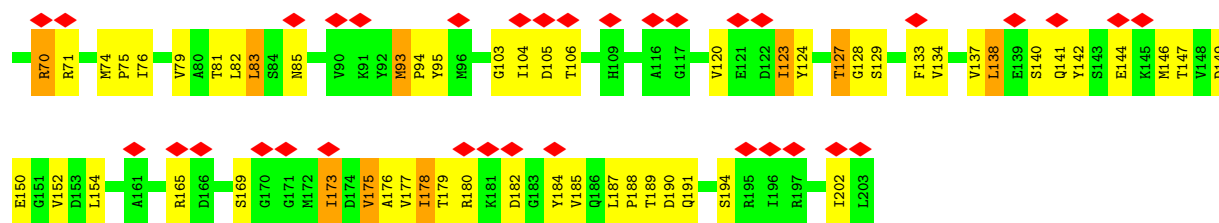


• Molecule 2: Proteasome subunit beta

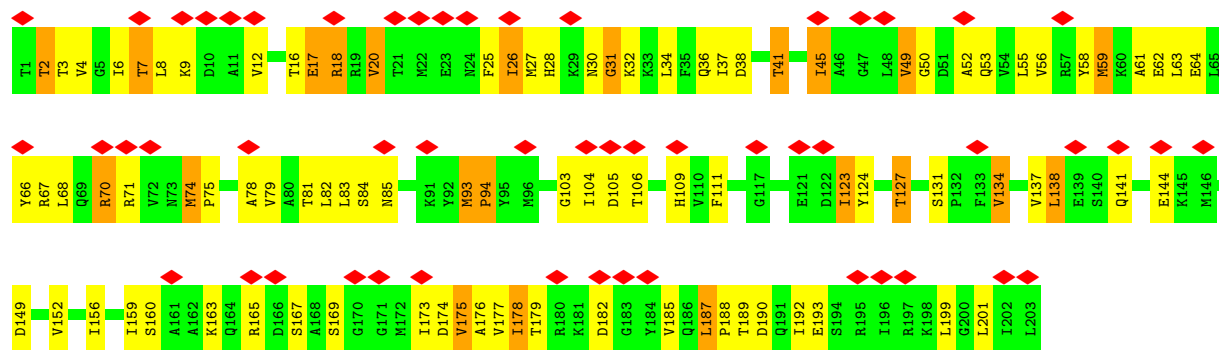


• Molecule 2: Proteasome subunit beta

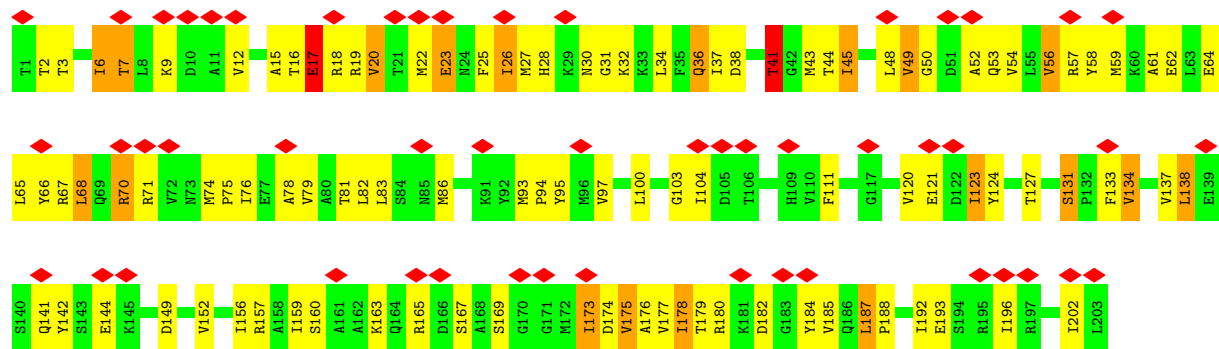




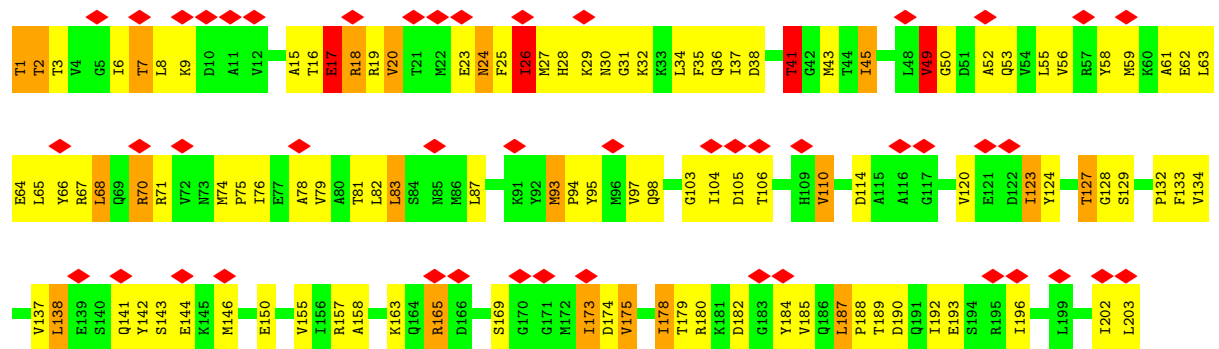
• Molecule 2: Proteasome subunit beta



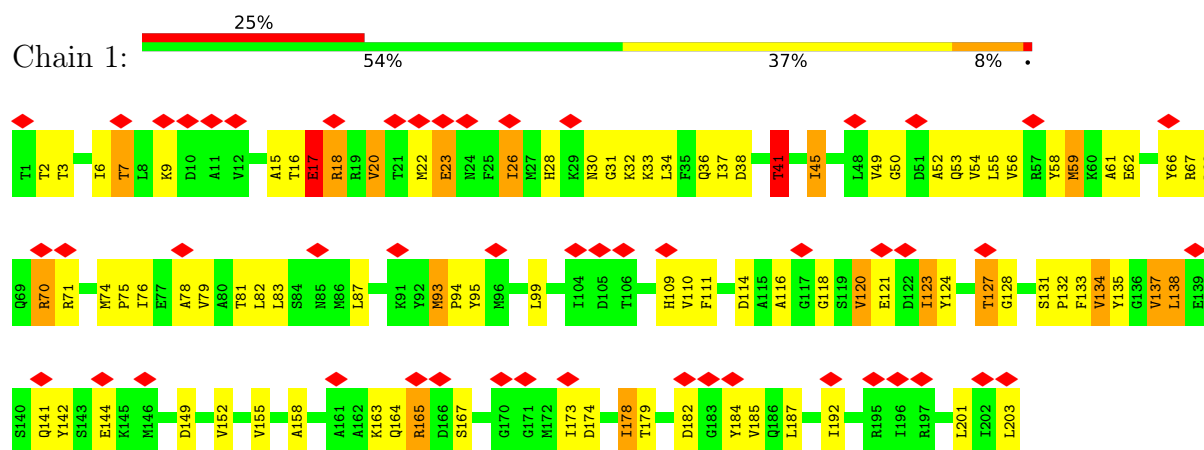
• Molecule 2: Proteasome subunit beta



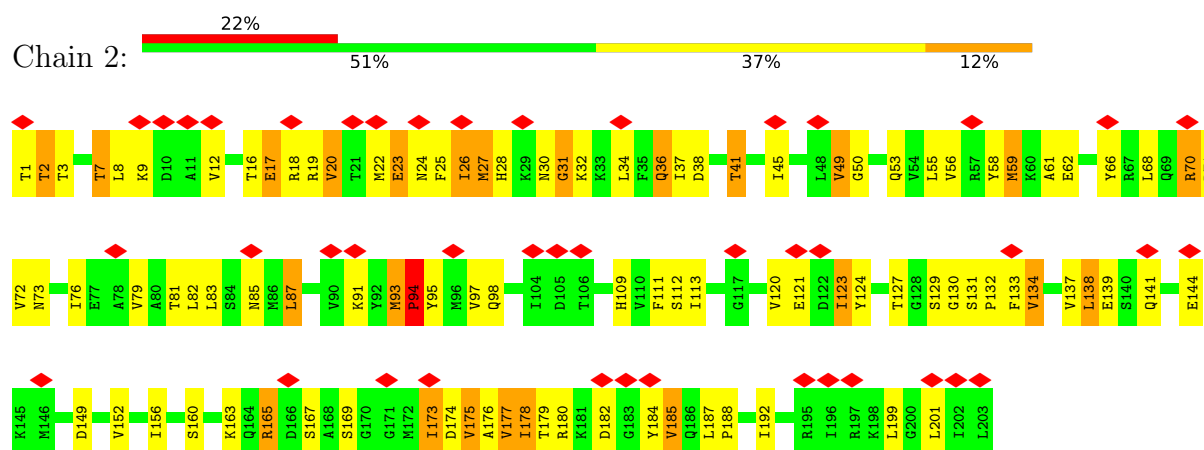
• Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, D7                 | Depositor |
| Number of particles used             | 44794                     | Depositor |
| Resolution determination method      | Not provided              |           |
| CTF correction method                | PHASE AND AMPLITUDE       | Depositor |
| Microscope                           | FEI TECNAI F20            | Depositor |
| Voltage (kV)                         | 200                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20.00                     | Depositor |
| Minimum defocus (nm)                 | -1500.00                  | Depositor |
| Maximum defocus (nm)                 | -3500.00                  | Depositor |
| Magnification                        | 51159                     | Depositor |
| Image detector                       | KODAK SO-163 FILM         | Depositor |
| Maximum map value                    | 9.018                     | Depositor |
| Minimum map value                    | -4.980                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 1.000                     | Depositor |
| Recommended contour level            | 2.5                       | Depositor |
| Map size ( $\text{\AA}$ )            | 197.028, 197.028, 197.028 | wwPDB     |
| Map dimensions                       | 144, 144, 144             | wwPDB     |
| Map angles ( $^\circ$ )              | 90, 90, 90                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.36825, 1.36825, 1.36825 | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 1   | A     | 0.67         | 0/1793         | 1.11        | 8/2416 (0.3%)    |
| 1   | B     | 0.67         | 0/1793         | 1.11        | 8/2416 (0.3%)    |
| 1   | C     | 0.67         | 0/1793         | 1.12        | 9/2416 (0.4%)    |
| 1   | D     | 0.67         | 0/1793         | 1.11        | 9/2416 (0.4%)    |
| 1   | E     | 0.67         | 0/1793         | 1.12        | 9/2416 (0.4%)    |
| 1   | F     | 0.67         | 0/1793         | 1.11        | 9/2416 (0.4%)    |
| 1   | G     | 0.67         | 0/1793         | 1.11        | 8/2416 (0.3%)    |
| 1   | O     | 0.67         | 0/1793         | 1.11        | 8/2416 (0.3%)    |
| 1   | P     | 0.67         | 0/1793         | 1.11        | 8/2416 (0.3%)    |
| 1   | Q     | 0.67         | 0/1793         | 1.11        | 9/2416 (0.4%)    |
| 1   | R     | 0.67         | 0/1793         | 1.12        | 8/2416 (0.3%)    |
| 1   | S     | 0.67         | 0/1793         | 1.12        | 9/2416 (0.4%)    |
| 1   | T     | 0.67         | 0/1793         | 1.11        | 9/2416 (0.4%)    |
| 1   | U     | 0.67         | 0/1793         | 1.12        | 8/2416 (0.3%)    |
| 2   | 1     | 0.73         | 0/1577         | 1.11        | 12/2129 (0.6%)   |
| 2   | 2     | 0.72         | 0/1577         | 1.11        | 11/2129 (0.5%)   |
| 2   | H     | 0.75         | 0/1577         | 1.12        | 11/2129 (0.5%)   |
| 2   | I     | 0.72         | 1/1577 (0.1%)  | 1.14        | 12/2129 (0.6%)   |
| 2   | J     | 0.71         | 0/1577         | 1.15        | 13/2129 (0.6%)   |
| 2   | K     | 0.74         | 0/1577         | 1.13        | 11/2129 (0.5%)   |
| 2   | L     | 0.75         | 1/1577 (0.1%)  | 1.14        | 15/2129 (0.7%)   |
| 2   | M     | 0.73         | 0/1577         | 1.11        | 12/2129 (0.6%)   |
| 2   | N     | 0.72         | 0/1577         | 1.11        | 11/2129 (0.5%)   |
| 2   | V     | 0.75         | 0/1577         | 1.12        | 11/2129 (0.5%)   |
| 2   | W     | 0.72         | 1/1577 (0.1%)  | 1.14        | 12/2129 (0.6%)   |
| 2   | X     | 0.71         | 0/1577         | 1.14        | 13/2129 (0.6%)   |
| 2   | Y     | 0.74         | 0/1577         | 1.13        | 11/2129 (0.5%)   |
| 2   | Z     | 0.75         | 1/1577 (0.1%)  | 1.14        | 15/2129 (0.7%)   |
| All | All   | 0.70         | 4/47180 (0.0%) | 1.12        | 289/63630 (0.5%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | Z     | 26  | ILE  | CA-CB | 6.71 | 1.60        | 1.53     |
| 2   | L     | 26  | ILE  | CA-CB | 6.69 | 1.60        | 1.53     |
| 2   | I     | 93  | MET  | SD-CE | 5.13 | 1.92        | 1.79     |
| 2   | W     | 93  | MET  | SD-CE | 5.10 | 1.92        | 1.79     |

All (289) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | E     | 13  | THR  | CA-C-N | -16.33 | 92.58       | 121.97   |
| 1   | E     | 13  | THR  | C-N-CA | -16.33 | 92.58       | 121.97   |
| 1   | S     | 13  | THR  | CA-C-N | -16.33 | 92.58       | 121.97   |
| 1   | S     | 13  | THR  | C-N-CA | -16.33 | 92.58       | 121.97   |
| 1   | B     | 13  | THR  | CA-C-N | -16.30 | 92.62       | 121.97   |
| 1   | B     | 13  | THR  | C-N-CA | -16.30 | 92.62       | 121.97   |
| 1   | P     | 13  | THR  | CA-C-N | -16.30 | 92.62       | 121.97   |
| 1   | P     | 13  | THR  | C-N-CA | -16.30 | 92.62       | 121.97   |
| 1   | R     | 13  | THR  | CA-C-N | -16.30 | 92.63       | 121.97   |
| 1   | R     | 13  | THR  | C-N-CA | -16.30 | 92.63       | 121.97   |
| 1   | A     | 13  | THR  | CA-C-N | -16.30 | 92.63       | 121.97   |
| 1   | A     | 13  | THR  | C-N-CA | -16.30 | 92.63       | 121.97   |
| 1   | G     | 13  | THR  | CA-C-N | -16.29 | 92.65       | 121.97   |
| 1   | G     | 13  | THR  | C-N-CA | -16.29 | 92.65       | 121.97   |
| 1   | U     | 13  | THR  | CA-C-N | -16.29 | 92.65       | 121.97   |
| 1   | U     | 13  | THR  | C-N-CA | -16.29 | 92.65       | 121.97   |
| 1   | D     | 13  | THR  | CA-C-N | -16.29 | 92.66       | 121.97   |
| 1   | D     | 13  | THR  | C-N-CA | -16.29 | 92.66       | 121.97   |
| 1   | C     | 13  | THR  | CA-C-N | -16.28 | 92.66       | 121.97   |
| 1   | C     | 13  | THR  | C-N-CA | -16.28 | 92.66       | 121.97   |
| 1   | O     | 13  | THR  | CA-C-N | -16.28 | 92.66       | 121.97   |
| 1   | O     | 13  | THR  | C-N-CA | -16.28 | 92.66       | 121.97   |
| 1   | T     | 13  | THR  | CA-C-N | -16.28 | 92.67       | 121.97   |
| 1   | T     | 13  | THR  | C-N-CA | -16.28 | 92.67       | 121.97   |
| 1   | Q     | 13  | THR  | CA-C-N | -16.27 | 92.68       | 121.97   |
| 1   | Q     | 13  | THR  | C-N-CA | -16.27 | 92.68       | 121.97   |
| 1   | F     | 13  | THR  | CA-C-N | -16.27 | 92.69       | 121.97   |
| 1   | F     | 13  | THR  | C-N-CA | -16.27 | 92.69       | 121.97   |
| 1   | E     | 203 | GLU  | N-CA-C | -9.90  | 100.33      | 111.82   |
| 1   | O     | 203 | GLU  | N-CA-C | -9.90  | 100.34      | 111.82   |
| 2   | J     | 93  | MET  | CA-C-N | 9.89   | 130.51      | 119.92   |
| 2   | J     | 93  | MET  | C-N-CA | 9.89   | 130.51      | 119.92   |
| 1   | Q     | 203 | GLU  | N-CA-C | -9.88  | 100.36      | 111.82   |
| 1   | C     | 203 | GLU  | N-CA-C | -9.88  | 100.36      | 111.82   |
| 1   | S     | 203 | GLU  | N-CA-C | -9.88  | 100.36      | 111.82   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | X     | 93  | MET  | CA-C-N | 9.88  | 130.49      | 119.92   |
| 2   | X     | 93  | MET  | C-N-CA | 9.88  | 130.49      | 119.92   |
| 1   | A     | 203 | GLU  | N-CA-C | -9.86 | 100.38      | 111.82   |
| 1   | T     | 203 | GLU  | N-CA-C | -9.86 | 100.38      | 111.82   |
| 1   | P     | 203 | GLU  | N-CA-C | -9.86 | 100.39      | 111.82   |
| 1   | B     | 203 | GLU  | N-CA-C | -9.85 | 100.39      | 111.82   |
| 1   | F     | 203 | GLU  | N-CA-C | -9.85 | 100.39      | 111.82   |
| 1   | G     | 203 | GLU  | N-CA-C | -9.85 | 100.39      | 111.82   |
| 1   | U     | 203 | GLU  | N-CA-C | -9.84 | 100.40      | 111.82   |
| 1   | R     | 203 | GLU  | N-CA-C | -9.83 | 100.42      | 111.82   |
| 1   | D     | 203 | GLU  | N-CA-C | -9.82 | 100.43      | 111.82   |
| 2   | I     | 93  | MET  | CA-C-N | 9.68  | 130.28      | 119.92   |
| 2   | I     | 93  | MET  | C-N-CA | 9.68  | 130.28      | 119.92   |
| 2   | W     | 93  | MET  | CA-C-N | 9.65  | 130.24      | 119.92   |
| 2   | W     | 93  | MET  | C-N-CA | 9.65  | 130.24      | 119.92   |
| 2   | 1     | 18  | ARG  | N-CA-C | 9.58  | 121.72      | 110.41   |
| 2   | Z     | 18  | ARG  | N-CA-C | 9.56  | 121.69      | 110.41   |
| 2   | L     | 18  | ARG  | N-CA-C | 9.55  | 121.68      | 110.41   |
| 2   | M     | 18  | ARG  | N-CA-C | 9.55  | 121.67      | 110.41   |
| 2   | X     | 18  | ARG  | N-CA-C | 8.52  | 120.47      | 110.41   |
| 2   | J     | 18  | ARG  | N-CA-C | 8.50  | 120.44      | 110.41   |
| 1   | D     | 161 | LYS  | N-CA-C | -8.50 | 103.04      | 113.41   |
| 1   | U     | 161 | LYS  | N-CA-C | -8.49 | 103.05      | 113.41   |
| 1   | R     | 161 | LYS  | N-CA-C | -8.49 | 103.06      | 113.41   |
| 1   | A     | 161 | LYS  | N-CA-C | -8.48 | 103.07      | 113.41   |
| 1   | G     | 161 | LYS  | N-CA-C | -8.48 | 103.07      | 113.41   |
| 1   | O     | 161 | LYS  | N-CA-C | -8.47 | 103.07      | 113.41   |
| 1   | E     | 161 | LYS  | N-CA-C | -8.46 | 103.08      | 113.41   |
| 1   | C     | 161 | LYS  | N-CA-C | -8.46 | 103.09      | 113.41   |
| 1   | F     | 161 | LYS  | N-CA-C | -8.46 | 103.09      | 113.41   |
| 1   | S     | 161 | LYS  | N-CA-C | -8.45 | 103.10      | 113.41   |
| 1   | T     | 161 | LYS  | N-CA-C | -8.45 | 103.10      | 113.41   |
| 1   | B     | 161 | LYS  | N-CA-C | -8.45 | 103.10      | 113.41   |
| 1   | P     | 161 | LYS  | N-CA-C | -8.44 | 103.11      | 113.41   |
| 1   | Q     | 161 | LYS  | N-CA-C | -8.42 | 103.14      | 113.41   |
| 2   | K     | 95  | TYR  | N-CA-C | -8.25 | 95.13       | 108.41   |
| 2   | Y     | 95  | TYR  | N-CA-C | -8.24 | 95.14       | 108.41   |
| 2   | N     | 93  | MET  | CA-C-N | 8.03  | 128.52      | 119.92   |
| 2   | N     | 93  | MET  | C-N-CA | 8.03  | 128.52      | 119.92   |
| 2   | 2     | 93  | MET  | CA-C-N | 8.03  | 128.51      | 119.92   |
| 2   | 2     | 93  | MET  | C-N-CA | 8.03  | 128.51      | 119.92   |
| 2   | H     | 93  | MET  | CA-C-N | 8.03  | 128.51      | 119.92   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | H     | 93  | MET  | C-N-CA | 8.03  | 128.51      | 119.92   |
| 2   | I     | 18  | ARG  | N-CA-C | 8.01  | 119.86      | 110.41   |
| 2   | V     | 93  | MET  | CA-C-N | 8.00  | 128.48      | 119.92   |
| 2   | V     | 93  | MET  | C-N-CA | 8.00  | 128.48      | 119.92   |
| 2   | W     | 18  | ARG  | N-CA-C | 7.97  | 119.82      | 110.41   |
| 2   | M     | 31  | GLY  | N-CA-C | -7.79 | 101.90      | 112.57   |
| 2   | 1     | 31  | GLY  | N-CA-C | -7.78 | 101.91      | 112.57   |
| 2   | J     | 31  | GLY  | N-CA-C | -7.50 | 100.73      | 112.58   |
| 2   | 1     | 93  | MET  | CA-C-N | 7.44  | 129.14      | 119.84   |
| 2   | 1     | 93  | MET  | C-N-CA | 7.44  | 129.14      | 119.84   |
| 2   | M     | 93  | MET  | CA-C-N | 7.43  | 129.13      | 119.84   |
| 2   | M     | 93  | MET  | C-N-CA | 7.43  | 129.13      | 119.84   |
| 2   | X     | 36  | GLN  | N-CA-C | -7.27 | 99.72       | 110.48   |
| 2   | J     | 36  | GLN  | N-CA-C | -7.25 | 99.74       | 110.48   |
| 2   | K     | 36  | GLN  | N-CA-C | -7.18 | 98.86       | 110.20   |
| 2   | Y     | 36  | GLN  | N-CA-C | -7.17 | 98.87       | 110.20   |
| 2   | J     | 17  | GLU  | N-CA-C | -7.01 | 99.36       | 109.31   |
| 2   | X     | 17  | GLU  | N-CA-C | -7.00 | 99.36       | 109.31   |
| 2   | L     | 17  | GLU  | N-CA-C | -7.00 | 98.96       | 109.94   |
| 2   | N     | 17  | GLU  | N-CA-C | -6.99 | 99.38       | 109.31   |
| 2   | 2     | 17  | GLU  | N-CA-C | -6.99 | 99.39       | 109.31   |
| 2   | Z     | 17  | GLU  | N-CA-C | -6.97 | 98.99       | 109.94   |
| 2   | Y     | 17  | GLU  | N-CA-C | -6.93 | 99.47       | 109.31   |
| 2   | L     | 93  | MET  | CA-C-N | 6.91  | 128.48      | 119.84   |
| 2   | L     | 93  | MET  | C-N-CA | 6.91  | 128.48      | 119.84   |
| 2   | Z     | 93  | MET  | CA-C-N | 6.91  | 128.48      | 119.84   |
| 2   | Z     | 93  | MET  | C-N-CA | 6.91  | 128.48      | 119.84   |
| 2   | X     | 31  | GLY  | N-CA-C | -6.91 | 100.70      | 112.51   |
| 2   | K     | 17  | GLU  | N-CA-C | -6.91 | 99.50       | 109.31   |
| 2   | 1     | 95  | TYR  | N-CA-C | -6.87 | 97.35       | 108.41   |
| 2   | M     | 95  | TYR  | N-CA-C | -6.85 | 97.39       | 108.41   |
| 2   | V     | 36  | GLN  | N-CA-C | -6.80 | 99.46       | 110.20   |
| 2   | H     | 36  | GLN  | N-CA-C | -6.79 | 99.47       | 110.20   |
| 2   | N     | 36  | GLN  | N-CA-C | -6.79 | 99.47       | 110.20   |
| 2   | 2     | 36  | GLN  | N-CA-C | -6.78 | 99.49       | 110.20   |
| 2   | 1     | 17  | GLU  | N-CA-C | -6.68 | 99.45       | 109.94   |
| 2   | M     | 17  | GLU  | N-CA-C | -6.67 | 99.47       | 109.94   |
| 2   | X     | 94  | PRO  | N-CA-C | 6.63  | 121.62      | 111.34   |
| 2   | J     | 94  | PRO  | N-CA-C | 6.61  | 121.59      | 111.34   |
| 1   | P     | 57  | ARG  | N-CA-C | -6.59 | 104.72      | 112.89   |
| 1   | F     | 57  | ARG  | N-CA-C | -6.58 | 104.73      | 112.89   |
| 1   | B     | 57  | ARG  | N-CA-C | -6.57 | 104.74      | 112.89   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | R     | 57  | ARG  | N-CA-C | -6.57 | 104.74      | 112.89   |
| 1   | D     | 57  | ARG  | N-CA-C | -6.57 | 104.74      | 112.89   |
| 1   | T     | 57  | ARG  | N-CA-C | -6.56 | 104.76      | 112.89   |
| 1   | A     | 57  | ARG  | N-CA-C | -6.55 | 104.76      | 112.89   |
| 1   | S     | 57  | ARG  | N-CA-C | -6.55 | 104.77      | 112.89   |
| 1   | E     | 57  | ARG  | N-CA-C | -6.55 | 104.77      | 112.89   |
| 1   | C     | 57  | ARG  | N-CA-C | -6.55 | 104.77      | 112.89   |
| 1   | G     | 57  | ARG  | N-CA-C | -6.55 | 104.77      | 112.89   |
| 2   | K     | 93  | MET  | CA-C-N | 6.54  | 128.02      | 119.84   |
| 2   | K     | 93  | MET  | C-N-CA | 6.54  | 128.02      | 119.84   |
| 1   | U     | 57  | ARG  | N-CA-C | -6.54 | 104.78      | 112.89   |
| 1   | O     | 57  | ARG  | N-CA-C | -6.54 | 104.79      | 112.89   |
| 2   | Y     | 93  | MET  | CA-C-N | 6.53  | 128.00      | 119.84   |
| 2   | Y     | 93  | MET  | C-N-CA | 6.53  | 128.00      | 119.84   |
| 2   | V     | 80  | ALA  | N-CA-C | -6.53 | 103.86      | 110.97   |
| 2   | L     | 187 | LEU  | CA-C-N | 6.53  | 126.88      | 119.83   |
| 2   | L     | 187 | LEU  | C-N-CA | 6.53  | 126.88      | 119.83   |
| 1   | Q     | 57  | ARG  | N-CA-C | -6.53 | 104.80      | 112.89   |
| 2   | H     | 80  | ALA  | N-CA-C | -6.51 | 103.87      | 110.97   |
| 2   | Z     | 187 | LEU  | CA-C-N | 6.51  | 126.86      | 119.83   |
| 2   | Z     | 187 | LEU  | C-N-CA | 6.51  | 126.86      | 119.83   |
| 2   | I     | 128 | GLY  | N-CA-C | 6.41  | 118.58      | 112.04   |
| 2   | W     | 128 | GLY  | N-CA-C | 6.39  | 118.56      | 112.04   |
| 2   | 1     | 36  | GLN  | N-CA-C | -6.39 | 101.02      | 110.48   |
| 2   | M     | 36  | GLN  | N-CA-C | -6.39 | 101.02      | 110.48   |
| 2   | H     | 128 | GLY  | N-CA-C | 6.32  | 118.49      | 112.04   |
| 2   | W     | 95  | TYR  | N-CA-C | -6.32 | 98.87       | 108.67   |
| 2   | I     | 95  | TYR  | N-CA-C | -6.32 | 98.88       | 108.67   |
| 2   | V     | 128 | GLY  | N-CA-C | 6.30  | 118.46      | 112.04   |
| 2   | L     | 128 | GLY  | N-CA-C | 6.06  | 119.46      | 111.70   |
| 2   | Z     | 128 | GLY  | N-CA-C | 6.04  | 119.43      | 111.70   |
| 2   | 2     | 94  | PRO  | N-CA-C | 6.00  | 120.64      | 111.34   |
| 2   | I     | 30  | ASN  | N-CA-C | 5.99  | 116.99      | 108.54   |
| 2   | N     | 94  | PRO  | N-CA-C | 5.99  | 120.62      | 111.34   |
| 2   | W     | 30  | ASN  | N-CA-C | 5.98  | 116.97      | 108.54   |
| 2   | M     | 118 | GLY  | N-CA-C | -5.88 | 100.80      | 111.15   |
| 2   | 1     | 118 | GLY  | N-CA-C | -5.86 | 100.83      | 111.15   |
| 2   | L     | 95  | TYR  | N-CA-C | -5.85 | 98.20       | 108.20   |
| 2   | V     | 150 | GLU  | N-CA-C | -5.85 | 104.90      | 111.28   |
| 2   | X     | 187 | LEU  | CA-C-N | 5.85  | 126.04      | 119.90   |
| 2   | X     | 187 | LEU  | C-N-CA | 5.85  | 126.04      | 119.90   |
| 2   | Z     | 95  | TYR  | N-CA-C | -5.84 | 98.21       | 108.20   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | H     | 150 | GLU  | N-CA-C | -5.82 | 104.94      | 111.28   |
| 2   | J     | 187 | LEU  | CA-C-N | 5.82  | 126.01      | 119.90   |
| 2   | J     | 187 | LEU  | C-N-CA | 5.82  | 126.01      | 119.90   |
| 2   | M     | 187 | LEU  | CA-C-N | 5.81  | 126.72      | 119.98   |
| 2   | M     | 187 | LEU  | C-N-CA | 5.81  | 126.72      | 119.98   |
| 2   | W     | 17  | GLU  | N-CA-C | -5.81 | 100.97      | 109.63   |
| 2   | H     | 95  | TYR  | N-CA-C | -5.81 | 97.77       | 107.99   |
| 2   | 1     | 187 | LEU  | CA-C-N | 5.81  | 126.72      | 119.98   |
| 2   | 1     | 187 | LEU  | C-N-CA | 5.81  | 126.72      | 119.98   |
| 2   | V     | 95  | TYR  | N-CA-C | -5.80 | 97.78       | 107.99   |
| 2   | I     | 17  | GLU  | N-CA-C | -5.80 | 100.99      | 109.63   |
| 2   | Y     | 131 | SER  | N-CA-C | 5.79  | 120.78      | 113.25   |
| 2   | J     | 4   | VAL  | N-CA-C | 5.78  | 116.19      | 108.27   |
| 2   | K     | 131 | SER  | N-CA-C | 5.76  | 120.74      | 113.25   |
| 2   | X     | 4   | VAL  | N-CA-C | 5.75  | 116.15      | 108.27   |
| 2   | 2     | 27  | MET  | N-CA-C | 5.75  | 120.43      | 112.90   |
| 2   | X     | 74  | MET  | CA-C-N | 5.74  | 125.69      | 119.78   |
| 2   | X     | 74  | MET  | C-N-CA | 5.74  | 125.69      | 119.78   |
| 2   | N     | 27  | MET  | N-CA-C | 5.74  | 120.42      | 112.90   |
| 2   | J     | 74  | MET  | CA-C-N | 5.74  | 125.69      | 119.78   |
| 2   | J     | 74  | MET  | C-N-CA | 5.74  | 125.69      | 119.78   |
| 2   | K     | 187 | LEU  | CA-C-N | 5.73  | 125.91      | 119.90   |
| 2   | K     | 187 | LEU  | C-N-CA | 5.73  | 125.91      | 119.90   |
| 2   | Y     | 187 | LEU  | CA-C-N | 5.72  | 125.91      | 119.90   |
| 2   | Y     | 187 | LEU  | C-N-CA | 5.72  | 125.91      | 119.90   |
| 2   | N     | 31  | GLY  | N-CA-C | -5.65 | 103.65      | 112.58   |
| 2   | 2     | 31  | GLY  | N-CA-C | -5.65 | 103.66      | 112.58   |
| 2   | W     | 202 | ILE  | N-CA-C | 5.64  | 116.49      | 108.42   |
| 2   | I     | 202 | ILE  | N-CA-C | 5.64  | 116.48      | 108.42   |
| 1   | G     | 219 | ASN  | N-CA-C | 5.61  | 116.48      | 108.74   |
| 1   | Q     | 219 | ASN  | N-CA-C | 5.61  | 116.48      | 108.74   |
| 1   | B     | 219 | ASN  | N-CA-C | 5.61  | 116.47      | 108.74   |
| 1   | S     | 219 | ASN  | N-CA-C | 5.60  | 116.47      | 108.74   |
| 1   | O     | 219 | ASN  | N-CA-C | 5.60  | 116.47      | 108.74   |
| 1   | D     | 219 | ASN  | N-CA-C | 5.60  | 116.46      | 108.74   |
| 1   | C     | 219 | ASN  | N-CA-C | 5.59  | 116.46      | 108.74   |
| 1   | P     | 219 | ASN  | N-CA-C | 5.59  | 116.46      | 108.74   |
| 1   | A     | 219 | ASN  | N-CA-C | 5.59  | 116.46      | 108.74   |
| 1   | R     | 219 | ASN  | N-CA-C | 5.59  | 116.46      | 108.74   |
| 1   | U     | 219 | ASN  | N-CA-C | 5.59  | 116.45      | 108.74   |
| 1   | P     | 179 | GLU  | N-CA-C | 5.58  | 119.18      | 112.93   |
| 1   | B     | 179 | GLU  | N-CA-C | 5.58  | 119.18      | 112.93   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 219 | ASN  | N-CA-C  | 5.57  | 116.42      | 108.74   |
| 1   | T     | 219 | ASN  | N-CA-C  | 5.56  | 116.42      | 108.74   |
| 1   | E     | 219 | ASN  | N-CA-C  | 5.56  | 116.42      | 108.74   |
| 1   | C     | 179 | GLU  | N-CA-C  | 5.55  | 119.15      | 112.93   |
| 1   | U     | 179 | GLU  | N-CA-C  | 5.55  | 119.14      | 112.93   |
| 1   | G     | 179 | GLU  | N-CA-C  | 5.54  | 119.14      | 112.93   |
| 1   | Q     | 179 | GLU  | N-CA-C  | 5.54  | 119.14      | 112.93   |
| 2   | W     | 36  | GLN  | N-CA-C  | -5.54 | 101.44      | 110.20   |
| 1   | A     | 179 | GLU  | N-CA-C  | 5.54  | 119.13      | 112.93   |
| 1   | D     | 179 | GLU  | N-CA-C  | 5.53  | 119.13      | 112.93   |
| 2   | Z     | 26  | ILE  | CB-CA-C | 5.53  | 117.66      | 111.80   |
| 2   | I     | 36  | GLN  | N-CA-C  | -5.52 | 101.47      | 110.20   |
| 1   | O     | 179 | GLU  | N-CA-C  | 5.52  | 119.11      | 112.93   |
| 1   | R     | 179 | GLU  | N-CA-C  | 5.52  | 119.11      | 112.93   |
| 2   | L     | 26  | ILE  | CB-CA-C | 5.50  | 117.64      | 111.80   |
| 1   | E     | 179 | GLU  | N-CA-C  | 5.50  | 119.09      | 112.93   |
| 1   | F     | 179 | GLU  | N-CA-C  | 5.50  | 119.09      | 112.93   |
| 1   | T     | 179 | GLU  | N-CA-C  | 5.49  | 119.08      | 112.93   |
| 2   | K     | 41  | THR  | N-CA-C  | 5.49  | 117.43      | 108.76   |
| 2   | L     | 202 | ILE  | N-CA-C  | 5.49  | 117.70      | 108.81   |
| 1   | S     | 179 | GLU  | N-CA-C  | 5.48  | 119.07      | 112.93   |
| 2   | Y     | 41  | THR  | N-CA-C  | 5.48  | 117.42      | 108.76   |
| 2   | K     | 31  | GLY  | N-CA-C  | -5.48 | 104.22      | 112.60   |
| 2   | Y     | 31  | GLY  | N-CA-C  | -5.47 | 104.23      | 112.60   |
| 2   | Z     | 202 | ILE  | N-CA-C  | 5.47  | 117.67      | 108.81   |
| 2   | 2     | 95  | TYR  | N-CA-C  | -5.46 | 100.20      | 108.67   |
| 2   | N     | 95  | TYR  | N-CA-C  | -5.46 | 100.21      | 108.67   |
| 2   | V     | 94  | PRO  | N-CA-C  | 5.42  | 119.75      | 111.34   |
| 2   | N     | 49  | VAL  | N-CA-C  | 5.41  | 115.86      | 110.23   |
| 2   | H     | 94  | PRO  | N-CA-C  | 5.41  | 119.72      | 111.34   |
| 2   | Z     | 27  | MET  | N-CA-C  | 5.39  | 118.32      | 111.69   |
| 1   | R     | 128 | GLY  | N-CA-C  | 5.39  | 125.94      | 113.18   |
| 2   | 2     | 49  | VAL  | N-CA-C  | 5.39  | 115.83      | 110.23   |
| 2   | W     | 41  | THR  | N-CA-C  | 5.38  | 117.26      | 108.76   |
| 2   | I     | 41  | THR  | N-CA-C  | 5.38  | 117.26      | 108.76   |
| 1   | D     | 128 | GLY  | N-CA-C  | 5.37  | 125.91      | 113.18   |
| 1   | B     | 128 | GLY  | N-CA-C  | 5.37  | 125.91      | 113.18   |
| 1   | P     | 128 | GLY  | N-CA-C  | 5.37  | 125.91      | 113.18   |
| 1   | Q     | 128 | GLY  | N-CA-C  | 5.37  | 125.91      | 113.18   |
| 1   | C     | 128 | GLY  | N-CA-C  | 5.37  | 125.90      | 113.18   |
| 1   | O     | 128 | GLY  | N-CA-C  | 5.36  | 125.89      | 113.18   |
| 1   | A     | 128 | GLY  | N-CA-C  | 5.36  | 125.88      | 113.18   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | L     | 27  | MET  | N-CA-C | 5.36  | 118.28      | 111.69   |
| 1   | E     | 128 | GLY  | N-CA-C | 5.35  | 125.87      | 113.18   |
| 1   | G     | 128 | GLY  | N-CA-C | 5.35  | 125.86      | 113.18   |
| 1   | F     | 128 | GLY  | N-CA-C | 5.35  | 125.85      | 113.18   |
| 1   | S     | 128 | GLY  | N-CA-C | 5.34  | 125.84      | 113.18   |
| 1   | T     | 128 | GLY  | N-CA-C | 5.34  | 125.84      | 113.18   |
| 1   | U     | 128 | GLY  | N-CA-C | 5.34  | 125.83      | 113.18   |
| 2   | L     | 41  | THR  | N-CA-C | 5.33  | 117.37      | 108.99   |
| 2   | H     | 187 | LEU  | CA-C-N | 5.33  | 125.09      | 119.76   |
| 2   | H     | 187 | LEU  | C-N-CA | 5.33  | 125.09      | 119.76   |
| 2   | Z     | 41  | THR  | N-CA-C | 5.32  | 117.35      | 108.99   |
| 2   | V     | 187 | LEU  | CA-C-N | 5.30  | 125.06      | 119.76   |
| 2   | V     | 187 | LEU  | C-N-CA | 5.30  | 125.06      | 119.76   |
| 2   | J     | 27  | MET  | N-CA-C | 5.29  | 118.89      | 112.23   |
| 2   | V     | 17  | GLU  | N-CA-C | -5.28 | 99.55       | 110.80   |
| 2   | X     | 27  | MET  | N-CA-C | 5.28  | 118.89      | 112.23   |
| 2   | H     | 17  | GLU  | N-CA-C | -5.28 | 99.55       | 110.80   |
| 2   | N     | 24  | ASN  | N-CA-C | -5.23 | 107.06      | 113.50   |
| 2   | M     | 128 | GLY  | N-CA-C | 5.22  | 118.38      | 111.70   |
| 2   | 2     | 24  | ASN  | N-CA-C | -5.21 | 107.10      | 113.50   |
| 2   | K     | 202 | ILE  | N-CA-C | 5.19  | 117.21      | 108.81   |
| 2   | 1     | 128 | GLY  | N-CA-C | 5.18  | 118.33      | 111.70   |
| 2   | Y     | 202 | ILE  | N-CA-C | 5.18  | 117.20      | 108.81   |
| 2   | Z     | 24  | ASN  | N-CA-C | -5.17 | 107.35      | 113.97   |
| 2   | L     | 24  | ASN  | N-CA-C | -5.17 | 107.35      | 113.97   |
| 2   | Z     | 150 | GLU  | N-CA-C | -5.13 | 105.68      | 111.28   |
| 2   | L     | 150 | GLU  | N-CA-C | -5.12 | 105.70      | 111.28   |
| 2   | L     | 36  | GLN  | N-CA-C | -5.11 | 102.13      | 110.20   |
| 2   | M     | 41  | THR  | N-CA-C | 5.10  | 116.81      | 108.55   |
| 2   | Z     | 36  | GLN  | N-CA-C | -5.10 | 102.15      | 110.20   |
| 2   | 1     | 41  | THR  | N-CA-C | 5.07  | 116.77      | 108.55   |
| 2   | W     | 140 | SER  | N-CA-C | 5.04  | 117.89      | 111.69   |
| 1   | T     | 13  | THR  | O-C-N  | -5.04 | 117.15      | 123.04   |
| 2   | 2     | 87  | LEU  | N-CA-C | 5.04  | 116.77      | 111.28   |
| 1   | F     | 13  | THR  | O-C-N  | -5.02 | 117.16      | 123.04   |
| 2   | N     | 87  | LEU  | N-CA-C | 5.02  | 116.75      | 111.28   |
| 1   | E     | 13  | THR  | CA-C-O | -5.02 | 114.97      | 120.69   |
| 1   | S     | 13  | THR  | CA-C-O | -5.02 | 114.97      | 120.69   |
| 2   | I     | 140 | SER  | N-CA-C | 5.01  | 117.86      | 111.69   |
| 1   | D     | 13  | THR  | O-C-N  | -5.01 | 117.18      | 123.04   |
| 1   | C     | 13  | THR  | CA-C-O | -5.00 | 114.98      | 120.69   |
| 2   | W     | 49  | VAL  | N-CA-C | 5.00  | 115.61      | 110.36   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | I     | 49  | VAL  | N-CA-C | 5.00  | 115.61      | 110.36   |
| 1   | Q     | 13  | THR  | CA-C-O | -5.00 | 114.99      | 120.69   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1769  | 0        | 1799     | 279     | 0            |
| 1   | B     | 1769  | 0        | 1799     | 267     | 0            |
| 1   | C     | 1769  | 0        | 1798     | 291     | 0            |
| 1   | D     | 1769  | 0        | 1799     | 306     | 0            |
| 1   | E     | 1769  | 0        | 1798     | 311     | 0            |
| 1   | F     | 1769  | 0        | 1797     | 306     | 0            |
| 1   | G     | 1769  | 0        | 1799     | 339     | 0            |
| 1   | O     | 1769  | 0        | 1799     | 284     | 0            |
| 1   | P     | 1769  | 0        | 1799     | 270     | 0            |
| 1   | Q     | 1769  | 0        | 1798     | 285     | 0            |
| 1   | R     | 1769  | 0        | 1799     | 306     | 0            |
| 1   | S     | 1769  | 0        | 1798     | 309     | 0            |
| 1   | T     | 1769  | 0        | 1797     | 310     | 0            |
| 1   | U     | 1769  | 0        | 1799     | 340     | 0            |
| 2   | 1     | 1558  | 0        | 1609     | 131     | 0            |
| 2   | 2     | 1558  | 0        | 1609     | 129     | 0            |
| 2   | H     | 1558  | 0        | 1609     | 147     | 0            |
| 2   | I     | 1558  | 0        | 1609     | 100     | 0            |
| 2   | J     | 1558  | 0        | 1609     | 114     | 0            |
| 2   | K     | 1558  | 0        | 1609     | 124     | 0            |
| 2   | L     | 1558  | 0        | 1609     | 137     | 0            |
| 2   | M     | 1558  | 0        | 1609     | 135     | 0            |
| 2   | N     | 1558  | 0        | 1609     | 129     | 0            |
| 2   | V     | 1558  | 0        | 1609     | 145     | 0            |
| 2   | W     | 1558  | 0        | 1609     | 105     | 0            |
| 2   | X     | 1558  | 0        | 1609     | 104     | 0            |
| 2   | Y     | 1558  | 0        | 1609     | 130     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | Z     | 1558  | 0        | 1609     | 136     | 0            |
| All | All   | 46578 | 0        | 47704    | 4166    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (4166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:177:GLU:HA  | 1:D:58:LEU:CG   | 1.26                     | 1.65              |
| 1:T:12:ILE:CD1  | 1:T:23:GLN:CG   | 1.74                     | 1.64              |
| 1:O:177:GLU:HA  | 1:P:58:LEU:CD1  | 1.21                     | 1.64              |
| 1:S:12:ILE:CD1  | 1:S:23:GLN:CG   | 1.74                     | 1.64              |
| 1:R:12:ILE:CD1  | 1:R:23:GLN:CG   | 1.74                     | 1.63              |
| 1:Q:177:GLU:HB2 | 1:R:58:LEU:CD2  | 1.19                     | 1.62              |
| 1:A:177:GLU:HA  | 1:B:58:LEU:CD1  | 1.21                     | 1.62              |
| 1:A:12:ILE:CD1  | 1:A:23:GLN:CG   | 1.74                     | 1.62              |
| 1:G:12:ILE:CD1  | 1:G:23:GLN:CG   | 1.74                     | 1.62              |
| 1:D:12:ILE:CG1  | 1:D:23:GLN:CB   | 1.78                     | 1.61              |
| 1:Q:177:GLU:CB  | 1:R:58:LEU:CD2  | 1.76                     | 1.61              |
| 1:F:12:ILE:CD1  | 1:F:23:GLN:CG   | 1.74                     | 1.61              |
| 1:B:12:ILE:CD1  | 1:B:23:GLN:CG   | 1.74                     | 1.60              |
| 1:C:177:GLU:CB  | 1:D:58:LEU:CD2  | 1.76                     | 1.60              |
| 1:Q:12:ILE:CD1  | 1:Q:23:GLN:CG   | 1.74                     | 1.60              |
| 1:Q:177:GLU:HA  | 1:R:58:LEU:CD1  | 1.18                     | 1.60              |
| 1:E:12:ILE:CG1  | 1:E:23:GLN:CB   | 1.78                     | 1.59              |
| 1:D:12:ILE:CD1  | 1:D:23:GLN:CG   | 1.74                     | 1.59              |
| 1:O:12:ILE:CG1  | 1:O:23:GLN:CB   | 1.78                     | 1.59              |
| 1:G:108:ASN:CB  | 2:H:70:ARG:HG2  | 1.28                     | 1.58              |
| 1:C:12:ILE:CG1  | 1:C:23:GLN:CB   | 1.78                     | 1.57              |
| 1:U:12:ILE:CD1  | 1:U:23:GLN:CG   | 1.74                     | 1.57              |
| 1:R:12:ILE:CD1  | 1:R:23:GLN:CA   | 1.83                     | 1.57              |
| 1:C:177:GLU:HA  | 1:D:58:LEU:CD1  | 1.18                     | 1.57              |
| 1:G:12:ILE:CD1  | 1:G:23:GLN:CA   | 1.83                     | 1.57              |
| 1:F:12:ILE:CB   | 1:F:23:GLN:HG3  | 1.11                     | 1.56              |
| 1:Q:12:ILE:CG1  | 1:Q:23:GLN:CB   | 1.78                     | 1.56              |
| 1:Q:177:GLU:HA  | 1:R:58:LEU:CG   | 1.26                     | 1.56              |
| 1:U:12:ILE:CG1  | 1:U:23:GLN:CB   | 1.78                     | 1.56              |
| 1:E:12:ILE:CB   | 1:E:23:GLN:HG3  | 1.11                     | 1.56              |
| 1:Q:177:GLU:CA  | 1:R:58:LEU:HD11 | 1.32                     | 1.56              |
| 1:C:12:ILE:CD1  | 1:C:23:GLN:CG   | 1.74                     | 1.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:P:12:ILE:CB   | 1:P:23:GLN:HG3  | 1.11                     | 1.56              |
| 1:P:12:ILE:CD1  | 1:P:23:GLN:CG   | 1.74                     | 1.56              |
| 1:P:12:ILE:CG1  | 1:P:23:GLN:CB   | 1.78                     | 1.56              |
| 1:U:12:ILE:CD1  | 1:U:23:GLN:CA   | 1.83                     | 1.56              |
| 1:B:12:ILE:CD1  | 1:B:23:GLN:CA   | 1.83                     | 1.56              |
| 1:C:177:GLU:CA  | 1:D:58:LEU:HD21 | 1.30                     | 1.56              |
| 1:C:177:GLU:HB2 | 1:D:58:LEU:CD2  | 1.19                     | 1.56              |
| 1:G:12:ILE:CG1  | 1:G:23:GLN:CB   | 1.78                     | 1.56              |
| 1:G:12:ILE:CB   | 1:G:23:GLN:HG3  | 1.11                     | 1.56              |
| 1:Q:12:ILE:CB   | 1:Q:23:GLN:HG3  | 1.11                     | 1.56              |
| 1:T:12:ILE:CB   | 1:T:23:GLN:HG3  | 1.11                     | 1.56              |
| 1:E:12:ILE:CD1  | 1:E:23:GLN:CG   | 1.74                     | 1.55              |
| 1:O:12:ILE:CD1  | 1:O:23:GLN:CG   | 1.74                     | 1.55              |
| 1:C:12:ILE:CD1  | 1:C:23:GLN:CA   | 1.83                     | 1.55              |
| 1:T:12:ILE:CD1  | 1:T:23:GLN:CA   | 1.83                     | 1.55              |
| 1:U:108:ASN:CB  | 2:V:70:ARG:HG2  | 1.28                     | 1.55              |
| 1:F:12:ILE:CG1  | 1:F:23:GLN:CB   | 1.78                     | 1.55              |
| 1:C:12:ILE:CB   | 1:C:23:GLN:HG3  | 1.11                     | 1.54              |
| 1:R:12:ILE:CG1  | 1:R:23:GLN:CB   | 1.78                     | 1.54              |
| 1:R:12:ILE:CB   | 1:R:23:GLN:HG3  | 1.11                     | 1.54              |
| 1:S:12:ILE:CD1  | 1:S:23:GLN:CA   | 1.83                     | 1.54              |
| 1:T:12:ILE:CG1  | 1:T:23:GLN:CB   | 1.78                     | 1.54              |
| 1:U:12:ILE:CB   | 1:U:23:GLN:HG3  | 1.11                     | 1.54              |
| 1:A:12:ILE:CD1  | 1:A:23:GLN:CA   | 1.83                     | 1.54              |
| 1:C:177:GLU:CA  | 1:D:58:LEU:HD11 | 1.32                     | 1.54              |
| 1:B:12:ILE:CB   | 1:B:23:GLN:HG3  | 1.11                     | 1.54              |
| 1:B:177:GLU:CA  | 1:C:58:LEU:HD11 | 1.30                     | 1.54              |
| 1:P:177:GLU:CA  | 1:Q:58:LEU:HD11 | 1.30                     | 1.54              |
| 1:D:12:ILE:HD12 | 1:D:23:GLN:CA   | 1.38                     | 1.53              |
| 1:O:12:ILE:CB   | 1:O:23:GLN:HG3  | 1.11                     | 1.53              |
| 1:A:12:ILE:CB   | 1:A:23:GLN:HG3  | 1.11                     | 1.53              |
| 1:D:12:ILE:CB   | 1:D:23:GLN:HG3  | 1.11                     | 1.53              |
| 1:O:12:ILE:HD12 | 1:O:23:GLN:CA   | 1.38                     | 1.53              |
| 1:A:12:ILE:CG1  | 1:A:23:GLN:CB   | 1.78                     | 1.52              |
| 1:S:12:ILE:CG1  | 1:S:23:GLN:CB   | 1.78                     | 1.52              |
| 1:B:12:ILE:CG1  | 1:B:23:GLN:CB   | 1.78                     | 1.52              |
| 1:P:177:GLU:HA  | 1:Q:58:LEU:CD1  | 1.06                     | 1.52              |
| 1:Q:177:GLU:CA  | 1:R:58:LEU:HD21 | 1.30                     | 1.52              |
| 1:F:12:ILE:HD12 | 1:F:23:GLN:CA   | 1.38                     | 1.52              |
| 1:S:12:ILE:CB   | 1:S:23:GLN:HG3  | 1.11                     | 1.52              |
| 1:B:12:ILE:HD12 | 1:B:23:GLN:CA   | 1.38                     | 1.51              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:12:ILE:CB   | 1:C:23:GLN:CG   | 1.88                     | 1.51              |
| 1:F:177:GLU:HA  | 1:G:58:LEU:CD1  | 1.04                     | 1.51              |
| 1:O:12:ILE:CD1  | 1:O:23:GLN:CA   | 1.83                     | 1.51              |
| 1:R:12:ILE:CB   | 1:R:23:GLN:CG   | 1.89                     | 1.51              |
| 1:U:12:ILE:CB   | 1:U:23:GLN:CG   | 1.89                     | 1.51              |
| 1:Q:12:ILE:HD12 | 1:Q:23:GLN:CA   | 1.38                     | 1.51              |
| 1:B:177:GLU:HA  | 1:C:58:LEU:CD1  | 1.06                     | 1.51              |
| 1:T:177:GLU:HA  | 1:U:58:LEU:CD1  | 1.04                     | 1.50              |
| 1:D:12:ILE:CB   | 1:D:23:GLN:CG   | 1.88                     | 1.50              |
| 1:G:12:ILE:CB   | 1:G:23:GLN:CG   | 1.89                     | 1.50              |
| 1:E:12:ILE:CD1  | 1:E:23:GLN:CA   | 1.83                     | 1.50              |
| 1:T:12:ILE:HD12 | 1:T:23:GLN:CA   | 1.38                     | 1.50              |
| 1:T:12:ILE:CB   | 1:T:23:GLN:CG   | 1.89                     | 1.50              |
| 1:B:12:ILE:CB   | 1:B:23:GLN:CG   | 1.89                     | 1.50              |
| 1:P:12:ILE:CD1  | 1:P:23:GLN:CA   | 1.83                     | 1.49              |
| 1:E:12:ILE:CB   | 1:E:23:GLN:CG   | 1.89                     | 1.49              |
| 1:P:12:ILE:CB   | 1:P:23:GLN:CG   | 1.89                     | 1.49              |
| 1:P:12:ILE:HD12 | 1:P:23:GLN:CA   | 1.38                     | 1.49              |
| 1:B:108:ASN:CB  | 2:J:70:ARG:HG2  | 1.38                     | 1.49              |
| 1:P:108:ASN:CB  | 2:X:70:ARG:HG2  | 1.38                     | 1.48              |
| 1:D:12:ILE:CD1  | 1:D:23:GLN:CA   | 1.83                     | 1.47              |
| 1:R:12:ILE:HD12 | 1:R:23:GLN:CA   | 1.38                     | 1.47              |
| 1:G:12:ILE:HD12 | 1:G:23:GLN:CA   | 1.38                     | 1.47              |
| 1:E:12:ILE:HD12 | 1:E:23:GLN:CA   | 1.38                     | 1.47              |
| 1:O:12:ILE:CB   | 1:O:23:GLN:CG   | 1.88                     | 1.47              |
| 1:S:12:ILE:CB   | 1:S:23:GLN:CG   | 1.89                     | 1.47              |
| 1:Q:12:ILE:CD1  | 1:Q:23:GLN:CA   | 1.83                     | 1.46              |
| 1:A:12:ILE:CB   | 1:A:23:GLN:CG   | 1.88                     | 1.46              |
| 1:F:12:ILE:CD1  | 1:F:23:GLN:CA   | 1.83                     | 1.46              |
| 1:F:12:ILE:CB   | 1:F:23:GLN:CG   | 1.89                     | 1.46              |
| 1:Q:12:ILE:CB   | 1:Q:23:GLN:CG   | 1.88                     | 1.45              |
| 1:T:177:GLU:N   | 1:U:58:LEU:HD21 | 1.26                     | 1.45              |
| 1:C:12:ILE:HD12 | 1:C:23:GLN:CA   | 1.38                     | 1.45              |
| 1:Q:177:GLU:CA  | 1:R:58:LEU:CD1  | 1.89                     | 1.45              |
| 1:Q:108:ASN:CB  | 2:Y:70:ARG:HG2  | 1.46                     | 1.44              |
| 1:Q:177:GLU:CA  | 1:R:58:LEU:CD2  | 1.88                     | 1.44              |
| 1:F:177:GLU:N   | 1:G:58:LEU:HD21 | 1.26                     | 1.44              |
| 1:U:12:ILE:HD12 | 1:U:23:GLN:CA   | 1.38                     | 1.44              |
| 1:F:177:GLU:CA  | 1:G:58:LEU:HD11 | 1.46                     | 1.43              |
| 1:A:57:ARG:HH21 | 1:G:178:ARG:CA  | 1.30                     | 1.43              |
| 1:P:12:ILE:HB   | 1:P:23:GLN:CG   | 1.47                     | 1.42              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:U:12:ILE:HB   | 1:U:23:GLN:CG   | 1.47                     | 1.42              |
| 1:T:177:GLU:CA  | 1:U:58:LEU:HD11 | 1.46                     | 1.42              |
| 1:C:12:ILE:HB   | 1:C:23:GLN:CG   | 1.47                     | 1.42              |
| 1:C:108:ASN:CB  | 2:K:70:ARG:HG2  | 1.46                     | 1.41              |
| 1:E:12:ILE:HB   | 1:E:23:GLN:CG   | 1.47                     | 1.41              |
| 1:A:12:ILE:HB   | 1:A:23:GLN:CG   | 1.47                     | 1.40              |
| 1:R:12:ILE:HB   | 1:R:23:GLN:CG   | 1.47                     | 1.40              |
| 1:G:12:ILE:HB   | 1:G:23:GLN:CG   | 1.47                     | 1.40              |
| 1:O:57:ARG:HH21 | 1:U:178:ARG:CA  | 1.30                     | 1.40              |
| 1:S:12:ILE:HB   | 1:S:23:GLN:CG   | 1.47                     | 1.40              |
| 1:T:12:ILE:HB   | 1:T:23:GLN:CG   | 1.47                     | 1.39              |
| 1:F:177:GLU:CA  | 1:G:58:LEU:CD1  | 1.99                     | 1.39              |
| 1:S:12:ILE:HD12 | 1:S:23:GLN:CA   | 1.38                     | 1.39              |
| 1:T:177:GLU:CA  | 1:U:58:LEU:CD1  | 1.98                     | 1.39              |
| 1:A:12:ILE:HD12 | 1:A:23:GLN:CA   | 1.38                     | 1.38              |
| 1:B:12:ILE:HB   | 1:B:23:GLN:CG   | 1.47                     | 1.38              |
| 1:Q:177:GLU:N   | 1:R:58:LEU:HD21 | 1.35                     | 1.38              |
| 1:C:177:GLU:N   | 1:D:58:LEU:HD21 | 1.35                     | 1.38              |
| 1:A:57:ARG:NH2  | 1:G:178:ARG:CA  | 1.87                     | 1.38              |
| 1:C:108:ASN:CG  | 2:K:70:ARG:HG2  | 1.50                     | 1.37              |
| 1:Q:177:GLU:C   | 1:R:58:LEU:HD11 | 1.46                     | 1.37              |
| 1:C:177:GLU:CA  | 1:D:58:LEU:CD2  | 1.88                     | 1.37              |
| 1:A:57:ARG:NE   | 1:G:177:GLU:O   | 1.58                     | 1.37              |
| 1:C:177:GLU:C   | 1:D:58:LEU:HD11 | 1.46                     | 1.37              |
| 1:F:108:ASN:CB  | 2:N:70:ARG:HG2  | 1.55                     | 1.36              |
| 1:C:155:GLY:O   | 1:D:86:ARG:NH2  | 1.59                     | 1.35              |
| 1:A:60:GLU:OE2  | 1:G:161:LYS:HB2 | 1.21                     | 1.35              |
| 1:C:178:ARG:HA  | 1:D:57:ARG:NH2  | 1.42                     | 1.35              |
| 1:O:57:ARG:NE   | 1:U:177:GLU:O   | 1.58                     | 1.35              |
| 1:Q:12:ILE:HB   | 1:Q:23:GLN:CG   | 1.47                     | 1.34              |
| 1:O:57:ARG:NH2  | 1:U:178:ARG:CA  | 1.87                     | 1.34              |
| 1:O:57:ARG:NH2  | 1:U:178:ARG:C   | 1.85                     | 1.34              |
| 1:U:108:ASN:CG  | 2:V:70:ARG:HG2  | 1.52                     | 1.34              |
| 1:Q:108:ASN:CG  | 2:Y:70:ARG:HG2  | 1.50                     | 1.34              |
| 1:Q:155:GLY:O   | 1:R:86:ARG:NH2  | 1.59                     | 1.34              |
| 1:O:12:ILE:HB   | 1:O:23:GLN:CG   | 1.47                     | 1.34              |
| 1:A:177:GLU:CA  | 1:B:58:LEU:HD11 | 1.58                     | 1.33              |
| 1:A:57:ARG:NH2  | 1:G:178:ARG:C   | 1.85                     | 1.33              |
| 1:O:60:GLU:OE2  | 1:U:161:LYS:HD2 | 1.28                     | 1.33              |
| 1:T:108:ASN:CB  | 2:2:70:ARG:HG2  | 1.55                     | 1.33              |
| 1:O:177:GLU:CA  | 1:P:58:LEU:HD11 | 1.58                     | 1.32              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:12:ILE:HB    | 1:F:23:GLN:CG   | 1.47                     | 1.32              |
| 1:G:108:ASN:CG   | 2:H:70:ARG:HG2  | 1.52                     | 1.31              |
| 1:F:101:VAL:CG2  | 2:M:58:TYR:CD1  | 2.14                     | 1.30              |
| 1:D:101:VAL:CG2  | 2:K:58:TYR:HD1  | 1.45                     | 1.30              |
| 1:Q:178:ARG:HA   | 1:R:57:ARG:NH2  | 1.42                     | 1.30              |
| 1:A:60:GLU:OE2   | 1:G:161:LYS:HD2 | 1.28                     | 1.30              |
| 1:A:108:ASN:CB   | 2:I:70:ARG:HG2  | 1.62                     | 1.29              |
| 1:D:12:ILE:HB    | 1:D:23:GLN:CG   | 1.47                     | 1.29              |
| 1:S:161:LYS:CB   | 1:T:60:GLU:OE2  | 1.80                     | 1.29              |
| 1:D:101:VAL:CG2  | 2:K:58:TYR:CD1  | 2.14                     | 1.29              |
| 1:E:161:LYS:CB   | 1:F:60:GLU:OE2  | 1.80                     | 1.29              |
| 1:R:101:VAL:CG2  | 2:Y:58:TYR:CD1  | 2.14                     | 1.29              |
| 1:T:101:VAL:CG2  | 2:I:58:TYR:CD1  | 2.14                     | 1.29              |
| 1:O:107:VAL:HG11 | 2:W:66:TYR:OH   | 1.33                     | 1.29              |
| 1:G:108:ASN:CB   | 2:H:70:ARG:CG   | 2.09                     | 1.28              |
| 1:U:108:ASN:CB   | 2:V:70:ARG:CG   | 2.09                     | 1.28              |
| 1:C:101:VAL:HG21 | 2:J:58:TYR:CD1  | 1.68                     | 1.28              |
| 1:R:101:VAL:CG2  | 2:Y:58:TYR:HD1  | 1.45                     | 1.28              |
| 1:S:101:VAL:CG2  | 2:Z:58:TYR:CD1  | 2.17                     | 1.27              |
| 1:A:57:ARG:CZ    | 1:G:177:GLU:O   | 1.82                     | 1.27              |
| 1:O:108:ASN:CB   | 2:W:70:ARG:HG2  | 1.62                     | 1.27              |
| 1:O:177:GLU:O    | 1:P:57:ARG:NH2  | 1.66                     | 1.27              |
| 1:E:101:VAL:CG2  | 2:L:58:TYR:CD1  | 2.17                     | 1.27              |
| 1:P:107:VAL:HG11 | 2:X:66:TYR:OH   | 1.32                     | 1.27              |
| 1:G:108:ASN:HB3  | 2:H:70:ARG:CG   | 1.65                     | 1.26              |
| 1:B:9:ASP:HB2    | 1:B:26:TYR:OH   | 1.09                     | 1.26              |
| 1:Q:101:VAL:HG21 | 2:X:58:TYR:CD1  | 1.68                     | 1.26              |
| 1:O:60:GLU:OE2   | 1:U:161:LYS:HB2 | 1.21                     | 1.26              |
| 1:O:86:ARG:NH2   | 1:U:155:GLY:O   | 1.68                     | 1.26              |
| 1:D:155:GLY:O    | 1:E:86:ARG:NH2  | 1.69                     | 1.26              |
| 1:U:9:ASP:HB2    | 1:U:26:TYR:OH   | 1.09                     | 1.26              |
| 1:A:12:ILE:HD13  | 1:A:23:GLN:CG   | 1.47                     | 1.25              |
| 1:B:107:VAL:HG11 | 2:J:66:TYR:OH   | 1.32                     | 1.25              |
| 1:C:9:ASP:HB2    | 1:C:26:TYR:OH   | 1.09                     | 1.25              |
| 1:T:9:ASP:HB2    | 1:T:26:TYR:OH   | 1.09                     | 1.25              |
| 1:D:177:GLU:OE1  | 1:E:57:ARG:N    | 1.68                     | 1.25              |
| 1:T:101:VAL:HG21 | 2:I:58:TYR:CD1  | 1.72                     | 1.25              |
| 1:A:177:GLU:O    | 1:B:57:ARG:NH2  | 1.66                     | 1.25              |
| 1:C:12:ILE:HD13  | 1:C:23:GLN:CG   | 1.47                     | 1.25              |
| 1:D:9:ASP:HB2    | 1:D:26:TYR:OH   | 1.09                     | 1.25              |
| 1:O:57:ARG:CZ    | 1:U:177:GLU:O   | 1.82                     | 1.25              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:S:9:ASP:HB2    | 1:S:26:TYR:OH   | 1.09                     | 1.25              |
| 1:T:102:THR:O    | 2:2:85:ASN:OD1  | 1.53                     | 1.25              |
| 1:Q:101:VAL:CG2  | 2:X:58:TYR:CD1  | 2.19                     | 1.24              |
| 1:A:107:VAL:HG11 | 2:I:66:TYR:OH   | 1.33                     | 1.24              |
| 1:P:161:LYS:HB2  | 1:Q:60:GLU:OE2  | 1.36                     | 1.24              |
| 1:R:177:GLU:CD   | 1:S:57:ARG:H    | 1.45                     | 1.24              |
| 1:A:9:ASP:HB2    | 1:A:26:TYR:OH   | 1.09                     | 1.24              |
| 1:T:21:LEU:HD11  | 1:U:130:ARG:CD  | 1.68                     | 1.24              |
| 1:A:102:THR:O    | 2:I:85:ASN:OD1  | 1.54                     | 1.24              |
| 1:F:102:THR:O    | 2:N:85:ASN:OD1  | 1.52                     | 1.24              |
| 1:O:9:ASP:HB2    | 1:O:26:TYR:OH   | 1.09                     | 1.24              |
| 1:S:12:ILE:HD13  | 1:S:23:GLN:CG   | 1.48                     | 1.24              |
| 1:U:12:ILE:HD13  | 1:U:23:GLN:CG   | 1.47                     | 1.24              |
| 1:C:101:VAL:CG2  | 2:J:58:TYR:CD1  | 2.19                     | 1.23              |
| 1:P:177:GLU:OE2  | 1:Q:56:SER:OG   | 1.56                     | 1.23              |
| 1:Q:9:ASP:HB2    | 1:Q:26:TYR:OH   | 1.09                     | 1.23              |
| 1:R:177:GLU:OE1  | 1:S:57:ARG:N    | 1.68                     | 1.23              |
| 1:A:57:ARG:HH21  | 1:G:178:ARG:N   | 1.36                     | 1.23              |
| 1:E:173:VAL:O    | 1:F:58:LEU:HD21 | 1.38                     | 1.23              |
| 1:P:9:ASP:HB2    | 1:P:26:TYR:OH   | 1.09                     | 1.23              |
| 1:P:101:VAL:HG21 | 2:W:58:TYR:CD1  | 1.72                     | 1.23              |
| 1:B:101:VAL:HG21 | 2:I:58:TYR:CD1  | 1.72                     | 1.23              |
| 1:A:86:ARG:NH2   | 1:G:155:GLY:O   | 1.68                     | 1.23              |
| 1:D:161:LYS:CB   | 1:E:60:GLU:OE2  | 1.86                     | 1.23              |
| 1:F:12:ILE:HD13  | 1:F:23:GLN:CG   | 1.47                     | 1.23              |
| 1:E:9:ASP:HB2    | 1:E:26:TYR:OH   | 1.09                     | 1.23              |
| 1:Q:177:GLU:CB   | 1:R:58:LEU:HD21 | 1.50                     | 1.23              |
| 1:R:12:ILE:HD13  | 1:R:23:GLN:CG   | 1.47                     | 1.23              |
| 1:R:155:GLY:O    | 1:S:86:ARG:NH2  | 1.69                     | 1.23              |
| 1:U:107:VAL:HG11 | 2:V:66:TYR:OH   | 1.38                     | 1.23              |
| 1:O:102:THR:O    | 2:W:85:ASN:OD1  | 1.54                     | 1.22              |
| 1:C:177:GLU:CA   | 1:D:58:LEU:CD1  | 1.89                     | 1.22              |
| 1:D:177:GLU:CD   | 1:E:57:ARG:H    | 1.45                     | 1.22              |
| 1:F:101:VAL:HG21 | 2:M:58:TYR:CD1  | 1.72                     | 1.22              |
| 1:F:9:ASP:HB2    | 1:F:26:TYR:OH   | 1.09                     | 1.22              |
| 1:F:21:LEU:HD11  | 1:G:130:ARG:CD  | 1.68                     | 1.22              |
| 1:G:9:ASP:HB2    | 1:G:26:TYR:OH   | 1.09                     | 1.22              |
| 1:Q:12:ILE:HD13  | 1:Q:23:GLN:CG   | 1.48                     | 1.22              |
| 1:R:9:ASP:HB2    | 1:R:26:TYR:OH   | 1.09                     | 1.22              |
| 1:Q:177:GLU:CB   | 1:R:58:LEU:HD22 | 1.47                     | 1.22              |
| 1:A:57:ARG:N     | 1:G:177:GLU:OE1 | 1.73                     | 1.22              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:161:LYS:HB2  | 1:E:60:GLU:OE2  | 1.05                     | 1.22              |
| 1:O:57:ARG:HH21  | 1:U:178:ARG:N   | 1.36                     | 1.22              |
| 1:C:177:GLU:CB   | 1:D:58:LEU:HD22 | 1.47                     | 1.21              |
| 1:R:161:LYS:CB   | 1:S:60:GLU:OE2  | 1.86                     | 1.21              |
| 1:C:108:ASN:ND2  | 2:K:70:ARG:HG2  | 1.54                     | 1.21              |
| 1:F:177:GLU:OE1  | 1:G:58:LEU:HD13 | 1.41                     | 1.21              |
| 1:O:12:ILE:CG1   | 1:O:23:GLN:CG   | 2.11                     | 1.21              |
| 1:S:108:ASN:ND2  | 2:1:70:ARG:HG2  | 1.55                     | 1.21              |
| 1:T:12:ILE:HD13  | 1:T:23:GLN:CG   | 1.47                     | 1.21              |
| 1:B:161:LYS:HB2  | 1:C:60:GLU:OE2  | 1.36                     | 1.20              |
| 1:C:177:GLU:CB   | 1:D:58:LEU:HD21 | 1.50                     | 1.20              |
| 1:T:177:GLU:OE1  | 1:U:58:LEU:HD13 | 1.41                     | 1.20              |
| 1:U:108:ASN:HB3  | 2:V:70:ARG:CG   | 1.65                     | 1.20              |
| 1:E:12:ILE:HD13  | 1:E:23:GLN:CG   | 1.47                     | 1.20              |
| 1:G:102:THR:O    | 2:H:85:ASN:OD1  | 1.59                     | 1.20              |
| 1:R:101:VAL:HG21 | 2:Y:58:TYR:CD1  | 1.73                     | 1.20              |
| 1:E:108:ASN:ND2  | 2:M:70:ARG:HG2  | 1.55                     | 1.20              |
| 1:G:107:VAL:HG11 | 2:H:66:TYR:OH   | 1.38                     | 1.20              |
| 1:Q:108:ASN:ND2  | 2:Y:70:ARG:HG2  | 1.54                     | 1.20              |
| 1:D:177:GLU:N    | 1:E:58:LEU:HD21 | 1.49                     | 1.20              |
| 1:P:12:ILE:CG1   | 1:P:23:GLN:HG3  | 1.72                     | 1.20              |
| 1:Q:12:ILE:CG1   | 1:Q:23:GLN:HG3  | 1.72                     | 1.19              |
| 1:F:12:ILE:CG1   | 1:F:23:GLN:CG   | 2.10                     | 1.19              |
| 1:F:12:ILE:CG1   | 1:F:23:GLN:HG3  | 1.72                     | 1.19              |
| 1:D:101:VAL:HG21 | 2:K:58:TYR:CD1  | 1.73                     | 1.19              |
| 1:O:12:ILE:CG1   | 1:O:23:GLN:HG3  | 1.72                     | 1.19              |
| 1:S:173:VAL:O    | 1:T:58:LEU:HD21 | 1.38                     | 1.19              |
| 1:P:12:ILE:HD13  | 1:P:23:GLN:CG   | 1.48                     | 1.19              |
| 1:R:12:ILE:CG1   | 1:R:23:GLN:HG3  | 1.72                     | 1.19              |
| 1:A:177:GLU:N    | 1:B:58:LEU:HD21 | 1.58                     | 1.19              |
| 1:F:177:GLU:HA   | 1:G:58:LEU:CG   | 1.72                     | 1.19              |
| 1:E:101:VAL:HG21 | 2:L:58:TYR:CD1  | 1.79                     | 1.18              |
| 1:S:12:ILE:CG1   | 1:S:23:GLN:HG3  | 1.72                     | 1.18              |
| 1:A:58:LEU:HD21  | 1:G:177:GLU:N   | 1.35                     | 1.18              |
| 1:C:108:ASN:CB   | 2:K:70:ARG:CG   | 2.20                     | 1.18              |
| 1:Q:12:ILE:CG1   | 1:Q:23:GLN:CG   | 2.11                     | 1.18              |
| 1:Q:108:ASN:CB   | 2:Y:70:ARG:CG   | 2.20                     | 1.18              |
| 1:G:12:ILE:CG1   | 1:G:23:GLN:HG3  | 1.72                     | 1.18              |
| 1:T:177:GLU:HA   | 1:U:58:LEU:CG   | 1.72                     | 1.18              |
| 1:E:177:GLU:CD   | 1:F:57:ARG:H    | 1.52                     | 1.18              |
| 1:O:57:ARG:N     | 1:U:177:GLU:OE1 | 1.73                     | 1.18              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:173:VAL:O    | 1:T:58:LEU:CD2   | 1.92                     | 1.18              |
| 1:A:12:ILE:CG1   | 1:A:23:GLN:HG3   | 1.72                     | 1.18              |
| 1:A:57:ARG:HH22  | 1:G:178:ARG:C    | 1.48                     | 1.18              |
| 1:R:161:LYS:HB2  | 1:S:60:GLU:OE2   | 1.05                     | 1.18              |
| 1:A:177:GLU:CA   | 1:B:58:LEU:CD1   | 2.18                     | 1.17              |
| 1:C:12:ILE:CG1   | 1:C:23:GLN:HG3   | 1.72                     | 1.17              |
| 1:T:12:ILE:CG1   | 1:T:23:GLN:CG    | 2.11                     | 1.17              |
| 1:B:177:GLU:OE2  | 1:C:56:SER:OG    | 1.56                     | 1.17              |
| 1:T:155:GLY:O    | 1:U:86:ARG:NH2   | 1.76                     | 1.17              |
| 1:U:12:ILE:CG1   | 1:U:23:GLN:HG3   | 1.72                     | 1.17              |
| 1:E:173:VAL:O    | 1:F:58:LEU:CD2   | 1.92                     | 1.17              |
| 1:O:58:LEU:HD21  | 1:U:177:GLU:N    | 1.35                     | 1.17              |
| 1:S:101:VAL:HG21 | 2:Z:58:TYR:CD1   | 1.79                     | 1.17              |
| 1:F:155:GLY:O    | 1:G:86:ARG:NH2   | 1.76                     | 1.17              |
| 1:S:108:ASN:CG   | 2:1:70:ARG:HG2   | 1.70                     | 1.17              |
| 1:C:108:ASN:HB3  | 2:K:70:ARG:HD3   | 1.26                     | 1.16              |
| 1:U:102:THR:O    | 2:V:85:ASN:OD1   | 1.59                     | 1.16              |
| 1:A:12:ILE:CG1   | 1:A:23:GLN:CG    | 2.11                     | 1.16              |
| 1:O:177:GLU:CA   | 1:P:58:LEU:CD1   | 2.18                     | 1.16              |
| 1:A:60:GLU:OE2   | 1:G:161:LYS:CB   | 1.92                     | 1.16              |
| 1:A:21:LEU:HD11  | 1:B:130:ARG:HD2  | 1.27                     | 1.16              |
| 1:A:177:GLU:C    | 1:B:57:ARG:HH21  | 1.54                     | 1.16              |
| 1:O:60:GLU:OE2   | 1:U:161:LYS:CB   | 1.92                     | 1.16              |
| 1:O:177:GLU:N    | 1:P:58:LEU:HD21  | 1.58                     | 1.16              |
| 1:F:177:GLU:CA   | 1:G:58:LEU:CD2   | 2.24                     | 1.16              |
| 1:D:12:ILE:HD13  | 1:D:23:GLN:CG    | 1.47                     | 1.15              |
| 1:B:12:ILE:CG1   | 1:B:23:GLN:HG3   | 1.72                     | 1.15              |
| 1:S:12:ILE:CG1   | 1:S:23:GLN:CG    | 2.10                     | 1.15              |
| 1:S:177:GLU:CD   | 1:T:57:ARG:H     | 1.52                     | 1.15              |
| 1:T:177:GLU:CA   | 1:U:58:LEU:CD2   | 2.24                     | 1.15              |
| 1:E:108:ASN:CG   | 2:M:70:ARG:HG2   | 1.70                     | 1.15              |
| 1:R:103:TYR:C    | 2:Z:81:THR:HG21  | 1.70                     | 1.15              |
| 1:D:103:TYR:C    | 2:L:81:THR:HG21  | 1.70                     | 1.14              |
| 1:B:178:ARG:CA   | 1:C:57:ARG:NH2   | 2.11                     | 1.14              |
| 1:D:124:THR:HG22 | 1:E:130:ARG:HH21 | 1.05                     | 1.14              |
| 1:B:177:GLU:CA   | 1:C:58:LEU:CD1   | 2.01                     | 1.14              |
| 1:O:177:GLU:C    | 1:P:57:ARG:HH21  | 1.54                     | 1.14              |
| 1:P:12:ILE:CG1   | 1:P:23:GLN:HB2   | 1.59                     | 1.14              |
| 1:P:101:VAL:CG2  | 2:W:58:TYR:CD1   | 2.31                     | 1.14              |
| 1:U:108:ASN:HB3  | 2:V:70:ARG:HG2   | 1.17                     | 1.14              |
| 1:A:177:GLU:O    | 1:B:57:ARG:CZ    | 1.95                     | 1.14              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:103:TYR:C    | 2:M:81:THR:HG21  | 1.72                     | 1.14              |
| 1:G:101:VAL:HG21 | 2:N:58:TYR:CD1   | 1.83                     | 1.14              |
| 1:T:12:ILE:CG1   | 1:T:23:GLN:HG3   | 1.72                     | 1.14              |
| 1:O:12:ILE:HD13  | 1:O:23:GLN:CG    | 1.47                     | 1.13              |
| 1:O:177:GLU:O    | 1:P:57:ARG:CZ    | 1.95                     | 1.13              |
| 1:P:178:ARG:CA   | 1:Q:57:ARG:NH2   | 2.11                     | 1.13              |
| 1:T:161:LYS:HD2  | 1:U:60:GLU:OE2   | 1.45                     | 1.13              |
| 1:B:12:ILE:HD13  | 1:B:23:GLN:CG    | 1.47                     | 1.13              |
| 1:F:161:LYS:HD2  | 1:G:60:GLU:OE2   | 1.45                     | 1.13              |
| 1:Q:101:VAL:CG2  | 2:X:58:TYR:CE1   | 2.31                     | 1.13              |
| 1:S:103:TYR:C    | 2:1:81:THR:HG21  | 1.72                     | 1.13              |
| 1:S:177:GLU:OE1  | 1:T:57:ARG:HB2   | 1.48                     | 1.13              |
| 1:T:177:GLU:CA   | 1:U:58:LEU:HD21  | 1.78                     | 1.13              |
| 1:E:177:GLU:OE1  | 1:F:57:ARG:CB    | 1.97                     | 1.13              |
| 1:G:12:ILE:HD13  | 1:G:23:GLN:CG    | 1.47                     | 1.13              |
| 1:P:108:ASN:HB3  | 2:X:70:ARG:HG2   | 1.24                     | 1.13              |
| 1:E:155:GLY:O    | 1:F:86:ARG:NH2   | 1.82                     | 1.13              |
| 1:E:177:GLU:OE1  | 1:F:57:ARG:HB2   | 1.48                     | 1.13              |
| 1:P:108:ASN:HB3  | 2:X:70:ARG:CG    | 1.79                     | 1.13              |
| 1:U:107:VAL:CG1  | 2:V:66:TYR:OH    | 1.96                     | 1.13              |
| 1:B:101:VAL:CG2  | 2:I:58:TYR:CD1   | 2.31                     | 1.13              |
| 1:G:107:VAL:CG1  | 2:H:66:TYR:OH    | 1.96                     | 1.12              |
| 1:O:57:ARG:HH22  | 1:U:178:ARG:C    | 1.48                     | 1.12              |
| 1:P:108:ASN:CB   | 2:X:70:ARG:CG    | 2.27                     | 1.12              |
| 1:Q:21:LEU:HD11  | 1:R:130:ARG:HD2  | 1.14                     | 1.12              |
| 1:R:177:GLU:N    | 1:S:58:LEU:HD21  | 1.49                     | 1.13              |
| 1:T:101:VAL:CG2  | 2:1:58:TYR:CE1   | 2.32                     | 1.12              |
| 1:T:108:ASN:CB   | 2:2:70:ARG:CG    | 2.28                     | 1.12              |
| 1:C:101:VAL:CG2  | 2:J:58:TYR:CE1   | 2.31                     | 1.12              |
| 1:D:12:ILE:CG1   | 1:D:23:GLN:HB2   | 1.59                     | 1.12              |
| 1:F:101:VAL:CG2  | 2:M:58:TYR:CE1   | 2.32                     | 1.12              |
| 1:F:108:ASN:CG   | 2:N:70:ARG:HG2   | 1.75                     | 1.12              |
| 1:F:177:GLU:HB2  | 1:G:58:LEU:HD22  | 1.21                     | 1.12              |
| 1:Q:108:ASN:HB3  | 2:Y:70:ARG:HD3   | 1.26                     | 1.12              |
| 1:S:155:GLY:O    | 1:T:86:ARG:NH2   | 1.82                     | 1.12              |
| 1:Q:177:GLU:OE1  | 1:R:58:LEU:N     | 1.83                     | 1.12              |
| 1:R:124:THR:HG22 | 1:S:130:ARG:HH21 | 1.05                     | 1.12              |
| 1:U:101:VAL:HG21 | 2:2:58:TYR:CD1   | 1.83                     | 1.12              |
| 1:B:108:ASN:HB3  | 2:J:70:ARG:CG    | 1.79                     | 1.12              |
| 1:P:177:GLU:CA   | 1:Q:58:LEU:CD1   | 2.01                     | 1.12              |
| 1:S:177:GLU:OE1  | 1:T:57:ARG:CB    | 1.97                     | 1.12              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:108:ASN:ND2  | 2:L:70:ARG:HG2  | 1.65                     | 1.11              |
| 1:U:108:ASN:HB3  | 2:V:70:ARG:CD   | 1.80                     | 1.11              |
| 1:C:161:LYS:HB2  | 1:D:60:GLU:OE2  | 1.51                     | 1.11              |
| 1:E:12:ILE:CG1   | 1:E:23:GLN:HB2  | 1.59                     | 1.11              |
| 1:E:12:ILE:CG1   | 1:E:23:GLN:HG3  | 1.72                     | 1.11              |
| 1:F:177:GLU:CA   | 1:G:58:LEU:HD21 | 1.78                     | 1.11              |
| 1:S:97:GLN:OE1   | 2:Z:61:ALA:HB1  | 1.50                     | 1.11              |
| 1:B:108:ASN:CB   | 2:J:70:ARG:CG   | 2.27                     | 1.11              |
| 1:B:108:ASN:HB3  | 2:J:70:ARG:HG2  | 1.24                     | 1.11              |
| 1:D:12:ILE:CG1   | 1:D:23:GLN:HG3  | 1.72                     | 1.11              |
| 1:A:177:GLU:OE1  | 1:B:58:LEU:HD13 | 1.50                     | 1.10              |
| 1:R:161:LYS:HD2  | 1:S:60:GLU:OE2  | 1.51                     | 1.10              |
| 1:C:177:GLU:OE1  | 1:D:58:LEU:N    | 1.83                     | 1.10              |
| 1:E:97:GLN:OE1   | 2:L:61:ALA:HB1  | 1.51                     | 1.10              |
| 1:C:108:ASN:HB3  | 2:K:70:ARG:CD   | 1.81                     | 1.10              |
| 1:D:161:LYS:HD2  | 1:E:60:GLU:OE2  | 1.51                     | 1.10              |
| 1:G:108:ASN:HB3  | 2:H:70:ARG:CD   | 1.80                     | 1.10              |
| 1:Q:161:LYS:HB2  | 1:R:60:GLU:OE2  | 1.51                     | 1.10              |
| 1:R:108:ASN:ND2  | 2:Z:70:ARG:HG2  | 1.65                     | 1.10              |
| 1:T:108:ASN:CG   | 2:2:70:ARG:HG2  | 1.75                     | 1.10              |
| 1:C:12:ILE:CG1   | 1:C:23:GLN:CG   | 2.11                     | 1.10              |
| 1:F:108:ASN:CB   | 2:N:70:ARG:CG   | 2.28                     | 1.10              |
| 1:F:108:ASN:ND2  | 2:N:70:ARG:HG2  | 1.66                     | 1.10              |
| 1:S:108:ASN:CB   | 2:1:70:ARG:HG2  | 1.82                     | 1.10              |
| 1:E:108:ASN:CB   | 2:M:70:ARG:HG2  | 1.82                     | 1.09              |
| 1:O:130:ARG:HD2  | 1:U:21:LEU:HD11 | 1.11                     | 1.09              |
| 1:O:101:VAL:HG21 | 2:V:58:TYR:CD1  | 1.88                     | 1.09              |
| 1:R:108:ASN:CG   | 2:Z:70:ARG:HG2  | 1.77                     | 1.09              |
| 1:S:101:VAL:CG2  | 2:Z:58:TYR:HD1  | 1.61                     | 1.09              |
| 1:G:108:ASN:HB3  | 2:H:70:ARG:HG2  | 1.17                     | 1.09              |
| 1:O:177:GLU:OE1  | 1:P:58:LEU:HD13 | 1.50                     | 1.09              |
| 1:C:21:LEU:HD11  | 1:D:130:ARG:HD2 | 1.14                     | 1.09              |
| 1:Q:108:ASN:HB3  | 2:Y:70:ARG:CD   | 1.81                     | 1.09              |
| 1:U:12:ILE:CG1   | 1:U:23:GLN:CG   | 2.10                     | 1.09              |
| 1:D:177:GLU:H    | 1:E:58:LEU:HD21 | 0.95                     | 1.09              |
| 1:S:12:ILE:CG1   | 1:S:23:GLN:HB2  | 1.59                     | 1.09              |
| 1:T:178:ARG:CA   | 1:U:57:ARG:HH21 | 1.66                     | 1.09              |
| 1:A:101:VAL:HG21 | 2:H:58:TYR:CD1  | 1.88                     | 1.08              |
| 1:D:173:VAL:O    | 1:E:58:LEU:CD2  | 2.01                     | 1.08              |
| 1:O:21:LEU:HD11  | 1:P:130:ARG:HD2 | 1.27                     | 1.08              |
| 1:R:173:VAL:O    | 1:S:58:LEU:CD2  | 2.01                     | 1.08              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:T:108:ASN:ND2  | 2:2:70:ARG:HG2  | 1.66                     | 1.08              |
| 1:E:161:LYS:HB2  | 1:F:60:GLU:OE2  | 0.90                     | 1.08              |
| 1:G:12:ILE:CG1   | 1:G:23:GLN:HB2  | 1.59                     | 1.08              |
| 1:O:57:ARG:NH2   | 1:U:178:ARG:HA  | 1.67                     | 1.08              |
| 1:A:130:ARG:HD2  | 1:G:21:LEU:HD11 | 1.11                     | 1.08              |
| 1:B:177:GLU:HA   | 1:C:58:LEU:HD13 | 1.35                     | 1.08              |
| 1:S:161:LYS:HB2  | 1:T:60:GLU:OE2  | 0.90                     | 1.08              |
| 1:S:177:GLU:H    | 1:T:58:LEU:HD21 | 1.19                     | 1.08              |
| 1:A:12:ILE:CG1   | 1:A:23:GLN:HB2  | 1.59                     | 1.08              |
| 1:R:12:ILE:CG1   | 1:R:23:GLN:HB2  | 1.59                     | 1.08              |
| 1:R:177:GLU:H    | 1:S:58:LEU:HD21 | 0.95                     | 1.08              |
| 1:A:57:ARG:NH2   | 1:G:178:ARG:HA  | 1.67                     | 1.08              |
| 1:D:108:ASN:CG   | 2:L:70:ARG:HG2  | 1.76                     | 1.08              |
| 1:E:177:GLU:CD   | 1:F:58:LEU:HD13 | 1.77                     | 1.08              |
| 1:F:161:LYS:HB2  | 1:G:60:GLU:OE2  | 1.55                     | 1.07              |
| 1:O:57:ARG:HH21  | 1:U:177:GLU:C   | 1.62                     | 1.07              |
| 1:A:57:ARG:HH21  | 1:G:177:GLU:C   | 1.62                     | 1.07              |
| 1:F:178:ARG:CA   | 1:G:57:ARG:HH21 | 1.66                     | 1.07              |
| 1:P:101:VAL:CG2  | 2:W:58:TYR:HD1  | 1.65                     | 1.07              |
| 1:Q:12:ILE:CG1   | 1:Q:23:GLN:HB2  | 1.59                     | 1.07              |
| 1:F:177:GLU:O    | 1:G:57:ARG:NH2  | 1.88                     | 1.07              |
| 1:T:177:GLU:HB2  | 1:U:58:LEU:HD22 | 1.21                     | 1.07              |
| 1:O:107:VAL:CG1  | 2:W:66:TYR:OH   | 2.03                     | 1.07              |
| 1:S:177:GLU:CD   | 1:T:58:LEU:HD13 | 1.77                     | 1.07              |
| 1:T:161:LYS:HB2  | 1:U:60:GLU:OE2  | 1.54                     | 1.07              |
| 1:U:12:ILE:CG1   | 1:U:23:GLN:HB2  | 1.59                     | 1.07              |
| 1:G:12:ILE:CG1   | 1:G:23:GLN:CG   | 2.10                     | 1.07              |
| 1:P:12:ILE:CG1   | 1:P:23:GLN:CG   | 2.11                     | 1.07              |
| 1:T:177:GLU:HA   | 1:U:58:LEU:HD13 | 1.30                     | 1.07              |
| 1:U:108:ASN:HD22 | 2:V:70:ARG:CB   | 1.67                     | 1.07              |
| 1:C:177:GLU:O    | 1:D:58:LEU:HD11 | 1.54                     | 1.06              |
| 1:F:177:GLU:HA   | 1:G:58:LEU:HD13 | 1.30                     | 1.06              |
| 1:O:161:LYS:HD2  | 1:P:60:GLU:OE2  | 1.54                     | 1.06              |
| 1:C:101:VAL:HG21 | 2:J:58:TYR:CE1  | 1.91                     | 1.06              |
| 1:R:21:LEU:HD11  | 1:S:130:ARG:HD2 | 1.09                     | 1.06              |
| 1:Q:177:GLU:O    | 1:R:58:LEU:HD11 | 1.54                     | 1.06              |
| 1:T:13:THR:CB    | 1:T:14:VAL:HG23 | 1.77                     | 1.06              |
| 1:C:12:ILE:CG1   | 1:C:23:GLN:HB2  | 1.59                     | 1.06              |
| 1:D:13:THR:HB    | 1:D:14:VAL:HG23 | 1.36                     | 1.06              |
| 1:O:60:GLU:OE2   | 1:U:161:LYS:CD  | 2.03                     | 1.06              |
| 1:T:177:GLU:O    | 1:U:57:ARG:NH2  | 1.88                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:107:VAL:CG1  | 2:I:66:TYR:OH    | 2.03                     | 1.06              |
| 1:A:177:GLU:O    | 1:B:57:ARG:NE    | 1.89                     | 1.06              |
| 1:O:58:LEU:CD2   | 1:U:177:GLU:N    | 2.16                     | 1.06              |
| 1:T:177:GLU:N    | 1:U:58:LEU:CD2   | 2.19                     | 1.06              |
| 2:V:38:ASP:HB3   | 2:V:41:THR:HG23  | 1.38                     | 1.06              |
| 1:G:108:ASN:HD22 | 2:H:70:ARG:CB    | 1.67                     | 1.05              |
| 1:B:101:VAL:CG2  | 2:I:58:TYR:HD1   | 1.64                     | 1.05              |
| 1:O:13:THR:CB    | 1:O:14:VAL:HG23  | 1.77                     | 1.05              |
| 1:O:57:ARG:H     | 1:U:177:GLU:CD   | 1.64                     | 1.05              |
| 1:O:130:ARG:HH21 | 1:U:124:THR:HG22 | 0.90                     | 1.05              |
| 1:Q:13:THR:CB    | 1:Q:14:VAL:HG23  | 1.77                     | 1.05              |
| 1:U:101:VAL:CG2  | 2:2:58:TYR:CD1   | 2.40                     | 1.05              |
| 1:U:103:TYR:CE1  | 2:V:82:LEU:HD13  | 1.92                     | 1.05              |
| 1:A:60:GLU:OE2   | 1:G:161:LYS:CD   | 2.03                     | 1.05              |
| 1:E:13:THR:HB    | 1:E:14:VAL:HG23  | 1.36                     | 1.05              |
| 1:F:12:ILE:CG1   | 1:F:23:GLN:HB2   | 1.59                     | 1.05              |
| 1:A:58:LEU:CD2   | 1:G:177:GLU:N    | 2.16                     | 1.05              |
| 1:B:13:THR:CB    | 1:B:14:VAL:HG23  | 1.77                     | 1.05              |
| 1:A:130:ARG:HH21 | 1:G:124:THR:HG22 | 0.90                     | 1.04              |
| 1:D:21:LEU:HD11  | 1:E:130:ARG:HD2  | 1.09                     | 1.04              |
| 1:E:177:GLU:H    | 1:F:58:LEU:HD21  | 1.18                     | 1.04              |
| 1:G:101:VAL:CG2  | 2:N:58:TYR:CD1   | 2.40                     | 1.04              |
| 1:Q:101:VAL:HG21 | 2:X:58:TYR:CE1   | 1.91                     | 1.04              |
| 1:R:12:ILE:CG1   | 1:R:23:GLN:CG    | 2.11                     | 1.04              |
| 1:A:57:ARG:H     | 1:G:177:GLU:CD   | 1.64                     | 1.04              |
| 1:A:161:LYS:HD2  | 1:B:60:GLU:OE2   | 1.54                     | 1.04              |
| 1:E:101:VAL:CG2  | 2:L:58:TYR:HD1   | 1.60                     | 1.04              |
| 1:F:13:THR:HB    | 1:F:14:VAL:HG23  | 1.36                     | 1.04              |
| 1:G:103:TYR:CE1  | 2:H:82:LEU:HD13  | 1.92                     | 1.04              |
| 2:H:38:ASP:HB3   | 2:H:41:THR:HG23  | 1.38                     | 1.04              |
| 1:O:177:GLU:HA   | 1:P:58:LEU:HD13  | 1.36                     | 1.04              |
| 1:R:13:THR:HB    | 1:R:14:VAL:HG23  | 1.36                     | 1.04              |
| 1:U:12:ILE:CA    | 1:U:23:GLN:CG    | 2.36                     | 1.04              |
| 1:P:12:ILE:CA    | 1:P:23:GLN:CG    | 2.36                     | 1.03              |
| 1:Q:9:ASP:CB     | 1:Q:26:TYR:OH    | 2.06                     | 1.03              |
| 1:T:12:ILE:CG1   | 1:T:23:GLN:HB2   | 1.59                     | 1.03              |
| 1:T:12:ILE:CA    | 1:T:23:GLN:CG    | 2.36                     | 1.03              |
| 1:C:12:ILE:CA    | 1:C:23:GLN:CG    | 2.36                     | 1.03              |
| 1:D:177:GLU:HB2  | 1:E:58:LEU:HD22  | 1.40                     | 1.03              |
| 1:E:12:ILE:CA    | 1:E:23:GLN:CG    | 2.36                     | 1.03              |
| 1:F:12:ILE:CA    | 1:F:23:GLN:CG    | 2.36                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:177:GLU:N    | 1:G:58:LEU:CD2   | 2.19                     | 1.03              |
| 1:O:124:THR:HG22 | 1:P:130:ARG:HH21 | 1.24                     | 1.03              |
| 1:O:177:GLU:O    | 1:P:57:ARG:NE    | 1.89                     | 1.03              |
| 1:Q:12:ILE:CA    | 1:Q:23:GLN:CG    | 2.36                     | 1.03              |
| 1:A:58:LEU:HD22  | 1:G:177:GLU:HB2  | 1.40                     | 1.03              |
| 1:B:12:ILE:CG1   | 1:B:23:GLN:HB2   | 1.59                     | 1.03              |
| 1:D:12:ILE:CA    | 1:D:23:GLN:CG    | 2.36                     | 1.03              |
| 1:F:9:ASP:CB     | 1:F:26:TYR:OH    | 2.06                     | 1.03              |
| 1:F:13:THR:CB    | 1:F:14:VAL:HG23  | 1.76                     | 1.03              |
| 1:O:12:ILE:CA    | 1:O:23:GLN:CG    | 2.36                     | 1.03              |
| 1:P:9:ASP:CB     | 1:P:26:TYR:OH    | 2.06                     | 1.03              |
| 1:A:57:ARG:NH2   | 1:G:177:GLU:O    | 1.92                     | 1.03              |
| 1:G:9:ASP:CB     | 1:G:26:TYR:OH    | 2.06                     | 1.03              |
| 1:G:12:ILE:CA    | 1:G:23:GLN:CG    | 2.36                     | 1.03              |
| 1:G:13:THR:HB    | 1:G:14:VAL:HG23  | 1.36                     | 1.03              |
| 1:S:21:LEU:HD11  | 1:T:130:ARG:HD2  | 1.40                     | 1.03              |
| 1:T:108:ASN:HB2  | 2:2:70:ARG:HG2   | 1.38                     | 1.03              |
| 1:A:108:ASN:HB3  | 2:I:70:ARG:HG2   | 1.38                     | 1.03              |
| 1:C:21:LEU:HD11  | 1:D:130:ARG:CD   | 1.89                     | 1.03              |
| 1:C:178:ARG:CA   | 1:D:57:ARG:NH2   | 2.22                     | 1.03              |
| 1:E:9:ASP:CB     | 1:E:26:TYR:OH    | 2.06                     | 1.03              |
| 1:O:13:THR:HB    | 1:O:14:VAL:HG23  | 1.36                     | 1.03              |
| 1:R:9:ASP:CB     | 1:R:26:TYR:OH    | 2.06                     | 1.03              |
| 1:S:177:GLU:OE1  | 1:T:57:ARG:CA    | 2.07                     | 1.03              |
| 1:A:13:THR:HB    | 1:A:14:VAL:HG23  | 1.36                     | 1.02              |
| 1:A:130:ARG:HH21 | 1:G:124:THR:CG2  | 1.72                     | 1.02              |
| 1:C:9:ASP:CB     | 1:C:26:TYR:OH    | 2.06                     | 1.02              |
| 1:D:13:THR:CB    | 1:D:14:VAL:HG23  | 1.76                     | 1.02              |
| 1:D:108:ASN:CB   | 2:L:70:ARG:HG2   | 1.89                     | 1.02              |
| 1:E:177:GLU:OE1  | 1:F:57:ARG:CA    | 2.07                     | 1.02              |
| 1:P:13:THR:HB    | 1:P:14:VAL:HG23  | 1.36                     | 1.02              |
| 1:P:102:THR:O    | 2:X:85:ASN:OD1   | 1.77                     | 1.02              |
| 1:U:9:ASP:CB     | 1:U:26:TYR:OH    | 2.06                     | 1.02              |
| 1:B:12:ILE:CA    | 1:B:23:GLN:CG    | 2.36                     | 1.02              |
| 1:C:13:THR:HB    | 1:C:14:VAL:HG23  | 1.36                     | 1.02              |
| 1:Q:12:ILE:CA    | 1:Q:23:GLN:HG2   | 1.89                     | 1.02              |
| 1:Q:13:THR:HB    | 1:Q:14:VAL:HG23  | 1.36                     | 1.02              |
| 1:Q:21:LEU:HD11  | 1:R:130:ARG:CD   | 1.89                     | 1.02              |
| 1:Q:108:ASN:ND2  | 2:Y:70:ARG:CG    | 2.22                     | 1.02              |
| 1:U:13:THR:HB    | 1:U:14:VAL:HG23  | 1.36                     | 1.02              |
| 1:C:108:ASN:ND2  | 2:K:70:ARG:CG    | 2.22                     | 1.02              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:177:GLU:CD  | 1:E:57:ARG:N     | 2.14                     | 1.02              |
| 1:F:12:ILE:CA   | 1:F:23:GLN:HG2   | 1.89                     | 1.02              |
| 1:Q:108:ASN:HB3 | 2:Y:70:ARG:CG    | 1.89                     | 1.02              |
| 1:R:12:ILE:CA   | 1:R:23:GLN:CG    | 2.36                     | 1.02              |
| 1:R:108:ASN:CB  | 2:Z:70:ARG:HG2   | 1.89                     | 1.02              |
| 1:S:9:ASP:CB    | 1:S:26:TYR:OH    | 2.06                     | 1.02              |
| 1:A:9:ASP:CB    | 1:A:26:TYR:OH    | 2.06                     | 1.02              |
| 1:A:12:ILE:CA   | 1:A:23:GLN:CG    | 2.36                     | 1.02              |
| 1:B:9:ASP:CB    | 1:B:26:TYR:OH    | 2.06                     | 1.02              |
| 1:G:12:ILE:CA   | 1:G:23:GLN:HG2   | 1.89                     | 1.02              |
| 1:O:58:LEU:HD22 | 1:U:177:GLU:HB2  | 1.40                     | 1.02              |
| 1:P:12:ILE:CA   | 1:P:23:GLN:HG2   | 1.89                     | 1.02              |
| 1:P:108:ASN:CG  | 2:X:70:ARG:HG2   | 1.85                     | 1.02              |
| 1:S:13:THR:HB   | 1:S:14:VAL:HG23  | 1.36                     | 1.02              |
| 1:C:12:ILE:CA   | 1:C:23:GLN:HG2   | 1.89                     | 1.02              |
| 1:O:9:ASP:CB    | 1:O:26:TYR:OH    | 2.06                     | 1.02              |
| 1:R:177:GLU:OE1 | 1:S:57:ARG:CA    | 2.08                     | 1.02              |
| 1:S:12:ILE:CA   | 1:S:23:GLN:CG    | 2.36                     | 1.02              |
| 1:T:9:ASP:CB    | 1:T:26:TYR:OH    | 2.06                     | 1.02              |
| 1:U:12:ILE:CA   | 1:U:23:GLN:HG2   | 1.89                     | 1.02              |
| 1:A:177:GLU:HA  | 1:B:58:LEU:HD13  | 1.36                     | 1.01              |
| 1:D:9:ASP:CB    | 1:D:26:TYR:OH    | 2.06                     | 1.01              |
| 1:E:12:ILE:CA   | 1:E:23:GLN:HG2   | 1.89                     | 1.01              |
| 1:G:108:ASN:HB3 | 2:H:70:ARG:HD3   | 1.41                     | 1.01              |
| 1:O:108:ASN:HB3 | 2:W:70:ARG:HG2   | 1.38                     | 1.01              |
| 1:P:177:GLU:HA  | 1:Q:58:LEU:HD13  | 1.35                     | 1.01              |
| 1:R:12:ILE:CA   | 1:R:23:GLN:HG2   | 1.89                     | 1.01              |
| 1:T:13:THR:HB   | 1:T:14:VAL:HG23  | 1.36                     | 1.01              |
| 1:B:108:ASN:HB2 | 2:J:70:ARG:HG2   | 1.39                     | 1.01              |
| 1:B:13:THR:HB   | 1:B:14:VAL:HG23  | 1.36                     | 1.01              |
| 1:E:177:GLU:HB2 | 1:F:58:LEU:HD22  | 1.42                     | 1.01              |
| 1:O:130:ARG:NH2 | 1:U:124:THR:HG22 | 1.75                     | 1.01              |
| 1:S:108:ASN:HB3 | 2:1:70:ARG:HD3   | 1.38                     | 1.01              |
| 1:B:107:VAL:CG1 | 2:J:66:TYR:OH    | 2.07                     | 1.01              |
| 1:P:107:VAL:CG1 | 2:X:66:TYR:OH    | 2.08                     | 1.01              |
| 1:A:12:ILE:CA   | 1:A:23:GLN:HG2   | 1.89                     | 1.01              |
| 1:E:21:LEU:HD11 | 1:F:130:ARG:HD2  | 1.40                     | 1.01              |
| 1:O:12:ILE:CA   | 1:O:23:GLN:HG2   | 1.89                     | 1.01              |
| 1:P:108:ASN:HB2 | 2:X:70:ARG:HG2   | 1.39                     | 1.01              |
| 1:T:12:ILE:CA   | 1:T:23:GLN:HG2   | 1.89                     | 1.01              |
| 1:O:57:ARG:NH2  | 1:U:177:GLU:O    | 1.92                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:130:ARG:HH21 | 1:U:124:THR:CG2  | 1.72                     | 1.00              |
| 1:P:107:VAL:HG11 | 2:X:66:TYR:HH    | 1.24                     | 1.00              |
| 1:Q:178:ARG:CA   | 1:R:57:ARG:NH2   | 2.22                     | 1.00              |
| 1:S:12:ILE:CA    | 1:S:23:GLN:HG2   | 1.89                     | 1.00              |
| 1:A:130:ARG:NH2  | 1:G:124:THR:HG22 | 1.75                     | 1.00              |
| 1:B:102:THR:O    | 2:J:85:ASN:OD1   | 1.77                     | 1.00              |
| 1:B:177:GLU:OE1  | 1:C:58:LEU:HD13  | 1.62                     | 1.00              |
| 1:C:108:ASN:HD22 | 2:K:70:ARG:CB    | 1.75                     | 1.00              |
| 1:E:108:ASN:HB3  | 2:M:70:ARG:HD3   | 1.38                     | 1.00              |
| 1:P:177:GLU:OE1  | 1:Q:58:LEU:HD13  | 1.62                     | 1.00              |
| 1:R:177:GLU:CD   | 1:S:57:ARG:N     | 2.14                     | 1.00              |
| 1:R:177:GLU:HB2  | 1:S:58:LEU:HD22  | 1.40                     | 1.00              |
| 1:A:101:VAL:CG2  | 2:H:58:TYR:CD1   | 2.45                     | 1.00              |
| 1:B:108:ASN:CG   | 2:J:70:ARG:HG2   | 1.85                     | 1.00              |
| 1:Q:178:ARG:CA   | 1:R:57:ARG:HH21  | 1.74                     | 1.00              |
| 1:T:21:LEU:CD1   | 1:U:130:ARG:HD2  | 1.91                     | 1.00              |
| 1:C:178:ARG:HA   | 1:D:57:ARG:HH21  | 0.95                     | 1.00              |
| 2:M:38:ASP:HB3   | 2:M:41:THR:HG23  | 1.44                     | 1.00              |
| 1:Q:177:GLU:O    | 1:R:57:ARG:NH2   | 1.94                     | 1.00              |
| 1:B:12:ILE:CA    | 1:B:23:GLN:HG2   | 1.89                     | 1.00              |
| 1:D:12:ILE:CA    | 1:D:23:GLN:HG2   | 1.89                     | 1.00              |
| 1:G:101:VAL:HG21 | 2:N:58:TYR:CE1   | 1.97                     | 1.00              |
| 1:C:101:VAL:CG2  | 2:J:58:TYR:HD1   | 1.65                     | 1.00              |
| 1:T:101:VAL:HG22 | 2:1:58:TYR:CE1   | 1.97                     | 1.00              |
| 1:C:177:GLU:O    | 1:D:57:ARG:NH2   | 1.94                     | 0.99              |
| 1:O:57:ARG:NH2   | 1:U:178:ARG:O    | 1.88                     | 0.99              |
| 1:S:177:GLU:HB2  | 1:T:58:LEU:HD22  | 1.42                     | 0.99              |
| 1:Q:108:ASN:HD22 | 2:Y:70:ARG:CB    | 1.74                     | 0.99              |
| 1:D:177:GLU:OE1  | 1:E:57:ARG:CA    | 2.08                     | 0.99              |
| 1:Q:124:THR:HG22 | 1:R:130:ARG:HH21 | 1.24                     | 0.99              |
| 1:U:108:ASN:HB3  | 2:V:70:ARG:HD3   | 1.41                     | 0.99              |
| 1:F:101:VAL:CG2  | 2:M:58:TYR:HD1   | 1.62                     | 0.99              |
| 1:O:101:VAL:CG2  | 2:V:58:TYR:CD1   | 2.45                     | 0.99              |
| 1:Q:177:GLU:CA   | 1:R:58:LEU:CG    | 2.08                     | 0.99              |
| 1:C:178:ARG:CA   | 1:D:57:ARG:HH21  | 1.74                     | 0.99              |
| 1:F:108:ASN:HB2  | 2:N:70:ARG:HG2   | 1.38                     | 0.99              |
| 1:C:124:THR:HG22 | 1:D:130:ARG:HH21 | 1.24                     | 0.99              |
| 1:A:124:THR:HG22 | 1:B:130:ARG:HH21 | 1.24                     | 0.99              |
| 1:F:21:LEU:CD1   | 1:G:130:ARG:HD2  | 1.91                     | 0.99              |
| 2:X:45:ILE:HG12  | 2:X:52:ALA:HB1   | 1.44                     | 0.99              |
| 1:S:13:THR:CB    | 1:S:14:VAL:HG23  | 1.76                     | 0.98              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:57:ARG:NH2   | 1:G:178:ARG:O   | 1.88                     | 0.98              |
| 1:B:12:ILE:CG1   | 1:B:23:GLN:CG   | 2.11                     | 0.98              |
| 2:K:38:ASP:HB3   | 2:K:41:THR:HG23 | 1.45                     | 0.98              |
| 1:U:101:VAL:HG21 | 2:2:58:TYR:CE1  | 1.97                     | 0.98              |
| 2:1:38:ASP:HB3   | 2:1:41:THR:HG23 | 1.44                     | 0.98              |
| 1:C:177:GLU:H    | 1:D:58:LEU:HD21 | 1.22                     | 0.98              |
| 1:S:177:GLU:OE1  | 1:T:57:ARG:N    | 1.97                     | 0.98              |
| 1:F:101:VAL:HG22 | 2:M:58:TYR:CE1  | 1.97                     | 0.98              |
| 1:C:108:ASN:CB   | 2:K:70:ARG:CD   | 2.42                     | 0.98              |
| 1:G:13:THR:CB    | 1:G:14:VAL:HG23 | 1.77                     | 0.97              |
| 1:A:13:THR:CB    | 1:A:14:VAL:HG23 | 1.77                     | 0.97              |
| 1:S:12:ILE:CG1   | 1:S:23:GLN:HB3  | 1.67                     | 0.97              |
| 1:O:12:ILE:CG1   | 1:O:23:GLN:HB2  | 1.59                     | 0.97              |
| 1:E:13:THR:CB    | 1:E:14:VAL:HG23 | 1.77                     | 0.97              |
| 1:Q:108:ASN:CB   | 2:Y:70:ARG:CD   | 2.42                     | 0.97              |
| 1:R:13:THR:CB    | 1:R:14:VAL:HG23 | 1.76                     | 0.97              |
| 1:T:12:ILE:CG1   | 1:T:23:GLN:HB3  | 1.67                     | 0.97              |
| 1:A:12:ILE:CG1   | 1:A:23:GLN:HB3  | 1.67                     | 0.97              |
| 1:E:177:GLU:CD   | 1:F:57:ARG:N    | 2.21                     | 0.97              |
| 1:E:177:GLU:OE1  | 1:F:57:ARG:N    | 1.97                     | 0.97              |
| 1:E:177:GLU:HB2  | 1:F:58:LEU:CD2  | 1.95                     | 0.97              |
| 1:S:177:GLU:CD   | 1:T:57:ARG:N    | 2.21                     | 0.97              |
| 1:G:101:VAL:CG2  | 2:N:58:TYR:CE1  | 2.48                     | 0.97              |
| 2:M:45:ILE:HG12  | 2:M:52:ALA:HB1  | 1.46                     | 0.97              |
| 1:T:177:GLU:C    | 1:U:58:LEU:HD11 | 1.90                     | 0.97              |
| 1:D:21:LEU:HD11  | 1:E:130:ARG:CD  | 1.95                     | 0.97              |
| 1:U:101:VAL:CG2  | 2:2:58:TYR:CE1  | 2.48                     | 0.97              |
| 1:T:101:VAL:HG23 | 2:1:58:TYR:HD1  | 1.26                     | 0.97              |
| 2:1:45:ILE:HG12  | 2:1:52:ALA:HB1  | 1.46                     | 0.97              |
| 1:B:12:ILE:CG1   | 1:B:23:GLN:HB3  | 1.67                     | 0.96              |
| 2:J:45:ILE:HG12  | 2:J:52:ALA:HB1  | 1.44                     | 0.96              |
| 1:O:161:LYS:HB2  | 1:P:60:GLU:OE2  | 1.65                     | 0.96              |
| 1:U:9:ASP:HB2    | 1:U:26:TYR:HH   | 1.24                     | 0.96              |
| 1:P:177:GLU:N    | 1:Q:58:LEU:HD21 | 1.80                     | 0.96              |
| 1:A:101:VAL:CG2  | 2:H:58:TYR:HD1  | 1.78                     | 0.96              |
| 1:F:101:VAL:HG23 | 2:M:58:TYR:HD1  | 1.26                     | 0.96              |
| 1:P:13:THR:CB    | 1:P:14:VAL:HG23 | 1.76                     | 0.96              |
| 1:C:12:ILE:CG1   | 1:C:23:GLN:HB3  | 1.67                     | 0.96              |
| 1:F:103:TYR:CE1  | 2:N:82:LEU:HD13 | 2.01                     | 0.96              |
| 1:Q:101:VAL:CG2  | 2:X:58:TYR:HD1  | 1.65                     | 0.96              |
| 1:R:21:LEU:HD11  | 1:S:130:ARG:CD  | 1.95                     | 0.96              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:178:ARG:CA   | 1:G:57:ARG:NH2  | 2.29                     | 0.96              |
| 1:T:178:ARG:CA   | 1:U:57:ARG:NH2  | 2.29                     | 0.96              |
| 1:U:13:THR:CB    | 1:U:14:VAL:HG23 | 1.77                     | 0.96              |
| 2:Y:38:ASP:HB3   | 2:Y:41:THR:HG23 | 1.45                     | 0.96              |
| 1:U:12:ILE:HD13  | 1:U:23:GLN:CD   | 1.91                     | 0.95              |
| 1:C:12:ILE:HD13  | 1:C:23:GLN:CD   | 1.91                     | 0.95              |
| 1:U:12:ILE:CG1   | 1:U:23:GLN:HB3  | 1.67                     | 0.95              |
| 1:B:177:GLU:N    | 1:C:58:LEU:HD21 | 1.80                     | 0.95              |
| 1:E:12:ILE:HD13  | 1:E:23:GLN:CD   | 1.91                     | 0.95              |
| 2:J:38:ASP:HB3   | 2:J:41:THR:HG23 | 1.46                     | 0.95              |
| 1:A:12:ILE:HD13  | 1:A:23:GLN:CD   | 1.91                     | 0.95              |
| 1:F:108:ASN:HB3  | 2:N:70:ARG:HD3  | 1.49                     | 0.95              |
| 1:F:177:GLU:C    | 1:G:58:LEU:HD11 | 1.90                     | 0.95              |
| 1:O:107:VAL:HG11 | 2:W:66:TYR:HH   | 1.30                     | 0.95              |
| 1:S:12:ILE:HD13  | 1:S:23:GLN:CD   | 1.91                     | 0.95              |
| 1:O:12:ILE:HD13  | 1:O:23:GLN:CD   | 1.91                     | 0.95              |
| 1:O:101:VAL:CG2  | 2:V:58:TYR:HD1  | 1.78                     | 0.95              |
| 1:T:103:TYR:CE1  | 2:2:82:LEU:HD13 | 2.01                     | 0.95              |
| 1:T:12:ILE:HD13  | 1:T:23:GLN:CD   | 1.91                     | 0.95              |
| 1:T:21:LEU:HD11  | 1:U:130:ARG:HD2 | 0.96                     | 0.95              |
| 1:F:12:ILE:HD13  | 1:F:23:GLN:CD   | 1.91                     | 0.95              |
| 2:W:38:ASP:HB3   | 2:W:41:THR:HG23 | 1.49                     | 0.95              |
| 1:A:161:LYS:HB2  | 1:B:60:GLU:OE2  | 1.65                     | 0.94              |
| 1:B:12:ILE:HD13  | 1:B:23:GLN:CD   | 1.91                     | 0.94              |
| 1:D:12:ILE:CG1   | 1:D:23:GLN:CG   | 2.10                     | 0.94              |
| 1:D:12:ILE:HD13  | 1:D:23:GLN:CD   | 1.91                     | 0.94              |
| 2:X:38:ASP:HB3   | 2:X:41:THR:HG23 | 1.46                     | 0.94              |
| 1:C:13:THR:CB    | 1:C:14:VAL:HG23 | 1.77                     | 0.94              |
| 1:C:108:ASN:HB3  | 2:K:70:ARG:CG   | 1.89                     | 0.94              |
| 1:P:12:ILE:HD13  | 1:P:23:GLN:CD   | 1.91                     | 0.94              |
| 1:Q:178:ARG:HA   | 1:R:57:ARG:HH21 | 0.95                     | 0.94              |
| 2:2:38:ASP:HB3   | 2:2:41:THR:HG23 | 1.47                     | 0.94              |
| 1:Q:12:ILE:HD13  | 1:Q:23:GLN:CD   | 1.91                     | 0.94              |
| 1:T:177:GLU:O    | 1:U:57:ARG:CZ   | 2.15                     | 0.94              |
| 1:D:103:TYR:O    | 2:L:81:THR:HG21 | 1.68                     | 0.94              |
| 1:F:15:PHE:HB2   | 1:G:23:GLN:HE22 | 1.32                     | 0.94              |
| 1:F:21:LEU:HD11  | 1:G:130:ARG:HD2 | 0.96                     | 0.94              |
| 1:O:57:ARG:NH2   | 1:U:177:GLU:C   | 2.25                     | 0.94              |
| 1:R:12:ILE:HD13  | 1:R:23:GLN:CD   | 1.91                     | 0.94              |
| 2:N:38:ASP:HB3   | 2:N:41:THR:HG23 | 1.47                     | 0.94              |
| 1:P:161:LYS:CB   | 1:Q:60:GLU:OE2  | 2.16                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:101:VAL:CG2  | 2:1:58:TYR:HD1   | 1.62                     | 0.94              |
| 1:C:177:GLU:HA   | 1:D:58:LEU:HG    | 1.50                     | 0.94              |
| 1:D:12:ILE:CG1   | 1:D:23:GLN:HB3   | 1.67                     | 0.94              |
| 1:D:21:LEU:CD1   | 1:E:130:ARG:HD2  | 1.97                     | 0.94              |
| 1:F:125:GLN:O    | 1:G:129:VAL:HG23 | 1.68                     | 0.94              |
| 1:G:12:ILE:HD13  | 1:G:23:GLN:CD    | 1.91                     | 0.94              |
| 1:R:12:ILE:CG1   | 1:R:23:GLN:HB3   | 1.67                     | 0.94              |
| 1:R:103:TYR:O    | 2:Z:81:THR:HG21  | 1.68                     | 0.94              |
| 1:O:155:GLY:O    | 1:P:86:ARG:NH2   | 2.00                     | 0.94              |
| 1:R:21:LEU:CD1   | 1:S:130:ARG:HD2  | 1.97                     | 0.94              |
| 1:F:177:GLU:CB   | 1:G:58:LEU:HD22  | 1.97                     | 0.94              |
| 2:I:38:ASP:HB3   | 2:I:41:THR:HG23  | 1.49                     | 0.94              |
| 1:Q:177:GLU:H    | 1:R:58:LEU:HD21  | 1.22                     | 0.94              |
| 1:R:173:VAL:O    | 1:S:58:LEU:HD21  | 1.67                     | 0.94              |
| 1:T:108:ASN:HD22 | 2:2:70:ARG:HG2   | 1.32                     | 0.94              |
| 1:T:177:GLU:CB   | 1:U:58:LEU:HD22  | 1.97                     | 0.94              |
| 1:D:173:VAL:O    | 1:E:58:LEU:HD21  | 1.67                     | 0.93              |
| 1:T:108:ASN:HB3  | 2:2:70:ARG:CG    | 1.97                     | 0.93              |
| 1:U:107:VAL:HG11 | 2:V:66:TYR:HH    | 1.31                     | 0.93              |
| 1:B:161:LYS:CB   | 1:C:60:GLU:OE2   | 2.16                     | 0.93              |
| 1:C:108:ASN:CB   | 2:K:70:ARG:HD3   | 1.99                     | 0.93              |
| 1:T:125:GLN:O    | 1:U:129:VAL:HG23 | 1.68                     | 0.93              |
| 1:F:177:GLU:H    | 1:G:58:LEU:HD21  | 1.13                     | 0.93              |
| 1:S:177:GLU:HB2  | 1:T:58:LEU:CD2   | 1.94                     | 0.93              |
| 1:U:108:ASN:ND2  | 2:V:70:ARG:HG2   | 1.83                     | 0.93              |
| 1:A:155:GLY:O    | 1:B:86:ARG:NH2   | 2.00                     | 0.93              |
| 1:T:177:GLU:H    | 1:U:58:LEU:HD21  | 1.13                     | 0.93              |
| 1:G:108:ASN:ND2  | 2:H:70:ARG:HG2   | 1.83                     | 0.93              |
| 1:O:12:ILE:CG1   | 1:O:23:GLN:HB3   | 1.67                     | 0.93              |
| 1:R:108:ASN:HB3  | 2:Z:70:ARG:HD3   | 1.50                     | 0.93              |
| 1:E:177:GLU:N    | 1:F:58:LEU:HD21  | 1.82                     | 0.93              |
| 1:F:101:VAL:HG21 | 2:M:58:TYR:CE1   | 2.00                     | 0.93              |
| 1:F:124:THR:HG22 | 1:G:130:ARG:HH21 | 1.34                     | 0.93              |
| 1:Q:177:GLU:HA   | 1:R:58:LEU:HG    | 1.50                     | 0.93              |
| 1:R:161:LYS:HB2  | 1:S:60:GLU:CD    | 1.94                     | 0.93              |
| 1:T:177:GLU:HB2  | 1:U:58:LEU:CD2   | 1.99                     | 0.93              |
| 1:C:177:GLU:HA   | 1:D:58:LEU:CD2   | 1.77                     | 0.93              |
| 1:F:103:TYR:C    | 2:N:81:THR:HG21  | 1.94                     | 0.93              |
| 1:F:177:GLU:O    | 1:G:57:ARG:CZ    | 2.15                     | 0.93              |
| 1:G:9:ASP:HB2    | 1:G:26:TYR:HH    | 1.32                     | 0.93              |
| 1:T:108:ASN:HB3  | 2:2:70:ARG:HD3   | 1.49                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:12:ILE:CG1   | 1:G:23:GLN:HB3   | 1.67                     | 0.93              |
| 1:S:124:THR:HG22 | 1:T:130:ARG:HH21 | 1.33                     | 0.93              |
| 1:F:101:VAL:HG22 | 2:M:58:TYR:HE1   | 1.32                     | 0.92              |
| 1:P:178:ARG:HA   | 1:Q:57:ARG:NH2   | 1.84                     | 0.92              |
| 1:A:130:ARG:CD   | 1:G:21:LEU:HD11  | 2.00                     | 0.92              |
| 1:A:57:ARG:NH2   | 1:G:177:GLU:C    | 2.25                     | 0.92              |
| 1:Q:108:ASN:CB   | 2:Y:70:ARG:HD3   | 1.99                     | 0.92              |
| 1:O:108:ASN:HB3  | 2:W:70:ARG:CG    | 1.99                     | 0.92              |
| 1:Q:101:VAL:HG22 | 2:X:58:TYR:HE1   | 1.34                     | 0.92              |
| 1:T:15:PHE:HB2   | 1:U:23:GLN:HE22  | 1.32                     | 0.92              |
| 1:B:177:GLU:OE2  | 1:C:56:SER:CB    | 2.18                     | 0.92              |
| 1:O:58:LEU:HD21  | 1:U:177:GLU:H    | 0.95                     | 0.92              |
| 1:P:177:GLU:CD   | 1:Q:58:LEU:HD13  | 1.94                     | 0.92              |
| 1:D:108:ASN:HB3  | 2:L:70:ARG:HD3   | 1.50                     | 0.92              |
| 1:S:103:TYR:C    | 2:1:81:THR:CG2   | 2.41                     | 0.92              |
| 1:O:108:ASN:CG   | 2:W:70:ARG:HG2   | 1.94                     | 0.92              |
| 1:A:108:ASN:CG   | 2:I:70:ARG:HG2   | 1.94                     | 0.91              |
| 1:B:161:LYS:HD2  | 1:C:60:GLU:OE2   | 1.69                     | 0.91              |
| 1:D:161:LYS:HB2  | 1:E:60:GLU:CD    | 1.94                     | 0.91              |
| 1:E:101:VAL:HG23 | 2:L:58:TYR:HD1   | 1.35                     | 0.91              |
| 1:Q:101:VAL:HG22 | 2:X:58:TYR:CE1   | 2.04                     | 0.91              |
| 1:E:103:TYR:C    | 2:M:81:THR:CG2   | 2.41                     | 0.91              |
| 1:F:177:GLU:HB2  | 1:G:58:LEU:CD2   | 1.99                     | 0.91              |
| 1:F:178:ARG:C    | 1:G:57:ARG:NH2   | 2.28                     | 0.91              |
| 1:T:101:VAL:HG22 | 2:1:58:TYR:HE1   | 1.32                     | 0.91              |
| 1:S:177:GLU:N    | 1:T:58:LEU:HD21  | 1.82                     | 0.91              |
| 1:T:178:ARG:HA   | 1:U:57:ARG:HH21  | 1.32                     | 0.91              |
| 1:C:108:ASN:CG   | 2:K:70:ARG:CG    | 2.42                     | 0.91              |
| 1:Q:107:VAL:HG11 | 2:Y:66:TYR:OH    | 1.69                     | 0.91              |
| 1:T:107:VAL:HG11 | 2:2:66:TYR:OH    | 1.71                     | 0.91              |
| 1:B:177:GLU:CD   | 1:C:58:LEU:HD13  | 1.94                     | 0.91              |
| 1:D:177:GLU:N    | 1:E:58:LEU:CD2   | 2.25                     | 0.91              |
| 1:F:108:ASN:HB3  | 2:N:70:ARG:CG    | 1.97                     | 0.91              |
| 1:F:178:ARG:O    | 1:G:57:ARG:NH2   | 2.03                     | 0.91              |
| 1:F:107:VAL:HG11 | 2:N:66:TYR:OH    | 1.71                     | 0.91              |
| 1:T:103:TYR:C    | 2:2:81:THR:HG21  | 1.94                     | 0.91              |
| 1:T:108:ASN:ND2  | 2:2:70:ARG:CG    | 2.33                     | 0.91              |
| 1:F:12:ILE:CG1   | 1:F:23:GLN:HB3   | 1.67                     | 0.91              |
| 1:P:161:LYS:HD2  | 1:Q:60:GLU:OE2   | 1.69                     | 0.91              |
| 1:S:101:VAL:HG23 | 2:Z:58:TYR:HD1   | 1.35                     | 0.91              |
| 1:T:178:ARG:C    | 1:U:57:ARG:NH2   | 2.28                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:108:ASN:HB3  | 2:I:70:ARG:CG    | 1.99                     | 0.91              |
| 1:O:58:LEU:CD2   | 1:U:173:VAL:O    | 2.19                     | 0.91              |
| 1:T:178:ARG:HA   | 1:U:57:ARG:NH2   | 1.85                     | 0.91              |
| 1:A:58:LEU:CD2   | 1:G:173:VAL:O    | 2.19                     | 0.91              |
| 1:E:124:THR:HG22 | 1:F:130:ARG:HH21 | 1.34                     | 0.91              |
| 1:T:124:THR:HG22 | 1:U:130:ARG:HH21 | 1.34                     | 0.90              |
| 1:A:10:ARG:HH11  | 1:G:7:ALA:HB1    | 1.36                     | 0.90              |
| 1:A:130:ARG:HD2  | 1:G:21:LEU:CD1   | 2.00                     | 0.90              |
| 1:F:178:ARG:HA   | 1:G:57:ARG:NH2   | 1.85                     | 0.90              |
| 1:Q:101:VAL:HG23 | 2:X:58:TYR:HD1   | 1.35                     | 0.90              |
| 1:O:10:ARG:HH11  | 1:U:7:ALA:HB1    | 1.36                     | 0.90              |
| 1:O:60:GLU:CD    | 1:U:161:LYS:HB2  | 1.97                     | 0.90              |
| 1:O:177:GLU:HB2  | 1:P:58:LEU:HD22  | 1.52                     | 0.90              |
| 1:P:177:GLU:OE2  | 1:Q:56:SER:CB    | 2.18                     | 0.90              |
| 1:Q:9:ASP:HB2    | 1:Q:26:TYR:HH    | 1.32                     | 0.90              |
| 1:T:178:ARG:O    | 1:U:57:ARG:NH2   | 2.03                     | 0.90              |
| 1:C:108:ASN:HD22 | 2:K:70:ARG:CG    | 1.82                     | 0.90              |
| 1:E:12:ILE:CG1   | 1:E:23:GLN:HB3   | 1.67                     | 0.90              |
| 1:E:101:VAL:CG2  | 2:L:58:TYR:CE1   | 2.54                     | 0.90              |
| 1:F:108:ASN:HD22 | 2:N:70:ARG:HG2   | 1.32                     | 0.90              |
| 1:R:177:GLU:N    | 1:S:58:LEU:CD2   | 2.25                     | 0.90              |
| 1:O:130:ARG:CD   | 1:U:21:LEU:HD11  | 2.00                     | 0.90              |
| 1:E:108:ASN:ND2  | 2:M:70:ARG:CG    | 2.35                     | 0.90              |
| 1:O:108:ASN:CB   | 2:W:70:ARG:CG    | 2.50                     | 0.90              |
| 1:R:9:ASP:HB2    | 1:R:26:TYR:HH    | 1.29                     | 0.90              |
| 1:S:101:VAL:CG2  | 2:Z:58:TYR:CE1   | 2.54                     | 0.90              |
| 1:S:177:GLU:OE2  | 1:T:57:ARG:N     | 2.05                     | 0.90              |
| 1:A:178:ARG:CA   | 1:B:57:ARG:HH21  | 1.85                     | 0.90              |
| 1:F:108:ASN:ND2  | 2:N:70:ARG:CG    | 2.33                     | 0.90              |
| 1:F:178:ARG:HA   | 1:G:57:ARG:HH21  | 1.32                     | 0.90              |
| 1:U:108:ASN:HB2  | 2:V:70:ARG:HG2   | 1.53                     | 0.90              |
| 1:A:177:GLU:HB2  | 1:B:58:LEU:HD22  | 1.52                     | 0.89              |
| 1:C:107:VAL:HG11 | 2:K:66:TYR:OH    | 1.69                     | 0.89              |
| 1:P:21:LEU:HD11  | 1:Q:130:ARG:HD2  | 1.54                     | 0.89              |
| 1:Q:12:ILE:CG1   | 1:Q:23:GLN:HB3   | 1.67                     | 0.89              |
| 1:Q:108:ASN:HB2  | 2:Y:70:ARG:HG2   | 1.52                     | 0.89              |
| 1:S:101:VAL:HG22 | 2:Z:58:TYR:CE1   | 2.07                     | 0.89              |
| 1:S:108:ASN:ND2  | 2:1:70:ARG:CG    | 2.35                     | 0.89              |
| 1:P:12:ILE:CG1   | 1:P:23:GLN:HB3   | 1.67                     | 0.89              |
| 1:Q:177:GLU:N    | 1:R:58:LEU:CD2   | 2.23                     | 0.89              |
| 1:T:12:ILE:HA    | 1:T:23:GLN:HG2   | 1.55                     | 0.89              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:101:VAL:HG22 | 2:J:58:TYR:CE1  | 2.04                     | 0.89              |
| 1:D:161:LYS:CD   | 1:E:60:GLU:OE2  | 2.21                     | 0.89              |
| 1:C:101:VAL:HG23 | 2:J:58:TYR:HD1  | 1.35                     | 0.89              |
| 1:A:60:GLU:CD    | 1:G:161:LYS:HB2 | 1.97                     | 0.89              |
| 1:B:178:ARG:HA   | 1:C:57:ARG:NH2  | 1.84                     | 0.89              |
| 1:R:161:LYS:CD   | 1:S:60:GLU:OE2  | 2.21                     | 0.89              |
| 1:S:12:ILE:HA    | 1:S:23:GLN:HG2  | 1.55                     | 0.89              |
| 1:T:101:VAL:HG21 | 2:1:58:TYR:CE1  | 2.00                     | 0.89              |
| 1:T:108:ASN:HB3  | 2:2:70:ARG:CD   | 2.03                     | 0.89              |
| 1:A:12:ILE:HA    | 1:A:23:GLN:HG2  | 1.55                     | 0.89              |
| 1:D:101:VAL:HG22 | 2:K:58:TYR:CD1  | 2.06                     | 0.89              |
| 1:Q:108:ASN:HD22 | 2:Y:70:ARG:CG   | 1.82                     | 0.89              |
| 1:S:108:ASN:HB3  | 2:1:70:ARG:CD   | 2.02                     | 0.89              |
| 1:A:108:ASN:CB   | 2:I:70:ARG:CG   | 2.50                     | 0.89              |
| 1:B:12:ILE:HA    | 1:B:23:GLN:HG2  | 1.55                     | 0.89              |
| 1:E:108:ASN:HD22 | 2:M:70:ARG:HG2  | 1.35                     | 0.89              |
| 1:O:130:ARG:HD2  | 1:U:21:LEU:CD1  | 2.00                     | 0.89              |
| 1:E:177:GLU:OE2  | 1:F:57:ARG:N    | 2.05                     | 0.89              |
| 1:R:12:ILE:HA    | 1:R:23:GLN:HG2  | 1.55                     | 0.88              |
| 1:C:101:VAL:HG22 | 2:J:58:TYR:HE1  | 1.34                     | 0.88              |
| 1:O:178:ARG:CA   | 1:P:57:ARG:HH21 | 1.85                     | 0.88              |
| 1:R:177:GLU:OE1  | 1:S:57:ARG:CB   | 2.21                     | 0.88              |
| 1:E:108:ASN:HB3  | 2:M:70:ARG:CD   | 2.02                     | 0.88              |
| 1:F:177:GLU:C    | 1:G:57:ARG:HH21 | 1.80                     | 0.88              |
| 1:U:12:ILE:HA    | 1:U:23:GLN:HG2  | 1.55                     | 0.88              |
| 2:1:37:ILE:HD11  | 2:1:59:MET:HB3  | 1.56                     | 0.88              |
| 1:C:108:ASN:HB2  | 2:K:70:ARG:HG2  | 1.52                     | 0.88              |
| 1:P:155:GLY:O    | 1:Q:86:ARG:NH2  | 2.06                     | 0.88              |
| 1:G:12:ILE:HA    | 1:G:23:GLN:HG2  | 1.55                     | 0.88              |
| 1:U:103:TYR:C    | 2:V:81:THR:HG21 | 1.99                     | 0.88              |
| 1:D:177:GLU:OE1  | 1:E:57:ARG:CB   | 2.21                     | 0.88              |
| 1:F:12:ILE:HA    | 1:F:23:GLN:HG2  | 1.55                     | 0.88              |
| 1:G:101:VAL:CG2  | 2:N:58:TYR:HD1  | 1.83                     | 0.88              |
| 1:T:177:GLU:C    | 1:U:57:ARG:HH21 | 1.80                     | 0.88              |
| 1:T:177:GLU:CB   | 1:U:58:LEU:CD2  | 2.52                     | 0.88              |
| 1:E:12:ILE:HA    | 1:E:23:GLN:HG2  | 1.55                     | 0.88              |
| 1:G:103:TYR:C    | 2:H:81:THR:HG21 | 1.98                     | 0.88              |
| 1:E:101:VAL:HG22 | 2:L:58:TYR:CE1  | 2.07                     | 0.88              |
| 1:G:108:ASN:HD22 | 2:H:70:ARG:HB3  | 1.38                     | 0.88              |
| 1:C:12:ILE:HA    | 1:C:23:GLN:HG2  | 1.55                     | 0.88              |
| 1:G:108:ASN:CB   | 2:H:70:ARG:CD   | 2.47                     | 0.88              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:P:177:GLU:H    | 1:Q:58:LEU:HD21 | 1.38                     | 0.88              |
| 1:B:21:LEU:HD11  | 1:C:130:ARG:HD2 | 1.54                     | 0.87              |
| 1:D:177:GLU:OE1  | 1:E:58:LEU:N    | 2.07                     | 0.87              |
| 1:U:108:ASN:HD22 | 2:V:70:ARG:HB3  | 1.38                     | 0.87              |
| 1:A:58:LEU:HD21  | 1:G:177:GLU:H   | 0.95                     | 0.87              |
| 1:D:12:ILE:HD13  | 1:D:23:GLN:NE2  | 1.89                     | 0.87              |
| 1:U:101:VAL:CG2  | 2:2:58:TYR:HD1  | 1.83                     | 0.87              |
| 1:A:107:VAL:HG11 | 2:I:66:TYR:HH   | 1.34                     | 0.87              |
| 1:R:177:GLU:H    | 1:S:58:LEU:CD2  | 1.84                     | 0.87              |
| 1:P:9:ASP:HB2    | 1:P:26:TYR:HH   | 1.37                     | 0.87              |
| 1:B:101:VAL:CG2  | 2:I:58:TYR:CE1  | 2.57                     | 0.87              |
| 1:D:177:GLU:H    | 1:E:58:LEU:CD2  | 1.84                     | 0.87              |
| 1:S:108:ASN:HD22 | 2:1:70:ARG:HG2  | 1.35                     | 0.87              |
| 1:C:12:ILE:HD13  | 1:C:23:GLN:NE2  | 1.89                     | 0.87              |
| 1:D:124:THR:HG22 | 1:E:130:ARG:NH2 | 1.89                     | 0.87              |
| 1:G:12:ILE:HD13  | 1:G:23:GLN:NE2  | 1.89                     | 0.87              |
| 1:P:101:VAL:CG2  | 2:W:58:TYR:CE1  | 2.57                     | 0.87              |
| 1:B:101:VAL:HG21 | 2:I:58:TYR:CE1  | 2.10                     | 0.87              |
| 1:D:12:ILE:HA    | 1:D:23:GLN:HG2  | 1.55                     | 0.87              |
| 1:O:12:ILE:HA    | 1:O:23:GLN:HG2  | 1.55                     | 0.87              |
| 1:Q:12:ILE:HD13  | 1:Q:23:GLN:NE2  | 1.89                     | 0.87              |
| 1:R:177:GLU:OE1  | 1:S:58:LEU:N    | 2.06                     | 0.87              |
| 1:A:97:GLN:OE1   | 2:H:61:ALA:HB1  | 1.75                     | 0.87              |
| 1:S:103:TYR:HE1  | 2:1:82:LEU:HD22 | 1.39                     | 0.87              |
| 1:F:12:ILE:HD13  | 1:F:23:GLN:NE2  | 1.89                     | 0.86              |
| 1:G:108:ASN:HB2  | 2:H:70:ARG:HG2  | 1.53                     | 0.86              |
| 1:P:12:ILE:HA    | 1:P:23:GLN:HG2  | 1.55                     | 0.86              |
| 1:P:101:VAL:HG21 | 2:W:58:TYR:CE1  | 2.10                     | 0.86              |
| 1:Q:12:ILE:HA    | 1:Q:23:GLN:HG2  | 1.55                     | 0.86              |
| 1:E:12:ILE:CG1   | 1:E:23:GLN:CG   | 2.10                     | 0.86              |
| 1:O:12:ILE:HD13  | 1:O:23:GLN:NE2  | 1.89                     | 0.86              |
| 1:T:108:ASN:HD22 | 2:2:70:ARG:CG   | 1.87                     | 0.86              |
| 1:F:108:ASN:HB3  | 2:N:70:ARG:CD   | 2.03                     | 0.86              |
| 1:R:12:ILE:HD13  | 1:R:23:GLN:NE2  | 1.89                     | 0.86              |
| 1:A:12:ILE:HD13  | 1:A:23:GLN:NE2  | 1.89                     | 0.86              |
| 1:B:177:GLU:HB2  | 1:C:58:LEU:HD22 | 1.57                     | 0.86              |
| 1:D:9:ASP:HB2    | 1:D:26:TYR:HH   | 1.40                     | 0.86              |
| 1:T:177:GLU:CD   | 1:U:58:LEU:HD13 | 2.00                     | 0.86              |
| 1:U:12:ILE:HD13  | 1:U:23:GLN:NE2  | 1.89                     | 0.86              |
| 1:G:107:VAL:HG11 | 2:H:66:TYR:HH   | 1.36                     | 0.86              |
| 1:S:9:ASP:HB2    | 1:S:26:TYR:HH   | 1.38                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:12:ILE:HD13  | 1:S:23:GLN:NE2   | 1.89                     | 0.86              |
| 1:T:177:GLU:O    | 1:U:57:ARG:NE    | 2.08                     | 0.86              |
| 1:B:155:GLY:O    | 1:C:86:ARG:NH2   | 2.06                     | 0.86              |
| 1:E:12:ILE:HD13  | 1:E:23:GLN:NE2   | 1.89                     | 0.86              |
| 1:B:12:ILE:HD13  | 1:B:23:GLN:NE2   | 1.89                     | 0.86              |
| 1:Q:108:ASN:CG   | 2:Y:70:ARG:CG    | 2.42                     | 0.86              |
| 1:R:124:THR:HG22 | 1:S:130:ARG:NH2  | 1.89                     | 0.86              |
| 1:P:178:ARG:C    | 1:Q:57:ARG:NH2   | 2.33                     | 0.86              |
| 1:Q:103:TYR:C    | 2:Y:81:THR:HG21  | 2.00                     | 0.86              |
| 1:T:12:ILE:HD13  | 1:T:23:GLN:NE2   | 1.89                     | 0.86              |
| 1:A:21:LEU:HD11  | 1:B:130:ARG:CD   | 2.05                     | 0.86              |
| 1:O:21:LEU:HD11  | 1:P:130:ARG:CD   | 2.05                     | 0.85              |
| 1:U:108:ASN:CB   | 2:V:70:ARG:CD    | 2.47                     | 0.85              |
| 1:B:9:ASP:HB2    | 1:B:26:TYR:HH    | 1.39                     | 0.85              |
| 1:P:12:ILE:HD13  | 1:P:23:GLN:NE2   | 1.89                     | 0.85              |
| 1:S:177:GLU:OE1  | 1:T:58:LEU:N     | 2.09                     | 0.85              |
| 1:B:178:ARG:C    | 1:C:57:ARG:NH2   | 2.33                     | 0.85              |
| 1:C:177:GLU:CA   | 1:D:58:LEU:CG    | 2.08                     | 0.85              |
| 1:F:177:GLU:CD   | 1:G:58:LEU:HD13  | 2.00                     | 0.85              |
| 1:R:101:VAL:HG22 | 2:Y:58:TYR:CD1   | 2.06                     | 0.85              |
| 1:C:103:TYR:C    | 2:K:81:THR:HG21  | 2.00                     | 0.85              |
| 1:E:177:GLU:OE1  | 1:F:58:LEU:N     | 2.09                     | 0.85              |
| 1:F:108:ASN:HD22 | 2:N:70:ARG:CG    | 1.87                     | 0.85              |
| 2:M:37:ILE:HD11  | 2:M:59:MET:HB3   | 1.56                     | 0.85              |
| 2:L:38:ASP:HB3   | 2:L:41:THR:HG23  | 1.59                     | 0.85              |
| 1:T:161:LYS:CD   | 1:U:60:GLU:OE2   | 2.25                     | 0.85              |
| 1:F:177:GLU:HA   | 1:G:58:LEU:HD11  | 0.86                     | 0.85              |
| 1:R:124:THR:CG2  | 1:S:130:ARG:HH21 | 1.89                     | 0.85              |
| 1:U:108:ASN:CG   | 2:V:70:ARG:CG    | 2.44                     | 0.85              |
| 1:E:97:GLN:OE1   | 2:L:61:ALA:CB    | 2.25                     | 0.85              |
| 1:T:177:GLU:HA   | 1:U:58:LEU:HD11  | 0.86                     | 0.85              |
| 1:B:177:GLU:H    | 1:C:58:LEU:HD21  | 1.38                     | 0.85              |
| 1:D:7:ALA:HB1    | 1:E:10:ARG:HH11  | 1.40                     | 0.85              |
| 1:F:21:LEU:CD1   | 1:G:130:ARG:CD   | 2.52                     | 0.85              |
| 1:R:7:ALA:HB1    | 1:S:10:ARG:HH11  | 1.40                     | 0.85              |
| 1:E:103:TYR:HE1  | 2:M:82:LEU:HD22  | 1.40                     | 0.85              |
| 1:F:177:GLU:CB   | 1:G:58:LEU:CD2   | 2.52                     | 0.85              |
| 1:E:161:LYS:HB2  | 1:F:60:GLU:CD    | 2.00                     | 0.84              |
| 1:F:177:GLU:O    | 1:G:57:ARG:NE    | 2.08                     | 0.84              |
| 1:A:177:GLU:HA   | 1:B:58:LEU:CG    | 2.07                     | 0.84              |
| 1:C:9:ASP:HB2    | 1:C:26:TYR:HH    | 1.38                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:177:GLU:HB2  | 1:Q:58:LEU:HD22  | 1.57                     | 0.84              |
| 1:T:9:ASP:HB2    | 1:T:26:TYR:HH    | 1.39                     | 0.84              |
| 2:Z:38:ASP:HB3   | 2:Z:41:THR:HG23  | 1.59                     | 0.84              |
| 1:E:9:ASP:HB2    | 1:E:26:TYR:HH    | 1.38                     | 0.84              |
| 1:S:161:LYS:HB2  | 1:T:60:GLU:CD    | 2.00                     | 0.84              |
| 1:G:108:ASN:ND2  | 2:H:70:ARG:CB    | 2.41                     | 0.84              |
| 1:O:97:GLN:OE1   | 2:V:61:ALA:HB1   | 1.75                     | 0.84              |
| 1:D:103:TYR:C    | 2:L:81:THR:CG2   | 2.51                     | 0.84              |
| 1:A:177:GLU:H    | 1:B:58:LEU:HD21  | 1.38                     | 0.84              |
| 1:C:177:GLU:N    | 1:D:58:LEU:CD2   | 2.23                     | 0.84              |
| 1:O:178:ARG:CA   | 1:P:57:ARG:NH2   | 2.41                     | 0.84              |
| 1:S:97:GLN:OE1   | 2:Z:61:ALA:CB    | 2.25                     | 0.84              |
| 1:G:108:ASN:ND2  | 2:H:70:ARG:CG    | 2.41                     | 0.83              |
| 1:C:108:ASN:HD22 | 2:K:70:ARG:HG2   | 1.38                     | 0.83              |
| 1:E:108:ASN:CB   | 2:M:70:ARG:CG    | 2.56                     | 0.83              |
| 1:F:15:PHE:CZ    | 1:G:130:ARG:NH1  | 2.46                     | 0.83              |
| 1:B:12:ILE:CD1   | 1:B:23:GLN:C     | 2.52                     | 0.83              |
| 1:S:108:ASN:CB   | 2:I:70:ARG:CG    | 2.56                     | 0.83              |
| 1:U:108:ASN:ND2  | 2:V:70:ARG:CG    | 2.41                     | 0.83              |
| 1:T:12:ILE:CD1   | 1:T:23:GLN:C     | 2.52                     | 0.83              |
| 1:O:129:VAL:HG23 | 1:U:125:GLN:O    | 1.79                     | 0.83              |
| 2:2:53:GLN:O     | 2:2:56:VAL:HG12  | 1.78                     | 0.83              |
| 1:F:161:LYS:CD   | 1:G:60:GLU:OE2   | 2.25                     | 0.83              |
| 1:C:125:GLN:O    | 1:D:129:VAL:HG23 | 1.78                     | 0.83              |
| 1:G:107:VAL:CG2  | 2:H:66:TYR:OH    | 2.27                     | 0.83              |
| 2:N:53:GLN:O     | 2:N:56:VAL:HG12  | 1.78                     | 0.83              |
| 1:P:124:THR:HG22 | 1:Q:130:ARG:HH21 | 1.43                     | 0.83              |
| 1:F:97:GLN:OE1   | 2:M:61:ALA:HB1   | 1.78                     | 0.83              |
| 1:O:60:GLU:HG2   | 1:U:161:LYS:N    | 1.93                     | 0.83              |
| 1:O:178:ARG:N    | 1:P:57:ARG:HH21  | 1.76                     | 0.83              |
| 1:T:21:LEU:CD1   | 1:U:130:ARG:CD   | 2.52                     | 0.83              |
| 1:O:9:ASP:HB2    | 1:O:26:TYR:HH    | 1.40                     | 0.83              |
| 1:S:12:ILE:CD1   | 1:S:23:GLN:C     | 2.52                     | 0.83              |
| 1:A:60:GLU:HG2   | 1:G:161:LYS:N    | 1.93                     | 0.83              |
| 1:A:178:ARG:CA   | 1:B:57:ARG:NH2   | 2.41                     | 0.83              |
| 1:D:124:THR:CG2  | 1:E:130:ARG:HH21 | 1.89                     | 0.83              |
| 1:O:177:GLU:CA   | 1:P:58:LEU:HD21  | 2.09                     | 0.83              |
| 1:P:12:ILE:CD1   | 1:P:23:GLN:C     | 2.52                     | 0.83              |
| 2:W:123:ILE:HG12 | 2:W:124:TYR:HD1  | 1.44                     | 0.83              |
| 1:A:12:ILE:CD1   | 1:A:23:GLN:C     | 2.52                     | 0.82              |
| 1:D:101:VAL:HG23 | 2:K:58:TYR:HD1   | 1.43                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:12:ILE:CD1   | 1:E:23:GLN:C     | 2.52                     | 0.82              |
| 1:G:108:ASN:CG   | 2:H:70:ARG:CG    | 2.44                     | 0.82              |
| 1:P:178:ARG:C    | 1:Q:57:ARG:HH22  | 1.87                     | 0.82              |
| 1:R:12:ILE:CD1   | 1:R:23:GLN:C     | 2.52                     | 0.82              |
| 1:T:97:GLN:OE1   | 2:1:61:ALA:HB1   | 1.78                     | 0.82              |
| 1:A:9:ASP:HB2    | 1:A:26:TYR:HH    | 1.39                     | 0.82              |
| 1:A:129:VAL:HG23 | 1:G:125:GLN:O    | 1.79                     | 0.82              |
| 1:F:9:ASP:HB2    | 1:F:26:TYR:HH    | 1.39                     | 0.82              |
| 1:G:12:ILE:CD1   | 1:G:23:GLN:C     | 2.52                     | 0.82              |
| 1:O:177:GLU:H    | 1:P:58:LEU:HD21  | 1.38                     | 0.82              |
| 1:A:58:LEU:CD2   | 1:G:177:GLU:H    | 1.83                     | 0.82              |
| 1:Q:125:GLN:O    | 1:R:129:VAL:HG23 | 1.78                     | 0.82              |
| 1:C:12:ILE:CD1   | 1:C:23:GLN:C     | 2.52                     | 0.82              |
| 1:T:177:GLU:HA   | 1:U:58:LEU:CD2   | 1.98                     | 0.82              |
| 1:A:177:GLU:CA   | 1:B:58:LEU:HD21  | 2.09                     | 0.82              |
| 1:C:107:VAL:HG21 | 2:K:66:TYR:OH    | 1.80                     | 0.82              |
| 1:O:12:ILE:CD1   | 1:O:23:GLN:C     | 2.52                     | 0.82              |
| 1:O:177:GLU:HA   | 1:P:58:LEU:CG    | 2.07                     | 0.82              |
| 1:U:108:ASN:ND2  | 2:V:70:ARG:CB    | 2.41                     | 0.82              |
| 1:D:101:VAL:HG22 | 2:K:58:TYR:CE1   | 2.15                     | 0.82              |
| 1:F:177:GLU:OE1  | 1:G:58:LEU:CD1   | 2.27                     | 0.82              |
| 1:U:12:ILE:CD1   | 1:U:23:GLN:C     | 2.52                     | 0.82              |
| 1:T:15:PHE:CZ    | 1:U:130:ARG:NH1  | 2.46                     | 0.82              |
| 1:A:178:ARG:N    | 1:B:57:ARG:HH21  | 1.76                     | 0.81              |
| 1:B:124:THR:HG22 | 1:C:130:ARG:HH21 | 1.43                     | 0.81              |
| 1:C:97:GLN:OE1   | 2:J:61:ALA:HB1   | 1.80                     | 0.81              |
| 1:F:12:ILE:CD1   | 1:F:23:GLN:C     | 2.52                     | 0.81              |
| 1:B:178:ARG:C    | 1:C:57:ARG:HH22  | 1.87                     | 0.81              |
| 1:D:12:ILE:CD1   | 1:D:23:GLN:C     | 2.52                     | 0.81              |
| 1:D:108:ASN:ND2  | 2:L:70:ARG:CG    | 2.43                     | 0.81              |
| 2:J:37:ILE:HD11  | 2:J:59:MET:HB3   | 1.61                     | 0.81              |
| 1:R:101:VAL:HG23 | 2:Y:58:TYR:HD1   | 1.43                     | 0.81              |
| 2:1:20:VAL:HG13  | 2:1:28:HIS:HB2   | 1.62                     | 0.81              |
| 1:O:58:LEU:CD2   | 1:U:177:GLU:H    | 1.83                     | 0.81              |
| 1:Q:12:ILE:CD1   | 1:Q:23:GLN:C     | 2.52                     | 0.81              |
| 1:R:101:VAL:HG22 | 2:Y:58:TYR:CE1   | 2.15                     | 0.81              |
| 1:B:108:ASN:HB3  | 2:J:70:ARG:CD    | 2.11                     | 0.81              |
| 1:G:103:TYR:C    | 2:H:81:THR:CG2   | 2.54                     | 0.81              |
| 2:I:123:ILE:HG12 | 2:I:124:TYR:HD1  | 1.44                     | 0.81              |
| 1:O:177:GLU:CA   | 1:P:58:LEU:CD2   | 2.59                     | 0.81              |
| 1:U:107:VAL:CG2  | 2:V:66:TYR:OH    | 2.27                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:52:LYS:NZ    | 1:A:62:ASN:HA    | 1.96                     | 0.81              |
| 1:E:103:TYR:O    | 2:M:81:THR:HG21  | 1.80                     | 0.81              |
| 1:T:7:ALA:HB1    | 1:U:10:ARG:HH11  | 1.46                     | 0.81              |
| 1:S:177:GLU:OE1  | 1:T:58:LEU:HD13  | 1.80                     | 0.81              |
| 2:M:20:VAL:HG13  | 2:M:28:HIS:HB2   | 1.62                     | 0.81              |
| 1:S:52:LYS:NZ    | 1:S:62:ASN:HA    | 1.96                     | 0.81              |
| 1:U:52:LYS:NZ    | 1:U:62:ASN:HA    | 1.96                     | 0.81              |
| 2:X:37:ILE:HD11  | 2:X:59:MET:HB3   | 1.61                     | 0.81              |
| 1:C:52:LYS:NZ    | 1:C:62:ASN:HA    | 1.96                     | 0.80              |
| 1:Q:107:VAL:HG21 | 2:Y:66:TYR:OH    | 1.80                     | 0.80              |
| 1:Q:177:GLU:C    | 1:R:58:LEU:CD1   | 2.41                     | 0.80              |
| 1:R:103:TYR:C    | 2:Z:81:THR:CG2   | 2.51                     | 0.80              |
| 1:U:103:TYR:C    | 2:V:81:THR:CG2   | 2.54                     | 0.80              |
| 1:F:177:GLU:HA   | 1:G:58:LEU:CD2   | 1.98                     | 0.80              |
| 1:S:103:TYR:O    | 2:1:81:THR:HG21  | 1.80                     | 0.80              |
| 1:U:107:VAL:HG21 | 2:V:66:TYR:OH    | 1.82                     | 0.80              |
| 1:G:52:LYS:NZ    | 1:G:62:ASN:HA    | 1.96                     | 0.80              |
| 1:O:57:ARG:CA    | 1:U:177:GLU:OE1  | 2.30                     | 0.80              |
| 1:O:177:GLU:HA   | 1:P:58:LEU:HD11  | 0.80                     | 0.80              |
| 1:Q:97:GLN:OE1   | 2:X:61:ALA:HB1   | 1.80                     | 0.80              |
| 1:A:177:GLU:HA   | 1:B:58:LEU:HD11  | 0.80                     | 0.80              |
| 1:D:52:LYS:NZ    | 1:D:62:ASN:HA    | 1.96                     | 0.80              |
| 2:K:59:MET:HE2   | 2:K:79:VAL:HG23  | 1.64                     | 0.80              |
| 1:O:10:ARG:NH1   | 1:U:7:ALA:HB1    | 1.96                     | 0.80              |
| 1:Q:108:ASN:HD22 | 2:Y:70:ARG:HG2   | 1.38                     | 0.80              |
| 1:R:108:ASN:ND2  | 2:Z:70:ARG:CG    | 2.43                     | 0.80              |
| 1:B:52:LYS:NZ    | 1:B:62:ASN:HA    | 1.96                     | 0.80              |
| 1:D:12:ILE:HD12  | 1:D:23:GLN:CG    | 1.76                     | 0.80              |
| 1:D:125:GLN:O    | 1:E:129:VAL:HG23 | 1.81                     | 0.80              |
| 1:O:12:ILE:HD12  | 1:O:23:GLN:CG    | 1.76                     | 0.80              |
| 1:E:177:GLU:OE1  | 1:F:58:LEU:HD13  | 1.80                     | 0.80              |
| 1:O:52:LYS:NZ    | 1:O:62:ASN:HA    | 1.96                     | 0.80              |
| 1:R:177:GLU:HB2  | 1:S:58:LEU:CD2   | 2.12                     | 0.80              |
| 1:T:52:LYS:NZ    | 1:T:62:ASN:HA    | 1.96                     | 0.80              |
| 1:G:107:VAL:HG21 | 2:H:66:TYR:OH    | 1.82                     | 0.80              |
| 1:R:52:LYS:NZ    | 1:R:62:ASN:HA    | 1.96                     | 0.80              |
| 2:Y:59:MET:HE1   | 2:Y:82:LEU:HD23  | 1.63                     | 0.80              |
| 1:B:12:ILE:HD11  | 1:B:23:GLN:C     | 2.07                     | 0.79              |
| 1:E:52:LYS:NZ    | 1:E:62:ASN:HA    | 1.96                     | 0.79              |
| 1:P:108:ASN:HB3  | 2:X:70:ARG:CD    | 2.11                     | 0.79              |
| 1:R:155:GLY:C    | 1:S:86:ARG:HH22  | 1.90                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:12:ILE:HD11  | 1:C:23:GLN:C     | 2.07                     | 0.79              |
| 1:F:108:ASN:CB   | 2:N:70:ARG:CD    | 2.59                     | 0.79              |
| 1:Q:52:LYS:NZ    | 1:Q:62:ASN:HA    | 1.96                     | 0.79              |
| 1:Q:177:GLU:O    | 1:R:58:LEU:CD1   | 2.29                     | 0.79              |
| 1:T:12:ILE:HD11  | 1:T:23:GLN:C     | 2.07                     | 0.79              |
| 1:U:12:ILE:HD11  | 1:U:23:GLN:C     | 2.07                     | 0.79              |
| 1:C:177:GLU:O    | 1:D:58:LEU:CD1   | 2.29                     | 0.79              |
| 1:P:52:LYS:NZ    | 1:P:62:ASN:HA    | 1.96                     | 0.79              |
| 2:Y:123:ILE:HG12 | 2:Y:124:TYR:HD1  | 1.48                     | 0.79              |
| 1:A:57:ARG:CA    | 1:G:177:GLU:OE1  | 2.30                     | 0.79              |
| 1:B:177:GLU:CD   | 1:C:57:ARG:H     | 1.90                     | 0.79              |
| 1:O:177:GLU:C    | 1:P:57:ARG:NH2   | 2.30                     | 0.79              |
| 1:P:177:GLU:CD   | 1:Q:57:ARG:H     | 1.90                     | 0.79              |
| 1:A:177:GLU:CA   | 1:B:58:LEU:CD2   | 2.59                     | 0.79              |
| 1:D:177:GLU:HB2  | 1:E:58:LEU:CD2   | 2.12                     | 0.79              |
| 1:F:103:TYR:C    | 2:N:81:THR:CG2   | 2.56                     | 0.79              |
| 1:F:7:ALA:HB1    | 1:G:10:ARG:HH11  | 1.46                     | 0.79              |
| 1:F:52:LYS:NZ    | 1:F:62:ASN:HA    | 1.96                     | 0.79              |
| 1:A:10:ARG:NH1   | 1:G:7:ALA:HB1    | 1.96                     | 0.78              |
| 1:O:12:ILE:HD12  | 1:O:23:GLN:N     | 1.98                     | 0.78              |
| 1:P:12:ILE:HD12  | 1:P:23:GLN:N     | 1.98                     | 0.78              |
| 1:T:177:GLU:OE1  | 1:U:58:LEU:CD1   | 2.27                     | 0.78              |
| 1:C:103:TYR:C    | 2:K:81:THR:CG2   | 2.56                     | 0.78              |
| 1:E:12:ILE:HD11  | 1:E:23:GLN:C     | 2.07                     | 0.78              |
| 2:K:123:ILE:HG12 | 2:K:124:TYR:HD1  | 1.48                     | 0.78              |
| 1:P:12:ILE:HD11  | 1:P:23:GLN:C     | 2.07                     | 0.78              |
| 1:S:12:ILE:HD12  | 1:S:23:GLN:CG    | 1.75                     | 0.78              |
| 1:Q:107:VAL:CG1  | 2:Y:66:TYR:OH    | 2.31                     | 0.78              |
| 1:R:125:GLN:O    | 1:S:129:VAL:HG23 | 1.81                     | 0.78              |
| 1:A:12:ILE:HD11  | 1:A:23:GLN:C     | 2.07                     | 0.78              |
| 1:D:12:ILE:HD12  | 1:D:23:GLN:N     | 1.98                     | 0.78              |
| 1:O:186:GLU:O    | 1:O:190:VAL:HG12 | 1.84                     | 0.78              |
| 1:Q:12:ILE:HD11  | 1:Q:23:GLN:C     | 2.07                     | 0.78              |
| 1:R:7:ALA:HB1    | 1:S:10:ARG:NH1   | 1.99                     | 0.78              |
| 1:S:108:ASN:HD22 | 2:1:70:ARG:CG    | 1.95                     | 0.78              |
| 1:T:108:ASN:CB   | 2:2:70:ARG:CD    | 2.59                     | 0.78              |
| 1:U:12:ILE:HD12  | 1:U:23:GLN:N     | 1.98                     | 0.78              |
| 2:Y:59:MET:HE2   | 2:Y:79:VAL:HG23  | 1.64                     | 0.78              |
| 1:C:12:ILE:HD12  | 1:C:23:GLN:N     | 1.99                     | 0.78              |
| 1:C:124:THR:CG2  | 1:D:130:ARG:HH21 | 1.97                     | 0.78              |
| 1:D:186:GLU:O    | 1:D:190:VAL:HG12 | 1.84                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:12:ILE:HD12  | 1:E:23:GLN:N     | 1.98                     | 0.78              |
| 2:K:59:MET:HE1   | 2:K:82:LEU:HD23  | 1.63                     | 0.78              |
| 1:D:97:GLN:OE1   | 2:K:61:ALA:HB1   | 1.84                     | 0.78              |
| 1:G:108:ASN:ND2  | 2:H:70:ARG:CA    | 2.47                     | 0.78              |
| 1:Q:12:ILE:HD12  | 1:Q:23:GLN:N     | 1.98                     | 0.78              |
| 1:S:12:ILE:HD11  | 1:S:23:GLN:C     | 2.07                     | 0.78              |
| 1:T:103:TYR:C    | 2:2:81:THR:CG2   | 2.56                     | 0.78              |
| 2:V:43:MET:HE2   | 2:V:56:VAL:HG23  | 1.66                     | 0.78              |
| 2:V:123:ILE:HG12 | 2:V:124:TYR:HD1  | 1.49                     | 0.78              |
| 1:A:177:GLU:CD   | 1:B:58:LEU:HD13  | 2.08                     | 0.78              |
| 1:C:107:VAL:CG1  | 2:K:66:TYR:OH    | 2.31                     | 0.78              |
| 1:T:186:GLU:O    | 1:T:190:VAL:HG12 | 1.84                     | 0.78              |
| 2:W:53:GLN:O     | 2:W:56:VAL:HG12  | 1.83                     | 0.78              |
| 1:F:186:GLU:O    | 1:F:190:VAL:HG12 | 1.84                     | 0.78              |
| 1:G:108:ASN:HB2  | 2:H:70:ARG:CG    | 2.09                     | 0.78              |
| 1:O:86:ARG:HH22  | 1:U:155:GLY:C    | 1.92                     | 0.78              |
| 1:B:186:GLU:O    | 1:B:190:VAL:HG12 | 1.84                     | 0.78              |
| 1:D:12:ILE:HD11  | 1:D:23:GLN:HB3   | 0.80                     | 0.78              |
| 1:Q:103:TYR:C    | 2:Y:81:THR:CG2   | 2.56                     | 0.78              |
| 1:Q:186:GLU:O    | 1:Q:190:VAL:HG12 | 1.84                     | 0.78              |
| 1:F:12:ILE:HD12  | 1:F:23:GLN:N     | 1.98                     | 0.77              |
| 1:F:108:ASN:CG   | 2:N:70:ARG:CG    | 2.56                     | 0.77              |
| 1:Q:161:LYS:HD2  | 1:R:60:GLU:OE2   | 1.84                     | 0.77              |
| 1:T:52:LYS:HZ1   | 1:T:62:ASN:HA    | 1.47                     | 0.77              |
| 1:A:12:ILE:HD12  | 1:A:23:GLN:N     | 1.98                     | 0.77              |
| 1:D:7:ALA:HB1    | 1:E:10:ARG:NH1   | 1.99                     | 0.77              |
| 1:F:12:ILE:HD11  | 1:F:23:GLN:C     | 2.07                     | 0.77              |
| 1:O:12:ILE:HD11  | 1:O:23:GLN:HB3   | 0.80                     | 0.77              |
| 1:R:97:GLN:OE1   | 2:Y:61:ALA:HB1   | 1.84                     | 0.77              |
| 1:R:108:ASN:HB3  | 2:Z:70:ARG:CD    | 2.14                     | 0.77              |
| 1:B:12:ILE:HD12  | 1:B:23:GLN:N     | 1.98                     | 0.77              |
| 1:G:12:ILE:HD11  | 1:G:23:GLN:C     | 2.07                     | 0.77              |
| 1:P:177:GLU:OE1  | 1:Q:57:ARG:N     | 2.17                     | 0.77              |
| 1:U:186:GLU:O    | 1:U:190:VAL:HG12 | 1.84                     | 0.77              |
| 1:A:12:ILE:HD12  | 1:A:23:GLN:CG    | 1.76                     | 0.77              |
| 1:A:86:ARG:HH22  | 1:G:155:GLY:C    | 1.92                     | 0.77              |
| 1:O:177:GLU:CD   | 1:P:58:LEU:HD13  | 2.08                     | 0.77              |
| 1:R:12:ILE:HD11  | 1:R:23:GLN:C     | 2.07                     | 0.77              |
| 1:S:12:ILE:HD12  | 1:S:23:GLN:N     | 1.98                     | 0.77              |
| 1:T:12:ILE:HD12  | 1:T:23:GLN:N     | 1.98                     | 0.77              |
| 1:D:155:GLY:C    | 1:E:86:ARG:HH22  | 1.90                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:186:GLU:O    | 1:E:190:VAL:HG12 | 1.84                     | 0.77              |
| 1:G:186:GLU:O    | 1:G:190:VAL:HG12 | 1.84                     | 0.77              |
| 1:O:12:ILE:HD11  | 1:O:23:GLN:C     | 2.07                     | 0.77              |
| 1:D:108:ASN:HB3  | 2:L:70:ARG:CD    | 2.14                     | 0.77              |
| 1:P:12:ILE:HD11  | 1:P:23:GLN:HB3   | 0.80                     | 0.77              |
| 1:C:186:GLU:O    | 1:C:190:VAL:HG12 | 1.84                     | 0.77              |
| 2:N:32:LYS:HE2   | 2:N:34:LEU:O     | 1.85                     | 0.77              |
| 1:R:108:ASN:HD22 | 2:Z:70:ARG:HG2   | 1.49                     | 0.77              |
| 1:T:13:THR:CB    | 1:T:14:VAL:CG2   | 2.62                     | 0.77              |
| 1:U:12:ILE:HD11  | 1:U:23:GLN:HB3   | 0.80                     | 0.77              |
| 1:E:12:ILE:HD11  | 1:E:23:GLN:HB3   | 0.80                     | 0.77              |
| 1:A:186:GLU:O    | 1:A:190:VAL:HG12 | 1.84                     | 0.77              |
| 1:C:12:ILE:HD11  | 1:C:23:GLN:CB    | 1.31                     | 0.77              |
| 1:C:12:ILE:HD11  | 1:C:23:GLN:HB3   | 0.80                     | 0.77              |
| 1:C:161:LYS:HD2  | 1:D:60:GLU:OE2   | 1.84                     | 0.77              |
| 2:N:167:SER:HB2  | 2:Y:167:SER:HB2  | 1.65                     | 0.77              |
| 1:T:107:VAL:CG1  | 2:2:66:TYR:OH    | 2.32                     | 0.77              |
| 2:H:123:ILE:HG12 | 2:H:124:TYR:HD1  | 1.49                     | 0.77              |
| 2:I:53:GLN:O     | 2:I:56:VAL:HG12  | 1.83                     | 0.77              |
| 1:R:12:ILE:HD12  | 1:R:23:GLN:CG    | 1.76                     | 0.77              |
| 2:X:123:ILE:H    | 2:X:123:ILE:HD13 | 1.49                     | 0.77              |
| 1:B:177:GLU:OE1  | 1:C:57:ARG:N     | 2.17                     | 0.76              |
| 1:E:108:ASN:HD22 | 2:M:70:ARG:CG    | 1.96                     | 0.76              |
| 1:A:101:VAL:CG2  | 2:H:58:TYR:CE1   | 2.68                     | 0.76              |
| 1:D:13:THR:CB    | 1:D:14:VAL:CG2   | 2.62                     | 0.76              |
| 1:O:101:VAL:CG2  | 2:V:58:TYR:CE1   | 2.68                     | 0.76              |
| 1:Q:103:TYR:O    | 2:Y:81:THR:HG21  | 1.86                     | 0.76              |
| 1:U:12:ILE:HD11  | 1:U:23:GLN:CB    | 1.31                     | 0.76              |
| 1:B:12:ILE:HD11  | 1:B:23:GLN:CB    | 1.31                     | 0.76              |
| 1:F:12:ILE:HD11  | 1:F:23:GLN:CB    | 1.31                     | 0.76              |
| 1:G:12:ILE:HD11  | 1:G:23:GLN:CB    | 1.31                     | 0.76              |
| 1:O:12:ILE:HG13  | 1:O:23:GLN:HB2   | 1.67                     | 0.76              |
| 1:O:101:VAL:HG21 | 2:V:58:TYR:CE1   | 2.20                     | 0.76              |
| 1:O:178:ARG:C    | 1:P:57:ARG:NH2   | 2.43                     | 0.76              |
| 1:R:111:ASN:CG   | 2:Z:70:ARG:NH1   | 2.43                     | 0.76              |
| 1:R:161:LYS:N    | 1:S:60:GLU:HG2   | 2.01                     | 0.76              |
| 1:T:12:ILE:HD12  | 1:T:23:GLN:CG    | 1.76                     | 0.76              |
| 1:A:178:ARG:C    | 1:B:57:ARG:NH2   | 2.43                     | 0.76              |
| 1:D:12:ILE:HD11  | 1:D:23:GLN:C     | 2.07                     | 0.76              |
| 1:E:177:GLU:OE1  | 1:F:57:ARG:C     | 2.28                     | 0.76              |
| 1:F:108:ASN:CB   | 2:N:70:ARG:HD3   | 2.15                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:12:ILE:HG13  | 1:G:23:GLN:HB2   | 1.67                     | 0.76              |
| 1:P:186:GLU:O    | 1:P:190:VAL:HG12 | 1.84                     | 0.76              |
| 1:Q:124:THR:CG2  | 1:R:130:ARG:HH21 | 1.97                     | 0.76              |
| 1:R:186:GLU:O    | 1:R:190:VAL:HG12 | 1.84                     | 0.76              |
| 1:S:186:GLU:O    | 1:S:190:VAL:HG12 | 1.84                     | 0.76              |
| 2:2:32:LYS:HE2   | 2:2:34:LEU:O     | 1.85                     | 0.76              |
| 2:K:167:SER:HB2  | 2:2:167:SER:HB2  | 1.68                     | 0.76              |
| 1:S:107:VAL:HG11 | 2:1:66:TYR:OH    | 1.86                     | 0.76              |
| 1:U:108:ASN:ND2  | 2:V:70:ARG:CA    | 2.47                     | 0.76              |
| 1:Q:12:ILE:HD11  | 1:Q:23:GLN:HB3   | 0.80                     | 0.76              |
| 1:R:12:ILE:HD12  | 1:R:23:GLN:N     | 1.98                     | 0.76              |
| 1:D:111:ASN:CG   | 2:L:70:ARG:NH1   | 2.43                     | 0.76              |
| 1:O:13:THR:CB    | 1:O:14:VAL:CG2   | 2.62                     | 0.76              |
| 2:H:43:MET:HE2   | 2:H:56:VAL:HG23  | 1.66                     | 0.76              |
| 1:R:12:ILE:HG13  | 1:R:23:GLN:HB2   | 1.67                     | 0.76              |
| 1:B:101:VAL:HG21 | 2:I:58:TYR:HD1   | 1.24                     | 0.76              |
| 1:E:101:VAL:HG22 | 2:L:58:TYR:CD1   | 2.19                     | 0.76              |
| 2:J:123:ILE:H    | 2:J:123:ILE:HD13 | 1.49                     | 0.76              |
| 1:P:173:VAL:O    | 1:Q:58:LEU:HD21  | 1.86                     | 0.76              |
| 1:P:177:GLU:OE1  | 1:Q:57:ARG:HB2   | 1.86                     | 0.76              |
| 1:S:177:GLU:OE1  | 1:T:57:ARG:C     | 2.28                     | 0.76              |
| 1:A:101:VAL:HG21 | 2:H:58:TYR:CE1   | 2.21                     | 0.76              |
| 1:C:103:TYR:O    | 2:K:81:THR:HG21  | 1.86                     | 0.76              |
| 1:D:13:THR:HB    | 1:D:14:VAL:CG2   | 2.16                     | 0.76              |
| 1:F:12:ILE:HD11  | 1:F:23:GLN:HB3   | 0.80                     | 0.76              |
| 1:F:107:VAL:CG1  | 2:N:66:TYR:OH    | 2.32                     | 0.76              |
| 1:E:107:VAL:HG11 | 2:M:66:TYR:OH    | 1.86                     | 0.75              |
| 1:G:12:ILE:HD12  | 1:G:23:GLN:N     | 1.98                     | 0.75              |
| 1:P:159:GLU:O    | 1:Q:60:GLU:HB2   | 1.87                     | 0.75              |
| 1:R:177:GLU:CD   | 1:S:58:LEU:HD13  | 2.10                     | 0.75              |
| 1:S:21:LEU:HD11  | 1:T:130:ARG:CD   | 2.16                     | 0.75              |
| 1:R:13:THR:CB    | 1:R:14:VAL:CG2   | 2.62                     | 0.75              |
| 1:T:12:ILE:HD11  | 1:T:23:GLN:HB3   | 0.80                     | 0.75              |
| 1:P:97:GLN:OE1   | 2:W:61:ALA:HB1   | 1.86                     | 0.75              |
| 1:Q:12:ILE:HD11  | 1:Q:23:GLN:CB    | 1.31                     | 0.75              |
| 1:B:177:GLU:OE1  | 1:C:57:ARG:HB2   | 1.86                     | 0.75              |
| 1:D:108:ASN:HD22 | 2:L:70:ARG:HG2   | 1.49                     | 0.75              |
| 1:D:161:LYS:N    | 1:E:60:GLU:HG2   | 2.01                     | 0.75              |
| 1:D:177:GLU:CD   | 1:E:58:LEU:HD13  | 2.10                     | 0.75              |
| 1:G:13:THR:CB    | 1:G:14:VAL:CG2   | 2.62                     | 0.75              |
| 1:O:13:THR:HB    | 1:O:14:VAL:CG2   | 2.16                     | 0.75              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:R:12:ILE:HD11  | 1:R:23:GLN:HB3  | 0.80                     | 0.75              |
| 1:S:12:ILE:HD11  | 1:S:23:GLN:HB3  | 0.80                     | 0.75              |
| 1:B:12:ILE:HD11  | 1:B:23:GLN:HB3  | 0.80                     | 0.75              |
| 1:B:12:ILE:HG13  | 1:B:23:GLN:HB2  | 1.66                     | 0.75              |
| 1:D:12:ILE:HG13  | 1:D:23:GLN:HB2  | 1.66                     | 0.75              |
| 1:P:12:ILE:HD11  | 1:P:23:GLN:CB   | 1.31                     | 0.75              |
| 1:R:12:ILE:HD11  | 1:R:23:GLN:CB   | 1.31                     | 0.75              |
| 1:A:58:LEU:HD13  | 1:G:177:GLU:OE1 | 1.86                     | 0.75              |
| 1:B:173:VAL:O    | 1:C:58:LEU:HD21 | 1.86                     | 0.75              |
| 1:E:12:ILE:HD11  | 1:E:23:GLN:CB   | 1.31                     | 0.75              |
| 1:Q:103:TYR:O    | 2:Y:81:THR:CG2  | 2.35                     | 0.75              |
| 1:U:108:ASN:CB   | 2:V:70:ARG:HD3  | 2.16                     | 0.75              |
| 2:Z:53:GLN:O     | 2:Z:56:VAL:HG12 | 1.87                     | 0.75              |
| 1:A:13:THR:HB    | 1:A:14:VAL:CG2  | 2.16                     | 0.75              |
| 1:A:86:ARG:CZ    | 1:G:155:GLY:O   | 2.35                     | 0.75              |
| 1:E:103:TYR:O    | 2:M:81:THR:CG2  | 2.35                     | 0.75              |
| 1:D:12:ILE:HD13  | 1:D:23:GLN:HE21 | 1.51                     | 0.74              |
| 1:F:178:ARG:C    | 1:G:57:ARG:HH22 | 1.92                     | 0.74              |
| 1:G:12:ILE:HD12  | 1:G:23:GLN:CG   | 1.76                     | 0.74              |
| 1:Q:13:THR:CB    | 1:Q:14:VAL:CG2  | 2.62                     | 0.74              |
| 1:R:177:GLU:OE1  | 1:S:57:ARG:HB2  | 1.86                     | 0.74              |
| 1:S:13:THR:HB    | 1:S:14:VAL:CG2  | 2.16                     | 0.74              |
| 1:C:103:TYR:O    | 2:K:81:THR:CG2  | 2.35                     | 0.74              |
| 1:E:104:GLY:N    | 2:M:81:THR:HG21 | 2.02                     | 0.74              |
| 1:Q:161:LYS:CB   | 1:R:60:GLU:OE2  | 2.34                     | 0.74              |
| 1:T:108:ASN:HD22 | 2:2:70:ARG:CB   | 2.00                     | 0.74              |
| 1:A:60:GLU:OE2   | 1:G:161:LYS:CG  | 2.35                     | 0.74              |
| 1:T:12:ILE:HG13  | 1:T:23:GLN:HB2  | 1.66                     | 0.74              |
| 1:T:178:ARG:N    | 1:U:57:ARG:HH21 | 1.84                     | 0.74              |
| 1:A:12:ILE:HD11  | 1:A:23:GLN:HB3  | 0.80                     | 0.74              |
| 1:B:12:ILE:HD12  | 1:B:23:GLN:CG   | 1.75                     | 0.74              |
| 1:B:97:GLN:OE1   | 2:I:61:ALA:HB1  | 1.86                     | 0.74              |
| 1:F:13:THR:HB    | 1:F:14:VAL:CG2  | 2.16                     | 0.74              |
| 1:G:12:ILE:HD11  | 1:G:23:GLN:HB3  | 0.80                     | 0.74              |
| 1:B:177:GLU:HB2  | 1:C:58:LEU:CD2  | 2.17                     | 0.74              |
| 1:C:161:LYS:CB   | 1:D:60:GLU:OE2  | 2.34                     | 0.74              |
| 1:E:21:LEU:HD11  | 1:F:130:ARG:CD  | 2.16                     | 0.74              |
| 1:F:13:THR:CB    | 1:F:14:VAL:CG2  | 2.62                     | 0.74              |
| 1:Q:12:ILE:HD12  | 1:Q:23:GLN:CG   | 1.75                     | 0.74              |
| 1:T:12:ILE:HD11  | 1:T:23:GLN:CB   | 1.31                     | 0.74              |
| 1:T:108:ASN:CB   | 2:2:70:ARG:HD3  | 2.15                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:62:GLU:HG2   | 2:2:82:LEU:HD21  | 1.70                     | 0.74              |
| 1:P:12:ILE:HG13  | 1:P:23:GLN:HB2   | 1.66                     | 0.74              |
| 1:U:97:GLN:OE1   | 2:2:61:ALA:HB1   | 1.88                     | 0.74              |
| 2:2:123:ILE:H    | 2:2:123:ILE:HD13 | 1.52                     | 0.74              |
| 1:A:58:LEU:N     | 1:G:177:GLU:OE1  | 2.21                     | 0.74              |
| 1:D:177:GLU:OE1  | 1:E:57:ARG:HB2   | 1.86                     | 0.74              |
| 1:F:178:ARG:N    | 1:G:57:ARG:HH21  | 1.84                     | 0.74              |
| 1:B:108:ASN:ND2  | 2:J:70:ARG:HG2   | 2.03                     | 0.74              |
| 1:B:177:GLU:OE1  | 1:C:57:ARG:CB    | 2.36                     | 0.74              |
| 1:F:108:ASN:HD22 | 2:N:70:ARG:CB    | 2.00                     | 0.74              |
| 1:G:108:ASN:CB   | 2:H:70:ARG:HD3   | 2.16                     | 0.74              |
| 2:M:123:ILE:HG12 | 2:M:124:TYR:HD1  | 1.53                     | 0.74              |
| 1:O:58:LEU:HD13  | 1:U:177:GLU:OE1  | 1.86                     | 0.74              |
| 1:O:86:ARG:CZ    | 1:U:155:GLY:O    | 2.34                     | 0.74              |
| 1:O:108:ASN:HB2  | 2:W:70:ARG:HG2   | 1.66                     | 0.74              |
| 1:S:108:ASN:CB   | 2:1:70:ARG:CD    | 2.66                     | 0.74              |
| 1:E:108:ASN:CB   | 2:M:70:ARG:HD3   | 2.18                     | 0.74              |
| 1:F:177:GLU:OE1  | 1:G:57:ARG:N     | 2.21                     | 0.74              |
| 1:A:108:ASN:ND2  | 2:I:70:ARG:HG2   | 2.02                     | 0.73              |
| 1:O:60:GLU:OE2   | 1:U:161:LYS:CG   | 2.35                     | 0.73              |
| 1:P:177:GLU:HB2  | 1:Q:58:LEU:CD2   | 2.17                     | 0.73              |
| 1:T:12:ILE:HD13  | 1:T:23:GLN:HE21  | 1.51                     | 0.73              |
| 1:E:12:ILE:HD13  | 1:E:23:GLN:HE21  | 1.51                     | 0.73              |
| 1:E:78:THR:HG21  | 1:E:85:ALA:HB1   | 1.71                     | 0.73              |
| 2:L:53:GLN:O     | 2:L:56:VAL:HG12  | 1.87                     | 0.73              |
| 1:P:78:THR:HG21  | 1:P:85:ALA:HB1   | 1.70                     | 0.73              |
| 1:P:177:GLU:CD   | 1:Q:56:SER:OG    | 2.31                     | 0.73              |
| 1:S:103:TYR:O    | 2:1:81:THR:CG2   | 2.35                     | 0.73              |
| 1:S:104:GLY:N    | 2:1:81:THR:HG21  | 2.02                     | 0.73              |
| 1:A:13:THR:CB    | 1:A:14:VAL:CG2   | 2.62                     | 0.73              |
| 1:B:159:GLU:O    | 1:C:60:GLU:HB2   | 1.87                     | 0.73              |
| 1:F:78:THR:HG21  | 1:F:85:ALA:HB1   | 1.70                     | 0.73              |
| 1:O:58:LEU:N     | 1:U:177:GLU:OE1  | 2.21                     | 0.73              |
| 1:Q:78:THR:HG21  | 1:Q:85:ALA:HB1   | 1.70                     | 0.73              |
| 1:S:108:ASN:HB3  | 2:1:70:ARG:CG    | 2.18                     | 0.73              |
| 1:B:177:GLU:CD   | 1:C:56:SER:OG    | 2.31                     | 0.73              |
| 1:C:13:THR:HB    | 1:C:14:VAL:CG2   | 2.16                     | 0.73              |
| 1:E:108:ASN:CB   | 2:M:70:ARG:CD    | 2.66                     | 0.73              |
| 1:G:97:GLN:OE1   | 2:N:61:ALA:HB1   | 1.88                     | 0.73              |
| 1:S:13:THR:CB    | 1:S:14:VAL:CG2   | 2.62                     | 0.73              |
| 1:D:78:THR:HG21  | 1:D:85:ALA:HB1   | 1.70                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:161:LYS:CB   | 1:G:60:GLU:OE2   | 2.36                     | 0.73              |
| 1:O:108:ASN:ND2  | 2:W:70:ARG:HG2   | 2.02                     | 0.73              |
| 1:Q:13:THR:HB    | 1:Q:14:VAL:CG2   | 2.16                     | 0.73              |
| 1:S:155:GLY:C    | 1:T:86:ARG:HH22  | 1.96                     | 0.73              |
| 1:U:13:THR:HB    | 1:U:14:VAL:CG2   | 2.16                     | 0.73              |
| 1:U:108:ASN:HD22 | 2:V:70:ARG:CA    | 2.00                     | 0.73              |
| 1:A:57:ARG:N     | 1:G:177:GLU:CD   | 2.33                     | 0.73              |
| 1:G:108:ASN:HD22 | 2:H:70:ARG:CA    | 2.00                     | 0.73              |
| 1:P:177:GLU:OE1  | 1:Q:57:ARG:CB    | 2.36                     | 0.73              |
| 1:R:155:GLY:O    | 1:S:86:ARG:CZ    | 2.36                     | 0.73              |
| 2:Z:2:THR:HG22   | 2:Z:169:SER:OG   | 1.89                     | 0.73              |
| 1:E:13:THR:CB    | 1:E:14:VAL:CG2   | 2.62                     | 0.73              |
| 1:O:12:ILE:HD13  | 1:O:23:GLN:HE21  | 1.51                     | 0.73              |
| 1:O:78:THR:HG21  | 1:O:85:ALA:HB1   | 1.70                     | 0.73              |
| 1:S:52:LYS:HZ1   | 1:S:62:ASN:HA    | 1.51                     | 0.73              |
| 1:C:12:ILE:HD13  | 1:C:23:GLN:HE21  | 1.51                     | 0.73              |
| 1:E:155:GLY:O    | 1:F:86:ARG:CZ    | 2.36                     | 0.73              |
| 1:G:78:THR:HG21  | 1:G:85:ALA:HB1   | 1.70                     | 0.73              |
| 2:L:2:THR:HG22   | 2:L:169:SER:OG   | 1.89                     | 0.73              |
| 1:P:13:THR:CB    | 1:P:14:VAL:CG2   | 2.62                     | 0.73              |
| 1:Q:107:VAL:CG2  | 2:Y:66:TYR:OH    | 2.37                     | 0.73              |
| 1:Q:108:ASN:HB2  | 2:Y:70:ARG:CG    | 2.12                     | 0.73              |
| 1:R:177:GLU:OE2  | 1:S:57:ARG:N     | 2.22                     | 0.73              |
| 1:S:108:ASN:HD22 | 2:I:70:ARG:CB    | 2.02                     | 0.73              |
| 1:S:155:GLY:O    | 1:T:86:ARG:CZ    | 2.36                     | 0.73              |
| 1:T:177:GLU:OE1  | 1:U:57:ARG:N     | 2.21                     | 0.73              |
| 1:C:72:ASP:OD1   | 2:J:67:ARG:NH2   | 2.22                     | 0.73              |
| 1:G:12:ILE:HD13  | 1:G:23:GLN:HE21  | 1.51                     | 0.73              |
| 1:P:108:ASN:ND2  | 2:X:70:ARG:HG2   | 2.03                     | 0.73              |
| 1:R:12:ILE:HD13  | 1:R:23:GLN:HE21  | 1.51                     | 0.73              |
| 1:R:78:THR:HG21  | 1:R:85:ALA:HB1   | 1.70                     | 0.73              |
| 1:S:12:ILE:HD13  | 1:S:23:GLN:HE21  | 1.51                     | 0.73              |
| 1:A:58:LEU:HD21  | 1:G:173:VAL:O    | 1.89                     | 0.73              |
| 1:E:108:ASN:HB3  | 2:M:70:ARG:CG    | 2.18                     | 0.73              |
| 1:O:58:LEU:CD2   | 1:U:177:GLU:HB2  | 2.19                     | 0.73              |
| 1:P:12:ILE:HD13  | 1:P:23:GLN:HE21  | 1.51                     | 0.73              |
| 2:W:103:GLY:HA2  | 2:W:178:ILE:HD11 | 1.71                     | 0.73              |
| 2:Z:20:VAL:HG13  | 2:Z:28:HIS:HB2   | 1.71                     | 0.73              |
| 1:C:13:THR:CB    | 1:C:14:VAL:CG2   | 2.62                     | 0.72              |
| 1:C:108:ASN:HD22 | 2:K:70:ARG:HB3   | 1.54                     | 0.72              |
| 1:D:101:VAL:CG2  | 2:K:58:TYR:CE1   | 2.68                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:111:ASN:CB   | 2:L:70:ARG:NH1   | 2.52                     | 0.72              |
| 1:O:57:ARG:N     | 1:U:177:GLU:CD   | 2.33                     | 0.72              |
| 1:O:168:GLY:O    | 1:O:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:S:161:LYS:HD2  | 1:T:60:GLU:OE2   | 1.88                     | 0.72              |
| 2:V:32:LYS:HE2   | 2:V:34:LEU:O     | 1.89                     | 0.72              |
| 1:D:168:GLY:O    | 1:D:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:E:12:ILE:HG13  | 1:E:23:GLN:HB2   | 1.66                     | 0.72              |
| 1:E:108:ASN:HD22 | 2:M:70:ARG:CB    | 2.02                     | 0.72              |
| 1:E:155:GLY:C    | 1:F:86:ARG:HH22  | 1.96                     | 0.72              |
| 1:F:12:ILE:HD13  | 1:F:23:GLN:HE21  | 1.51                     | 0.72              |
| 1:F:168:GLY:O    | 1:F:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:Q:72:ASP:OD1   | 2:X:67:ARG:NH2   | 2.22                     | 0.72              |
| 1:Q:168:GLY:O    | 1:Q:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:T:108:ASN:HB2  | 2:2:70:ARG:CG    | 2.11                     | 0.72              |
| 2:V:53:GLN:O     | 2:V:56:VAL:HG12  | 1.89                     | 0.72              |
| 2:1:18:ARG:HE    | 2:1:30:ASN:HD22  | 1.37                     | 0.72              |
| 1:D:108:ASN:CB   | 2:L:70:ARG:CG    | 2.66                     | 0.72              |
| 1:D:177:GLU:OE2  | 1:E:57:ARG:N     | 2.22                     | 0.72              |
| 1:P:101:VAL:HG21 | 2:W:58:TYR:HD1   | 1.24                     | 0.72              |
| 1:S:103:TYR:O    | 2:1:81:THR:CB    | 2.38                     | 0.72              |
| 1:C:78:THR:HG21  | 1:C:85:ALA:HB1   | 1.70                     | 0.72              |
| 1:D:155:GLY:O    | 1:E:86:ARG:CZ    | 2.36                     | 0.72              |
| 2:L:20:VAL:HG13  | 2:L:28:HIS:HB2   | 1.71                     | 0.72              |
| 2:N:62:GLU:HG2   | 2:N:82:LEU:HD21  | 1.69                     | 0.72              |
| 1:Q:12:ILE:HD13  | 1:Q:23:GLN:HE21  | 1.51                     | 0.72              |
| 1:Q:101:VAL:HG23 | 2:X:58:TYR:CD1   | 2.15                     | 0.72              |
| 1:Q:104:GLY:HA3  | 2:Y:81:THR:HG21  | 1.70                     | 0.72              |
| 1:Q:108:ASN:HD22 | 2:Y:70:ARG:HB3   | 1.54                     | 0.72              |
| 2:W:38:ASP:HB3   | 2:W:41:THR:CG2   | 2.18                     | 0.72              |
| 1:E:168:GLY:O    | 1:E:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:F:12:ILE:HD12  | 1:F:23:GLN:CG    | 1.75                     | 0.72              |
| 2:M:18:ARG:HE    | 2:M:30:ASN:HD22  | 1.37                     | 0.72              |
| 1:Q:108:ASN:ND2  | 2:Y:70:ARG:CB    | 2.50                     | 0.72              |
| 1:S:168:GLY:O    | 1:S:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:A:168:GLY:O    | 1:A:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:B:107:VAL:HG11 | 2:J:66:TYR:HH    | 1.51                     | 0.72              |
| 1:C:104:GLY:HA3  | 2:K:81:THR:HG21  | 1.70                     | 0.72              |
| 1:F:107:VAL:HG11 | 2:N:66:TYR:HH    | 1.54                     | 0.72              |
| 2:H:53:GLN:O     | 2:H:56:VAL:HG12  | 1.89                     | 0.72              |
| 1:P:168:GLY:O    | 1:P:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:R:111:ASN:ND2  | 2:Z:70:ARG:CZ    | 2.53                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:72:ASP:OD1   | 2:1:67:ARG:NH2   | 2.22                     | 0.72              |
| 2:1:123:ILE:HG12 | 2:1:124:TYR:HD1  | 1.53                     | 0.72              |
| 1:A:12:ILE:HD13  | 1:A:23:GLN:HE21  | 1.51                     | 0.72              |
| 1:R:111:ASN:CB   | 2:Z:70:ARG:NH1   | 2.52                     | 0.72              |
| 1:S:108:ASN:CB   | 2:1:70:ARG:HD3   | 2.18                     | 0.72              |
| 1:T:168:GLY:O    | 1:T:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:U:12:ILE:HD13  | 1:U:23:GLN:HE21  | 1.52                     | 0.72              |
| 1:U:13:THR:CB    | 1:U:14:VAL:CG2   | 2.62                     | 0.72              |
| 1:A:12:ILE:HD11  | 1:A:23:GLN:CB    | 1.31                     | 0.72              |
| 1:D:16:SER:O     | 1:E:26:TYR:HB3   | 1.90                     | 0.72              |
| 1:E:19:GLY:CA    | 1:F:30:ALA:HB2   | 2.20                     | 0.72              |
| 1:G:104:GLY:HA3  | 2:H:81:THR:HG21  | 1.71                     | 0.72              |
| 2:I:38:ASP:HB3   | 2:I:41:THR:CG2   | 2.19                     | 0.72              |
| 2:N:123:ILE:HD13 | 2:N:123:ILE:H    | 1.52                     | 0.72              |
| 1:O:12:ILE:HD11  | 1:O:23:GLN:CB    | 1.31                     | 0.72              |
| 1:R:108:ASN:CB   | 2:Z:70:ARG:CG    | 2.66                     | 0.72              |
| 1:U:78:THR:HG21  | 1:U:85:ALA:HB1   | 1.71                     | 0.72              |
| 1:B:12:ILE:HD13  | 1:B:23:GLN:HE21  | 1.51                     | 0.72              |
| 1:B:168:GLY:O    | 1:B:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:G:168:GLY:O    | 1:G:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:T:78:THR:HG21  | 1:T:85:ALA:HB1   | 1.70                     | 0.72              |
| 1:C:168:GLY:O    | 1:C:172:VAL:HG12 | 1.89                     | 0.72              |
| 1:E:103:TYR:O    | 2:M:81:THR:CB    | 2.38                     | 0.72              |
| 1:E:161:LYS:HD2  | 1:F:60:GLU:OE2   | 1.88                     | 0.72              |
| 1:S:12:ILE:HG13  | 1:S:23:GLN:HB2   | 1.66                     | 0.72              |
| 1:U:12:ILE:HD12  | 1:U:23:GLN:CG    | 1.75                     | 0.72              |
| 1:A:52:LYS:HZ1   | 1:A:62:ASN:HA    | 1.52                     | 0.71              |
| 1:C:107:VAL:CG2  | 2:K:66:TYR:OH    | 2.37                     | 0.71              |
| 1:D:12:ILE:HD11  | 1:D:23:GLN:CB    | 1.31                     | 0.71              |
| 1:T:161:LYS:CB   | 1:U:60:GLU:OE2   | 2.36                     | 0.71              |
| 1:U:168:GLY:O    | 1:U:172:VAL:HG12 | 1.89                     | 0.71              |
| 1:A:78:THR:HG21  | 1:A:85:ALA:HB1   | 1.70                     | 0.71              |
| 1:D:111:ASN:ND2  | 2:L:70:ARG:CZ    | 2.53                     | 0.71              |
| 1:S:78:THR:HG21  | 1:S:85:ALA:HB1   | 1.70                     | 0.71              |
| 1:T:178:ARG:C    | 1:U:57:ARG:HH22  | 1.92                     | 0.71              |
| 1:D:103:TYR:O    | 2:L:81:THR:CG2   | 2.39                     | 0.71              |
| 1:F:108:ASN:HB2  | 2:N:70:ARG:CG    | 2.11                     | 0.71              |
| 1:P:101:VAL:HG23 | 2:W:58:TYR:HD1   | 1.55                     | 0.71              |
| 1:A:12:ILE:HG13  | 1:A:23:GLN:HB2   | 1.67                     | 0.71              |
| 1:B:78:THR:HG21  | 1:B:85:ALA:HB1   | 1.70                     | 0.71              |
| 1:R:101:VAL:CG2  | 2:Y:58:TYR:CE1   | 2.68                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:13:THR:CB    | 1:B:14:VAL:CG2   | 2.62                     | 0.71              |
| 1:F:72:ASP:OD1   | 2:M:67:ARG:NH2   | 2.22                     | 0.71              |
| 2:I:103:GLY:HA2  | 2:I:178:ILE:HD11 | 1.71                     | 0.71              |
| 1:S:103:TYR:CE1  | 2:1:82:LEU:HD13  | 2.26                     | 0.71              |
| 1:D:17:PRO:O     | 1:E:29:GLU:HG3   | 1.90                     | 0.71              |
| 1:D:177:GLU:OE1  | 1:E:58:LEU:HD13  | 1.91                     | 0.71              |
| 2:L:7:THR:HB     | 2:L:123:ILE:O    | 1.90                     | 0.71              |
| 1:R:17:PRO:O     | 1:S:29:GLU:HG3   | 1.90                     | 0.71              |
| 1:R:168:GLY:O    | 1:R:172:VAL:HG12 | 1.89                     | 0.71              |
| 1:T:108:ASN:CG   | 2:2:70:ARG:CG    | 2.56                     | 0.71              |
| 1:G:101:VAL:CG2  | 2:N:58:TYR:HE1   | 2.02                     | 0.71              |
| 1:U:108:ASN:HB2  | 2:V:70:ARG:CG    | 2.09                     | 0.71              |
| 1:U:107:VAL:HG11 | 2:V:66:TYR:CZ    | 2.26                     | 0.71              |
| 2:Z:7:THR:HB     | 2:Z:123:ILE:O    | 1.90                     | 0.71              |
| 1:C:12:ILE:HD12  | 1:C:23:GLN:CG    | 1.75                     | 0.71              |
| 1:S:19:GLY:CA    | 1:T:30:ALA:HB2   | 2.20                     | 0.71              |
| 1:U:101:VAL:CG2  | 2:2:58:TYR:HE1   | 2.02                     | 0.71              |
| 1:A:178:ARG:HA   | 1:B:57:ARG:NH2   | 2.06                     | 0.70              |
| 1:B:13:THR:HB    | 1:B:14:VAL:CG2   | 2.16                     | 0.70              |
| 2:H:32:LYS:HE2   | 2:H:34:LEU:O     | 1.89                     | 0.70              |
| 1:O:58:LEU:HD21  | 1:U:173:VAL:O    | 1.89                     | 0.70              |
| 1:O:86:ARG:NH1   | 1:U:157:ILE:HG22 | 2.06                     | 0.70              |
| 1:Q:108:ASN:HB2  | 2:Y:70:ARG:CD    | 2.20                     | 0.70              |
| 1:S:12:ILE:HD11  | 1:S:23:GLN:CB    | 1.31                     | 0.70              |
| 1:U:104:GLY:HA3  | 2:V:81:THR:HG21  | 1.71                     | 0.70              |
| 1:A:86:ARG:NH1   | 1:G:157:ILE:HG22 | 2.06                     | 0.70              |
| 1:G:107:VAL:HG11 | 2:H:66:TYR:CZ    | 2.26                     | 0.70              |
| 1:U:104:GLY:CA   | 2:V:81:THR:HG21  | 2.21                     | 0.70              |
| 1:E:13:THR:HB    | 1:E:14:VAL:CG2   | 2.16                     | 0.70              |
| 1:E:103:TYR:CE1  | 2:M:82:LEU:HD22  | 2.26                     | 0.70              |
| 1:E:103:TYR:CE1  | 2:M:82:LEU:HD13  | 2.26                     | 0.70              |
| 2:N:38:ASP:HB3   | 2:N:41:THR:CG2   | 2.21                     | 0.70              |
| 2:X:53:GLN:O     | 2:X:56:VAL:HG12  | 1.91                     | 0.70              |
| 1:R:16:SER:O     | 1:S:26:TYR:HB3   | 1.90                     | 0.70              |
| 1:R:177:GLU:OE1  | 1:S:58:LEU:HD13  | 1.91                     | 0.70              |
| 1:A:108:ASN:HB2  | 2:I:70:ARG:HG2   | 1.66                     | 0.70              |
| 1:T:13:THR:HB    | 1:T:14:VAL:CG2   | 2.16                     | 0.70              |
| 2:V:59:MET:HE1   | 2:V:82:LEU:HD23  | 1.73                     | 0.70              |
| 1:C:108:ASN:ND2  | 2:K:70:ARG:CB    | 2.50                     | 0.70              |
| 1:G:13:THR:HB    | 1:G:14:VAL:CG2   | 2.16                     | 0.70              |
| 1:Q:12:ILE:HG13  | 1:Q:23:GLN:HB2   | 1.67                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:103:TYR:O    | 2:Z:81:THR:CG2   | 2.39                     | 0.70              |
| 1:S:101:VAL:HG22 | 2:Z:58:TYR:CD1   | 2.19                     | 0.70              |
| 1:A:58:LEU:CD2   | 1:G:177:GLU:HB2  | 2.19                     | 0.70              |
| 1:O:57:ARG:HH21  | 1:U:178:ARG:HA   | 1.32                     | 0.70              |
| 1:T:72:ASP:OD2   | 2:1:67:ARG:NH2   | 2.23                     | 0.70              |
| 1:U:12:ILE:HG13  | 1:U:23:GLN:HB2   | 1.67                     | 0.70              |
| 1:C:108:ASN:HB2  | 2:K:70:ARG:CG    | 2.12                     | 0.70              |
| 2:I:62:GLU:HG2   | 2:I:82:LEU:HD21  | 1.74                     | 0.70              |
| 1:P:108:ASN:HB3  | 2:X:70:ARG:HD3   | 1.72                     | 0.70              |
| 1:R:13:THR:HB    | 1:R:14:VAL:CG2   | 2.16                     | 0.70              |
| 1:U:103:TYR:CZ   | 2:V:82:LEU:HD13  | 2.27                     | 0.70              |
| 1:B:101:VAL:HG22 | 2:I:58:TYR:CE1   | 2.27                     | 0.69              |
| 2:V:38:ASP:HB3   | 2:V:41:THR:CG2   | 2.20                     | 0.69              |
| 2:W:62:GLU:HG2   | 2:W:82:LEU:HD21  | 1.74                     | 0.69              |
| 1:B:108:ASN:HB3  | 2:J:70:ARG:HD3   | 1.72                     | 0.69              |
| 1:B:173:VAL:O    | 1:C:58:LEU:CD2   | 2.39                     | 0.69              |
| 2:H:45:ILE:HG12  | 2:H:52:ALA:HB1   | 1.74                     | 0.69              |
| 1:P:173:VAL:O    | 1:Q:58:LEU:CD2   | 2.39                     | 0.69              |
| 2:Y:12:VAL:HG13  | 2:Y:178:ILE:HG23 | 1.74                     | 0.69              |
| 1:G:103:TYR:CZ   | 2:H:82:LEU:HD13  | 2.27                     | 0.69              |
| 2:W:103:GLY:HA2  | 2:W:178:ILE:CD1  | 2.22                     | 0.69              |
| 1:C:12:ILE:HG13  | 1:C:23:GLN:HB2   | 1.67                     | 0.69              |
| 1:G:104:GLY:CA   | 2:H:81:THR:HG21  | 2.21                     | 0.69              |
| 2:N:37:ILE:HD11  | 2:N:59:MET:HB3   | 1.73                     | 0.69              |
| 1:P:13:THR:HB    | 1:P:14:VAL:CG2   | 2.16                     | 0.69              |
| 1:D:184:LEU:HD23 | 1:D:189:ALA:HA   | 1.75                     | 0.69              |
| 1:Q:156:THR:HA   | 1:R:86:ARG:HH12  | 1.58                     | 0.69              |
| 1:G:101:VAL:HG22 | 2:N:58:TYR:CE1   | 2.27                     | 0.69              |
| 2:J:45:ILE:CG1   | 2:J:52:ALA:HB1   | 2.22                     | 0.69              |
| 2:K:7:THR:HB     | 2:K:123:ILE:O    | 1.93                     | 0.69              |
| 1:R:108:ASN:HD22 | 2:Z:70:ARG:CB    | 2.05                     | 0.69              |
| 1:T:103:TYR:O    | 2:2:81:THR:HG21  | 1.93                     | 0.69              |
| 2:M:141:GLN:NE2  | 2:1:141:GLN:NE2  | 2.41                     | 0.69              |
| 1:O:178:ARG:HA   | 1:P:57:ARG:NH2   | 2.06                     | 0.69              |
| 1:O:184:LEU:HD23 | 1:O:189:ALA:HA   | 1.75                     | 0.69              |
| 1:P:52:LYS:HZ1   | 1:P:62:ASN:HA    | 1.55                     | 0.69              |
| 1:Q:161:LYS:CD   | 1:R:60:GLU:OE2   | 2.41                     | 0.69              |
| 1:S:107:VAL:CG1  | 2:1:66:TYR:OH    | 2.41                     | 0.69              |
| 1:C:156:THR:HA   | 1:D:86:ARG:HH12  | 1.58                     | 0.69              |
| 1:D:161:LYS:CG   | 1:E:60:GLU:OE2   | 2.41                     | 0.69              |
| 1:E:101:VAL:HG21 | 2:L:58:TYR:CE1   | 2.26                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:72:ASP:OD2   | 2:M:67:ARG:NH2   | 2.23                     | 0.69              |
| 1:G:104:GLY:N    | 2:H:81:THR:HG21  | 2.08                     | 0.69              |
| 2:I:103:GLY:HA2  | 2:I:178:ILE:CD1  | 2.22                     | 0.69              |
| 2:J:53:GLN:O     | 2:J:56:VAL:HG12  | 1.91                     | 0.69              |
| 2:K:12:VAL:HG13  | 2:K:178:ILE:HG23 | 1.74                     | 0.69              |
| 1:O:178:ARG:O    | 1:P:57:ARG:NH2   | 2.26                     | 0.69              |
| 1:C:184:LEU:HD23 | 1:C:189:ALA:HA   | 1.75                     | 0.69              |
| 1:E:184:LEU:HD23 | 1:E:189:ALA:HA   | 1.75                     | 0.69              |
| 1:F:12:ILE:HG13  | 1:F:23:GLN:HB2   | 1.66                     | 0.69              |
| 2:H:59:MET:HE1   | 2:H:82:LEU:HD23  | 1.73                     | 0.69              |
| 1:P:12:ILE:HD12  | 1:P:23:GLN:CG    | 1.75                     | 0.69              |
| 1:P:101:VAL:HG22 | 2:W:58:TYR:CE1   | 2.27                     | 0.69              |
| 1:R:17:PRO:HA    | 1:S:26:TYR:CD1   | 2.28                     | 0.69              |
| 1:S:103:TYR:O    | 2:I:81:THR:HB    | 1.93                     | 0.69              |
| 1:R:161:LYS:CG   | 1:S:60:GLU:OE2   | 2.41                     | 0.68              |
| 1:U:184:LEU:HD23 | 1:U:189:ALA:HA   | 1.75                     | 0.68              |
| 2:V:45:ILE:HG12  | 2:V:52:ALA:HB1   | 1.74                     | 0.68              |
| 1:A:129:VAL:HG23 | 1:G:126:TYR:HA   | 1.74                     | 0.68              |
| 1:B:101:VAL:HG23 | 2:I:58:TYR:HD1   | 1.55                     | 0.68              |
| 1:G:101:VAL:HG22 | 2:N:58:TYR:HE1   | 1.57                     | 0.68              |
| 1:P:184:LEU:HD23 | 1:P:189:ALA:HA   | 1.75                     | 0.68              |
| 1:F:103:TYR:HE1  | 2:N:82:LEU:HD22  | 1.58                     | 0.68              |
| 2:L:193:GLU:HA   | 2:L:196:ILE:HD12 | 1.74                     | 0.68              |
| 2:I:3:THR:OG1    | 2:I:127:THR:HG22 | 1.93                     | 0.68              |
| 1:D:19:GLY:CA    | 1:E:30:ALA:HB2   | 2.24                     | 0.68              |
| 1:E:52:LYS:HZ1   | 1:E:62:ASN:HA    | 1.57                     | 0.68              |
| 1:S:177:GLU:OE1  | 1:T:58:LEU:CD1   | 2.41                     | 0.68              |
| 2:X:149:ASP:O    | 2:X:152:VAL:HG12 | 1.94                     | 0.68              |
| 1:D:108:ASN:HD22 | 2:L:70:ARG:CB    | 2.05                     | 0.68              |
| 1:E:15:PHE:CZ    | 1:F:130:ARG:NH1  | 2.62                     | 0.68              |
| 1:S:101:VAL:HG21 | 2:Z:58:TYR:CE1   | 2.26                     | 0.68              |
| 1:S:161:LYS:N    | 1:T:60:GLU:HG2   | 2.08                     | 0.68              |
| 2:Y:7:THR:HB     | 2:Y:123:ILE:O    | 1.93                     | 0.68              |
| 2:I:53:GLN:O     | 2:I:56:VAL:HG12  | 1.93                     | 0.68              |
| 2:2:37:ILE:HD11  | 2:2:59:MET:HB3   | 1.73                     | 0.68              |
| 1:A:178:ARG:O    | 1:B:57:ARG:NH2   | 2.26                     | 0.68              |
| 1:F:177:GLU:OE1  | 1:G:58:LEU:N     | 2.26                     | 0.68              |
| 2:J:149:ASP:O    | 2:J:152:VAL:HG12 | 1.94                     | 0.68              |
| 1:S:101:VAL:HG22 | 2:Z:58:TYR:HE1   | 1.59                     | 0.68              |
| 1:U:104:GLY:N    | 2:V:81:THR:HG21  | 2.08                     | 0.68              |
| 1:E:177:GLU:OE1  | 1:F:58:LEU:CD1   | 2.41                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:103:TYR:O    | 2:N:81:THR:HG21  | 1.93                     | 0.68              |
| 1:O:125:GLN:O    | 1:P:129:VAL:HG23 | 1.94                     | 0.68              |
| 1:O:177:GLU:OE1  | 1:P:57:ARG:N     | 2.27                     | 0.68              |
| 1:Q:125:GLN:O    | 1:R:129:VAL:HA   | 1.94                     | 0.68              |
| 1:E:161:LYS:N    | 1:F:60:GLU:HG2   | 2.08                     | 0.68              |
| 1:O:7:ALA:HB1    | 1:P:10:ARG:HH11  | 1.59                     | 0.68              |
| 1:Q:177:GLU:CD   | 1:R:58:LEU:H     | 2.01                     | 0.68              |
| 1:S:15:PHE:CZ    | 1:T:130:ARG:NH1  | 2.62                     | 0.68              |
| 2:X:18:ARG:HE    | 2:X:30:ASN:HD22  | 1.41                     | 0.68              |
| 2:Z:193:GLU:HA   | 2:Z:196:ILE:HD12 | 1.74                     | 0.68              |
| 1:D:17:PRO:HA    | 1:E:26:TYR:CD1   | 2.28                     | 0.68              |
| 1:E:103:TYR:O    | 2:M:81:THR:HB    | 1.93                     | 0.68              |
| 1:C:177:GLU:CD   | 1:D:58:LEU:H     | 2.01                     | 0.68              |
| 1:T:184:LEU:HD23 | 1:T:189:ALA:HA   | 1.75                     | 0.68              |
| 1:U:101:VAL:HG22 | 2:2:58:TYR:HE1   | 1.57                     | 0.68              |
| 1:A:7:ALA:HB1    | 1:B:10:ARG:HH11  | 1.59                     | 0.67              |
| 1:A:184:LEU:HD23 | 1:A:189:ALA:HA   | 1.75                     | 0.67              |
| 1:C:125:GLN:O    | 1:D:129:VAL:HA   | 1.94                     | 0.67              |
| 1:D:103:TYR:CE1  | 2:L:82:LEU:HD13  | 2.29                     | 0.67              |
| 1:E:12:ILE:HD12  | 1:E:23:GLN:CG    | 1.75                     | 0.67              |
| 1:F:184:LEU:HD23 | 1:F:189:ALA:HA   | 1.75                     | 0.67              |
| 1:O:129:VAL:HG23 | 1:U:126:TYR:HA   | 1.74                     | 0.67              |
| 1:P:177:GLU:N    | 1:Q:58:LEU:HD11  | 2.06                     | 0.67              |
| 1:Q:184:LEU:HD23 | 1:Q:189:ALA:HA   | 1.75                     | 0.67              |
| 1:C:161:LYS:CD   | 1:D:60:GLU:OE2   | 2.41                     | 0.67              |
| 2:M:3:THR:OG1    | 2:M:127:THR:HG22 | 1.93                     | 0.67              |
| 1:S:184:LEU:HD23 | 1:S:189:ALA:HA   | 1.75                     | 0.67              |
| 1:T:177:GLU:OE1  | 1:U:58:LEU:N     | 2.27                     | 0.67              |
| 1:A:125:GLN:O    | 1:B:129:VAL:HG23 | 1.94                     | 0.67              |
| 1:E:107:VAL:CG1  | 2:M:66:TYR:OH    | 2.41                     | 0.67              |
| 1:G:103:TYR:O    | 2:H:81:THR:HB    | 1.94                     | 0.67              |
| 1:G:108:ASN:ND2  | 2:H:70:ARG:HA    | 2.10                     | 0.67              |
| 1:G:184:LEU:HD23 | 1:G:189:ALA:HA   | 1.75                     | 0.67              |
| 2:H:59:MET:SD    | 2:H:83:LEU:HD13  | 2.35                     | 0.67              |
| 1:P:177:GLU:OE1  | 1:Q:58:LEU:CD1   | 2.40                     | 0.67              |
| 1:B:184:LEU:HD23 | 1:B:189:ALA:HA   | 1.75                     | 0.67              |
| 1:D:8:TYR:OH     | 1:E:9:ASP:OD2    | 2.12                     | 0.67              |
| 1:G:101:VAL:HG23 | 2:N:58:TYR:HD1   | 1.59                     | 0.67              |
| 1:D:177:GLU:OE1  | 1:E:57:ARG:C     | 2.37                     | 0.67              |
| 2:M:53:GLN:O     | 2:M:56:VAL:HG12  | 1.93                     | 0.67              |
| 1:O:177:GLU:HB2  | 1:P:58:LEU:CD2   | 2.23                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:177:GLU:OE1  | 1:S:57:ARG:C     | 2.37                     | 0.67              |
| 1:R:184:LEU:HD23 | 1:R:189:ALA:HA   | 1.75                     | 0.67              |
| 1:S:103:TYR:CE1  | 2:1:82:LEU:HD22  | 2.26                     | 0.67              |
| 1:R:19:GLY:CA    | 1:S:30:ALA:HB2   | 2.24                     | 0.67              |
| 1:A:177:GLU:OE1  | 1:B:57:ARG:N     | 2.27                     | 0.67              |
| 1:C:177:GLU:CB   | 1:D:58:LEU:CG    | 2.58                     | 0.67              |
| 2:X:45:ILE:CG1   | 2:X:52:ALA:HB1   | 2.22                     | 0.67              |
| 1:B:52:LYS:HZ1   | 1:B:62:ASN:HA    | 1.59                     | 0.67              |
| 2:I:133:PHE:CZ   | 2:I:165:ARG:HB3  | 2.30                     | 0.67              |
| 1:U:101:VAL:HG22 | 2:2:58:TYR:CE1   | 2.27                     | 0.67              |
| 1:B:177:GLU:N    | 1:C:58:LEU:HD11  | 2.06                     | 0.66              |
| 1:D:108:ASN:HB3  | 2:L:70:ARG:CG    | 2.25                     | 0.66              |
| 1:E:159:GLU:O    | 1:F:60:GLU:HB2   | 1.95                     | 0.66              |
| 1:R:103:TYR:CE1  | 2:Z:82:LEU:HD13  | 2.29                     | 0.66              |
| 1:R:108:ASN:HB3  | 2:Z:70:ARG:CG    | 2.25                     | 0.66              |
| 2:2:38:ASP:HB3   | 2:2:41:THR:CG2   | 2.21                     | 0.66              |
| 2:M:123:ILE:H    | 2:M:123:ILE:HD13 | 1.60                     | 0.66              |
| 1:T:103:TYR:HE1  | 2:2:82:LEU:HD22  | 1.58                     | 0.66              |
| 1:U:103:TYR:O    | 2:V:81:THR:HB    | 1.94                     | 0.66              |
| 1:A:177:GLU:HB2  | 1:B:58:LEU:CD2   | 2.23                     | 0.66              |
| 1:F:16:SER:O     | 1:G:26:TYR:HB3   | 1.95                     | 0.66              |
| 2:H:38:ASP:HB3   | 2:H:41:THR:CG2   | 2.20                     | 0.66              |
| 1:O:52:LYS:HZ1   | 1:O:62:ASN:HA    | 1.60                     | 0.66              |
| 1:O:58:LEU:HD13  | 1:U:177:GLU:CD   | 2.21                     | 0.66              |
| 1:R:8:TYR:OH     | 1:S:9:ASP:OD2    | 2.12                     | 0.66              |
| 1:T:16:SER:O     | 1:U:26:TYR:HB3   | 1.95                     | 0.66              |
| 1:T:61:GLN:O     | 1:T:64:ILE:HG22  | 1.96                     | 0.66              |
| 2:I:7:THR:HB     | 2:I:123:ILE:O    | 1.96                     | 0.66              |
| 2:L:59:MET:SD    | 2:L:83:LEU:HD13  | 2.36                     | 0.66              |
| 1:O:61:GLN:O     | 1:O:64:ILE:HG22  | 1.95                     | 0.66              |
| 1:R:111:ASN:ND2  | 2:Z:70:ARG:NH2   | 2.43                     | 0.66              |
| 1:S:159:GLU:O    | 1:T:60:GLU:HB2   | 1.96                     | 0.66              |
| 2:W:7:THR:HB     | 2:W:123:ILE:O    | 1.96                     | 0.66              |
| 2:W:133:PHE:CZ   | 2:W:165:ARG:HB3  | 2.30                     | 0.66              |
| 1:A:108:ASN:HB3  | 2:I:70:ARG:CD    | 2.24                     | 0.66              |
| 1:C:21:LEU:CD1   | 1:D:130:ARG:CD   | 2.72                     | 0.66              |
| 2:V:59:MET:SD    | 2:V:83:LEU:HD13  | 2.35                     | 0.66              |
| 1:C:61:GLN:O     | 1:C:64:ILE:HG22  | 1.95                     | 0.66              |
| 1:C:107:VAL:HG11 | 2:K:66:TYR:HH    | 1.61                     | 0.66              |
| 1:C:198:LYS:O    | 1:C:202:GLU:HB2  | 1.96                     | 0.66              |
| 1:O:108:ASN:HB3  | 2:W:70:ARG:CD    | 2.24                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:198:LYS:O    | 1:U:202:GLU:HB2  | 1.96                     | 0.66              |
| 2:Z:43:MET:HE2   | 2:Z:56:VAL:HG23  | 1.78                     | 0.66              |
| 1:D:61:GLN:O     | 1:D:64:ILE:HG22  | 1.96                     | 0.66              |
| 2:J:18:ARG:HE    | 2:J:30:ASN:HD22  | 1.41                     | 0.66              |
| 1:P:21:LEU:HD11  | 1:Q:130:ARG:CD   | 2.26                     | 0.66              |
| 1:R:108:ASN:HD22 | 2:Z:70:ARG:CG    | 2.06                     | 0.66              |
| 1:U:108:ASN:ND2  | 2:V:70:ARG:HA    | 2.10                     | 0.66              |
| 2:X:2:THR:HG22   | 2:X:169:SER:OG   | 1.96                     | 0.66              |
| 2:X:75:PRO:O     | 2:X:78:ALA:HB3   | 1.96                     | 0.66              |
| 1:B:61:GLN:O     | 1:B:64:ILE:HG22  | 1.95                     | 0.66              |
| 1:C:15:PHE:HB2   | 1:D:23:GLN:HE22  | 1.59                     | 0.66              |
| 2:M:164:GLN:NE2  | 2:Z:29:LYS:NZ    | 2.44                     | 0.66              |
| 1:O:57:ARG:CB    | 1:U:177:GLU:OE1  | 2.44                     | 0.66              |
| 1:U:61:GLN:O     | 1:U:64:ILE:HG22  | 1.95                     | 0.66              |
| 2:Z:59:MET:SD    | 2:Z:83:LEU:HD13  | 2.36                     | 0.66              |
| 1:A:61:GLN:O     | 1:A:64:ILE:HG22  | 1.95                     | 0.66              |
| 1:A:177:GLU:OE1  | 1:B:58:LEU:CD1   | 2.38                     | 0.66              |
| 1:B:177:GLU:OE1  | 1:C:58:LEU:CD1   | 2.40                     | 0.66              |
| 1:O:198:LYS:O    | 1:O:202:GLU:HB2  | 1.96                     | 0.66              |
| 1:Q:61:GLN:O     | 1:Q:64:ILE:HG22  | 1.95                     | 0.66              |
| 1:Q:177:GLU:O    | 1:R:57:ARG:CZ    | 2.43                     | 0.66              |
| 1:T:72:ASP:CG    | 2:1:67:ARG:NH2   | 2.54                     | 0.66              |
| 1:A:198:LYS:O    | 1:A:202:GLU:HB2  | 1.96                     | 0.66              |
| 1:E:61:GLN:O     | 1:E:64:ILE:HG22  | 1.95                     | 0.66              |
| 1:F:72:ASP:CG    | 2:M:67:ARG:NH2   | 2.54                     | 0.66              |
| 1:G:198:LYS:O    | 1:G:202:GLU:HB2  | 1.96                     | 0.66              |
| 2:J:2:THR:HG22   | 2:J:169:SER:OG   | 1.96                     | 0.66              |
| 1:R:61:GLN:O     | 1:R:64:ILE:HG22  | 1.96                     | 0.66              |
| 1:R:198:LYS:O    | 1:R:202:GLU:HB2  | 1.96                     | 0.66              |
| 1:U:52:LYS:HZ1   | 1:U:62:ASN:HA    | 1.61                     | 0.66              |
| 1:C:108:ASN:HB2  | 2:K:70:ARG:CD    | 2.20                     | 0.65              |
| 1:Q:15:PHE:HB2   | 1:R:23:GLN:HE22  | 1.59                     | 0.65              |
| 1:S:61:GLN:O     | 1:S:64:ILE:HG22  | 1.95                     | 0.65              |
| 2:1:123:ILE:HD13 | 2:1:123:ILE:H    | 1.60                     | 0.65              |
| 1:R:52:LYS:HZ3   | 1:R:62:ASN:HA    | 1.59                     | 0.65              |
| 1:A:57:ARG:CZ    | 1:G:178:ARG:HA   | 2.26                     | 0.65              |
| 1:B:198:LYS:O    | 1:B:202:GLU:HB2  | 1.96                     | 0.65              |
| 1:C:177:GLU:O    | 1:D:57:ARG:CZ    | 2.43                     | 0.65              |
| 2:L:123:ILE:HG12 | 2:L:124:TYR:HD1  | 1.61                     | 0.65              |
| 2:M:124:TYR:CD2  | 2:M:138:LEU:HD23 | 2.31                     | 0.65              |
| 1:O:57:ARG:CZ    | 1:U:178:ARG:HA   | 2.27                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:198:LYS:O    | 1:S:202:GLU:HB2  | 1.96                     | 0.65              |
| 2:Y:28:HIS:CD2   | 2:Z:120:VAL:HG11 | 2.31                     | 0.65              |
| 1:A:23:GLN:HE22  | 1:G:15:PHE:HB2   | 1.62                     | 0.65              |
| 1:D:198:LYS:O    | 1:D:202:GLU:HB2  | 1.96                     | 0.65              |
| 2:L:29:LYS:NZ    | 2:1:164:GLN:NE2  | 2.45                     | 0.65              |
| 2:M:164:GLN:NE2  | 2:Z:29:LYS:HZ1   | 1.93                     | 0.65              |
| 1:G:61:GLN:O     | 1:G:64:ILE:HG22  | 1.95                     | 0.65              |
| 1:Q:177:GLU:CG   | 1:R:58:LEU:HD22  | 2.25                     | 0.65              |
| 2:W:45:ILE:HG12  | 2:W:52:ALA:HB1   | 1.79                     | 0.65              |
| 1:O:108:ASN:HB3  | 2:W:70:ARG:HD3   | 1.79                     | 0.65              |
| 1:P:61:GLN:O     | 1:P:64:ILE:HG22  | 1.96                     | 0.65              |
| 2:Z:123:ILE:HG12 | 2:Z:124:TYR:HD1  | 1.62                     | 0.65              |
| 1:A:177:GLU:N    | 1:B:58:LEU:CD2   | 2.49                     | 0.65              |
| 1:D:111:ASN:ND2  | 2:L:70:ARG:NH2   | 2.43                     | 0.65              |
| 1:E:198:LYS:O    | 1:E:202:GLU:HB2  | 1.96                     | 0.65              |
| 1:F:124:THR:CG2  | 1:G:130:ARG:HH21 | 2.08                     | 0.65              |
| 2:K:28:HIS:CD2   | 2:L:120:VAL:HG11 | 2.31                     | 0.65              |
| 1:Q:198:LYS:O    | 1:Q:202:GLU:HB2  | 1.96                     | 0.65              |
| 1:T:198:LYS:O    | 1:T:202:GLU:HB2  | 1.96                     | 0.65              |
| 1:O:26:TYR:HB3   | 1:U:16:SER:O     | 1.97                     | 0.65              |
| 1:O:101:VAL:HG21 | 2:V:58:TYR:HD1   | 1.40                     | 0.65              |
| 1:T:103:TYR:O    | 2:2:81:THR:CG2   | 2.45                     | 0.65              |
| 1:T:107:VAL:HG21 | 2:2:66:TYR:OH    | 1.97                     | 0.65              |
| 1:T:124:THR:CG2  | 1:U:130:ARG:HH21 | 2.08                     | 0.65              |
| 2:W:123:ILE:HD13 | 2:W:123:ILE:H    | 1.62                     | 0.65              |
| 1:A:57:ARG:CB    | 1:G:177:GLU:OE1  | 2.44                     | 0.65              |
| 1:F:61:GLN:O     | 1:F:64:ILE:HG22  | 1.95                     | 0.65              |
| 1:O:23:GLN:HE22  | 1:U:15:PHE:HB2   | 1.62                     | 0.65              |
| 1:B:108:ASN:HD22 | 2:J:70:ARG:CB    | 2.10                     | 0.65              |
| 1:F:17:PRO:HA    | 1:G:26:TYR:CD1   | 2.32                     | 0.65              |
| 1:F:103:TYR:O    | 2:N:81:THR:CG2   | 2.45                     | 0.65              |
| 2:I:124:TYR:CD2  | 2:I:138:LEU:HD23 | 2.32                     | 0.65              |
| 1:Q:21:LEU:CD1   | 1:R:130:ARG:CD   | 2.72                     | 0.65              |
| 2:W:20:VAL:HG13  | 2:W:28:HIS:HB2   | 1.79                     | 0.65              |
| 1:C:52:LYS:HZ1   | 1:C:62:ASN:HA    | 1.62                     | 0.64              |
| 1:F:198:LYS:O    | 1:F:202:GLU:HB2  | 1.96                     | 0.64              |
| 1:O:177:GLU:C    | 1:P:58:LEU:HD11  | 2.22                     | 0.64              |
| 1:P:198:LYS:O    | 1:P:202:GLU:HB2  | 1.96                     | 0.64              |
| 1:A:58:LEU:HD13  | 1:G:177:GLU:CD   | 2.21                     | 0.64              |
| 2:I:20:VAL:HG13  | 2:I:28:HIS:HB2   | 1.79                     | 0.64              |
| 1:R:108:ASN:HB3  | 2:Z:70:ARG:HG2   | 1.74                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:15:PHE:CE2   | 1:U:131:PRO:O    | 2.51                     | 0.64              |
| 1:F:15:PHE:CE2   | 1:G:131:PRO:O    | 2.51                     | 0.64              |
| 1:G:52:LYS:HZ3   | 1:G:62:ASN:HA    | 1.60                     | 0.64              |
| 2:N:123:ILE:HG12 | 2:N:124:TYR:HD2  | 1.61                     | 0.64              |
| 1:T:155:GLY:C    | 1:U:86:ARG:HH22  | 2.00                     | 0.64              |
| 2:Y:123:ILE:HG12 | 2:Y:124:TYR:CD1  | 2.31                     | 0.64              |
| 2:1:49:VAL:HG23  | 2:1:50:GLY:H     | 1.63                     | 0.64              |
| 2:1:124:TYR:CD2  | 2:1:138:LEU:HD23 | 2.31                     | 0.64              |
| 2:J:75:PRO:O     | 2:J:78:ALA:HB3   | 1.96                     | 0.64              |
| 2:L:124:TYR:CD2  | 2:L:138:LEU:HD23 | 2.33                     | 0.64              |
| 1:U:101:VAL:HG23 | 2:2:58:TYR:HD1   | 1.59                     | 0.64              |
| 2:W:124:TYR:CD2  | 2:W:138:LEU:HD23 | 2.32                     | 0.64              |
| 1:B:21:LEU:HD11  | 1:C:130:ARG:CD   | 2.26                     | 0.64              |
| 1:D:156:THR:HA   | 1:E:86:ARG:HH12  | 1.62                     | 0.64              |
| 2:I:45:ILE:HG12  | 2:I:52:ALA:HB1   | 1.79                     | 0.64              |
| 1:O:177:GLU:OE1  | 1:P:58:LEU:CD1   | 2.38                     | 0.64              |
| 2:V:124:TYR:CD2  | 2:V:138:LEU:HD23 | 2.33                     | 0.64              |
| 2:M:123:ILE:HG12 | 2:M:124:TYR:CD1  | 2.33                     | 0.64              |
| 2:1:45:ILE:CG1   | 2:1:52:ALA:HB1   | 2.26                     | 0.64              |
| 1:A:26:TYR:HB3   | 1:G:16:SER:O     | 1.97                     | 0.64              |
| 1:A:108:ASN:HB3  | 2:I:70:ARG:HD3   | 1.79                     | 0.64              |
| 2:L:18:ARG:HB2   | 2:L:31:GLY:O     | 1.98                     | 0.64              |
| 1:R:100:LYS:NZ   | 2:Y:64:GLU:OE1   | 2.28                     | 0.64              |
| 2:V:55:LEU:HD21  | 2:V:87:LEU:HD11  | 1.80                     | 0.64              |
| 2:2:123:ILE:HG12 | 2:2:124:TYR:HD2  | 1.61                     | 0.64              |
| 1:A:177:GLU:C    | 1:B:57:ARG:NH2   | 2.30                     | 0.64              |
| 1:D:52:LYS:HZ1   | 1:D:62:ASN:HA    | 1.63                     | 0.64              |
| 2:K:3:THR:HB     | 2:K:16:THR:HG22  | 1.80                     | 0.64              |
| 1:S:19:GLY:HA3   | 1:T:30:ALA:HB2   | 1.80                     | 0.64              |
| 2:1:123:ILE:HG12 | 2:1:124:TYR:CD1  | 2.33                     | 0.64              |
| 2:I:123:ILE:HD13 | 2:I:123:ILE:H    | 1.62                     | 0.64              |
| 2:L:29:LYS:HZ1   | 2:1:164:GLN:NE2  | 1.96                     | 0.64              |
| 1:S:72:ASP:OD1   | 2:Z:67:ARG:NH2   | 2.31                     | 0.64              |
| 1:T:17:PRO:HA    | 1:U:26:TYR:CD1   | 2.32                     | 0.64              |
| 1:E:72:ASP:OD1   | 2:L:67:ARG:NH2   | 2.31                     | 0.63              |
| 1:E:177:GLU:CD   | 1:F:58:LEU:H     | 2.06                     | 0.63              |
| 1:Q:177:GLU:HB2  | 1:R:58:LEU:HD22  | 0.63                     | 0.63              |
| 1:R:156:THR:HA   | 1:S:86:ARG:HH12  | 1.62                     | 0.63              |
| 1:F:52:LYS:HZ1   | 1:F:62:ASN:HA    | 1.61                     | 0.63              |
| 2:L:43:MET:HE2   | 2:L:56:VAL:HG23  | 1.78                     | 0.63              |
| 1:O:97:GLN:OE1   | 2:V:61:ALA:CB    | 2.46                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:15:PHE:CZ    | 1:Q:130:ARG:NH1  | 2.66                     | 0.63              |
| 2:V:123:ILE:HD13 | 2:V:123:ILE:H    | 1.62                     | 0.63              |
| 1:A:23:GLN:HE22  | 1:G:15:PHE:H     | 1.46                     | 0.63              |
| 2:I:59:MET:HE1   | 2:I:82:LEU:HD23  | 1.79                     | 0.63              |
| 2:I:123:ILE:HG12 | 2:I:124:TYR:CD1  | 2.32                     | 0.63              |
| 2:M:141:GLN:NE2  | 2:1:141:GLN:HE21 | 1.96                     | 0.63              |
| 1:O:23:GLN:HE22  | 1:U:15:PHE:H     | 1.46                     | 0.63              |
| 1:P:108:ASN:HD22 | 2:X:70:ARG:CB    | 2.10                     | 0.63              |
| 1:Q:52:LYS:HZ1   | 1:Q:62:ASN:HA    | 1.61                     | 0.63              |
| 1:S:177:GLU:CD   | 1:T:58:LEU:H     | 2.06                     | 0.63              |
| 2:W:59:MET:HE1   | 2:W:82:LEU:HD23  | 1.79                     | 0.63              |
| 2:Z:37:ILE:HD11  | 2:Z:59:MET:HB3   | 1.79                     | 0.63              |
| 1:E:19:GLY:HA3   | 1:F:30:ALA:HB2   | 1.80                     | 0.63              |
| 2:J:103:GLY:HA2  | 2:J:178:ILE:HD13 | 1.81                     | 0.63              |
| 2:K:193:GLU:HA   | 2:K:196:ILE:HD12 | 1.81                     | 0.63              |
| 2:M:45:ILE:CG1   | 2:M:52:ALA:HB1   | 2.26                     | 0.63              |
| 2:M:49:VAL:HG23  | 2:M:50:GLY:H     | 1.62                     | 0.63              |
| 2:Y:193:GLU:HA   | 2:Y:196:ILE:HD12 | 1.81                     | 0.63              |
| 2:Z:18:ARG:HB2   | 2:Z:31:GLY:O     | 1.98                     | 0.63              |
| 2:Z:124:TYR:CD2  | 2:Z:138:LEU:HD23 | 2.33                     | 0.63              |
| 1:A:177:GLU:C    | 1:B:58:LEU:HD11  | 2.22                     | 0.63              |
| 1:B:15:PHE:CZ    | 1:C:130:ARG:NH1  | 2.66                     | 0.63              |
| 1:G:103:TYR:O    | 2:H:81:THR:CG2   | 2.47                     | 0.63              |
| 2:H:167:SER:HB2  | 2:X:167:SER:HB2  | 1.79                     | 0.63              |
| 2:N:179:THR:HG23 | 2:N:182:ASP:H    | 1.63                     | 0.63              |
| 2:X:103:GLY:HA2  | 2:X:178:ILE:HD13 | 1.81                     | 0.63              |
| 1:D:100:LYS:NZ   | 2:K:64:GLU:OE1   | 2.28                     | 0.63              |
| 1:E:160:TYR:C    | 1:F:60:GLU:HG3   | 2.24                     | 0.63              |
| 1:F:107:VAL:HG21 | 2:N:66:TYR:OH    | 1.97                     | 0.63              |
| 1:C:104:GLY:CA   | 2:K:81:THR:HG21  | 2.28                     | 0.63              |
| 1:C:177:GLU:HB2  | 1:D:58:LEU:HD22  | 0.63                     | 0.63              |
| 2:H:124:TYR:CD2  | 2:H:138:LEU:HD23 | 2.33                     | 0.63              |
| 1:S:160:TYR:C    | 1:T:60:GLU:HG3   | 2.24                     | 0.63              |
| 1:C:52:LYS:HZ3   | 1:C:62:ASN:HA    | 1.62                     | 0.63              |
| 1:B:177:GLU:OE2  | 1:C:56:SER:CA    | 2.47                     | 0.63              |
| 1:C:177:GLU:CG   | 1:D:58:LEU:HD22  | 2.25                     | 0.63              |
| 1:C:178:ARG:C    | 1:D:57:ARG:HH22  | 2.07                     | 0.63              |
| 2:H:123:ILE:HD13 | 2:H:123:ILE:H    | 1.62                     | 0.63              |
| 2:N:133:PHE:CZ   | 2:N:165:ARG:HB3  | 2.34                     | 0.63              |
| 1:U:103:TYR:O    | 2:V:81:THR:CG2   | 2.47                     | 0.63              |
| 1:A:26:TYR:CD1   | 1:G:17:PRO:HA    | 2.34                     | 0.62              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:103:TYR:HE1  | 2:H:82:LEU:HD22 | 1.64                     | 0.62              |
| 2:J:103:GLY:HA2  | 2:J:178:ILE:CD1 | 2.29                     | 0.62              |
| 1:O:161:LYS:CB   | 1:P:60:GLU:OE2  | 2.45                     | 0.62              |
| 1:R:173:VAL:O    | 1:S:58:LEU:HD22 | 1.99                     | 0.62              |
| 1:U:103:TYR:HE1  | 2:V:82:LEU:HD22 | 1.64                     | 0.62              |
| 2:2:133:PHE:CZ   | 2:2:165:ARG:HB3 | 2.34                     | 0.62              |
| 1:B:177:GLU:CA   | 1:C:58:LEU:HD13 | 2.08                     | 0.62              |
| 1:D:103:TYR:HE1  | 2:L:82:LEU:HD22 | 1.64                     | 0.62              |
| 2:L:37:ILE:HD11  | 2:L:59:MET:HB3  | 1.79                     | 0.62              |
| 1:O:177:GLU:HA   | 1:P:58:LEU:CD2  | 2.28                     | 0.62              |
| 1:E:101:VAL:HG22 | 2:L:58:TYR:HE1  | 1.59                     | 0.62              |
| 1:Q:104:GLY:CA   | 2:Y:81:THR:HG21 | 2.28                     | 0.62              |
| 2:Z:15:ALA:HB2   | 2:Z:175:VAL:HB  | 1.82                     | 0.62              |
| 1:E:177:GLU:CB   | 1:F:58:LEU:CD2  | 2.70                     | 0.62              |
| 2:K:123:ILE:HD13 | 2:K:123:ILE:H   | 1.63                     | 0.62              |
| 1:T:14:VAL:H     | 1:U:130:ARG:HB2 | 1.64                     | 0.62              |
| 2:W:1:THR:H3     | 2:W:129:SER:HB3 | 1.65                     | 0.62              |
| 1:A:129:VAL:CG2  | 1:G:125:GLN:O   | 2.48                     | 0.62              |
| 1:C:121:GLN:O    | 1:C:124:THR:HB  | 2.00                     | 0.62              |
| 1:T:17:PRO:HA    | 1:U:26:TYR:CG   | 2.35                     | 0.62              |
| 1:C:97:GLN:OE1   | 2:J:61:ALA:CB   | 2.48                     | 0.62              |
| 1:D:52:LYS:HZ3   | 1:D:62:ASN:HA   | 1.61                     | 0.62              |
| 1:D:108:ASN:HD22 | 2:L:70:ARG:CG   | 2.06                     | 0.62              |
| 1:E:107:VAL:HG21 | 2:M:66:TYR:OH   | 1.99                     | 0.62              |
| 1:F:17:PRO:HA    | 1:G:26:TYR:CG   | 2.34                     | 0.62              |
| 2:I:76:ILE:O     | 2:I:79:VAL:HG12 | 2.00                     | 0.62              |
| 1:O:26:TYR:CD1   | 1:U:17:PRO:HA   | 2.34                     | 0.62              |
| 1:Q:121:GLN:O    | 1:Q:124:THR:HB  | 2.00                     | 0.62              |
| 1:U:121:GLN:O    | 1:U:124:THR:HB  | 2.00                     | 0.62              |
| 2:M:141:GLN:HE21 | 2:1:141:GLN:NE2 | 1.97                     | 0.62              |
| 1:Q:178:ARG:C    | 1:R:57:ARG:HH22 | 2.07                     | 0.62              |
| 2:Y:3:THR:HB     | 2:Y:16:THR:HG22 | 1.80                     | 0.62              |
| 1:F:52:LYS:HZ3   | 1:F:62:ASN:HA   | 1.64                     | 0.62              |
| 2:H:2:THR:HG22   | 2:H:169:SER:OG  | 2.00                     | 0.62              |
| 2:H:55:LEU:HD21  | 2:H:87:LEU:HD11 | 1.80                     | 0.62              |
| 2:J:167:SER:HB2  | 2:V:167:SER:HB2 | 1.82                     | 0.62              |
| 1:Q:52:LYS:HZ3   | 1:Q:62:ASN:HA   | 1.63                     | 0.62              |
| 1:T:121:GLN:O    | 1:T:124:THR:HB  | 2.00                     | 0.62              |
| 2:V:43:MET:CE    | 2:V:56:VAL:HG23 | 2.29                     | 0.62              |
| 2:X:103:GLY:HA2  | 2:X:178:ILE:CD1 | 2.29                     | 0.62              |
| 1:B:121:GLN:O    | 1:B:124:THR:HB  | 2.00                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:125:GLN:C    | 1:D:129:VAL:HG23 | 2.25                     | 0.62              |
| 1:F:121:GLN:O    | 1:F:124:THR:HB   | 2.00                     | 0.62              |
| 1:P:177:GLU:OE2  | 1:Q:56:SER:CA    | 2.47                     | 0.62              |
| 1:P:177:GLU:CB   | 1:Q:58:LEU:CD1   | 2.77                     | 0.62              |
| 2:1:149:ASP:O    | 2:1:152:VAL:HG12 | 1.99                     | 0.62              |
| 1:F:155:GLY:C    | 1:G:86:ARG:HH22  | 2.00                     | 0.62              |
| 2:H:123:ILE:HG12 | 2:H:124:TYR:CD1  | 2.33                     | 0.62              |
| 1:P:121:GLN:O    | 1:P:124:THR:HB   | 2.00                     | 0.62              |
| 1:Q:97:GLN:OE1   | 2:X:61:ALA:CB    | 2.48                     | 0.62              |
| 1:R:121:GLN:O    | 1:R:124:THR:HB   | 2.00                     | 0.62              |
| 2:2:179:THR:HG23 | 2:2:182:ASP:H    | 1.63                     | 0.62              |
| 2:M:149:ASP:O    | 2:M:152:VAL:HG12 | 1.99                     | 0.61              |
| 1:U:52:LYS:HZ3   | 1:U:62:ASN:HA    | 1.63                     | 0.61              |
| 1:D:61:GLN:OE1   | 1:D:62:ASN:HB3   | 2.00                     | 0.61              |
| 1:G:12:ILE:HA    | 1:G:23:GLN:CG    | 2.21                     | 0.61              |
| 1:S:121:GLN:O    | 1:S:124:THR:HB   | 2.00                     | 0.61              |
| 1:G:121:GLN:O    | 1:G:124:THR:HB   | 2.00                     | 0.61              |
| 2:K:38:ASP:HB3   | 2:K:41:THR:CG2   | 2.26                     | 0.61              |
| 1:O:102:THR:C    | 2:W:85:ASN:OD1   | 2.42                     | 0.61              |
| 1:P:88:LEU:HD21  | 1:P:120:MET:SD   | 2.41                     | 0.61              |
| 1:S:107:VAL:HG21 | 2:1:66:TYR:OH    | 1.99                     | 0.61              |
| 2:V:2:THR:HG22   | 2:V:169:SER:OG   | 2.00                     | 0.61              |
| 2:W:76:ILE:O     | 2:W:79:VAL:HG12  | 1.99                     | 0.61              |
| 1:A:88:LEU:HD21  | 1:A:120:MET:SD   | 2.41                     | 0.61              |
| 1:E:121:GLN:O    | 1:E:124:THR:HB   | 2.00                     | 0.61              |
| 1:F:14:VAL:H     | 1:G:130:ARG:HB2  | 1.64                     | 0.61              |
| 1:O:49:ILE:HD12  | 1:O:211:GLU:O    | 2.01                     | 0.61              |
| 1:P:49:ILE:HD12  | 1:P:211:GLU:O    | 2.01                     | 0.61              |
| 1:P:177:GLU:CB   | 1:Q:58:LEU:HD13  | 2.30                     | 0.61              |
| 1:Q:15:PHE:CZ    | 1:R:130:ARG:NH1  | 2.68                     | 0.61              |
| 1:B:88:LEU:HD21  | 1:B:120:MET:SD   | 2.41                     | 0.61              |
| 1:C:49:ILE:HD12  | 1:C:211:GLU:O    | 2.01                     | 0.61              |
| 2:N:76:ILE:O     | 2:N:79:VAL:HG12  | 2.00                     | 0.61              |
| 1:O:88:LEU:HD21  | 1:O:120:MET:SD   | 2.41                     | 0.61              |
| 1:Q:49:ILE:HD12  | 1:Q:211:GLU:O    | 2.01                     | 0.61              |
| 1:Q:88:LEU:HD21  | 1:Q:120:MET:SD   | 2.41                     | 0.61              |
| 2:Y:123:ILE:HD13 | 2:Y:123:ILE:H    | 1.63                     | 0.61              |
| 1:A:121:GLN:O    | 1:A:124:THR:HB   | 2.00                     | 0.61              |
| 1:C:15:PHE:CZ    | 1:D:130:ARG:NH1  | 2.68                     | 0.61              |
| 1:C:88:LEU:HD21  | 1:C:120:MET:SD   | 2.41                     | 0.61              |
| 1:D:121:GLN:O    | 1:D:124:THR:HB   | 2.00                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:88:LEU:HD21  | 1:E:120:MET:SD   | 2.41                     | 0.61              |
| 1:G:108:ASN:ND2  | 2:H:70:ARG:O     | 2.33                     | 0.61              |
| 2:K:123:ILE:HG12 | 2:K:124:TYR:CD1  | 2.31                     | 0.61              |
| 1:A:97:GLN:OE1   | 2:H:61:ALA:CB    | 2.46                     | 0.61              |
| 1:D:49:ILE:HD12  | 1:D:211:GLU:O    | 2.01                     | 0.61              |
| 1:F:88:LEU:HD21  | 1:F:120:MET:SD   | 2.41                     | 0.61              |
| 1:O:121:GLN:O    | 1:O:124:THR:HB   | 2.00                     | 0.61              |
| 1:S:49:ILE:HD12  | 1:S:211:GLU:O    | 2.01                     | 0.61              |
| 1:T:61:GLN:OE1   | 1:T:62:ASN:HB3   | 2.00                     | 0.61              |
| 1:U:88:LEU:HD21  | 1:U:120:MET:SD   | 2.41                     | 0.61              |
| 2:W:123:ILE:HG12 | 2:W:124:TYR:CD1  | 2.32                     | 0.61              |
| 1:A:49:ILE:HD12  | 1:A:211:GLU:O    | 2.01                     | 0.61              |
| 1:B:61:GLN:OE1   | 1:B:62:ASN:HB3   | 2.00                     | 0.61              |
| 1:D:88:LEU:HD21  | 1:D:120:MET:SD   | 2.41                     | 0.61              |
| 1:E:49:ILE:HD12  | 1:E:211:GLU:O    | 2.01                     | 0.61              |
| 1:F:61:GLN:OE1   | 1:F:62:ASN:HB3   | 2.00                     | 0.61              |
| 1:O:61:GLN:OE1   | 1:O:62:ASN:HB3   | 2.00                     | 0.61              |
| 1:S:88:LEU:HD21  | 1:S:120:MET:SD   | 2.41                     | 0.61              |
| 1:T:88:LEU:HD21  | 1:T:120:MET:SD   | 2.41                     | 0.61              |
| 1:U:49:ILE:HD12  | 1:U:211:GLU:O    | 2.01                     | 0.61              |
| 1:A:178:ARG:C    | 1:B:57:ARG:HH22  | 2.08                     | 0.61              |
| 1:E:61:GLN:OE1   | 1:E:62:ASN:HB3   | 2.00                     | 0.61              |
| 1:G:61:GLN:OE1   | 1:G:62:ASN:HB3   | 2.00                     | 0.61              |
| 2:L:15:ALA:HB2   | 2:L:175:VAL:HB   | 1.82                     | 0.61              |
| 2:N:3:THR:HB     | 2:N:16:THR:HG22  | 1.83                     | 0.61              |
| 1:O:129:VAL:CG2  | 1:U:125:GLN:O    | 2.48                     | 0.61              |
| 1:Q:12:ILE:HA    | 1:Q:23:GLN:CG    | 2.21                     | 0.61              |
| 1:R:103:TYR:HE1  | 2:Z:82:LEU:HD22  | 1.64                     | 0.61              |
| 1:U:108:ASN:ND2  | 2:V:70:ARG:O     | 2.33                     | 0.61              |
| 2:W:37:ILE:HD11  | 2:W:59:MET:HB3   | 1.82                     | 0.61              |
| 2:I:37:ILE:HD11  | 2:I:59:MET:HB3   | 1.83                     | 0.60              |
| 1:P:61:GLN:OE1   | 1:P:62:ASN:HB3   | 2.00                     | 0.60              |
| 1:Q:61:GLN:OE1   | 1:Q:62:ASN:HB3   | 2.00                     | 0.60              |
| 1:U:61:GLN:OE1   | 1:U:62:ASN:HB3   | 2.00                     | 0.60              |
| 2:L:3:THR:HB     | 2:L:16:THR:HG22  | 1.83                     | 0.60              |
| 1:R:49:ILE:HD12  | 1:R:211:GLU:O    | 2.01                     | 0.60              |
| 1:S:125:GLN:O    | 1:T:129:VAL:HG23 | 2.02                     | 0.60              |
| 1:C:178:ARG:HA   | 1:D:57:ARG:HH22  | 1.59                     | 0.60              |
| 1:F:49:ILE:HD12  | 1:F:211:GLU:O    | 2.01                     | 0.60              |
| 1:R:61:GLN:OE1   | 1:R:62:ASN:HB3   | 2.00                     | 0.60              |
| 2:Z:32:LYS:HE2   | 2:Z:34:LEU:O     | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:107:VAL:HG11 | 2:L:66:TYR:OH    | 2.01                     | 0.60              |
| 1:E:125:GLN:O    | 1:F:129:VAL:HG23 | 2.02                     | 0.60              |
| 1:E:160:TYR:C    | 1:F:60:GLU:CG    | 2.75                     | 0.60              |
| 2:H:43:MET:CE    | 2:H:56:VAL:HG23  | 2.30                     | 0.60              |
| 2:L:133:PHE:HE1  | 2:2:132:PRO:HA   | 1.65                     | 0.60              |
| 1:O:15:PHE:HB2   | 1:P:23:GLN:HE22  | 1.66                     | 0.60              |
| 1:R:12:ILE:HA    | 1:R:23:GLN:CG    | 2.21                     | 0.60              |
| 1:S:111:ASN:CG   | 2:1:70:ARG:NH1   | 2.60                     | 0.60              |
| 1:B:177:GLU:CB   | 1:C:58:LEU:CD1   | 2.77                     | 0.60              |
| 1:C:61:GLN:OE1   | 1:C:62:ASN:HB3   | 2.00                     | 0.60              |
| 1:F:108:ASN:HB2  | 2:N:70:ARG:CD    | 2.31                     | 0.60              |
| 1:G:49:ILE:HD12  | 1:G:211:GLU:O    | 2.01                     | 0.60              |
| 2:N:26:ILE:HD13  | 2:N:26:ILE:C     | 2.27                     | 0.60              |
| 1:R:28:ARG:O     | 1:R:31:VAL:HG22  | 2.02                     | 0.60              |
| 1:R:88:LEU:HD21  | 1:R:120:MET:SD   | 2.41                     | 0.60              |
| 2:2:76:ILE:O     | 2:2:79:VAL:HG12  | 2.00                     | 0.60              |
| 1:A:61:GLN:OE1   | 1:A:62:ASN:HB3   | 2.00                     | 0.60              |
| 1:B:161:LYS:N    | 1:C:60:GLU:HG2   | 2.16                     | 0.60              |
| 1:F:71:ASP:HA    | 2:M:68:LEU:HD21  | 1.82                     | 0.60              |
| 1:G:28:ARG:O     | 1:G:31:VAL:HG22  | 2.02                     | 0.60              |
| 1:G:52:LYS:HZ1   | 1:G:62:ASN:HA    | 1.65                     | 0.60              |
| 1:G:103:TYR:O    | 2:H:81:THR:HG21  | 2.02                     | 0.60              |
| 2:K:124:TYR:CD2  | 2:K:138:LEU:HD23 | 2.37                     | 0.60              |
| 1:O:52:LYS:HZ3   | 1:O:62:ASN:HA    | 1.65                     | 0.60              |
| 1:R:107:VAL:HG11 | 2:Z:66:TYR:OH    | 2.01                     | 0.60              |
| 1:B:177:GLU:CB   | 1:C:58:LEU:HD13  | 2.30                     | 0.60              |
| 1:S:28:ARG:O     | 1:S:31:VAL:HG22  | 2.02                     | 0.60              |
| 1:S:160:TYR:C    | 1:T:60:GLU:CG    | 2.75                     | 0.60              |
| 1:T:104:GLY:N    | 2:2:81:THR:HG21  | 2.17                     | 0.60              |
| 1:T:107:VAL:HG11 | 2:2:66:TYR:HH    | 1.66                     | 0.60              |
| 2:1:133:PHE:CZ   | 2:1:165:ARG:HB3  | 2.37                     | 0.60              |
| 1:E:108:ASN:HB3  | 2:M:70:ARG:HG2   | 1.76                     | 0.60              |
| 1:G:88:LEU:HD21  | 1:G:120:MET:SD   | 2.41                     | 0.60              |
| 1:R:52:LYS:HZ1   | 1:R:62:ASN:HA    | 1.66                     | 0.60              |
| 1:S:107:VAL:CG2  | 2:1:66:TYR:OH    | 2.50                     | 0.60              |
| 1:T:15:PHE:HB2   | 1:U:23:GLN:NE2   | 2.11                     | 0.60              |
| 1:T:71:ASP:HA    | 2:1:68:LEU:HD21  | 1.83                     | 0.60              |
| 2:Y:159:ILE:O    | 2:Y:163:LYS:HG3  | 2.02                     | 0.60              |
| 1:F:8:TYR:CE2    | 1:G:10:ARG:HD3   | 2.37                     | 0.60              |
| 1:O:178:ARG:C    | 1:P:57:ARG:HH22  | 2.08                     | 0.60              |
| 1:S:61:GLN:OE1   | 1:S:62:ASN:HB3   | 2.00                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:107:VAL:CB   | 2:V:66:TYR:OH    | 2.49                     | 0.60              |
| 2:2:3:THR:HB     | 2:2:16:THR:HG22  | 1.83                     | 0.60              |
| 1:B:49:ILE:HD12  | 1:B:211:GLU:O    | 2.01                     | 0.60              |
| 1:D:97:GLN:OE1   | 2:K:61:ALA:CB    | 2.50                     | 0.60              |
| 1:E:111:ASN:CG   | 2:M:70:ARG:NH1   | 2.60                     | 0.60              |
| 1:P:161:LYS:N    | 1:Q:60:GLU:HG2   | 2.16                     | 0.60              |
| 1:T:42:PHE:HD1   | 1:T:43:ALA:N     | 2.00                     | 0.60              |
| 1:U:12:ILE:HB    | 1:U:23:GLN:HG3   | 0.60                     | 0.60              |
| 1:D:28:ARG:O     | 1:D:31:VAL:HG22  | 2.02                     | 0.59              |
| 1:Q:28:ARG:O     | 1:Q:31:VAL:HG22  | 2.02                     | 0.59              |
| 1:Q:125:GLN:C    | 1:R:129:VAL:HG23 | 2.25                     | 0.59              |
| 1:Q:177:GLU:CB   | 1:R:58:LEU:CG    | 2.59                     | 0.59              |
| 1:U:102:THR:C    | 2:V:85:ASN:OD1   | 2.43                     | 0.59              |
| 1:A:15:PHE:HB2   | 1:B:23:GLN:HE22  | 1.66                     | 0.59              |
| 1:A:28:ARG:O     | 1:A:31:VAL:HG22  | 2.02                     | 0.59              |
| 1:A:42:PHE:HD1   | 1:A:43:ALA:N     | 2.00                     | 0.59              |
| 1:O:28:ARG:O     | 1:O:31:VAL:HG22  | 2.02                     | 0.59              |
| 1:T:49:ILE:HD12  | 1:T:211:GLU:O    | 2.01                     | 0.59              |
| 2:V:123:ILE:HG12 | 2:V:124:TYR:CD1  | 2.33                     | 0.59              |
| 2:X:38:ASP:HB2   | 2:X:63:LEU:HD23  | 1.84                     | 0.59              |
| 2:Z:3:THR:HB     | 2:Z:16:THR:HG22  | 1.83                     | 0.59              |
| 1:B:12:ILE:HB    | 1:B:23:GLN:HG3   | 0.60                     | 0.59              |
| 1:C:12:ILE:HB    | 1:C:23:GLN:HG3   | 0.59                     | 0.59              |
| 1:F:28:ARG:O     | 1:F:31:VAL:HG22  | 2.02                     | 0.59              |
| 1:F:42:PHE:HD1   | 1:F:43:ALA:N     | 2.00                     | 0.59              |
| 1:G:107:VAL:CB   | 2:H:66:TYR:OH    | 2.49                     | 0.59              |
| 2:K:32:LYS:HE2   | 2:K:34:LEU:O     | 2.02                     | 0.59              |
| 2:M:133:PHE:CZ   | 2:M:165:ARG:HB3  | 2.37                     | 0.59              |
| 1:P:12:ILE:HB    | 1:P:23:GLN:HG3   | 0.60                     | 0.59              |
| 1:Q:72:ASP:CG    | 2:X:67:ARG:NH2   | 2.61                     | 0.59              |
| 1:T:103:TYR:CZ   | 2:2:82:LEU:HD13  | 2.37                     | 0.59              |
| 2:V:37:ILE:HD11  | 2:V:59:MET:HB3   | 1.82                     | 0.59              |
| 1:D:15:PHE:HB2   | 1:E:23:GLN:HE22  | 1.67                     | 0.59              |
| 1:D:19:GLY:HA3   | 1:E:30:ALA:HB2   | 1.84                     | 0.59              |
| 1:F:107:VAL:CG2  | 2:N:66:TYR:OH    | 2.51                     | 0.59              |
| 1:G:42:PHE:HD1   | 1:G:43:ALA:N     | 2.00                     | 0.59              |
| 2:K:1:THR:H3     | 2:K:129:SER:HB3  | 1.68                     | 0.59              |
| 1:O:12:ILE:HB    | 1:O:23:GLN:HG3   | 0.59                     | 0.59              |
| 1:Q:12:ILE:HB    | 1:Q:23:GLN:HG3   | 0.59                     | 0.59              |
| 1:R:42:PHE:HD1   | 1:R:43:ALA:N     | 2.00                     | 0.59              |
| 1:S:42:PHE:HD1   | 1:S:43:ALA:N     | 2.00                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:12:ILE:HB    | 1:T:23:GLN:HG3   | 0.60                     | 0.59              |
| 1:T:28:ARG:O     | 1:T:31:VAL:HG22  | 2.02                     | 0.59              |
| 2:W:149:ASP:O    | 2:W:152:VAL:HG12 | 2.03                     | 0.59              |
| 2:Y:18:ARG:HE    | 2:Y:30:ASN:HD22  | 1.51                     | 0.59              |
| 2:2:26:ILE:C     | 2:2:26:ILE:HD13  | 2.27                     | 0.59              |
| 1:A:49:ILE:HD11  | 1:A:210:PRO:HB3  | 1.85                     | 0.59              |
| 1:A:178:ARG:HA   | 1:B:57:ARG:HH21  | 1.62                     | 0.59              |
| 1:D:108:ASN:HD22 | 2:L:70:ARG:HB3   | 1.68                     | 0.59              |
| 1:F:177:GLU:CA   | 1:G:58:LEU:HD13  | 2.02                     | 0.59              |
| 2:K:152:VAL:O    | 2:K:156:ILE:HG13 | 2.03                     | 0.59              |
| 1:S:12:ILE:HB    | 1:S:23:GLN:HG3   | 0.60                     | 0.59              |
| 1:U:42:PHE:HD1   | 1:U:43:ALA:N     | 2.00                     | 0.59              |
| 1:A:12:ILE:HB    | 1:A:23:GLN:HG3   | 0.59                     | 0.59              |
| 1:B:49:ILE:HD11  | 1:B:210:PRO:HB3  | 1.85                     | 0.59              |
| 1:D:12:ILE:HB    | 1:D:23:GLN:HG3   | 0.59                     | 0.59              |
| 1:D:173:VAL:O    | 1:E:58:LEU:HD22  | 1.99                     | 0.59              |
| 1:F:12:ILE:HA    | 1:F:23:GLN:CG    | 2.21                     | 0.59              |
| 1:F:104:GLY:N    | 2:N:81:THR:HG21  | 2.17                     | 0.59              |
| 1:G:12:ILE:HB    | 1:G:23:GLN:HG3   | 0.60                     | 0.59              |
| 1:G:49:ILE:HD11  | 1:G:210:PRO:HB3  | 1.85                     | 0.59              |
| 1:O:15:PHE:CZ    | 1:P:130:ARG:NH1  | 2.71                     | 0.59              |
| 1:P:108:ASN:ND2  | 2:X:70:ARG:CG    | 2.66                     | 0.59              |
| 1:R:15:PHE:HB2   | 1:S:23:GLN:HE22  | 1.67                     | 0.59              |
| 1:T:8:TYR:CE2    | 1:U:10:ARG:HD3   | 2.37                     | 0.59              |
| 2:V:59:MET:HE2   | 2:V:79:VAL:HG23  | 1.83                     | 0.59              |
| 1:B:42:PHE:HD1   | 1:B:43:ALA:N     | 2.00                     | 0.59              |
| 1:E:111:ASN:CB   | 2:M:70:ARG:NH1   | 2.66                     | 0.59              |
| 2:L:32:LYS:HE2   | 2:L:34:LEU:O     | 2.01                     | 0.59              |
| 1:Q:42:PHE:HD1   | 1:Q:43:ALA:N     | 2.00                     | 0.59              |
| 1:R:97:GLN:OE1   | 2:Y:61:ALA:CB    | 2.50                     | 0.59              |
| 2:1:38:ASP:HB3   | 2:1:41:THR:CG2   | 2.28                     | 0.59              |
| 1:A:15:PHE:CZ    | 1:B:130:ARG:NH1  | 2.71                     | 0.59              |
| 1:A:161:LYS:CB   | 1:B:60:GLU:OE2   | 2.45                     | 0.59              |
| 1:D:108:ASN:HB3  | 2:L:70:ARG:HG2   | 1.74                     | 0.59              |
| 1:E:42:PHE:HD1   | 1:E:43:ALA:N     | 2.00                     | 0.59              |
| 1:E:107:VAL:CG2  | 2:M:66:TYR:OH    | 2.50                     | 0.59              |
| 2:H:59:MET:HE2   | 2:H:79:VAL:HG23  | 1.83                     | 0.59              |
| 1:R:19:GLY:HA3   | 1:S:30:ALA:HB2   | 1.84                     | 0.59              |
| 1:R:49:ILE:HD11  | 1:R:210:PRO:HB3  | 1.85                     | 0.59              |
| 1:R:177:GLU:CD   | 1:S:58:LEU:H     | 2.11                     | 0.59              |
| 1:S:49:ILE:HD11  | 1:S:210:PRO:HB3  | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:42:PHE:HD1   | 1:C:43:ALA:N     | 2.00                     | 0.59              |
| 1:E:28:ARG:O     | 1:E:31:VAL:HG22  | 2.02                     | 0.59              |
| 1:F:49:ILE:HD11  | 1:F:210:PRO:HB3  | 1.85                     | 0.59              |
| 2:H:37:ILE:HD11  | 2:H:59:MET:HB3   | 1.82                     | 0.59              |
| 1:P:28:ARG:O     | 1:P:31:VAL:HG22  | 2.02                     | 0.59              |
| 1:T:107:VAL:CG2  | 2:2:66:TYR:OH    | 2.51                     | 0.59              |
| 1:A:101:VAL:HG21 | 2:H:58:TYR:HD1   | 1.40                     | 0.59              |
| 1:C:28:ARG:O     | 1:C:31:VAL:HG22  | 2.02                     | 0.59              |
| 1:C:35:SER:O     | 1:C:166:GLY:HA3  | 2.03                     | 0.59              |
| 1:C:72:ASP:CG    | 2:J:67:ARG:NH2   | 2.61                     | 0.59              |
| 2:L:38:ASP:HB3   | 2:L:41:THR:CG2   | 2.31                     | 0.59              |
| 1:Q:49:ILE:HD11  | 1:Q:210:PRO:HB3  | 1.85                     | 0.59              |
| 1:R:12:ILE:HB    | 1:R:23:GLN:HG3   | 0.59                     | 0.59              |
| 1:B:28:ARG:O     | 1:B:31:VAL:HG22  | 2.02                     | 0.58              |
| 1:D:42:PHE:HD1   | 1:D:43:ALA:N     | 2.00                     | 0.58              |
| 1:E:12:ILE:HD13  | 1:E:23:GLN:CA    | 1.93                     | 0.58              |
| 1:F:12:ILE:HB    | 1:F:23:GLN:HG3   | 0.59                     | 0.58              |
| 2:J:7:THR:HB     | 2:J:123:ILE:O    | 2.03                     | 0.58              |
| 2:N:165:ARG:C    | 2:Y:26:ILE:HG22  | 2.28                     | 0.58              |
| 1:R:108:ASN:CB   | 2:Z:70:ARG:CD    | 2.80                     | 0.58              |
| 1:T:35:SER:O     | 1:T:166:GLY:HA3  | 2.03                     | 0.58              |
| 2:Y:124:TYR:CD2  | 2:Y:138:LEU:HD23 | 2.37                     | 0.58              |
| 1:F:177:GLU:C    | 1:G:57:ARG:NH2   | 2.50                     | 0.58              |
| 2:J:38:ASP:HB2   | 2:J:63:LEU:HD23  | 1.84                     | 0.58              |
| 2:N:132:PRO:HA   | 2:Z:133:PHE:HE1  | 1.67                     | 0.58              |
| 1:O:42:PHE:HD1   | 1:O:43:ALA:N     | 2.00                     | 0.58              |
| 1:T:49:ILE:HD11  | 1:T:210:PRO:HB3  | 1.85                     | 0.58              |
| 2:V:26:ILE:HD13  | 2:V:26:ILE:C     | 2.28                     | 0.58              |
| 2:Z:123:ILE:H    | 2:Z:123:ILE:HD13 | 1.67                     | 0.58              |
| 1:B:35:SER:O     | 1:B:166:GLY:HA3  | 2.03                     | 0.58              |
| 1:B:52:LYS:HZ3   | 1:B:62:ASN:HA    | 1.66                     | 0.58              |
| 1:D:35:SER:O     | 1:D:166:GLY:HA3  | 2.03                     | 0.58              |
| 1:E:12:ILE:HB    | 1:E:23:GLN:HG3   | 0.60                     | 0.58              |
| 1:T:108:ASN:HB2  | 2:2:70:ARG:CD    | 2.31                     | 0.58              |
| 1:U:28:ARG:O     | 1:U:31:VAL:HG22  | 2.02                     | 0.58              |
| 2:Z:38:ASP:HB3   | 2:Z:41:THR:CG2   | 2.31                     | 0.58              |
| 2:2:178:ILE:HB   | 2:2:184:TYR:HA   | 1.84                     | 0.58              |
| 1:A:101:VAL:HG22 | 2:H:58:TYR:CE1   | 2.38                     | 0.58              |
| 2:H:26:ILE:C     | 2:H:26:ILE:HD13  | 2.28                     | 0.58              |
| 2:K:159:ILE:O    | 2:K:163:LYS:HG3  | 2.02                     | 0.58              |
| 2:L:123:ILE:HD13 | 2:L:123:ILE:H    | 1.67                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:42:PHE:HD1   | 1:P:43:ALA:N     | 2.00                     | 0.58              |
| 1:R:108:ASN:HD22 | 2:Z:70:ARG:HB3   | 1.68                     | 0.58              |
| 1:S:35:SER:O     | 1:S:166:GLY:HA3  | 2.03                     | 0.58              |
| 1:U:35:SER:O     | 1:U:166:GLY:HA3  | 2.03                     | 0.58              |
| 2:X:7:THR:HB     | 2:X:123:ILE:O    | 2.03                     | 0.58              |
| 2:X:199:LEU:HB3  | 2:X:201:LEU:HD13 | 1.85                     | 0.58              |
| 2:Y:152:VAL:O    | 2:Y:156:ILE:HG13 | 2.03                     | 0.58              |
| 1:B:101:VAL:HG22 | 2:I:58:TYR:HE1   | 1.67                     | 0.58              |
| 1:B:108:ASN:CG   | 2:J:70:ARG:CG    | 2.72                     | 0.58              |
| 1:C:49:ILE:HD11  | 1:C:210:PRO:HB3  | 1.85                     | 0.58              |
| 1:E:49:ILE:HD11  | 1:E:210:PRO:HB3  | 1.85                     | 0.58              |
| 1:F:103:TYR:CZ   | 2:N:82:LEU:HD13  | 2.37                     | 0.58              |
| 1:F:135:SER:OG   | 1:F:153:PRO:HD3  | 2.04                     | 0.58              |
| 2:L:28:HIS:CD2   | 2:M:120:VAL:HG11 | 2.39                     | 0.58              |
| 1:R:35:SER:O     | 1:R:166:GLY:HA3  | 2.03                     | 0.58              |
| 1:S:111:ASN:CB   | 2:1:70:ARG:NH1   | 2.66                     | 0.58              |
| 1:U:49:ILE:HD11  | 1:U:210:PRO:HB3  | 1.85                     | 0.58              |
| 2:Y:20:VAL:HG22  | 2:Y:28:HIS:HB2   | 1.86                     | 0.58              |
| 1:A:35:SER:O     | 1:A:166:GLY:HA3  | 2.03                     | 0.58              |
| 1:B:160:TYR:C    | 1:C:60:GLU:HG2   | 2.29                     | 0.58              |
| 1:D:177:GLU:CD   | 1:E:58:LEU:H     | 2.11                     | 0.58              |
| 1:E:135:SER:OG   | 1:E:153:PRO:HD3  | 2.04                     | 0.58              |
| 1:P:135:SER:OG   | 1:P:153:PRO:HD3  | 2.04                     | 0.58              |
| 1:T:177:GLU:C    | 1:U:57:ARG:NH2   | 2.50                     | 0.58              |
| 1:U:144:ILE:HD11 | 2:V:70:ARG:O     | 2.03                     | 0.58              |
| 1:D:97:GLN:HG3   | 2:K:65:LEU:HB2   | 1.85                     | 0.58              |
| 1:E:15:PHE:CZ    | 1:F:133:GLY:HA3  | 2.39                     | 0.58              |
| 1:P:49:ILE:HD11  | 1:P:210:PRO:HB3  | 1.84                     | 0.58              |
| 1:U:103:TYR:O    | 2:V:81:THR:HG21  | 2.02                     | 0.58              |
| 2:V:152:VAL:O    | 2:V:156:ILE:HG13 | 2.04                     | 0.58              |
| 2:Y:25:PHE:C     | 2:Y:25:PHE:CD1   | 2.80                     | 0.58              |
| 2:Y:32:LYS:HE2   | 2:Y:34:LEU:O     | 2.02                     | 0.58              |
| 1:A:177:GLU:HA   | 1:B:58:LEU:CD2   | 2.28                     | 0.58              |
| 1:F:35:SER:O     | 1:F:166:GLY:HA3  | 2.03                     | 0.58              |
| 2:H:8:LEU:HD12   | 2:H:8:LEU:O      | 2.03                     | 0.58              |
| 1:O:135:SER:OG   | 1:O:153:PRO:HD3  | 2.04                     | 0.58              |
| 1:Q:135:SER:OG   | 1:Q:153:PRO:HD3  | 2.04                     | 0.58              |
| 1:C:72:ASP:OD2   | 2:J:67:ARG:NH2   | 2.36                     | 0.58              |
| 1:D:111:ASN:CG   | 2:L:70:ARG:CZ    | 2.76                     | 0.58              |
| 1:D:135:SER:OG   | 1:D:153:PRO:HD3  | 2.04                     | 0.58              |
| 1:E:35:SER:O     | 1:E:166:GLY:HA3  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:35:SER:O     | 1:G:166:GLY:HA3  | 2.03                     | 0.58              |
| 1:G:135:SER:OG   | 1:G:153:PRO:HD3  | 2.04                     | 0.58              |
| 2:I:149:ASP:O    | 2:I:152:VAL:HG12 | 2.03                     | 0.58              |
| 1:P:160:TYR:C    | 1:Q:60:GLU:HG2   | 2.29                     | 0.58              |
| 2:X:59:MET:HE1   | 2:X:82:LEU:HD23  | 1.86                     | 0.58              |
| 2:Y:38:ASP:HB3   | 2:Y:41:THR:CG2   | 2.26                     | 0.58              |
| 1:B:108:ASN:ND2  | 2:J:70:ARG:CG    | 2.66                     | 0.58              |
| 1:D:19:GLY:O     | 1:E:30:ALA:HB2   | 2.04                     | 0.58              |
| 1:G:144:ILE:HD11 | 2:H:70:ARG:O     | 2.03                     | 0.58              |
| 2:K:18:ARG:HE    | 2:K:30:ASN:HD22  | 1.51                     | 0.58              |
| 1:O:49:ILE:HD11  | 1:O:210:PRO:HB3  | 1.85                     | 0.58              |
| 2:X:123:ILE:HG12 | 2:X:124:TYR:HD1  | 1.69                     | 0.58              |
| 1:O:86:ARG:HH12  | 1:U:156:THR:HA   | 1.69                     | 0.57              |
| 1:Q:72:ASP:OD2   | 2:X:67:ARG:NH2   | 2.36                     | 0.57              |
| 1:B:177:GLU:HA   | 1:C:58:LEU:CG    | 2.19                     | 0.57              |
| 2:J:3:THR:OG1    | 2:J:127:THR:HG22 | 2.05                     | 0.57              |
| 2:J:26:ILE:C     | 2:J:26:ILE:HD13  | 2.30                     | 0.57              |
| 2:M:28:HIS:CD2   | 2:N:120:VAL:HG11 | 2.39                     | 0.57              |
| 2:N:178:ILE:HB   | 2:N:184:TYR:HA   | 1.84                     | 0.57              |
| 1:O:35:SER:O     | 1:O:166:GLY:HA3  | 2.03                     | 0.57              |
| 1:O:101:VAL:HG22 | 2:V:58:TYR:CE1   | 2.38                     | 0.57              |
| 1:R:15:PHE:H     | 1:S:23:GLN:HE22  | 1.51                     | 0.57              |
| 1:S:15:PHE:CZ    | 1:T:133:GLY:HA3  | 2.39                     | 0.57              |
| 2:X:160:SER:O    | 2:X:163:LYS:HB2  | 2.04                     | 0.57              |
| 1:D:15:PHE:H     | 1:E:23:GLN:HE22  | 1.51                     | 0.57              |
| 2:I:51:ASP:O     | 2:I:55:LEU:HB2   | 2.04                     | 0.57              |
| 2:J:59:MET:HE1   | 2:J:82:LEU:HD23  | 1.86                     | 0.57              |
| 2:K:26:ILE:C     | 2:K:26:ILE:HD13  | 2.29                     | 0.57              |
| 1:P:12:ILE:HD13  | 1:P:23:GLN:CA    | 1.93                     | 0.57              |
| 1:P:12:ILE:HA    | 1:P:23:GLN:CG    | 2.21                     | 0.57              |
| 1:Q:35:SER:O     | 1:Q:166:GLY:HA3  | 2.03                     | 0.57              |
| 1:R:135:SER:OG   | 1:R:153:PRO:HD3  | 2.04                     | 0.57              |
| 2:1:28:HIS:CD2   | 2:2:120:VAL:HG11 | 2.39                     | 0.57              |
| 1:A:86:ARG:HH12  | 1:G:156:THR:HA   | 1.69                     | 0.57              |
| 1:A:102:THR:C    | 2:I:85:ASN:OD1   | 2.42                     | 0.57              |
| 1:C:135:SER:OG   | 1:C:153:PRO:HD3  | 2.04                     | 0.57              |
| 2:M:75:PRO:O     | 2:M:78:ALA:HB3   | 2.05                     | 0.57              |
| 1:O:12:ILE:CD1   | 1:O:23:GLN:HB2   | 1.06                     | 0.57              |
| 2:X:3:THR:OG1    | 2:X:127:THR:HG22 | 2.05                     | 0.57              |
| 2:Z:28:HIS:CD2   | 2:1:120:VAL:HG11 | 2.39                     | 0.57              |
| 1:G:108:ASN:HD22 | 2:H:70:ARG:CG    | 2.08                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:20:VAL:HG22  | 2:K:28:HIS:HB2   | 1.86                     | 0.57              |
| 2:K:173:ILE:HD13 | 2:K:173:ILE:C    | 2.30                     | 0.57              |
| 2:N:124:TYR:CD1  | 2:N:138:LEU:HD23 | 2.40                     | 0.57              |
| 1:R:97:GLN:HG3   | 2:Y:65:LEU:HB2   | 1.85                     | 0.57              |
| 1:T:103:TYR:O    | 2:2:81:THR:HB    | 2.05                     | 0.57              |
| 2:V:8:LEU:HD12   | 2:V:8:LEU:O      | 2.03                     | 0.57              |
| 2:Y:26:ILE:HD13  | 2:Y:26:ILE:C     | 2.29                     | 0.57              |
| 2:Y:131:SER:O    | 2:Y:134:VAL:HG13 | 2.04                     | 0.57              |
| 1:D:12:ILE:HA    | 1:D:23:GLN:CG    | 2.21                     | 0.57              |
| 1:D:108:ASN:CB   | 2:L:70:ARG:CD    | 2.80                     | 0.57              |
| 1:E:12:ILE:HA    | 1:E:23:GLN:CG    | 2.21                     | 0.57              |
| 2:K:26:ILE:HG22  | 2:2:165:ARG:C    | 2.30                     | 0.57              |
| 2:K:131:SER:O    | 2:K:134:VAL:HG13 | 2.04                     | 0.57              |
| 1:R:19:GLY:O     | 1:S:30:ALA:HB2   | 2.04                     | 0.57              |
| 1:T:15:PHE:HE2   | 1:U:131:PRO:O    | 1.87                     | 0.57              |
| 1:T:177:GLU:CA   | 1:U:58:LEU:HD13  | 2.02                     | 0.57              |
| 1:B:12:ILE:CD1   | 1:B:23:GLN:HB2   | 1.05                     | 0.57              |
| 1:C:100:LYS:NZ   | 2:J:64:GLU:OE1   | 2.38                     | 0.57              |
| 1:E:52:LYS:HZ3   | 1:E:62:ASN:HA    | 1.68                     | 0.57              |
| 2:H:152:VAL:O    | 2:H:156:ILE:HG13 | 2.04                     | 0.57              |
| 1:P:35:SER:O     | 1:P:166:GLY:HA3  | 2.03                     | 0.57              |
| 1:T:12:ILE:CD1   | 1:T:23:GLN:HB2   | 1.06                     | 0.57              |
| 1:U:135:SER:OG   | 1:U:153:PRO:HD3  | 2.04                     | 0.57              |
| 2:W:51:ASP:O     | 2:W:55:LEU:HB2   | 2.05                     | 0.57              |
| 2:X:26:ILE:C     | 2:X:26:ILE:HD13  | 2.30                     | 0.57              |
| 1:D:49:ILE:HD11  | 1:D:210:PRO:HB3  | 1.85                     | 0.57              |
| 1:F:15:PHE:HE2   | 1:G:131:PRO:O    | 1.87                     | 0.57              |
| 1:F:143:GLN:HA   | 1:F:143:GLN:HE21 | 1.70                     | 0.57              |
| 1:G:102:THR:C    | 2:H:85:ASN:OD1   | 2.43                     | 0.57              |
| 2:M:178:ILE:HB   | 2:M:184:TYR:HA   | 1.87                     | 0.57              |
| 1:P:143:GLN:HE21 | 1:P:143:GLN:HA   | 1.70                     | 0.57              |
| 1:P:177:GLU:CA   | 1:Q:58:LEU:CD2   | 2.83                     | 0.57              |
| 1:Q:177:GLU:C    | 1:R:57:ARG:HH21  | 2.13                     | 0.57              |
| 1:E:143:GLN:HE21 | 1:E:143:GLN:HA   | 1.70                     | 0.57              |
| 2:H:37:ILE:HD11  | 2:H:59:MET:CG    | 2.35                     | 0.57              |
| 1:Q:12:ILE:HD13  | 1:Q:23:GLN:CA    | 1.93                     | 0.57              |
| 1:R:21:LEU:CD1   | 1:S:130:ARG:CD   | 2.71                     | 0.57              |
| 1:S:12:ILE:CD1   | 1:S:23:GLN:HB2   | 1.06                     | 0.57              |
| 1:F:103:TYR:O    | 2:N:81:THR:HB    | 2.05                     | 0.57              |
| 1:R:111:ASN:CG   | 2:Z:70:ARG:CZ    | 2.77                     | 0.57              |
| 2:V:62:GLU:HG2   | 2:V:82:LEU:HD21  | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Y:173:ILE:C    | 2:Y:173:ILE:HD13 | 2.30                     | 0.57              |
| 2:1:178:ILE:HB   | 2:1:184:TYR:HA   | 1.87                     | 0.57              |
| 2:2:152:VAL:O    | 2:2:156:ILE:HG13 | 2.05                     | 0.57              |
| 1:A:9:ASP:OD2    | 1:G:8:TYR:OH     | 2.23                     | 0.56              |
| 1:A:12:ILE:CD1   | 1:A:23:GLN:HB2   | 1.05                     | 0.56              |
| 1:B:135:SER:OG   | 1:B:153:PRO:HD3  | 2.04                     | 0.56              |
| 1:C:125:GLN:O    | 1:D:129:VAL:CG2  | 2.51                     | 0.56              |
| 1:C:177:GLU:C    | 1:D:57:ARG:HH21  | 2.13                     | 0.56              |
| 2:K:45:ILE:HG12  | 2:K:52:ALA:HB1   | 1.87                     | 0.56              |
| 1:O:101:VAL:HG23 | 2:V:58:TYR:HD1   | 1.66                     | 0.56              |
| 1:P:107:VAL:HG11 | 2:X:66:TYR:CZ    | 2.35                     | 0.56              |
| 1:Q:143:GLN:HA   | 1:Q:143:GLN:HE21 | 1.70                     | 0.56              |
| 1:T:101:VAL:HG23 | 2:1:58:TYR:CD1   | 2.09                     | 0.56              |
| 1:T:143:GLN:HA   | 1:T:143:GLN:HE21 | 1.70                     | 0.56              |
| 1:A:177:GLU:CB   | 1:B:58:LEU:CD2   | 2.83                     | 0.56              |
| 1:C:103:TYR:CE1  | 2:K:82:LEU:HD13  | 2.40                     | 0.56              |
| 1:E:12:ILE:CD1   | 1:E:23:GLN:HB2   | 1.05                     | 0.56              |
| 1:G:103:TYR:CD1  | 2:H:82:LEU:HD13  | 2.40                     | 0.56              |
| 2:L:179:THR:HG23 | 2:L:182:ASP:H    | 1.70                     | 0.56              |
| 2:M:76:ILE:HG21  | 2:M:109:HIS:HB2  | 1.88                     | 0.56              |
| 1:R:143:GLN:HA   | 1:R:143:GLN:HE21 | 1.70                     | 0.56              |
| 1:S:143:GLN:HE21 | 1:S:143:GLN:HA   | 1.70                     | 0.56              |
| 2:2:124:TYR:CD1  | 2:2:138:LEU:HD23 | 2.40                     | 0.56              |
| 1:A:60:GLU:CG    | 1:G:160:TYR:C    | 2.78                     | 0.56              |
| 1:A:135:SER:OG   | 1:A:153:PRO:HD3  | 2.04                     | 0.56              |
| 1:A:143:GLN:HA   | 1:A:143:GLN:HE21 | 1.70                     | 0.56              |
| 1:A:177:GLU:CB   | 1:B:58:LEU:HD22  | 2.32                     | 0.56              |
| 1:B:143:GLN:HA   | 1:B:143:GLN:HE21 | 1.70                     | 0.56              |
| 1:C:161:LYS:HB2  | 1:D:60:GLU:CD    | 2.29                     | 0.56              |
| 1:G:143:GLN:HA   | 1:G:143:GLN:HE21 | 1.70                     | 0.56              |
| 2:H:174:ASP:HA   | 2:H:192:ILE:HD13 | 1.88                     | 0.56              |
| 2:J:160:SER:O    | 2:J:163:LYS:HB2  | 2.04                     | 0.56              |
| 2:L:1:THR:H3     | 2:L:129:SER:HB3  | 1.70                     | 0.56              |
| 2:M:38:ASP:HB3   | 2:M:41:THR:CG2   | 2.28                     | 0.56              |
| 2:N:152:VAL:O    | 2:N:156:ILE:HG13 | 2.05                     | 0.56              |
| 1:O:12:ILE:HD12  | 1:O:23:GLN:HB2   | 0.74                     | 0.56              |
| 1:O:124:THR:CG2  | 1:P:130:ARG:HH21 | 2.09                     | 0.56              |
| 1:Q:103:TYR:CE1  | 2:Y:82:LEU:HD13  | 2.41                     | 0.56              |
| 1:S:12:ILE:HD13  | 1:S:23:GLN:CA    | 1.93                     | 0.56              |
| 1:C:12:ILE:CD1   | 1:C:23:GLN:HB2   | 1.06                     | 0.56              |
| 1:C:101:VAL:HG23 | 2:J:58:TYR:CD1   | 2.15                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:100:LYS:NZ   | 2:L:64:GLU:OE1   | 2.38                     | 0.56              |
| 2:J:199:LEU:HB3  | 2:J:201:LEU:HD13 | 1.85                     | 0.56              |
| 1:P:101:VAL:HG22 | 2:W:58:TYR:HE1   | 1.68                     | 0.56              |
| 1:Q:100:LYS:NZ   | 2:X:64:GLU:OE1   | 2.38                     | 0.56              |
| 1:U:108:ASN:HD22 | 2:V:70:ARG:CG    | 2.08                     | 0.56              |
| 2:V:37:ILE:HD11  | 2:V:59:MET:CG    | 2.35                     | 0.56              |
| 1:D:43:ALA:HB2   | 1:D:185:PRO:HA   | 1.88                     | 0.56              |
| 1:G:97:GLN:OE1   | 2:N:61:ALA:CB    | 2.53                     | 0.56              |
| 1:Q:104:GLY:N    | 2:Y:81:THR:HG21  | 2.21                     | 0.56              |
| 1:U:103:TYR:CD1  | 2:V:82:LEU:HD13  | 2.40                     | 0.56              |
| 2:V:174:ASP:HA   | 2:V:192:ILE:HD13 | 1.88                     | 0.56              |
| 2:K:25:PHE:CD1   | 2:K:25:PHE:C     | 2.80                     | 0.56              |
| 1:O:60:GLU:CG    | 1:U:160:TYR:C    | 2.78                     | 0.56              |
| 1:O:143:GLN:HA   | 1:O:143:GLN:HE21 | 1.70                     | 0.56              |
| 1:O:177:GLU:CB   | 1:P:58:LEU:CD2   | 2.83                     | 0.56              |
| 1:P:12:ILE:CD1   | 1:P:23:GLN:HB2   | 1.05                     | 0.56              |
| 1:R:12:ILE:CD1   | 1:R:23:GLN:HB2   | 1.05                     | 0.56              |
| 1:S:177:GLU:CB   | 1:T:58:LEU:CD2   | 2.70                     | 0.56              |
| 2:Z:179:THR:HG23 | 2:Z:182:ASP:H    | 1.70                     | 0.56              |
| 2:L:43:MET:CE    | 2:L:56:VAL:HG23  | 2.35                     | 0.56              |
| 2:N:174:ASP:HA   | 2:N:192:ILE:HD13 | 1.87                     | 0.56              |
| 1:U:103:TYR:O    | 2:V:81:THR:CB    | 2.54                     | 0.56              |
| 1:A:12:ILE:HD13  | 1:A:23:GLN:CA    | 1.93                     | 0.56              |
| 1:D:177:GLU:CB   | 1:E:58:LEU:CD2   | 2.75                     | 0.56              |
| 2:H:173:ILE:HD13 | 2:H:173:ILE:C    | 2.31                     | 0.56              |
| 2:M:32:LYS:HE2   | 2:M:34:LEU:O     | 2.06                     | 0.56              |
| 1:O:9:ASP:OD2    | 1:U:8:TYR:OH     | 2.23                     | 0.56              |
| 1:P:177:GLU:CA   | 1:Q:58:LEU:HD21  | 2.35                     | 0.56              |
| 1:T:135:SER:OG   | 1:T:153:PRO:HD3  | 2.04                     | 0.56              |
| 1:U:12:ILE:CD1   | 1:U:23:GLN:HB2   | 1.05                     | 0.56              |
| 1:B:103:TYR:C    | 2:J:81:THR:HG21  | 2.31                     | 0.56              |
| 1:B:177:GLU:CA   | 1:C:58:LEU:CD2   | 2.83                     | 0.56              |
| 1:C:104:GLY:N    | 2:K:81:THR:HG21  | 2.21                     | 0.56              |
| 1:S:135:SER:OG   | 1:S:153:PRO:HD3  | 2.04                     | 0.56              |
| 1:T:97:GLN:OE1   | 2:1:61:ALA:CB    | 2.53                     | 0.56              |
| 2:V:120:VAL:HG11 | 2:2:28:HIS:CD2   | 2.41                     | 0.56              |
| 2:V:173:ILE:HD13 | 2:V:173:ILE:C    | 2.31                     | 0.56              |
| 2:1:75:PRO:O     | 2:1:78:ALA:HB3   | 2.04                     | 0.56              |
| 1:D:14:VAL:H     | 1:E:130:ARG:HB2  | 1.70                     | 0.56              |
| 1:P:103:TYR:C    | 2:X:81:THR:HG21  | 2.31                     | 0.56              |
| 1:S:43:ALA:HB2   | 1:S:185:PRO:HA   | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Y:43:MET:HE2   | 2:Y:56:VAL:HG23  | 1.88                     | 0.56              |
| 1:G:103:TYR:O    | 2:H:81:THR:CB    | 2.54                     | 0.55              |
| 2:N:66:TYR:CZ    | 2:N:70:ARG:HD2   | 2.41                     | 0.55              |
| 1:O:43:ALA:HB2   | 1:O:185:PRO:HA   | 1.88                     | 0.55              |
| 1:P:52:LYS:HZ3   | 1:P:62:ASN:HA    | 1.70                     | 0.55              |
| 1:Q:125:GLN:O    | 1:R:129:VAL:CG2  | 2.51                     | 0.55              |
| 1:R:14:VAL:H     | 1:S:130:ARG:HB2  | 1.70                     | 0.55              |
| 1:R:14:VAL:HG13  | 1:S:23:GLN:OE1   | 2.06                     | 0.55              |
| 2:Z:43:MET:CE    | 2:Z:56:VAL:HG23  | 2.35                     | 0.55              |
| 1:A:43:ALA:HB2   | 1:A:185:PRO:HA   | 1.88                     | 0.55              |
| 1:B:12:ILE:HD12  | 1:B:23:GLN:HB2   | 0.74                     | 0.55              |
| 1:E:72:ASP:OD2   | 2:L:67:ARG:NH2   | 2.39                     | 0.55              |
| 1:F:104:GLY:HA3  | 2:N:81:THR:HG21  | 1.89                     | 0.55              |
| 1:G:12:ILE:CD1   | 1:G:23:GLN:HB2   | 1.05                     | 0.55              |
| 1:G:70:ILE:HD12  | 1:G:74:VAL:HG22  | 1.88                     | 0.55              |
| 2:H:62:GLU:HG2   | 2:H:82:LEU:HD21  | 1.87                     | 0.55              |
| 2:J:123:ILE:HG12 | 2:J:124:TYR:HD1  | 1.69                     | 0.55              |
| 1:O:60:GLU:CG    | 1:U:161:LYS:N    | 2.68                     | 0.55              |
| 1:Q:12:ILE:CD1   | 1:Q:23:GLN:HB2   | 1.06                     | 0.55              |
| 1:R:43:ALA:HB2   | 1:R:185:PRO:HA   | 1.88                     | 0.55              |
| 1:T:156:THR:HA   | 1:U:86:ARG:HH12  | 1.71                     | 0.55              |
| 2:V:6:ILE:HD11   | 2:V:142:TYR:CD1  | 2.42                     | 0.55              |
| 2:2:174:ASP:HA   | 2:2:192:ILE:HD13 | 1.87                     | 0.55              |
| 1:A:161:LYS:CD   | 1:B:60:GLU:OE2   | 2.41                     | 0.55              |
| 1:B:175:PHE:CD1  | 1:B:175:PHE:C    | 2.85                     | 0.55              |
| 1:B:177:GLU:CA   | 1:C:58:LEU:HD21  | 2.35                     | 0.55              |
| 1:C:43:ALA:HB2   | 1:C:185:PRO:HA   | 1.88                     | 0.55              |
| 1:D:14:VAL:HG13  | 1:E:23:GLN:OE1   | 2.06                     | 0.55              |
| 1:F:12:ILE:CD1   | 1:F:23:GLN:HB2   | 1.05                     | 0.55              |
| 2:L:173:ILE:C    | 2:L:173:ILE:HD13 | 2.32                     | 0.55              |
| 1:T:43:ALA:HB2   | 1:T:185:PRO:HA   | 1.88                     | 0.55              |
| 1:A:70:ILE:HD12  | 1:A:74:VAL:HG22  | 1.88                     | 0.55              |
| 1:C:143:GLN:HA   | 1:C:143:GLN:HE21 | 1.70                     | 0.55              |
| 1:E:43:ALA:HB2   | 1:E:185:PRO:HA   | 1.88                     | 0.55              |
| 1:F:12:ILE:HD12  | 1:F:23:GLN:HB2   | 0.74                     | 0.55              |
| 1:F:15:PHE:HB2   | 1:G:23:GLN:NE2   | 2.11                     | 0.55              |
| 1:F:70:ILE:HD12  | 1:F:74:VAL:HG22  | 1.88                     | 0.55              |
| 1:F:156:THR:HA   | 1:G:86:ARG:HH12  | 1.71                     | 0.55              |
| 1:G:108:ASN:HB2  | 2:H:70:ARG:CD    | 2.31                     | 0.55              |
| 2:H:120:VAL:HG11 | 2:N:28:HIS:CD2   | 2.41                     | 0.55              |
| 2:M:167:SER:OG   | 2:Z:24:ASN:HA    | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:43:ALA:HB2   | 1:P:185:PRO:HA   | 1.88                     | 0.55              |
| 1:R:15:PHE:CZ    | 1:S:130:ARG:NH1  | 2.74                     | 0.55              |
| 1:R:70:ILE:HD12  | 1:R:74:VAL:HG22  | 1.88                     | 0.55              |
| 2:1:76:ILE:HG21  | 2:1:109:HIS:HB2  | 1.88                     | 0.55              |
| 1:A:123:TYR:OH   | 1:G:126:TYR:OH   | 2.24                     | 0.55              |
| 1:B:70:ILE:HD12  | 1:B:74:VAL:HG22  | 1.88                     | 0.55              |
| 1:B:160:TYR:C    | 1:C:60:GLU:CG    | 2.80                     | 0.55              |
| 1:D:12:ILE:CD1   | 1:D:23:GLN:HB2   | 1.05                     | 0.55              |
| 1:D:72:ASP:OD2   | 2:K:67:ARG:NH2   | 2.40                     | 0.55              |
| 1:E:175:PHE:C    | 1:E:175:PHE:HD1  | 2.15                     | 0.55              |
| 1:E:198:LYS:HG2  | 1:E:202:GLU:HG2  | 1.88                     | 0.55              |
| 1:G:175:PHE:HD1  | 1:G:175:PHE:C    | 2.15                     | 0.55              |
| 1:P:175:PHE:CD1  | 1:P:175:PHE:C    | 2.85                     | 0.55              |
| 1:P:177:GLU:OE1  | 1:Q:57:ARG:CA    | 2.54                     | 0.55              |
| 1:Q:175:PHE:C    | 1:Q:175:PHE:CD1  | 2.84                     | 0.55              |
| 1:U:143:GLN:HE21 | 1:U:143:GLN:HA   | 1.70                     | 0.55              |
| 2:2:66:TYR:CZ    | 2:2:70:ARG:HD2   | 2.41                     | 0.55              |
| 1:A:177:GLU:CD   | 1:B:57:ARG:H     | 2.14                     | 0.55              |
| 1:B:95:SER:OG    | 1:B:115:ARG:HD3  | 2.07                     | 0.55              |
| 1:E:173:VAL:HG22 | 1:F:58:LEU:HD23  | 1.89                     | 0.55              |
| 1:F:43:ALA:HB2   | 1:F:185:PRO:HA   | 1.88                     | 0.55              |
| 1:P:175:PHE:C    | 1:P:175:PHE:HD1  | 2.15                     | 0.55              |
| 1:Q:161:LYS:HB2  | 1:R:60:GLU:CD    | 2.29                     | 0.55              |
| 1:Q:175:PHE:C    | 1:Q:175:PHE:HD1  | 2.15                     | 0.55              |
| 1:S:95:SER:OG    | 1:S:115:ARG:HD3  | 2.07                     | 0.55              |
| 1:S:175:PHE:C    | 1:S:175:PHE:CD1  | 2.85                     | 0.55              |
| 1:U:97:GLN:OE1   | 2:2:61:ALA:CB    | 2.53                     | 0.55              |
| 1:A:95:SER:OG    | 1:A:115:ARG:HD3  | 2.07                     | 0.55              |
| 1:C:103:TYR:CD1  | 2:K:82:LEU:HB2   | 2.42                     | 0.55              |
| 1:C:175:PHE:C    | 1:C:175:PHE:CD1  | 2.84                     | 0.55              |
| 1:D:15:PHE:CZ    | 1:E:130:ARG:NH1  | 2.74                     | 0.55              |
| 1:D:95:SER:OG    | 1:D:115:ARG:HD3  | 2.07                     | 0.55              |
| 1:D:198:LYS:HG2  | 1:D:202:GLU:HG2  | 1.88                     | 0.55              |
| 1:E:95:SER:OG    | 1:E:115:ARG:HD3  | 2.07                     | 0.55              |
| 2:H:179:THR:HG23 | 2:H:182:ASP:H    | 1.72                     | 0.55              |
| 1:P:95:SER:OG    | 1:P:115:ARG:HD3  | 2.07                     | 0.55              |
| 2:Y:45:ILE:HG12  | 2:Y:52:ALA:HB1   | 1.87                     | 0.55              |
| 1:B:43:ALA:HB2   | 1:B:185:PRO:HA   | 1.88                     | 0.55              |
| 1:B:177:GLU:OE1  | 1:C:57:ARG:CA    | 2.54                     | 0.55              |
| 1:C:12:ILE:HD12  | 1:C:23:GLN:HB2   | 0.74                     | 0.55              |
| 1:D:143:GLN:HA   | 1:D:143:GLN:HE21 | 1.70                     | 0.55              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:175:PHE:HD1  | 1:F:175:PHE:C   | 2.15                     | 0.55              |
| 1:G:43:ALA:HB2   | 1:G:185:PRO:HA  | 1.88                     | 0.55              |
| 2:I:17:GLU:O     | 2:I:33:LYS:HD2  | 2.07                     | 0.55              |
| 2:K:43:MET:HE2   | 2:K:56:VAL:HG23 | 1.88                     | 0.55              |
| 1:O:95:SER:OG    | 1:O:115:ARG:HD3 | 2.07                     | 0.55              |
| 1:O:175:PHE:CD1  | 1:O:175:PHE:C   | 2.85                     | 0.55              |
| 1:P:160:TYR:C    | 1:Q:60:GLU:CG   | 2.80                     | 0.55              |
| 1:R:12:ILE:HD12  | 1:R:23:GLN:HB2  | 0.74                     | 0.55              |
| 1:R:95:SER:OG    | 1:R:115:ARG:HD3 | 2.07                     | 0.55              |
| 1:R:175:PHE:CD1  | 1:R:175:PHE:C   | 2.84                     | 0.55              |
| 1:S:70:ILE:HD12  | 1:S:74:VAL:HG22 | 1.88                     | 0.55              |
| 1:T:175:PHE:CD1  | 1:T:175:PHE:C   | 2.85                     | 0.55              |
| 1:U:43:ALA:HB2   | 1:U:185:PRO:HA  | 1.88                     | 0.55              |
| 1:U:70:ILE:HD12  | 1:U:74:VAL:HG22 | 1.88                     | 0.55              |
| 1:C:124:THR:HG22 | 1:D:130:ARG:NH2 | 2.08                     | 0.55              |
| 1:D:175:PHE:CD1  | 1:D:175:PHE:C   | 2.84                     | 0.55              |
| 1:E:70:ILE:HD12  | 1:E:74:VAL:HG22 | 1.88                     | 0.55              |
| 1:F:198:LYS:HG2  | 1:F:202:GLU:HG2 | 1.88                     | 0.55              |
| 1:Q:43:ALA:HB2   | 1:Q:185:PRO:HA  | 1.88                     | 0.55              |
| 1:Q:95:SER:OG    | 1:Q:115:ARG:HD3 | 2.07                     | 0.55              |
| 1:Q:103:TYR:O    | 2:Y:81:THR:HB   | 2.07                     | 0.55              |
| 1:R:111:ASN:HB2  | 2:Z:70:ARG:NH1  | 2.21                     | 0.55              |
| 1:T:70:ILE:HD12  | 1:T:74:VAL:HG22 | 1.88                     | 0.55              |
| 1:A:12:ILE:HD12  | 1:A:23:GLN:HB2  | 0.74                     | 0.55              |
| 1:B:108:ASN:HB2  | 2:J:70:ARG:CG   | 2.19                     | 0.55              |
| 1:C:95:SER:OG    | 1:C:115:ARG:HD3 | 2.07                     | 0.55              |
| 1:D:12:ILE:HD12  | 1:D:23:GLN:HB2  | 0.74                     | 0.55              |
| 1:D:70:ILE:HD12  | 1:D:74:VAL:HG22 | 1.88                     | 0.55              |
| 1:E:175:PHE:C    | 1:E:175:PHE:CD1 | 2.84                     | 0.55              |
| 1:F:175:PHE:C    | 1:F:175:PHE:CD1 | 2.85                     | 0.55              |
| 1:P:12:ILE:HD12  | 1:P:23:GLN:HB2  | 0.74                     | 0.55              |
| 1:P:198:LYS:HG2  | 1:P:202:GLU:HG2 | 1.88                     | 0.55              |
| 1:R:49:ILE:HD13  | 1:R:212:ILE:HB  | 1.89                     | 0.55              |
| 1:R:175:PHE:C    | 1:R:175:PHE:HD1 | 2.15                     | 0.55              |
| 1:T:12:ILE:HD12  | 1:T:23:GLN:HB2  | 0.74                     | 0.55              |
| 1:T:104:GLY:HA3  | 2:2:81:THR:HG21 | 1.89                     | 0.55              |
| 1:U:12:ILE:HD12  | 1:U:23:GLN:HB2  | 0.74                     | 0.55              |
| 1:A:175:PHE:CD1  | 1:A:175:PHE:C   | 2.85                     | 0.54              |
| 1:C:70:ILE:HD12  | 1:C:74:VAL:HG22 | 1.88                     | 0.54              |
| 1:D:49:ILE:HD13  | 1:D:212:ILE:HB  | 1.89                     | 0.54              |
| 1:G:175:PHE:C    | 1:G:175:PHE:CD1 | 2.85                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:70:ILE:HD12  | 1:O:74:VAL:HG22  | 1.88                     | 0.54              |
| 1:O:177:GLU:CD   | 1:P:57:ARG:H     | 2.14                     | 0.54              |
| 1:S:12:ILE:HD12  | 1:S:23:GLN:HB2   | 0.74                     | 0.54              |
| 1:T:95:SER:OG    | 1:T:115:ARG:HD3  | 2.07                     | 0.54              |
| 1:U:12:ILE:HD13  | 1:U:23:GLN:CA    | 1.93                     | 0.54              |
| 2:V:179:THR:HG23 | 2:V:182:ASP:H    | 1.71                     | 0.54              |
| 2:Z:173:ILE:C    | 2:Z:173:ILE:HD13 | 2.32                     | 0.54              |
| 2:2:25:PHE:CD1   | 2:2:25:PHE:C     | 2.84                     | 0.54              |
| 1:C:12:ILE:HA    | 1:C:23:GLN:CG    | 2.21                     | 0.54              |
| 1:C:175:PHE:C    | 1:C:175:PHE:HD1  | 2.15                     | 0.54              |
| 1:F:49:ILE:HD13  | 1:F:212:ILE:HB   | 1.89                     | 0.54              |
| 1:F:95:SER:OG    | 1:F:115:ARG:HD3  | 2.07                     | 0.54              |
| 1:G:49:ILE:HD13  | 1:G:212:ILE:HB   | 1.89                     | 0.54              |
| 1:O:12:ILE:HA    | 1:O:23:GLN:CG    | 2.21                     | 0.54              |
| 1:O:49:ILE:HD13  | 1:O:212:ILE:HB   | 1.89                     | 0.54              |
| 1:Q:70:ILE:HD12  | 1:Q:74:VAL:HG22  | 1.88                     | 0.54              |
| 1:S:155:GLY:O    | 1:T:86:ARG:NH1   | 2.41                     | 0.54              |
| 1:S:173:VAL:HG22 | 1:T:58:LEU:HD23  | 1.89                     | 0.54              |
| 1:T:175:PHE:C    | 1:T:175:PHE:HD1  | 2.15                     | 0.54              |
| 1:U:95:SER:OG    | 1:U:115:ARG:HD3  | 2.07                     | 0.54              |
| 1:U:108:ASN:HB2  | 2:V:70:ARG:CD    | 2.31                     | 0.54              |
| 1:D:21:LEU:CD1   | 1:E:130:ARG:CD   | 2.71                     | 0.54              |
| 1:G:12:ILE:HD13  | 1:G:23:GLN:CA    | 1.93                     | 0.54              |
| 2:H:6:ILE:HD11   | 2:H:142:TYR:CD1  | 2.42                     | 0.54              |
| 1:Q:49:ILE:HD13  | 1:Q:212:ILE:HB   | 1.89                     | 0.54              |
| 1:Q:108:ASN:ND2  | 2:Y:70:ARG:CA    | 2.71                     | 0.54              |
| 1:S:49:ILE:HD13  | 1:S:212:ILE:HB   | 1.89                     | 0.54              |
| 1:U:175:PHE:CD1  | 1:U:175:PHE:C    | 2.85                     | 0.54              |
| 2:W:17:GLU:O     | 2:W:33:LYS:HD2   | 2.07                     | 0.54              |
| 1:A:49:ILE:HD13  | 1:A:212:ILE:HB   | 1.89                     | 0.54              |
| 1:B:161:LYS:CD   | 1:C:60:GLU:OE2   | 2.51                     | 0.54              |
| 1:E:49:ILE:HD13  | 1:E:212:ILE:HB   | 1.89                     | 0.54              |
| 1:G:95:SER:OG    | 1:G:115:ARG:HD3  | 2.07                     | 0.54              |
| 1:G:198:LYS:HG2  | 1:G:202:GLU:HG2  | 1.88                     | 0.54              |
| 1:P:49:ILE:HD13  | 1:P:212:ILE:HB   | 1.89                     | 0.54              |
| 1:P:70:ILE:HD12  | 1:P:74:VAL:HG22  | 1.88                     | 0.54              |
| 1:Q:198:LYS:HG2  | 1:Q:202:GLU:HG2  | 1.88                     | 0.54              |
| 1:U:175:PHE:C    | 1:U:175:PHE:HD1  | 2.15                     | 0.54              |
| 1:A:198:LYS:HG2  | 1:A:202:GLU:HG2  | 1.88                     | 0.54              |
| 1:B:108:ASN:ND2  | 2:J:70:ARG:O     | 2.41                     | 0.54              |
| 1:Q:103:TYR:CD1  | 2:Y:82:LEU:HB2   | 2.42                     | 0.54              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:175:PHE:C    | 1:A:175:PHE:HD1 | 2.15                     | 0.54              |
| 1:B:107:VAL:HG11 | 2:J:66:TYR:CZ   | 2.35                     | 0.54              |
| 1:B:198:LYS:HG2  | 1:B:202:GLU:HG2 | 1.88                     | 0.54              |
| 1:C:103:TYR:O    | 2:K:81:THR:HB   | 2.07                     | 0.54              |
| 1:E:156:THR:HA   | 1:F:86:ARG:HH12 | 1.72                     | 0.54              |
| 1:F:12:ILE:HD13  | 1:F:23:GLN:CA   | 1.92                     | 0.54              |
| 2:I:3:THR:HB     | 2:I:16:THR:HG22 | 1.90                     | 0.54              |
| 2:K:62:GLU:HG2   | 2:K:82:LEU:HD21 | 1.90                     | 0.54              |
| 2:M:37:ILE:HD11  | 2:M:59:MET:CB   | 2.35                     | 0.54              |
| 2:M:164:GLN:HE21 | 2:Z:29:LYS:HZ1  | 1.54                     | 0.54              |
| 1:O:175:PHE:C    | 1:O:175:PHE:HD1 | 2.15                     | 0.54              |
| 1:O:198:LYS:HG2  | 1:O:202:GLU:HG2 | 1.88                     | 0.54              |
| 2:1:32:LYS:HE2   | 2:1:34:LEU:O    | 2.06                     | 0.54              |
| 2:H:159:ILE:O    | 2:H:163:LYS:HG3 | 2.08                     | 0.54              |
| 2:K:37:ILE:HD11  | 2:K:59:MET:HB3  | 1.90                     | 0.54              |
| 2:K:141:GLN:NE2  | 2:V:141:GLN:NE2 | 2.55                     | 0.54              |
| 1:R:198:LYS:HG2  | 1:R:202:GLU:HG2 | 1.88                     | 0.54              |
| 1:S:72:ASP:OD2   | 2:Z:67:ARG:NH2  | 2.39                     | 0.54              |
| 1:S:161:LYS:CD   | 1:T:60:GLU:OE2  | 2.56                     | 0.54              |
| 1:S:198:LYS:HG2  | 1:S:202:GLU:HG2 | 1.88                     | 0.54              |
| 1:T:198:LYS:HG2  | 1:T:202:GLU:HG2 | 1.88                     | 0.54              |
| 2:W:3:THR:HB     | 2:W:16:THR:HG22 | 1.90                     | 0.54              |
| 2:Y:37:ILE:HD11  | 2:Y:59:MET:HB3  | 1.90                     | 0.54              |
| 2:Z:1:THR:H3     | 2:Z:129:SER:HB3 | 1.73                     | 0.54              |
| 1:C:198:LYS:HG2  | 1:C:202:GLU:HG2 | 1.88                     | 0.54              |
| 1:D:19:GLY:HA3   | 1:E:30:ALA:N    | 2.23                     | 0.54              |
| 2:I:63:LEU:HD11  | 2:I:74:MET:SD   | 2.48                     | 0.54              |
| 2:L:45:ILE:HG12  | 2:L:52:ALA:HB1  | 1.90                     | 0.54              |
| 1:S:156:THR:HA   | 1:T:86:ARG:HH12 | 1.72                     | 0.54              |
| 1:S:175:PHE:C    | 1:S:175:PHE:HD1 | 2.15                     | 0.54              |
| 1:B:175:PHE:C    | 1:B:175:PHE:HD1 | 2.15                     | 0.54              |
| 1:C:108:ASN:ND2  | 2:K:70:ARG:CA   | 2.71                     | 0.54              |
| 1:D:175:PHE:C    | 1:D:175:PHE:HD1 | 2.15                     | 0.54              |
| 2:K:141:GLN:HE21 | 2:V:141:GLN:NE2 | 2.06                     | 0.54              |
| 1:S:161:LYS:N    | 1:T:60:GLU:CG   | 2.71                     | 0.54              |
| 1:U:42:PHE:HB2   | 1:U:184:LEU:O   | 2.08                     | 0.54              |
| 2:W:63:LEU:HD11  | 2:W:74:MET:SD   | 2.48                     | 0.54              |
| 2:Z:35:PHE:CE2   | 2:Z:45:ILE:HD12 | 2.43                     | 0.54              |
| 1:A:52:LYS:HZ3   | 1:A:62:ASN:HA   | 1.73                     | 0.54              |
| 1:C:42:PHE:HB2   | 1:C:184:LEU:O   | 2.09                     | 0.54              |
| 2:J:32:LYS:HE2   | 2:J:34:LEU:O    | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:141:GLN:NE2  | 2:2:141:GLN:NE2  | 2.56                     | 0.54              |
| 1:Q:126:TYR:HA   | 1:R:129:VAL:HG23 | 1.90                     | 0.54              |
| 1:S:108:ASN:HB3  | 2:1:70:ARG:HG2   | 1.76                     | 0.54              |
| 2:Y:36:GLN:HB2   | 2:Y:184:TYR:CE1  | 2.43                     | 0.54              |
| 2:1:37:ILE:HD11  | 2:1:59:MET:CB    | 2.35                     | 0.54              |
| 1:C:144:ILE:HD12 | 1:C:147:ARG:NH1  | 2.24                     | 0.53              |
| 1:E:107:VAL:HG11 | 2:M:66:TYR:HH    | 1.73                     | 0.53              |
| 2:H:3:THR:HB     | 2:H:16:THR:HG22  | 1.90                     | 0.53              |
| 2:J:131:SER:O    | 2:J:134:VAL:HG13 | 2.08                     | 0.53              |
| 1:O:42:PHE:HB2   | 1:O:184:LEU:O    | 2.08                     | 0.53              |
| 1:O:129:VAL:HA   | 1:U:125:GLN:O    | 2.08                     | 0.53              |
| 1:R:161:LYS:N    | 1:S:60:GLU:CG    | 2.71                     | 0.53              |
| 1:T:177:GLU:CA   | 1:U:58:LEU:CG    | 2.53                     | 0.53              |
| 1:U:12:ILE:HA    | 1:U:23:GLN:CG    | 2.21                     | 0.53              |
| 2:V:159:ILE:O    | 2:V:163:LYS:HG3  | 2.08                     | 0.53              |
| 1:A:129:VAL:HA   | 1:G:125:GLN:O    | 2.08                     | 0.53              |
| 1:B:49:ILE:HD13  | 1:B:212:ILE:HB   | 1.89                     | 0.53              |
| 1:B:107:VAL:HG21 | 2:J:66:TYR:OH    | 2.08                     | 0.53              |
| 1:C:177:GLU:C    | 1:D:57:ARG:NH2   | 2.65                     | 0.53              |
| 1:E:144:ILE:HD12 | 1:E:147:ARG:NH1  | 2.23                     | 0.53              |
| 1:E:161:LYS:N    | 1:F:60:GLU:CG    | 2.71                     | 0.53              |
| 1:G:42:PHE:HB2   | 1:G:184:LEU:O    | 2.08                     | 0.53              |
| 2:M:55:LEU:HD23  | 2:M:99:LEU:HD11  | 1.91                     | 0.53              |
| 2:N:25:PHE:C     | 2:N:25:PHE:CD1   | 2.84                     | 0.53              |
| 1:O:23:GLN:OE1   | 1:U:14:VAL:HG13  | 2.09                     | 0.53              |
| 1:O:57:ARG:NH2   | 1:U:178:ARG:N    | 2.20                     | 0.53              |
| 1:P:144:ILE:HD12 | 1:P:147:ARG:NH1  | 2.24                     | 0.53              |
| 1:P:177:GLU:C    | 1:Q:58:LEU:HD11  | 2.24                     | 0.53              |
| 1:R:42:PHE:HB2   | 1:R:184:LEU:O    | 2.08                     | 0.53              |
| 1:T:177:GLU:O    | 1:U:58:LEU:HD11  | 2.07                     | 0.53              |
| 1:U:144:ILE:HD12 | 1:U:147:ARG:NH1  | 2.24                     | 0.53              |
| 2:2:199:LEU:HB3  | 2:2:201:LEU:HD13 | 1.90                     | 0.53              |
| 1:A:57:ARG:NH2   | 1:G:178:ARG:N    | 2.20                     | 0.53              |
| 1:A:101:VAL:HG23 | 2:H:58:TYR:HD1   | 1.65                     | 0.53              |
| 1:B:12:ILE:HA    | 1:B:23:GLN:CG    | 2.21                     | 0.53              |
| 1:B:42:PHE:HB2   | 1:B:184:LEU:O    | 2.08                     | 0.53              |
| 1:B:144:ILE:HD12 | 1:B:147:ARG:NH1  | 2.24                     | 0.53              |
| 1:C:177:GLU:CB   | 1:D:58:LEU:CD1   | 2.51                     | 0.53              |
| 1:E:161:LYS:CD   | 1:F:60:GLU:OE2   | 2.56                     | 0.53              |
| 2:K:36:GLN:HB2   | 2:K:184:TYR:CE1  | 2.43                     | 0.53              |
| 1:O:86:ARG:NH1   | 1:U:155:GLY:O    | 2.41                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:108:ASN:CG   | 2:X:70:ARG:CG    | 2.72                     | 0.53              |
| 1:R:12:ILE:HD13  | 1:R:23:GLN:CA    | 1.92                     | 0.53              |
| 1:R:72:ASP:OD2   | 2:Y:67:ARG:NH2   | 2.40                     | 0.53              |
| 1:U:49:ILE:HD13  | 1:U:212:ILE:HB   | 1.90                     | 0.53              |
| 1:U:198:LYS:HG2  | 1:U:202:GLU:HG2  | 1.88                     | 0.53              |
| 1:A:42:PHE:HB2   | 1:A:184:LEU:O    | 2.08                     | 0.53              |
| 1:C:12:ILE:HD13  | 1:C:23:GLN:CA    | 1.93                     | 0.53              |
| 1:C:49:ILE:HD13  | 1:C:212:ILE:HB   | 1.89                     | 0.53              |
| 1:C:143:GLN:OE1  | 2:K:75:PRO:HG2   | 2.09                     | 0.53              |
| 1:D:42:PHE:HB2   | 1:D:184:LEU:O    | 2.08                     | 0.53              |
| 1:E:12:ILE:HD12  | 1:E:23:GLN:HB2   | 0.74                     | 0.53              |
| 2:J:3:THR:HB     | 2:J:16:THR:HG22  | 1.90                     | 0.53              |
| 2:M:135:TYR:HB3  | 2:1:165:ARG:HG2  | 1.90                     | 0.53              |
| 2:N:149:ASP:O    | 2:N:152:VAL:HG12 | 2.08                     | 0.53              |
| 1:Q:42:PHE:HB2   | 1:Q:184:LEU:O    | 2.08                     | 0.53              |
| 1:S:42:PHE:HB2   | 1:S:184:LEU:O    | 2.09                     | 0.53              |
| 1:T:177:GLU:CD   | 1:U:57:ARG:H     | 2.16                     | 0.53              |
| 1:E:104:GLY:CA   | 2:M:81:THR:HG21  | 2.39                     | 0.53              |
| 1:F:177:GLU:CD   | 1:G:57:ARG:H     | 2.16                     | 0.53              |
| 2:H:133:PHE:CZ   | 2:H:165:ARG:HB3  | 2.43                     | 0.53              |
| 1:O:58:LEU:CD2   | 1:U:177:GLU:CB   | 2.76                     | 0.53              |
| 1:O:161:LYS:CD   | 1:P:60:GLU:OE2   | 2.41                     | 0.53              |
| 1:P:42:PHE:HB2   | 1:P:184:LEU:O    | 2.08                     | 0.53              |
| 1:P:108:ASN:ND2  | 2:X:70:ARG:O     | 2.41                     | 0.53              |
| 1:S:72:ASP:CG    | 2:Z:67:ARG:NH2   | 2.67                     | 0.53              |
| 2:Z:103:GLY:HA2  | 2:Z:178:ILE:CD1  | 2.39                     | 0.53              |
| 2:1:55:LEU:HD23  | 2:1:99:LEU:HD11  | 1.91                     | 0.53              |
| 1:B:178:ARG:O    | 1:C:57:ARG:NH2   | 2.40                     | 0.53              |
| 1:D:12:ILE:HD13  | 1:D:23:GLN:CA    | 1.93                     | 0.53              |
| 1:E:155:GLY:O    | 1:F:86:ARG:NH1   | 2.41                     | 0.53              |
| 1:Q:144:ILE:HD12 | 1:Q:147:ARG:NH1  | 2.24                     | 0.53              |
| 1:Q:157:ILE:HG22 | 1:R:86:ARG:CZ    | 2.39                     | 0.53              |
| 1:R:19:GLY:HA3   | 1:S:30:ALA:N     | 2.23                     | 0.53              |
| 1:R:144:ILE:HD12 | 1:R:147:ARG:NH1  | 2.24                     | 0.53              |
| 1:T:19:GLY:HA3   | 1:U:30:ALA:HB2   | 1.90                     | 0.53              |
| 2:X:3:THR:HB     | 2:X:16:THR:HG22  | 1.90                     | 0.53              |
| 1:C:126:TYR:HA   | 1:D:129:VAL:HG23 | 1.90                     | 0.53              |
| 1:E:72:ASP:CG    | 2:L:67:ARG:NH2   | 2.67                     | 0.53              |
| 1:F:144:ILE:HD12 | 1:F:147:ARG:NH1  | 2.24                     | 0.53              |
| 2:L:35:PHE:CE2   | 2:L:45:ILE:HD12  | 2.43                     | 0.53              |
| 1:S:100:LYS:NZ   | 2:Z:64:GLU:OE1   | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:42:PHE:HB2   | 1:T:184:LEU:O    | 2.09                     | 0.53              |
| 1:T:104:GLY:CA   | 2:2:81:THR:HG21  | 2.39                     | 0.53              |
| 2:Z:45:ILE:HG12  | 2:Z:52:ALA:HB1   | 1.90                     | 0.53              |
| 2:2:149:ASP:O    | 2:2:152:VAL:HG12 | 2.08                     | 0.53              |
| 2:L:103:GLY:HA2  | 2:L:178:ILE:CD1  | 2.39                     | 0.53              |
| 1:O:129:VAL:HG23 | 1:U:125:GLN:C    | 2.33                     | 0.53              |
| 1:Q:124:THR:HG22 | 1:R:130:ARG:NH2  | 2.08                     | 0.53              |
| 1:S:104:GLY:CA   | 2:1:81:THR:HG21  | 2.39                     | 0.53              |
| 1:S:124:THR:HG22 | 1:T:130:ARG:NH2  | 2.15                     | 0.53              |
| 2:V:133:PHE:CZ   | 2:V:165:ARG:HB3  | 2.43                     | 0.53              |
| 2:2:123:ILE:HG12 | 2:2:124:TYR:CD2  | 2.44                     | 0.53              |
| 1:B:108:ASN:CB   | 2:J:70:ARG:CD    | 2.79                     | 0.53              |
| 1:G:144:ILE:HD12 | 1:G:147:ARG:NH1  | 2.24                     | 0.53              |
| 1:T:49:ILE:HD13  | 1:T:212:ILE:HB   | 1.89                     | 0.53              |
| 1:T:144:ILE:HD12 | 1:T:147:ARG:NH1  | 2.24                     | 0.53              |
| 1:U:103:TYR:CE1  | 2:V:82:LEU:HD22  | 2.44                     | 0.53              |
| 2:X:32:LYS:HE2   | 2:X:34:LEU:O     | 2.08                     | 0.53              |
| 2:Y:15:ALA:HB2   | 2:Y:175:VAL:HB   | 1.91                     | 0.53              |
| 2:Z:26:ILE:O     | 2:Z:26:ILE:HD13  | 2.09                     | 0.53              |
| 2:1:6:ILE:HD11   | 2:1:142:TYR:CD1  | 2.44                     | 0.53              |
| 1:B:12:ILE:HG13  | 1:B:12:ILE:O     | 2.09                     | 0.53              |
| 1:D:144:ILE:HD12 | 1:D:147:ARG:NH1  | 2.24                     | 0.53              |
| 1:D:160:TYR:C    | 1:E:60:GLU:CG    | 2.82                     | 0.53              |
| 1:F:42:PHE:HB2   | 1:F:184:LEU:O    | 2.09                     | 0.53              |
| 1:O:57:ARG:HB2   | 1:U:177:GLU:OE1  | 2.09                     | 0.53              |
| 2:V:3:THR:HB     | 2:V:16:THR:HG22  | 1.90                     | 0.53              |
| 1:D:108:ASN:CB   | 2:L:70:ARG:HD3   | 2.30                     | 0.52              |
| 1:E:42:PHE:HB2   | 1:E:184:LEU:O    | 2.09                     | 0.52              |
| 1:G:107:VAL:HG21 | 2:H:66:TYR:HH    | 1.74                     | 0.52              |
| 1:O:108:ASN:ND2  | 2:W:70:ARG:O     | 2.42                     | 0.52              |
| 1:O:178:ARG:HA   | 1:P:57:ARG:HH21  | 1.62                     | 0.52              |
| 1:P:107:VAL:HG21 | 2:X:66:TYR:OH    | 2.08                     | 0.52              |
| 1:P:108:ASN:HB2  | 2:X:70:ARG:CG    | 2.19                     | 0.52              |
| 1:S:144:ILE:HD12 | 1:S:147:ARG:NH1  | 2.23                     | 0.52              |
| 1:A:57:ARG:HB2   | 1:G:177:GLU:OE1  | 2.09                     | 0.52              |
| 1:B:177:GLU:N    | 1:C:58:LEU:CD2   | 2.66                     | 0.52              |
| 2:K:103:GLY:HA2  | 2:K:178:ILE:HD13 | 1.91                     | 0.52              |
| 2:M:131:SER:O    | 2:M:134:VAL:HG13 | 2.10                     | 0.52              |
| 2:N:131:SER:O    | 2:N:134:VAL:HG13 | 2.09                     | 0.52              |
| 2:N:199:LEU:HB3  | 2:N:201:LEU:HD13 | 1.90                     | 0.52              |
| 1:O:12:ILE:HG13  | 1:O:12:ILE:O     | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:60:GLU:HG2   | 1:U:160:TYR:C    | 2.34                     | 0.52              |
| 1:O:144:ILE:HD12 | 1:O:147:ARG:NH1  | 2.23                     | 0.52              |
| 2:X:28:HIS:CD2   | 2:Y:120:VAL:HG11 | 2.44                     | 0.52              |
| 2:X:131:SER:O    | 2:X:134:VAL:HG13 | 2.08                     | 0.52              |
| 2:Z:59:MET:HE1   | 2:Z:82:LEU:HD23  | 1.91                     | 0.52              |
| 2:2:131:SER:O    | 2:2:134:VAL:HG13 | 2.09                     | 0.52              |
| 1:A:124:THR:CG2  | 1:B:130:ARG:HH21 | 2.09                     | 0.52              |
| 1:C:42:PHE:CD1   | 1:C:43:ALA:N     | 2.78                     | 0.52              |
| 1:C:157:ILE:HG22 | 1:D:86:ARG:CZ    | 2.39                     | 0.52              |
| 1:D:12:ILE:HG13  | 1:D:12:ILE:O     | 2.09                     | 0.52              |
| 2:J:124:TYR:CD2  | 2:J:138:LEU:HD23 | 2.45                     | 0.52              |
| 2:K:15:ALA:HB2   | 2:K:175:VAL:HB   | 1.91                     | 0.52              |
| 2:L:26:ILE:O     | 2:L:26:ILE:HD13  | 2.09                     | 0.52              |
| 1:P:178:ARG:O    | 1:Q:57:ARG:NH2   | 2.40                     | 0.52              |
| 1:R:160:TYR:C    | 1:S:60:GLU:CG    | 2.82                     | 0.52              |
| 1:S:12:ILE:HA    | 1:S:23:GLN:CG    | 2.21                     | 0.52              |
| 1:S:12:ILE:HG13  | 1:S:12:ILE:O     | 2.09                     | 0.52              |
| 1:S:107:VAL:HG21 | 2:1:66:TYR:HH    | 1.73                     | 0.52              |
| 1:T:12:ILE:HG13  | 1:T:12:ILE:O     | 2.09                     | 0.52              |
| 1:U:42:PHE:CD1   | 1:U:43:ALA:N     | 2.78                     | 0.52              |
| 2:V:45:ILE:CG1   | 2:V:52:ALA:HB1   | 2.39                     | 0.52              |
| 1:A:86:ARG:NH1   | 1:G:155:GLY:O    | 2.41                     | 0.52              |
| 1:A:108:ASN:ND2  | 2:I:70:ARG:O     | 2.42                     | 0.52              |
| 1:D:108:ASN:ND2  | 2:L:70:ARG:CB    | 2.72                     | 0.52              |
| 1:F:97:GLN:OE1   | 2:M:61:ALA:CB    | 2.53                     | 0.52              |
| 2:H:141:GLN:NE2  | 2:Y:141:GLN:NE2  | 2.58                     | 0.52              |
| 1:O:42:PHE:CD1   | 1:O:43:ALA:N     | 2.78                     | 0.52              |
| 1:Q:107:VAL:HG21 | 2:Y:66:TYR:HH    | 1.74                     | 0.52              |
| 1:Q:143:GLN:OE1  | 2:Y:75:PRO:HG2   | 2.09                     | 0.52              |
| 2:W:26:ILE:HD13  | 2:W:26:ILE:C     | 2.35                     | 0.52              |
| 1:D:111:ASN:HB2  | 2:L:70:ARG:NH1   | 2.21                     | 0.52              |
| 1:F:125:GLN:O    | 1:G:129:VAL:CG2  | 2.51                     | 0.52              |
| 2:J:28:HIS:CD2   | 2:K:120:VAL:HG11 | 2.44                     | 0.52              |
| 2:M:26:ILE:C     | 2:M:26:ILE:HD13  | 2.34                     | 0.52              |
| 1:Q:178:ARG:C    | 1:R:57:ARG:NH2   | 2.67                     | 0.52              |
| 1:U:160:TYR:CD2  | 1:U:163:THR:HB   | 2.45                     | 0.52              |
| 2:X:124:TYR:CD2  | 2:X:138:LEU:HD23 | 2.44                     | 0.52              |
| 1:A:12:ILE:HG13  | 1:A:12:ILE:O     | 2.09                     | 0.52              |
| 1:A:129:VAL:HG23 | 1:G:125:GLN:C    | 2.33                     | 0.52              |
| 1:A:144:ILE:HD12 | 1:A:147:ARG:NH1  | 2.24                     | 0.52              |
| 1:C:160:TYR:CD2  | 1:C:163:THR:HB   | 2.45                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:21:LEU:O     | 1:D:24:VAL:HG12  | 2.10                     | 0.52              |
| 1:D:160:TYR:C    | 1:E:60:GLU:HG3   | 2.35                     | 0.52              |
| 1:D:160:TYR:CD2  | 1:D:163:THR:HB   | 2.45                     | 0.52              |
| 2:I:45:ILE:CG1   | 2:I:52:ALA:HB1   | 2.39                     | 0.52              |
| 2:J:37:ILE:HD11  | 2:J:59:MET:CB    | 2.38                     | 0.52              |
| 2:L:29:LYS:HZ1   | 2:1:164:GLN:HE21 | 1.57                     | 0.52              |
| 2:M:6:ILE:HD11   | 2:M:142:TYR:CD1  | 2.44                     | 0.52              |
| 1:O:21:LEU:O     | 1:O:24:VAL:HG12  | 2.10                     | 0.52              |
| 1:O:60:GLU:HG3   | 1:U:160:TYR:C    | 2.35                     | 0.52              |
| 1:R:108:ASN:CB   | 2:Z:70:ARG:HD3   | 2.30                     | 0.52              |
| 1:S:19:GLY:HA3   | 1:T:30:ALA:CA    | 2.39                     | 0.52              |
| 1:S:173:VAL:HG22 | 1:T:58:LEU:CD2   | 2.40                     | 0.52              |
| 1:T:160:TYR:CD2  | 1:T:163:THR:HB   | 2.45                     | 0.52              |
| 2:X:189:THR:HG23 | 2:X:190:ASP:N    | 2.25                     | 0.52              |
| 2:1:20:VAL:CG1   | 2:1:28:HIS:HB2   | 2.36                     | 0.52              |
| 1:A:60:GLU:HG2   | 1:G:160:TYR:C    | 2.33                     | 0.52              |
| 1:A:130:ARG:CD   | 1:G:21:LEU:CD1   | 2.75                     | 0.52              |
| 2:H:45:ILE:CG1   | 2:H:52:ALA:HB1   | 2.39                     | 0.52              |
| 2:I:26:ILE:HD13  | 2:I:26:ILE:C     | 2.35                     | 0.52              |
| 2:L:24:ASN:HA    | 2:1:167:SER:OG   | 2.09                     | 0.52              |
| 2:L:59:MET:HE1   | 2:L:82:LEU:HD23  | 1.91                     | 0.52              |
| 2:L:62:GLU:HG2   | 2:L:82:LEU:HD21  | 1.91                     | 0.52              |
| 1:O:108:ASN:HD22 | 2:W:70:ARG:CB    | 2.22                     | 0.52              |
| 1:O:160:TYR:CD2  | 1:O:163:THR:HB   | 2.45                     | 0.52              |
| 1:R:21:LEU:O     | 1:R:24:VAL:HG12  | 2.10                     | 0.52              |
| 1:R:111:ASN:CG   | 2:Z:70:ARG:HH12  | 2.17                     | 0.52              |
| 1:S:52:LYS:HZ3   | 1:S:62:ASN:HA    | 1.74                     | 0.52              |
| 2:2:18:ARG:HE    | 2:2:30:ASN:HD22  | 1.57                     | 0.52              |
| 1:A:23:GLN:OE1   | 1:G:14:VAL:HG13  | 2.09                     | 0.52              |
| 1:C:70:ILE:HB    | 1:C:74:VAL:HG13  | 1.92                     | 0.52              |
| 1:F:104:GLY:CA   | 2:N:81:THR:HG21  | 2.39                     | 0.52              |
| 1:G:21:LEU:O     | 1:G:24:VAL:HG12  | 2.10                     | 0.52              |
| 2:H:141:GLN:NE2  | 2:Y:141:GLN:HE21 | 2.08                     | 0.52              |
| 1:Q:103:TYR:O    | 2:Y:81:THR:CB    | 2.58                     | 0.52              |
| 1:Q:160:TYR:CD2  | 1:Q:163:THR:HB   | 2.45                     | 0.52              |
| 1:T:12:ILE:HA    | 1:T:23:GLN:CG    | 2.21                     | 0.52              |
| 2:W:45:ILE:CG1   | 2:W:52:ALA:HB1   | 2.39                     | 0.52              |
| 2:1:26:ILE:HD13  | 2:1:26:ILE:C     | 2.34                     | 0.52              |
| 1:A:60:GLU:HG3   | 1:G:160:TYR:C    | 2.35                     | 0.52              |
| 1:E:21:LEU:CD1   | 1:F:130:ARG:HD2  | 2.27                     | 0.52              |
| 1:E:70:ILE:HB    | 1:E:74:VAL:HG13  | 1.92                     | 0.52              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:21:LEU:O    | 1:F:24:VAL:HG12  | 2.10                     | 0.52              |
| 1:F:42:PHE:CD1  | 1:F:43:ALA:N     | 2.78                     | 0.52              |
| 1:F:70:ILE:HB   | 1:F:74:VAL:HG13  | 1.92                     | 0.52              |
| 1:F:103:TYR:O   | 2:N:81:THR:CB    | 2.58                     | 0.52              |
| 1:P:12:ILE:HG13 | 1:P:12:ILE:O     | 2.09                     | 0.52              |
| 1:Q:70:ILE:HB   | 1:Q:74:VAL:HG13  | 1.92                     | 0.52              |
| 1:R:70:ILE:HB   | 1:R:74:VAL:HG13  | 1.92                     | 0.52              |
| 1:U:12:ILE:HG13 | 1:U:12:ILE:O     | 2.09                     | 0.52              |
| 1:U:70:ILE:HB   | 1:U:74:VAL:HG13  | 1.92                     | 0.52              |
| 2:Y:62:GLU:HG2  | 2:Y:82:LEU:HD21  | 1.90                     | 0.52              |
| 2:Y:103:GLY:HA2 | 2:Y:178:ILE:HD13 | 1.91                     | 0.52              |
| 2:Z:55:LEU:HD21 | 2:Z:87:LEU:HD11  | 1.92                     | 0.52              |
| 1:A:85:ALA:O    | 1:A:89:VAL:HG23  | 2.10                     | 0.52              |
| 1:B:42:PHE:CD1  | 1:B:43:ALA:N     | 2.78                     | 0.52              |
| 1:B:72:ASP:OD1  | 2:I:67:ARG:NH2   | 2.43                     | 0.52              |
| 1:D:42:PHE:CD1  | 1:D:43:ALA:N     | 2.78                     | 0.52              |
| 1:E:12:ILE:HG13 | 1:E:12:ILE:O     | 2.09                     | 0.52              |
| 1:E:42:PHE:CD1  | 1:E:43:ALA:N     | 2.78                     | 0.52              |
| 1:E:160:TYR:CD2 | 1:E:163:THR:HB   | 2.45                     | 0.52              |
| 1:G:85:ALA:O    | 1:G:89:VAL:HG23  | 2.10                     | 0.52              |
| 1:O:70:ILE:HB   | 1:O:74:VAL:HG13  | 1.92                     | 0.52              |
| 1:O:85:ALA:O    | 1:O:89:VAL:HG23  | 2.10                     | 0.52              |
| 1:P:70:ILE:HB   | 1:P:74:VAL:HG13  | 1.92                     | 0.52              |
| 1:Q:21:LEU:O    | 1:Q:24:VAL:HG12  | 2.10                     | 0.52              |
| 1:R:85:ALA:O    | 1:R:89:VAL:HG23  | 2.10                     | 0.52              |
| 1:R:108:ASN:ND2 | 2:Z:70:ARG:CB    | 2.72                     | 0.52              |
| 1:S:85:ALA:O    | 1:S:89:VAL:HG23  | 2.10                     | 0.52              |
| 1:T:103:TYR:O   | 2:2:81:THR:CB    | 2.58                     | 0.52              |
| 2:Z:62:GLU:HG2  | 2:Z:82:LEU:HD21  | 1.91                     | 0.52              |
| 2:2:2:THR:HG22  | 2:2:169:SER:OG   | 2.10                     | 0.52              |
| 1:A:60:GLU:CG   | 1:G:161:LYS:N    | 2.68                     | 0.51              |
| 1:C:12:ILE:HG13 | 1:C:12:ILE:O     | 2.09                     | 0.51              |
| 1:D:85:ALA:O    | 1:D:89:VAL:HG23  | 2.10                     | 0.51              |
| 1:F:160:TYR:CD2 | 1:F:163:THR:HB   | 2.45                     | 0.51              |
| 1:P:72:ASP:OD1  | 2:W:67:ARG:NH2   | 2.44                     | 0.51              |
| 1:P:160:TYR:CD2 | 1:P:163:THR:HB   | 2.45                     | 0.51              |
| 1:P:177:GLU:CB  | 1:Q:58:LEU:CD2   | 2.88                     | 0.51              |
| 1:Q:177:GLU:C   | 1:R:57:ARG:NH2   | 2.65                     | 0.51              |
| 1:R:42:PHE:CD1  | 1:R:43:ALA:N     | 2.78                     | 0.51              |
| 2:V:176:ALA:HA  | 2:V:186:GLN:HA   | 1.92                     | 0.51              |
| 1:B:85:ALA:O    | 1:B:89:VAL:HG23  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:160:TYR:CD2  | 1:B:163:THR:HB   | 2.45                     | 0.51              |
| 1:D:70:ILE:HB    | 1:D:74:VAL:HG13  | 1.92                     | 0.51              |
| 2:J:189:THR:HG23 | 2:J:190:ASP:N    | 2.25                     | 0.51              |
| 2:K:174:ASP:HA   | 2:K:192:ILE:HD13 | 1.92                     | 0.51              |
| 2:M:165:ARG:HG2  | 2:1:135:TYR:HB3  | 1.91                     | 0.51              |
| 2:N:141:GLN:NE2  | 2:Z:141:GLN:NE2  | 2.58                     | 0.51              |
| 2:N:165:ARG:HA   | 2:Y:26:ILE:HG23  | 1.92                     | 0.51              |
| 1:P:108:ASN:CB   | 2:X:70:ARG:CD    | 2.79                     | 0.51              |
| 1:Q:12:ILE:HG13  | 1:Q:12:ILE:O     | 2.09                     | 0.51              |
| 1:Q:42:PHE:CD1   | 1:Q:43:ALA:N     | 2.78                     | 0.51              |
| 1:S:161:LYS:CA   | 1:T:60:GLU:OE2   | 2.56                     | 0.51              |
| 1:T:42:PHE:CD1   | 1:T:43:ALA:N     | 2.78                     | 0.51              |
| 2:Y:174:ASP:HA   | 2:Y:192:ILE:HD13 | 1.92                     | 0.51              |
| 1:B:21:LEU:O     | 1:B:24:VAL:HG12  | 2.10                     | 0.51              |
| 1:C:103:TYR:O    | 2:K:81:THR:CB    | 2.58                     | 0.51              |
| 1:E:173:VAL:HG22 | 1:F:58:LEU:CD2   | 2.40                     | 0.51              |
| 1:G:70:ILE:HB    | 1:G:74:VAL:HG13  | 1.92                     | 0.51              |
| 2:L:29:LYS:NZ    | 2:1:164:GLN:HE21 | 2.08                     | 0.51              |
| 1:Q:191:THR:O    | 1:Q:194:ILE:HG22 | 2.11                     | 0.51              |
| 1:T:70:ILE:HB    | 1:T:74:VAL:HG13  | 1.92                     | 0.51              |
| 2:W:18:ARG:HE    | 2:W:30:ASN:HD22  | 1.57                     | 0.51              |
| 2:1:124:TYR:HD2  | 2:1:138:LEU:HD23 | 1.76                     | 0.51              |
| 1:B:70:ILE:HB    | 1:B:74:VAL:HG13  | 1.92                     | 0.51              |
| 1:E:19:GLY:HA3   | 1:F:30:ALA:CA    | 2.39                     | 0.51              |
| 1:F:102:THR:O    | 2:N:85:ASN:CG    | 2.47                     | 0.51              |
| 1:G:42:PHE:CD1   | 1:G:43:ALA:N     | 2.78                     | 0.51              |
| 1:G:160:TYR:CD2  | 1:G:163:THR:HB   | 2.45                     | 0.51              |
| 2:I:179:THR:HG23 | 2:I:182:ASP:H    | 1.75                     | 0.51              |
| 2:N:2:THR:HG22   | 2:N:169:SER:OG   | 2.10                     | 0.51              |
| 1:P:21:LEU:O     | 1:P:24:VAL:HG12  | 2.10                     | 0.51              |
| 1:R:12:ILE:HG13  | 1:R:12:ILE:O     | 2.09                     | 0.51              |
| 1:R:125:GLN:O    | 1:S:129:VAL:CG2  | 2.56                     | 0.51              |
| 1:T:85:ALA:O     | 1:T:89:VAL:HG23  | 2.10                     | 0.51              |
| 1:A:21:LEU:O     | 1:A:24:VAL:HG12  | 2.10                     | 0.51              |
| 1:A:42:PHE:CD1   | 1:A:43:ALA:N     | 2.78                     | 0.51              |
| 1:A:103:TYR:O    | 2:I:81:THR:HB    | 2.11                     | 0.51              |
| 1:B:180:TYR:HA   | 1:B:192:LEU:HD21 | 1.93                     | 0.51              |
| 1:E:85:ALA:O     | 1:E:89:VAL:HG23  | 2.10                     | 0.51              |
| 1:F:19:GLY:HA3   | 1:G:30:ALA:HB2   | 1.91                     | 0.51              |
| 1:F:191:THR:O    | 1:F:194:ILE:HG22 | 2.11                     | 0.51              |
| 1:P:42:PHE:CD1   | 1:P:43:ALA:N     | 2.78                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:160:TYR:CD2  | 1:R:163:THR:HB   | 2.45                     | 0.51              |
| 1:S:42:PHE:CD1   | 1:S:43:ALA:N     | 2.78                     | 0.51              |
| 2:Z:124:TYR:HD2  | 2:Z:138:LEU:HD23 | 1.76                     | 0.51              |
| 1:A:7:ALA:HB1    | 1:B:10:ARG:NH1   | 2.25                     | 0.51              |
| 1:A:108:ASN:HD22 | 2:I:70:ARG:CB    | 2.22                     | 0.51              |
| 1:C:21:LEU:O     | 1:C:24:VAL:HG12  | 2.10                     | 0.51              |
| 1:C:180:TYR:HA   | 1:C:192:LEU:HD21 | 1.93                     | 0.51              |
| 1:E:191:THR:O    | 1:E:194:ILE:HG22 | 2.11                     | 0.51              |
| 1:F:177:GLU:O    | 1:G:58:LEU:HD11  | 2.07                     | 0.51              |
| 1:G:191:THR:O    | 1:G:194:ILE:HG22 | 2.11                     | 0.51              |
| 2:L:141:GLN:NE2  | 2:2:141:GLN:HE21 | 2.09                     | 0.51              |
| 2:M:164:GLN:HE21 | 2:Z:29:LYS:NZ    | 2.07                     | 0.51              |
| 1:O:180:TYR:HA   | 1:O:192:LEU:HD21 | 1.93                     | 0.51              |
| 1:O:191:THR:O    | 1:O:194:ILE:HG22 | 2.11                     | 0.51              |
| 1:Q:85:ALA:O     | 1:Q:89:VAL:HG23  | 2.10                     | 0.51              |
| 1:Q:107:VAL:HG11 | 2:Y:66:TYR:HH    | 1.75                     | 0.51              |
| 1:R:191:THR:O    | 1:R:194:ILE:HG22 | 2.11                     | 0.51              |
| 1:S:191:THR:O    | 1:S:194:ILE:HG22 | 2.11                     | 0.51              |
| 2:V:116:ALA:O    | 2:2:50:GLY:HA3   | 2.11                     | 0.51              |
| 1:A:70:ILE:HB    | 1:A:74:VAL:HG13  | 1.92                     | 0.51              |
| 1:A:101:VAL:HG22 | 2:H:58:TYR:HE1   | 1.76                     | 0.51              |
| 1:B:191:THR:O    | 1:B:194:ILE:HG22 | 2.11                     | 0.51              |
| 1:D:149:PHE:CE1  | 1:D:159:GLU:HB2  | 2.46                     | 0.51              |
| 2:I:18:ARG:HE    | 2:I:30:ASN:HD22  | 1.57                     | 0.51              |
| 2:K:53:GLN:O     | 2:K:56:VAL:HG12  | 2.10                     | 0.51              |
| 2:L:55:LEU:HD21  | 2:L:87:LEU:HD11  | 1.92                     | 0.51              |
| 1:P:191:THR:O    | 1:P:194:ILE:HG22 | 2.11                     | 0.51              |
| 1:R:19:GLY:HA3   | 1:S:30:ALA:CA    | 2.41                     | 0.51              |
| 1:R:160:TYR:C    | 1:S:60:GLU:HG3   | 2.35                     | 0.51              |
| 1:S:21:LEU:CD1   | 1:T:130:ARG:HD2  | 2.27                     | 0.51              |
| 1:S:70:ILE:HB    | 1:S:74:VAL:HG13  | 1.92                     | 0.51              |
| 1:S:180:TYR:HA   | 1:S:192:LEU:HD21 | 1.93                     | 0.51              |
| 1:T:191:THR:O    | 1:T:194:ILE:HG22 | 2.11                     | 0.51              |
| 1:U:180:TYR:HA   | 1:U:192:LEU:HD21 | 1.93                     | 0.51              |
| 2:2:36:GLN:HB2   | 2:2:184:TYR:CE1  | 2.46                     | 0.51              |
| 1:A:191:THR:O    | 1:A:194:ILE:HG22 | 2.11                     | 0.51              |
| 1:C:177:GLU:H    | 1:D:58:LEU:CD2   | 2.06                     | 0.51              |
| 1:F:7:ALA:HB1    | 1:G:10:ARG:NH1   | 2.22                     | 0.51              |
| 1:F:12:ILE:HG13  | 1:F:12:ILE:O     | 2.09                     | 0.51              |
| 2:H:116:ALA:O    | 2:N:50:GLY:HA3   | 2.11                     | 0.51              |
| 2:N:36:GLN:HB2   | 2:N:184:TYR:CE1  | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:7:ALA:HB1    | 1:P:10:ARG:NH1   | 2.25                     | 0.51              |
| 1:O:177:GLU:CA   | 1:P:58:LEU:HD13  | 2.17                     | 0.51              |
| 1:P:161:LYS:CD   | 1:Q:60:GLU:OE2   | 2.51                     | 0.51              |
| 1:R:180:TYR:HA   | 1:R:192:LEU:HD21 | 1.93                     | 0.51              |
| 1:S:160:TYR:CD2  | 1:S:163:THR:HB   | 2.45                     | 0.51              |
| 1:T:180:TYR:HA   | 1:T:192:LEU:HD21 | 1.93                     | 0.51              |
| 2:W:59:MET:CE    | 2:W:82:LEU:HD23  | 2.41                     | 0.51              |
| 2:1:131:SER:O    | 2:1:134:VAL:HG13 | 2.10                     | 0.51              |
| 1:D:15:PHE:HZ    | 1:E:133:GLY:N    | 2.09                     | 0.51              |
| 1:D:107:VAL:CG1  | 2:L:66:TYR:OH    | 2.59                     | 0.51              |
| 1:D:180:TYR:HA   | 1:D:192:LEU:HD21 | 1.93                     | 0.51              |
| 1:E:21:LEU:O     | 1:E:24:VAL:HG12  | 2.10                     | 0.51              |
| 1:E:160:TYR:HA   | 1:F:60:GLU:CG    | 2.41                     | 0.51              |
| 1:F:85:ALA:O     | 1:F:89:VAL:HG23  | 2.11                     | 0.51              |
| 1:F:180:TYR:HA   | 1:F:192:LEU:HD21 | 1.93                     | 0.51              |
| 2:I:59:MET:CE    | 2:I:82:LEU:HD23  | 2.41                     | 0.51              |
| 2:M:62:GLU:HG2   | 2:M:82:LEU:HD21  | 1.93                     | 0.51              |
| 2:N:123:ILE:HG12 | 2:N:124:TYR:CD2  | 2.44                     | 0.51              |
| 1:O:149:PHE:CE1  | 1:O:159:GLU:HB2  | 2.46                     | 0.51              |
| 1:R:107:VAL:CG1  | 2:Z:66:TYR:OH    | 2.59                     | 0.51              |
| 1:S:21:LEU:O     | 1:S:24:VAL:HG12  | 2.10                     | 0.51              |
| 1:S:160:TYR:HA   | 1:T:60:GLU:CG    | 2.41                     | 0.51              |
| 1:C:85:ALA:O     | 1:C:89:VAL:HG23  | 2.10                     | 0.51              |
| 1:E:180:TYR:HA   | 1:E:192:LEU:HD21 | 1.93                     | 0.51              |
| 1:P:85:ALA:O     | 1:P:89:VAL:HG23  | 2.11                     | 0.51              |
| 1:P:180:TYR:HA   | 1:P:192:LEU:HD21 | 1.93                     | 0.51              |
| 1:T:21:LEU:O     | 1:T:24:VAL:HG12  | 2.10                     | 0.51              |
| 1:U:21:LEU:O     | 1:U:24:VAL:HG12  | 2.10                     | 0.51              |
| 2:W:15:ALA:HB2   | 2:W:175:VAL:HB   | 1.93                     | 0.51              |
| 2:Y:53:GLN:O     | 2:Y:56:VAL:HG12  | 2.10                     | 0.51              |
| 2:2:20:VAL:HG13  | 2:2:28:HIS:HB2   | 1.93                     | 0.51              |
| 1:A:12:ILE:HA    | 1:A:23:GLN:CG    | 2.21                     | 0.50              |
| 1:A:108:ASN:ND2  | 2:I:70:ARG:CG    | 2.73                     | 0.50              |
| 1:A:160:TYR:CD2  | 1:A:163:THR:HB   | 2.45                     | 0.50              |
| 1:D:19:GLY:C     | 1:E:30:ALA:HB2   | 2.36                     | 0.50              |
| 1:D:161:LYS:N    | 1:E:60:GLU:CG    | 2.71                     | 0.50              |
| 1:G:12:ILE:HG13  | 1:G:12:ILE:O     | 2.09                     | 0.50              |
| 2:H:176:ALA:HA   | 2:H:186:GLN:HA   | 1.92                     | 0.50              |
| 2:J:160:SER:HA   | 2:J:163:LYS:HD3  | 1.93                     | 0.50              |
| 1:U:85:ALA:O     | 1:U:89:VAL:HG23  | 2.11                     | 0.50              |
| 1:A:180:TYR:HA   | 1:A:192:LEU:HD21 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:149:PHE:CE1  | 1:G:159:GLU:HB2  | 2.46                     | 0.50              |
| 1:G:180:TYR:HA   | 1:G:192:LEU:HD21 | 1.93                     | 0.50              |
| 2:N:20:VAL:HG13  | 2:N:28:HIS:HB2   | 1.93                     | 0.50              |
| 1:Q:149:PHE:CE1  | 1:Q:159:GLU:HB2  | 2.46                     | 0.50              |
| 1:S:108:ASN:HD22 | 2:1:70:ARG:HB3   | 1.75                     | 0.50              |
| 2:W:3:THR:OG1    | 2:W:127:THR:HG22 | 2.12                     | 0.50              |
| 2:W:179:THR:HG23 | 2:W:182:ASP:H    | 1.75                     | 0.50              |
| 1:A:149:PHE:CE1  | 1:A:159:GLU:HB2  | 2.46                     | 0.50              |
| 1:C:191:THR:O    | 1:C:194:ILE:HG22 | 2.11                     | 0.50              |
| 1:E:103:TYR:CD1  | 2:M:82:LEU:HB2   | 2.46                     | 0.50              |
| 2:M:49:VAL:HG23  | 2:M:50:GLY:N     | 2.25                     | 0.50              |
| 1:Q:157:ILE:HG22 | 1:R:86:ARG:NH1   | 2.26                     | 0.50              |
| 1:U:191:THR:O    | 1:U:194:ILE:HG22 | 2.11                     | 0.50              |
| 2:V:124:TYR:HD2  | 2:V:138:LEU:HD23 | 1.76                     | 0.50              |
| 2:1:62:GLU:HG2   | 2:1:82:LEU:HD21  | 1.93                     | 0.50              |
| 1:D:191:THR:O    | 1:D:194:ILE:HG22 | 2.11                     | 0.50              |
| 1:E:149:PHE:CE1  | 1:E:159:GLU:HB2  | 2.46                     | 0.50              |
| 1:E:177:GLU:N    | 1:F:58:LEU:CD2   | 2.58                     | 0.50              |
| 1:F:149:PHE:CE1  | 1:F:159:GLU:HB2  | 2.46                     | 0.50              |
| 1:G:103:TYR:CE1  | 2:H:82:LEU:HD22  | 2.44                     | 0.50              |
| 1:R:149:PHE:CE1  | 1:R:159:GLU:HB2  | 2.46                     | 0.50              |
| 2:2:112:SER:O    | 2:2:113:ILE:HD13 | 2.12                     | 0.50              |
| 1:D:15:PHE:CE2   | 1:E:131:PRO:O    | 2.65                     | 0.50              |
| 2:H:124:TYR:HD2  | 2:H:138:LEU:HD23 | 1.76                     | 0.50              |
| 2:J:174:ASP:HA   | 2:J:192:ILE:HD13 | 1.94                     | 0.50              |
| 1:O:12:ILE:HD13  | 1:O:23:GLN:CA    | 1.93                     | 0.50              |
| 1:P:149:PHE:CE1  | 1:P:159:GLU:HB2  | 2.46                     | 0.50              |
| 1:Q:180:TYR:HA   | 1:Q:192:LEU:HD21 | 1.93                     | 0.50              |
| 2:1:49:VAL:HG23  | 2:1:50:GLY:N     | 2.25                     | 0.50              |
| 1:C:157:ILE:HG22 | 1:D:86:ARG:NH1   | 2.26                     | 0.50              |
| 1:E:93:ARG:HB3   | 2:L:65:LEU:HD11  | 1.94                     | 0.50              |
| 1:F:15:PHE:HZ    | 1:G:130:ARG:NH1  | 2.07                     | 0.50              |
| 1:F:173:VAL:O    | 1:G:58:LEU:CD2   | 2.60                     | 0.50              |
| 2:M:20:VAL:CG1   | 2:M:28:HIS:HB2   | 2.36                     | 0.50              |
| 1:R:15:PHE:HZ    | 1:S:133:GLY:N    | 2.10                     | 0.50              |
| 1:S:71:ASP:HA    | 2:Z:68:LEU:HD21  | 1.94                     | 0.50              |
| 1:S:103:TYR:CD1  | 2:1:82:LEU:HB2   | 2.46                     | 0.50              |
| 2:X:160:SER:HA   | 2:X:163:LYS:HD3  | 1.94                     | 0.50              |
| 2:Z:133:PHE:CZ   | 2:Z:165:ARG:HB3  | 2.47                     | 0.50              |
| 1:D:19:GLY:HA3   | 1:E:30:ALA:CA    | 2.41                     | 0.50              |
| 1:E:15:PHE:CZ    | 1:F:133:GLY:CA   | 2.95                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:15:ALA:HB2   | 2:I:175:VAL:HB   | 1.93                     | 0.50              |
| 2:M:132:PRO:HA   | 2:1:133:PHE:CE1  | 2.47                     | 0.50              |
| 2:M:133:PHE:CE1  | 2:1:132:PRO:HA   | 2.47                     | 0.50              |
| 1:R:15:PHE:CE2   | 1:S:131:PRO:O    | 2.65                     | 0.50              |
| 1:R:126:TYR:HA   | 1:S:129:VAL:HG23 | 1.94                     | 0.50              |
| 1:S:149:PHE:CE1  | 1:S:159:GLU:HB2  | 2.46                     | 0.50              |
| 1:T:173:VAL:O    | 1:U:58:LEU:CD2   | 2.60                     | 0.50              |
| 1:U:103:TYR:CE1  | 2:V:82:LEU:CD1   | 2.83                     | 0.50              |
| 2:X:123:ILE:H    | 2:X:123:ILE:CD1  | 2.23                     | 0.50              |
| 1:B:177:GLU:CB   | 1:C:58:LEU:CD2   | 2.88                     | 0.50              |
| 2:I:59:MET:HE1   | 2:I:82:LEU:CD2   | 2.42                     | 0.50              |
| 2:I:173:ILE:C    | 2:I:173:ILE:HD13 | 2.37                     | 0.50              |
| 2:N:123:ILE:H    | 2:N:123:ILE:CD1  | 2.24                     | 0.50              |
| 1:O:100:LYS:NZ   | 2:V:64:GLU:OE1   | 2.43                     | 0.50              |
| 1:O:177:GLU:CB   | 1:P:58:LEU:HD22  | 2.32                     | 0.50              |
| 2:W:66:TYR:CZ    | 2:W:70:ARG:HD2   | 2.46                     | 0.50              |
| 2:W:173:ILE:C    | 2:W:173:ILE:HD13 | 2.37                     | 0.50              |
| 1:A:21:LEU:CD1   | 1:B:130:ARG:HD2  | 2.20                     | 0.50              |
| 2:M:26:ILE:HD13  | 2:M:26:ILE:O     | 2.11                     | 0.50              |
| 1:O:103:TYR:O    | 2:W:81:THR:HB    | 2.11                     | 0.50              |
| 1:B:149:PHE:CE1  | 1:B:159:GLU:HB2  | 2.46                     | 0.49              |
| 1:D:125:GLN:O    | 1:E:129:VAL:CG2  | 2.56                     | 0.49              |
| 1:E:107:VAL:HG21 | 2:M:66:TYR:HH    | 1.76                     | 0.49              |
| 2:I:66:TYR:CZ    | 2:I:70:ARG:HD2   | 2.46                     | 0.49              |
| 2:N:18:ARG:HE    | 2:N:30:ASN:HD22  | 1.57                     | 0.49              |
| 1:R:137:ILE:HG22 | 1:R:150:ASP:HB2  | 1.94                     | 0.49              |
| 1:S:137:ILE:HG22 | 1:S:150:ASP:HB2  | 1.94                     | 0.49              |
| 2:1:26:ILE:HD13  | 2:1:26:ILE:O     | 2.11                     | 0.49              |
| 1:A:23:GLN:NE2   | 1:G:15:PHE:H     | 2.10                     | 0.49              |
| 1:A:108:ASN:HD22 | 2:I:70:ARG:HG2   | 1.77                     | 0.49              |
| 1:A:137:ILE:HG22 | 1:A:150:ASP:HB2  | 1.95                     | 0.49              |
| 1:A:177:GLU:CA   | 1:B:58:LEU:HD13  | 2.17                     | 0.49              |
| 1:C:110:GLU:O    | 1:C:113:VAL:HG12 | 2.13                     | 0.49              |
| 1:G:137:ILE:HG22 | 1:G:150:ASP:HB2  | 1.94                     | 0.49              |
| 2:L:133:PHE:CZ   | 2:L:165:ARG:HB3  | 2.47                     | 0.49              |
| 1:O:170:ASP:O    | 1:O:173:VAL:HG12 | 2.13                     | 0.49              |
| 1:P:137:ILE:HG22 | 1:P:150:ASP:HB2  | 1.95                     | 0.49              |
| 1:U:149:PHE:CE1  | 1:U:159:GLU:HB2  | 2.46                     | 0.49              |
| 2:V:178:ILE:HB   | 2:V:184:TYR:HA   | 1.93                     | 0.49              |
| 1:D:126:TYR:HA   | 1:E:129:VAL:HG23 | 1.94                     | 0.49              |
| 2:I:3:THR:OG1    | 2:I:127:THR:HG22 | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:132:PRO:HA   | 2:2:133:PHE:CE1  | 2.47                     | 0.49              |
| 1:O:137:ILE:HG22 | 1:O:150:ASP:HB2  | 1.94                     | 0.49              |
| 1:Q:137:ILE:HG22 | 1:Q:150:ASP:CB   | 2.43                     | 0.49              |
| 1:Q:170:ASP:O    | 1:Q:173:VAL:HG12 | 2.13                     | 0.49              |
| 1:S:15:PHE:CZ    | 1:T:133:GLY:CA   | 2.95                     | 0.49              |
| 1:S:93:ARG:HB3   | 2:Z:65:LEU:HD11  | 1.94                     | 0.49              |
| 1:U:110:GLU:O    | 1:U:113:VAL:HG12 | 2.13                     | 0.49              |
| 1:A:110:GLU:O    | 1:A:113:VAL:HG12 | 2.13                     | 0.49              |
| 1:B:137:ILE:HG22 | 1:B:150:ASP:HB2  | 1.94                     | 0.49              |
| 1:C:149:PHE:CE1  | 1:C:159:GLU:HB2  | 2.46                     | 0.49              |
| 1:D:170:ASP:O    | 1:D:173:VAL:HG12 | 2.13                     | 0.49              |
| 1:E:137:ILE:HG22 | 1:E:150:ASP:HB2  | 1.95                     | 0.49              |
| 1:G:137:ILE:HG22 | 1:G:150:ASP:CB   | 2.43                     | 0.49              |
| 1:O:101:VAL:HG22 | 2:V:58:TYR:HE1   | 1.76                     | 0.49              |
| 1:Q:137:ILE:HG22 | 1:Q:150:ASP:HB2  | 1.94                     | 0.49              |
| 1:R:19:GLY:C     | 1:S:30:ALA:HB2   | 2.36                     | 0.49              |
| 1:S:110:GLU:O    | 1:S:113:VAL:HG12 | 2.13                     | 0.49              |
| 2:X:174:ASP:HA   | 2:X:192:ILE:HD13 | 1.94                     | 0.49              |
| 1:B:62:ASN:O     | 1:B:65:GLU:HG2   | 2.13                     | 0.49              |
| 1:C:137:ILE:HG22 | 1:C:150:ASP:HB2  | 1.94                     | 0.49              |
| 1:C:178:ARG:C    | 1:D:57:ARG:NH2   | 2.67                     | 0.49              |
| 1:D:62:ASN:O     | 1:D:65:GLU:HG2   | 2.12                     | 0.49              |
| 1:D:137:ILE:HG22 | 1:D:150:ASP:CB   | 2.43                     | 0.49              |
| 1:F:137:ILE:HG22 | 1:F:150:ASP:HB2  | 1.94                     | 0.49              |
| 1:F:170:ASP:O    | 1:F:173:VAL:HG12 | 2.13                     | 0.49              |
| 2:K:179:THR:HG23 | 2:K:182:ASP:H    | 1.77                     | 0.49              |
| 1:P:155:GLY:O    | 1:Q:86:ARG:CZ    | 2.61                     | 0.49              |
| 1:R:110:GLU:O    | 1:R:113:VAL:HG12 | 2.13                     | 0.49              |
| 1:R:137:ILE:HG22 | 1:R:150:ASP:CB   | 2.43                     | 0.49              |
| 1:T:149:PHE:CE1  | 1:T:159:GLU:HB2  | 2.46                     | 0.49              |
| 2:Z:189:THR:HG23 | 2:Z:190:ASP:N    | 2.28                     | 0.49              |
| 1:B:228:GLU:O    | 1:B:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:C:62:ASN:O     | 1:C:65:GLU:HG2   | 2.12                     | 0.49              |
| 1:C:228:GLU:O    | 1:C:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:G:110:GLU:O    | 1:G:113:VAL:HG12 | 2.13                     | 0.49              |
| 1:G:228:GLU:O    | 1:G:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:O:110:GLU:O    | 1:O:113:VAL:HG12 | 2.13                     | 0.49              |
| 1:R:170:ASP:O    | 1:R:173:VAL:HG12 | 2.13                     | 0.49              |
| 1:R:228:GLU:O    | 1:R:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:T:137:ILE:HG22 | 1:T:150:ASP:HB2  | 1.95                     | 0.49              |
| 1:U:137:ILE:HG22 | 1:U:150:ASP:HB2  | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:62:ASN:O     | 1:A:65:GLU:HG2   | 2.13                     | 0.49              |
| 1:A:228:GLU:O    | 1:A:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:C:177:GLU:C    | 1:D:58:LEU:CD1   | 2.41                     | 0.49              |
| 1:D:137:ILE:HG22 | 1:D:150:ASP:HB2  | 1.94                     | 0.49              |
| 1:E:110:GLU:O    | 1:E:113:VAL:HG12 | 2.13                     | 0.49              |
| 1:P:177:GLU:HA   | 1:Q:58:LEU:CG    | 2.19                     | 0.49              |
| 1:S:228:GLU:O    | 1:S:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:U:62:ASN:O     | 1:U:65:GLU:HG2   | 2.13                     | 0.49              |
| 1:U:228:GLU:O    | 1:U:231:LYS:HB3  | 2.13                     | 0.49              |
| 2:W:59:MET:HE1   | 2:W:82:LEU:CD2   | 2.42                     | 0.49              |
| 2:X:62:GLU:HG2   | 2:X:82:LEU:HD21  | 1.94                     | 0.49              |
| 1:A:137:ILE:HG22 | 1:A:150:ASP:CB   | 2.43                     | 0.49              |
| 1:C:170:ASP:O    | 1:C:173:VAL:HG12 | 2.13                     | 0.49              |
| 1:D:228:GLU:O    | 1:D:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:E:228:GLU:O    | 1:E:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:F:137:ILE:HG22 | 1:F:150:ASP:CB   | 2.43                     | 0.49              |
| 2:K:26:ILE:HG23  | 2:2:165:ARG:HA   | 1.94                     | 0.49              |
| 1:O:228:GLU:O    | 1:O:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:P:228:GLU:O    | 1:P:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:T:228:GLU:O    | 1:T:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:U:170:ASP:O    | 1:U:173:VAL:HG12 | 2.13                     | 0.49              |
| 1:B:110:GLU:O    | 1:B:113:VAL:HG12 | 2.13                     | 0.49              |
| 1:B:155:GLY:O    | 1:C:86:ARG:CZ    | 2.61                     | 0.49              |
| 1:F:228:GLU:O    | 1:F:231:LYS:HB3  | 2.13                     | 0.49              |
| 1:G:170:ASP:O    | 1:G:173:VAL:HG12 | 2.13                     | 0.49              |
| 2:H:26:ILE:HG23  | 2:X:165:ARG:HA   | 1.94                     | 0.49              |
| 2:H:178:ILE:HB   | 2:H:184:TYR:HA   | 1.93                     | 0.49              |
| 1:O:62:ASN:O     | 1:O:65:GLU:HG2   | 2.12                     | 0.49              |
| 1:P:101:VAL:CG2  | 2:W:58:TYR:HE1   | 2.21                     | 0.49              |
| 1:Q:12:ILE:HD12  | 1:Q:23:GLN:HB2   | 0.74                     | 0.49              |
| 1:Q:62:ASN:O     | 1:Q:65:GLU:HG2   | 2.13                     | 0.49              |
| 1:R:62:ASN:O     | 1:R:65:GLU:HG2   | 2.13                     | 0.49              |
| 1:T:7:ALA:HB1    | 1:U:10:ARG:NH1   | 2.22                     | 0.49              |
| 1:T:62:ASN:O     | 1:T:65:GLU:HG2   | 2.13                     | 0.49              |
| 2:W:124:TYR:HD2  | 2:W:138:LEU:HD23 | 1.78                     | 0.49              |
| 1:B:170:ASP:O    | 1:B:173:VAL:HG12 | 2.13                     | 0.49              |
| 1:C:126:TYR:HH   | 1:D:123:TYR:HH   | 1.61                     | 0.49              |
| 1:D:110:GLU:O    | 1:D:113:VAL:HG12 | 2.13                     | 0.49              |
| 1:E:15:PHE:HE2   | 1:F:131:PRO:O    | 1.96                     | 0.49              |
| 1:G:62:ASN:O     | 1:G:65:GLU:HG2   | 2.13                     | 0.49              |
| 1:S:62:ASN:O     | 1:S:65:GLU:HG2   | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:170:ASP:O    | 1:T:173:VAL:HG12 | 2.13                     | 0.49              |
| 2:X:66:TYR:CD2   | 2:X:74:MET:HE2   | 2.48                     | 0.49              |
| 1:C:137:ILE:HG22 | 1:C:150:ASP:CB   | 2.43                     | 0.48              |
| 1:F:62:ASN:O     | 1:F:65:GLU:HG2   | 2.13                     | 0.48              |
| 2:J:18:ARG:HB2   | 2:J:31:GLY:O     | 2.13                     | 0.48              |
| 2:M:76:ILE:O     | 2:M:79:VAL:HG12  | 2.13                     | 0.48              |
| 2:N:112:SER:O    | 2:N:113:ILE:HD13 | 2.12                     | 0.48              |
| 2:N:141:GLN:HE21 | 2:Z:141:GLN:NE2  | 2.11                     | 0.48              |
| 1:O:137:ILE:HG22 | 1:O:150:ASP:CB   | 2.43                     | 0.48              |
| 1:Q:110:GLU:O    | 1:Q:113:VAL:HG12 | 2.13                     | 0.48              |
| 1:S:137:ILE:HG22 | 1:S:150:ASP:CB   | 2.43                     | 0.48              |
| 1:T:110:GLU:O    | 1:T:113:VAL:HG12 | 2.13                     | 0.48              |
| 1:B:107:VAL:CG2  | 2:J:66:TYR:OH    | 2.62                     | 0.48              |
| 1:B:177:GLU:CA   | 1:C:58:LEU:CG    | 2.88                     | 0.48              |
| 1:C:103:TYR:C    | 2:K:81:THR:HG22  | 2.37                     | 0.48              |
| 1:E:17:PRO:O     | 1:F:29:GLU:HG3   | 2.13                     | 0.48              |
| 1:E:62:ASN:O     | 1:E:65:GLU:HG2   | 2.13                     | 0.48              |
| 1:E:71:ASP:HA    | 2:L:68:LEU:HD21  | 1.94                     | 0.48              |
| 1:E:137:ILE:HG22 | 1:E:150:ASP:CB   | 2.43                     | 0.48              |
| 1:Q:228:GLU:O    | 1:Q:231:LYS:HB3  | 2.13                     | 0.48              |
| 2:Y:175:VAL:CG2  | 2:Y:176:ALA:N    | 2.75                     | 0.48              |
| 2:1:76:ILE:O     | 2:1:79:VAL:HG12  | 2.13                     | 0.48              |
| 1:E:170:ASP:O    | 1:E:173:VAL:HG12 | 2.13                     | 0.48              |
| 2:N:1:THR:H3     | 2:N:129:SER:HB3  | 1.79                     | 0.48              |
| 1:P:110:GLU:O    | 1:P:113:VAL:HG12 | 2.13                     | 0.48              |
| 1:S:14:VAL:H     | 1:T:130:ARG:HB2  | 1.78                     | 0.48              |
| 1:S:17:PRO:O     | 1:T:29:GLU:HG3   | 2.13                     | 0.48              |
| 2:Y:179:THR:HG23 | 2:Y:182:ASP:H    | 1.77                     | 0.48              |
| 1:A:30:ALA:HB2   | 1:G:19:GLY:O     | 2.13                     | 0.48              |
| 1:A:170:ASP:O    | 1:A:173:VAL:HG12 | 2.13                     | 0.48              |
| 1:D:148:LEU:O    | 1:D:159:GLU:HG3  | 2.14                     | 0.48              |
| 2:H:12:VAL:HG13  | 2:H:178:ILE:HG23 | 1.96                     | 0.48              |
| 2:I:189:THR:HG23 | 2:I:190:ASP:N    | 2.28                     | 0.48              |
| 1:S:170:ASP:O    | 1:S:173:VAL:HG12 | 2.13                     | 0.48              |
| 2:V:36:GLN:HB2   | 2:V:184:TYR:CE1  | 2.48                     | 0.48              |
| 1:E:14:VAL:H     | 1:F:130:ARG:HB2  | 1.79                     | 0.48              |
| 2:H:36:GLN:HB2   | 2:H:184:TYR:CE1  | 2.48                     | 0.48              |
| 2:K:175:VAL:CG2  | 2:K:176:ALA:N    | 2.75                     | 0.48              |
| 1:P:107:VAL:CG2  | 2:X:66:TYR:OH    | 2.62                     | 0.48              |
| 1:P:137:ILE:HG22 | 1:P:150:ASP:CB   | 2.43                     | 0.48              |
| 1:U:137:ILE:HG22 | 1:U:150:ASP:CB   | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:123:ILE:HD13 | 2:2:123:ILE:N    | 2.26                     | 0.48              |
| 1:F:110:GLU:O    | 1:F:113:VAL:HG12 | 2.13                     | 0.48              |
| 2:H:17:GLU:HB2   | 2:H:170:GLY:O    | 2.14                     | 0.48              |
| 2:L:18:ARG:HE    | 2:L:30:ASN:HD22  | 1.61                     | 0.48              |
| 2:L:189:THR:HG23 | 2:L:190:ASP:N    | 2.28                     | 0.48              |
| 2:N:139:GLU:OE1  | 2:Z:165:ARG:NE   | 2.46                     | 0.48              |
| 1:O:30:ALA:HB2   | 1:U:19:GLY:O     | 2.13                     | 0.48              |
| 1:O:148:LEU:O    | 1:O:159:GLU:HG3  | 2.14                     | 0.48              |
| 1:P:97:GLN:OE1   | 2:W:61:ALA:CB    | 2.60                     | 0.48              |
| 1:P:170:ASP:O    | 1:P:173:VAL:HG12 | 2.13                     | 0.48              |
| 1:A:148:LEU:O    | 1:A:159:GLU:HG3  | 2.14                     | 0.48              |
| 1:B:137:ILE:HG22 | 1:B:150:ASP:CB   | 2.43                     | 0.48              |
| 1:D:111:ASN:CG   | 2:L:70:ARG:HH12  | 2.17                     | 0.48              |
| 1:E:108:ASN:HD22 | 2:M:70:ARG:HB3   | 1.75                     | 0.48              |
| 1:E:160:TYR:C    | 1:F:60:GLU:HG2   | 2.39                     | 0.48              |
| 1:G:101:VAL:HG21 | 2:N:58:TYR:HD1   | 1.47                     | 0.48              |
| 1:G:148:LEU:O    | 1:G:159:GLU:HG3  | 2.14                     | 0.48              |
| 2:J:66:TYR:CD2   | 2:J:74:MET:HE2   | 2.48                     | 0.48              |
| 1:P:103:TYR:HE1  | 2:X:82:LEU:HD22  | 1.79                     | 0.48              |
| 1:P:177:GLU:HA   | 1:Q:58:LEU:HD11  | 0.48                     | 0.48              |
| 1:S:148:LEU:O    | 1:S:159:GLU:HG3  | 2.14                     | 0.48              |
| 1:B:177:GLU:HA   | 1:C:58:LEU:HD11  | 0.48                     | 0.48              |
| 1:P:62:ASN:O     | 1:P:65:GLU:HG2   | 2.13                     | 0.48              |
| 1:R:148:LEU:O    | 1:R:159:GLU:HG3  | 2.14                     | 0.48              |
| 1:R:157:ILE:HG22 | 1:S:86:ARG:NH1   | 2.29                     | 0.48              |
| 1:T:137:ILE:HG22 | 1:T:150:ASP:CB   | 2.43                     | 0.48              |
| 2:V:103:GLY:HA2  | 2:V:178:ILE:CD1  | 2.44                     | 0.48              |
| 2:Z:174:ASP:HA   | 2:Z:192:ILE:HD13 | 1.96                     | 0.48              |
| 1:A:21:LEU:CD1   | 1:B:130:ARG:CD   | 2.87                     | 0.48              |
| 1:F:101:VAL:HG23 | 2:M:58:TYR:CD1   | 2.09                     | 0.48              |
| 2:J:45:ILE:HD11  | 2:J:52:ALA:O     | 2.14                     | 0.48              |
| 2:J:165:ARG:HA   | 2:V:26:ILE:HG23  | 1.96                     | 0.48              |
| 1:P:108:ASN:HD22 | 2:X:70:ARG:CA    | 2.27                     | 0.48              |
| 1:T:134:VAL:O    | 1:T:153:PRO:HG3  | 2.14                     | 0.48              |
| 2:X:109:HIS:HB3  | 2:X:111:PHE:HE1  | 1.79                     | 0.48              |
| 1:B:134:VAL:O    | 1:B:153:PRO:HG3  | 2.14                     | 0.48              |
| 1:D:155:GLY:O    | 1:E:86:ARG:NH1   | 2.46                     | 0.48              |
| 1:G:61:GLN:CD    | 1:G:62:ASN:H     | 2.22                     | 0.48              |
| 2:I:32:LYS:HE2   | 2:I:34:LEU:O     | 2.14                     | 0.48              |
| 2:K:44:THR:OG1   | 2:K:100:LEU:HB3  | 2.14                     | 0.48              |
| 1:Q:148:LEU:O    | 1:Q:159:GLU:HG3  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:134:VAL:O    | 1:U:153:PRO:HG3  | 2.14                     | 0.48              |
| 2:Z:178:ILE:O    | 2:Z:178:ILE:HG12 | 2.14                     | 0.48              |
| 2:1:179:THR:HG23 | 2:1:182:ASP:H    | 1.79                     | 0.48              |
| 1:A:134:VAL:O    | 1:A:153:PRO:HG3  | 2.14                     | 0.47              |
| 1:B:103:TYR:HE1  | 2:J:82:LEU:HD22  | 1.79                     | 0.47              |
| 1:C:173:VAL:O    | 1:D:58:LEU:CD2   | 2.62                     | 0.47              |
| 1:E:161:LYS:CA   | 1:F:60:GLU:OE2   | 2.56                     | 0.47              |
| 2:H:25:PHE:CD1   | 2:H:25:PHE:C     | 2.90                     | 0.47              |
| 2:J:141:GLN:NE2  | 2:W:141:GLN:HE21 | 2.11                     | 0.47              |
| 2:J:152:VAL:O    | 2:J:156:ILE:HG13 | 2.14                     | 0.47              |
| 1:P:108:ASN:HD22 | 2:X:70:ARG:CG    | 2.26                     | 0.47              |
| 1:Q:134:VAL:O    | 1:Q:153:PRO:HG3  | 2.14                     | 0.47              |
| 1:R:101:VAL:HA   | 2:Y:57:ARG:HB3   | 1.96                     | 0.47              |
| 1:R:155:GLY:O    | 1:S:86:ARG:NH1   | 2.46                     | 0.47              |
| 1:S:108:ASN:ND2  | 2:1:70:ARG:CB    | 2.72                     | 0.47              |
| 1:S:177:GLU:N    | 1:T:58:LEU:CD2   | 2.58                     | 0.47              |
| 1:T:107:VAL:HG21 | 2:2:66:TYR:HH    | 1.79                     | 0.47              |
| 2:Z:25:PHE:CD1   | 2:Z:25:PHE:C     | 2.91                     | 0.47              |
| 2:1:74:MET:HG2   | 2:1:78:ALA:HB3   | 1.96                     | 0.47              |
| 1:A:58:LEU:HD22  | 1:G:173:VAL:O    | 2.11                     | 0.47              |
| 1:B:61:GLN:CD    | 1:B:62:ASN:H     | 2.22                     | 0.47              |
| 1:C:134:VAL:O    | 1:C:153:PRO:HG3  | 2.14                     | 0.47              |
| 1:F:134:VAL:O    | 1:F:153:PRO:HG3  | 2.14                     | 0.47              |
| 1:F:148:LEU:O    | 1:F:159:GLU:HG3  | 2.14                     | 0.47              |
| 1:O:108:ASN:ND2  | 2:W:70:ARG:CG    | 2.73                     | 0.47              |
| 1:R:101:VAL:HG23 | 2:Y:58:TYR:N     | 2.29                     | 0.47              |
| 1:S:134:VAL:O    | 1:S:153:PRO:HG3  | 2.14                     | 0.47              |
| 1:T:61:GLN:CD    | 1:T:62:ASN:H     | 2.23                     | 0.47              |
| 2:V:66:TYR:CZ    | 2:V:70:ARG:HD2   | 2.49                     | 0.47              |
| 2:V:126:SER:HB3  | 2:V:135:TYR:CE2  | 2.49                     | 0.47              |
| 2:W:32:LYS:HE2   | 2:W:34:LEU:O     | 2.14                     | 0.47              |
| 2:W:189:THR:HG23 | 2:W:190:ASP:N    | 2.28                     | 0.47              |
| 2:X:45:ILE:HD11  | 2:X:52:ALA:O     | 2.14                     | 0.47              |
| 2:Y:44:THR:OG1   | 2:Y:100:LEU:HB3  | 2.14                     | 0.47              |
| 1:B:148:LEU:O    | 1:B:159:GLU:HG3  | 2.14                     | 0.47              |
| 1:D:15:PHE:CZ    | 1:E:133:GLY:CA   | 2.97                     | 0.47              |
| 2:J:62:GLU:HG2   | 2:J:82:LEU:HD21  | 1.94                     | 0.47              |
| 2:J:159:ILE:O    | 2:J:163:LYS:HG3  | 2.14                     | 0.47              |
| 2:K:103:GLY:HA2  | 2:K:178:ILE:CD1  | 2.44                     | 0.47              |
| 2:L:25:PHE:CD1   | 2:L:25:PHE:C     | 2.91                     | 0.47              |
| 1:O:23:GLN:NE2   | 1:U:15:PHE:H     | 2.10                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:61:GLN:CD    | 1:P:62:ASN:H     | 2.22                     | 0.47              |
| 1:P:177:GLU:CA   | 1:Q:58:LEU:HD13  | 2.08                     | 0.47              |
| 1:U:61:GLN:CD    | 1:U:62:ASN:H     | 2.22                     | 0.47              |
| 2:W:25:PHE:CD1   | 2:W:25:PHE:C     | 2.91                     | 0.47              |
| 2:Y:124:TYR:HD2  | 2:Y:138:LEU:HD23 | 1.80                     | 0.47              |
| 2:2:76:ILE:HG21  | 2:2:109:HIS:HB2  | 1.96                     | 0.47              |
| 1:B:108:ASN:ND2  | 2:J:70:ARG:CA    | 2.77                     | 0.47              |
| 2:K:133:PHE:CZ   | 2:K:165:ARG:HB3  | 2.48                     | 0.47              |
| 2:M:7:THR:HB     | 2:M:123:ILE:O    | 2.14                     | 0.47              |
| 2:M:74:MET:HG2   | 2:M:78:ALA:HB3   | 1.95                     | 0.47              |
| 1:S:15:PHE:HE2   | 1:T:131:PRO:O    | 1.96                     | 0.47              |
| 1:T:148:LEU:O    | 1:T:159:GLU:HG3  | 2.14                     | 0.47              |
| 2:V:55:LEU:HD12  | 2:V:55:LEU:HA    | 1.50                     | 0.47              |
| 2:W:22:MET:O     | 2:W:23:GLU:HB2   | 2.14                     | 0.47              |
| 1:D:61:GLN:CD    | 1:D:62:ASN:H     | 2.23                     | 0.47              |
| 1:D:157:ILE:HG22 | 1:E:86:ARG:NH1   | 2.29                     | 0.47              |
| 1:E:61:GLN:CD    | 1:E:62:ASN:H     | 2.23                     | 0.47              |
| 2:H:6:ILE:HD11   | 2:H:142:TYR:HD1  | 1.79                     | 0.47              |
| 2:H:103:GLY:HA2  | 2:H:178:ILE:CD1  | 2.44                     | 0.47              |
| 2:I:22:MET:O     | 2:I:23:GLU:HB2   | 2.14                     | 0.47              |
| 2:I:124:TYR:HD2  | 2:I:138:LEU:HD23 | 1.78                     | 0.47              |
| 2:N:133:PHE:CE1  | 2:Z:132:PRO:HA   | 2.50                     | 0.47              |
| 2:V:12:VAL:HG13  | 2:V:178:ILE:HG23 | 1.96                     | 0.47              |
| 2:X:159:ILE:O    | 2:X:163:LYS:HG3  | 2.14                     | 0.47              |
| 1:A:57:ARG:N     | 1:G:177:GLU:OE2  | 2.48                     | 0.47              |
| 1:B:12:ILE:HD11  | 1:B:24:VAL:N     | 2.30                     | 0.47              |
| 1:B:108:ASN:HD22 | 2:J:70:ARG:CA    | 2.27                     | 0.47              |
| 1:B:177:GLU:C    | 1:C:58:LEU:HD11  | 2.24                     | 0.47              |
| 1:O:134:VAL:O    | 1:O:153:PRO:HG3  | 2.14                     | 0.47              |
| 1:P:44:ASN:HD22  | 1:P:44:ASN:HA    | 1.56                     | 0.47              |
| 1:S:19:GLY:HA3   | 1:T:30:ALA:CB    | 2.44                     | 0.47              |
| 1:T:177:GLU:C    | 1:U:58:LEU:CD1   | 2.68                     | 0.47              |
| 1:U:148:LEU:O    | 1:U:159:GLU:HG3  | 2.14                     | 0.47              |
| 2:Y:50:GLY:O     | 2:Y:54:VAL:HG12  | 2.14                     | 0.47              |
| 2:Y:133:PHE:CZ   | 2:Y:165:ARG:HB3  | 2.49                     | 0.47              |
| 1:A:12:ILE:HD11  | 1:A:24:VAL:N     | 2.30                     | 0.47              |
| 1:A:111:ASN:CG   | 2:I:70:ARG:NH1   | 2.73                     | 0.47              |
| 1:A:175:PHE:CD2  | 1:A:196:ALA:HA   | 2.50                     | 0.47              |
| 1:B:175:PHE:CD2  | 1:B:196:ALA:HA   | 2.50                     | 0.47              |
| 1:C:12:ILE:HD11  | 1:C:24:VAL:N     | 2.30                     | 0.47              |
| 1:C:61:GLN:CD    | 1:C:62:ASN:H     | 2.22                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:175:PHE:CD2  | 1:C:196:ALA:HA   | 2.50                     | 0.47              |
| 1:D:134:VAL:O    | 1:D:153:PRO:HG3  | 2.14                     | 0.47              |
| 1:E:44:ASN:HD22  | 1:E:44:ASN:HA    | 1.56                     | 0.47              |
| 1:E:93:ARG:HB3   | 2:L:65:LEU:CD1   | 2.45                     | 0.47              |
| 1:F:61:GLN:CD    | 1:F:62:ASN:H     | 2.23                     | 0.47              |
| 1:F:108:ASN:ND2  | 2:N:70:ARG:CA    | 2.78                     | 0.47              |
| 2:H:20:VAL:HG22  | 2:H:28:HIS:HB2   | 1.97                     | 0.47              |
| 2:H:66:TYR:CZ    | 2:H:70:ARG:HD2   | 2.49                     | 0.47              |
| 2:H:126:SER:HB3  | 2:H:135:TYR:CE2  | 2.49                     | 0.47              |
| 2:H:165:ARG:C    | 2:X:26:ILE:HG22  | 2.39                     | 0.47              |
| 2:I:141:GLN:HE21 | 2:X:141:GLN:NE2  | 2.12                     | 0.47              |
| 2:J:109:HIS:HB3  | 2:J:111:PHE:HE1  | 1.79                     | 0.47              |
| 2:L:178:ILE:O    | 2:L:178:ILE:HG12 | 2.14                     | 0.47              |
| 2:M:184:TYR:CD1  | 2:M:184:TYR:C    | 2.93                     | 0.47              |
| 1:O:61:GLN:CD    | 1:O:62:ASN:H     | 2.22                     | 0.47              |
| 1:P:148:LEU:O    | 1:P:159:GLU:HG3  | 2.14                     | 0.47              |
| 1:P:175:PHE:CD2  | 1:P:196:ALA:HA   | 2.50                     | 0.47              |
| 1:R:12:ILE:HD11  | 1:R:24:VAL:N     | 2.30                     | 0.47              |
| 1:R:61:GLN:CD    | 1:R:62:ASN:H     | 2.23                     | 0.47              |
| 1:S:160:TYR:HA   | 1:T:60:GLU:HG2   | 1.96                     | 0.47              |
| 1:S:175:PHE:CD2  | 1:S:196:ALA:HA   | 2.50                     | 0.47              |
| 1:T:125:GLN:O    | 1:U:129:VAL:CG2  | 2.51                     | 0.47              |
| 1:T:175:PHE:CD2  | 1:T:196:ALA:HA   | 2.50                     | 0.47              |
| 1:U:175:PHE:CD2  | 1:U:196:ALA:HA   | 2.50                     | 0.47              |
| 2:V:17:GLU:HB2   | 2:V:170:GLY:O    | 2.14                     | 0.47              |
| 2:V:25:PHE:C     | 2:V:25:PHE:CD1   | 2.90                     | 0.47              |
| 2:W:189:THR:HG23 | 2:W:190:ASP:H    | 1.79                     | 0.47              |
| 2:X:18:ARG:HB2   | 2:X:31:GLY:O     | 2.13                     | 0.47              |
| 2:X:37:ILE:HD11  | 2:X:59:MET:CB    | 2.37                     | 0.47              |
| 2:X:175:VAL:CG2  | 2:X:176:ALA:N    | 2.78                     | 0.47              |
| 2:Y:74:MET:HG2   | 2:Y:78:ALA:HB3   | 1.97                     | 0.47              |
| 2:Y:103:GLY:HA2  | 2:Y:178:ILE:CD1  | 2.44                     | 0.47              |
| 2:Z:18:ARG:HE    | 2:Z:30:ASN:HD22  | 1.61                     | 0.47              |
| 1:G:12:ILE:HD11  | 1:G:24:VAL:N     | 2.30                     | 0.47              |
| 2:L:174:ASP:HA   | 2:L:192:ILE:HD13 | 1.96                     | 0.47              |
| 2:N:18:ARG:HB2   | 2:N:31:GLY:O     | 2.15                     | 0.47              |
| 2:N:76:ILE:HG21  | 2:N:109:HIS:HB2  | 1.96                     | 0.47              |
| 2:N:91:LYS:O     | 2:N:94:PRO:HD3   | 2.15                     | 0.47              |
| 1:P:108:ASN:ND2  | 2:X:70:ARG:CA    | 2.77                     | 0.47              |
| 1:P:134:VAL:O    | 1:P:153:PRO:HG3  | 2.14                     | 0.47              |
| 1:T:12:ILE:HD11  | 1:T:24:VAL:N     | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:1:THR:H3     | 2:2:129:SER:HB3  | 1.78                     | 0.47              |
| 1:C:148:LEU:O    | 1:C:159:GLU:HG3  | 2.14                     | 0.47              |
| 1:E:148:LEU:O    | 1:E:159:GLU:HG3  | 2.14                     | 0.47              |
| 1:E:160:TYR:HA   | 1:F:60:GLU:HG2   | 1.96                     | 0.47              |
| 1:E:175:PHE:CD2  | 1:E:196:ALA:HA   | 2.50                     | 0.47              |
| 2:K:141:GLN:NE2  | 2:V:141:GLN:HE21 | 2.13                     | 0.47              |
| 2:L:124:TYR:HD2  | 2:L:138:LEU:HD23 | 1.76                     | 0.47              |
| 2:M:179:THR:HG23 | 2:M:182:ASP:H    | 1.79                     | 0.47              |
| 2:N:175:VAL:CG2  | 2:N:176:ALA:N    | 2.78                     | 0.47              |
| 1:O:111:ASN:CG   | 2:W:70:ARG:NH1   | 2.73                     | 0.47              |
| 1:Q:61:GLN:CD    | 1:Q:62:ASN:H     | 2.22                     | 0.47              |
| 1:R:175:PHE:CD2  | 1:R:196:ALA:HA   | 2.50                     | 0.47              |
| 1:S:12:ILE:HD11  | 1:S:24:VAL:N     | 2.30                     | 0.47              |
| 1:U:9:ASP:CB     | 1:U:26:TYR:HH    | 2.09                     | 0.47              |
| 1:U:12:ILE:HD11  | 1:U:24:VAL:N     | 2.30                     | 0.47              |
| 1:U:98:GLN:O     | 1:U:102:THR:HG23 | 2.15                     | 0.47              |
| 2:V:37:ILE:HD11  | 2:V:59:MET:CB    | 2.45                     | 0.47              |
| 2:W:175:VAL:CG2  | 2:W:176:ALA:N    | 2.78                     | 0.47              |
| 2:2:55:LEU:HD21  | 2:2:87:LEU:HD11  | 1.97                     | 0.47              |
| 2:2:93:MET:N     | 2:2:94:PRO:CD    | 2.77                     | 0.47              |
| 1:A:130:ARG:NH2  | 1:G:124:THR:CG2  | 2.54                     | 0.47              |
| 1:D:12:ILE:HD11  | 1:D:24:VAL:N     | 2.30                     | 0.47              |
| 1:D:15:PHE:CZ    | 1:E:133:GLY:HA3  | 2.50                     | 0.47              |
| 1:E:103:TYR:CZ   | 2:M:82:LEU:HD13  | 2.49                     | 0.47              |
| 1:F:12:ILE:HD11  | 1:F:24:VAL:N     | 2.30                     | 0.47              |
| 2:I:35:PHE:CE2   | 2:I:45:ILE:HD12  | 2.50                     | 0.47              |
| 2:I:189:THR:HG23 | 2:I:190:ASP:H    | 1.79                     | 0.47              |
| 1:R:15:PHE:CZ    | 1:S:133:GLY:CA   | 2.97                     | 0.47              |
| 1:S:93:ARG:HB3   | 2:Z:65:LEU:CD1   | 2.45                     | 0.47              |
| 1:S:98:GLN:O     | 1:S:102:THR:HG23 | 2.15                     | 0.47              |
| 1:T:108:ASN:ND2  | 2:2:70:ARG:CA    | 2.78                     | 0.47              |
| 2:1:7:THR:HB     | 2:1:123:ILE:O    | 2.14                     | 0.47              |
| 1:E:19:GLY:HA3   | 1:F:30:ALA:CB    | 2.44                     | 0.46              |
| 1:E:98:GLN:O     | 1:E:102:THR:HG23 | 2.16                     | 0.46              |
| 1:F:21:LEU:CD1   | 1:G:130:ARG:HD3  | 2.43                     | 0.46              |
| 1:G:175:PHE:CD2  | 1:G:196:ALA:HA   | 2.50                     | 0.46              |
| 2:H:193:GLU:HA   | 2:H:196:ILE:HD12 | 1.98                     | 0.46              |
| 2:M:22:MET:O     | 2:M:23:GLU:HB2   | 2.15                     | 0.46              |
| 2:N:55:LEU:HD21  | 2:N:87:LEU:HD11  | 1.97                     | 0.46              |
| 2:N:123:ILE:HD13 | 2:N:123:ILE:N    | 2.26                     | 0.46              |
| 1:O:12:ILE:HD11  | 1:O:24:VAL:N     | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:57:ARG:N     | 1:U:177:GLU:OE2  | 2.48                     | 0.46              |
| 1:O:103:TYR:CE1  | 2:W:82:LEU:HD13  | 2.50                     | 0.46              |
| 1:R:7:ALA:CB     | 1:S:10:ARG:NH1   | 2.76                     | 0.46              |
| 2:X:20:VAL:HG13  | 2:X:28:HIS:HB2   | 1.97                     | 0.46              |
| 2:X:81:THR:O     | 2:X:84:SER:HB3   | 2.15                     | 0.46              |
| 2:Y:43:MET:CE    | 2:Y:56:VAL:HG23  | 2.45                     | 0.46              |
| 2:1:22:MET:O     | 2:1:23:GLU:HB2   | 2.15                     | 0.46              |
| 1:A:61:GLN:CD    | 1:A:62:ASN:H     | 2.22                     | 0.46              |
| 1:A:98:GLN:O     | 1:A:102:THR:HG23 | 2.16                     | 0.46              |
| 1:A:100:LYS:NZ   | 2:H:64:GLU:OE1   | 2.43                     | 0.46              |
| 1:D:98:GLN:O     | 1:D:102:THR:HG23 | 2.16                     | 0.46              |
| 1:D:101:VAL:HA   | 2:K:57:ARG:HB3   | 1.96                     | 0.46              |
| 1:D:175:PHE:CD2  | 1:D:196:ALA:HA   | 2.50                     | 0.46              |
| 1:E:12:ILE:HD11  | 1:E:24:VAL:N     | 2.30                     | 0.46              |
| 2:H:37:ILE:HD11  | 2:H:59:MET:CB    | 2.45                     | 0.46              |
| 2:I:25:PHE:C     | 2:I:25:PHE:CD1   | 2.91                     | 0.46              |
| 2:J:138:LEU:HD12 | 2:J:138:LEU:HA   | 1.68                     | 0.46              |
| 2:K:27:MET:HG2   | 2:K:27:MET:O     | 2.16                     | 0.46              |
| 2:K:50:GLY:O     | 2:K:54:VAL:HG12  | 2.14                     | 0.46              |
| 2:M:124:TYR:HD2  | 2:M:138:LEU:HD23 | 1.76                     | 0.46              |
| 1:P:98:GLN:O     | 1:P:102:THR:HG23 | 2.16                     | 0.46              |
| 1:Q:173:VAL:O    | 1:R:58:LEU:CD2   | 2.62                     | 0.46              |
| 1:R:15:PHE:CZ    | 1:S:133:GLY:HA3  | 2.50                     | 0.46              |
| 1:S:15:PHE:CE2   | 1:T:131:PRO:O    | 2.68                     | 0.46              |
| 1:S:61:GLN:CD    | 1:S:62:ASN:H     | 2.23                     | 0.46              |
| 2:V:177:VAL:HG12 | 2:V:187:LEU:CD1  | 2.46                     | 0.46              |
| 1:C:98:GLN:O     | 1:C:102:THR:HG23 | 2.16                     | 0.46              |
| 1:D:101:VAL:HG23 | 2:K:58:TYR:N     | 2.29                     | 0.46              |
| 1:E:15:PHE:CE2   | 1:F:131:PRO:O    | 2.68                     | 0.46              |
| 1:E:134:VAL:O    | 1:E:153:PRO:HG3  | 2.14                     | 0.46              |
| 2:H:177:VAL:HG12 | 2:H:187:LEU:CD1  | 2.46                     | 0.46              |
| 2:I:175:VAL:CG2  | 2:I:176:ALA:N    | 2.78                     | 0.46              |
| 2:K:74:MET:HG2   | 2:K:78:ALA:HB3   | 1.97                     | 0.46              |
| 2:M:110:VAL:O    | 2:M:110:VAL:HG13 | 2.16                     | 0.46              |
| 2:N:93:MET:N     | 2:N:94:PRO:CD    | 2.77                     | 0.46              |
| 1:O:175:PHE:CD2  | 1:O:196:ALA:HA   | 2.50                     | 0.46              |
| 2:W:35:PHE:CE2   | 2:W:45:ILE:HD12  | 2.50                     | 0.46              |
| 2:2:18:ARG:HB2   | 2:2:31:GLY:O     | 2.15                     | 0.46              |
| 2:2:175:VAL:CG2  | 2:2:176:ALA:N    | 2.78                     | 0.46              |
| 2:J:175:VAL:CG2  | 2:J:176:ALA:N    | 2.78                     | 0.46              |
| 2:J:179:THR:HG23 | 2:J:182:ASP:H    | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:48:LEU:HD12  | 2:K:49:VAL:N     | 2.31                     | 0.46              |
| 2:N:109:HIS:HB3  | 2:N:111:PHE:HE1  | 1.81                     | 0.46              |
| 1:P:12:ILE:HD11  | 1:P:24:VAL:N     | 2.30                     | 0.46              |
| 1:Q:175:PHE:CD2  | 1:Q:196:ALA:HA   | 2.50                     | 0.46              |
| 1:R:104:GLY:N    | 2:Z:81:THR:HG21  | 2.28                     | 0.46              |
| 1:R:134:VAL:O    | 1:R:153:PRO:HG3  | 2.14                     | 0.46              |
| 2:X:138:LEU:HD12 | 2:X:138:LEU:HA   | 1.68                     | 0.46              |
| 2:2:91:LYS:O     | 2:2:94:PRO:HD3   | 2.15                     | 0.46              |
| 1:G:134:VAL:O    | 1:G:153:PRO:HG3  | 2.14                     | 0.46              |
| 1:G:198:LYS:O    | 1:G:199:SER:C    | 2.59                     | 0.46              |
| 2:I:20:VAL:CG1   | 2:I:28:HIS:HB2   | 2.44                     | 0.46              |
| 2:J:26:ILE:HG22  | 2:V:165:ARG:C    | 2.40                     | 0.46              |
| 2:L:132:PRO:HA   | 2:2:133:PHE:HE1  | 1.81                     | 0.46              |
| 2:N:37:ILE:HD11  | 2:N:59:MET:CG    | 2.46                     | 0.46              |
| 1:O:130:ARG:HB2  | 1:U:14:VAL:H     | 1.81                     | 0.46              |
| 1:P:103:TYR:CE1  | 2:X:82:LEU:HD22  | 2.51                     | 0.46              |
| 1:Q:12:ILE:HD11  | 1:Q:24:VAL:N     | 2.30                     | 0.46              |
| 1:S:103:TYR:CZ   | 2:1:82:LEU:HD13  | 2.49                     | 0.46              |
| 2:X:152:VAL:O    | 2:X:156:ILE:HG13 | 2.14                     | 0.46              |
| 2:2:109:HIS:HB3  | 2:2:111:PHE:HE1  | 1.81                     | 0.46              |
| 1:B:108:ASN:HD22 | 2:J:70:ARG:HG2   | 1.79                     | 0.46              |
| 1:E:108:ASN:HB2  | 2:M:70:ARG:HG2   | 1.90                     | 0.46              |
| 2:I:138:LEU:HD12 | 2:I:154:LEU:HD11 | 1.98                     | 0.46              |
| 1:Q:108:ASN:ND2  | 2:Y:70:ARG:HA    | 2.31                     | 0.46              |
| 1:S:104:GLY:HA3  | 2:1:81:THR:HG21  | 1.97                     | 0.46              |
| 2:V:7:THR:HB     | 2:V:123:ILE:O    | 2.16                     | 0.46              |
| 2:V:193:GLU:HA   | 2:V:196:ILE:HD12 | 1.97                     | 0.46              |
| 2:2:37:ILE:HD11  | 2:2:59:MET:CG    | 2.46                     | 0.46              |
| 1:A:198:LYS:O    | 1:A:199:SER:C    | 2.59                     | 0.46              |
| 1:F:175:PHE:CD2  | 1:F:196:ALA:HA   | 2.50                     | 0.46              |
| 1:G:103:TYR:CE1  | 2:H:82:LEU:CD1   | 2.83                     | 0.46              |
| 2:L:103:GLY:HA2  | 2:L:178:ILE:HD11 | 1.98                     | 0.46              |
| 2:L:165:ARG:NE   | 2:2:139:GLU:OE1  | 2.49                     | 0.46              |
| 1:O:98:GLN:O     | 1:O:102:THR:HG23 | 2.16                     | 0.46              |
| 1:O:177:GLU:N    | 1:P:58:LEU:CD2   | 2.49                     | 0.46              |
| 1:T:177:GLU:CG   | 1:U:58:LEU:HD13  | 2.46                     | 0.46              |
| 2:V:72:VAL:HG22  | 2:V:73:ASN:N     | 2.31                     | 0.46              |
| 2:W:20:VAL:CG1   | 2:W:28:HIS:HB2   | 2.44                     | 0.46              |
| 2:X:179:THR:HG23 | 2:X:182:ASP:H    | 1.80                     | 0.46              |
| 2:1:184:TYR:CD1  | 2:1:184:TYR:C    | 2.93                     | 0.46              |
| 1:D:198:LYS:O    | 1:D:199:SER:C    | 2.59                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:12:ILE:HD12  | 1:G:23:GLN:HB2   | 0.74                     | 0.46              |
| 1:G:98:GLN:O     | 1:G:102:THR:HG23 | 2.15                     | 0.46              |
| 2:N:27:MET:O     | 2:N:27:MET:HG2   | 2.15                     | 0.46              |
| 1:O:130:ARG:CD   | 1:U:21:LEU:CD1   | 2.75                     | 0.46              |
| 1:Q:12:ILE:HD13  | 1:Q:23:GLN:CB    | 1.03                     | 0.46              |
| 1:R:98:GLN:O     | 1:R:102:THR:HG23 | 2.16                     | 0.46              |
| 1:R:107:VAL:HG21 | 2:Z:66:TYR:HH    | 1.80                     | 0.46              |
| 1:R:198:LYS:O    | 1:R:199:SER:C    | 2.59                     | 0.46              |
| 1:T:108:ASN:ND2  | 2:2:70:ARG:HA    | 2.31                     | 0.46              |
| 1:T:177:GLU:H    | 1:U:58:LEU:CD2   | 2.03                     | 0.46              |
| 2:1:174:ASP:HA   | 2:1:192:ILE:HD13 | 1.98                     | 0.46              |
| 1:D:44:ASN:HD22  | 1:D:44:ASN:HA    | 1.56                     | 0.46              |
| 2:K:17:GLU:HA    | 2:K:173:ILE:HA   | 1.98                     | 0.46              |
| 2:K:160:SER:HA   | 2:K:163:LYS:HD3  | 1.98                     | 0.46              |
| 1:O:44:ASN:HD22  | 1:O:44:ASN:HA    | 1.56                     | 0.46              |
| 1:Q:198:LYS:O    | 1:Q:199:SER:C    | 2.59                     | 0.46              |
| 1:S:44:ASN:HD22  | 1:S:44:ASN:HA    | 1.56                     | 0.46              |
| 1:S:198:LYS:O    | 1:S:199:SER:C    | 2.59                     | 0.46              |
| 2:X:189:THR:HG23 | 2:X:190:ASP:H    | 1.81                     | 0.46              |
| 2:2:27:MET:O     | 2:2:27:MET:HG2   | 2.15                     | 0.46              |
| 1:A:29:GLU:HG3   | 1:G:17:PRO:O     | 2.16                     | 0.46              |
| 1:D:160:TYR:C    | 1:E:60:GLU:HG2   | 2.41                     | 0.46              |
| 1:F:125:GLN:C    | 1:G:129:VAL:HG23 | 2.38                     | 0.46              |
| 1:F:177:GLU:H    | 1:G:58:LEU:CD2   | 2.03                     | 0.46              |
| 1:F:198:LYS:O    | 1:F:199:SER:C    | 2.59                     | 0.46              |
| 1:O:21:LEU:CD1   | 1:P:130:ARG:HD2  | 2.20                     | 0.46              |
| 1:Q:98:GLN:O     | 1:Q:102:THR:HG23 | 2.16                     | 0.46              |
| 1:R:107:VAL:HG21 | 2:Z:66:TYR:OH    | 2.15                     | 0.46              |
| 1:T:125:GLN:C    | 1:U:129:VAL:HG23 | 2.38                     | 0.46              |
| 1:T:177:GLU:CB   | 1:U:58:LEU:HD13  | 2.45                     | 0.46              |
| 2:V:20:VAL:HG22  | 2:V:28:HIS:HB2   | 1.96                     | 0.46              |
| 2:I:105:ASP:OD1  | 2:I:106:THR:N    | 2.49                     | 0.45              |
| 2:N:97:VAL:HG22  | 2:N:98:GLN:H     | 1.81                     | 0.45              |
| 1:U:198:LYS:O    | 1:U:199:SER:C    | 2.59                     | 0.45              |
| 1:A:103:TYR:CE1  | 2:I:82:LEU:HD13  | 2.50                     | 0.45              |
| 1:D:107:VAL:HG11 | 2:L:66:TYR:HH    | 1.81                     | 0.45              |
| 1:D:107:VAL:HG21 | 2:L:66:TYR:OH    | 2.15                     | 0.45              |
| 1:F:98:GLN:O     | 1:F:102:THR:HG23 | 2.16                     | 0.45              |
| 2:H:111:PHE:CE2  | 2:H:121:GLU:HB2  | 2.51                     | 0.45              |
| 2:J:81:THR:O     | 2:J:84:SER:HB3   | 2.15                     | 0.45              |
| 2:K:111:PHE:CE2  | 2:K:121:GLU:HB2  | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:6:ILE:HG23   | 2:M:6:ILE:O      | 2.16                     | 0.45              |
| 2:M:15:ALA:HB3   | 2:M:155:VAL:HG11 | 1.98                     | 0.45              |
| 1:S:160:TYR:C    | 1:T:60:GLU:HG2   | 2.39                     | 0.45              |
| 1:U:108:ASN:ND2  | 2:V:70:ARG:C     | 2.75                     | 0.45              |
| 2:Y:17:GLU:HA    | 2:Y:173:ILE:HA   | 1.98                     | 0.45              |
| 2:Y:27:MET:HG2   | 2:Y:27:MET:O     | 2.16                     | 0.45              |
| 2:2:97:VAL:HG22  | 2:2:98:GLN:N     | 2.32                     | 0.45              |
| 1:B:108:ASN:HD22 | 2:J:70:ARG:CG    | 2.26                     | 0.45              |
| 1:C:49:ILE:HD11  | 1:C:210:PRO:CB   | 2.47                     | 0.45              |
| 1:C:198:LYS:O    | 1:C:199:SER:C    | 2.59                     | 0.45              |
| 1:F:177:GLU:CG   | 1:G:58:LEU:HD13  | 2.46                     | 0.45              |
| 2:J:105:ASP:OD1  | 2:J:106:THR:N    | 2.50                     | 0.45              |
| 2:K:43:MET:CE    | 2:K:56:VAL:HG23  | 2.45                     | 0.45              |
| 2:L:19:ARG:HE    | 2:L:26:ILE:HG13  | 1.81                     | 0.45              |
| 2:M:174:ASP:HA   | 2:M:192:ILE:HD13 | 1.98                     | 0.45              |
| 2:N:124:TYR:HD1  | 2:N:138:LEU:HD23 | 1.81                     | 0.45              |
| 1:O:21:LEU:CD1   | 1:P:130:ARG:CD   | 2.87                     | 0.45              |
| 1:T:98:GLN:O     | 1:T:102:THR:HG23 | 2.16                     | 0.45              |
| 1:U:49:ILE:HD11  | 1:U:210:PRO:CB   | 2.47                     | 0.45              |
| 2:Y:48:LEU:HD12  | 2:Y:49:VAL:N     | 2.31                     | 0.45              |
| 2:2:123:ILE:H    | 2:2:123:ILE:CD1  | 2.24                     | 0.45              |
| 1:B:198:LYS:O    | 1:B:199:SER:C    | 2.59                     | 0.45              |
| 1:C:108:ASN:ND2  | 2:K:70:ARG:HA    | 2.31                     | 0.45              |
| 1:E:104:GLY:HA3  | 2:M:81:THR:HG21  | 1.97                     | 0.45              |
| 2:L:19:ARG:NE    | 2:L:26:ILE:HG13  | 2.32                     | 0.45              |
| 2:L:75:PRO:O     | 2:L:78:ALA:HB3   | 2.16                     | 0.45              |
| 1:T:52:LYS:HE3   | 1:T:64:ILE:HG23  | 1.99                     | 0.45              |
| 1:T:198:LYS:O    | 1:T:199:SER:C    | 2.59                     | 0.45              |
| 2:V:111:PHE:CE2  | 2:V:121:GLU:HB2  | 2.51                     | 0.45              |
| 2:X:105:ASP:OD1  | 2:X:106:THR:N    | 2.50                     | 0.45              |
| 2:Y:149:ASP:O    | 2:Y:152:VAL:HG12 | 2.17                     | 0.45              |
| 2:1:110:VAL:O    | 2:1:110:VAL:HG13 | 2.16                     | 0.45              |
| 2:2:37:ILE:HD11  | 2:2:59:MET:CB    | 2.43                     | 0.45              |
| 1:B:98:GLN:O     | 1:B:102:THR:HG23 | 2.16                     | 0.45              |
| 1:B:103:TYR:CE1  | 2:J:82:LEU:HD22  | 2.51                     | 0.45              |
| 1:D:12:ILE:N     | 1:D:23:GLN:HG2   | 2.31                     | 0.45              |
| 1:E:198:LYS:O    | 1:E:199:SER:C    | 2.59                     | 0.45              |
| 2:H:22:MET:O     | 2:H:23:GLU:HB2   | 2.17                     | 0.45              |
| 2:H:66:TYR:CD1   | 2:H:66:TYR:C     | 2.94                     | 0.45              |
| 2:H:141:GLN:HE21 | 2:Y:141:GLN:NE2  | 2.15                     | 0.45              |
| 2:J:20:VAL:HG13  | 2:J:28:HIS:HB2   | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:55:LEU:HD12  | 2:M:55:LEU:HA    | 1.76                     | 0.45              |
| 2:N:8:LEU:HD12   | 2:N:8:LEU:O      | 2.17                     | 0.45              |
| 1:O:12:ILE:N     | 1:O:23:GLN:HG2   | 2.31                     | 0.45              |
| 1:Q:18:ASP:OD2   | 1:Q:20:ARG:HD3   | 2.17                     | 0.45              |
| 1:S:12:ILE:CD1   | 1:S:23:GLN:CB    | 0.48                     | 0.45              |
| 2:Y:75:PRO:O     | 2:Y:78:ALA:HB3   | 2.16                     | 0.45              |
| 2:2:180:ARG:HD2  | 2:2:180:ARG:HA   | 1.80                     | 0.45              |
| 1:D:103:TYR:HA   | 2:L:81:THR:HG22  | 1.99                     | 0.45              |
| 1:F:108:ASN:ND2  | 2:N:70:ARG:HA    | 2.31                     | 0.45              |
| 2:H:7:THR:HB     | 2:H:123:ILE:O    | 2.16                     | 0.45              |
| 2:H:72:VAL:HG22  | 2:H:73:ASN:N     | 2.31                     | 0.45              |
| 2:K:75:PRO:O     | 2:K:78:ALA:HB3   | 2.16                     | 0.45              |
| 2:L:6:ILE:HD11   | 2:L:142:TYR:CD1  | 2.52                     | 0.45              |
| 2:L:110:VAL:O    | 2:L:110:VAL:HG13 | 2.16                     | 0.45              |
| 1:T:18:ASP:OD2   | 1:T:20:ARG:HD3   | 2.17                     | 0.45              |
| 2:W:105:ASP:OD1  | 2:W:106:THR:N    | 2.49                     | 0.45              |
| 2:Z:19:ARG:HE    | 2:Z:26:ILE:HG13  | 1.82                     | 0.45              |
| 2:Z:110:VAL:O    | 2:Z:110:VAL:HG13 | 2.16                     | 0.45              |
| 2:Z:187:LEU:HA   | 2:Z:188:PRO:HD3  | 1.77                     | 0.45              |
| 1:B:18:ASP:OD2   | 1:B:20:ARG:HD3   | 2.17                     | 0.45              |
| 1:D:78:THR:CG2   | 1:D:85:ALA:HB1   | 2.45                     | 0.45              |
| 1:E:18:ASP:OD2   | 1:E:20:ARG:HD3   | 2.17                     | 0.45              |
| 1:E:124:THR:HG22 | 1:F:130:ARG:NH2  | 2.15                     | 0.45              |
| 1:F:18:ASP:OD2   | 1:F:20:ARG:HD3   | 2.17                     | 0.45              |
| 2:N:97:VAL:HG22  | 2:N:98:GLN:N     | 2.32                     | 0.45              |
| 2:N:180:ARG:HD2  | 2:N:180:ARG:HA   | 1.80                     | 0.45              |
| 1:O:29:GLU:HG3   | 1:U:17:PRO:O     | 2.16                     | 0.45              |
| 1:O:198:LYS:O    | 1:O:199:SER:C    | 2.59                     | 0.45              |
| 1:P:198:LYS:O    | 1:P:199:SER:C    | 2.59                     | 0.45              |
| 1:Q:12:ILE:CD1   | 1:Q:23:GLN:CB    | 0.48                     | 0.45              |
| 1:Q:78:THR:CG2   | 1:Q:85:ALA:HB1   | 2.45                     | 0.45              |
| 1:R:103:TYR:HA   | 2:Z:81:THR:HG22  | 1.99                     | 0.45              |
| 1:R:177:GLU:CB   | 1:S:58:LEU:CD2   | 2.75                     | 0.45              |
| 2:V:66:TYR:CD1   | 2:V:66:TYR:C     | 2.94                     | 0.45              |
| 2:W:2:THR:HG22   | 2:W:169:SER:OG   | 2.17                     | 0.45              |
| 2:2:97:VAL:HG22  | 2:2:98:GLN:H     | 1.81                     | 0.45              |
| 1:B:24:VAL:O     | 1:B:28:ARG:HG3   | 2.17                     | 0.45              |
| 1:B:177:GLU:CG   | 1:C:58:LEU:HD13  | 2.46                     | 0.45              |
| 1:C:12:ILE:HD13  | 1:C:23:GLN:HB3   | 0.88                     | 0.45              |
| 1:C:126:TYR:OH   | 1:D:123:TYR:OH   | 2.32                     | 0.45              |
| 1:D:49:ILE:HD11  | 1:D:210:PRO:CB   | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:177:GLU:CB   | 1:G:58:LEU:HD13  | 2.45                     | 0.45              |
| 1:G:143:GLN:OE1  | 2:H:75:PRO:HG3   | 2.17                     | 0.45              |
| 2:K:55:LEU:HD12  | 2:K:55:LEU:HA    | 1.79                     | 0.45              |
| 2:K:149:ASP:O    | 2:K:152:VAL:HG12 | 2.17                     | 0.45              |
| 2:M:180:ARG:HA   | 2:M:180:ARG:HD2  | 1.77                     | 0.45              |
| 1:P:12:ILE:HD12  | 1:P:23:GLN:CB    | 0.59                     | 0.45              |
| 1:R:19:GLY:HA3   | 1:S:30:ALA:CB    | 2.47                     | 0.45              |
| 1:S:52:LYS:HE3   | 1:S:64:ILE:HG23  | 1.99                     | 0.45              |
| 2:W:146:MET:HA   | 2:W:150:GLU:OE1  | 2.17                     | 0.45              |
| 2:1:6:ILE:HG23   | 2:1:6:ILE:O      | 2.16                     | 0.45              |
| 1:B:97:GLN:OE1   | 2:I:61:ALA:CB    | 2.60                     | 0.45              |
| 1:C:18:ASP:OD2   | 1:C:20:ARG:HD3   | 2.17                     | 0.45              |
| 1:E:24:VAL:O     | 1:E:28:ARG:HG3   | 2.17                     | 0.45              |
| 1:E:78:THR:CG2   | 1:E:85:ALA:HB1   | 2.45                     | 0.45              |
| 1:F:12:ILE:CD1   | 1:F:23:GLN:CB    | 0.48                     | 0.45              |
| 1:F:161:LYS:HB2  | 1:G:60:GLU:CD    | 2.37                     | 0.45              |
| 2:L:141:GLN:HE21 | 2:2:141:GLN:NE2  | 2.14                     | 0.45              |
| 1:O:57:ARG:C     | 1:U:177:GLU:OE1  | 2.60                     | 0.45              |
| 1:P:177:GLU:CA   | 1:Q:58:LEU:CG    | 2.88                     | 0.45              |
| 1:S:18:ASP:OD2   | 1:S:20:ARG:HD3   | 2.17                     | 0.45              |
| 1:S:111:ASN:ND2  | 2:1:70:ARG:CZ    | 2.80                     | 0.45              |
| 1:T:102:THR:O    | 2:2:85:ASN:CG    | 2.47                     | 0.45              |
| 2:X:49:VAL:HG23  | 2:X:50:GLY:H     | 1.82                     | 0.45              |
| 2:1:15:ALA:HB3   | 2:1:155:VAL:HG11 | 1.98                     | 0.45              |
| 1:A:52:LYS:HE3   | 1:A:64:ILE:HG23  | 1.99                     | 0.45              |
| 1:C:78:THR:CG2   | 1:C:85:ALA:HB1   | 2.45                     | 0.45              |
| 2:I:2:THR:HG22   | 2:I:169:SER:OG   | 2.17                     | 0.45              |
| 2:L:17:GLU:HA    | 2:L:173:ILE:HA   | 1.99                     | 0.45              |
| 2:N:37:ILE:HD11  | 2:N:59:MET:CB    | 2.43                     | 0.45              |
| 1:O:108:ASN:HD22 | 2:W:70:ARG:HG2   | 1.77                     | 0.45              |
| 1:P:18:ASP:OD2   | 1:P:20:ARG:HD3   | 2.17                     | 0.45              |
| 1:P:24:VAL:O     | 1:P:28:ARG:HG3   | 2.17                     | 0.45              |
| 1:Q:143:GLN:OE1  | 2:Y:75:PRO:CG    | 2.65                     | 0.45              |
| 1:R:177:GLU:OE1  | 1:S:58:LEU:CD1   | 2.63                     | 0.45              |
| 1:T:24:VAL:O     | 1:T:28:ARG:HG3   | 2.17                     | 0.45              |
| 1:U:18:ASP:OD2   | 1:U:20:ARG:HD3   | 2.17                     | 0.45              |
| 1:U:24:VAL:O     | 1:U:28:ARG:HG3   | 2.16                     | 0.45              |
| 2:V:6:ILE:HD11   | 2:V:142:TYR:HD1  | 1.79                     | 0.45              |
| 2:V:22:MET:O     | 2:V:23:GLU:HB2   | 2.17                     | 0.45              |
| 2:V:27:MET:HG2   | 2:V:27:MET:O     | 2.17                     | 0.45              |
| 2:Y:160:SER:HA   | 2:Y:163:LYS:HD3  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:Z:75:PRO:O     | 2:Z:78:ALA:HB3  | 2.16                     | 0.45              |
| 1:A:44:ASN:HD22  | 1:A:44:ASN:HA   | 1.56                     | 0.44              |
| 1:A:159:GLU:O    | 1:B:60:GLU:HB2  | 2.17                     | 0.44              |
| 1:B:52:LYS:HE3   | 1:B:64:ILE:HG23 | 1.99                     | 0.44              |
| 2:J:123:ILE:HG12 | 2:J:124:TYR:CD1 | 2.51                     | 0.44              |
| 2:J:189:THR:HG23 | 2:J:190:ASP:H   | 1.81                     | 0.44              |
| 1:Q:72:ASP:CG    | 2:X:67:ARG:HH22 | 2.22                     | 0.44              |
| 1:R:72:ASP:CG    | 2:Y:67:ARG:NH2  | 2.75                     | 0.44              |
| 1:S:107:VAL:HG11 | 2:1:66:TYR:HH   | 1.81                     | 0.44              |
| 1:T:108:ASN:ND2  | 2:2:70:ARG:CB   | 2.75                     | 0.44              |
| 1:U:143:GLN:OE1  | 2:V:75:PRO:HG3  | 2.17                     | 0.44              |
| 2:Y:111:PHE:CE2  | 2:Y:121:GLU:HB2 | 2.51                     | 0.44              |
| 2:Z:8:LEU:HD12   | 2:Z:8:LEU:O     | 2.17                     | 0.44              |
| 2:Z:19:ARG:NE    | 2:Z:26:ILE:HG13 | 2.32                     | 0.44              |
| 2:2:19:ARG:HD2   | 2:2:169:SER:C   | 2.43                     | 0.44              |
| 1:A:18:ASP:OD2   | 1:A:20:ARG:HD3  | 2.17                     | 0.44              |
| 1:D:177:GLU:OE1  | 1:E:58:LEU:CD1  | 2.63                     | 0.44              |
| 2:L:8:LEU:O      | 2:L:8:LEU:HD12  | 2.17                     | 0.44              |
| 2:N:7:THR:HB     | 2:N:123:ILE:O   | 2.18                     | 0.44              |
| 1:P:78:THR:CG2   | 1:P:85:ALA:HB1  | 2.45                     | 0.44              |
| 1:P:177:GLU:CG   | 1:Q:58:LEU:HD13 | 2.46                     | 0.44              |
| 1:T:21:LEU:CD1   | 1:U:130:ARG:HD3 | 2.43                     | 0.44              |
| 2:V:15:ALA:HB2   | 2:V:175:VAL:HB  | 1.99                     | 0.44              |
| 2:Y:187:LEU:HA   | 2:Y:188:PRO:HD3 | 1.76                     | 0.44              |
| 2:2:8:LEU:HD12   | 2:2:8:LEU:O     | 2.17                     | 0.44              |
| 1:A:24:VAL:O     | 1:A:28:ARG:HG3  | 2.17                     | 0.44              |
| 1:A:130:ARG:HB2  | 1:G:14:VAL:H    | 1.81                     | 0.44              |
| 1:B:177:GLU:OE1  | 1:C:58:LEU:N    | 2.50                     | 0.44              |
| 1:C:12:ILE:N     | 1:C:23:GLN:HG2  | 2.31                     | 0.44              |
| 1:C:24:VAL:O     | 1:C:28:ARG:HG3  | 2.17                     | 0.44              |
| 1:D:12:ILE:HD13  | 1:D:23:GLN:HB3  | 0.88                     | 0.44              |
| 1:E:52:LYS:HE3   | 1:E:64:ILE:HG23 | 1.99                     | 0.44              |
| 1:E:111:ASN:ND2  | 2:M:70:ARG:CZ   | 2.80                     | 0.44              |
| 1:G:103:TYR:C    | 2:H:81:THR:HG22 | 2.39                     | 0.44              |
| 2:L:93:MET:N     | 2:L:94:PRO:CD   | 2.81                     | 0.44              |
| 1:O:78:THR:CG2   | 1:O:85:ALA:HB1  | 2.45                     | 0.44              |
| 1:R:9:ASP:CB     | 1:R:26:TYR:HH   | 2.14                     | 0.44              |
| 1:A:57:ARG:C     | 1:G:177:GLU:OE1 | 2.60                     | 0.44              |
| 1:E:173:VAL:CG2  | 1:F:58:LEU:HD23 | 2.47                     | 0.44              |
| 1:G:18:ASP:OD2   | 1:G:20:ARG:HD3  | 2.17                     | 0.44              |
| 1:G:49:ILE:HD11  | 1:G:210:PRO:CB  | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:27:MET:O     | 2:H:27:MET:HG2   | 2.17                     | 0.44              |
| 2:K:124:TYR:HD2  | 2:K:138:LEU:HD23 | 1.80                     | 0.44              |
| 1:O:24:VAL:O     | 1:O:28:ARG:HG3   | 2.17                     | 0.44              |
| 1:Q:177:GLU:H    | 1:R:58:LEU:CD2   | 2.06                     | 0.44              |
| 1:R:18:ASP:OD2   | 1:R:20:ARG:HD3   | 2.17                     | 0.44              |
| 2:W:138:LEU:HD12 | 2:W:154:LEU:HD11 | 1.98                     | 0.44              |
| 2:Y:76:ILE:O     | 2:Y:79:VAL:HG12  | 2.18                     | 0.44              |
| 2:Z:103:GLY:HA2  | 2:Z:178:ILE:HD11 | 1.98                     | 0.44              |
| 2:2:130:GLY:O    | 2:2:134:VAL:HG12 | 2.17                     | 0.44              |
| 1:F:12:ILE:HD13  | 1:F:23:GLN:CB    | 1.02                     | 0.44              |
| 1:G:103:TYR:CD1  | 2:H:82:LEU:HB2   | 2.53                     | 0.44              |
| 1:O:49:ILE:HD11  | 1:O:210:PRO:CB   | 2.47                     | 0.44              |
| 1:R:52:LYS:HE3   | 1:R:64:ILE:HG23  | 1.99                     | 0.44              |
| 1:S:49:ILE:HD11  | 1:S:210:PRO:CB   | 2.47                     | 0.44              |
| 1:U:12:ILE:HD13  | 1:U:23:GLN:HB3   | 0.88                     | 0.44              |
| 1:U:103:TYR:CD1  | 2:V:82:LEU:HB2   | 2.53                     | 0.44              |
| 2:Z:59:MET:HE1   | 2:Z:82:LEU:CD2   | 2.48                     | 0.44              |
| 2:2:173:ILE:HD13 | 2:2:173:ILE:C    | 2.43                     | 0.44              |
| 1:B:12:ILE:CD1   | 1:B:23:GLN:CB    | 0.48                     | 0.44              |
| 1:D:19:GLY:HA3   | 1:E:30:ALA:CB    | 2.47                     | 0.44              |
| 1:D:24:VAL:O     | 1:D:28:ARG:HG3   | 2.17                     | 0.44              |
| 1:D:52:LYS:HE3   | 1:D:64:ILE:HG23  | 1.99                     | 0.44              |
| 1:D:72:ASP:CG    | 2:K:67:ARG:NH2   | 2.75                     | 0.44              |
| 1:E:111:ASN:HB2  | 2:M:70:ARG:NH1   | 2.33                     | 0.44              |
| 1:E:173:VAL:O    | 1:F:58:LEU:HD23  | 2.06                     | 0.44              |
| 1:F:24:VAL:O     | 1:F:28:ARG:HG3   | 2.17                     | 0.44              |
| 2:H:187:LEU:HA   | 2:H:188:PRO:HD3  | 1.77                     | 0.44              |
| 2:I:6:ILE:HD11   | 2:I:142:TYR:CD1  | 2.52                     | 0.44              |
| 2:J:123:ILE:H    | 2:J:123:ILE:CD1  | 2.23                     | 0.44              |
| 2:L:74:MET:HG2   | 2:L:78:ALA:HB3   | 2.00                     | 0.44              |
| 2:N:19:ARG:HD2   | 2:N:169:SER:C    | 2.42                     | 0.44              |
| 2:N:49:VAL:O     | 2:N:50:GLY:C     | 2.61                     | 0.44              |
| 2:N:130:GLY:O    | 2:N:134:VAL:HG12 | 2.17                     | 0.44              |
| 1:O:58:LEU:HD22  | 1:U:177:GLU:CB   | 2.20                     | 0.44              |
| 1:P:177:GLU:OE1  | 1:Q:58:LEU:N     | 2.50                     | 0.44              |
| 1:Q:24:VAL:O     | 1:Q:28:ARG:HG3   | 2.17                     | 0.44              |
| 1:Q:49:ILE:HD11  | 1:Q:210:PRO:CB   | 2.47                     | 0.44              |
| 1:S:24:VAL:O     | 1:S:28:ARG:HG3   | 2.17                     | 0.44              |
| 1:U:12:ILE:N     | 1:U:23:GLN:HG2   | 2.31                     | 0.44              |
| 1:U:52:LYS:HE3   | 1:U:64:ILE:HG23  | 1.99                     | 0.44              |
| 1:U:78:THR:CG2   | 1:U:85:ALA:HB1   | 2.45                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Z:17:GLU:HA    | 2:Z:173:ILE:HA   | 1.99                     | 0.44              |
| 1:B:125:GLN:O    | 1:C:129:VAL:HG23 | 2.18                     | 0.44              |
| 1:C:52:LYS:HE3   | 1:C:64:ILE:HG23  | 1.99                     | 0.44              |
| 1:C:143:GLN:OE1  | 2:K:75:PRO:CG    | 2.65                     | 0.44              |
| 1:C:178:ARG:N    | 1:D:57:ARG:HH21  | 2.15                     | 0.44              |
| 1:D:18:ASP:OD2   | 1:D:20:ARG:HD3   | 2.17                     | 0.44              |
| 1:F:49:ILE:HD11  | 1:F:210:PRO:CB   | 2.47                     | 0.44              |
| 2:H:59:MET:HE2   | 2:H:79:VAL:CG2   | 2.47                     | 0.44              |
| 2:N:25:PHE:C     | 2:N:25:PHE:HD1   | 2.26                     | 0.44              |
| 1:P:52:LYS:HE3   | 1:P:64:ILE:HG23  | 1.99                     | 0.44              |
| 2:W:6:ILE:HD11   | 2:W:142:TYR:CD1  | 2.53                     | 0.44              |
| 2:Z:74:MET:HG2   | 2:Z:78:ALA:HB3   | 2.00                     | 0.44              |
| 1:D:17:PRO:HA    | 1:E:26:TYR:CG    | 2.53                     | 0.44              |
| 1:E:15:PHE:HZ    | 1:F:133:GLY:N    | 2.15                     | 0.44              |
| 1:G:108:ASN:ND2  | 2:H:70:ARG:C     | 2.75                     | 0.44              |
| 2:K:19:ARG:HD2   | 2:K:169:SER:C    | 2.43                     | 0.44              |
| 1:S:15:PHE:HZ    | 1:T:133:GLY:N    | 2.15                     | 0.44              |
| 1:T:52:LYS:HZ3   | 1:T:62:ASN:HA    | 1.78                     | 0.44              |
| 2:V:90:VAL:O     | 2:V:90:VAL:HG22  | 2.18                     | 0.44              |
| 2:Z:76:ILE:HA    | 2:Z:79:VAL:HG12  | 2.00                     | 0.44              |
| 1:A:49:ILE:HD11  | 1:A:210:PRO:CB   | 2.47                     | 0.44              |
| 1:C:108:ASN:HD22 | 2:K:70:ARG:CA    | 2.24                     | 0.44              |
| 1:F:108:ASN:HD22 | 2:N:70:ARG:CA    | 2.31                     | 0.44              |
| 2:H:15:ALA:HB2   | 2:H:175:VAL:HB   | 1.99                     | 0.44              |
| 2:K:76:ILE:O     | 2:K:79:VAL:HG12  | 2.18                     | 0.44              |
| 1:O:109:ILE:CG2  | 1:O:147:ARG:HD3  | 2.48                     | 0.44              |
| 1:R:49:ILE:HD11  | 1:R:210:PRO:CB   | 2.47                     | 0.44              |
| 1:T:108:ASN:HD22 | 2:2:70:ARG:CA    | 2.30                     | 0.44              |
| 2:Y:34:LEU:HD21  | 2:Y:176:ALA:HB3  | 2.00                     | 0.44              |
| 2:2:124:TYR:HD1  | 2:2:138:LEU:HD23 | 1.81                     | 0.44              |
| 2:2:160:SER:HA   | 2:2:163:LYS:HD3  | 2.00                     | 0.44              |
| 1:D:72:ASP:OD1   | 2:K:67:ARG:NH2   | 2.52                     | 0.43              |
| 1:E:32:LYS:O     | 1:E:167:SER:HA   | 2.18                     | 0.43              |
| 1:E:109:ILE:CG2  | 1:E:147:ARG:HD3  | 2.48                     | 0.43              |
| 1:F:187:LYS:O    | 1:F:190:VAL:HG13 | 2.18                     | 0.43              |
| 1:G:52:LYS:HE3   | 1:G:64:ILE:HG23  | 1.99                     | 0.43              |
| 2:L:59:MET:HE1   | 2:L:82:LEU:CD2   | 2.48                     | 0.43              |
| 2:M:93:MET:N     | 2:M:94:PRO:CD    | 2.81                     | 0.43              |
| 2:N:83:LEU:HD12  | 2:N:83:LEU:HA    | 1.85                     | 0.43              |
| 1:P:49:ILE:HD11  | 1:P:210:PRO:CB   | 2.47                     | 0.43              |
| 1:P:109:ILE:CG2  | 1:P:147:ARG:HD3  | 2.48                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:Q:103:TYR:C   | 2:Y:81:THR:HG22  | 2.37                     | 0.43              |
| 1:Q:109:ILE:CG2 | 1:Q:147:ARG:HD3  | 2.48                     | 0.43              |
| 1:Q:111:ASN:CB  | 2:Y:70:ARG:NH1   | 2.80                     | 0.43              |
| 1:S:108:ASN:HB2 | 2:1:70:ARG:CD    | 2.48                     | 0.43              |
| 1:T:12:ILE:CD1  | 1:T:23:GLN:CB    | 0.48                     | 0.43              |
| 2:W:187:LEU:HA  | 2:W:188:PRO:HD3  | 1.83                     | 0.43              |
| 1:B:108:ASN:ND2 | 2:J:70:ARG:HA    | 2.34                     | 0.43              |
| 1:B:130:ARG:NH1 | 1:B:131:PRO:O    | 2.51                     | 0.43              |
| 1:C:109:ILE:CG2 | 1:C:147:ARG:HD3  | 2.48                     | 0.43              |
| 1:E:49:ILE:HD11 | 1:E:210:PRO:CB   | 2.47                     | 0.43              |
| 1:F:16:SER:HB3  | 1:F:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:G:24:VAL:O    | 1:G:28:ARG:HG3   | 2.17                     | 0.43              |
| 1:G:143:GLN:OE1 | 2:H:75:PRO:CG    | 2.66                     | 0.43              |
| 1:G:187:LYS:O   | 1:G:190:VAL:HG13 | 2.18                     | 0.43              |
| 2:I:146:MET:HA  | 2:I:150:GLU:OE1  | 2.17                     | 0.43              |
| 2:L:76:ILE:HA   | 2:L:79:VAL:HG12  | 2.00                     | 0.43              |
| 2:L:178:ILE:HB  | 2:L:184:TYR:HA   | 2.00                     | 0.43              |
| 2:N:165:ARG:HA  | 2:Y:26:ILE:CG2   | 2.48                     | 0.43              |
| 1:O:18:ASP:OD2  | 1:O:20:ARG:HD3   | 2.17                     | 0.43              |
| 1:O:52:LYS:HE3  | 1:O:64:ILE:HG23  | 1.99                     | 0.43              |
| 1:O:130:ARG:NH1 | 1:O:131:PRO:O    | 2.52                     | 0.43              |
| 1:O:159:GLU:O   | 1:P:60:GLU:HB2   | 2.17                     | 0.43              |
| 1:Q:16:SER:HB3  | 1:Q:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:Q:32:LYS:O    | 1:Q:167:SER:HA   | 2.18                     | 0.43              |
| 1:Q:52:LYS:HE3  | 1:Q:64:ILE:HG23  | 1.99                     | 0.43              |
| 1:Q:187:LYS:O   | 1:Q:190:VAL:HG13 | 2.19                     | 0.43              |
| 1:R:72:ASP:OD1  | 2:Y:67:ARG:NH2   | 2.51                     | 0.43              |
| 1:S:173:VAL:CG2 | 1:T:58:LEU:HD23  | 2.47                     | 0.43              |
| 1:T:16:SER:HB3  | 1:T:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:T:32:LYS:O    | 1:T:167:SER:HA   | 2.18                     | 0.43              |
| 1:T:49:ILE:HD11 | 1:T:210:PRO:CB   | 2.47                     | 0.43              |
| 1:T:130:ARG:NH1 | 1:T:131:PRO:O    | 2.52                     | 0.43              |
| 1:U:109:ILE:CG2 | 1:U:147:ARG:HD3  | 2.48                     | 0.43              |
| 1:U:130:ARG:NH1 | 1:U:131:PRO:O    | 2.51                     | 0.43              |
| 2:Y:19:ARG:HD2  | 2:Y:169:SER:C    | 2.43                     | 0.43              |
| 2:2:111:PHE:CE2 | 2:2:121:GLU:HB2  | 2.53                     | 0.43              |
| 1:A:130:ARG:NH1 | 1:A:131:PRO:O    | 2.51                     | 0.43              |
| 1:D:32:LYS:O    | 1:D:167:SER:HA   | 2.18                     | 0.43              |
| 1:D:109:ILE:CG2 | 1:D:147:ARG:HD3  | 2.48                     | 0.43              |
| 1:D:130:ARG:NH1 | 1:D:131:PRO:O    | 2.51                     | 0.43              |
| 1:E:130:ARG:NH1 | 1:E:131:PRO:O    | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:32:LYS:O     | 1:F:167:SER:HA   | 2.18                     | 0.43              |
| 1:F:52:LYS:HE3   | 1:F:64:ILE:HG23  | 1.99                     | 0.43              |
| 1:F:109:ILE:CG2  | 1:F:147:ARG:HD3  | 2.48                     | 0.43              |
| 2:J:49:VAL:HG23  | 2:J:50:GLY:H     | 1.82                     | 0.43              |
| 2:M:133:PHE:HE1  | 2:1:132:PRO:HA   | 1.81                     | 0.43              |
| 2:N:138:LEU:HD12 | 2:N:138:LEU:HA   | 1.71                     | 0.43              |
| 1:P:32:LYS:O     | 1:P:167:SER:HA   | 2.18                     | 0.43              |
| 1:R:17:PRO:HA    | 1:S:26:TYR:CG    | 2.53                     | 0.43              |
| 1:R:187:LYS:O    | 1:R:190:VAL:HG13 | 2.19                     | 0.43              |
| 1:S:130:ARG:NH1  | 1:S:131:PRO:O    | 2.52                     | 0.43              |
| 1:U:16:SER:HB3   | 1:U:22:PHE:CE2   | 2.53                     | 0.43              |
| 2:V:17:GLU:HA    | 2:V:173:ILE:HA   | 2.01                     | 0.43              |
| 2:W:184:TYR:CD1  | 2:W:184:TYR:C    | 2.97                     | 0.43              |
| 2:2:49:VAL:O     | 2:2:50:GLY:C     | 2.61                     | 0.43              |
| 1:B:12:ILE:N     | 1:B:23:GLN:HG2   | 2.31                     | 0.43              |
| 1:C:16:SER:HB3   | 1:C:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:D:81:LEU:HD23  | 1:D:133:GLY:HA3  | 2.00                     | 0.43              |
| 1:E:187:LYS:O    | 1:E:190:VAL:HG13 | 2.18                     | 0.43              |
| 1:F:19:GLY:CA    | 1:G:30:ALA:HB2   | 2.49                     | 0.43              |
| 1:G:12:ILE:HD13  | 1:G:23:GLN:CB    | 1.02                     | 0.43              |
| 2:H:90:VAL:O     | 2:H:90:VAL:HG22  | 2.18                     | 0.43              |
| 2:L:189:THR:HG23 | 2:L:190:ASP:H    | 1.83                     | 0.43              |
| 2:N:141:GLN:NE2  | 2:Z:141:GLN:HE21 | 2.15                     | 0.43              |
| 2:N:173:ILE:HD13 | 2:N:173:ILE:C    | 2.43                     | 0.43              |
| 1:O:10:ARG:NH1   | 1:U:7:ALA:CB     | 2.77                     | 0.43              |
| 1:P:160:TYR:C    | 1:Q:60:GLU:HG3   | 2.43                     | 0.43              |
| 1:R:130:ARG:NH1  | 1:R:131:PRO:O    | 2.52                     | 0.43              |
| 1:S:111:ASN:HB2  | 2:1:70:ARG:NH1   | 2.33                     | 0.43              |
| 1:U:143:GLN:OE1  | 2:V:75:PRO:CG    | 2.66                     | 0.43              |
| 2:V:19:ARG:HE    | 2:V:26:ILE:HG13  | 1.84                     | 0.43              |
| 2:Z:6:ILE:HD11   | 2:Z:142:TYR:CD1  | 2.52                     | 0.43              |
| 1:B:160:TYR:C    | 1:C:60:GLU:HG3   | 2.43                     | 0.43              |
| 1:C:130:ARG:NH1  | 1:C:131:PRO:O    | 2.52                     | 0.43              |
| 1:D:16:SER:HB3   | 1:D:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:G:130:ARG:NH1  | 1:G:131:PRO:O    | 2.51                     | 0.43              |
| 2:H:17:GLU:HA    | 2:H:173:ILE:HA   | 2.01                     | 0.43              |
| 2:M:66:TYR:CZ    | 2:M:70:ARG:HD2   | 2.54                     | 0.43              |
| 1:O:58:LEU:HD22  | 1:U:173:VAL:O    | 2.11                     | 0.43              |
| 1:P:16:SER:HB3   | 1:P:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:P:177:GLU:N    | 1:Q:58:LEU:CD2   | 2.66                     | 0.43              |
| 1:P:187:LYS:O    | 1:P:190:VAL:HG13 | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:108:ASN:HD22 | 2:Y:70:ARG:CA    | 2.24                     | 0.43              |
| 1:T:19:GLY:CA    | 1:U:30:ALA:HB2   | 2.49                     | 0.43              |
| 2:Y:59:MET:CE    | 2:Y:82:LEU:HD23  | 2.43                     | 0.43              |
| 1:B:32:LYS:O     | 1:B:167:SER:HA   | 2.18                     | 0.43              |
| 1:B:109:ILE:CG2  | 1:B:147:ARG:HD3  | 2.48                     | 0.43              |
| 1:C:111:ASN:CB   | 2:K:70:ARG:NH1   | 2.80                     | 0.43              |
| 1:E:108:ASN:ND2  | 2:M:70:ARG:CB    | 2.72                     | 0.43              |
| 1:F:130:ARG:NH1  | 1:F:131:PRO:O    | 2.52                     | 0.43              |
| 1:F:177:GLU:O    | 1:G:58:LEU:CD1   | 2.67                     | 0.43              |
| 2:H:19:ARG:HE    | 2:H:26:ILE:HG13  | 1.84                     | 0.43              |
| 2:L:3:THR:OG1    | 2:L:127:THR:HG22 | 2.19                     | 0.43              |
| 1:R:24:VAL:O     | 1:R:28:ARG:HG3   | 2.17                     | 0.43              |
| 1:S:32:LYS:O     | 1:S:167:SER:HA   | 2.18                     | 0.43              |
| 1:T:52:LYS:HB3   | 1:T:209:ALA:O    | 2.19                     | 0.43              |
| 2:Y:6:ILE:HD11   | 2:Y:142:TYR:CD1  | 2.53                     | 0.43              |
| 2:Z:105:ASP:OD1  | 2:Z:106:THR:N    | 2.52                     | 0.43              |
| 2:Z:189:THR:HG23 | 2:Z:190:ASP:H    | 1.84                     | 0.43              |
| 2:1:66:TYR:CZ    | 2:1:70:ARG:HD2   | 2.53                     | 0.43              |
| 2:1:93:MET:N     | 2:1:94:PRO:CD    | 2.81                     | 0.43              |
| 1:D:187:LYS:O    | 1:D:190:VAL:HG13 | 2.19                     | 0.43              |
| 1:E:16:SER:HB3   | 1:E:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:G:16:SER:HB3   | 1:G:22:PHE:CE2   | 2.53                     | 0.43              |
| 2:H:103:GLY:HA2  | 2:H:178:ILE:HD13 | 2.01                     | 0.43              |
| 2:J:105:ASP:CG   | 2:J:106:THR:H    | 2.26                     | 0.43              |
| 2:M:49:VAL:O     | 2:M:50:GLY:C     | 2.61                     | 0.43              |
| 1:O:32:LYS:O     | 1:O:167:SER:HA   | 2.18                     | 0.43              |
| 1:P:130:ARG:NH1  | 1:P:131:PRO:O    | 2.51                     | 0.43              |
| 1:Q:12:ILE:HD12  | 1:Q:23:GLN:CB    | 0.59                     | 0.43              |
| 1:Q:81:LEU:HD23  | 1:Q:133:GLY:HA3  | 2.00                     | 0.43              |
| 1:S:187:LYS:O    | 1:S:190:VAL:HG13 | 2.19                     | 0.43              |
| 2:V:83:LEU:HD12  | 2:V:83:LEU:HA    | 1.69                     | 0.43              |
| 2:V:103:GLY:HA2  | 2:V:178:ILE:HD13 | 2.01                     | 0.43              |
| 2:Z:55:LEU:HD12  | 2:Z:55:LEU:HA    | 1.67                     | 0.43              |
| 1:A:16:SER:HB3   | 1:A:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:A:32:LYS:O     | 1:A:167:SER:HA   | 2.18                     | 0.43              |
| 1:B:16:SER:HB3   | 1:B:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:B:177:GLU:CD   | 1:C:57:ARG:N     | 2.66                     | 0.43              |
| 1:D:103:TYR:O    | 2:L:81:THR:CB    | 2.66                     | 0.43              |
| 1:E:52:LYS:HB3   | 1:E:209:ALA:O    | 2.19                     | 0.43              |
| 1:G:12:ILE:N     | 1:G:23:GLN:HG2   | 2.31                     | 0.43              |
| 2:H:131:SER:O    | 2:H:134:VAL:HG13 | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:45:ILE:CD1   | 2:I:52:ALA:HB1   | 2.49                     | 0.43              |
| 2:L:180:ARG:HA   | 2:L:180:ARG:HD2  | 1.72                     | 0.43              |
| 2:L:187:LEU:HA   | 2:L:188:PRO:HD3  | 1.77                     | 0.43              |
| 2:M:109:HIS:HB3  | 2:M:111:PHE:HE1  | 1.84                     | 0.43              |
| 2:M:132:PRO:HA   | 2:1:133:PHE:HE1  | 1.81                     | 0.43              |
| 2:N:160:SER:HA   | 2:N:163:LYS:HD3  | 2.00                     | 0.43              |
| 1:T:15:PHE:HZ    | 1:U:130:ARG:NH1  | 2.07                     | 0.43              |
| 2:Y:157:ARG:O    | 2:Y:160:SER:HB2  | 2.19                     | 0.43              |
| 2:Z:15:ALA:HB3   | 2:Z:155:VAL:HG11 | 2.00                     | 0.43              |
| 2:Z:26:ILE:HD13  | 2:Z:26:ILE:C     | 2.44                     | 0.43              |
| 2:Z:178:ILE:HB   | 2:Z:184:TYR:HA   | 2.01                     | 0.43              |
| 1:A:12:ILE:N     | 1:A:23:GLN:HG2   | 2.31                     | 0.43              |
| 1:A:60:GLU:CG    | 1:G:161:LYS:HB2  | 2.48                     | 0.43              |
| 1:B:49:ILE:HD11  | 1:B:210:PRO:CB   | 2.47                     | 0.43              |
| 1:B:52:LYS:HB3   | 1:B:209:ALA:O    | 2.19                     | 0.43              |
| 1:C:12:ILE:CD1   | 1:C:23:GLN:CB    | 0.48                     | 0.43              |
| 1:F:52:LYS:HB3   | 1:F:209:ALA:O    | 2.19                     | 0.43              |
| 2:H:202:ILE:HG12 | 2:H:203:LEU:N    | 2.34                     | 0.43              |
| 2:K:34:LEU:HD21  | 2:K:176:ALA:HB3  | 2.00                     | 0.43              |
| 2:M:87:LEU:HD23  | 2:M:114:ASP:O    | 2.19                     | 0.43              |
| 1:P:108:ASN:ND2  | 2:X:70:ARG:HA    | 2.34                     | 0.43              |
| 1:Q:7:ALA:HB1    | 1:R:10:ARG:HH11  | 1.84                     | 0.43              |
| 1:Q:52:LYS:HB3   | 1:Q:209:ALA:O    | 2.19                     | 0.43              |
| 1:Q:130:ARG:NH1  | 1:Q:131:PRO:O    | 2.52                     | 0.43              |
| 1:R:15:PHE:H     | 1:S:23:GLN:NE2   | 2.17                     | 0.43              |
| 1:R:16:SER:HB3   | 1:R:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:R:103:TYR:O    | 2:Z:81:THR:CB    | 2.66                     | 0.43              |
| 1:R:109:ILE:CG2  | 1:R:147:ARG:HD3  | 2.48                     | 0.43              |
| 1:S:81:LEU:HD23  | 1:S:133:GLY:HA3  | 2.00                     | 0.43              |
| 1:T:109:ILE:CG2  | 1:T:147:ARG:HD3  | 2.48                     | 0.43              |
| 1:U:12:ILE:CD1   | 1:U:23:GLN:CB    | 0.48                     | 0.43              |
| 2:V:3:THR:OG1    | 2:V:127:THR:HG22 | 2.19                     | 0.43              |
| 2:V:18:ARG:HE    | 2:V:30:ASN:HD22  | 1.67                     | 0.43              |
| 2:V:28:HIS:CD2   | 2:W:120:VAL:HG11 | 2.54                     | 0.43              |
| 2:Y:180:ARG:HD2  | 2:Y:180:ARG:HA   | 1.78                     | 0.43              |
| 2:2:7:THR:HB     | 2:2:123:ILE:O    | 2.18                     | 0.43              |
| 1:A:81:LEU:HD23  | 1:A:133:GLY:HA3  | 2.00                     | 0.43              |
| 1:A:107:VAL:HG13 | 2:I:66:TYR:OH    | 2.09                     | 0.43              |
| 1:A:109:ILE:CG2  | 1:A:147:ARG:HD3  | 2.48                     | 0.43              |
| 1:A:187:LYS:O    | 1:A:190:VAL:HG13 | 2.19                     | 0.43              |
| 1:C:81:LEU:HD23  | 1:C:133:GLY:HA3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:25:PHE:CD1   | 2:J:25:PHE:C     | 2.96                     | 0.43              |
| 2:L:26:ILE:HD13  | 2:L:26:ILE:C     | 2.44                     | 0.43              |
| 2:L:55:LEU:HD12  | 2:L:55:LEU:HA    | 1.68                     | 0.43              |
| 1:O:57:ARG:HE    | 1:U:177:GLU:C    | 2.16                     | 0.43              |
| 1:O:187:LYS:O    | 1:O:190:VAL:HG13 | 2.18                     | 0.43              |
| 1:P:125:GLN:O    | 1:Q:129:VAL:HG23 | 2.18                     | 0.43              |
| 1:S:16:SER:HB3   | 1:S:22:PHE:CE2   | 2.53                     | 0.43              |
| 1:T:187:LYS:O    | 1:T:190:VAL:HG13 | 2.19                     | 0.43              |
| 1:U:103:TYR:C    | 2:V:81:THR:HG22  | 2.39                     | 0.43              |
| 2:Z:15:ALA:HB3   | 2:Z:155:VAL:CG1  | 2.49                     | 0.43              |
| 1:B:187:LYS:O    | 1:B:190:VAL:HG13 | 2.19                     | 0.42              |
| 1:C:32:LYS:O     | 1:C:167:SER:HA   | 2.18                     | 0.42              |
| 1:C:107:VAL:HG21 | 2:K:66:TYR:HH    | 1.81                     | 0.42              |
| 1:D:15:PHE:CZ    | 1:E:133:GLY:N    | 2.87                     | 0.42              |
| 1:G:107:VAL:HG13 | 2:H:66:TYR:OH    | 2.08                     | 0.42              |
| 1:S:12:ILE:N     | 1:S:23:GLN:HG2   | 2.31                     | 0.42              |
| 2:V:59:MET:HE2   | 2:V:79:VAL:CG2   | 2.47                     | 0.42              |
| 2:W:180:ARG:HD2  | 2:W:180:ARG:HA   | 1.81                     | 0.42              |
| 2:2:59:MET:HE1   | 2:2:82:LEU:HD23  | 2.01                     | 0.42              |
| 1:C:54:VAL:HG22  | 1:C:55:ARG:N     | 2.35                     | 0.42              |
| 1:D:104:GLY:N    | 2:L:81:THR:HG21  | 2.28                     | 0.42              |
| 1:F:103:TYR:CE1  | 2:N:82:LEU:HD22  | 2.46                     | 0.42              |
| 1:F:155:GLY:O    | 1:G:86:ARG:CZ    | 2.58                     | 0.42              |
| 1:G:81:LEU:HD23  | 1:G:133:GLY:HA3  | 2.00                     | 0.42              |
| 1:G:109:ILE:CG2  | 1:G:147:ARG:HD3  | 2.48                     | 0.42              |
| 2:H:28:HIS:CD2   | 2:I:120:VAL:HG11 | 2.54                     | 0.42              |
| 2:K:6:ILE:HD11   | 2:K:142:TYR:CD1  | 2.53                     | 0.42              |
| 1:O:81:LEU:HD23  | 1:O:133:GLY:HA3  | 2.00                     | 0.42              |
| 1:O:173:VAL:O    | 1:P:58:LEU:CD2   | 2.67                     | 0.42              |
| 1:P:52:LYS:HB3   | 1:P:209:ALA:O    | 2.19                     | 0.42              |
| 1:R:12:ILE:HD13  | 1:R:23:GLN:CB    | 1.02                     | 0.42              |
| 1:R:12:ILE:N     | 1:R:23:GLN:HG2   | 2.31                     | 0.42              |
| 1:R:81:LEU:HD23  | 1:R:133:GLY:HA3  | 2.00                     | 0.42              |
| 1:T:81:LEU:HD23  | 1:T:133:GLY:HA3  | 2.00                     | 0.42              |
| 1:U:32:LYS:O     | 1:U:167:SER:HA   | 2.18                     | 0.42              |
| 1:U:54:VAL:HG22  | 1:U:55:ARG:N     | 2.35                     | 0.42              |
| 1:U:81:LEU:HD23  | 1:U:133:GLY:HA3  | 2.00                     | 0.42              |
| 2:Z:49:VAL:O     | 2:Z:50:GLY:C     | 2.62                     | 0.42              |
| 2:Z:157:ARG:O    | 2:Z:158:ALA:C    | 2.63                     | 0.42              |
| 2:1:74:MET:HA    | 2:1:75:PRO:HD3   | 1.87                     | 0.42              |
| 1:B:54:VAL:HG22  | 1:B:55:ARG:N     | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:187:LYS:O    | 1:C:190:VAL:HG13 | 2.19                     | 0.42              |
| 1:D:52:LYS:HB3   | 1:D:209:ALA:O    | 2.19                     | 0.42              |
| 1:E:81:LEU:HD23  | 1:E:133:GLY:HA3  | 2.00                     | 0.42              |
| 1:G:32:LYS:O     | 1:G:167:SER:HA   | 2.18                     | 0.42              |
| 2:H:55:LEU:HA    | 2:H:55:LEU:HD12  | 1.50                     | 0.42              |
| 2:L:15:ALA:HB3   | 2:L:155:VAL:HG11 | 2.00                     | 0.42              |
| 2:M:114:ASP:OD1  | 2:M:116:ALA:HB3  | 2.20                     | 0.42              |
| 2:N:111:PHE:CE2  | 2:N:121:GLU:HB2  | 2.53                     | 0.42              |
| 1:O:16:SER:HB3   | 1:O:22:PHE:CE2   | 2.53                     | 0.42              |
| 1:O:60:GLU:CG    | 1:U:161:LYS:HB2  | 2.48                     | 0.42              |
| 1:T:12:ILE:N     | 1:T:23:GLN:HG2   | 2.31                     | 0.42              |
| 1:U:187:LYS:O    | 1:U:190:VAL:HG13 | 2.18                     | 0.42              |
| 1:E:102:THR:O    | 2:M:81:THR:HG22  | 2.19                     | 0.42              |
| 1:F:81:LEU:HD23  | 1:F:133:GLY:HA3  | 2.00                     | 0.42              |
| 2:I:123:ILE:H    | 2:I:123:ILE:CD1  | 2.31                     | 0.42              |
| 2:I:184:TYR:CD1  | 2:I:184:TYR:C    | 2.97                     | 0.42              |
| 2:K:157:ARG:O    | 2:K:160:SER:HB2  | 2.19                     | 0.42              |
| 2:L:15:ALA:HB3   | 2:L:155:VAL:CG1  | 2.49                     | 0.42              |
| 2:N:22:MET:O     | 2:N:23:GLU:HB2   | 2.20                     | 0.42              |
| 1:Q:54:VAL:HG22  | 1:Q:55:ARG:N     | 2.35                     | 0.42              |
| 1:R:32:LYS:O     | 1:R:167:SER:HA   | 2.18                     | 0.42              |
| 1:S:52:LYS:HB3   | 1:S:209:ALA:O    | 2.19                     | 0.42              |
| 1:S:109:ILE:CG2  | 1:S:147:ARG:HD3  | 2.48                     | 0.42              |
| 1:T:12:ILE:HD13  | 1:T:23:GLN:CA    | 1.93                     | 0.42              |
| 1:T:54:VAL:HG22  | 1:T:55:ARG:N     | 2.35                     | 0.42              |
| 2:V:131:SER:O    | 2:V:134:VAL:HG13 | 2.19                     | 0.42              |
| 2:V:202:ILE:HG12 | 2:V:203:LEU:N    | 2.34                     | 0.42              |
| 2:Z:93:MET:N     | 2:Z:94:PRO:CD    | 2.81                     | 0.42              |
| 1:C:58:LEU:CD1   | 1:C:58:LEU:N     | 2.82                     | 0.42              |
| 1:C:101:VAL:CG2  | 2:J:58:TYR:HE1   | 1.92                     | 0.42              |
| 1:D:12:ILE:CD1   | 1:D:23:GLN:CB    | 0.48                     | 0.42              |
| 1:G:107:VAL:HG11 | 2:H:66:TYR:CE2   | 2.55                     | 0.42              |
| 2:H:83:LEU:HD12  | 2:H:83:LEU:HA    | 1.69                     | 0.42              |
| 2:H:179:THR:O    | 2:H:183:GLY:N    | 2.50                     | 0.42              |
| 2:J:34:LEU:HD21  | 2:J:176:ALA:CB   | 2.50                     | 0.42              |
| 1:P:177:GLU:CD   | 1:Q:57:ARG:N     | 2.66                     | 0.42              |
| 2:W:93:MET:N     | 2:W:94:PRO:CD    | 2.82                     | 0.42              |
| 2:1:109:HIS:HB3  | 2:1:111:PHE:HE1  | 1.84                     | 0.42              |
| 2:1:138:LEU:HD12 | 2:1:138:LEU:HA   | 1.86                     | 0.42              |
| 1:A:52:LYS:HB3   | 1:A:209:ALA:O    | 2.19                     | 0.42              |
| 1:B:56:SER:OG    | 1:B:58:LEU:HB2   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:123:TYR:N    | 1:B:123:TYR:CD1  | 2.88                     | 0.42              |
| 1:G:52:LYS:HB3   | 1:G:209:ALA:O    | 2.19                     | 0.42              |
| 2:H:3:THR:OG1    | 2:H:127:THR:HG22 | 2.19                     | 0.42              |
| 2:J:55:LEU:HD12  | 2:J:55:LEU:HA    | 1.85                     | 0.42              |
| 2:J:199:LEU:CB   | 2:J:201:LEU:HD13 | 2.50                     | 0.42              |
| 2:L:105:ASP:OD1  | 2:L:106:THR:N    | 2.52                     | 0.42              |
| 1:R:54:VAL:HG22  | 1:R:55:ARG:N     | 2.34                     | 0.42              |
| 1:R:159:GLU:O    | 1:S:60:GLU:HB2   | 2.19                     | 0.42              |
| 1:T:155:GLY:O    | 1:U:86:ARG:CZ    | 2.58                     | 0.42              |
| 1:U:107:VAL:HG21 | 2:V:66:TYR:HH    | 1.78                     | 0.42              |
| 2:X:109:HIS:HB3  | 2:X:111:PHE:CE1  | 2.54                     | 0.42              |
| 2:Z:3:THR:OG1    | 2:Z:127:THR:HG22 | 2.19                     | 0.42              |
| 2:2:187:LEU:HA   | 2:2:188:PRO:HD3  | 1.81                     | 0.42              |
| 1:C:7:ALA:HB1    | 1:D:10:ARG:HH11  | 1.84                     | 0.42              |
| 1:C:52:LYS:HB3   | 1:C:209:ALA:O    | 2.19                     | 0.42              |
| 1:F:12:ILE:N     | 1:F:23:GLN:HG2   | 2.31                     | 0.42              |
| 1:G:54:VAL:HG22  | 1:G:55:ARG:N     | 2.34                     | 0.42              |
| 2:J:187:LEU:HA   | 2:J:188:PRO:HD3  | 1.79                     | 0.42              |
| 1:O:52:LYS:HB3   | 1:O:209:ALA:O    | 2.19                     | 0.42              |
| 1:P:81:LEU:HD23  | 1:P:133:GLY:HA3  | 2.00                     | 0.42              |
| 1:R:52:LYS:HB3   | 1:R:209:ALA:O    | 2.19                     | 0.42              |
| 1:T:56:SER:OG    | 1:T:58:LEU:HB2   | 2.20                     | 0.42              |
| 1:U:58:LEU:CD1   | 1:U:58:LEU:N     | 2.83                     | 0.42              |
| 2:W:191:GLN:O    | 2:W:194:SER:HB3  | 2.20                     | 0.42              |
| 2:X:25:PHE:C     | 2:X:25:PHE:CD1   | 2.96                     | 0.42              |
| 2:X:187:LEU:HA   | 2:X:188:PRO:HD3  | 1.79                     | 0.42              |
| 2:Z:143:SER:O    | 2:Z:146:MET:HG3  | 2.20                     | 0.42              |
| 2:Z:190:ASP:HA   | 2:Z:193:GLU:HG2  | 2.02                     | 0.42              |
| 2:2:25:PHE:C     | 2:2:25:PHE:HD1   | 2.26                     | 0.42              |
| 1:A:72:ASP:OD1   | 2:H:67:ARG:NH2   | 2.53                     | 0.42              |
| 1:B:81:LEU:HD23  | 1:B:133:GLY:HA3  | 2.00                     | 0.42              |
| 1:C:123:TYR:CD1  | 1:C:123:TYR:N    | 2.88                     | 0.42              |
| 1:E:54:VAL:HG22  | 1:E:55:ARG:N     | 2.35                     | 0.42              |
| 1:F:54:VAL:HG22  | 1:F:55:ARG:N     | 2.35                     | 0.42              |
| 1:F:56:SER:OG    | 1:F:58:LEU:HB2   | 2.20                     | 0.42              |
| 2:L:2:THR:HG23   | 2:L:17:GLU:HG3   | 2.02                     | 0.42              |
| 1:O:108:ASN:CB   | 2:W:70:ARG:CD    | 2.93                     | 0.42              |
| 1:P:72:ASP:OD2   | 2:W:67:ARG:NH2   | 2.52                     | 0.42              |
| 1:P:103:TYR:O    | 2:X:81:THR:HB    | 2.19                     | 0.42              |
| 1:T:103:TYR:CE1  | 2:2:82:LEU:HD22  | 2.46                     | 0.42              |
| 1:T:123:TYR:N    | 1:T:123:TYR:CD1  | 2.88                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:52:LYS:HB3   | 1:U:209:ALA:O    | 2.19                     | 0.42              |
| 1:A:108:ASN:HD22 | 2:I:70:ARG:CG    | 2.33                     | 0.42              |
| 1:A:173:VAL:O    | 1:B:58:LEU:CD2   | 2.67                     | 0.42              |
| 1:D:56:SER:OG    | 1:D:58:LEU:HB2   | 2.20                     | 0.42              |
| 1:G:56:SER:OG    | 1:G:58:LEU:HB2   | 2.20                     | 0.42              |
| 2:I:180:ARG:HD2  | 2:I:180:ARG:HA   | 1.81                     | 0.42              |
| 2:I:191:GLN:O    | 2:I:194:SER:HB3  | 2.20                     | 0.42              |
| 1:O:123:TYR:N    | 1:O:123:TYR:CD1  | 2.88                     | 0.42              |
| 1:O:155:GLY:O    | 1:P:86:ARG:CZ    | 2.66                     | 0.42              |
| 1:R:56:SER:OG    | 1:R:58:LEU:HB2   | 2.20                     | 0.42              |
| 1:R:101:VAL:HG22 | 2:Y:58:TYR:HE1   | 1.76                     | 0.42              |
| 2:W:188:PRO:O    | 2:W:189:THR:C    | 2.63                     | 0.42              |
| 2:2:22:MET:O     | 2:2:23:GLU:HB2   | 2.20                     | 0.42              |
| 1:A:58:LEU:N     | 1:A:58:LEU:CD1   | 2.82                     | 0.42              |
| 1:E:58:LEU:N     | 1:E:58:LEU:CD1   | 2.82                     | 0.42              |
| 1:E:123:TYR:CD1  | 1:E:123:TYR:N    | 2.88                     | 0.42              |
| 2:J:74:MET:HA    | 2:J:75:PRO:HD3   | 1.88                     | 0.42              |
| 1:O:58:LEU:N     | 1:O:58:LEU:CD1   | 2.82                     | 0.42              |
| 1:S:102:THR:O    | 2:1:81:THR:HG22  | 2.19                     | 0.42              |
| 1:U:123:TYR:N    | 1:U:123:TYR:CD1  | 2.88                     | 0.42              |
| 2:Z:163:LYS:CE   | 2:Z:203:LEU:HD23 | 2.50                     | 0.42              |
| 1:A:14:VAL:H     | 1:B:130:ARG:HB2  | 1.85                     | 0.41              |
| 1:B:58:LEU:CD1   | 1:B:58:LEU:N     | 2.83                     | 0.41              |
| 1:C:177:GLU:CD   | 1:D:58:LEU:HB2   | 2.44                     | 0.41              |
| 1:D:15:PHE:HE2   | 1:E:131:PRO:O    | 2.03                     | 0.41              |
| 2:I:188:PRO:O    | 2:I:189:THR:C    | 2.63                     | 0.41              |
| 2:M:17:GLU:O     | 2:M:33:LYS:HD2   | 2.20                     | 0.41              |
| 1:T:58:LEU:N     | 1:T:58:LEU:CD1   | 2.82                     | 0.41              |
| 1:T:198:LYS:CG   | 1:T:202:GLU:HG2  | 2.50                     | 0.41              |
| 2:W:45:ILE:CD1   | 2:W:52:ALA:HB1   | 2.49                     | 0.41              |
| 2:X:34:LEU:HD21  | 2:X:176:ALA:CB   | 2.50                     | 0.41              |
| 2:X:123:ILE:HG12 | 2:X:124:TYR:CD1  | 2.51                     | 0.41              |
| 2:Z:180:ARG:HA   | 2:Z:180:ARG:HD2  | 1.71                     | 0.41              |
| 1:B:198:LYS:CG   | 1:B:202:GLU:HG2  | 2.50                     | 0.41              |
| 1:D:107:VAL:CG2  | 2:L:66:TYR:OH    | 2.68                     | 0.41              |
| 1:G:58:LEU:CD1   | 1:G:58:LEU:N     | 2.82                     | 0.41              |
| 2:I:147:THR:OG1  | 2:I:150:GLU:HG3  | 2.21                     | 0.41              |
| 2:L:157:ARG:O    | 2:L:158:ALA:C    | 2.63                     | 0.41              |
| 2:M:111:PHE:CE2  | 2:M:121:GLU:HB2  | 2.55                     | 0.41              |
| 1:O:72:ASP:OD1   | 2:V:67:ARG:NH2   | 2.53                     | 0.41              |
| 1:O:102:THR:O    | 2:W:81:THR:HG22  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:108:ASN:HD22 | 2:W:70:ARG:CG    | 2.33                     | 0.41              |
| 1:P:54:VAL:HG22  | 1:P:55:ARG:N     | 2.35                     | 0.41              |
| 2:1:87:LEU:HD23  | 2:1:114:ASP:O    | 2.19                     | 0.41              |
| 1:A:57:ARG:CZ    | 1:G:178:ARG:O    | 2.63                     | 0.41              |
| 1:A:126:TYR:HA   | 1:B:129:VAL:HG23 | 2.03                     | 0.41              |
| 1:B:12:ILE:HD13  | 1:B:23:GLN:CA    | 1.92                     | 0.41              |
| 1:D:159:GLU:O    | 1:E:60:GLU:HB2   | 2.19                     | 0.41              |
| 1:E:56:SER:OG    | 1:E:58:LEU:HB2   | 2.20                     | 0.41              |
| 1:F:21:LEU:HD21  | 1:G:130:ARG:CZ   | 2.50                     | 0.41              |
| 1:G:107:VAL:CG1  | 2:H:66:TYR:CZ    | 2.94                     | 0.41              |
| 2:J:190:ASP:HA   | 2:J:193:GLU:HG2  | 2.02                     | 0.41              |
| 2:M:59:MET:HE1   | 2:M:82:LEU:HD23  | 2.01                     | 0.41              |
| 2:M:163:LYS:CE   | 2:M:203:LEU:HD23 | 2.50                     | 0.41              |
| 2:N:59:MET:HE1   | 2:N:82:LEU:HD23  | 2.01                     | 0.41              |
| 1:P:123:TYR:CD1  | 1:P:123:TYR:N    | 2.88                     | 0.41              |
| 1:U:44:ASN:HD22  | 1:U:44:ASN:HA    | 1.56                     | 0.41              |
| 1:U:56:SER:OG    | 1:U:58:LEU:HB2   | 2.20                     | 0.41              |
| 2:W:123:ILE:H    | 2:W:123:ILE:CD1  | 2.31                     | 0.41              |
| 2:1:59:MET:HE1   | 2:1:82:LEU:HD23  | 2.01                     | 0.41              |
| 1:E:15:PHE:CZ    | 1:F:133:GLY:N    | 2.88                     | 0.41              |
| 2:I:19:ARG:NE    | 2:I:26:ILE:HG13  | 2.36                     | 0.41              |
| 2:I:93:MET:N     | 2:I:94:PRO:CD    | 2.82                     | 0.41              |
| 2:I:175:VAL:HG22 | 2:I:176:ALA:N    | 2.35                     | 0.41              |
| 2:L:143:SER:O    | 2:L:146:MET:HG3  | 2.20                     | 0.41              |
| 2:L:163:LYS:CE   | 2:L:203:LEU:HD23 | 2.50                     | 0.41              |
| 2:M:3:THR:HB     | 2:M:16:THR:HG22  | 2.03                     | 0.41              |
| 1:R:15:PHE:CZ    | 1:S:133:GLY:N    | 2.87                     | 0.41              |
| 1:R:107:VAL:CG2  | 2:Z:66:TYR:OH    | 2.68                     | 0.41              |
| 1:R:160:TYR:C    | 1:S:60:GLU:HG2   | 2.41                     | 0.41              |
| 1:T:21:LEU:HD21  | 1:U:130:ARG:CZ   | 2.50                     | 0.41              |
| 2:V:180:ARG:HA   | 2:V:180:ARG:HD2  | 1.79                     | 0.41              |
| 2:1:114:ASP:OD1  | 2:1:116:ALA:HB3  | 2.20                     | 0.41              |
| 1:A:102:THR:O    | 2:I:81:THR:HG22  | 2.20                     | 0.41              |
| 1:C:56:SER:OG    | 1:C:58:LEU:HB2   | 2.20                     | 0.41              |
| 1:D:123:TYR:N    | 1:D:123:TYR:CD1  | 2.88                     | 0.41              |
| 1:E:12:ILE:N     | 1:E:23:GLN:HG2   | 2.31                     | 0.41              |
| 2:K:26:ILE:CG2   | 2:2:165:ARG:HA   | 2.50                     | 0.41              |
| 2:M:187:LEU:HA   | 2:M:188:PRO:HD3  | 1.82                     | 0.41              |
| 2:N:59:MET:SD    | 2:N:83:LEU:HD13  | 2.60                     | 0.41              |
| 2:N:158:ALA:O    | 2:N:161:ALA:HB3  | 2.21                     | 0.41              |
| 1:Q:56:SER:OG    | 1:Q:58:LEU:HB2   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:12:ILE:CD1   | 1:R:23:GLN:CB    | 0.48                     | 0.41              |
| 1:S:54:VAL:HG22  | 1:S:55:ARG:N     | 2.35                     | 0.41              |
| 1:S:58:LEU:N     | 1:S:58:LEU:CD1   | 2.82                     | 0.41              |
| 1:T:161:LYS:HB2  | 1:U:60:GLU:CD    | 2.37                     | 0.41              |
| 2:Y:49:VAL:O     | 2:Y:50:GLY:C     | 2.64                     | 0.41              |
| 2:1:49:VAL:O     | 2:1:50:GLY:C     | 2.61                     | 0.41              |
| 2:1:137:VAL:HG21 | 2:1:158:ALA:HA   | 2.01                     | 0.41              |
| 2:1:163:LYS:CE   | 2:1:203:LEU:HD23 | 2.50                     | 0.41              |
| 1:A:54:VAL:HG22  | 1:A:55:ARG:N     | 2.35                     | 0.41              |
| 1:A:198:LYS:CG   | 1:A:202:GLU:HG2  | 2.50                     | 0.41              |
| 1:G:123:TYR:N    | 1:G:123:TYR:CD1  | 2.88                     | 0.41              |
| 2:L:66:TYR:CZ    | 2:L:70:ARG:HD2   | 2.56                     | 0.41              |
| 1:O:56:SER:OG    | 1:O:58:LEU:HB2   | 2.20                     | 0.41              |
| 1:Q:12:ILE:N     | 1:Q:23:GLN:HG2   | 2.31                     | 0.41              |
| 1:Q:58:LEU:CD1   | 1:Q:58:LEU:N     | 2.82                     | 0.41              |
| 1:Q:177:GLU:CD   | 1:R:58:LEU:HB2   | 2.44                     | 0.41              |
| 1:R:101:VAL:HG21 | 2:Y:58:TYR:CE1   | 2.41                     | 0.41              |
| 1:S:15:PHE:CZ    | 1:T:133:GLY:N    | 2.88                     | 0.41              |
| 1:U:107:VAL:HG11 | 2:V:66:TYR:CE2   | 2.55                     | 0.41              |
| 2:V:187:LEU:HA   | 2:V:188:PRO:HD3  | 1.77                     | 0.41              |
| 2:X:105:ASP:CG   | 2:X:106:THR:H    | 2.26                     | 0.41              |
| 2:1:17:GLU:O     | 2:1:33:LYS:HD2   | 2.20                     | 0.41              |
| 2:1:111:PHE:CE2  | 2:1:121:GLU:HB2  | 2.55                     | 0.41              |
| 1:B:103:TYR:O    | 2:J:81:THR:HB    | 2.19                     | 0.41              |
| 1:G:78:THR:CG2   | 1:G:85:ALA:HB1   | 2.45                     | 0.41              |
| 1:G:176:LEU:C    | 1:G:178:ARG:N    | 2.79                     | 0.41              |
| 2:H:18:ARG:HE    | 2:H:30:ASN:HD22  | 1.67                     | 0.41              |
| 2:I:105:ASP:CG   | 2:I:106:THR:H    | 2.28                     | 0.41              |
| 2:K:22:MET:O     | 2:K:23:GLU:HB2   | 2.21                     | 0.41              |
| 2:K:49:VAL:HG23  | 2:K:50:GLY:H     | 1.86                     | 0.41              |
| 2:L:20:VAL:CG1   | 2:L:28:HIS:HB2   | 2.44                     | 0.41              |
| 2:L:97:VAL:HG22  | 2:L:98:GLN:N     | 2.36                     | 0.41              |
| 2:M:165:ARG:NH2  | 2:1:135:TYR:HE1  | 2.18                     | 0.41              |
| 1:P:56:SER:OG    | 1:P:58:LEU:HB2   | 2.20                     | 0.41              |
| 1:P:58:LEU:CD1   | 1:P:58:LEU:N     | 2.83                     | 0.41              |
| 2:Y:86:MET:HE2   | 2:Y:86:MET:HB3   | 2.00                     | 0.41              |
| 2:1:3:THR:HB     | 2:1:16:THR:HG22  | 2.03                     | 0.41              |
| 2:2:177:VAL:HG13 | 2:2:185:VAL:HG13 | 2.03                     | 0.41              |
| 1:A:56:SER:OG    | 1:A:58:LEU:HB2   | 2.20                     | 0.41              |
| 1:A:165:ILE:HD12 | 1:A:169:LYS:HD2  | 2.03                     | 0.41              |
| 2:I:56:VAL:CG1   | 2:I:57:ARG:N     | 2.84                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:59:MET:HE2   | 2:J:79:VAL:HG23  | 2.03                     | 0.41              |
| 2:J:203:LEU:HD12 | 2:J:203:LEU:HA   | 1.86                     | 0.41              |
| 2:N:133:PHE:HE1  | 2:Z:132:PRO:HA   | 1.83                     | 0.41              |
| 2:N:187:LEU:HA   | 2:N:188:PRO:HD3  | 1.81                     | 0.41              |
| 1:R:58:LEU:CD1   | 1:R:58:LEU:N     | 2.82                     | 0.41              |
| 1:S:198:LYS:CG   | 1:S:202:GLU:HG2  | 2.50                     | 0.41              |
| 2:W:56:VAL:CG1   | 2:W:57:ARG:N     | 2.84                     | 0.41              |
| 2:Z:20:VAL:CG1   | 2:Z:28:HIS:HB2   | 2.44                     | 0.41              |
| 2:Z:97:VAL:HG22  | 2:Z:98:GLN:N     | 2.36                     | 0.41              |
| 1:D:54:VAL:HG22  | 1:D:55:ARG:N     | 2.34                     | 0.41              |
| 1:E:227:GLU:N    | 1:E:227:GLU:CD   | 2.79                     | 0.41              |
| 2:J:141:GLN:HE21 | 2:W:141:GLN:HE21 | 1.69                     | 0.41              |
| 2:J:190:ASP:O    | 2:J:193:GLU:HG2  | 2.21                     | 0.41              |
| 2:L:138:LEU:HD12 | 2:L:138:LEU:HA   | 1.90                     | 0.41              |
| 2:M:86:MET:HE2   | 2:M:86:MET:HB3   | 1.91                     | 0.41              |
| 2:M:135:TYR:HE1  | 2:1:165:ARG:NH2  | 2.19                     | 0.41              |
| 2:M:137:VAL:HG21 | 2:M:158:ALA:HA   | 2.01                     | 0.41              |
| 2:N:74:MET:HA    | 2:N:75:PRO:HD3   | 1.95                     | 0.41              |
| 1:O:126:TYR:HA   | 1:P:129:VAL:HG23 | 2.03                     | 0.41              |
| 1:R:123:TYR:CD1  | 1:R:123:TYR:N    | 2.88                     | 0.41              |
| 1:R:176:LEU:C    | 1:R:178:ARG:N    | 2.79                     | 0.41              |
| 1:S:56:SER:OG    | 1:S:58:LEU:HB2   | 2.20                     | 0.41              |
| 1:S:165:ILE:HD12 | 1:S:169:LYS:HD2  | 2.03                     | 0.41              |
| 1:T:12:ILE:CD1   | 1:T:23:GLN:HB3   | 0.55                     | 0.41              |
| 1:T:165:ILE:HD12 | 1:T:169:LYS:HD2  | 2.03                     | 0.41              |
| 2:W:19:ARG:NE    | 2:W:26:ILE:HG13  | 2.36                     | 0.41              |
| 2:Y:19:ARG:NH1   | 2:Y:169:SER:O    | 2.54                     | 0.41              |
| 2:Z:66:TYR:CZ    | 2:Z:70:ARG:HD2   | 2.56                     | 0.41              |
| 2:2:72:VAL:HG22  | 2:2:73:ASN:N     | 2.36                     | 0.41              |
| 1:A:12:ILE:CD1   | 1:A:23:GLN:CB    | 0.48                     | 0.41              |
| 1:B:165:ILE:HD12 | 1:B:169:LYS:HD2  | 2.03                     | 0.41              |
| 1:D:198:LYS:CG   | 1:D:202:GLU:HG2  | 2.50                     | 0.41              |
| 1:E:177:GLU:OE2  | 1:F:56:SER:C     | 2.45                     | 0.41              |
| 1:F:58:LEU:N     | 1:F:58:LEU:CD1   | 2.82                     | 0.41              |
| 2:H:81:THR:O     | 2:H:84:SER:HB3   | 2.21                     | 0.41              |
| 2:J:26:ILE:HG23  | 2:V:165:ARG:HA   | 2.03                     | 0.41              |
| 2:J:109:HIS:HB3  | 2:J:111:PHE:CE1  | 2.55                     | 0.41              |
| 2:M:165:ARG:CZ   | 2:1:135:TYR:CD1  | 3.04                     | 0.41              |
| 1:O:14:VAL:H     | 1:P:130:ARG:HB2  | 1.85                     | 0.41              |
| 1:P:198:LYS:CG   | 1:P:202:GLU:HG2  | 2.50                     | 0.41              |
| 1:R:19:GLY:O     | 1:S:30:ALA:CB    | 2.69                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:71:ASP:HA    | 2:Y:68:LEU:HD21  | 2.03                     | 0.41              |
| 1:T:177:GLU:O    | 1:U:58:LEU:CD1   | 2.67                     | 0.41              |
| 1:U:101:VAL:HG23 | 2:2:58:TYR:CD1   | 2.39                     | 0.41              |
| 2:Y:34:LEU:HD21  | 2:Y:176:ALA:CB   | 2.51                     | 0.41              |
| 1:A:86:ARG:CZ    | 1:G:157:ILE:HG22 | 2.51                     | 0.40              |
| 1:C:177:GLU:CD   | 1:D:58:LEU:CB    | 2.91                     | 0.40              |
| 1:F:123:TYR:CD1  | 1:F:123:TYR:N    | 2.88                     | 0.40              |
| 1:F:177:GLU:CA   | 1:G:58:LEU:CG    | 2.53                     | 0.40              |
| 1:G:227:GLU:CD   | 1:G:227:GLU:N    | 2.80                     | 0.40              |
| 2:I:178:ILE:HB   | 2:I:184:TYR:HA   | 2.03                     | 0.40              |
| 2:J:103:GLY:HA2  | 2:J:178:ILE:HD11 | 2.02                     | 0.40              |
| 2:K:34:LEU:HD21  | 2:K:176:ALA:CB   | 2.51                     | 0.40              |
| 2:L:49:VAL:O     | 2:L:50:GLY:C     | 2.62                     | 0.40              |
| 2:M:76:ILE:HA    | 2:M:79:VAL:HG12  | 2.04                     | 0.40              |
| 1:O:54:VAL:HG22  | 1:O:55:ARG:N     | 2.34                     | 0.40              |
| 1:P:227:GLU:N    | 1:P:227:GLU:CD   | 2.80                     | 0.40              |
| 1:R:78:THR:CG2   | 1:R:85:ALA:HB1   | 2.45                     | 0.40              |
| 1:R:165:ILE:HD12 | 1:R:169:LYS:HD2  | 2.03                     | 0.40              |
| 2:W:178:ILE:HB   | 2:W:184:TYR:HA   | 2.03                     | 0.40              |
| 2:X:93:MET:N     | 2:X:94:PRO:CD    | 2.85                     | 0.40              |
| 2:Y:22:MET:O     | 2:Y:23:GLU:HB2   | 2.21                     | 0.40              |
| 2:Z:2:THR:HG23   | 2:Z:17:GLU:HG3   | 2.02                     | 0.40              |
| 2:Z:87:LEU:HD23  | 2:Z:114:ASP:O    | 2.20                     | 0.40              |
| 1:B:72:ASP:OD2   | 2:I:67:ARG:NH2   | 2.52                     | 0.40              |
| 1:E:198:LYS:CG   | 1:E:202:GLU:HG2  | 2.50                     | 0.40              |
| 1:F:124:THR:HG22 | 1:G:130:ARG:NH2  | 2.17                     | 0.40              |
| 1:G:165:ILE:HD12 | 1:G:169:LYS:HD2  | 2.03                     | 0.40              |
| 2:L:190:ASP:HA   | 2:L:193:GLU:HG2  | 2.02                     | 0.40              |
| 2:M:135:TYR:CD1  | 2:1:165:ARG:CZ   | 3.04                     | 0.40              |
| 1:P:12:ILE:CD1   | 1:P:23:GLN:CB    | 0.48                     | 0.40              |
| 1:R:15:PHE:HE2   | 1:S:131:PRO:O    | 2.03                     | 0.40              |
| 1:S:161:LYS:CG   | 1:T:60:GLU:OE2   | 2.60                     | 0.40              |
| 2:W:26:ILE:HD13  | 2:W:26:ILE:O     | 2.22                     | 0.40              |
| 2:W:105:ASP:CG   | 2:W:106:THR:H    | 2.28                     | 0.40              |
| 2:2:59:MET:SD    | 2:2:83:LEU:HD13  | 2.60                     | 0.40              |
| 1:B:102:THR:O    | 2:J:81:THR:HG22  | 2.22                     | 0.40              |
| 1:C:44:ASN:HD22  | 1:C:44:ASN:HA    | 1.56                     | 0.40              |
| 1:F:227:GLU:N    | 1:F:227:GLU:CD   | 2.79                     | 0.40              |
| 1:G:111:ASN:CB   | 2:H:70:ARG:NH1   | 2.84                     | 0.40              |
| 2:I:59:MET:SD    | 2:I:83:LEU:HD13  | 2.61                     | 0.40              |
| 2:N:190:ASP:HA   | 2:N:193:GLU:HG2  | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:103:TYR:C    | 2:X:81:THR:CG2   | 2.95                     | 0.40              |
| 1:Q:227:GLU:CD   | 1:Q:227:GLU:N    | 2.80                     | 0.40              |
| 1:S:123:TYR:CD1  | 1:S:123:TYR:N    | 2.88                     | 0.40              |
| 1:T:12:ILE:HD13  | 1:T:23:GLN:HB3   | 0.88                     | 0.40              |
| 1:U:12:ILE:CD1   | 1:U:23:GLN:HB3   | 0.55                     | 0.40              |
| 2:V:81:THR:O     | 2:V:84:SER:HB3   | 2.21                     | 0.40              |
| 2:W:59:MET:SD    | 2:W:83:LEU:HD13  | 2.61                     | 0.40              |
| 2:W:147:THR:OG1  | 2:W:150:GLU:HG3  | 2.21                     | 0.40              |
| 2:X:190:ASP:HA   | 2:X:193:GLU:HG2  | 2.02                     | 0.40              |
| 1:B:176:LEU:C    | 1:B:178:ARG:N    | 2.79                     | 0.40              |
| 1:D:15:PHE:H     | 1:E:23:GLN:NE2   | 2.17                     | 0.40              |
| 1:E:12:ILE:CD1   | 1:E:23:GLN:CB    | 0.48                     | 0.40              |
| 1:G:130:ARG:HA   | 1:G:131:PRO:HD3  | 1.96                     | 0.40              |
| 2:H:86:MET:HE2   | 2:H:86:MET:HB3   | 1.97                     | 0.40              |
| 2:L:87:LEU:HD23  | 2:L:114:ASP:O    | 2.20                     | 0.40              |
| 1:O:198:LYS:CG   | 1:O:202:GLU:HG2  | 2.50                     | 0.40              |
| 1:O:227:GLU:N    | 1:O:227:GLU:CD   | 2.80                     | 0.40              |
| 1:R:227:GLU:CD   | 1:R:227:GLU:N    | 2.80                     | 0.40              |
| 2:V:202:ILE:CG1  | 2:V:203:LEU:N    | 2.85                     | 0.40              |
| 1:B:227:GLU:N    | 1:B:227:GLU:CD   | 2.80                     | 0.40              |
| 1:D:125:GLN:C    | 1:E:129:VAL:HG23 | 2.46                     | 0.40              |
| 1:D:227:GLU:N    | 1:D:227:GLU:CD   | 2.80                     | 0.40              |
| 1:E:161:LYS:CG   | 1:F:60:GLU:OE2   | 2.60                     | 0.40              |
| 2:I:26:ILE:HD13  | 2:I:26:ILE:O     | 2.22                     | 0.40              |
| 2:J:141:GLN:HE21 | 2:W:141:GLN:NE2  | 2.19                     | 0.40              |
| 2:M:188:PRO:O    | 2:M:189:THR:C    | 2.65                     | 0.40              |
| 1:O:16:SER:O     | 1:P:26:TYR:HB3   | 2.21                     | 0.40              |
| 1:O:86:ARG:CZ    | 1:U:157:ILE:HG22 | 2.51                     | 0.40              |
| 1:P:176:LEU:C    | 1:P:178:ARG:N    | 2.79                     | 0.40              |
| 1:Q:177:GLU:CD   | 1:R:58:LEU:HD22  | 2.47                     | 0.40              |
| 1:T:15:PHE:CB    | 1:U:23:GLN:HE22  | 2.18                     | 0.40              |
| 1:T:157:ILE:HG22 | 1:U:86:ARG:NH1   | 2.37                     | 0.40              |
| 2:W:74:MET:HA    | 2:W:75:PRO:HD3   | 1.94                     | 0.40              |
| 2:2:76:ILE:O     | 2:2:79:VAL:CG1   | 2.69                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 225/233 (97%) | 189 (84%) | 26 (12%) | 10 (4%)  | 2           | 17 |
| 1   | B     | 225/233 (97%) | 189 (84%) | 26 (12%) | 10 (4%)  | 2           | 17 |
| 1   | C     | 225/233 (97%) | 188 (84%) | 27 (12%) | 10 (4%)  | 2           | 17 |
| 1   | D     | 225/233 (97%) | 189 (84%) | 26 (12%) | 10 (4%)  | 2           | 17 |
| 1   | E     | 225/233 (97%) | 189 (84%) | 26 (12%) | 10 (4%)  | 2           | 17 |
| 1   | F     | 225/233 (97%) | 188 (84%) | 27 (12%) | 10 (4%)  | 2           | 17 |
| 1   | G     | 225/233 (97%) | 189 (84%) | 26 (12%) | 10 (4%)  | 2           | 17 |
| 1   | O     | 225/233 (97%) | 189 (84%) | 26 (12%) | 10 (4%)  | 2           | 17 |
| 1   | P     | 225/233 (97%) | 189 (84%) | 26 (12%) | 10 (4%)  | 2           | 17 |
| 1   | Q     | 225/233 (97%) | 188 (84%) | 27 (12%) | 10 (4%)  | 2           | 17 |
| 1   | R     | 225/233 (97%) | 189 (84%) | 26 (12%) | 10 (4%)  | 2           | 17 |
| 1   | S     | 225/233 (97%) | 189 (84%) | 26 (12%) | 10 (4%)  | 2           | 17 |
| 1   | T     | 225/233 (97%) | 188 (84%) | 27 (12%) | 10 (4%)  | 2           | 17 |
| 1   | U     | 225/233 (97%) | 189 (84%) | 26 (12%) | 10 (4%)  | 2           | 17 |
| 2   | 1     | 201/203 (99%) | 176 (88%) | 23 (11%) | 2 (1%)   | 12          | 48 |
| 2   | 2     | 201/203 (99%) | 184 (92%) | 15 (8%)  | 2 (1%)   | 12          | 48 |
| 2   | H     | 201/203 (99%) | 184 (92%) | 15 (8%)  | 2 (1%)   | 12          | 48 |
| 2   | I     | 201/203 (99%) | 183 (91%) | 16 (8%)  | 2 (1%)   | 12          | 48 |
| 2   | J     | 201/203 (99%) | 180 (90%) | 20 (10%) | 1 (0%)   | 24          | 63 |
| 2   | K     | 201/203 (99%) | 184 (92%) | 15 (8%)  | 2 (1%)   | 12          | 48 |
| 2   | L     | 201/203 (99%) | 181 (90%) | 16 (8%)  | 4 (2%)   | 6           | 31 |
| 2   | M     | 201/203 (99%) | 176 (88%) | 23 (11%) | 2 (1%)   | 12          | 48 |
| 2   | N     | 201/203 (99%) | 184 (92%) | 15 (8%)  | 2 (1%)   | 12          | 48 |
| 2   | V     | 201/203 (99%) | 185 (92%) | 14 (7%)  | 2 (1%)   | 12          | 48 |
| 2   | W     | 201/203 (99%) | 183 (91%) | 16 (8%)  | 2 (1%)   | 12          | 48 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 2   | X     | 201/203 (99%)   | 180 (90%)  | 20 (10%)  | 1 (0%)   | 24          | 63 |
| 2   | Y     | 201/203 (99%)   | 184 (92%)  | 15 (8%)   | 2 (1%)   | 12          | 48 |
| 2   | Z     | 201/203 (99%)   | 181 (90%)  | 16 (8%)   | 4 (2%)   | 6           | 31 |
| All | All   | 5964/6104 (98%) | 5187 (87%) | 607 (10%) | 170 (3%) | 5           | 23 |

All (170) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | VAL  |
| 1   | A     | 128 | GLY  |
| 1   | A     | 182 | GLU  |
| 1   | A     | 200 | SER  |
| 1   | B     | 14  | VAL  |
| 1   | B     | 128 | GLY  |
| 1   | B     | 182 | GLU  |
| 1   | B     | 200 | SER  |
| 1   | C     | 14  | VAL  |
| 1   | C     | 128 | GLY  |
| 1   | C     | 182 | GLU  |
| 1   | C     | 200 | SER  |
| 1   | D     | 14  | VAL  |
| 1   | D     | 128 | GLY  |
| 1   | D     | 182 | GLU  |
| 1   | D     | 200 | SER  |
| 1   | E     | 14  | VAL  |
| 1   | E     | 128 | GLY  |
| 1   | E     | 182 | GLU  |
| 1   | E     | 200 | SER  |
| 1   | F     | 14  | VAL  |
| 1   | F     | 128 | GLY  |
| 1   | F     | 182 | GLU  |
| 1   | F     | 200 | SER  |
| 1   | G     | 14  | VAL  |
| 1   | G     | 128 | GLY  |
| 1   | G     | 182 | GLU  |
| 1   | G     | 200 | SER  |
| 2   | I     | 9   | LYS  |
| 2   | L     | 9   | LYS  |
| 2   | M     | 9   | LYS  |
| 1   | O     | 14  | VAL  |
| 1   | O     | 128 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 182 | GLU  |
| 1   | O     | 200 | SER  |
| 1   | P     | 14  | VAL  |
| 1   | P     | 128 | GLY  |
| 1   | P     | 182 | GLU  |
| 1   | P     | 200 | SER  |
| 1   | Q     | 14  | VAL  |
| 1   | Q     | 128 | GLY  |
| 1   | Q     | 182 | GLU  |
| 1   | Q     | 200 | SER  |
| 1   | R     | 14  | VAL  |
| 1   | R     | 128 | GLY  |
| 1   | R     | 182 | GLU  |
| 1   | R     | 200 | SER  |
| 1   | S     | 14  | VAL  |
| 1   | S     | 128 | GLY  |
| 1   | S     | 182 | GLU  |
| 1   | S     | 200 | SER  |
| 1   | T     | 14  | VAL  |
| 1   | T     | 128 | GLY  |
| 1   | T     | 182 | GLU  |
| 1   | T     | 200 | SER  |
| 1   | U     | 14  | VAL  |
| 1   | U     | 128 | GLY  |
| 1   | U     | 182 | GLU  |
| 1   | U     | 200 | SER  |
| 2   | W     | 9   | LYS  |
| 2   | Z     | 9   | LYS  |
| 2   | 1     | 9   | LYS  |
| 1   | A     | 43  | ALA  |
| 1   | A     | 72  | ASP  |
| 1   | A     | 205 | GLU  |
| 1   | B     | 43  | ALA  |
| 1   | B     | 72  | ASP  |
| 1   | B     | 205 | GLU  |
| 1   | C     | 43  | ALA  |
| 1   | C     | 72  | ASP  |
| 1   | C     | 205 | GLU  |
| 1   | D     | 43  | ALA  |
| 1   | D     | 72  | ASP  |
| 1   | D     | 205 | GLU  |
| 1   | E     | 43  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 72  | ASP  |
| 1   | E     | 205 | GLU  |
| 1   | F     | 43  | ALA  |
| 1   | F     | 72  | ASP  |
| 1   | F     | 205 | GLU  |
| 1   | G     | 43  | ALA  |
| 1   | G     | 72  | ASP  |
| 1   | G     | 205 | GLU  |
| 2   | H     | 9   | LYS  |
| 2   | J     | 9   | LYS  |
| 2   | K     | 9   | LYS  |
| 2   | N     | 9   | LYS  |
| 1   | O     | 43  | ALA  |
| 1   | O     | 72  | ASP  |
| 1   | O     | 205 | GLU  |
| 1   | P     | 43  | ALA  |
| 1   | P     | 72  | ASP  |
| 1   | P     | 205 | GLU  |
| 1   | Q     | 43  | ALA  |
| 1   | Q     | 72  | ASP  |
| 1   | Q     | 205 | GLU  |
| 1   | R     | 43  | ALA  |
| 1   | R     | 72  | ASP  |
| 1   | R     | 205 | GLU  |
| 1   | S     | 43  | ALA  |
| 1   | S     | 72  | ASP  |
| 1   | S     | 205 | GLU  |
| 1   | T     | 43  | ALA  |
| 1   | T     | 72  | ASP  |
| 1   | T     | 205 | GLU  |
| 1   | U     | 43  | ALA  |
| 1   | U     | 72  | ASP  |
| 1   | U     | 205 | GLU  |
| 2   | V     | 9   | LYS  |
| 2   | X     | 9   | LYS  |
| 2   | Y     | 9   | LYS  |
| 2   | 2     | 9   | LYS  |
| 2   | H     | 23  | GLU  |
| 2   | K     | 23  | GLU  |
| 2   | V     | 23  | GLU  |
| 2   | Y     | 23  | GLU  |
| 2   | M     | 23  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1     | 23  | GLU  |
| 1   | A     | 198 | LYS  |
| 1   | A     | 202 | GLU  |
| 1   | B     | 198 | LYS  |
| 1   | B     | 202 | GLU  |
| 1   | C     | 198 | LYS  |
| 1   | C     | 202 | GLU  |
| 1   | D     | 198 | LYS  |
| 1   | D     | 202 | GLU  |
| 1   | E     | 198 | LYS  |
| 1   | E     | 202 | GLU  |
| 1   | F     | 198 | LYS  |
| 1   | F     | 202 | GLU  |
| 1   | G     | 198 | LYS  |
| 1   | G     | 202 | GLU  |
| 2   | L     | 23  | GLU  |
| 2   | N     | 23  | GLU  |
| 1   | O     | 198 | LYS  |
| 1   | O     | 202 | GLU  |
| 1   | P     | 198 | LYS  |
| 1   | P     | 202 | GLU  |
| 1   | Q     | 198 | LYS  |
| 1   | Q     | 202 | GLU  |
| 1   | R     | 198 | LYS  |
| 1   | R     | 202 | GLU  |
| 1   | S     | 198 | LYS  |
| 1   | S     | 202 | GLU  |
| 1   | T     | 198 | LYS  |
| 1   | T     | 202 | GLU  |
| 1   | U     | 198 | LYS  |
| 1   | U     | 202 | GLU  |
| 2   | Z     | 23  | GLU  |
| 2   | 2     | 23  | GLU  |
| 2   | I     | 23  | GLU  |
| 2   | L     | 49  | VAL  |
| 2   | W     | 23  | GLU  |
| 2   | Z     | 49  | VAL  |
| 2   | L     | 110 | VAL  |
| 2   | Z     | 110 | VAL  |
| 1   | A     | 129 | VAL  |
| 1   | B     | 129 | VAL  |
| 1   | C     | 129 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 129 | VAL  |
| 1   | E     | 129 | VAL  |
| 1   | F     | 129 | VAL  |
| 1   | G     | 129 | VAL  |
| 1   | O     | 129 | VAL  |
| 1   | P     | 129 | VAL  |
| 1   | Q     | 129 | VAL  |
| 1   | R     | 129 | VAL  |
| 1   | S     | 129 | VAL  |
| 1   | T     | 129 | VAL  |
| 1   | U     | 129 | VAL  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | B     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | C     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | D     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | E     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | F     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | G     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | O     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | P     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | Q     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | R     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | S     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | T     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 1   | U     | 188/193 (97%)  | 160 (85%) | 28 (15%) | 3           | 13 |
| 2   | 1     | 170/170 (100%) | 146 (86%) | 24 (14%) | 3           | 13 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2   | 2     | 170/170 (100%)  | 145 (85%)  | 25 (15%)  | 3           | 13 |
| 2   | H     | 170/170 (100%)  | 142 (84%)  | 28 (16%)  | 2           | 10 |
| 2   | I     | 170/170 (100%)  | 143 (84%)  | 27 (16%)  | 2           | 11 |
| 2   | J     | 170/170 (100%)  | 140 (82%)  | 30 (18%)  | 2           | 9  |
| 2   | K     | 170/170 (100%)  | 142 (84%)  | 28 (16%)  | 2           | 10 |
| 2   | L     | 170/170 (100%)  | 144 (85%)  | 26 (15%)  | 3           | 12 |
| 2   | M     | 170/170 (100%)  | 146 (86%)  | 24 (14%)  | 3           | 13 |
| 2   | N     | 170/170 (100%)  | 145 (85%)  | 25 (15%)  | 3           | 13 |
| 2   | V     | 170/170 (100%)  | 142 (84%)  | 28 (16%)  | 2           | 10 |
| 2   | W     | 170/170 (100%)  | 143 (84%)  | 27 (16%)  | 2           | 11 |
| 2   | X     | 170/170 (100%)  | 140 (82%)  | 30 (18%)  | 2           | 9  |
| 2   | Y     | 170/170 (100%)  | 142 (84%)  | 28 (16%)  | 2           | 10 |
| 2   | Z     | 170/170 (100%)  | 144 (85%)  | 26 (15%)  | 3           | 12 |
| All | All   | 5012/5082 (99%) | 4244 (85%) | 768 (15%) | 5           | 12 |

All (768) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 13  | THR  |
| 1   | A     | 21  | LEU  |
| 1   | A     | 23  | GLN  |
| 1   | A     | 24  | VAL  |
| 1   | A     | 31  | VAL  |
| 1   | A     | 44  | ASN  |
| 1   | A     | 47  | LEU  |
| 1   | A     | 48  | LEU  |
| 1   | A     | 62  | ASN  |
| 1   | A     | 71  | ASP  |
| 1   | A     | 82  | VAL  |
| 1   | A     | 102 | THR  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 107 | VAL  |
| 1   | A     | 111 | ASN  |
| 1   | A     | 119 | GLN  |
| 1   | A     | 134 | VAL  |
| 1   | A     | 136 | LEU  |
| 1   | A     | 141 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 143 | GLN  |
| 1   | A     | 157 | ILE  |
| 1   | A     | 161 | LYS  |
| 1   | A     | 175 | PHE  |
| 1   | A     | 176 | LEU  |
| 1   | A     | 190 | VAL  |
| 1   | A     | 201 | LEU  |
| 1   | A     | 202 | GLU  |
| 1   | A     | 212 | ILE  |
| 1   | B     | 13  | THR  |
| 1   | B     | 21  | LEU  |
| 1   | B     | 23  | GLN  |
| 1   | B     | 24  | VAL  |
| 1   | B     | 31  | VAL  |
| 1   | B     | 44  | ASN  |
| 1   | B     | 47  | LEU  |
| 1   | B     | 48  | LEU  |
| 1   | B     | 62  | ASN  |
| 1   | B     | 71  | ASP  |
| 1   | B     | 82  | VAL  |
| 1   | B     | 102 | THR  |
| 1   | B     | 106 | LEU  |
| 1   | B     | 107 | VAL  |
| 1   | B     | 111 | ASN  |
| 1   | B     | 119 | GLN  |
| 1   | B     | 134 | VAL  |
| 1   | B     | 136 | LEU  |
| 1   | B     | 141 | ILE  |
| 1   | B     | 143 | GLN  |
| 1   | B     | 157 | ILE  |
| 1   | B     | 161 | LYS  |
| 1   | B     | 175 | PHE  |
| 1   | B     | 176 | LEU  |
| 1   | B     | 190 | VAL  |
| 1   | B     | 201 | LEU  |
| 1   | B     | 202 | GLU  |
| 1   | B     | 212 | ILE  |
| 1   | C     | 13  | THR  |
| 1   | C     | 21  | LEU  |
| 1   | C     | 23  | GLN  |
| 1   | C     | 24  | VAL  |
| 1   | C     | 31  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 44  | ASN  |
| 1   | C     | 47  | LEU  |
| 1   | C     | 48  | LEU  |
| 1   | C     | 62  | ASN  |
| 1   | C     | 71  | ASP  |
| 1   | C     | 82  | VAL  |
| 1   | C     | 102 | THR  |
| 1   | C     | 106 | LEU  |
| 1   | C     | 107 | VAL  |
| 1   | C     | 111 | ASN  |
| 1   | C     | 119 | GLN  |
| 1   | C     | 134 | VAL  |
| 1   | C     | 136 | LEU  |
| 1   | C     | 141 | ILE  |
| 1   | C     | 143 | GLN  |
| 1   | C     | 157 | ILE  |
| 1   | C     | 161 | LYS  |
| 1   | C     | 175 | PHE  |
| 1   | C     | 176 | LEU  |
| 1   | C     | 190 | VAL  |
| 1   | C     | 201 | LEU  |
| 1   | C     | 202 | GLU  |
| 1   | C     | 212 | ILE  |
| 1   | D     | 13  | THR  |
| 1   | D     | 21  | LEU  |
| 1   | D     | 23  | GLN  |
| 1   | D     | 24  | VAL  |
| 1   | D     | 31  | VAL  |
| 1   | D     | 44  | ASN  |
| 1   | D     | 47  | LEU  |
| 1   | D     | 48  | LEU  |
| 1   | D     | 62  | ASN  |
| 1   | D     | 71  | ASP  |
| 1   | D     | 82  | VAL  |
| 1   | D     | 102 | THR  |
| 1   | D     | 106 | LEU  |
| 1   | D     | 107 | VAL  |
| 1   | D     | 111 | ASN  |
| 1   | D     | 119 | GLN  |
| 1   | D     | 134 | VAL  |
| 1   | D     | 136 | LEU  |
| 1   | D     | 141 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 143 | GLN  |
| 1   | D     | 157 | ILE  |
| 1   | D     | 161 | LYS  |
| 1   | D     | 175 | PHE  |
| 1   | D     | 176 | LEU  |
| 1   | D     | 190 | VAL  |
| 1   | D     | 201 | LEU  |
| 1   | D     | 202 | GLU  |
| 1   | D     | 212 | ILE  |
| 1   | E     | 13  | THR  |
| 1   | E     | 21  | LEU  |
| 1   | E     | 23  | GLN  |
| 1   | E     | 24  | VAL  |
| 1   | E     | 31  | VAL  |
| 1   | E     | 44  | ASN  |
| 1   | E     | 47  | LEU  |
| 1   | E     | 48  | LEU  |
| 1   | E     | 62  | ASN  |
| 1   | E     | 71  | ASP  |
| 1   | E     | 82  | VAL  |
| 1   | E     | 102 | THR  |
| 1   | E     | 106 | LEU  |
| 1   | E     | 107 | VAL  |
| 1   | E     | 111 | ASN  |
| 1   | E     | 119 | GLN  |
| 1   | E     | 134 | VAL  |
| 1   | E     | 136 | LEU  |
| 1   | E     | 141 | ILE  |
| 1   | E     | 143 | GLN  |
| 1   | E     | 157 | ILE  |
| 1   | E     | 161 | LYS  |
| 1   | E     | 175 | PHE  |
| 1   | E     | 176 | LEU  |
| 1   | E     | 190 | VAL  |
| 1   | E     | 201 | LEU  |
| 1   | E     | 202 | GLU  |
| 1   | E     | 212 | ILE  |
| 1   | F     | 13  | THR  |
| 1   | F     | 21  | LEU  |
| 1   | F     | 23  | GLN  |
| 1   | F     | 24  | VAL  |
| 1   | F     | 31  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 44  | ASN  |
| 1   | F     | 47  | LEU  |
| 1   | F     | 48  | LEU  |
| 1   | F     | 62  | ASN  |
| 1   | F     | 71  | ASP  |
| 1   | F     | 82  | VAL  |
| 1   | F     | 102 | THR  |
| 1   | F     | 106 | LEU  |
| 1   | F     | 107 | VAL  |
| 1   | F     | 111 | ASN  |
| 1   | F     | 119 | GLN  |
| 1   | F     | 134 | VAL  |
| 1   | F     | 136 | LEU  |
| 1   | F     | 141 | ILE  |
| 1   | F     | 143 | GLN  |
| 1   | F     | 157 | ILE  |
| 1   | F     | 161 | LYS  |
| 1   | F     | 175 | PHE  |
| 1   | F     | 176 | LEU  |
| 1   | F     | 190 | VAL  |
| 1   | F     | 201 | LEU  |
| 1   | F     | 202 | GLU  |
| 1   | F     | 212 | ILE  |
| 1   | G     | 13  | THR  |
| 1   | G     | 21  | LEU  |
| 1   | G     | 23  | GLN  |
| 1   | G     | 24  | VAL  |
| 1   | G     | 31  | VAL  |
| 1   | G     | 44  | ASN  |
| 1   | G     | 47  | LEU  |
| 1   | G     | 48  | LEU  |
| 1   | G     | 62  | ASN  |
| 1   | G     | 71  | ASP  |
| 1   | G     | 82  | VAL  |
| 1   | G     | 102 | THR  |
| 1   | G     | 106 | LEU  |
| 1   | G     | 107 | VAL  |
| 1   | G     | 111 | ASN  |
| 1   | G     | 119 | GLN  |
| 1   | G     | 134 | VAL  |
| 1   | G     | 136 | LEU  |
| 1   | G     | 141 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 143 | GLN  |
| 1   | G     | 157 | ILE  |
| 1   | G     | 161 | LYS  |
| 1   | G     | 175 | PHE  |
| 1   | G     | 176 | LEU  |
| 1   | G     | 190 | VAL  |
| 1   | G     | 201 | LEU  |
| 1   | G     | 202 | GLU  |
| 1   | G     | 212 | ILE  |
| 2   | H     | 2   | THR  |
| 2   | H     | 4   | VAL  |
| 2   | H     | 7   | THR  |
| 2   | H     | 17  | GLU  |
| 2   | H     | 20  | VAL  |
| 2   | H     | 26  | ILE  |
| 2   | H     | 41  | THR  |
| 2   | H     | 45  | ILE  |
| 2   | H     | 49  | VAL  |
| 2   | H     | 56  | VAL  |
| 2   | H     | 63  | LEU  |
| 2   | H     | 68  | LEU  |
| 2   | H     | 83  | LEU  |
| 2   | H     | 94  | PRO  |
| 2   | H     | 97  | VAL  |
| 2   | H     | 104 | ILE  |
| 2   | H     | 123 | ILE  |
| 2   | H     | 127 | THR  |
| 2   | H     | 134 | VAL  |
| 2   | H     | 137 | VAL  |
| 2   | H     | 138 | LEU  |
| 2   | H     | 144 | GLU  |
| 2   | H     | 173 | ILE  |
| 2   | H     | 175 | VAL  |
| 2   | H     | 177 | VAL  |
| 2   | H     | 178 | ILE  |
| 2   | H     | 185 | VAL  |
| 2   | H     | 201 | LEU  |
| 2   | I     | 2   | THR  |
| 2   | I     | 7   | THR  |
| 2   | I     | 17  | GLU  |
| 2   | I     | 20  | VAL  |
| 2   | I     | 26  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 41  | THR  |
| 2   | I     | 45  | ILE  |
| 2   | I     | 49  | VAL  |
| 2   | I     | 54  | VAL  |
| 2   | I     | 55  | LEU  |
| 2   | I     | 59  | MET  |
| 2   | I     | 63  | LEU  |
| 2   | I     | 70  | ARG  |
| 2   | I     | 71  | ARG  |
| 2   | I     | 83  | LEU  |
| 2   | I     | 104 | ILE  |
| 2   | I     | 123 | ILE  |
| 2   | I     | 127 | THR  |
| 2   | I     | 134 | VAL  |
| 2   | I     | 137 | VAL  |
| 2   | I     | 138 | LEU  |
| 2   | I     | 144 | GLU  |
| 2   | I     | 173 | ILE  |
| 2   | I     | 175 | VAL  |
| 2   | I     | 177 | VAL  |
| 2   | I     | 178 | ILE  |
| 2   | I     | 185 | VAL  |
| 2   | J     | 2   | THR  |
| 2   | J     | 6   | ILE  |
| 2   | J     | 7   | THR  |
| 2   | J     | 8   | LEU  |
| 2   | J     | 12  | VAL  |
| 2   | J     | 17  | GLU  |
| 2   | J     | 20  | VAL  |
| 2   | J     | 26  | ILE  |
| 2   | J     | 41  | THR  |
| 2   | J     | 45  | ILE  |
| 2   | J     | 49  | VAL  |
| 2   | J     | 55  | LEU  |
| 2   | J     | 59  | MET  |
| 2   | J     | 68  | LEU  |
| 2   | J     | 70  | ARG  |
| 2   | J     | 71  | ARG  |
| 2   | J     | 79  | VAL  |
| 2   | J     | 83  | LEU  |
| 2   | J     | 104 | ILE  |
| 2   | J     | 123 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 127 | THR  |
| 2   | J     | 134 | VAL  |
| 2   | J     | 137 | VAL  |
| 2   | J     | 138 | LEU  |
| 2   | J     | 144 | GLU  |
| 2   | J     | 173 | ILE  |
| 2   | J     | 175 | VAL  |
| 2   | J     | 177 | VAL  |
| 2   | J     | 178 | ILE  |
| 2   | J     | 185 | VAL  |
| 2   | K     | 2   | THR  |
| 2   | K     | 6   | ILE  |
| 2   | K     | 7   | THR  |
| 2   | K     | 17  | GLU  |
| 2   | K     | 20  | VAL  |
| 2   | K     | 26  | ILE  |
| 2   | K     | 41  | THR  |
| 2   | K     | 45  | ILE  |
| 2   | K     | 49  | VAL  |
| 2   | K     | 56  | VAL  |
| 2   | K     | 68  | LEU  |
| 2   | K     | 70  | ARG  |
| 2   | K     | 71  | ARG  |
| 2   | K     | 83  | LEU  |
| 2   | K     | 94  | PRO  |
| 2   | K     | 97  | VAL  |
| 2   | K     | 104 | ILE  |
| 2   | K     | 123 | ILE  |
| 2   | K     | 127 | THR  |
| 2   | K     | 134 | VAL  |
| 2   | K     | 137 | VAL  |
| 2   | K     | 138 | LEU  |
| 2   | K     | 144 | GLU  |
| 2   | K     | 173 | ILE  |
| 2   | K     | 175 | VAL  |
| 2   | K     | 177 | VAL  |
| 2   | K     | 178 | ILE  |
| 2   | K     | 185 | VAL  |
| 2   | L     | 1   | THR  |
| 2   | L     | 2   | THR  |
| 2   | L     | 7   | THR  |
| 2   | L     | 17  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 20  | VAL  |
| 2   | L     | 26  | ILE  |
| 2   | L     | 41  | THR  |
| 2   | L     | 45  | ILE  |
| 2   | L     | 49  | VAL  |
| 2   | L     | 63  | LEU  |
| 2   | L     | 68  | LEU  |
| 2   | L     | 70  | ARG  |
| 2   | L     | 71  | ARG  |
| 2   | L     | 83  | LEU  |
| 2   | L     | 104 | ILE  |
| 2   | L     | 123 | ILE  |
| 2   | L     | 127 | THR  |
| 2   | L     | 134 | VAL  |
| 2   | L     | 137 | VAL  |
| 2   | L     | 138 | LEU  |
| 2   | L     | 144 | GLU  |
| 2   | L     | 165 | ARG  |
| 2   | L     | 173 | ILE  |
| 2   | L     | 175 | VAL  |
| 2   | L     | 178 | ILE  |
| 2   | L     | 185 | VAL  |
| 2   | M     | 2   | THR  |
| 2   | M     | 7   | THR  |
| 2   | M     | 17  | GLU  |
| 2   | M     | 20  | VAL  |
| 2   | M     | 26  | ILE  |
| 2   | M     | 41  | THR  |
| 2   | M     | 45  | ILE  |
| 2   | M     | 54  | VAL  |
| 2   | M     | 59  | MET  |
| 2   | M     | 70  | ARG  |
| 2   | M     | 71  | ARG  |
| 2   | M     | 83  | LEU  |
| 2   | M     | 120 | VAL  |
| 2   | M     | 123 | ILE  |
| 2   | M     | 127 | THR  |
| 2   | M     | 134 | VAL  |
| 2   | M     | 137 | VAL  |
| 2   | M     | 138 | LEU  |
| 2   | M     | 144 | GLU  |
| 2   | M     | 165 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 173 | ILE  |
| 2   | M     | 178 | ILE  |
| 2   | M     | 185 | VAL  |
| 2   | M     | 201 | LEU  |
| 2   | N     | 2   | THR  |
| 2   | N     | 7   | THR  |
| 2   | N     | 12  | VAL  |
| 2   | N     | 17  | GLU  |
| 2   | N     | 20  | VAL  |
| 2   | N     | 26  | ILE  |
| 2   | N     | 41  | THR  |
| 2   | N     | 45  | ILE  |
| 2   | N     | 59  | MET  |
| 2   | N     | 68  | LEU  |
| 2   | N     | 70  | ARG  |
| 2   | N     | 71  | ARG  |
| 2   | N     | 94  | PRO  |
| 2   | N     | 123 | ILE  |
| 2   | N     | 127 | THR  |
| 2   | N     | 134 | VAL  |
| 2   | N     | 137 | VAL  |
| 2   | N     | 138 | LEU  |
| 2   | N     | 144 | GLU  |
| 2   | N     | 165 | ARG  |
| 2   | N     | 173 | ILE  |
| 2   | N     | 175 | VAL  |
| 2   | N     | 177 | VAL  |
| 2   | N     | 178 | ILE  |
| 2   | N     | 185 | VAL  |
| 1   | O     | 13  | THR  |
| 1   | O     | 21  | LEU  |
| 1   | O     | 23  | GLN  |
| 1   | O     | 24  | VAL  |
| 1   | O     | 31  | VAL  |
| 1   | O     | 44  | ASN  |
| 1   | O     | 47  | LEU  |
| 1   | O     | 48  | LEU  |
| 1   | O     | 62  | ASN  |
| 1   | O     | 71  | ASP  |
| 1   | O     | 82  | VAL  |
| 1   | O     | 102 | THR  |
| 1   | O     | 106 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 107 | VAL  |
| 1   | O     | 111 | ASN  |
| 1   | O     | 119 | GLN  |
| 1   | O     | 134 | VAL  |
| 1   | O     | 136 | LEU  |
| 1   | O     | 141 | ILE  |
| 1   | O     | 143 | GLN  |
| 1   | O     | 157 | ILE  |
| 1   | O     | 161 | LYS  |
| 1   | O     | 175 | PHE  |
| 1   | O     | 176 | LEU  |
| 1   | O     | 190 | VAL  |
| 1   | O     | 201 | LEU  |
| 1   | O     | 202 | GLU  |
| 1   | O     | 212 | ILE  |
| 1   | P     | 13  | THR  |
| 1   | P     | 21  | LEU  |
| 1   | P     | 23  | GLN  |
| 1   | P     | 24  | VAL  |
| 1   | P     | 31  | VAL  |
| 1   | P     | 44  | ASN  |
| 1   | P     | 47  | LEU  |
| 1   | P     | 48  | LEU  |
| 1   | P     | 62  | ASN  |
| 1   | P     | 71  | ASP  |
| 1   | P     | 82  | VAL  |
| 1   | P     | 102 | THR  |
| 1   | P     | 106 | LEU  |
| 1   | P     | 107 | VAL  |
| 1   | P     | 111 | ASN  |
| 1   | P     | 119 | GLN  |
| 1   | P     | 134 | VAL  |
| 1   | P     | 136 | LEU  |
| 1   | P     | 141 | ILE  |
| 1   | P     | 143 | GLN  |
| 1   | P     | 157 | ILE  |
| 1   | P     | 161 | LYS  |
| 1   | P     | 175 | PHE  |
| 1   | P     | 176 | LEU  |
| 1   | P     | 190 | VAL  |
| 1   | P     | 201 | LEU  |
| 1   | P     | 202 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 212 | ILE  |
| 1   | Q     | 13  | THR  |
| 1   | Q     | 21  | LEU  |
| 1   | Q     | 23  | GLN  |
| 1   | Q     | 24  | VAL  |
| 1   | Q     | 31  | VAL  |
| 1   | Q     | 44  | ASN  |
| 1   | Q     | 47  | LEU  |
| 1   | Q     | 48  | LEU  |
| 1   | Q     | 62  | ASN  |
| 1   | Q     | 71  | ASP  |
| 1   | Q     | 82  | VAL  |
| 1   | Q     | 102 | THR  |
| 1   | Q     | 106 | LEU  |
| 1   | Q     | 107 | VAL  |
| 1   | Q     | 111 | ASN  |
| 1   | Q     | 119 | GLN  |
| 1   | Q     | 134 | VAL  |
| 1   | Q     | 136 | LEU  |
| 1   | Q     | 141 | ILE  |
| 1   | Q     | 143 | GLN  |
| 1   | Q     | 157 | ILE  |
| 1   | Q     | 161 | LYS  |
| 1   | Q     | 175 | PHE  |
| 1   | Q     | 176 | LEU  |
| 1   | Q     | 190 | VAL  |
| 1   | Q     | 201 | LEU  |
| 1   | Q     | 202 | GLU  |
| 1   | Q     | 212 | ILE  |
| 1   | R     | 13  | THR  |
| 1   | R     | 21  | LEU  |
| 1   | R     | 23  | GLN  |
| 1   | R     | 24  | VAL  |
| 1   | R     | 31  | VAL  |
| 1   | R     | 44  | ASN  |
| 1   | R     | 47  | LEU  |
| 1   | R     | 48  | LEU  |
| 1   | R     | 62  | ASN  |
| 1   | R     | 71  | ASP  |
| 1   | R     | 82  | VAL  |
| 1   | R     | 102 | THR  |
| 1   | R     | 106 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 107 | VAL  |
| 1   | R     | 111 | ASN  |
| 1   | R     | 119 | GLN  |
| 1   | R     | 134 | VAL  |
| 1   | R     | 136 | LEU  |
| 1   | R     | 141 | ILE  |
| 1   | R     | 143 | GLN  |
| 1   | R     | 157 | ILE  |
| 1   | R     | 161 | LYS  |
| 1   | R     | 175 | PHE  |
| 1   | R     | 176 | LEU  |
| 1   | R     | 190 | VAL  |
| 1   | R     | 201 | LEU  |
| 1   | R     | 202 | GLU  |
| 1   | R     | 212 | ILE  |
| 1   | S     | 13  | THR  |
| 1   | S     | 21  | LEU  |
| 1   | S     | 23  | GLN  |
| 1   | S     | 24  | VAL  |
| 1   | S     | 31  | VAL  |
| 1   | S     | 44  | ASN  |
| 1   | S     | 47  | LEU  |
| 1   | S     | 48  | LEU  |
| 1   | S     | 62  | ASN  |
| 1   | S     | 71  | ASP  |
| 1   | S     | 82  | VAL  |
| 1   | S     | 102 | THR  |
| 1   | S     | 106 | LEU  |
| 1   | S     | 107 | VAL  |
| 1   | S     | 111 | ASN  |
| 1   | S     | 119 | GLN  |
| 1   | S     | 134 | VAL  |
| 1   | S     | 136 | LEU  |
| 1   | S     | 141 | ILE  |
| 1   | S     | 143 | GLN  |
| 1   | S     | 157 | ILE  |
| 1   | S     | 161 | LYS  |
| 1   | S     | 175 | PHE  |
| 1   | S     | 176 | LEU  |
| 1   | S     | 190 | VAL  |
| 1   | S     | 201 | LEU  |
| 1   | S     | 202 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 212 | ILE  |
| 1   | T     | 13  | THR  |
| 1   | T     | 21  | LEU  |
| 1   | T     | 23  | GLN  |
| 1   | T     | 24  | VAL  |
| 1   | T     | 31  | VAL  |
| 1   | T     | 44  | ASN  |
| 1   | T     | 47  | LEU  |
| 1   | T     | 48  | LEU  |
| 1   | T     | 62  | ASN  |
| 1   | T     | 71  | ASP  |
| 1   | T     | 82  | VAL  |
| 1   | T     | 102 | THR  |
| 1   | T     | 106 | LEU  |
| 1   | T     | 107 | VAL  |
| 1   | T     | 111 | ASN  |
| 1   | T     | 119 | GLN  |
| 1   | T     | 134 | VAL  |
| 1   | T     | 136 | LEU  |
| 1   | T     | 141 | ILE  |
| 1   | T     | 143 | GLN  |
| 1   | T     | 157 | ILE  |
| 1   | T     | 161 | LYS  |
| 1   | T     | 175 | PHE  |
| 1   | T     | 176 | LEU  |
| 1   | T     | 190 | VAL  |
| 1   | T     | 201 | LEU  |
| 1   | T     | 202 | GLU  |
| 1   | T     | 212 | ILE  |
| 1   | U     | 13  | THR  |
| 1   | U     | 21  | LEU  |
| 1   | U     | 23  | GLN  |
| 1   | U     | 24  | VAL  |
| 1   | U     | 31  | VAL  |
| 1   | U     | 44  | ASN  |
| 1   | U     | 47  | LEU  |
| 1   | U     | 48  | LEU  |
| 1   | U     | 62  | ASN  |
| 1   | U     | 71  | ASP  |
| 1   | U     | 82  | VAL  |
| 1   | U     | 102 | THR  |
| 1   | U     | 106 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | U     | 107 | VAL  |
| 1   | U     | 111 | ASN  |
| 1   | U     | 119 | GLN  |
| 1   | U     | 134 | VAL  |
| 1   | U     | 136 | LEU  |
| 1   | U     | 141 | ILE  |
| 1   | U     | 143 | GLN  |
| 1   | U     | 157 | ILE  |
| 1   | U     | 161 | LYS  |
| 1   | U     | 175 | PHE  |
| 1   | U     | 176 | LEU  |
| 1   | U     | 190 | VAL  |
| 1   | U     | 201 | LEU  |
| 1   | U     | 202 | GLU  |
| 1   | U     | 212 | ILE  |
| 2   | V     | 2   | THR  |
| 2   | V     | 4   | VAL  |
| 2   | V     | 7   | THR  |
| 2   | V     | 17  | GLU  |
| 2   | V     | 20  | VAL  |
| 2   | V     | 26  | ILE  |
| 2   | V     | 41  | THR  |
| 2   | V     | 45  | ILE  |
| 2   | V     | 49  | VAL  |
| 2   | V     | 56  | VAL  |
| 2   | V     | 63  | LEU  |
| 2   | V     | 68  | LEU  |
| 2   | V     | 83  | LEU  |
| 2   | V     | 94  | PRO  |
| 2   | V     | 97  | VAL  |
| 2   | V     | 104 | ILE  |
| 2   | V     | 123 | ILE  |
| 2   | V     | 127 | THR  |
| 2   | V     | 134 | VAL  |
| 2   | V     | 137 | VAL  |
| 2   | V     | 138 | LEU  |
| 2   | V     | 144 | GLU  |
| 2   | V     | 173 | ILE  |
| 2   | V     | 175 | VAL  |
| 2   | V     | 177 | VAL  |
| 2   | V     | 178 | ILE  |
| 2   | V     | 185 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | V     | 201 | LEU  |
| 2   | W     | 2   | THR  |
| 2   | W     | 7   | THR  |
| 2   | W     | 17  | GLU  |
| 2   | W     | 20  | VAL  |
| 2   | W     | 26  | ILE  |
| 2   | W     | 41  | THR  |
| 2   | W     | 45  | ILE  |
| 2   | W     | 49  | VAL  |
| 2   | W     | 54  | VAL  |
| 2   | W     | 55  | LEU  |
| 2   | W     | 59  | MET  |
| 2   | W     | 63  | LEU  |
| 2   | W     | 70  | ARG  |
| 2   | W     | 71  | ARG  |
| 2   | W     | 83  | LEU  |
| 2   | W     | 104 | ILE  |
| 2   | W     | 123 | ILE  |
| 2   | W     | 127 | THR  |
| 2   | W     | 134 | VAL  |
| 2   | W     | 137 | VAL  |
| 2   | W     | 138 | LEU  |
| 2   | W     | 144 | GLU  |
| 2   | W     | 173 | ILE  |
| 2   | W     | 175 | VAL  |
| 2   | W     | 177 | VAL  |
| 2   | W     | 178 | ILE  |
| 2   | W     | 185 | VAL  |
| 2   | X     | 2   | THR  |
| 2   | X     | 6   | ILE  |
| 2   | X     | 7   | THR  |
| 2   | X     | 8   | LEU  |
| 2   | X     | 12  | VAL  |
| 2   | X     | 17  | GLU  |
| 2   | X     | 20  | VAL  |
| 2   | X     | 26  | ILE  |
| 2   | X     | 41  | THR  |
| 2   | X     | 45  | ILE  |
| 2   | X     | 49  | VAL  |
| 2   | X     | 55  | LEU  |
| 2   | X     | 59  | MET  |
| 2   | X     | 68  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | X     | 70  | ARG  |
| 2   | X     | 71  | ARG  |
| 2   | X     | 79  | VAL  |
| 2   | X     | 83  | LEU  |
| 2   | X     | 104 | ILE  |
| 2   | X     | 123 | ILE  |
| 2   | X     | 127 | THR  |
| 2   | X     | 134 | VAL  |
| 2   | X     | 137 | VAL  |
| 2   | X     | 138 | LEU  |
| 2   | X     | 144 | GLU  |
| 2   | X     | 173 | ILE  |
| 2   | X     | 175 | VAL  |
| 2   | X     | 177 | VAL  |
| 2   | X     | 178 | ILE  |
| 2   | X     | 185 | VAL  |
| 2   | Y     | 2   | THR  |
| 2   | Y     | 6   | ILE  |
| 2   | Y     | 7   | THR  |
| 2   | Y     | 17  | GLU  |
| 2   | Y     | 20  | VAL  |
| 2   | Y     | 26  | ILE  |
| 2   | Y     | 41  | THR  |
| 2   | Y     | 45  | ILE  |
| 2   | Y     | 49  | VAL  |
| 2   | Y     | 56  | VAL  |
| 2   | Y     | 68  | LEU  |
| 2   | Y     | 70  | ARG  |
| 2   | Y     | 71  | ARG  |
| 2   | Y     | 83  | LEU  |
| 2   | Y     | 94  | PRO  |
| 2   | Y     | 97  | VAL  |
| 2   | Y     | 104 | ILE  |
| 2   | Y     | 123 | ILE  |
| 2   | Y     | 127 | THR  |
| 2   | Y     | 134 | VAL  |
| 2   | Y     | 137 | VAL  |
| 2   | Y     | 138 | LEU  |
| 2   | Y     | 144 | GLU  |
| 2   | Y     | 173 | ILE  |
| 2   | Y     | 175 | VAL  |
| 2   | Y     | 177 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Y     | 178 | ILE  |
| 2   | Y     | 185 | VAL  |
| 2   | Z     | 1   | THR  |
| 2   | Z     | 2   | THR  |
| 2   | Z     | 7   | THR  |
| 2   | Z     | 17  | GLU  |
| 2   | Z     | 20  | VAL  |
| 2   | Z     | 26  | ILE  |
| 2   | Z     | 41  | THR  |
| 2   | Z     | 45  | ILE  |
| 2   | Z     | 49  | VAL  |
| 2   | Z     | 63  | LEU  |
| 2   | Z     | 68  | LEU  |
| 2   | Z     | 70  | ARG  |
| 2   | Z     | 71  | ARG  |
| 2   | Z     | 83  | LEU  |
| 2   | Z     | 104 | ILE  |
| 2   | Z     | 123 | ILE  |
| 2   | Z     | 127 | THR  |
| 2   | Z     | 134 | VAL  |
| 2   | Z     | 137 | VAL  |
| 2   | Z     | 138 | LEU  |
| 2   | Z     | 144 | GLU  |
| 2   | Z     | 165 | ARG  |
| 2   | Z     | 173 | ILE  |
| 2   | Z     | 175 | VAL  |
| 2   | Z     | 178 | ILE  |
| 2   | Z     | 185 | VAL  |
| 2   | 1     | 2   | THR  |
| 2   | 1     | 7   | THR  |
| 2   | 1     | 17  | GLU  |
| 2   | 1     | 20  | VAL  |
| 2   | 1     | 26  | ILE  |
| 2   | 1     | 41  | THR  |
| 2   | 1     | 45  | ILE  |
| 2   | 1     | 54  | VAL  |
| 2   | 1     | 59  | MET  |
| 2   | 1     | 70  | ARG  |
| 2   | 1     | 71  | ARG  |
| 2   | 1     | 83  | LEU  |
| 2   | 1     | 120 | VAL  |
| 2   | 1     | 123 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1     | 127 | THR  |
| 2   | 1     | 134 | VAL  |
| 2   | 1     | 137 | VAL  |
| 2   | 1     | 138 | LEU  |
| 2   | 1     | 144 | GLU  |
| 2   | 1     | 165 | ARG  |
| 2   | 1     | 173 | ILE  |
| 2   | 1     | 178 | ILE  |
| 2   | 1     | 185 | VAL  |
| 2   | 1     | 201 | LEU  |
| 2   | 2     | 2   | THR  |
| 2   | 2     | 7   | THR  |
| 2   | 2     | 12  | VAL  |
| 2   | 2     | 17  | GLU  |
| 2   | 2     | 20  | VAL  |
| 2   | 2     | 26  | ILE  |
| 2   | 2     | 41  | THR  |
| 2   | 2     | 45  | ILE  |
| 2   | 2     | 59  | MET  |
| 2   | 2     | 68  | LEU  |
| 2   | 2     | 70  | ARG  |
| 2   | 2     | 71  | ARG  |
| 2   | 2     | 94  | PRO  |
| 2   | 2     | 123 | ILE  |
| 2   | 2     | 127 | THR  |
| 2   | 2     | 134 | VAL  |
| 2   | 2     | 137 | VAL  |
| 2   | 2     | 138 | LEU  |
| 2   | 2     | 144 | GLU  |
| 2   | 2     | 165 | ARG  |
| 2   | 2     | 173 | ILE  |
| 2   | 2     | 175 | VAL  |
| 2   | 2     | 177 | VAL  |
| 2   | 2     | 178 | ILE  |
| 2   | 2     | 185 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (171) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 23  | GLN  |
| 1   | A     | 44  | ASN  |
| 1   | A     | 98  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 111 | ASN  |
| 1   | A     | 119 | GLN  |
| 1   | A     | 121 | GLN  |
| 1   | A     | 125 | GLN  |
| 1   | A     | 143 | GLN  |
| 1   | B     | 23  | GLN  |
| 1   | B     | 44  | ASN  |
| 1   | B     | 98  | GLN  |
| 1   | B     | 111 | ASN  |
| 1   | B     | 119 | GLN  |
| 1   | B     | 121 | GLN  |
| 1   | B     | 125 | GLN  |
| 1   | B     | 143 | GLN  |
| 1   | C     | 23  | GLN  |
| 1   | C     | 44  | ASN  |
| 1   | C     | 98  | GLN  |
| 1   | C     | 111 | ASN  |
| 1   | C     | 119 | GLN  |
| 1   | C     | 121 | GLN  |
| 1   | C     | 125 | GLN  |
| 1   | D     | 23  | GLN  |
| 1   | D     | 44  | ASN  |
| 1   | D     | 98  | GLN  |
| 1   | D     | 111 | ASN  |
| 1   | D     | 119 | GLN  |
| 1   | D     | 121 | GLN  |
| 1   | D     | 125 | GLN  |
| 1   | E     | 23  | GLN  |
| 1   | E     | 44  | ASN  |
| 1   | E     | 98  | GLN  |
| 1   | E     | 111 | ASN  |
| 1   | E     | 119 | GLN  |
| 1   | E     | 121 | GLN  |
| 1   | E     | 125 | GLN  |
| 1   | F     | 23  | GLN  |
| 1   | F     | 44  | ASN  |
| 1   | F     | 111 | ASN  |
| 1   | F     | 119 | GLN  |
| 1   | F     | 121 | GLN  |
| 1   | F     | 125 | GLN  |
| 1   | G     | 23  | GLN  |
| 1   | G     | 44  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 98  | GLN  |
| 1   | G     | 111 | ASN  |
| 1   | G     | 119 | GLN  |
| 1   | G     | 121 | GLN  |
| 1   | G     | 125 | GLN  |
| 2   | H     | 28  | HIS  |
| 2   | H     | 30  | ASN  |
| 2   | H     | 36  | GLN  |
| 2   | H     | 85  | ASN  |
| 2   | H     | 164 | GLN  |
| 2   | I     | 28  | HIS  |
| 2   | I     | 30  | ASN  |
| 2   | I     | 36  | GLN  |
| 2   | I     | 164 | GLN  |
| 2   | J     | 30  | ASN  |
| 2   | J     | 36  | GLN  |
| 2   | J     | 141 | GLN  |
| 2   | J     | 164 | GLN  |
| 2   | K     | 28  | HIS  |
| 2   | K     | 30  | ASN  |
| 2   | K     | 36  | GLN  |
| 2   | K     | 85  | ASN  |
| 2   | K     | 141 | GLN  |
| 2   | K     | 164 | GLN  |
| 2   | L     | 28  | HIS  |
| 2   | L     | 30  | ASN  |
| 2   | L     | 36  | GLN  |
| 2   | L     | 85  | ASN  |
| 2   | L     | 141 | GLN  |
| 2   | L     | 164 | GLN  |
| 2   | M     | 28  | HIS  |
| 2   | M     | 30  | ASN  |
| 2   | M     | 85  | ASN  |
| 2   | M     | 141 | GLN  |
| 2   | M     | 164 | GLN  |
| 2   | N     | 30  | ASN  |
| 2   | N     | 36  | GLN  |
| 2   | N     | 85  | ASN  |
| 2   | N     | 141 | GLN  |
| 2   | N     | 164 | GLN  |
| 1   | O     | 23  | GLN  |
| 1   | O     | 44  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 98  | GLN  |
| 1   | O     | 111 | ASN  |
| 1   | O     | 119 | GLN  |
| 1   | O     | 121 | GLN  |
| 1   | O     | 125 | GLN  |
| 1   | O     | 143 | GLN  |
| 1   | P     | 23  | GLN  |
| 1   | P     | 44  | ASN  |
| 1   | P     | 111 | ASN  |
| 1   | P     | 119 | GLN  |
| 1   | P     | 121 | GLN  |
| 1   | P     | 125 | GLN  |
| 1   | Q     | 23  | GLN  |
| 1   | Q     | 44  | ASN  |
| 1   | Q     | 98  | GLN  |
| 1   | Q     | 111 | ASN  |
| 1   | Q     | 119 | GLN  |
| 1   | Q     | 121 | GLN  |
| 1   | Q     | 125 | GLN  |
| 1   | R     | 23  | GLN  |
| 1   | R     | 44  | ASN  |
| 1   | R     | 98  | GLN  |
| 1   | R     | 111 | ASN  |
| 1   | R     | 119 | GLN  |
| 1   | R     | 121 | GLN  |
| 1   | R     | 125 | GLN  |
| 1   | S     | 23  | GLN  |
| 1   | S     | 44  | ASN  |
| 1   | S     | 98  | GLN  |
| 1   | S     | 111 | ASN  |
| 1   | S     | 119 | GLN  |
| 1   | S     | 121 | GLN  |
| 1   | S     | 125 | GLN  |
| 1   | T     | 23  | GLN  |
| 1   | T     | 44  | ASN  |
| 1   | T     | 98  | GLN  |
| 1   | T     | 111 | ASN  |
| 1   | T     | 119 | GLN  |
| 1   | T     | 121 | GLN  |
| 1   | T     | 125 | GLN  |
| 1   | U     | 23  | GLN  |
| 1   | U     | 44  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | U     | 98  | GLN  |
| 1   | U     | 111 | ASN  |
| 1   | U     | 119 | GLN  |
| 1   | U     | 121 | GLN  |
| 1   | U     | 125 | GLN  |
| 2   | V     | 28  | HIS  |
| 2   | V     | 30  | ASN  |
| 2   | V     | 36  | GLN  |
| 2   | V     | 85  | ASN  |
| 2   | V     | 164 | GLN  |
| 2   | W     | 28  | HIS  |
| 2   | W     | 30  | ASN  |
| 2   | W     | 36  | GLN  |
| 2   | W     | 141 | GLN  |
| 2   | W     | 164 | GLN  |
| 2   | X     | 30  | ASN  |
| 2   | X     | 36  | GLN  |
| 2   | X     | 141 | GLN  |
| 2   | X     | 164 | GLN  |
| 2   | Y     | 28  | HIS  |
| 2   | Y     | 30  | ASN  |
| 2   | Y     | 36  | GLN  |
| 2   | Y     | 85  | ASN  |
| 2   | Y     | 141 | GLN  |
| 2   | Y     | 164 | GLN  |
| 2   | Z     | 28  | HIS  |
| 2   | Z     | 30  | ASN  |
| 2   | Z     | 36  | GLN  |
| 2   | Z     | 85  | ASN  |
| 2   | Z     | 141 | GLN  |
| 2   | Z     | 164 | GLN  |
| 2   | 1     | 28  | HIS  |
| 2   | 1     | 30  | ASN  |
| 2   | 1     | 85  | ASN  |
| 2   | 1     | 141 | GLN  |
| 2   | 1     | 164 | GLN  |
| 2   | 2     | 28  | HIS  |
| 2   | 2     | 30  | ASN  |
| 2   | 2     | 36  | GLN  |
| 2   | 2     | 85  | ASN  |
| 2   | 2     | 141 | GLN  |
| 2   | 2     | 164 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

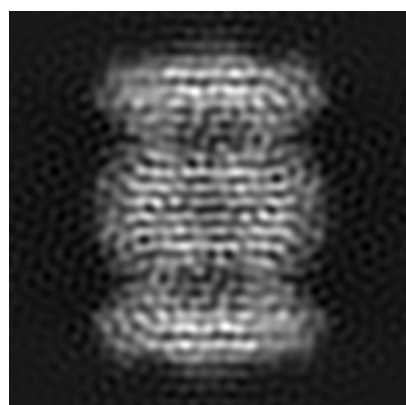
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1733. These allow visual inspection of the internal detail of the map and identification of artifacts.

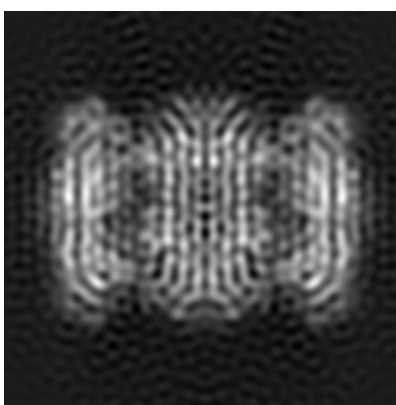
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

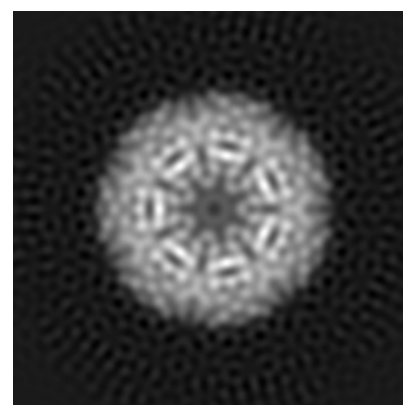
#### 6.1.1 Primary map



X



Y

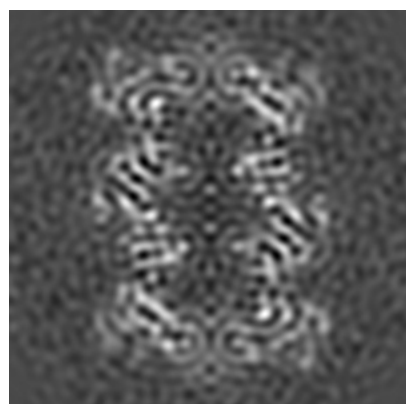


Z

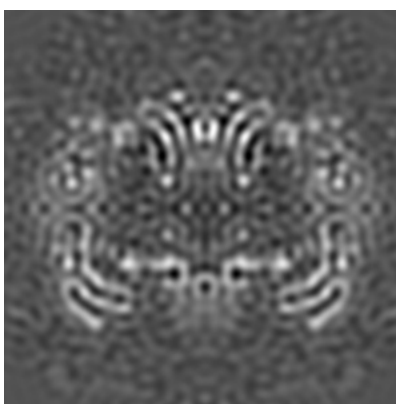
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

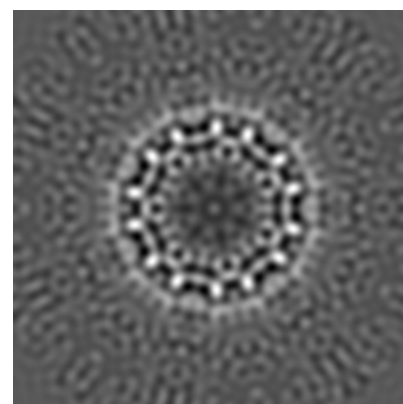
#### 6.2.1 Primary map



X Index: 72



Y Index: 72

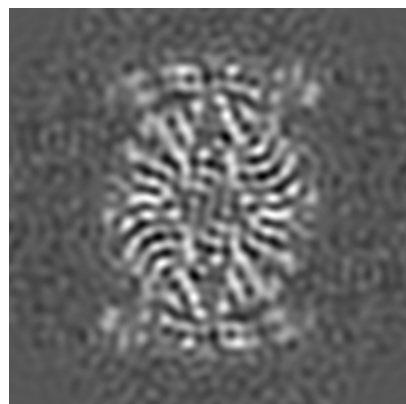


Z Index: 72

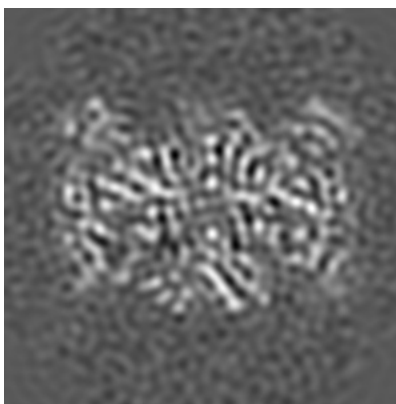
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

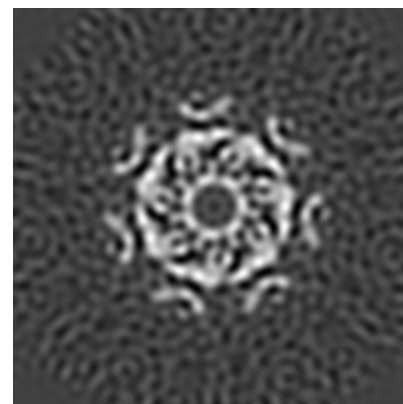
### 6.3.1 Primary map



X Index: 90



Y Index: 53

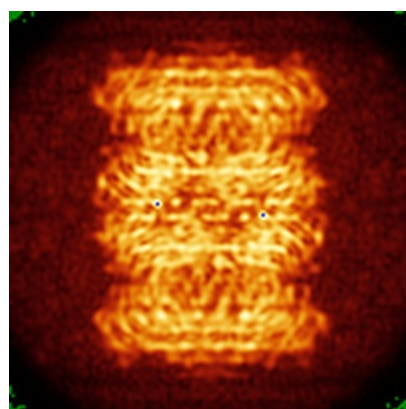


Z Index: 58

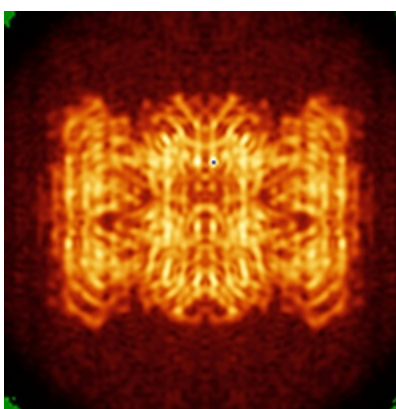
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

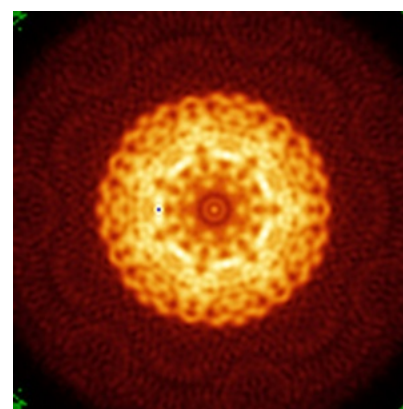
### 6.4.1 Primary map



X



Y

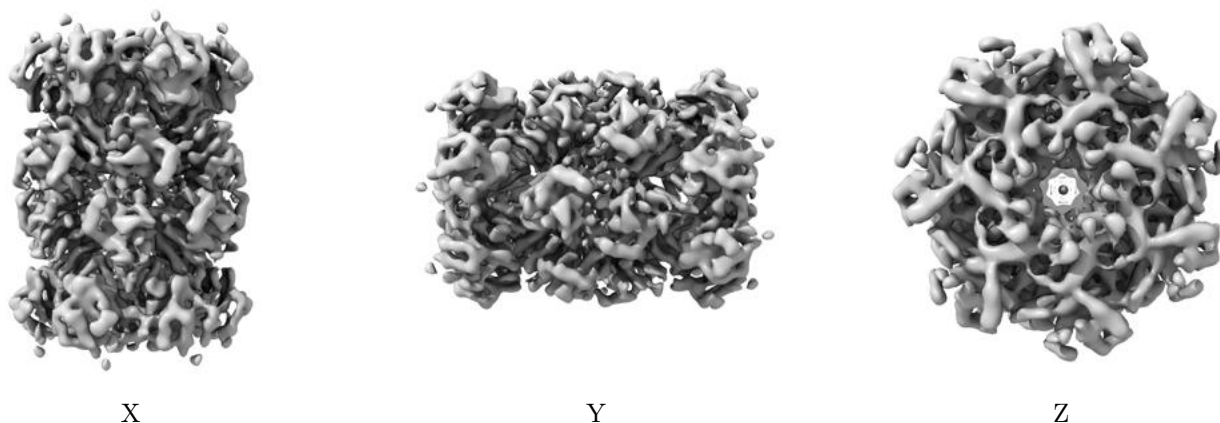


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

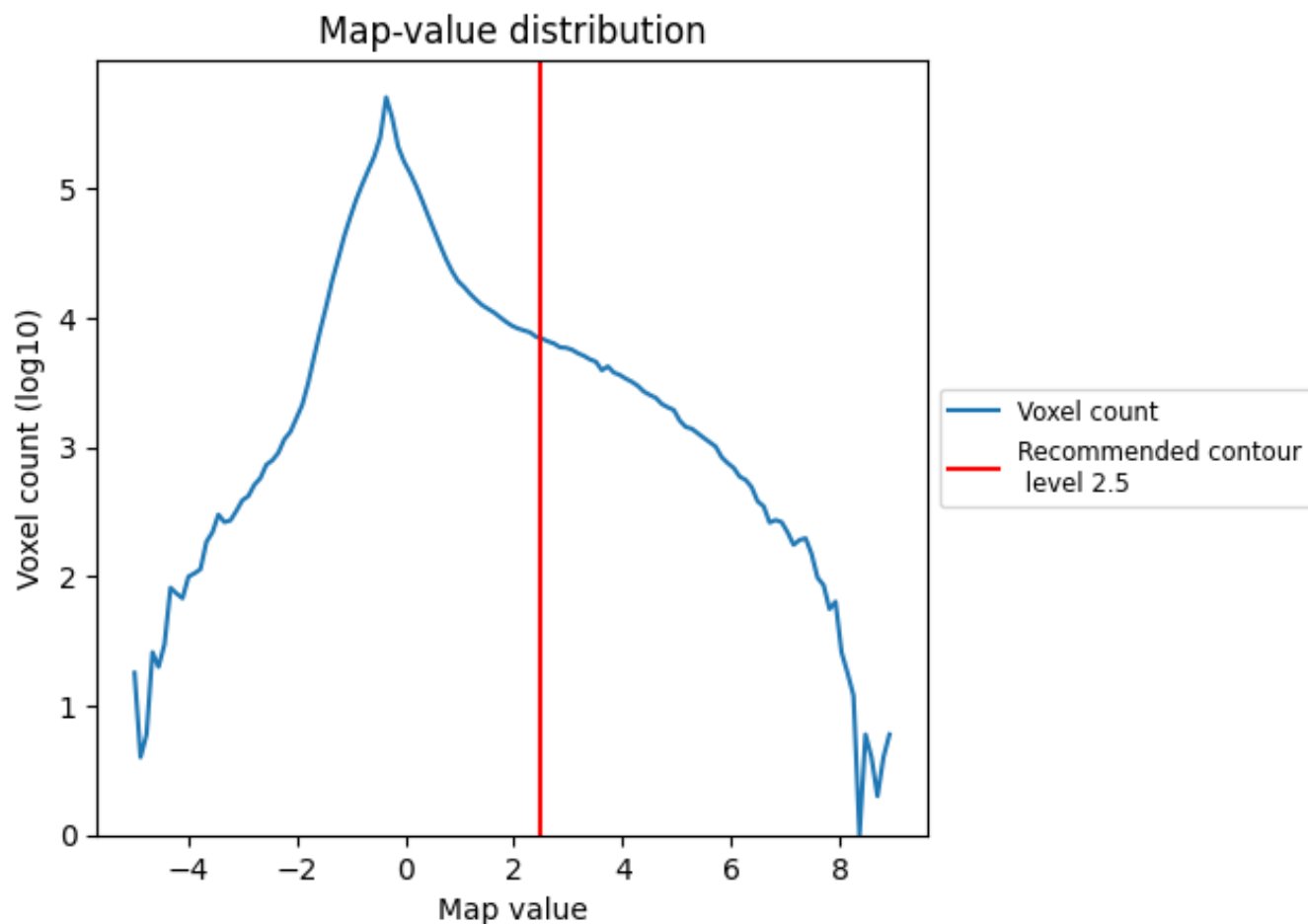
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

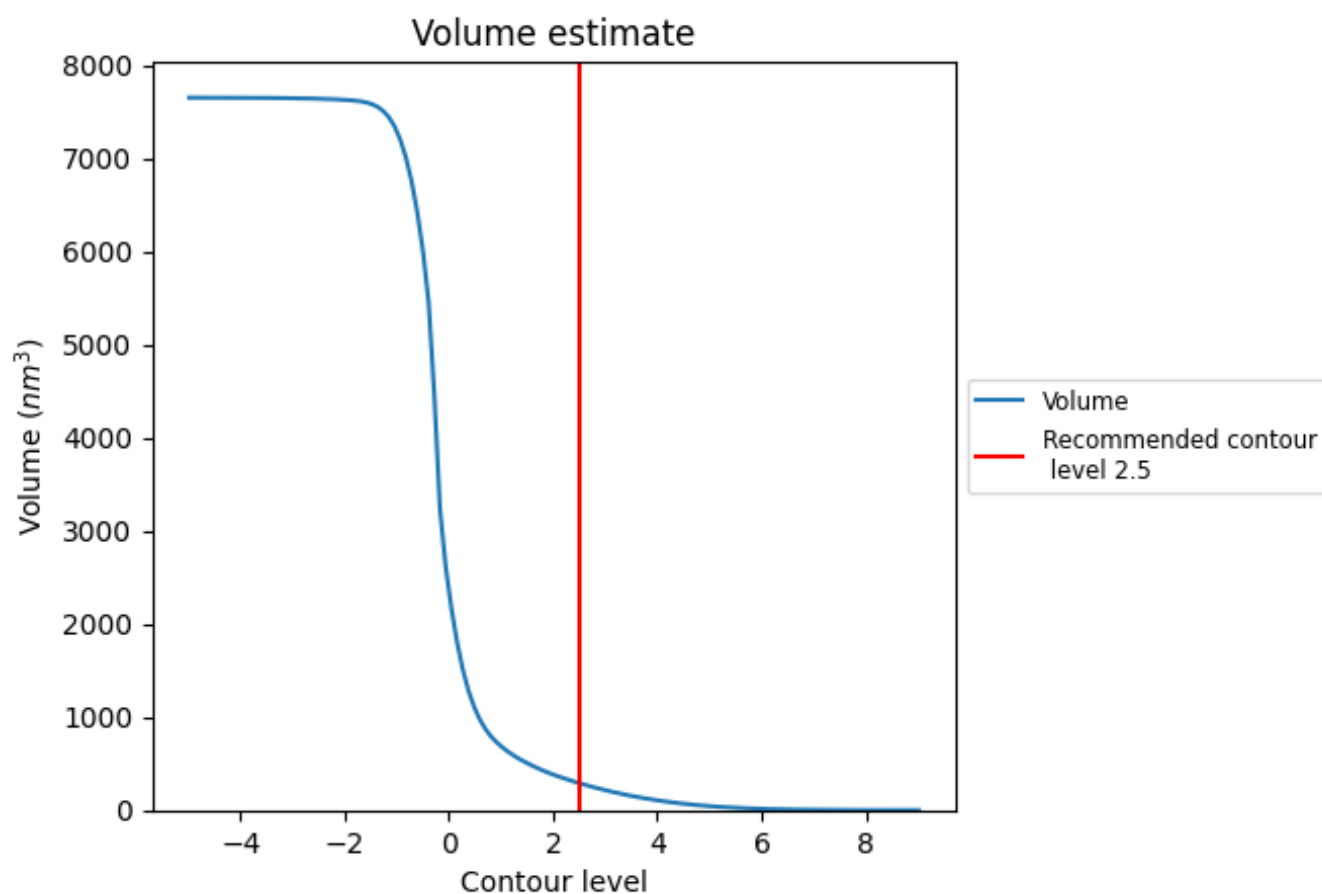
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

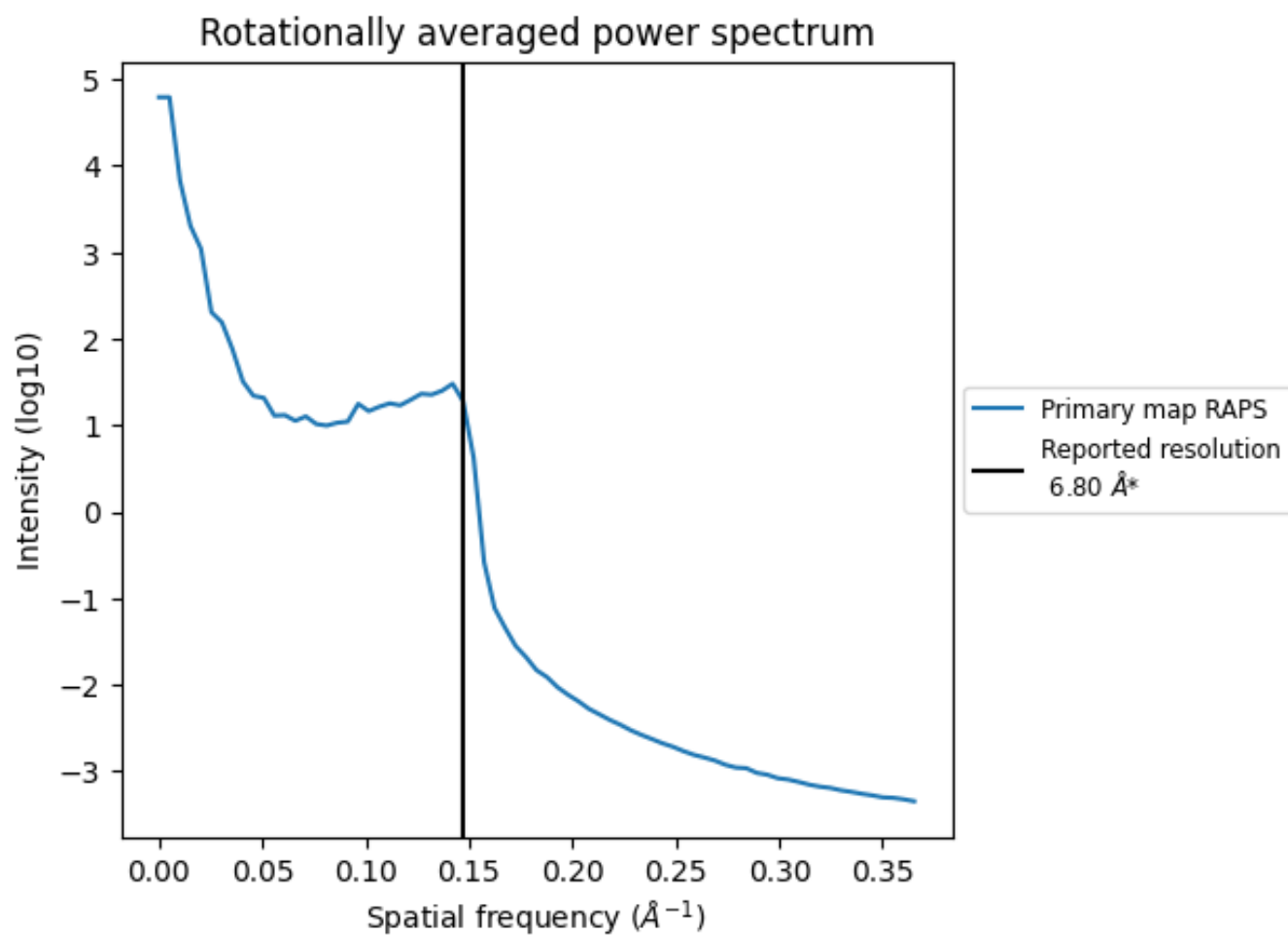
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290  $\text{nm}^3$ ; this corresponds to an approximate mass of 262 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.147 Å<sup>-1</sup>

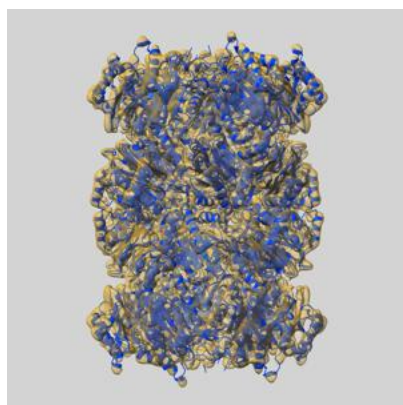
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

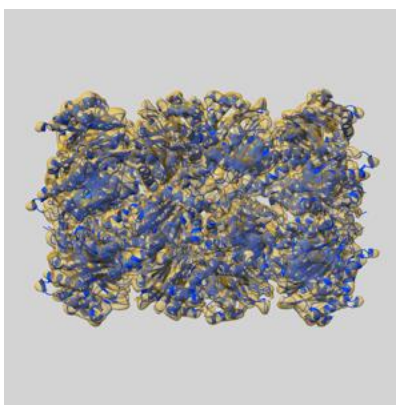
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1733 and PDB model 3C91. Per-residue inclusion information can be found in section [3](#) on page [6](#).

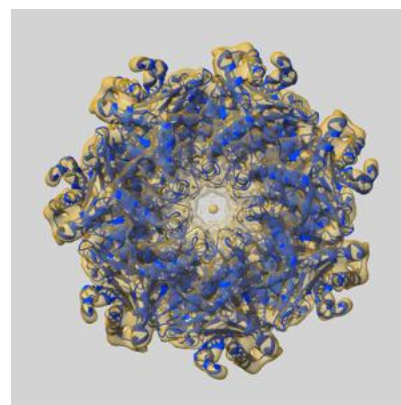
### 9.1 Map-model overlay [i](#)



X



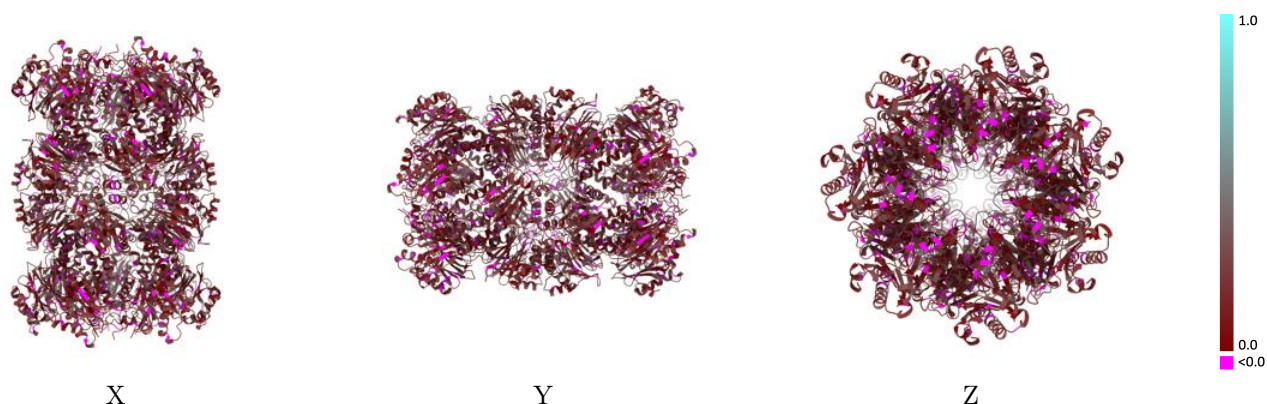
Y



Z

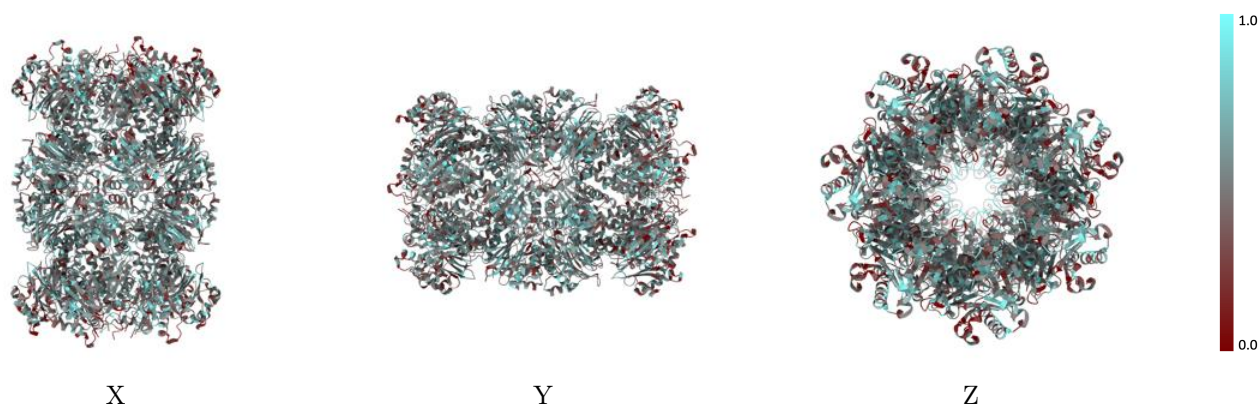
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



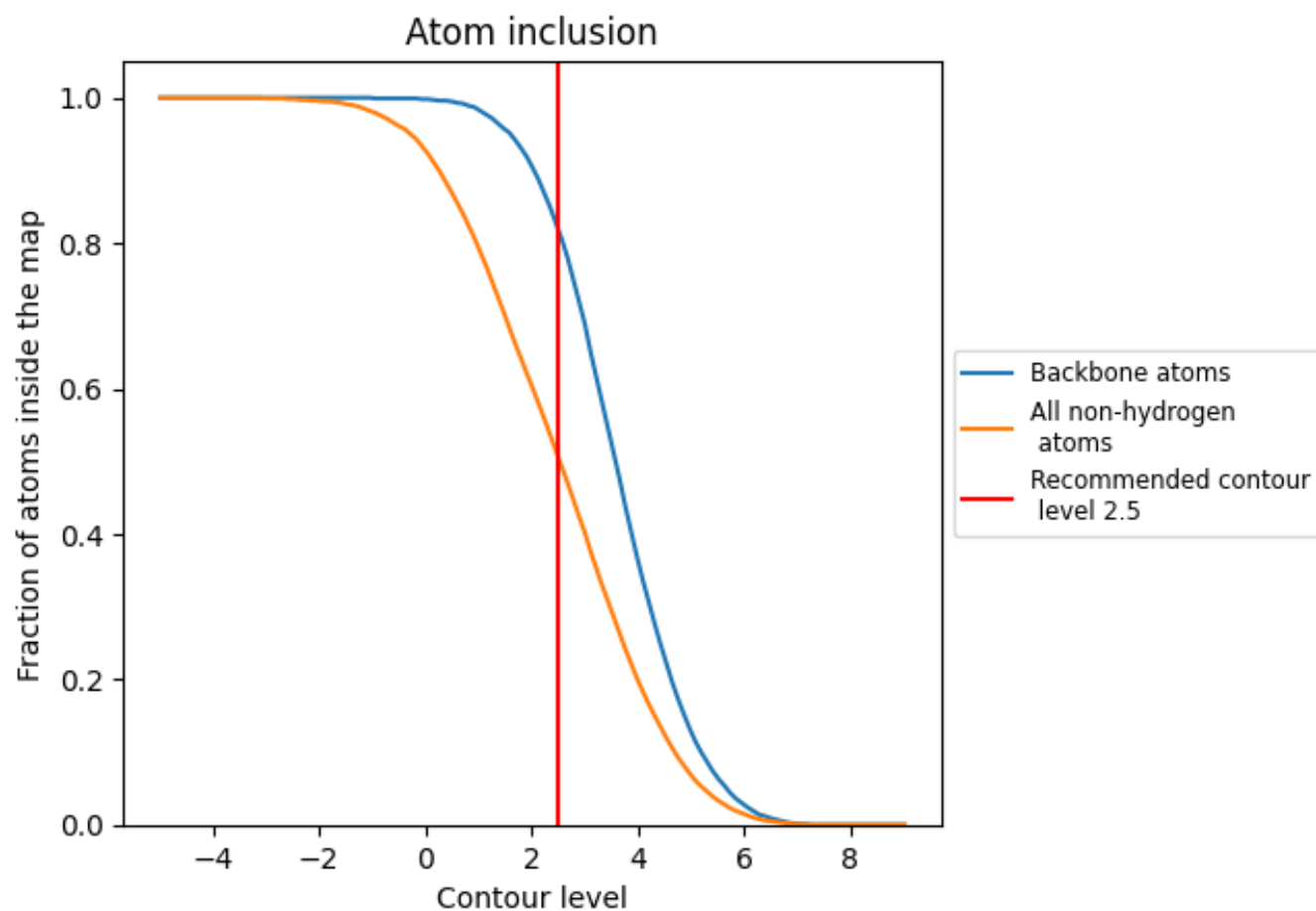
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.5060   |  0.1730   |
| 1     |  0.5250   |  0.1790   |
| 2     |  0.5300   |  0.1810   |
| A     |  0.4980   |  0.1720   |
| B     |  0.4980   |  0.1710   |
| C     |  0.4890   |  0.1700   |
| D     |  0.4900   |  0.1680   |
| E     |  0.4860   |  0.1710   |
| F     |  0.4760   |  0.1620   |
| G     |  0.4810   |  0.1680   |
| H     |  0.5340   |  0.1820   |
| I     |  0.5310   |  0.1810   |
| J     |  0.5280   |  0.1840   |
| K     |  0.5340   |  0.1810   |
| L     |  0.5340  |  0.1810  |
| M     |  0.5400 |  0.1840 |
| N     |  0.5390 |  0.1830 |
| O     |  0.4840 |  0.1640 |
| P     |  0.4840 |  0.1660 |
| Q     |  0.4820 |  0.1660 |
| R     |  0.4910 |  0.1660 |
| S     |  0.4770 |  0.1650 |
| T     |  0.4790 |  0.1590 |
| U     |  0.4970 |  0.1670 |
| V     |  0.5210 |  0.1770 |
| W     |  0.5220 |  0.1720 |
| X     |  0.5230 |  0.1740 |
| Y     |  0.5190 |  0.1760 |
| Z     |  0.5190 |  0.1770 |

