



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 04:45 PM UTC

PDB ID : 7EY6 / pdb\_00007ey6  
EMDB ID : EMD-31321  
Title : The portal protein (GP8) of bacteriophage T7  
Authors : Liu, H.R.; Chen, W.Y.  
Deposited on : 2021-05-30  
Resolution : 4.30 Å(reported)

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:

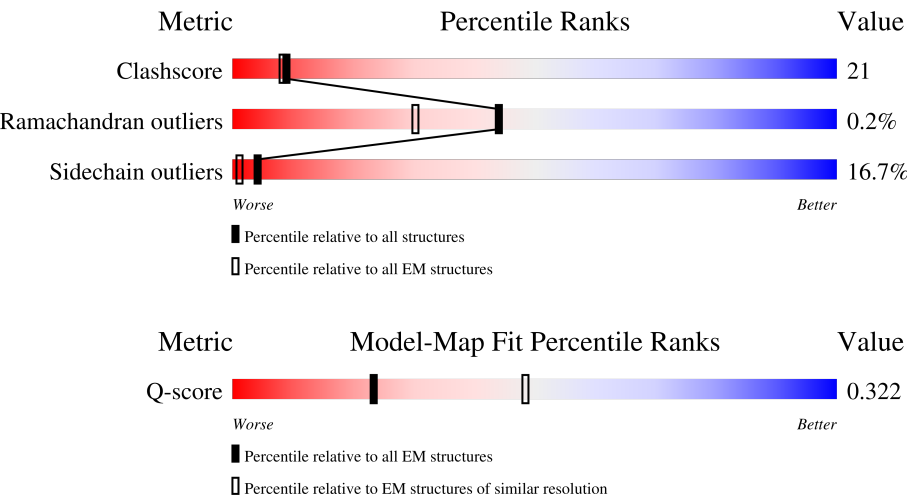
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 Å.

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



| Metric                | Whole archive<br>(#Entries) | 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                       | 4585 ( 3.80 - 4.80 )                                     |

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     | 536    |                  |
| 1   | B     | 536    |                  |
| 1   | C     | 536    |                  |
| 1   | D     | 536    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 536    |                  |
| 1   | F     | 536    |                  |
| 1   | G     | 536    |                  |
| 1   | H     | 536    |                  |
| 1   | I     | 536    |                  |
| 1   | J     | 536    |                  |
| 1   | K     | 536    |                  |
| 1   | L     | 536    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 44028 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.

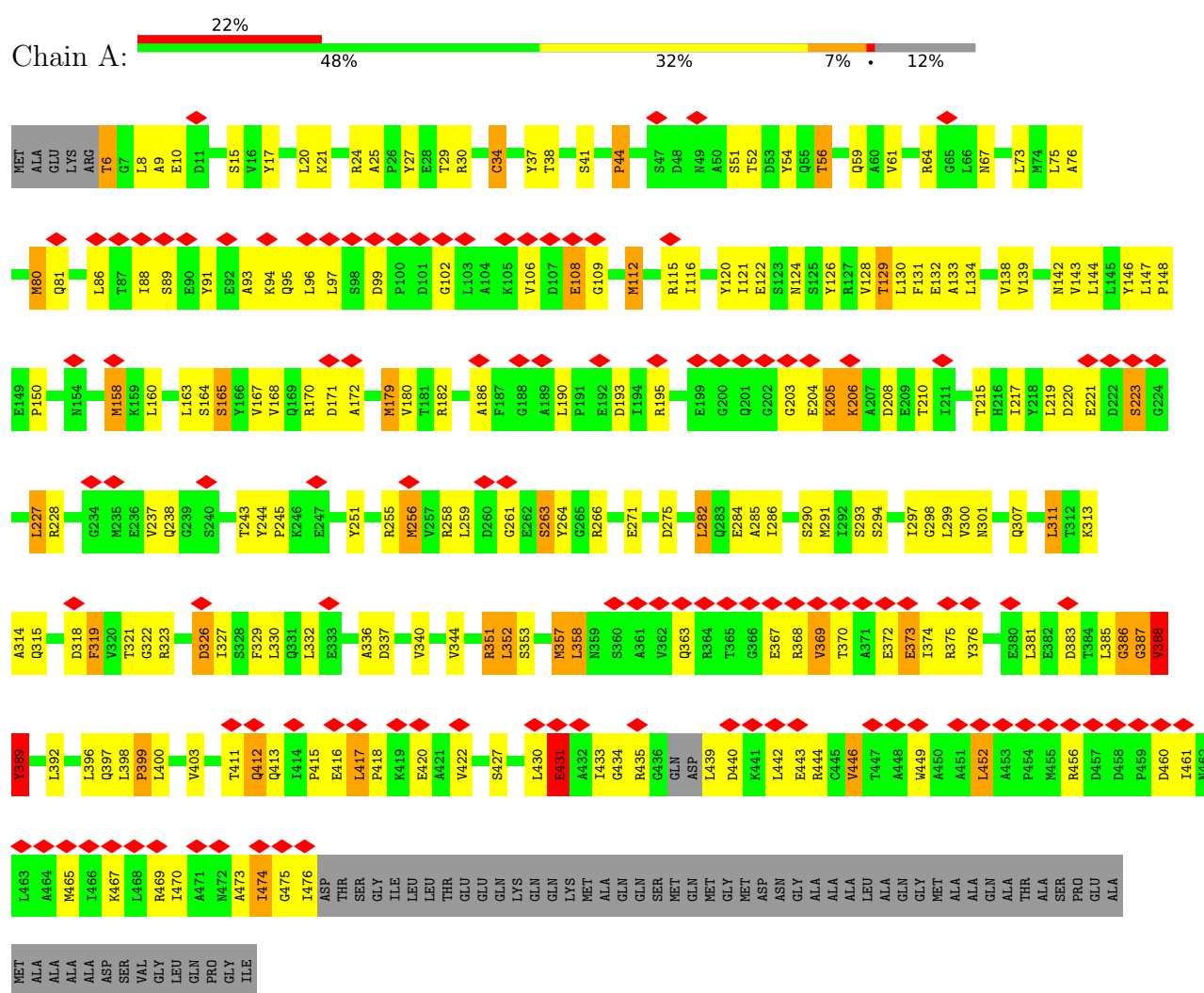
- Molecule 1 is a protein called Portal protein.

| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 1   | A     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | B     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | C     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | D     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | E     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | F     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | G     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | H     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | I     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | J     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | K     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |
| 1   | L     | 469      | Total<br>3669 | C<br>2313 | N<br>619 | O<br>720 | S<br>17 | 0       | 0     |

### 3 Residue-property plots

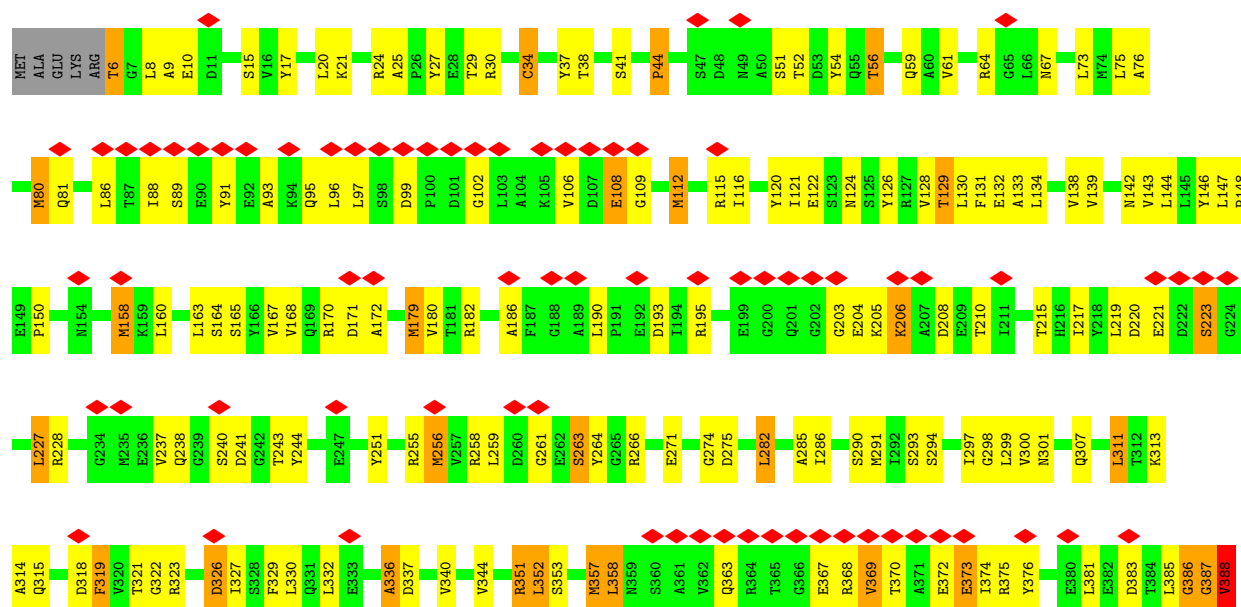
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

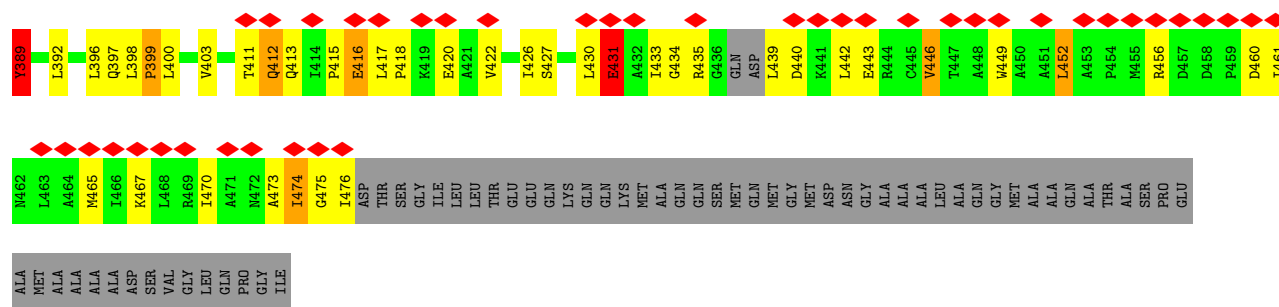
#### • Molecule 1: Portal protein



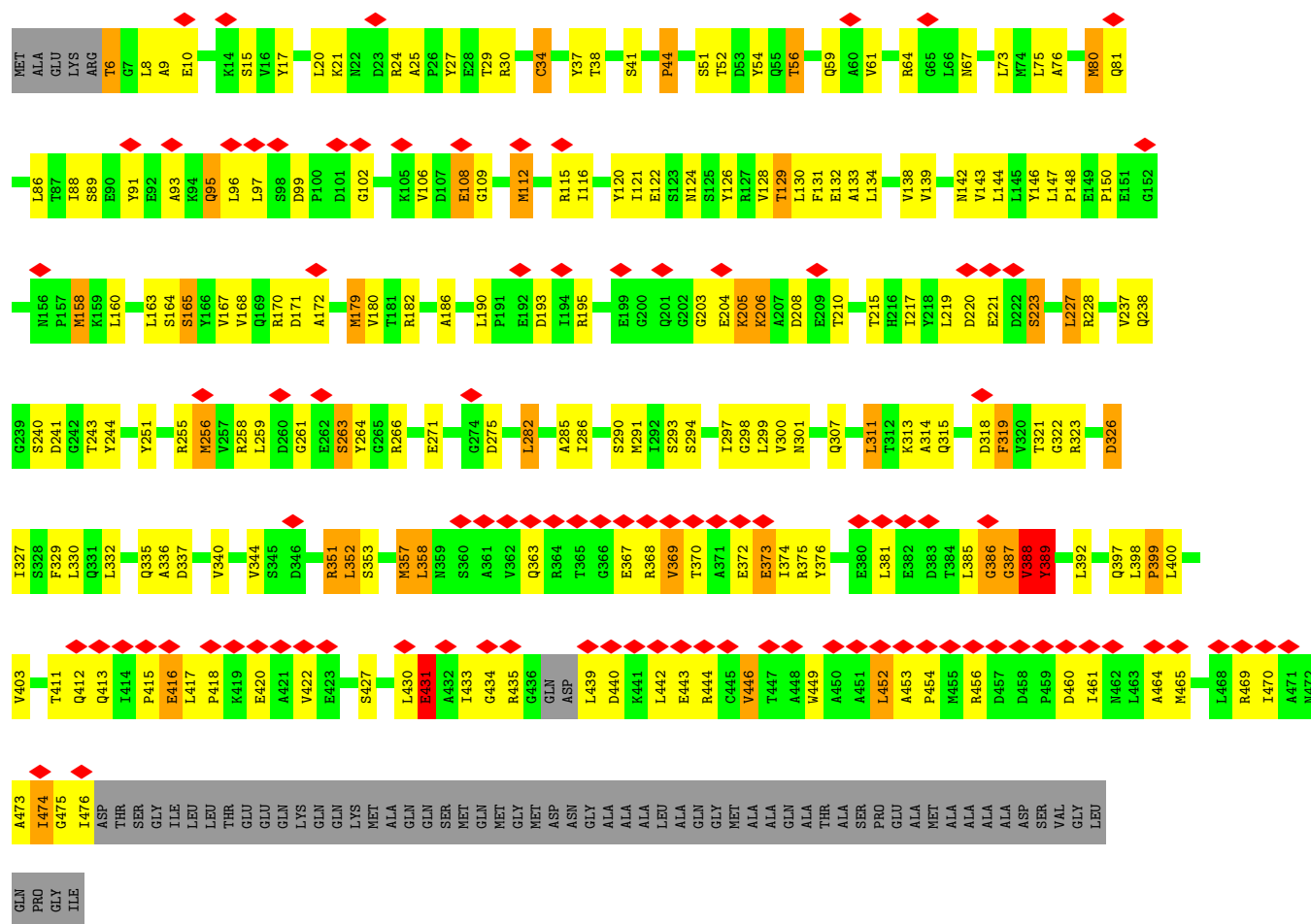
#### • Molecule 1: Portal protein





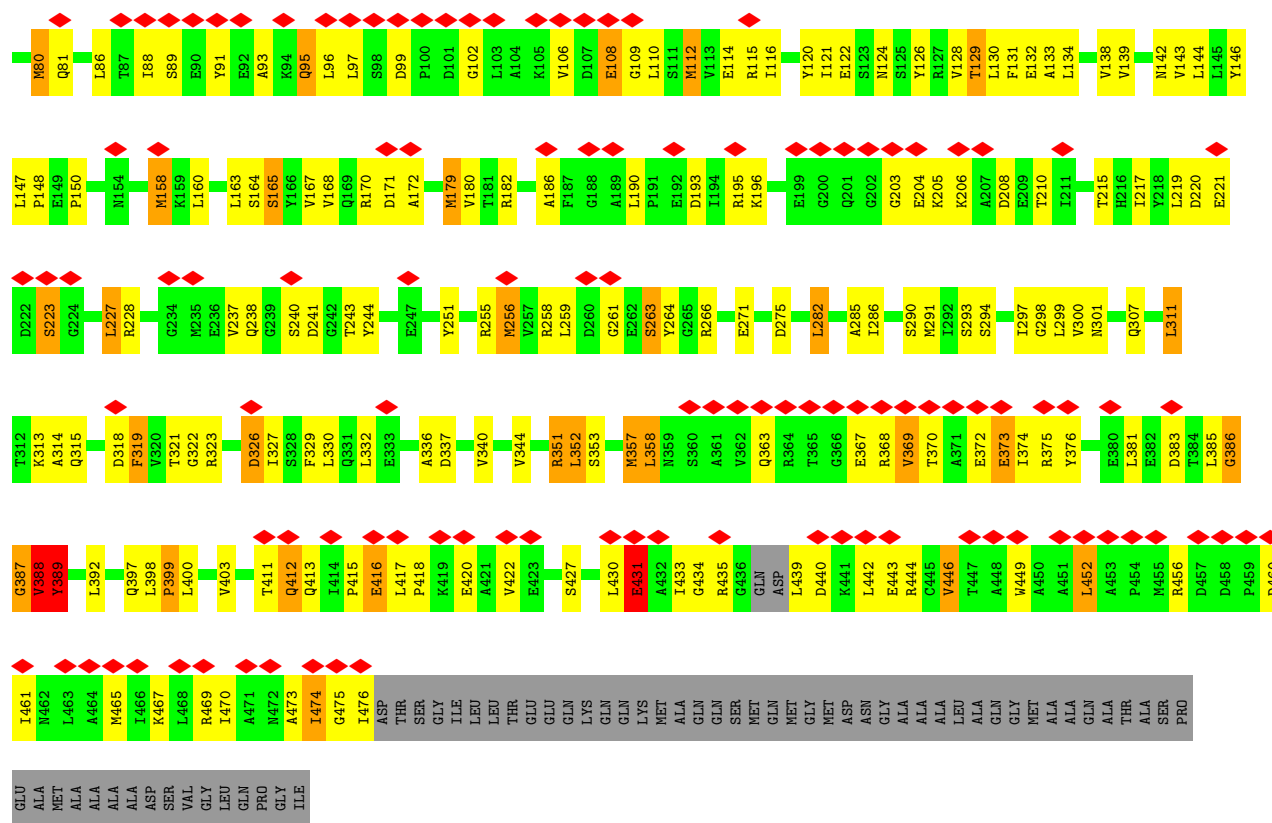


- Molecule 1: Portal protein

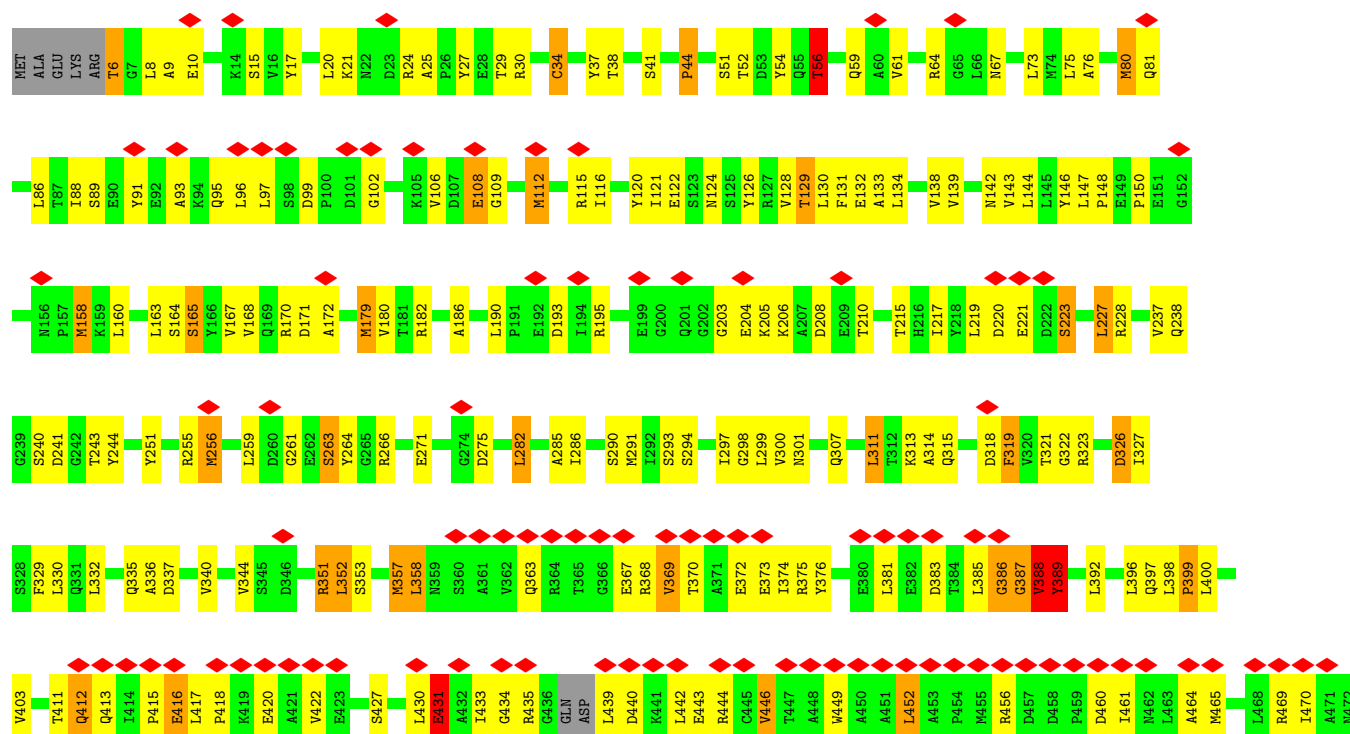


- Molecule 1: Portal protein

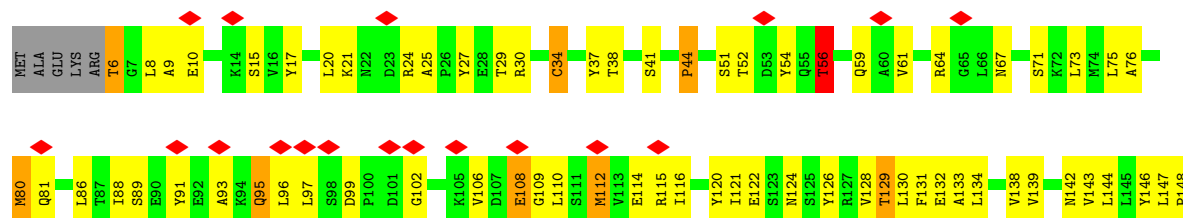


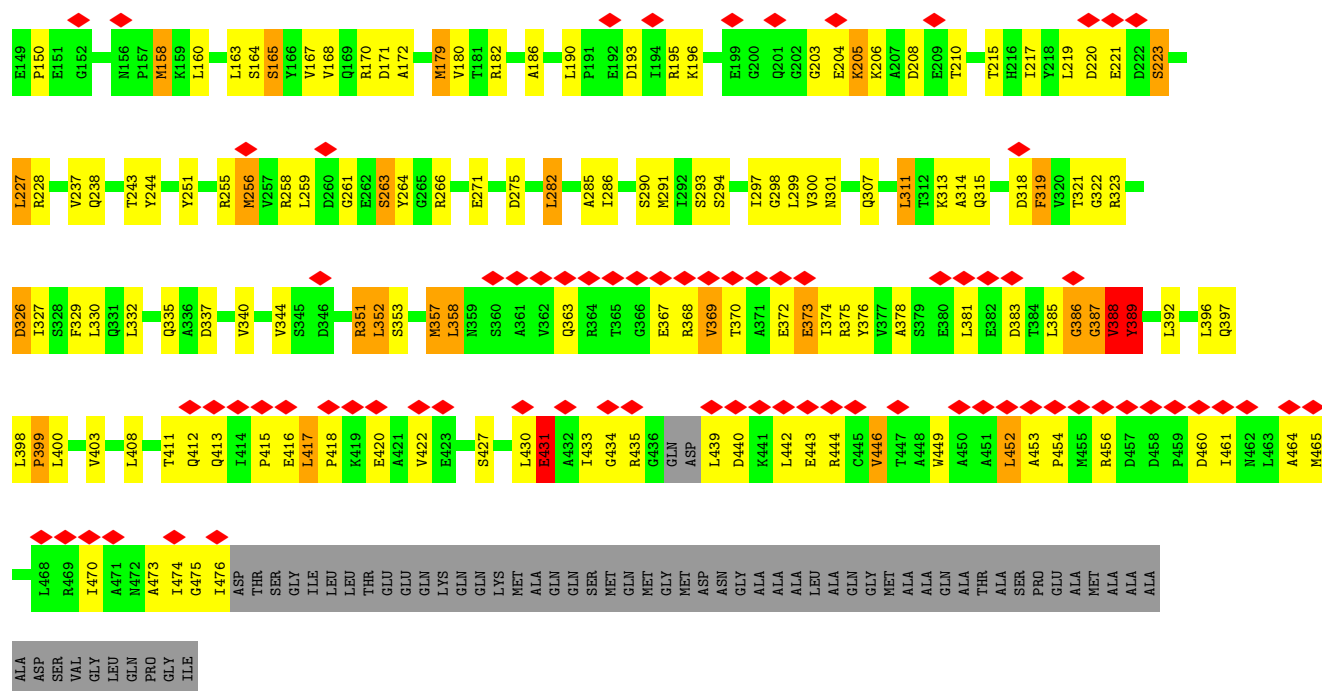


• Molecule 1: Portal protein

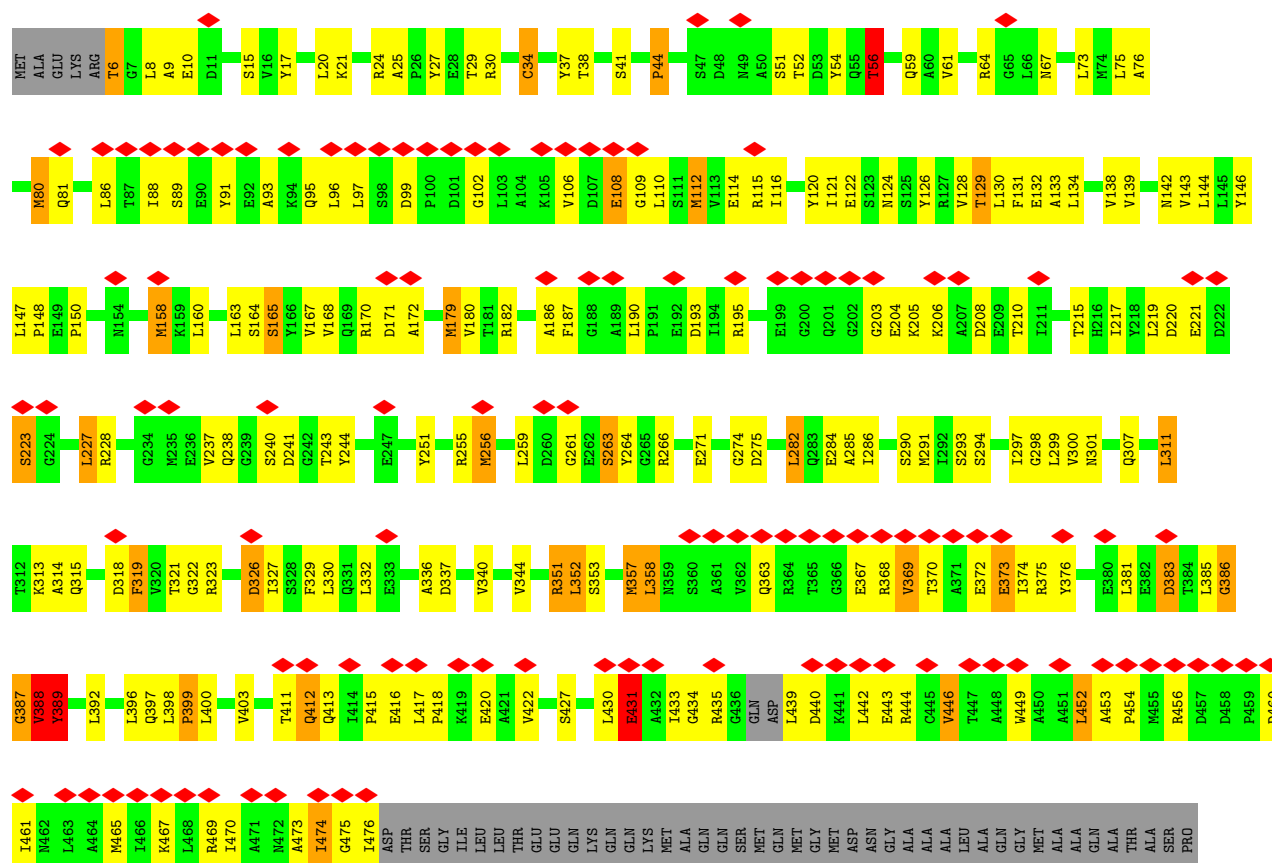






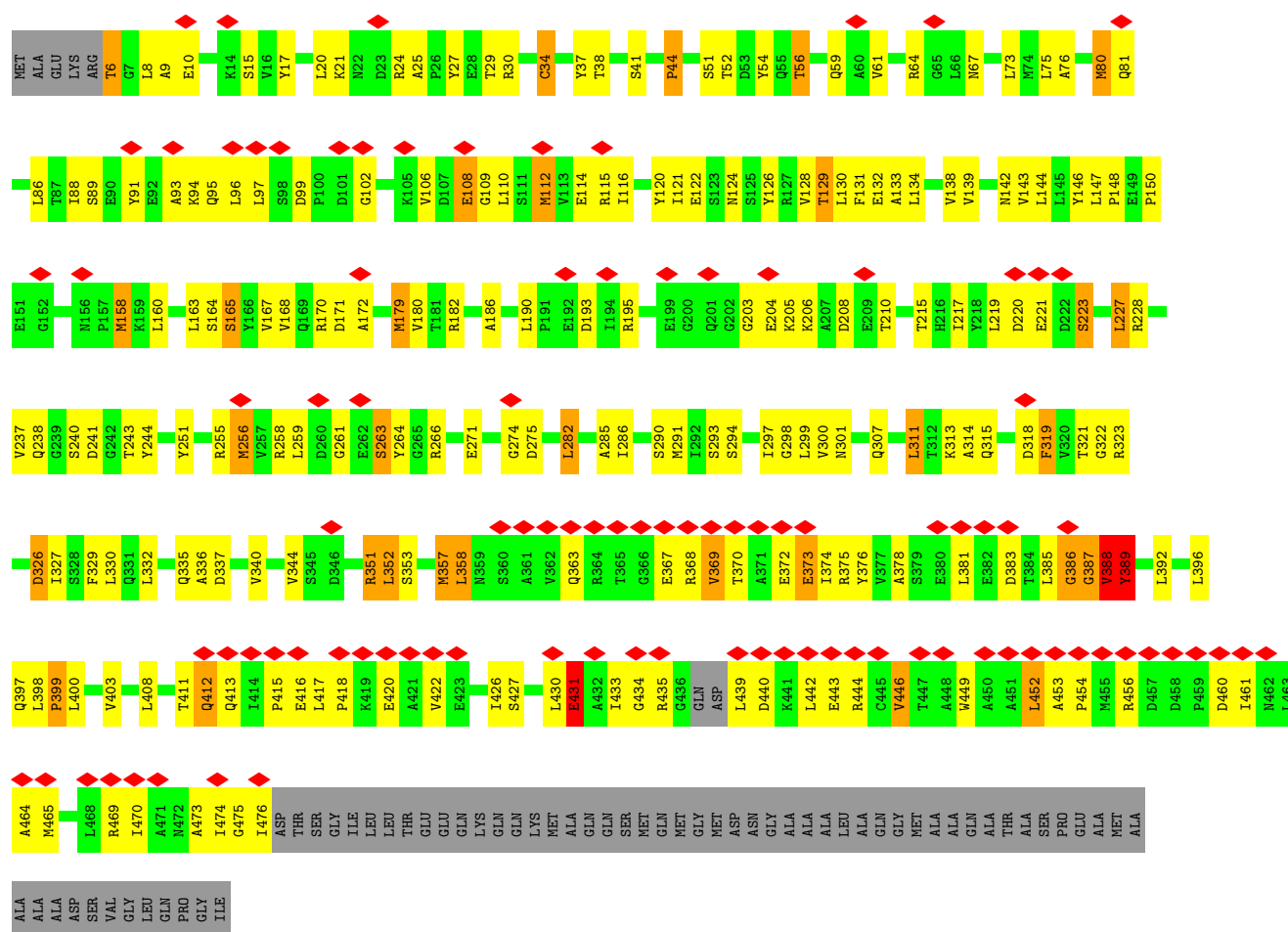


- Molecule 1: Portal protein

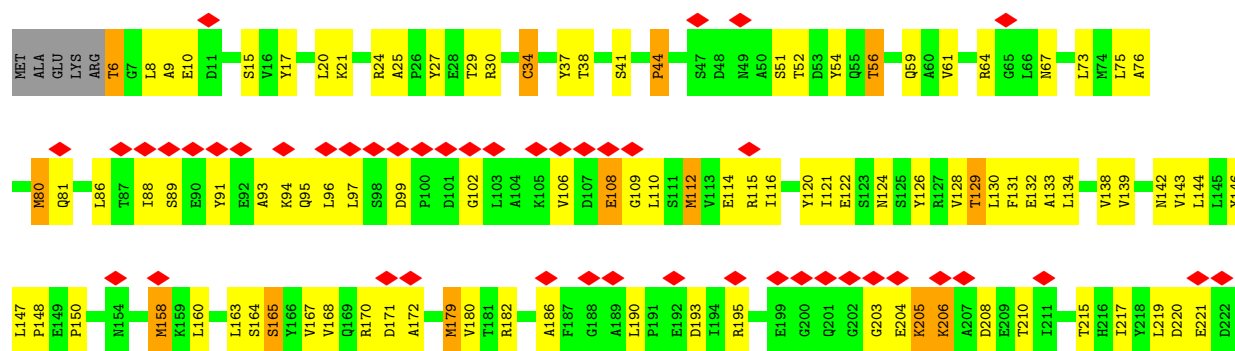


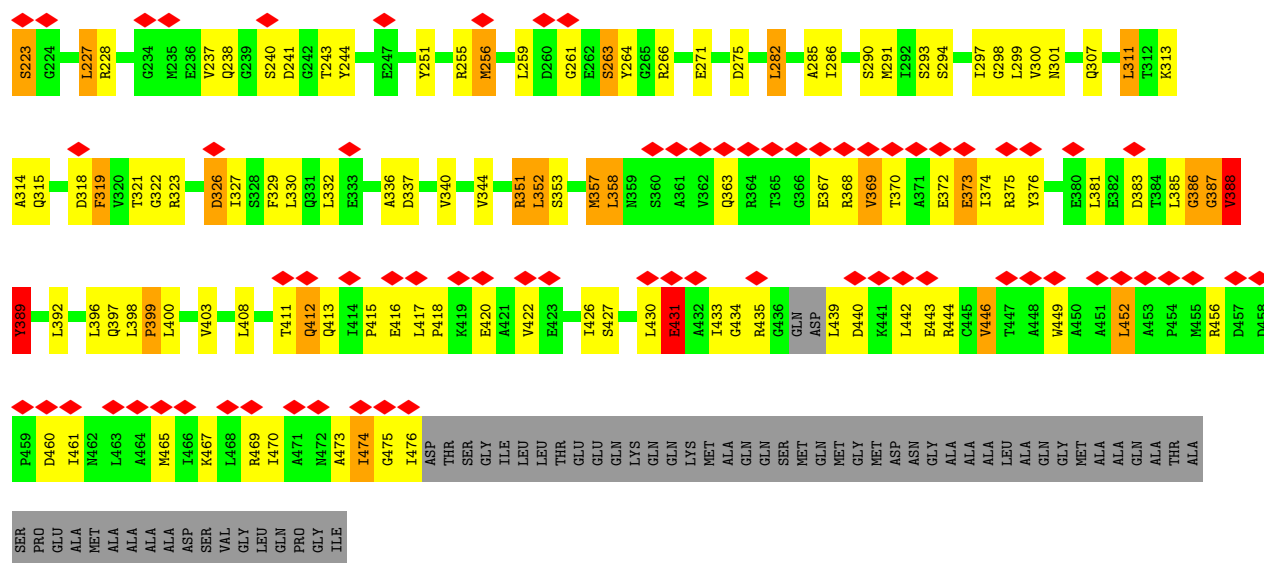
GLU  
ALA  
MET  
GLU  
ALA  
LYS  
ALA  
ARG  
ALA  
ASP  
SER  
VAL  
GLY  
LEU  
GLN  
PRO  
GLY  
ILE

• Molecule 1: Portal protein

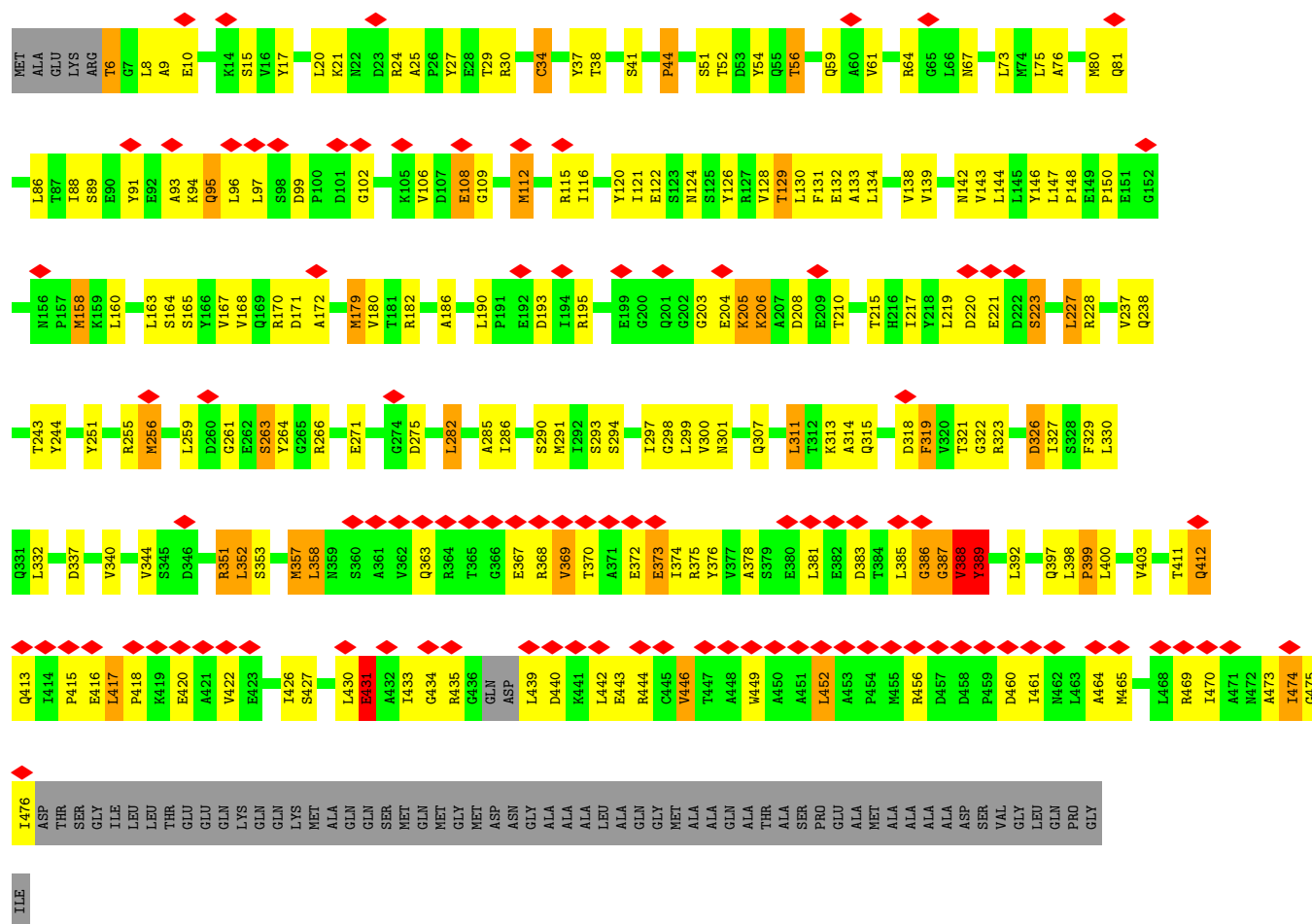


• Molecule 1: Portal protein





• Molecule 1: Portal protein



## 4 Experimental information

| Property                             | Value                   | Source    |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE         | Depositor |
| Imposed symmetry                     | POINT, Not provided     |           |
| Number of particles used             | 59985                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF       | Depositor |
| CTF correction method                | NONE                    | Depositor |
| Microscope                           | FEI TECNAI ARCTICA      | Depositor |
| Voltage (kV)                         | 200                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 25                      | Depositor |
| Minimum defocus (nm)                 | Not provided            |           |
| Maximum defocus (nm)                 | Not provided            |           |
| Magnification                        | Not provided            |           |
| Image detector                       | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value                    | 43.195                  | Depositor |
| Minimum map value                    | -27.980                 | Depositor |
| Average map value                    | 0.013                   | Depositor |
| Map value standard deviation         | 2.048                   | Depositor |
| Recommended contour level            | 8                       | Depositor |
| Map size ( $\text{\AA}$ )            | 508.0, 508.0, 508.0     | wwPDB     |
| Map dimensions                       | 400, 400, 400           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.27, 1.27, 1.27        | 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     | 0.69         | 0/3728  | 1.08        | 37/5049 (0.7%)   |
| 1   | B     | 0.68         | 0/3728  | 1.08        | 37/5049 (0.7%)   |
| 1   | C     | 0.68         | 0/3728  | 1.08        | 35/5049 (0.7%)   |
| 1   | D     | 0.68         | 0/3728  | 1.08        | 35/5049 (0.7%)   |
| 1   | E     | 0.68         | 0/3728  | 1.08        | 34/5049 (0.7%)   |
| 1   | F     | 0.68         | 0/3728  | 1.08        | 35/5049 (0.7%)   |
| 1   | G     | 0.68         | 0/3728  | 1.08        | 35/5049 (0.7%)   |
| 1   | H     | 0.68         | 0/3728  | 1.08        | 35/5049 (0.7%)   |
| 1   | I     | 0.68         | 0/3728  | 1.08        | 35/5049 (0.7%)   |
| 1   | J     | 0.68         | 0/3728  | 1.08        | 35/5049 (0.7%)   |
| 1   | K     | 0.68         | 0/3728  | 1.08        | 35/5049 (0.7%)   |
| 1   | L     | 0.68         | 0/3728  | 1.08        | 34/5049 (0.7%)   |
| All | All   | 0.68         | 0/44736 | 1.08        | 422/60588 (0.7%) |

There are no bond length outliers.

All (422) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 208 | ASP  | N-CA-C | 11.72 | 124.14      | 111.36   |
| 1   | A     | 208 | ASP  | N-CA-C | 11.72 | 124.13      | 111.36   |
| 1   | B     | 208 | ASP  | N-CA-C | 11.71 | 124.13      | 111.36   |
| 1   | E     | 208 | ASP  | N-CA-C | 11.69 | 124.11      | 111.36   |
| 1   | J     | 208 | ASP  | N-CA-C | 11.69 | 124.10      | 111.36   |
| 1   | F     | 208 | ASP  | N-CA-C | 11.68 | 124.09      | 111.36   |
| 1   | K     | 208 | ASP  | N-CA-C | 11.67 | 124.08      | 111.36   |
| 1   | H     | 208 | ASP  | N-CA-C | 11.66 | 124.07      | 111.36   |
| 1   | L     | 208 | ASP  | N-CA-C | 11.66 | 124.07      | 111.36   |
| 1   | G     | 208 | ASP  | N-CA-C | 11.66 | 124.07      | 111.36   |
| 1   | C     | 208 | ASP  | N-CA-C | 11.65 | 124.06      | 111.36   |
| 1   | I     | 208 | ASP  | N-CA-C | 11.63 | 124.04      | 111.36   |
| 1   | I     | 386 | GLY  | N-CA-C | -9.64 | 97.45       | 110.56   |
| 1   | F     | 386 | GLY  | N-CA-C | -9.63 | 97.47       | 110.56   |
| 1   | G     | 386 | GLY  | N-CA-C | -9.62 | 97.48       | 110.56   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | H     | 386 | GLY  | N-CA-C | -9.61 | 97.49       | 110.56   |
| 1   | B     | 386 | GLY  | N-CA-C | -9.61 | 97.49       | 110.56   |
| 1   | J     | 386 | GLY  | N-CA-C | -9.61 | 97.49       | 110.56   |
| 1   | L     | 386 | GLY  | N-CA-C | -9.60 | 97.50       | 110.56   |
| 1   | K     | 386 | GLY  | N-CA-C | -9.60 | 97.51       | 110.56   |
| 1   | D     | 386 | GLY  | N-CA-C | -9.58 | 97.53       | 110.56   |
| 1   | E     | 386 | GLY  | N-CA-C | -9.58 | 97.53       | 110.56   |
| 1   | A     | 386 | GLY  | N-CA-C | -9.58 | 97.53       | 110.56   |
| 1   | C     | 386 | GLY  | N-CA-C | -9.57 | 97.54       | 110.56   |
| 1   | C     | 9   | ALA  | N-CA-C | -9.43 | 101.00      | 111.28   |
| 1   | A     | 9   | ALA  | N-CA-C | -9.42 | 101.01      | 111.28   |
| 1   | F     | 9   | ALA  | N-CA-C | -9.41 | 101.02      | 111.28   |
| 1   | L     | 9   | ALA  | N-CA-C | -9.41 | 101.03      | 111.28   |
| 1   | E     | 9   | ALA  | N-CA-C | -9.39 | 101.04      | 111.28   |
| 1   | K     | 9   | ALA  | N-CA-C | -9.39 | 101.04      | 111.28   |
| 1   | I     | 9   | ALA  | N-CA-C | -9.39 | 101.04      | 111.28   |
| 1   | G     | 9   | ALA  | N-CA-C | -9.38 | 101.05      | 111.28   |
| 1   | J     | 9   | ALA  | N-CA-C | -9.38 | 101.05      | 111.28   |
| 1   | D     | 9   | ALA  | N-CA-C | -9.38 | 101.06      | 111.28   |
| 1   | H     | 9   | ALA  | N-CA-C | -9.37 | 101.06      | 111.28   |
| 1   | B     | 9   | ALA  | N-CA-C | -9.37 | 101.07      | 111.28   |
| 1   | K     | 465 | MET  | N-CA-C | 8.28  | 120.38      | 111.36   |
| 1   | E     | 465 | MET  | N-CA-C | 8.27  | 120.37      | 111.36   |
| 1   | A     | 465 | MET  | N-CA-C | 8.26  | 120.37      | 111.36   |
| 1   | B     | 465 | MET  | N-CA-C | 8.26  | 120.36      | 111.36   |
| 1   | D     | 465 | MET  | N-CA-C | 8.26  | 120.36      | 111.36   |
| 1   | H     | 465 | MET  | N-CA-C | 8.26  | 120.36      | 111.36   |
| 1   | I     | 465 | MET  | N-CA-C | 8.26  | 120.36      | 111.36   |
| 1   | F     | 465 | MET  | N-CA-C | 8.24  | 120.35      | 111.36   |
| 1   | L     | 465 | MET  | N-CA-C | 8.24  | 120.34      | 111.36   |
| 1   | J     | 465 | MET  | N-CA-C | 8.24  | 120.34      | 111.36   |
| 1   | C     | 465 | MET  | N-CA-C | 8.23  | 120.34      | 111.36   |
| 1   | G     | 465 | MET  | N-CA-C | 8.21  | 120.30      | 111.36   |
| 1   | B     | 91  | TYR  | N-CA-C | -8.13 | 100.09      | 113.50   |
| 1   | F     | 91  | TYR  | N-CA-C | -8.12 | 100.10      | 113.50   |
| 1   | D     | 91  | TYR  | N-CA-C | -8.12 | 100.10      | 113.50   |
| 1   | K     | 91  | TYR  | N-CA-C | -8.12 | 100.11      | 113.50   |
| 1   | L     | 91  | TYR  | N-CA-C | -8.12 | 100.11      | 113.50   |
| 1   | J     | 91  | TYR  | N-CA-C | -8.11 | 100.11      | 113.50   |
| 1   | A     | 91  | TYR  | N-CA-C | -8.11 | 100.11      | 113.50   |
| 1   | G     | 91  | TYR  | N-CA-C | -8.11 | 100.12      | 113.50   |
| 1   | H     | 91  | TYR  | N-CA-C | -8.11 | 100.12      | 113.50   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | I     | 91  | TYR  | N-CA-C  | -8.11 | 100.12      | 113.50   |
| 1   | C     | 91  | TYR  | N-CA-C  | -8.10 | 100.13      | 113.50   |
| 1   | E     | 91  | TYR  | N-CA-C  | -8.10 | 100.14      | 113.50   |
| 1   | C     | 315 | GLN  | N-CA-C  | -7.81 | 100.45      | 110.53   |
| 1   | K     | 315 | GLN  | N-CA-C  | -7.81 | 100.46      | 110.53   |
| 1   | D     | 315 | GLN  | N-CA-C  | -7.79 | 100.49      | 110.53   |
| 1   | E     | 315 | GLN  | N-CA-C  | -7.79 | 100.49      | 110.53   |
| 1   | G     | 315 | GLN  | N-CA-C  | -7.79 | 100.49      | 110.53   |
| 1   | A     | 315 | GLN  | N-CA-C  | -7.78 | 100.50      | 110.53   |
| 1   | F     | 315 | GLN  | N-CA-C  | -7.78 | 100.50      | 110.53   |
| 1   | L     | 315 | GLN  | N-CA-C  | -7.78 | 100.50      | 110.53   |
| 1   | I     | 315 | GLN  | N-CA-C  | -7.77 | 100.50      | 110.53   |
| 1   | H     | 315 | GLN  | N-CA-C  | -7.77 | 100.51      | 110.53   |
| 1   | B     | 315 | GLN  | N-CA-C  | -7.77 | 100.51      | 110.53   |
| 1   | J     | 315 | GLN  | N-CA-C  | -7.77 | 100.51      | 110.53   |
| 1   | K     | 10  | GLU  | CB-CA-C | -7.10 | 108.39      | 116.63   |
| 1   | L     | 10  | GLU  | CB-CA-C | -7.10 | 108.40      | 116.63   |
| 1   | G     | 10  | GLU  | CB-CA-C | -7.09 | 108.41      | 116.63   |
| 1   | J     | 387 | GLY  | N-CA-C  | -7.08 | 104.12      | 115.66   |
| 1   | C     | 10  | GLU  | CB-CA-C | -7.08 | 108.42      | 116.63   |
| 1   | F     | 10  | GLU  | CB-CA-C | -7.07 | 108.42      | 116.63   |
| 1   | H     | 10  | GLU  | CB-CA-C | -7.07 | 108.43      | 116.63   |
| 1   | J     | 10  | GLU  | CB-CA-C | -7.07 | 108.43      | 116.63   |
| 1   | A     | 10  | GLU  | CB-CA-C | -7.06 | 108.44      | 116.63   |
| 1   | I     | 10  | GLU  | CB-CA-C | -7.06 | 108.44      | 116.63   |
| 1   | L     | 387 | GLY  | N-CA-C  | -7.06 | 104.15      | 115.66   |
| 1   | E     | 10  | GLU  | CB-CA-C | -7.05 | 108.45      | 116.63   |
| 1   | K     | 387 | GLY  | N-CA-C  | -7.05 | 104.17      | 115.66   |
| 1   | I     | 387 | GLY  | N-CA-C  | -7.05 | 104.17      | 115.66   |
| 1   | B     | 10  | GLU  | CB-CA-C | -7.05 | 108.46      | 116.63   |
| 1   | D     | 10  | GLU  | CB-CA-C | -7.04 | 108.46      | 116.63   |
| 1   | D     | 387 | GLY  | N-CA-C  | -7.04 | 104.18      | 115.66   |
| 1   | A     | 112 | MET  | N-CA-C  | -6.89 | 103.70      | 111.07   |
| 1   | C     | 112 | MET  | N-CA-C  | -6.89 | 103.70      | 111.07   |
| 1   | F     | 112 | MET  | N-CA-C  | -6.89 | 103.70      | 111.07   |
| 1   | B     | 112 | MET  | N-CA-C  | -6.87 | 103.72      | 111.07   |
| 1   | H     | 112 | MET  | N-CA-C  | -6.87 | 103.72      | 111.07   |
| 1   | I     | 112 | MET  | N-CA-C  | -6.87 | 103.72      | 111.07   |
| 1   | E     | 112 | MET  | N-CA-C  | -6.87 | 103.72      | 111.07   |
| 1   | K     | 112 | MET  | N-CA-C  | -6.87 | 103.72      | 111.07   |
| 1   | D     | 112 | MET  | N-CA-C  | -6.86 | 103.73      | 111.07   |
| 1   | G     | 112 | MET  | N-CA-C  | -6.86 | 103.73      | 111.07   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | J     | 112 | MET  | N-CA-C | -6.86 | 103.73      | 111.07   |
| 1   | L     | 112 | MET  | N-CA-C | -6.83 | 103.76      | 111.07   |
| 1   | J     | 99  | ASP  | CA-C-N | -6.74 | 112.84      | 119.64   |
| 1   | J     | 99  | ASP  | C-N-CA | -6.74 | 112.84      | 119.64   |
| 1   | G     | 99  | ASP  | CA-C-N | -6.73 | 112.84      | 119.64   |
| 1   | G     | 99  | ASP  | C-N-CA | -6.73 | 112.84      | 119.64   |
| 1   | I     | 99  | ASP  | CA-C-N | -6.72 | 112.85      | 119.64   |
| 1   | I     | 99  | ASP  | C-N-CA | -6.72 | 112.85      | 119.64   |
| 1   | B     | 99  | ASP  | CA-C-N | -6.71 | 112.86      | 119.64   |
| 1   | B     | 99  | ASP  | C-N-CA | -6.71 | 112.86      | 119.64   |
| 1   | E     | 99  | ASP  | CA-C-N | -6.71 | 112.86      | 119.64   |
| 1   | E     | 99  | ASP  | C-N-CA | -6.71 | 112.86      | 119.64   |
| 1   | G     | 387 | GLY  | N-CA-C | -6.71 | 104.13      | 115.34   |
| 1   | E     | 387 | GLY  | N-CA-C | -6.71 | 104.14      | 115.34   |
| 1   | C     | 387 | GLY  | N-CA-C | -6.71 | 104.14      | 115.34   |
| 1   | K     | 99  | ASP  | CA-C-N | -6.71 | 112.87      | 119.64   |
| 1   | K     | 99  | ASP  | C-N-CA | -6.71 | 112.87      | 119.64   |
| 1   | H     | 387 | GLY  | N-CA-C | -6.70 | 104.14      | 115.34   |
| 1   | H     | 99  | ASP  | CA-C-N | -6.70 | 112.87      | 119.64   |
| 1   | H     | 99  | ASP  | C-N-CA | -6.70 | 112.87      | 119.64   |
| 1   | F     | 99  | ASP  | CA-C-N | -6.69 | 112.89      | 119.64   |
| 1   | F     | 99  | ASP  | C-N-CA | -6.69 | 112.89      | 119.64   |
| 1   | F     | 387 | GLY  | N-CA-C | -6.69 | 104.17      | 115.34   |
| 1   | A     | 387 | GLY  | N-CA-C | -6.68 | 104.18      | 115.34   |
| 1   | L     | 99  | ASP  | CA-C-N | -6.68 | 112.89      | 119.64   |
| 1   | L     | 99  | ASP  | C-N-CA | -6.68 | 112.89      | 119.64   |
| 1   | C     | 99  | ASP  | CA-C-N | -6.67 | 112.90      | 119.64   |
| 1   | C     | 99  | ASP  | C-N-CA | -6.67 | 112.90      | 119.64   |
| 1   | A     | 99  | ASP  | CA-C-N | -6.67 | 112.90      | 119.64   |
| 1   | A     | 99  | ASP  | C-N-CA | -6.67 | 112.90      | 119.64   |
| 1   | B     | 387 | GLY  | N-CA-C | -6.67 | 104.20      | 115.34   |
| 1   | D     | 99  | ASP  | CA-C-N | -6.66 | 112.91      | 119.64   |
| 1   | D     | 99  | ASP  | C-N-CA | -6.66 | 112.91      | 119.64   |
| 1   | G     | 204 | GLU  | N-CA-C | -6.66 | 100.17      | 110.10   |
| 1   | E     | 204 | GLU  | N-CA-C | -6.65 | 100.19      | 110.10   |
| 1   | B     | 204 | GLU  | N-CA-C | -6.64 | 100.20      | 110.10   |
| 1   | D     | 204 | GLU  | N-CA-C | -6.64 | 100.21      | 110.10   |
| 1   | F     | 204 | GLU  | N-CA-C | -6.63 | 100.21      | 110.10   |
| 1   | K     | 204 | GLU  | N-CA-C | -6.63 | 100.22      | 110.10   |
| 1   | H     | 204 | GLU  | N-CA-C | -6.62 | 100.23      | 110.10   |
| 1   | C     | 204 | GLU  | N-CA-C | -6.62 | 100.24      | 110.10   |
| 1   | I     | 204 | GLU  | N-CA-C | -6.62 | 100.24      | 110.10   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | J     | 204 | GLU  | N-CA-C | -6.62 | 100.24      | 110.10   |
| 1   | L     | 204 | GLU  | N-CA-C | -6.62 | 100.24      | 110.10   |
| 1   | A     | 204 | GLU  | N-CA-C | -6.61 | 100.25      | 110.10   |
| 1   | H     | 358 | LEU  | N-CA-C | -6.59 | 98.23       | 109.24   |
| 1   | B     | 358 | LEU  | N-CA-C | -6.58 | 98.25       | 109.24   |
| 1   | C     | 358 | LEU  | N-CA-C | -6.57 | 98.27       | 109.24   |
| 1   | G     | 358 | LEU  | N-CA-C | -6.56 | 98.28       | 109.24   |
| 1   | D     | 358 | LEU  | N-CA-C | -6.56 | 98.29       | 109.24   |
| 1   | L     | 358 | LEU  | N-CA-C | -6.56 | 98.28       | 109.24   |
| 1   | E     | 358 | LEU  | N-CA-C | -6.55 | 98.30       | 109.24   |
| 1   | F     | 358 | LEU  | N-CA-C | -6.55 | 98.30       | 109.24   |
| 1   | K     | 358 | LEU  | N-CA-C | -6.55 | 98.31       | 109.24   |
| 1   | I     | 358 | LEU  | N-CA-C | -6.55 | 98.31       | 109.24   |
| 1   | A     | 358 | LEU  | N-CA-C | -6.54 | 98.31       | 109.24   |
| 1   | J     | 358 | LEU  | N-CA-C | -6.54 | 98.31       | 109.24   |
| 1   | L     | 56  | THR  | CA-C-N | -6.48 | 113.61      | 120.03   |
| 1   | L     | 56  | THR  | C-N-CA | -6.48 | 113.61      | 120.03   |
| 1   | A     | 56  | THR  | CA-C-N | -6.47 | 113.62      | 120.03   |
| 1   | A     | 56  | THR  | C-N-CA | -6.47 | 113.62      | 120.03   |
| 1   | G     | 56  | THR  | CA-C-N | -6.47 | 113.62      | 120.03   |
| 1   | G     | 56  | THR  | C-N-CA | -6.47 | 113.62      | 120.03   |
| 1   | B     | 56  | THR  | CA-C-N | -6.46 | 113.63      | 120.03   |
| 1   | B     | 56  | THR  | C-N-CA | -6.46 | 113.63      | 120.03   |
| 1   | D     | 56  | THR  | CA-C-N | -6.46 | 113.64      | 120.03   |
| 1   | D     | 56  | THR  | C-N-CA | -6.46 | 113.64      | 120.03   |
| 1   | C     | 56  | THR  | CA-C-N | -6.46 | 113.64      | 120.03   |
| 1   | C     | 56  | THR  | C-N-CA | -6.46 | 113.64      | 120.03   |
| 1   | J     | 56  | THR  | CA-C-N | -6.45 | 113.64      | 120.03   |
| 1   | J     | 56  | THR  | C-N-CA | -6.45 | 113.64      | 120.03   |
| 1   | K     | 56  | THR  | CA-C-N | -6.44 | 113.66      | 120.03   |
| 1   | K     | 56  | THR  | C-N-CA | -6.44 | 113.66      | 120.03   |
| 1   | H     | 56  | THR  | CA-C-N | -6.44 | 113.66      | 120.03   |
| 1   | H     | 56  | THR  | C-N-CA | -6.44 | 113.66      | 120.03   |
| 1   | I     | 56  | THR  | CA-C-N | -6.42 | 113.68      | 120.03   |
| 1   | I     | 56  | THR  | C-N-CA | -6.42 | 113.68      | 120.03   |
| 1   | E     | 56  | THR  | CA-C-N | -6.40 | 113.69      | 120.03   |
| 1   | E     | 56  | THR  | C-N-CA | -6.40 | 113.69      | 120.03   |
| 1   | F     | 56  | THR  | CA-C-N | -6.40 | 113.70      | 120.03   |
| 1   | F     | 56  | THR  | C-N-CA | -6.40 | 113.70      | 120.03   |
| 1   | B     | 10  | GLU  | N-CA-C | 6.30  | 118.72      | 108.08   |
| 1   | C     | 10  | GLU  | N-CA-C | 6.29  | 118.71      | 108.08   |
| 1   | I     | 10  | GLU  | N-CA-C | 6.29  | 118.71      | 108.08   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 10  | GLU  | N-CA-C | 6.28  | 118.69      | 108.08   |
| 1   | K     | 10  | GLU  | N-CA-C | 6.28  | 118.69      | 108.08   |
| 1   | F     | 10  | GLU  | N-CA-C | 6.27  | 118.68      | 108.08   |
| 1   | D     | 10  | GLU  | N-CA-C | 6.27  | 118.68      | 108.08   |
| 1   | G     | 10  | GLU  | N-CA-C | 6.27  | 118.68      | 108.08   |
| 1   | H     | 10  | GLU  | N-CA-C | 6.27  | 118.68      | 108.08   |
| 1   | J     | 10  | GLU  | N-CA-C | 6.27  | 118.68      | 108.08   |
| 1   | A     | 10  | GLU  | N-CA-C | 6.26  | 118.66      | 108.08   |
| 1   | L     | 10  | GLU  | N-CA-C | 6.26  | 118.65      | 108.08   |
| 1   | K     | 431 | GLU  | N-CA-C | -6.24 | 104.53      | 111.71   |
| 1   | A     | 431 | GLU  | N-CA-C | -6.23 | 104.55      | 111.71   |
| 1   | D     | 431 | GLU  | N-CA-C | -6.23 | 104.55      | 111.71   |
| 1   | G     | 431 | GLU  | N-CA-C | -6.22 | 104.55      | 111.71   |
| 1   | J     | 431 | GLU  | N-CA-C | -6.22 | 104.56      | 111.71   |
| 1   | E     | 431 | GLU  | N-CA-C | -6.21 | 104.56      | 111.71   |
| 1   | L     | 431 | GLU  | N-CA-C | -6.20 | 104.58      | 111.71   |
| 1   | B     | 431 | GLU  | N-CA-C | -6.20 | 104.58      | 111.71   |
| 1   | H     | 431 | GLU  | N-CA-C | -6.19 | 104.59      | 111.71   |
| 1   | C     | 431 | GLU  | N-CA-C | -6.19 | 104.60      | 111.71   |
| 1   | F     | 431 | GLU  | N-CA-C | -6.19 | 104.60      | 111.71   |
| 1   | B     | 44  | PRO  | N-CA-C | 6.18  | 122.03      | 111.03   |
| 1   | I     | 431 | GLU  | N-CA-C | -6.18 | 104.60      | 111.71   |
| 1   | I     | 44  | PRO  | N-CA-C | 6.17  | 122.01      | 111.03   |
| 1   | J     | 44  | PRO  | N-CA-C | 6.16  | 122.00      | 111.03   |
| 1   | H     | 44  | PRO  | N-CA-C | 6.16  | 122.00      | 111.03   |
| 1   | C     | 44  | PRO  | N-CA-C | 6.16  | 121.99      | 111.03   |
| 1   | D     | 44  | PRO  | N-CA-C | 6.15  | 121.98      | 111.03   |
| 1   | G     | 400 | LEU  | N-CA-C | -6.15 | 104.58      | 111.28   |
| 1   | L     | 44  | PRO  | N-CA-C | 6.15  | 121.97      | 111.03   |
| 1   | K     | 44  | PRO  | N-CA-C | 6.14  | 121.97      | 111.03   |
| 1   | E     | 44  | PRO  | N-CA-C | 6.14  | 121.96      | 111.03   |
| 1   | G     | 44  | PRO  | N-CA-C | 6.14  | 121.96      | 111.03   |
| 1   | F     | 44  | PRO  | N-CA-C | 6.13  | 121.95      | 111.03   |
| 1   | A     | 44  | PRO  | N-CA-C | 6.13  | 121.94      | 111.03   |
| 1   | H     | 400 | LEU  | N-CA-C | -6.11 | 104.62      | 111.28   |
| 1   | I     | 400 | LEU  | N-CA-C | -6.10 | 104.63      | 111.28   |
| 1   | F     | 400 | LEU  | N-CA-C | -6.10 | 104.63      | 111.28   |
| 1   | E     | 400 | LEU  | N-CA-C | -6.10 | 104.63      | 111.28   |
| 1   | K     | 400 | LEU  | N-CA-C | -6.10 | 104.63      | 111.28   |
| 1   | B     | 400 | LEU  | N-CA-C | -6.09 | 104.64      | 111.28   |
| 1   | L     | 400 | LEU  | N-CA-C | -6.08 | 104.65      | 111.28   |
| 1   | C     | 400 | LEU  | N-CA-C | -6.08 | 104.65      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 400 | LEU  | N-CA-C | -6.08 | 104.65      | 111.28   |
| 1   | J     | 400 | LEU  | N-CA-C | -6.08 | 104.65      | 111.28   |
| 1   | F     | 37  | TYR  | N-CA-C | 6.07  | 117.98      | 111.36   |
| 1   | A     | 400 | LEU  | N-CA-C | -6.06 | 104.68      | 111.28   |
| 1   | B     | 37  | TYR  | N-CA-C | 6.04  | 117.95      | 111.36   |
| 1   | H     | 37  | TYR  | N-CA-C | 6.04  | 117.95      | 111.36   |
| 1   | C     | 37  | TYR  | N-CA-C | 6.04  | 117.94      | 111.36   |
| 1   | G     | 37  | TYR  | N-CA-C | 6.03  | 117.94      | 111.36   |
| 1   | K     | 37  | TYR  | N-CA-C | 6.03  | 117.94      | 111.36   |
| 1   | E     | 37  | TYR  | N-CA-C | 6.02  | 117.92      | 111.36   |
| 1   | A     | 37  | TYR  | N-CA-C | 6.02  | 117.92      | 111.36   |
| 1   | I     | 37  | TYR  | N-CA-C | 6.01  | 117.92      | 111.36   |
| 1   | J     | 37  | TYR  | N-CA-C | 6.01  | 117.91      | 111.36   |
| 1   | F     | 373 | GLU  | N-CA-C | -5.99 | 104.55      | 112.34   |
| 1   | D     | 37  | TYR  | N-CA-C | 5.99  | 117.89      | 111.36   |
| 1   | I     | 373 | GLU  | N-CA-C | -5.99 | 104.55      | 112.34   |
| 1   | L     | 37  | TYR  | N-CA-C | 5.98  | 117.88      | 111.36   |
| 1   | K     | 373 | GLU  | N-CA-C | -5.98 | 104.56      | 112.34   |
| 1   | D     | 373 | GLU  | N-CA-C | -5.97 | 104.58      | 112.34   |
| 1   | C     | 373 | GLU  | N-CA-C | -5.96 | 104.59      | 112.34   |
| 1   | J     | 373 | GLU  | N-CA-C | -5.96 | 104.59      | 112.34   |
| 1   | A     | 373 | GLU  | N-CA-C | -5.96 | 104.60      | 112.34   |
| 1   | G     | 373 | GLU  | N-CA-C | -5.95 | 104.60      | 112.34   |
| 1   | B     | 373 | GLU  | N-CA-C | -5.95 | 104.61      | 112.34   |
| 1   | H     | 373 | GLU  | N-CA-C | -5.95 | 104.60      | 112.34   |
| 1   | L     | 373 | GLU  | N-CA-C | -5.95 | 104.61      | 112.34   |
| 1   | E     | 373 | GLU  | N-CA-C | -5.94 | 104.62      | 112.34   |
| 1   | C     | 102 | GLY  | N-CA-C | -5.67 | 105.92      | 112.73   |
| 1   | L     | 102 | GLY  | N-CA-C | -5.63 | 105.98      | 112.73   |
| 1   | J     | 102 | GLY  | N-CA-C | -5.62 | 105.98      | 112.73   |
| 1   | K     | 102 | GLY  | N-CA-C | -5.62 | 105.99      | 112.73   |
| 1   | A     | 102 | GLY  | N-CA-C | -5.61 | 105.99      | 112.73   |
| 1   | G     | 102 | GLY  | N-CA-C | -5.61 | 105.99      | 112.73   |
| 1   | I     | 102 | GLY  | N-CA-C | -5.61 | 105.99      | 112.73   |
| 1   | B     | 102 | GLY  | N-CA-C | -5.60 | 106.01      | 112.73   |
| 1   | H     | 102 | GLY  | N-CA-C | -5.60 | 106.01      | 112.73   |
| 1   | D     | 102 | GLY  | N-CA-C | -5.59 | 106.02      | 112.73   |
| 1   | F     | 102 | GLY  | N-CA-C | -5.57 | 106.04      | 112.73   |
| 1   | E     | 102 | GLY  | N-CA-C | -5.57 | 106.05      | 112.73   |
| 1   | A     | 326 | ASP  | N-CA-C | 5.46  | 117.23      | 111.28   |
| 1   | G     | 51  | SER  | N-CA-C | 5.46  | 119.43      | 112.34   |
| 1   | K     | 51  | SER  | N-CA-C | 5.44  | 119.41      | 112.34   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | I     | 326 | ASP  | N-CA-C | 5.44  | 117.21      | 111.28   |
| 1   | E     | 326 | ASP  | N-CA-C | 5.43  | 117.20      | 111.28   |
| 1   | F     | 326 | ASP  | N-CA-C | 5.43  | 117.20      | 111.28   |
| 1   | D     | 51  | SER  | N-CA-C | 5.43  | 119.40      | 112.34   |
| 1   | J     | 51  | SER  | N-CA-C | 5.43  | 119.39      | 112.34   |
| 1   | B     | 326 | ASP  | N-CA-C | 5.42  | 117.19      | 111.28   |
| 1   | C     | 326 | ASP  | N-CA-C | 5.42  | 117.19      | 111.28   |
| 1   | E     | 51  | SER  | N-CA-C | 5.42  | 119.39      | 112.34   |
| 1   | G     | 326 | ASP  | N-CA-C | 5.42  | 117.19      | 111.28   |
| 1   | J     | 326 | ASP  | N-CA-C | 5.42  | 117.19      | 111.28   |
| 1   | F     | 51  | SER  | N-CA-C | 5.41  | 119.38      | 112.34   |
| 1   | H     | 326 | ASP  | N-CA-C | 5.41  | 117.18      | 111.28   |
| 1   | D     | 326 | ASP  | N-CA-C | 5.41  | 117.17      | 111.28   |
| 1   | L     | 326 | ASP  | N-CA-C | 5.41  | 117.17      | 111.28   |
| 1   | B     | 51  | SER  | N-CA-C | 5.40  | 119.37      | 112.34   |
| 1   | C     | 51  | SER  | N-CA-C | 5.40  | 119.36      | 112.34   |
| 1   | A     | 51  | SER  | N-CA-C | 5.39  | 119.35      | 112.34   |
| 1   | H     | 51  | SER  | N-CA-C | 5.39  | 119.35      | 112.34   |
| 1   | L     | 51  | SER  | N-CA-C | 5.39  | 119.35      | 112.34   |
| 1   | I     | 51  | SER  | N-CA-C | 5.38  | 119.33      | 112.34   |
| 1   | K     | 326 | ASP  | N-CA-C | 5.38  | 117.14      | 111.28   |
| 1   | J     | 34  | CYS  | N-CA-C | -5.37 | 105.42      | 111.28   |
| 1   | H     | 34  | CYS  | N-CA-C | -5.37 | 105.43      | 111.28   |
| 1   | G     | 34  | CYS  | N-CA-C | -5.36 | 105.43      | 111.28   |
| 1   | C     | 34  | CYS  | N-CA-C | -5.36 | 105.44      | 111.28   |
| 1   | B     | 34  | CYS  | N-CA-C | -5.35 | 105.45      | 111.28   |
| 1   | K     | 34  | CYS  | N-CA-C | -5.35 | 105.45      | 111.28   |
| 1   | A     | 34  | CYS  | N-CA-C | -5.35 | 105.45      | 111.28   |
| 1   | I     | 34  | CYS  | N-CA-C | -5.35 | 105.45      | 111.28   |
| 1   | L     | 34  | CYS  | N-CA-C | -5.33 | 105.47      | 111.28   |
| 1   | E     | 388 | VAL  | CA-C-N | -5.33 | 113.14      | 120.28   |
| 1   | E     | 388 | VAL  | C-N-CA | -5.33 | 113.14      | 120.28   |
| 1   | K     | 388 | VAL  | CA-C-N | -5.33 | 113.14      | 120.28   |
| 1   | K     | 388 | VAL  | C-N-CA | -5.33 | 113.14      | 120.28   |
| 1   | A     | 388 | VAL  | CA-C-N | -5.32 | 113.15      | 120.28   |
| 1   | A     | 388 | VAL  | C-N-CA | -5.32 | 113.15      | 120.28   |
| 1   | F     | 34  | CYS  | N-CA-C | -5.32 | 105.48      | 111.28   |
| 1   | E     | 34  | CYS  | N-CA-C | -5.31 | 105.49      | 111.28   |
| 1   | C     | 388 | VAL  | CA-C-N | -5.31 | 113.16      | 120.28   |
| 1   | C     | 388 | VAL  | C-N-CA | -5.31 | 113.16      | 120.28   |
| 1   | H     | 388 | VAL  | CA-C-N | -5.29 | 113.19      | 120.28   |
| 1   | H     | 388 | VAL  | C-N-CA | -5.29 | 113.19      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 388 | VAL  | CA-C-N | -5.29 | 113.19      | 120.28   |
| 1   | D     | 388 | VAL  | C-N-CA | -5.29 | 113.19      | 120.28   |
| 1   | J     | 388 | VAL  | CA-C-N | -5.29 | 113.19      | 120.28   |
| 1   | J     | 388 | VAL  | C-N-CA | -5.29 | 113.19      | 120.28   |
| 1   | L     | 388 | VAL  | CA-C-N | -5.29 | 113.20      | 120.28   |
| 1   | L     | 388 | VAL  | C-N-CA | -5.29 | 113.20      | 120.28   |
| 1   | D     | 34  | CYS  | N-CA-C | -5.28 | 105.53      | 111.28   |
| 1   | F     | 388 | VAL  | CA-C-N | -5.27 | 113.22      | 120.28   |
| 1   | F     | 388 | VAL  | C-N-CA | -5.27 | 113.22      | 120.28   |
| 1   | G     | 388 | VAL  | CA-C-N | -5.26 | 113.23      | 120.28   |
| 1   | G     | 388 | VAL  | C-N-CA | -5.26 | 113.23      | 120.28   |
| 1   | B     | 388 | VAL  | CA-C-N | -5.26 | 113.23      | 120.28   |
| 1   | B     | 388 | VAL  | C-N-CA | -5.26 | 113.23      | 120.28   |
| 1   | I     | 388 | VAL  | CA-C-N | -5.25 | 113.24      | 120.28   |
| 1   | I     | 388 | VAL  | C-N-CA | -5.25 | 113.24      | 120.28   |
| 1   | B     | 319 | PHE  | N-CA-C | 5.24  | 117.64      | 108.52   |
| 1   | E     | 319 | PHE  | N-CA-C | 5.24  | 117.64      | 108.52   |
| 1   | A     | 319 | PHE  | N-CA-C | 5.24  | 117.64      | 108.52   |
| 1   | H     | 319 | PHE  | N-CA-C | 5.23  | 117.63      | 108.52   |
| 1   | L     | 319 | PHE  | N-CA-C | 5.23  | 117.62      | 108.52   |
| 1   | J     | 319 | PHE  | N-CA-C | 5.23  | 117.62      | 108.52   |
| 1   | G     | 319 | PHE  | N-CA-C | 5.22  | 117.61      | 108.52   |
| 1   | D     | 319 | PHE  | N-CA-C | 5.22  | 117.60      | 108.52   |
| 1   | F     | 319 | PHE  | N-CA-C | 5.22  | 117.60      | 108.52   |
| 1   | C     | 319 | PHE  | N-CA-C | 5.21  | 117.59      | 108.52   |
| 1   | I     | 319 | PHE  | N-CA-C | 5.21  | 117.59      | 108.52   |
| 1   | D     | 81  | GLN  | N-CA-C | 5.21  | 116.64      | 111.07   |
| 1   | K     | 319 | PHE  | N-CA-C | 5.21  | 117.58      | 108.52   |
| 1   | F     | 120 | TYR  | N-CA-C | -5.18 | 105.75      | 111.71   |
| 1   | B     | 120 | TYR  | N-CA-C | -5.18 | 105.75      | 111.71   |
| 1   | H     | 120 | TYR  | N-CA-C | -5.18 | 105.75      | 111.71   |
| 1   | G     | 89  | SER  | N-CA-C | 5.18  | 116.94      | 109.07   |
| 1   | K     | 120 | TYR  | N-CA-C | -5.18 | 105.76      | 111.71   |
| 1   | A     | 120 | TYR  | N-CA-C | -5.17 | 105.76      | 111.71   |
| 1   | L     | 81  | GLN  | N-CA-C | 5.17  | 116.60      | 111.07   |
| 1   | D     | 89  | SER  | N-CA-C | 5.17  | 116.92      | 109.07   |
| 1   | B     | 81  | GLN  | N-CA-C | 5.16  | 116.59      | 111.07   |
| 1   | F     | 81  | GLN  | N-CA-C | 5.16  | 116.59      | 111.07   |
| 1   | A     | 81  | GLN  | N-CA-C | 5.16  | 116.59      | 111.07   |
| 1   | A     | 89  | SER  | N-CA-C | 5.16  | 116.92      | 109.07   |
| 1   | C     | 120 | TYR  | N-CA-C | -5.16 | 105.78      | 111.71   |
| 1   | E     | 81  | GLN  | N-CA-C | 5.16  | 116.59      | 111.07   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 89  | SER  | N-CA-C | 5.16  | 116.92      | 109.07   |
| 1   | I     | 120 | TYR  | N-CA-C | -5.16 | 105.78      | 111.71   |
| 1   | L     | 120 | TYR  | N-CA-C | -5.16 | 105.78      | 111.71   |
| 1   | C     | 81  | GLN  | N-CA-C | 5.16  | 116.59      | 111.07   |
| 1   | E     | 120 | TYR  | N-CA-C | -5.16 | 105.78      | 111.71   |
| 1   | L     | 89  | SER  | N-CA-C | 5.16  | 116.91      | 109.07   |
| 1   | I     | 89  | SER  | N-CA-C | 5.15  | 116.90      | 109.07   |
| 1   | J     | 89  | SER  | N-CA-C | 5.15  | 116.90      | 109.07   |
| 1   | K     | 81  | GLN  | N-CA-C | 5.15  | 116.58      | 111.07   |
| 1   | K     | 89  | SER  | N-CA-C | 5.15  | 116.89      | 109.07   |
| 1   | G     | 120 | TYR  | N-CA-C | -5.14 | 105.79      | 111.71   |
| 1   | H     | 81  | GLN  | N-CA-C | 5.14  | 116.58      | 111.07   |
| 1   | H     | 89  | SER  | N-CA-C | 5.14  | 116.89      | 109.07   |
| 1   | D     | 120 | TYR  | N-CA-C | -5.14 | 105.80      | 111.71   |
| 1   | C     | 89  | SER  | N-CA-C | 5.14  | 116.88      | 109.07   |
| 1   | J     | 120 | TYR  | N-CA-C | -5.14 | 105.80      | 111.71   |
| 1   | J     | 81  | GLN  | N-CA-C | 5.13  | 116.56      | 111.07   |
| 1   | J     | 389 | TYR  | N-CA-C | -5.13 | 105.69      | 111.28   |
| 1   | G     | 81  | GLN  | N-CA-C | 5.13  | 116.56      | 111.07   |
| 1   | D     | 389 | TYR  | N-CA-C | -5.13 | 105.69      | 111.28   |
| 1   | I     | 81  | GLN  | N-CA-C | 5.13  | 116.56      | 111.07   |
| 1   | E     | 89  | SER  | N-CA-C | 5.12  | 116.86      | 109.07   |
| 1   | B     | 89  | SER  | N-CA-C | 5.12  | 116.86      | 109.07   |
| 1   | I     | 389 | TYR  | N-CA-C | -5.12 | 105.70      | 111.28   |
| 1   | B     | 389 | TYR  | N-CA-C | -5.12 | 105.70      | 111.28   |
| 1   | L     | 389 | TYR  | N-CA-C | -5.10 | 105.72      | 111.28   |
| 1   | F     | 389 | TYR  | N-CA-C | -5.10 | 105.72      | 111.28   |
| 1   | C     | 389 | TYR  | N-CA-C | -5.10 | 105.72      | 111.28   |
| 1   | H     | 389 | TYR  | N-CA-C | -5.10 | 105.72      | 111.28   |
| 1   | G     | 389 | TYR  | N-CA-C | -5.09 | 105.73      | 111.28   |
| 1   | A     | 389 | TYR  | N-CA-C | -5.08 | 105.74      | 111.28   |
| 1   | J     | 336 | ALA  | N-CA-C | -5.08 | 105.74      | 111.28   |
| 1   | K     | 389 | TYR  | N-CA-C | -5.08 | 105.75      | 111.28   |
| 1   | A     | 383 | ASP  | N-CA-C | 5.07  | 116.50      | 111.07   |
| 1   | J     | 383 | ASP  | N-CA-C | 5.07  | 116.50      | 111.07   |
| 1   | I     | 383 | ASP  | N-CA-C | 5.07  | 116.50      | 111.07   |
| 1   | F     | 383 | ASP  | N-CA-C | 5.07  | 116.49      | 111.07   |
| 1   | I     | 80  | MET  | N-CA-C | 5.06  | 116.49      | 111.07   |
| 1   | G     | 383 | ASP  | N-CA-C | 5.06  | 116.48      | 111.07   |
| 1   | H     | 383 | ASP  | N-CA-C | 5.06  | 116.48      | 111.07   |
| 1   | E     | 389 | TYR  | N-CA-C | -5.05 | 105.77      | 111.28   |
| 1   | A     | 336 | ALA  | N-CA-C | -5.05 | 105.78      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | H     | 205 | LYS  | N-CA-C | 5.05  | 117.35      | 109.52   |
| 1   | D     | 336 | ALA  | N-CA-C | -5.05 | 105.78      | 111.28   |
| 1   | E     | 383 | ASP  | N-CA-C | 5.05  | 116.47      | 111.07   |
| 1   | F     | 80  | MET  | N-CA-C | 5.05  | 116.47      | 111.07   |
| 1   | D     | 80  | MET  | N-CA-C | 5.04  | 116.47      | 111.07   |
| 1   | J     | 80  | MET  | N-CA-C | 5.04  | 116.47      | 111.07   |
| 1   | K     | 383 | ASP  | N-CA-C | 5.04  | 116.47      | 111.07   |
| 1   | C     | 383 | ASP  | N-CA-C | 5.04  | 116.47      | 111.07   |
| 1   | C     | 80  | MET  | N-CA-C | 5.04  | 116.46      | 111.07   |
| 1   | D     | 205 | LYS  | N-CA-C | 5.04  | 117.33      | 109.52   |
| 1   | L     | 383 | ASP  | N-CA-C | 5.04  | 116.46      | 111.07   |
| 1   | K     | 205 | LYS  | N-CA-C | 5.03  | 117.32      | 109.52   |
| 1   | A     | 80  | MET  | N-CA-C | 5.03  | 116.45      | 111.07   |
| 1   | G     | 80  | MET  | N-CA-C | 5.03  | 116.45      | 111.07   |
| 1   | B     | 284 | GLU  | N-CA-C | -5.03 | 105.80      | 111.28   |
| 1   | G     | 205 | LYS  | N-CA-C | 5.03  | 117.31      | 109.52   |
| 1   | H     | 80  | MET  | N-CA-C | 5.02  | 116.45      | 111.07   |
| 1   | K     | 80  | MET  | N-CA-C | 5.02  | 116.44      | 111.07   |
| 1   | B     | 80  | MET  | N-CA-C | 5.02  | 116.44      | 111.07   |
| 1   | B     | 383 | ASP  | N-CA-C | 5.02  | 116.44      | 111.07   |
| 1   | B     | 205 | LYS  | N-CA-C | 5.02  | 117.29      | 109.52   |
| 1   | I     | 284 | GLU  | N-CA-C | -5.02 | 105.81      | 111.28   |
| 1   | A     | 284 | GLU  | N-CA-C | -5.01 | 105.81      | 111.28   |
| 1   | C     | 336 | ALA  | N-CA-C | -5.01 | 105.82      | 111.28   |
| 1   | B     | 336 | ALA  | N-CA-C | -5.01 | 105.82      | 111.28   |
| 1   | A     | 205 | LYS  | N-CA-C | 5.01  | 117.28      | 109.52   |
| 1   | F     | 336 | ALA  | N-CA-C | -5.01 | 105.82      | 111.28   |
| 1   | E     | 80  | MET  | N-CA-C | 5.00  | 116.42      | 111.07   |
| 1   | L     | 205 | LYS  | N-CA-C | 5.00  | 117.28      | 109.52   |

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     | 3669  | 0        | 3672     | 219     | 0            |
| 1   | B     | 3669  | 0        | 3672     | 221     | 0            |
| 1   | C     | 3669  | 0        | 3672     | 217     | 0            |
| 1   | D     | 3669  | 0        | 3672     | 223     | 0            |
| 1   | E     | 3669  | 0        | 3672     | 221     | 0            |
| 1   | F     | 3669  | 0        | 3672     | 221     | 0            |
| 1   | G     | 3669  | 0        | 3672     | 220     | 0            |
| 1   | H     | 3669  | 0        | 3672     | 219     | 0            |
| 1   | I     | 3669  | 0        | 3672     | 224     | 0            |
| 1   | J     | 3669  | 0        | 3672     | 223     | 0            |
| 1   | K     | 3669  | 0        | 3672     | 215     | 0            |
| 1   | L     | 3669  | 0        | 3672     | 216     | 0            |
| All | All   | 44028 | 0        | 44064    | 1829    | 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 21.

All (1829) 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:F:131:PHE:HE2 | 1:G:387:GLY:HA3 | 1.12                     | 1.14              |
| 1:D:126:TYR:CG  | 1:D:158:MET:SD  | 2.42                     | 1.13              |
| 1:E:126:TYR:CG  | 1:E:158:MET:SD  | 2.42                     | 1.13              |
| 1:G:126:TYR:CG  | 1:G:158:MET:SD  | 2.42                     | 1.13              |
| 1:H:126:TYR:CG  | 1:H:158:MET:SD  | 2.42                     | 1.13              |
| 1:J:126:TYR:CG  | 1:J:158:MET:SD  | 2.42                     | 1.13              |
| 1:B:126:TYR:CG  | 1:B:158:MET:SD  | 2.42                     | 1.13              |
| 1:I:126:TYR:CG  | 1:I:158:MET:SD  | 2.42                     | 1.13              |
| 1:A:126:TYR:CG  | 1:A:158:MET:SD  | 2.42                     | 1.13              |
| 1:C:126:TYR:CG  | 1:C:158:MET:SD  | 2.42                     | 1.13              |
| 1:F:126:TYR:CG  | 1:F:158:MET:SD  | 2.42                     | 1.13              |
| 1:L:126:TYR:CD1 | 1:L:158:MET:SD  | 2.42                     | 1.13              |
| 1:C:126:TYR:CD1 | 1:C:158:MET:SD  | 2.42                     | 1.12              |
| 1:I:126:TYR:CD1 | 1:I:158:MET:SD  | 2.42                     | 1.12              |
| 1:K:126:TYR:CG  | 1:K:158:MET:SD  | 2.42                     | 1.12              |
| 1:H:126:TYR:CD1 | 1:H:158:MET:SD  | 2.42                     | 1.12              |
| 1:J:126:TYR:CD1 | 1:J:158:MET:SD  | 2.42                     | 1.12              |
| 1:K:126:TYR:CD1 | 1:K:158:MET:SD  | 2.42                     | 1.12              |
| 1:A:126:TYR:CD1 | 1:A:158:MET:SD  | 2.42                     | 1.12              |
| 1:D:126:TYR:CD1 | 1:D:158:MET:SD  | 2.42                     | 1.12              |
| 1:E:126:TYR:CD1 | 1:E:158:MET:SD  | 2.42                     | 1.12              |
| 1:G:126:TYR:CD1 | 1:G:158:MET:SD  | 2.42                     | 1.12              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:126:TYR:CD1 | 1:B:158:MET:SD  | 2.42                     | 1.11              |
| 1:L:126:TYR:CG  | 1:L:158:MET:SD  | 2.42                     | 1.11              |
| 1:F:126:TYR:CD1 | 1:F:158:MET:SD  | 2.43                     | 1.11              |
| 1:B:131:PHE:HE2 | 1:C:387:GLY:HA3 | 1.12                     | 1.09              |
| 1:D:131:PHE:HE2 | 1:E:387:GLY:HA3 | 1.16                     | 1.09              |
| 1:H:131:PHE:HE2 | 1:I:387:GLY:HA3 | 1.13                     | 1.08              |
| 1:J:131:PHE:HE2 | 1:K:387:GLY:HA3 | 1.15                     | 1.07              |
| 1:A:387:GLY:HA3 | 1:L:131:PHE:HE2 | 1.16                     | 1.05              |
| 1:K:131:PHE:HE2 | 1:L:387:GLY:HA3 | 1.21                     | 1.03              |
| 1:C:131:PHE:HE2 | 1:D:387:GLY:HA3 | 1.23                     | 1.03              |
| 1:B:131:PHE:CE2 | 1:C:387:GLY:HA3 | 1.94                     | 1.02              |
| 1:A:291:MET:HG2 | 1:B:282:LEU:CD1 | 1.90                     | 1.02              |
| 1:G:131:PHE:HE2 | 1:H:387:GLY:HA3 | 1.25                     | 1.02              |
| 1:C:291:MET:HG2 | 1:D:282:LEU:CD1 | 1.90                     | 1.01              |
| 1:H:131:PHE:CE2 | 1:I:387:GLY:HA3 | 1.95                     | 1.01              |
| 1:I:291:MET:HG2 | 1:J:282:LEU:CD1 | 1.91                     | 1.01              |
| 1:E:131:PHE:HE2 | 1:F:387:GLY:HA3 | 1.23                     | 1.00              |
| 1:F:131:PHE:CE2 | 1:G:387:GLY:HA3 | 1.94                     | 1.00              |
| 1:J:131:PHE:CE2 | 1:K:387:GLY:HA3 | 1.96                     | 1.00              |
| 1:A:131:PHE:HE2 | 1:B:387:GLY:HA3 | 1.24                     | 1.00              |
| 1:A:387:GLY:HA3 | 1:L:131:PHE:CE2 | 1.97                     | 1.00              |
| 1:G:291:MET:HG2 | 1:H:282:LEU:CD1 | 1.90                     | 1.00              |
| 1:E:291:MET:HG2 | 1:F:282:LEU:CD1 | 1.92                     | 0.99              |
| 1:K:291:MET:HG2 | 1:L:282:LEU:CD1 | 1.91                     | 0.99              |
| 1:I:80:MET:HE1  | 1:J:431:GLU:CD  | 1.86                     | 0.99              |
| 1:C:80:MET:HE1  | 1:D:431:GLU:CD  | 1.88                     | 0.98              |
| 1:I:131:PHE:HE2 | 1:J:387:GLY:HA3 | 1.23                     | 0.98              |
| 1:F:413:GLN:HB2 | 1:G:93:ALA:CB   | 1.94                     | 0.98              |
| 1:D:131:PHE:CE2 | 1:E:387:GLY:HA3 | 1.97                     | 0.98              |
| 1:D:291:MET:HG2 | 1:E:282:LEU:CD1 | 1.94                     | 0.98              |
| 1:J:291:MET:HG2 | 1:K:282:LEU:CD1 | 1.92                     | 0.98              |
| 1:B:413:GLN:HB2 | 1:C:93:ALA:CB   | 1.95                     | 0.97              |
| 1:G:80:MET:HE1  | 1:H:431:GLU:CD  | 1.89                     | 0.97              |
| 1:B:413:GLN:HB2 | 1:C:93:ALA:HB3  | 1.43                     | 0.97              |
| 1:F:413:GLN:HB2 | 1:G:93:ALA:HB3  | 1.43                     | 0.97              |
| 1:I:439:LEU:HB2 | 1:J:473:ALA:CB  | 1.95                     | 0.97              |
| 1:A:80:MET:HE1  | 1:B:431:GLU:CD  | 1.90                     | 0.96              |
| 1:H:413:GLN:HB2 | 1:I:93:ALA:HB3  | 1.44                     | 0.96              |
| 1:F:291:MET:HG2 | 1:G:282:LEU:CD1 | 1.94                     | 0.96              |
| 1:J:413:GLN:HB2 | 1:K:93:ALA:HB3  | 1.47                     | 0.96              |
| 1:B:291:MET:HG2 | 1:C:282:LEU:CD1 | 1.96                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:80:MET:HE1   | 1:F:431:GLU:CD   | 1.90                     | 0.96              |
| 1:H:291:MET:HG2  | 1:I:282:LEU:CD1  | 1.95                     | 0.95              |
| 1:H:413:GLN:HB2  | 1:I:93:ALA:CB    | 1.96                     | 0.95              |
| 1:A:282:LEU:CD1  | 1:L:291:MET:HG2  | 1.95                     | 0.95              |
| 1:A:93:ALA:HB3   | 1:L:413:GLN:HB2  | 1.47                     | 0.95              |
| 1:K:291:MET:HG2  | 1:L:282:LEU:HD11 | 1.49                     | 0.95              |
| 1:K:131:PHE:CE2  | 1:L:387:GLY:HA3  | 2.02                     | 0.95              |
| 1:K:80:MET:HE1   | 1:L:431:GLU:CD   | 1.91                     | 0.94              |
| 1:I:291:MET:HG2  | 1:J:282:LEU:HD11 | 1.50                     | 0.94              |
| 1:J:413:GLN:HB2  | 1:K:93:ALA:CB    | 1.96                     | 0.94              |
| 1:D:413:GLN:HB2  | 1:E:93:ALA:HB3   | 1.48                     | 0.94              |
| 1:I:131:PHE:CE2  | 1:J:387:GLY:HA3  | 2.04                     | 0.93              |
| 1:I:439:LEU:HB2  | 1:J:473:ALA:HB1  | 1.50                     | 0.93              |
| 1:A:291:MET:HG2  | 1:B:282:LEU:HD11 | 1.49                     | 0.93              |
| 1:D:80:MET:HE1   | 1:E:431:GLU:CD   | 1.94                     | 0.93              |
| 1:G:291:MET:HG2  | 1:H:282:LEU:HD11 | 1.50                     | 0.93              |
| 1:D:413:GLN:HB2  | 1:E:93:ALA:CB    | 1.99                     | 0.93              |
| 1:E:131:PHE:CE2  | 1:F:387:GLY:HA3  | 2.03                     | 0.92              |
| 1:H:80:MET:HE1   | 1:I:431:GLU:CD   | 1.94                     | 0.92              |
| 1:A:93:ALA:CB    | 1:L:413:GLN:HB2  | 1.99                     | 0.92              |
| 1:A:431:GLU:CD   | 1:L:80:MET:HE1   | 1.93                     | 0.92              |
| 1:G:439:LEU:HB2  | 1:H:473:ALA:CB   | 2.00                     | 0.92              |
| 1:D:439:LEU:HB2  | 1:E:473:ALA:CB   | 1.99                     | 0.92              |
| 1:F:291:MET:HG2  | 1:G:282:LEU:HD11 | 1.51                     | 0.92              |
| 1:A:131:PHE:CE2  | 1:B:387:GLY:HA3  | 2.05                     | 0.91              |
| 1:C:323:ARG:HG3  | 1:D:301:ASN:ND2  | 1.86                     | 0.91              |
| 1:A:473:ALA:CB   | 1:L:439:LEU:HB2  | 1.99                     | 0.91              |
| 1:C:131:PHE:CE2  | 1:D:387:GLY:HA3  | 2.04                     | 0.91              |
| 1:B:80:MET:HE1   | 1:C:431:GLU:CD   | 1.94                     | 0.91              |
| 1:J:323:ARG:HG3  | 1:K:301:ASN:ND2  | 1.86                     | 0.91              |
| 1:C:439:LEU:HB2  | 1:D:473:ALA:CB   | 1.98                     | 0.91              |
| 1:C:291:MET:HG2  | 1:D:282:LEU:HD11 | 1.48                     | 0.91              |
| 1:E:439:LEU:HB2  | 1:F:473:ALA:CB   | 1.99                     | 0.91              |
| 1:G:131:PHE:CE2  | 1:H:387:GLY:HA3  | 2.06                     | 0.91              |
| 1:G:323:ARG:HG3  | 1:H:301:ASN:ND2  | 1.86                     | 0.90              |
| 1:E:291:MET:HG2  | 1:F:282:LEU:HD11 | 1.50                     | 0.90              |
| 1:J:291:MET:HG2  | 1:K:282:LEU:HD11 | 1.50                     | 0.90              |
| 1:A:282:LEU:HD11 | 1:L:291:MET:HG2  | 1.52                     | 0.90              |
| 1:C:439:LEU:HB2  | 1:D:473:ALA:HB1  | 1.53                     | 0.90              |
| 1:A:323:ARG:HG3  | 1:B:301:ASN:ND2  | 1.86                     | 0.90              |
| 1:H:439:LEU:HB2  | 1:I:473:ALA:HB1  | 1.54                     | 0.89              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:439:LEU:HB2 | 1:E:473:ALA:HB1  | 1.51                     | 0.89              |
| 1:J:439:LEU:HB2 | 1:K:473:ALA:CB   | 2.02                     | 0.89              |
| 1:A:439:LEU:HB2 | 1:B:473:ALA:CB   | 2.01                     | 0.89              |
| 1:D:291:MET:HG2 | 1:E:282:LEU:HD11 | 1.52                     | 0.89              |
| 1:F:323:ARG:HG3 | 1:G:301:ASN:ND2  | 1.86                     | 0.89              |
| 1:K:439:LEU:HB2 | 1:L:473:ALA:CB   | 2.03                     | 0.89              |
| 1:A:473:ALA:HB1 | 1:L:439:LEU:HB2  | 1.51                     | 0.89              |
| 1:J:80:MET:HE1  | 1:K:431:GLU:CD   | 1.96                     | 0.89              |
| 1:H:439:LEU:HB2 | 1:I:473:ALA:CB   | 2.03                     | 0.89              |
| 1:I:323:ARG:HG3 | 1:J:301:ASN:ND2  | 1.87                     | 0.89              |
| 1:K:323:ARG:HG3 | 1:L:301:ASN:ND2  | 1.87                     | 0.89              |
| 1:F:80:MET:HE1  | 1:G:431:GLU:CD   | 1.96                     | 0.89              |
| 1:E:413:GLN:HB2 | 1:F:93:ALA:HB3   | 1.55                     | 0.88              |
| 1:H:291:MET:HG2 | 1:I:282:LEU:HD11 | 1.52                     | 0.88              |
| 1:D:323:ARG:HG3 | 1:E:301:ASN:ND2  | 1.87                     | 0.88              |
| 1:B:323:ARG:HG3 | 1:C:301:ASN:ND2  | 1.88                     | 0.88              |
| 1:J:439:LEU:HB2 | 1:K:473:ALA:HB1  | 1.55                     | 0.88              |
| 1:A:301:ASN:ND2 | 1:L:323:ARG:HG3  | 1.89                     | 0.88              |
| 1:B:439:LEU:HB2 | 1:C:473:ALA:HB1  | 1.54                     | 0.87              |
| 1:K:413:GLN:HB2 | 1:L:93:ALA:HB3   | 1.54                     | 0.87              |
| 1:B:439:LEU:HB2 | 1:C:473:ALA:CB   | 2.04                     | 0.87              |
| 1:G:439:LEU:HB2 | 1:H:473:ALA:HB1  | 1.55                     | 0.87              |
| 1:E:439:LEU:HB2 | 1:F:473:ALA:HB1  | 1.54                     | 0.87              |
| 1:F:439:LEU:HB2 | 1:G:473:ALA:CB   | 2.05                     | 0.87              |
| 1:E:323:ARG:HG3 | 1:F:301:ASN:ND2  | 1.90                     | 0.87              |
| 1:B:291:MET:HG2 | 1:C:282:LEU:HD11 | 1.53                     | 0.87              |
| 1:H:323:ARG:HG3 | 1:I:301:ASN:ND2  | 1.88                     | 0.86              |
| 1:A:439:LEU:HB2 | 1:B:473:ALA:HB1  | 1.56                     | 0.86              |
| 1:K:439:LEU:HB2 | 1:L:473:ALA:HB1  | 1.56                     | 0.86              |
| 1:F:439:LEU:HB2 | 1:G:473:ALA:HB1  | 1.55                     | 0.86              |
| 1:C:413:GLN:HB2 | 1:D:93:ALA:HB3   | 1.57                     | 0.85              |
| 1:I:413:GLN:HB2 | 1:J:93:ALA:HB3   | 1.57                     | 0.84              |
| 1:A:413:GLN:HB2 | 1:B:93:ALA:HB3   | 1.57                     | 0.84              |
| 1:K:413:GLN:HB2 | 1:L:93:ALA:CB    | 2.07                     | 0.84              |
| 1:F:293:SER:OG  | 1:G:337:ASP:HB3  | 1.78                     | 0.84              |
| 1:I:80:MET:HE1  | 1:J:431:GLU:OE1  | 1.78                     | 0.83              |
| 1:J:293:SER:OG  | 1:K:337:ASP:HB3  | 1.77                     | 0.83              |
| 1:H:80:MET:HE1  | 1:I:431:GLU:OE1  | 1.78                     | 0.83              |
| 1:E:413:GLN:HB2 | 1:F:93:ALA:CB    | 2.09                     | 0.83              |
| 1:G:413:GLN:HB2 | 1:H:93:ALA:HB3   | 1.58                     | 0.83              |
| 1:H:293:SER:OG  | 1:I:337:ASP:HB3  | 1.79                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:80:MET:HE1   | 1:D:431:GLU:OE1  | 1.79                     | 0.83              |
| 1:D:293:SER:OG   | 1:E:337:ASP:HB3  | 1.79                     | 0.82              |
| 1:B:80:MET:HE1   | 1:C:431:GLU:OE1  | 1.78                     | 0.82              |
| 1:A:413:GLN:HB2  | 1:B:93:ALA:CB    | 2.10                     | 0.82              |
| 1:K:80:MET:HE1   | 1:L:431:GLU:OE1  | 1.80                     | 0.81              |
| 1:F:367:GLU:HG2  | 1:G:376:TYR:HE1  | 1.45                     | 0.81              |
| 1:H:367:GLU:HG2  | 1:I:376:TYR:HE1  | 1.45                     | 0.81              |
| 1:E:80:MET:HE1   | 1:F:431:GLU:OE1  | 1.81                     | 0.81              |
| 1:F:80:MET:HE1   | 1:G:431:GLU:OE1  | 1.79                     | 0.81              |
| 1:B:293:SER:OG   | 1:C:337:ASP:HB3  | 1.79                     | 0.81              |
| 1:G:413:GLN:HB2  | 1:H:93:ALA:CB    | 2.11                     | 0.81              |
| 1:A:431:GLU:OE1  | 1:L:80:MET:HE1   | 1.79                     | 0.81              |
| 1:C:413:GLN:HB2  | 1:D:93:ALA:CB    | 2.11                     | 0.81              |
| 1:D:442:LEU:HB3  | 1:E:470:ILE:HD11 | 1.63                     | 0.81              |
| 1:B:367:GLU:HG2  | 1:C:376:TYR:HE1  | 1.44                     | 0.80              |
| 1:A:293:SER:OG   | 1:B:337:ASP:HB3  | 1.81                     | 0.80              |
| 1:D:80:MET:HE1   | 1:E:431:GLU:OE1  | 1.80                     | 0.80              |
| 1:G:80:MET:HE1   | 1:H:431:GLU:OE1  | 1.82                     | 0.80              |
| 1:J:80:MET:HE1   | 1:K:431:GLU:OE1  | 1.82                     | 0.80              |
| 1:A:80:MET:HE1   | 1:B:431:GLU:OE1  | 1.81                     | 0.80              |
| 1:A:337:ASP:HB3  | 1:L:293:SER:OG   | 1.80                     | 0.80              |
| 1:J:367:GLU:HG2  | 1:K:376:TYR:HE1  | 1.45                     | 0.80              |
| 1:K:293:SER:OG   | 1:L:337:ASP:HB3  | 1.81                     | 0.80              |
| 1:C:293:SER:OG   | 1:D:337:ASP:HB3  | 1.81                     | 0.79              |
| 1:D:367:GLU:HG2  | 1:E:376:TYR:HE1  | 1.45                     | 0.79              |
| 1:J:442:LEU:HB3  | 1:K:470:ILE:HD11 | 1.65                     | 0.79              |
| 1:I:293:SER:OG   | 1:J:337:ASP:HB3  | 1.82                     | 0.79              |
| 1:A:97:LEU:HD22  | 1:L:112:MET:HE2  | 1.64                     | 0.79              |
| 1:A:376:TYR:HE1  | 1:L:367:GLU:HG2  | 1.46                     | 0.79              |
| 1:A:470:ILE:HD11 | 1:L:442:LEU:HB3  | 1.65                     | 0.78              |
| 1:H:112:MET:HE2  | 1:I:97:LEU:HD22  | 1.65                     | 0.78              |
| 1:D:112:MET:HE2  | 1:E:97:LEU:HD22  | 1.64                     | 0.78              |
| 1:I:413:GLN:HB2  | 1:J:93:ALA:CB    | 2.13                     | 0.78              |
| 1:I:439:LEU:HD12 | 1:J:473:ALA:HB3  | 1.64                     | 0.77              |
| 1:G:293:SER:OG   | 1:H:337:ASP:HB3  | 1.81                     | 0.77              |
| 1:F:59:GLN:HA    | 1:G:351:ARG:HH22 | 1.50                     | 0.77              |
| 1:F:112:MET:HE2  | 1:G:97:LEU:HD22  | 1.66                     | 0.77              |
| 1:J:112:MET:HE2  | 1:K:97:LEU:HD22  | 1.65                     | 0.77              |
| 1:C:439:LEU:HD12 | 1:D:473:ALA:HB3  | 1.66                     | 0.77              |
| 1:E:293:SER:OG   | 1:F:337:ASP:HB3  | 1.83                     | 0.77              |
| 1:B:112:MET:HE2  | 1:C:97:LEU:HD22  | 1.65                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:59:GLN:HA    | 1:K:351:ARG:HH22 | 1.48                     | 0.76              |
| 1:G:323:ARG:HG3  | 1:H:301:ASN:HD21 | 1.51                     | 0.76              |
| 1:I:467:LYS:HB2  | 1:J:460:ASP:OD2  | 1.84                     | 0.76              |
| 1:D:59:GLN:HA    | 1:E:351:ARG:HH22 | 1.50                     | 0.76              |
| 1:A:323:ARG:HG3  | 1:B:301:ASN:HD21 | 1.51                     | 0.75              |
| 1:A:291:MET:HG2  | 1:B:282:LEU:HD13 | 1.69                     | 0.75              |
| 1:H:59:GLN:HA    | 1:I:351:ARG:HH22 | 1.51                     | 0.75              |
| 1:A:351:ARG:HH22 | 1:L:59:GLN:HA    | 1.51                     | 0.75              |
| 1:B:442:LEU:HB3  | 1:C:470:ILE:HD11 | 1.69                     | 0.75              |
| 1:B:59:GLN:HA    | 1:C:351:ARG:HH22 | 1.51                     | 0.75              |
| 1:C:323:ARG:HG3  | 1:D:301:ASN:HD21 | 1.50                     | 0.75              |
| 1:G:439:LEU:HD12 | 1:H:473:ALA:HB3  | 1.68                     | 0.74              |
| 1:G:291:MET:HG2  | 1:H:282:LEU:HD13 | 1.67                     | 0.74              |
| 1:E:439:LEU:HD12 | 1:F:473:ALA:HB3  | 1.70                     | 0.74              |
| 1:C:467:LYS:HB2  | 1:D:460:ASP:OD2  | 1.86                     | 0.74              |
| 1:I:291:MET:HG2  | 1:J:282:LEU:HD13 | 1.69                     | 0.74              |
| 1:H:442:LEU:HB3  | 1:I:470:ILE:HD11 | 1.69                     | 0.73              |
| 1:A:439:LEU:HD12 | 1:B:473:ALA:HB3  | 1.69                     | 0.73              |
| 1:I:439:LEU:HD12 | 1:J:473:ALA:CB   | 2.17                     | 0.73              |
| 1:K:323:ARG:HG3  | 1:L:301:ASN:HD21 | 1.53                     | 0.73              |
| 1:C:439:LEU:HD12 | 1:D:473:ALA:CB   | 2.18                     | 0.73              |
| 1:F:442:LEU:HB3  | 1:G:470:ILE:HD11 | 1.69                     | 0.73              |
| 1:I:323:ARG:HG3  | 1:J:301:ASN:HD21 | 1.52                     | 0.73              |
| 1:K:186:ALA:HB2  | 1:L:171:ASP:HB3  | 1.71                     | 0.73              |
| 1:G:467:LYS:HB2  | 1:H:460:ASP:OD2  | 1.89                     | 0.72              |
| 1:E:186:ALA:HB2  | 1:F:171:ASP:HB3  | 1.72                     | 0.72              |
| 1:A:467:LYS:HB2  | 1:B:460:ASP:OD2  | 1.90                     | 0.71              |
| 1:C:291:MET:HG2  | 1:D:282:LEU:HD13 | 1.69                     | 0.71              |
| 1:K:439:LEU:HD12 | 1:L:473:ALA:HB3  | 1.71                     | 0.71              |
| 1:A:186:ALA:HB2  | 1:B:171:ASP:HB3  | 1.72                     | 0.71              |
| 1:B:398:LEU:HB3  | 1:B:399:PRO:HD3  | 1.73                     | 0.71              |
| 1:A:398:LEU:HB3  | 1:A:399:PRO:HD3  | 1.73                     | 0.71              |
| 1:C:398:LEU:HB3  | 1:C:399:PRO:HD3  | 1.73                     | 0.71              |
| 1:C:59:GLN:HA    | 1:D:351:ARG:HH22 | 1.56                     | 0.71              |
| 1:D:6:THR:O      | 1:D:6:THR:OG1    | 2.09                     | 0.71              |
| 1:G:186:ALA:HB2  | 1:H:171:ASP:HB3  | 1.73                     | 0.71              |
| 1:H:398:LEU:HB3  | 1:H:399:PRO:HD3  | 1.73                     | 0.71              |
| 1:K:291:MET:HG2  | 1:L:282:LEU:HD13 | 1.71                     | 0.71              |
| 1:E:291:MET:HG2  | 1:F:282:LEU:HD13 | 1.71                     | 0.70              |
| 1:G:439:LEU:HD12 | 1:H:473:ALA:CB   | 2.20                     | 0.70              |
| 1:L:398:LEU:HB3  | 1:L:399:PRO:HD3  | 1.73                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:186:ALA:HB2  | 1:D:171:ASP:HB3  | 1.73                     | 0.70              |
| 1:D:398:LEU:HB3  | 1:D:399:PRO:HD3  | 1.73                     | 0.70              |
| 1:E:323:ARG:HG3  | 1:F:301:ASN:HD21 | 1.55                     | 0.70              |
| 1:I:398:LEU:HB3  | 1:I:399:PRO:HD3  | 1.73                     | 0.70              |
| 1:E:467:LYS:HB2  | 1:F:460:ASP:OD2  | 1.91                     | 0.70              |
| 1:E:398:LEU:HB3  | 1:E:399:PRO:HD3  | 1.73                     | 0.70              |
| 1:G:290:SER:CB   | 1:H:344:VAL:HG11 | 2.22                     | 0.70              |
| 1:K:59:GLN:HA    | 1:L:351:ARG:HH22 | 1.55                     | 0.70              |
| 1:G:398:LEU:HB3  | 1:G:399:PRO:HD3  | 1.73                     | 0.70              |
| 1:C:109:GLY:HA2  | 1:C:112:MET:SD   | 2.32                     | 0.70              |
| 1:B:109:GLY:HA2  | 1:B:112:MET:SD   | 2.32                     | 0.69              |
| 1:H:109:GLY:HA2  | 1:H:112:MET:SD   | 2.32                     | 0.69              |
| 1:J:398:LEU:HB3  | 1:J:399:PRO:HD3  | 1.73                     | 0.69              |
| 1:L:109:GLY:HA2  | 1:L:112:MET:SD   | 2.32                     | 0.69              |
| 1:A:439:LEU:HD12 | 1:B:473:ALA:CB   | 2.21                     | 0.69              |
| 1:I:112:MET:HE2  | 1:J:97:LEU:HD22  | 1.73                     | 0.69              |
| 1:I:439:LEU:HB2  | 1:J:473:ALA:HB2  | 1.74                     | 0.69              |
| 1:A:109:GLY:HA2  | 1:A:112:MET:SD   | 2.32                     | 0.69              |
| 1:D:109:GLY:HA2  | 1:D:112:MET:SD   | 2.32                     | 0.69              |
| 1:E:59:GLN:HA    | 1:F:351:ARG:HH22 | 1.56                     | 0.69              |
| 1:F:109:GLY:HA2  | 1:F:112:MET:SD   | 2.32                     | 0.69              |
| 1:F:398:LEU:HB3  | 1:F:399:PRO:HD3  | 1.73                     | 0.69              |
| 1:A:59:GLN:HA    | 1:B:351:ARG:HH22 | 1.56                     | 0.69              |
| 1:B:126:TYR:CD2  | 1:B:158:MET:SD   | 2.86                     | 0.69              |
| 1:E:112:MET:HE2  | 1:F:97:LEU:HD22  | 1.73                     | 0.69              |
| 1:I:109:GLY:HA2  | 1:I:112:MET:SD   | 2.32                     | 0.69              |
| 1:I:186:ALA:HB2  | 1:J:171:ASP:HB3  | 1.74                     | 0.69              |
| 1:A:126:TYR:CD2  | 1:A:158:MET:SD   | 2.86                     | 0.69              |
| 1:K:398:LEU:HB3  | 1:K:399:PRO:HD3  | 1.73                     | 0.69              |
| 1:A:73:LEU:HD23  | 1:A:134:LEU:HD21 | 1.75                     | 0.69              |
| 1:E:109:GLY:HA2  | 1:E:112:MET:SD   | 2.32                     | 0.69              |
| 1:H:6:THR:O      | 1:H:6:THR:OG1    | 2.09                     | 0.69              |
| 1:I:6:THR:O      | 1:I:6:THR:OG1    | 2.09                     | 0.69              |
| 1:K:109:GLY:HA2  | 1:K:112:MET:SD   | 2.32                     | 0.69              |
| 1:K:467:LYS:HB2  | 1:L:460:ASP:OD2  | 1.93                     | 0.69              |
| 1:L:73:LEU:HD23  | 1:L:134:LEU:HD21 | 1.75                     | 0.69              |
| 1:L:126:TYR:CD2  | 1:L:158:MET:SD   | 2.86                     | 0.69              |
| 1:C:126:TYR:CD2  | 1:C:158:MET:SD   | 2.86                     | 0.69              |
| 1:B:6:THR:O      | 1:B:6:THR:OG1    | 2.09                     | 0.69              |
| 1:B:73:LEU:HD23  | 1:B:134:LEU:HD21 | 1.75                     | 0.69              |
| 1:G:6:THR:O      | 1:G:6:THR:OG1    | 2.09                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:73:LEU:HD23  | 1:C:134:LEU:HD21 | 1.75                     | 0.68              |
| 1:E:73:LEU:HD23  | 1:E:134:LEU:HD21 | 1.75                     | 0.68              |
| 1:D:73:LEU:HD23  | 1:D:134:LEU:HD21 | 1.75                     | 0.68              |
| 1:F:186:ALA:HB2  | 1:G:171:ASP:HB3  | 1.75                     | 0.68              |
| 1:G:59:GLN:HA    | 1:H:351:ARG:HH22 | 1.57                     | 0.68              |
| 1:G:109:GLY:HA2  | 1:G:112:MET:SD   | 2.32                     | 0.68              |
| 1:J:6:THR:O      | 1:J:6:THR:OG1    | 2.09                     | 0.68              |
| 1:K:73:LEU:HD23  | 1:K:134:LEU:HD21 | 1.75                     | 0.68              |
| 1:K:126:TYR:CD2  | 1:K:158:MET:SD   | 2.86                     | 0.68              |
| 1:C:290:SER:CB   | 1:D:344:VAL:HG11 | 2.23                     | 0.68              |
| 1:D:126:TYR:CD2  | 1:D:158:MET:SD   | 2.86                     | 0.68              |
| 1:I:59:GLN:HA    | 1:J:351:ARG:HH22 | 1.58                     | 0.68              |
| 1:J:73:LEU:HD23  | 1:J:134:LEU:HD21 | 1.75                     | 0.68              |
| 1:J:186:ALA:HB2  | 1:K:171:ASP:HB3  | 1.76                     | 0.68              |
| 1:E:439:LEU:HD12 | 1:F:473:ALA:CB   | 2.23                     | 0.68              |
| 1:F:73:LEU:HD23  | 1:F:134:LEU:HD21 | 1.75                     | 0.68              |
| 1:I:73:LEU:HD23  | 1:I:134:LEU:HD21 | 1.75                     | 0.68              |
| 1:I:126:TYR:CD2  | 1:I:158:MET:SD   | 2.86                     | 0.68              |
| 1:E:126:TYR:CD2  | 1:E:158:MET:SD   | 2.86                     | 0.68              |
| 1:G:73:LEU:HD23  | 1:G:134:LEU:HD21 | 1.75                     | 0.68              |
| 1:H:73:LEU:HD23  | 1:H:134:LEU:HD21 | 1.75                     | 0.68              |
| 1:I:290:SER:CB   | 1:J:344:VAL:HG11 | 2.24                     | 0.68              |
| 1:J:109:GLY:HA2  | 1:J:112:MET:SD   | 2.32                     | 0.68              |
| 1:J:126:TYR:CD2  | 1:J:158:MET:SD   | 2.86                     | 0.68              |
| 1:I:126:TYR:CE1  | 1:I:158:MET:SD   | 2.87                     | 0.68              |
| 1:K:439:LEU:HD12 | 1:L:473:ALA:CB   | 2.23                     | 0.68              |
| 1:H:126:TYR:CD2  | 1:H:158:MET:SD   | 2.86                     | 0.68              |
| 1:H:126:TYR:CE1  | 1:H:158:MET:SD   | 2.87                     | 0.67              |
| 1:H:186:ALA:HB2  | 1:I:171:ASP:HB3  | 1.76                     | 0.67              |
| 1:K:6:THR:O      | 1:K:6:THR:OG1    | 2.09                     | 0.67              |
| 1:A:290:SER:CB   | 1:B:344:VAL:HG11 | 2.23                     | 0.67              |
| 1:E:290:SER:CB   | 1:F:344:VAL:HG11 | 2.24                     | 0.67              |
| 1:G:126:TYR:CD2  | 1:G:158:MET:SD   | 2.86                     | 0.67              |
| 1:D:291:MET:HG2  | 1:E:282:LEU:HD13 | 1.74                     | 0.67              |
| 1:J:126:TYR:CE1  | 1:J:158:MET:SD   | 2.88                     | 0.67              |
| 1:C:291:MET:CG   | 1:D:282:LEU:HD11 | 2.24                     | 0.67              |
| 1:A:282:LEU:HD13 | 1:L:291:MET:HG2  | 1.76                     | 0.67              |
| 1:G:126:TYR:CE1  | 1:G:158:MET:SD   | 2.88                     | 0.67              |
| 1:F:6:THR:O      | 1:F:6:THR:OG1    | 2.09                     | 0.67              |
| 1:B:126:TYR:CE1  | 1:B:158:MET:SD   | 2.87                     | 0.67              |
| 1:B:186:ALA:HB2  | 1:C:171:ASP:HB3  | 1.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:126:TYR:CD2  | 1:F:158:MET:SD   | 2.86                     | 0.67              |
| 1:K:126:TYR:CE1  | 1:K:158:MET:SD   | 2.88                     | 0.67              |
| 1:A:171:ASP:HB3  | 1:L:186:ALA:HB2  | 1.77                     | 0.67              |
| 1:G:439:LEU:HB2  | 1:H:473:ALA:HB2  | 1.77                     | 0.67              |
| 1:G:327:ILE:HD12 | 1:H:330:LEU:CD1  | 2.25                     | 0.67              |
| 1:A:126:TYR:CE1  | 1:A:158:MET:SD   | 2.88                     | 0.66              |
| 1:E:20:LEU:HB2   | 1:E:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:H:20:LEU:HB2   | 1:H:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:K:112:MET:HE2  | 1:L:97:LEU:HD22  | 1.76                     | 0.66              |
| 1:K:291:MET:CG   | 1:L:282:LEU:HD11 | 2.25                     | 0.66              |
| 1:C:126:TYR:CE1  | 1:C:158:MET:SD   | 2.87                     | 0.66              |
| 1:L:126:TYR:CE1  | 1:L:158:MET:SD   | 2.87                     | 0.66              |
| 1:F:20:LEU:HB2   | 1:F:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:I:20:LEU:HB2   | 1:I:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:B:20:LEU:HB2   | 1:B:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:D:20:LEU:HB2   | 1:D:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:G:20:LEU:HB2   | 1:G:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:J:20:LEU:HB2   | 1:J:167:VAL:HG21 | 1.77                     | 0.66              |
| 1:A:20:LEU:HB2   | 1:A:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:C:20:LEU:HB2   | 1:C:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:C:112:MET:HE2  | 1:D:97:LEU:HD22  | 1.76                     | 0.66              |
| 1:F:126:TYR:CE1  | 1:F:158:MET:SD   | 2.88                     | 0.66              |
| 1:G:329:PHE:CE2  | 1:H:332:LEU:CD2  | 2.79                     | 0.66              |
| 1:L:6:THR:O      | 1:L:6:THR:OG1    | 2.09                     | 0.66              |
| 1:D:126:TYR:CE1  | 1:D:158:MET:SD   | 2.88                     | 0.66              |
| 1:E:126:TYR:CE1  | 1:E:158:MET:SD   | 2.88                     | 0.66              |
| 1:J:291:MET:HG2  | 1:K:282:LEU:HD13 | 1.73                     | 0.66              |
| 1:L:20:LEU:HB2   | 1:L:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:D:186:ALA:HB2  | 1:E:171:ASP:HB3  | 1.78                     | 0.66              |
| 1:K:20:LEU:HB2   | 1:K:167:VAL:HG21 | 1.78                     | 0.66              |
| 1:E:6:THR:OG1    | 1:E:6:THR:O      | 2.09                     | 0.65              |
| 1:A:327:ILE:HD12 | 1:B:330:LEU:CD1  | 2.27                     | 0.65              |
| 1:C:439:LEU:HB2  | 1:D:473:ALA:HB2  | 1.76                     | 0.65              |
| 1:F:367:GLU:HG2  | 1:G:376:TYR:CE1  | 2.31                     | 0.65              |
| 1:K:290:SER:CB   | 1:L:344:VAL:HG11 | 2.26                     | 0.65              |
| 1:J:367:GLU:HG2  | 1:K:376:TYR:CE1  | 2.29                     | 0.65              |
| 1:H:367:GLU:HG2  | 1:I:376:TYR:CE1  | 2.31                     | 0.65              |
| 1:E:439:LEU:HB2  | 1:F:473:ALA:HB2  | 1.78                     | 0.65              |
| 1:G:112:MET:HE2  | 1:H:97:LEU:HD22  | 1.78                     | 0.65              |
| 1:E:150:PRO:HG2  | 1:E:411:THR:HG21 | 1.79                     | 0.65              |
| 1:A:301:ASN:HD21 | 1:L:323:ARG:HG3  | 1.62                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:150:PRO:HG2  | 1:C:411:THR:HG21 | 1.79                     | 0.64              |
| 1:D:150:PRO:HG2  | 1:D:411:THR:HG21 | 1.79                     | 0.64              |
| 1:F:150:PRO:HG2  | 1:F:411:THR:HG21 | 1.79                     | 0.64              |
| 1:A:112:MET:HE2  | 1:B:97:LEU:HD22  | 1.78                     | 0.64              |
| 1:A:329:PHE:CE2  | 1:B:332:LEU:CD2  | 2.80                     | 0.64              |
| 1:C:327:ILE:HD12 | 1:D:330:LEU:HD12 | 1.80                     | 0.64              |
| 1:I:291:MET:CG   | 1:J:282:LEU:HD11 | 2.25                     | 0.64              |
| 1:A:6:THR:O      | 1:A:6:THR:OG1    | 2.09                     | 0.64              |
| 1:C:327:ILE:HD12 | 1:D:330:LEU:CD1  | 2.26                     | 0.64              |
| 1:H:291:MET:CG   | 1:I:282:LEU:HD11 | 2.27                     | 0.64              |
| 1:B:150:PRO:HG2  | 1:B:411:THR:HG21 | 1.79                     | 0.64              |
| 1:H:190:LEU:HB3  | 1:H:195:ARG:HG3  | 1.79                     | 0.64              |
| 1:I:190:LEU:HB3  | 1:I:195:ARG:HG3  | 1.79                     | 0.64              |
| 1:J:323:ARG:HG3  | 1:K:301:ASN:HD21 | 1.59                     | 0.64              |
| 1:F:291:MET:CG   | 1:G:282:LEU:HD11 | 2.26                     | 0.64              |
| 1:J:290:SER:CB   | 1:K:344:VAL:HG11 | 2.28                     | 0.64              |
| 1:J:293:SER:OG   | 1:K:337:ASP:CB   | 2.45                     | 0.64              |
| 1:G:190:LEU:HB3  | 1:G:195:ARG:HG3  | 1.79                     | 0.64              |
| 1:D:190:LEU:HB3  | 1:D:195:ARG:HG3  | 1.79                     | 0.64              |
| 1:F:413:GLN:CB   | 1:G:93:ALA:CB    | 2.74                     | 0.64              |
| 1:G:150:PRO:HG2  | 1:G:411:THR:HG21 | 1.79                     | 0.64              |
| 1:H:291:MET:HG2  | 1:I:282:LEU:HD13 | 1.77                     | 0.64              |
| 1:B:291:MET:HG2  | 1:C:282:LEU:HD13 | 1.77                     | 0.64              |
| 1:J:369:VAL:HB   | 1:K:375:ARG:HG2  | 1.80                     | 0.64              |
| 1:A:439:LEU:HB2  | 1:B:473:ALA:HB2  | 1.78                     | 0.64              |
| 1:C:190:LEU:HB3  | 1:C:195:ARG:HG3  | 1.79                     | 0.64              |
| 1:F:293:SER:OG   | 1:G:337:ASP:CB   | 2.45                     | 0.64              |
| 1:H:293:SER:OG   | 1:I:337:ASP:CB   | 2.46                     | 0.64              |
| 1:I:327:ILE:HD12 | 1:J:330:LEU:CD1  | 2.27                     | 0.64              |
| 1:J:190:LEU:HB3  | 1:J:195:ARG:HG3  | 1.79                     | 0.64              |
| 1:B:190:LEU:HB3  | 1:B:195:ARG:HG3  | 1.79                     | 0.64              |
| 1:I:168:VAL:HG22 | 1:I:179:MET:HB3  | 1.81                     | 0.64              |
| 1:J:115:ARG:NH2  | 1:K:476:ILE:N    | 2.46                     | 0.64              |
| 1:E:190:LEU:HB3  | 1:E:195:ARG:HG3  | 1.79                     | 0.63              |
| 1:F:291:MET:HG2  | 1:G:282:LEU:HD13 | 1.76                     | 0.63              |
| 1:A:150:PRO:HG2  | 1:A:411:THR:HG21 | 1.79                     | 0.63              |
| 1:D:367:GLU:HG2  | 1:E:376:TYR:CE1  | 2.30                     | 0.63              |
| 1:L:168:VAL:HG22 | 1:L:179:MET:HB3  | 1.81                     | 0.63              |
| 1:A:291:MET:CG   | 1:B:282:LEU:HD11 | 2.24                     | 0.63              |
| 1:B:293:SER:OG   | 1:C:337:ASP:CB   | 2.47                     | 0.63              |
| 1:D:369:VAL:HB   | 1:E:375:ARG:HG2  | 1.81                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:327:ILE:HD12 | 1:H:330:LEU:HD12 | 1.80                     | 0.63              |
| 1:H:413:GLN:HB2  | 1:I:93:ALA:HB1   | 1.80                     | 0.63              |
| 1:H:150:PRO:HG2  | 1:H:411:THR:HG21 | 1.79                     | 0.63              |
| 1:I:112:MET:HG2  | 1:J:97:LEU:HD21  | 1.80                     | 0.63              |
| 1:B:413:GLN:HB2  | 1:C:93:ALA:HB1   | 1.79                     | 0.63              |
| 1:D:290:SER:CB   | 1:E:344:VAL:HG11 | 2.28                     | 0.63              |
| 1:D:367:GLU:HB3  | 1:E:376:TYR:CE1  | 2.33                     | 0.63              |
| 1:J:291:MET:CG   | 1:K:282:LEU:HD11 | 2.25                     | 0.63              |
| 1:B:367:GLU:HB3  | 1:C:376:TYR:CE1  | 2.34                     | 0.63              |
| 1:F:190:LEU:HB3  | 1:F:195:ARG:HG3  | 1.79                     | 0.63              |
| 1:K:168:VAL:HG22 | 1:K:179:MET:HB3  | 1.81                     | 0.63              |
| 1:B:367:GLU:HG2  | 1:C:376:TYR:CE1  | 2.30                     | 0.63              |
| 1:C:329:PHE:CE2  | 1:D:332:LEU:CD2  | 2.81                     | 0.63              |
| 1:F:168:VAL:HG22 | 1:F:179:MET:HB3  | 1.80                     | 0.63              |
| 1:G:294:SER:HB2  | 1:H:285:ALA:CB   | 2.29                     | 0.63              |
| 1:K:190:LEU:HB3  | 1:K:195:ARG:HG3  | 1.79                     | 0.63              |
| 1:F:323:ARG:HG3  | 1:G:301:ASN:HD21 | 1.61                     | 0.63              |
| 1:A:190:LEU:HB3  | 1:A:195:ARG:HG3  | 1.79                     | 0.62              |
| 1:A:327:ILE:HD12 | 1:B:330:LEU:HD12 | 1.81                     | 0.62              |
| 1:A:376:TYR:CE1  | 1:L:367:GLU:HB3  | 2.34                     | 0.62              |
| 1:G:291:MET:CG   | 1:H:282:LEU:HD11 | 2.25                     | 0.62              |
| 1:H:168:VAL:HG22 | 1:H:179:MET:HB3  | 1.81                     | 0.62              |
| 1:I:150:PRO:HG2  | 1:I:411:THR:HG21 | 1.79                     | 0.62              |
| 1:J:168:VAL:HG22 | 1:J:179:MET:HB3  | 1.80                     | 0.62              |
| 1:K:150:PRO:HG2  | 1:K:411:THR:HG21 | 1.79                     | 0.62              |
| 1:L:150:PRO:HG2  | 1:L:411:THR:HG21 | 1.79                     | 0.62              |
| 1:A:282:LEU:HD11 | 1:L:291:MET:CG   | 2.28                     | 0.62              |
| 1:D:293:SER:OG   | 1:E:337:ASP:CB   | 2.47                     | 0.62              |
| 1:H:323:ARG:HG3  | 1:I:301:ASN:HD21 | 1.62                     | 0.62              |
| 1:I:327:ILE:HD12 | 1:J:330:LEU:HD12 | 1.81                     | 0.62              |
| 1:L:190:LEU:HB3  | 1:L:195:ARG:HG3  | 1.79                     | 0.62              |
| 1:B:64:ARG:HE    | 1:B:358:LEU:HD21 | 1.64                     | 0.62              |
| 1:C:6:THR:O      | 1:C:6:THR:OG1    | 2.09                     | 0.62              |
| 1:G:168:VAL:HG22 | 1:G:179:MET:HB3  | 1.81                     | 0.62              |
| 1:K:311:LEU:HD11 | 1:L:299:LEU:HD21 | 1.81                     | 0.62              |
| 1:C:168:VAL:HG22 | 1:C:179:MET:HB3  | 1.81                     | 0.62              |
| 1:D:323:ARG:HG3  | 1:E:301:ASN:HD21 | 1.60                     | 0.62              |
| 1:E:367:GLU:HG2  | 1:F:376:TYR:HE1  | 1.64                     | 0.62              |
| 1:F:115:ARG:NH2  | 1:G:476:ILE:N    | 2.47                     | 0.62              |
| 1:H:64:ARG:HE    | 1:H:358:LEU:HD21 | 1.64                     | 0.62              |
| 1:K:439:LEU:HB2  | 1:L:473:ALA:HB2  | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:168:VAL:HG22 | 1:B:179:MET:HB3  | 1.81                     | 0.62              |
| 1:G:64:ARG:HE    | 1:G:358:LEU:HD21 | 1.64                     | 0.62              |
| 1:J:150:PRO:HG2  | 1:J:411:THR:HG21 | 1.79                     | 0.62              |
| 1:A:344:VAL:HG11 | 1:L:290:SER:CB   | 2.29                     | 0.62              |
| 1:A:376:TYR:CE1  | 1:L:367:GLU:HG2  | 2.31                     | 0.62              |
| 1:F:413:GLN:HB2  | 1:G:93:ALA:HB1   | 1.78                     | 0.62              |
| 1:I:329:PHE:CE2  | 1:J:332:LEU:CD2  | 2.82                     | 0.62              |
| 1:E:168:VAL:HG22 | 1:E:179:MET:HB3  | 1.80                     | 0.62              |
| 1:I:64:ARG:HE    | 1:I:358:LEU:HD21 | 1.64                     | 0.62              |
| 1:I:439:LEU:CD1  | 1:J:473:ALA:CB   | 2.78                     | 0.62              |
| 1:J:413:GLN:HB2  | 1:K:93:ALA:HB1   | 1.79                     | 0.62              |
| 1:J:413:GLN:CB   | 1:K:93:ALA:CB    | 2.76                     | 0.62              |
| 1:D:291:MET:CG   | 1:E:282:LEU:HD11 | 2.27                     | 0.62              |
| 1:F:64:ARG:HE    | 1:F:358:LEU:HD21 | 1.64                     | 0.62              |
| 1:K:64:ARG:HE    | 1:K:358:LEU:HD21 | 1.64                     | 0.62              |
| 1:C:293:SER:OG   | 1:D:337:ASP:CB   | 2.48                     | 0.61              |
| 1:E:327:ILE:HD12 | 1:F:330:LEU:CD1  | 2.30                     | 0.61              |
| 1:J:367:GLU:HB3  | 1:K:376:TYR:CE1  | 2.35                     | 0.61              |
| 1:A:168:VAL:HG22 | 1:A:179:MET:HB3  | 1.81                     | 0.61              |
| 1:F:131:PHE:HE2  | 1:G:387:GLY:CA   | 2.02                     | 0.61              |
| 1:H:323:ARG:HG3  | 1:I:301:ASN:HD22 | 1.65                     | 0.61              |
| 1:I:367:GLU:HG2  | 1:J:376:TYR:HE1  | 1.64                     | 0.61              |
| 1:C:311:LEU:HD11 | 1:D:299:LEU:HD21 | 1.80                     | 0.61              |
| 1:E:64:ARG:HE    | 1:E:358:LEU:HD21 | 1.64                     | 0.61              |
| 1:H:115:ARG:NH2  | 1:I:476:ILE:N    | 2.49                     | 0.61              |
| 1:K:367:GLU:HG2  | 1:L:376:TYR:HE1  | 1.64                     | 0.61              |
| 1:L:64:ARG:HE    | 1:L:358:LEU:HD21 | 1.64                     | 0.61              |
| 1:A:64:ARG:HE    | 1:A:358:LEU:HD21 | 1.64                     | 0.61              |
| 1:E:311:LEU:HD11 | 1:F:299:LEU:HD21 | 1.82                     | 0.61              |
| 1:I:311:LEU:HD11 | 1:J:299:LEU:HD21 | 1.82                     | 0.61              |
| 1:J:64:ARG:HE    | 1:J:358:LEU:HD21 | 1.64                     | 0.61              |
| 1:D:168:VAL:HG22 | 1:D:179:MET:HB3  | 1.80                     | 0.61              |
| 1:D:442:LEU:HB3  | 1:E:470:ILE:CD1  | 2.29                     | 0.61              |
| 1:H:367:GLU:HB3  | 1:I:376:TYR:CE1  | 2.35                     | 0.61              |
| 1:A:476:ILE:N    | 1:L:115:ARG:NH2  | 2.49                     | 0.61              |
| 1:A:367:GLU:HG2  | 1:B:376:TYR:HE1  | 1.66                     | 0.61              |
| 1:K:327:ILE:HD12 | 1:L:330:LEU:CD1  | 2.30                     | 0.61              |
| 1:A:294:SER:HB2  | 1:B:285:ALA:CB   | 2.30                     | 0.61              |
| 1:A:375:ARG:HG2  | 1:L:369:VAL:HB   | 1.82                     | 0.61              |
| 1:B:413:GLN:CB   | 1:C:93:ALA:CB    | 2.75                     | 0.61              |
| 1:G:367:GLU:HG2  | 1:H:376:TYR:HE1  | 1.65                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:369:VAL:HB   | 1:C:375:ARG:HG2  | 1.83                     | 0.61              |
| 1:J:186:ALA:HB2  | 1:K:171:ASP:CB   | 2.31                     | 0.61              |
| 1:B:323:ARG:HG3  | 1:C:301:ASN:HD21 | 1.63                     | 0.60              |
| 1:E:327:ILE:HD12 | 1:F:330:LEU:HD12 | 1.83                     | 0.60              |
| 1:C:294:SER:HB2  | 1:D:285:ALA:CB   | 2.31                     | 0.60              |
| 1:I:294:SER:HB2  | 1:J:285:ALA:CB   | 2.31                     | 0.60              |
| 1:B:115:ARG:NH2  | 1:C:476:ILE:N    | 2.48                     | 0.60              |
| 1:D:64:ARG:HE    | 1:D:358:LEU:HD21 | 1.64                     | 0.60              |
| 1:A:293:SER:OG   | 1:B:337:ASP:CB   | 2.49                     | 0.60              |
| 1:C:112:MET:HG2  | 1:D:97:LEU:HD21  | 1.83                     | 0.60              |
| 1:G:449:TRP:CH2  | 1:H:461:ILE:HG12 | 2.36                     | 0.60              |
| 1:C:64:ARG:HE    | 1:C:358:LEU:HD21 | 1.64                     | 0.60              |
| 1:D:115:ARG:NH2  | 1:E:476:ILE:N    | 2.48                     | 0.60              |
| 1:G:293:SER:OG   | 1:H:337:ASP:CB   | 2.50                     | 0.60              |
| 1:K:327:ILE:HD12 | 1:L:330:LEU:HD12 | 1.83                     | 0.60              |
| 1:B:131:PHE:HE2  | 1:C:387:GLY:CA   | 2.02                     | 0.60              |
| 1:B:323:ARG:HG3  | 1:C:301:ASN:HD22 | 1.64                     | 0.60              |
| 1:C:367:GLU:HG2  | 1:D:376:TYR:HE1  | 1.65                     | 0.60              |
| 1:F:367:GLU:HB3  | 1:G:376:TYR:CE1  | 2.35                     | 0.60              |
| 1:F:369:VAL:HB   | 1:G:375:ARG:HG2  | 1.82                     | 0.60              |
| 1:G:21:LYS:HG3   | 1:G:24:ARG:HH12  | 1.67                     | 0.60              |
| 1:I:449:TRP:CH2  | 1:J:461:ILE:HG12 | 2.36                     | 0.60              |
| 1:J:21:LYS:HG3   | 1:J:24:ARG:HH12  | 1.67                     | 0.60              |
| 1:L:442:LEU:O    | 1:L:446:VAL:HG12 | 2.02                     | 0.60              |
| 1:A:21:LYS:HG3   | 1:A:24:ARG:HH12  | 1.67                     | 0.60              |
| 1:C:439:LEU:CD1  | 1:D:473:ALA:CB   | 2.80                     | 0.60              |
| 1:G:256:MET:HA   | 1:G:256:MET:HE2  | 1.84                     | 0.60              |
| 1:H:256:MET:HE2  | 1:H:256:MET:HA   | 1.84                     | 0.60              |
| 1:K:329:PHE:CE2  | 1:L:332:LEU:CD2  | 2.85                     | 0.60              |
| 1:K:442:LEU:O    | 1:K:446:VAL:HG12 | 2.02                     | 0.60              |
| 1:K:115:ARG:NH2  | 1:L:476:ILE:N    | 2.50                     | 0.60              |
| 1:A:470:ILE:CD1  | 1:L:442:LEU:HB3  | 2.30                     | 0.60              |
| 1:A:337:ASP:CB   | 1:L:293:SER:OG   | 2.48                     | 0.59              |
| 1:E:112:MET:HG2  | 1:F:97:LEU:HD21  | 1.83                     | 0.59              |
| 1:F:186:ALA:HB2  | 1:G:171:ASP:CB   | 2.30                     | 0.59              |
| 1:F:323:ARG:HG3  | 1:G:301:ASN:HD22 | 1.64                     | 0.59              |
| 1:H:290:SER:CB   | 1:I:344:VAL:HG11 | 2.32                     | 0.59              |
| 1:F:442:LEU:O    | 1:F:446:VAL:HG12 | 2.02                     | 0.59              |
| 1:H:369:VAL:HB   | 1:I:375:ARG:HG2  | 1.83                     | 0.59              |
| 1:J:131:PHE:HE2  | 1:K:387:GLY:CA   | 2.04                     | 0.59              |
| 1:A:442:LEU:O    | 1:A:446:VAL:HG12 | 2.02                     | 0.59              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:442:LEU:O   | 1:C:446:VAL:HG12 | 2.02                     | 0.59              |
| 1:D:256:MET:HE2 | 1:D:256:MET:HA   | 1.85                     | 0.59              |
| 1:E:21:LYS:HG3  | 1:E:24:ARG:HH12  | 1.67                     | 0.59              |
| 1:E:256:MET:HE2 | 1:E:256:MET:HA   | 1.85                     | 0.59              |
| 1:E:329:PHE:CE2 | 1:F:332:LEU:CD2  | 2.84                     | 0.59              |
| 1:E:442:LEU:O   | 1:E:446:VAL:HG12 | 2.02                     | 0.59              |
| 1:G:442:LEU:O   | 1:G:446:VAL:HG12 | 2.02                     | 0.59              |
| 1:I:256:MET:HE2 | 1:I:256:MET:HA   | 1.84                     | 0.59              |
| 1:I:293:SER:OG  | 1:J:337:ASP:CB   | 2.50                     | 0.59              |
| 1:A:20:LEU:CB   | 1:A:167:VAL:HG21 | 2.33                     | 0.59              |
| 1:A:115:ARG:NH2 | 1:B:476:ILE:N    | 2.50                     | 0.59              |
| 1:B:442:LEU:O   | 1:B:446:VAL:HG12 | 2.02                     | 0.59              |
| 1:C:21:LYS:HG3  | 1:C:24:ARG:HH12  | 1.67                     | 0.59              |
| 1:D:442:LEU:O   | 1:D:446:VAL:HG12 | 2.02                     | 0.59              |
| 1:F:256:MET:HE2 | 1:F:256:MET:HA   | 1.84                     | 0.59              |
| 1:G:112:MET:HG2 | 1:H:97:LEU:HD21  | 1.83                     | 0.59              |
| 1:J:294:SER:HB2 | 1:K:285:ALA:CB   | 2.33                     | 0.59              |
| 1:L:21:LYS:HG3  | 1:L:24:ARG:HH12  | 1.67                     | 0.59              |
| 1:B:20:LEU:CB   | 1:B:167:VAL:HG21 | 2.33                     | 0.59              |
| 1:C:256:MET:HE2 | 1:C:256:MET:HA   | 1.84                     | 0.59              |
| 1:C:449:TRP:CH2 | 1:D:461:ILE:HG12 | 2.37                     | 0.59              |
| 1:E:291:MET:CG  | 1:F:282:LEU:HD11 | 2.26                     | 0.59              |
| 1:F:413:GLN:CB  | 1:G:93:ALA:HB3   | 2.27                     | 0.59              |
| 1:G:329:PHE:CE2 | 1:H:332:LEU:HD22 | 2.38                     | 0.59              |
| 1:K:21:LYS:HG3  | 1:K:24:ARG:HH12  | 1.67                     | 0.59              |
| 1:K:293:SER:OG  | 1:L:337:ASP:CB   | 2.48                     | 0.59              |
| 1:C:20:LEU:CB   | 1:C:167:VAL:HG21 | 2.33                     | 0.59              |
| 1:H:442:LEU:O   | 1:H:446:VAL:HG12 | 2.02                     | 0.59              |
| 1:I:21:LYS:HG3  | 1:I:24:ARG:HH12  | 1.67                     | 0.59              |
| 1:K:20:LEU:CB   | 1:K:167:VAL:HG21 | 2.33                     | 0.59              |
| 1:L:20:LEU:CB   | 1:L:167:VAL:HG21 | 2.33                     | 0.59              |
| 1:D:439:LEU:HB2 | 1:E:473:ALA:HB2  | 1.85                     | 0.59              |
| 1:E:115:ARG:NH2 | 1:F:476:ILE:N    | 2.50                     | 0.59              |
| 1:E:294:SER:HB2 | 1:F:285:ALA:CB   | 2.33                     | 0.59              |
| 1:F:122:GLU:HG2 | 1:G:427:SER:HB3  | 1.84                     | 0.59              |
| 1:H:21:LYS:HG3  | 1:H:24:ARG:HH12  | 1.67                     | 0.59              |
| 1:H:186:ALA:HB2 | 1:I:171:ASP:CB   | 2.32                     | 0.59              |
| 1:A:449:TRP:CH2 | 1:B:461:ILE:HG12 | 2.37                     | 0.59              |
| 1:B:122:GLU:HG2 | 1:C:427:SER:HB3  | 1.84                     | 0.59              |
| 1:B:186:ALA:HB2 | 1:C:171:ASP:CB   | 2.32                     | 0.59              |
| 1:J:142:ASN:HB2 | 1:J:163:LEU:HD13 | 1.84                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:256:MET:HA   | 1:J:256:MET:HE2  | 1.84                     | 0.59              |
| 1:J:323:ARG:HG3  | 1:K:301:ASN:HD22 | 1.65                     | 0.59              |
| 1:J:442:LEU:O    | 1:J:446:VAL:HG12 | 2.02                     | 0.59              |
| 1:A:427:SER:HB3  | 1:L:122:GLU:HG2  | 1.85                     | 0.59              |
| 1:C:142:ASN:HB2  | 1:C:163:LEU:HD13 | 1.84                     | 0.59              |
| 1:D:21:LYS:HG3   | 1:D:24:ARG:HH12  | 1.67                     | 0.59              |
| 1:D:142:ASN:HB2  | 1:D:163:LEU:HD13 | 1.84                     | 0.59              |
| 1:D:294:SER:HB2  | 1:E:285:ALA:CB   | 2.33                     | 0.59              |
| 1:F:290:SER:CB   | 1:G:344:VAL:HG11 | 2.32                     | 0.59              |
| 1:J:20:LEU:CB    | 1:J:167:VAL:HG21 | 2.33                     | 0.59              |
| 1:K:294:SER:HB2  | 1:L:285:ALA:CB   | 2.32                     | 0.59              |
| 1:B:142:ASN:HB2  | 1:B:163:LEU:HD13 | 1.84                     | 0.59              |
| 1:D:20:LEU:CB    | 1:D:167:VAL:HG21 | 2.33                     | 0.59              |
| 1:F:21:LYS:HG3   | 1:F:24:ARG:HH12  | 1.67                     | 0.59              |
| 1:I:442:LEU:O    | 1:I:446:VAL:HG12 | 2.02                     | 0.59              |
| 1:B:256:MET:HA   | 1:B:256:MET:HE2  | 1.84                     | 0.58              |
| 1:D:439:LEU:HD12 | 1:E:473:ALA:HB3  | 1.85                     | 0.58              |
| 1:G:115:ARG:NH2  | 1:H:476:ILE:N    | 2.50                     | 0.58              |
| 1:J:144:LEU:HD11 | 1:J:251:TYR:HB3  | 1.85                     | 0.58              |
| 1:K:144:LEU:HD11 | 1:K:251:TYR:HB3  | 1.85                     | 0.58              |
| 1:E:20:LEU:CB    | 1:E:167:VAL:HG21 | 2.33                     | 0.58              |
| 1:K:256:MET:HE2  | 1:K:256:MET:HA   | 1.84                     | 0.58              |
| 1:L:144:LEU:HD11 | 1:L:251:TYR:HB3  | 1.85                     | 0.58              |
| 1:A:171:ASP:CB   | 1:L:186:ALA:HB2  | 2.33                     | 0.58              |
| 1:A:256:MET:HE2  | 1:A:256:MET:HA   | 1.84                     | 0.58              |
| 1:E:142:ASN:HB2  | 1:E:163:LEU:HD13 | 1.84                     | 0.58              |
| 1:H:122:GLU:HG2  | 1:I:427:SER:HB3  | 1.85                     | 0.58              |
| 1:I:20:LEU:CB    | 1:I:167:VAL:HG21 | 2.33                     | 0.58              |
| 1:I:144:LEU:HD11 | 1:I:251:TYR:HB3  | 1.85                     | 0.58              |
| 1:K:142:ASN:HB2  | 1:K:163:LEU:HD13 | 1.85                     | 0.58              |
| 1:A:144:LEU:HD11 | 1:A:251:TYR:HB3  | 1.85                     | 0.58              |
| 1:B:80:MET:HE3   | 1:C:430:LEU:HD23 | 1.84                     | 0.58              |
| 1:L:256:MET:HE2  | 1:L:256:MET:HA   | 1.84                     | 0.58              |
| 1:G:142:ASN:HB2  | 1:G:163:LEU:HD13 | 1.85                     | 0.58              |
| 1:H:131:PHE:HE2  | 1:I:387:GLY:CA   | 2.03                     | 0.58              |
| 1:I:142:ASN:HB2  | 1:I:163:LEU:HD13 | 1.84                     | 0.58              |
| 1:A:93:ALA:CB    | 1:L:413:GLN:CB   | 2.79                     | 0.58              |
| 1:A:112:MET:HG2  | 1:B:97:LEU:HD21  | 1.84                     | 0.58              |
| 1:A:142:ASN:HB2  | 1:A:163:LEU:HD13 | 1.84                     | 0.58              |
| 1:A:372:GLU:C    | 1:A:374:ILE:N    | 2.60                     | 0.58              |
| 1:H:144:LEU:HD11 | 1:H:251:TYR:HB3  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:144:LEU:HD11 | 1:B:251:TYR:HB3  | 1.85                     | 0.58              |
| 1:D:413:GLN:HB2  | 1:E:93:ALA:HB1   | 1.83                     | 0.58              |
| 1:E:449:TRP:CH2  | 1:F:461:ILE:HG12 | 2.38                     | 0.58              |
| 1:F:20:LEU:CB    | 1:F:167:VAL:HG21 | 2.33                     | 0.58              |
| 1:H:80:MET:HE3   | 1:I:430:LEU:HD23 | 1.85                     | 0.58              |
| 1:J:122:GLU:HG2  | 1:K:427:SER:HB3  | 1.84                     | 0.58              |
| 1:A:311:LEU:HD11 | 1:B:299:LEU:HD21 | 1.84                     | 0.58              |
| 1:A:439:LEU:CD1  | 1:B:473:ALA:CB   | 2.82                     | 0.58              |
| 1:F:80:MET:HE3   | 1:G:430:LEU:HD23 | 1.84                     | 0.58              |
| 1:G:439:LEU:CD1  | 1:H:473:ALA:CB   | 2.81                     | 0.58              |
| 1:J:442:LEU:HB3  | 1:K:470:ILE:CD1  | 2.31                     | 0.58              |
| 1:B:290:SER:CB   | 1:C:344:VAL:HG11 | 2.33                     | 0.58              |
| 1:G:20:LEU:CB    | 1:G:167:VAL:HG21 | 2.33                     | 0.58              |
| 1:B:21:LYS:HG3   | 1:B:24:ARG:HH12  | 1.67                     | 0.58              |
| 1:D:122:GLU:HG2  | 1:E:427:SER:HB3  | 1.85                     | 0.58              |
| 1:F:142:ASN:HB2  | 1:F:163:LEU:HD13 | 1.85                     | 0.58              |
| 1:G:144:LEU:HD11 | 1:G:251:TYR:HB3  | 1.85                     | 0.58              |
| 1:H:413:GLN:CB   | 1:I:93:ALA:CB    | 2.76                     | 0.58              |
| 1:B:228:ARG:HD2  | 1:B:244:TYR:HE2  | 1.69                     | 0.57              |
| 1:C:228:ARG:HD2  | 1:C:244:TYR:HE2  | 1.69                     | 0.57              |
| 1:G:372:GLU:C    | 1:G:374:ILE:N    | 2.60                     | 0.57              |
| 1:H:20:LEU:CB    | 1:H:167:VAL:HG21 | 2.33                     | 0.57              |
| 1:H:142:ASN:HB2  | 1:H:163:LEU:HD13 | 1.84                     | 0.57              |
| 1:A:473:ALA:HB3  | 1:L:439:LEU:HD12 | 1.84                     | 0.57              |
| 1:B:291:MET:CG   | 1:C:282:LEU:HD11 | 2.28                     | 0.57              |
| 1:C:144:LEU:HD11 | 1:C:251:TYR:HB3  | 1.86                     | 0.57              |
| 1:D:228:ARG:HD2  | 1:D:244:TYR:HE2  | 1.69                     | 0.57              |
| 1:A:228:ARG:HD2  | 1:A:244:TYR:HE2  | 1.69                     | 0.57              |
| 1:B:442:LEU:HB3  | 1:C:470:ILE:CD1  | 2.34                     | 0.57              |
| 1:D:122:GLU:HG2  | 1:E:427:SER:CB   | 2.35                     | 0.57              |
| 1:D:144:LEU:HD11 | 1:D:251:TYR:HB3  | 1.85                     | 0.57              |
| 1:E:293:SER:OG   | 1:F:337:ASP:CB   | 2.51                     | 0.57              |
| 1:F:144:LEU:HD11 | 1:F:251:TYR:HB3  | 1.85                     | 0.57              |
| 1:G:311:LEU:HD11 | 1:H:299:LEU:HD21 | 1.86                     | 0.57              |
| 1:K:186:ALA:HB2  | 1:L:171:ASP:CB   | 2.35                     | 0.57              |
| 1:D:131:PHE:HE2  | 1:E:387:GLY:CA   | 2.05                     | 0.57              |
| 1:K:41:SER:HB3   | 1:L:271:GLU:OE1  | 2.04                     | 0.57              |
| 1:L:142:ASN:HB2  | 1:L:163:LEU:HD13 | 1.84                     | 0.57              |
| 1:A:301:ASN:HD22 | 1:L:323:ARG:HG3  | 1.68                     | 0.57              |
| 1:D:186:ALA:HB2  | 1:E:171:ASP:CB   | 2.33                     | 0.57              |
| 1:E:144:LEU:HD11 | 1:E:251:TYR:HB3  | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:228:ARG:HD2  | 1:E:244:TYR:HE2  | 1.69                     | 0.57              |
| 1:I:442:LEU:HB3  | 1:J:470:ILE:HD11 | 1.87                     | 0.57              |
| 1:F:41:SER:HB3   | 1:G:271:GLU:OE1  | 2.05                     | 0.57              |
| 1:I:228:ARG:HD2  | 1:I:244:TYR:HE2  | 1.69                     | 0.57              |
| 1:J:41:SER:HB3   | 1:K:271:GLU:OE1  | 2.05                     | 0.57              |
| 1:K:449:TRP:CH2  | 1:L:461:ILE:HG12 | 2.40                     | 0.57              |
| 1:E:442:LEU:HB3  | 1:F:470:ILE:HD11 | 1.87                     | 0.57              |
| 1:H:228:ARG:HD2  | 1:H:244:TYR:HE2  | 1.69                     | 0.57              |
| 1:J:122:GLU:HG2  | 1:K:427:SER:CB   | 2.35                     | 0.57              |
| 1:F:294:SER:HB2  | 1:G:285:ALA:CB   | 2.35                     | 0.57              |
| 1:I:467:LYS:HD3  | 1:J:460:ASP:HB3  | 1.87                     | 0.57              |
| 1:L:228:ARG:HD2  | 1:L:244:TYR:HE2  | 1.70                     | 0.57              |
| 1:A:41:SER:HB3   | 1:B:271:GLU:OE1  | 2.05                     | 0.56              |
| 1:A:427:SER:CB   | 1:L:122:GLU:HG2  | 2.35                     | 0.56              |
| 1:A:387:GLY:CA   | 1:L:131:PHE:HE2  | 2.05                     | 0.56              |
| 1:C:372:GLU:C    | 1:C:374:ILE:N    | 2.60                     | 0.56              |
| 1:F:228:ARG:HD2  | 1:F:244:TYR:HE2  | 1.69                     | 0.56              |
| 1:H:413:GLN:CB   | 1:I:93:ALA:HB3   | 2.28                     | 0.56              |
| 1:A:329:PHE:CE2  | 1:B:332:LEU:HD22 | 2.40                     | 0.56              |
| 1:B:294:SER:HB2  | 1:C:285:ALA:CB   | 2.36                     | 0.56              |
| 1:G:41:SER:HB3   | 1:H:271:GLU:OE1  | 2.05                     | 0.56              |
| 1:G:228:ARG:HD2  | 1:G:244:TYR:HE2  | 1.69                     | 0.56              |
| 1:H:126:TYR:HE1  | 1:H:158:MET:H    | 1.53                     | 0.56              |
| 1:J:228:ARG:HD2  | 1:J:244:TYR:HE2  | 1.69                     | 0.56              |
| 1:A:285:ALA:CB   | 1:L:294:SER:HB2  | 2.35                     | 0.56              |
| 1:B:8:LEU:HD21   | 1:B:219:LEU:O    | 2.06                     | 0.56              |
| 1:C:41:SER:HB3   | 1:D:271:GLU:OE1  | 2.05                     | 0.56              |
| 1:C:329:PHE:CE2  | 1:D:332:LEU:HD22 | 2.41                     | 0.56              |
| 1:J:126:TYR:HE1  | 1:J:158:MET:H    | 1.53                     | 0.56              |
| 1:K:112:MET:HG2  | 1:L:97:LEU:HD21  | 1.87                     | 0.56              |
| 1:B:413:GLN:CB   | 1:C:93:ALA:HB3   | 2.27                     | 0.56              |
| 1:J:329:PHE:CE2  | 1:K:332:LEU:CD2  | 2.88                     | 0.56              |
| 1:L:372:GLU:C    | 1:L:374:ILE:N    | 2.60                     | 0.56              |
| 1:D:323:ARG:HG3  | 1:E:301:ASN:HD22 | 1.66                     | 0.56              |
| 1:E:41:SER:HB3   | 1:F:271:GLU:OE1  | 2.04                     | 0.56              |
| 1:I:41:SER:HB3   | 1:J:271:GLU:OE1  | 2.05                     | 0.56              |
| 1:J:80:MET:HE3   | 1:K:430:LEU:HD23 | 1.88                     | 0.56              |
| 1:K:126:TYR:HE1  | 1:K:158:MET:H    | 1.53                     | 0.56              |
| 1:B:439:LEU:HD12 | 1:C:473:ALA:HB3  | 1.87                     | 0.56              |
| 1:D:8:LEU:HD21   | 1:D:219:LEU:O    | 2.06                     | 0.56              |
| 1:F:8:LEU:HD21   | 1:F:219:LEU:O    | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:372:GLU:C    | 1:F:374:ILE:N    | 2.60                     | 0.56              |
| 1:H:8:LEU:HD21   | 1:H:219:LEU:O    | 2.06                     | 0.56              |
| 1:I:329:PHE:CE2  | 1:J:332:LEU:HD22 | 2.41                     | 0.56              |
| 1:K:8:LEU:HD21   | 1:K:219:LEU:O    | 2.06                     | 0.56              |
| 1:H:439:LEU:HD12 | 1:I:473:ALA:HB3  | 1.86                     | 0.56              |
| 1:J:372:GLU:C    | 1:J:374:ILE:N    | 2.60                     | 0.56              |
| 1:J:413:GLN:H    | 1:K:93:ALA:HB3   | 1.70                     | 0.56              |
| 1:K:372:GLU:C    | 1:K:374:ILE:N    | 2.60                     | 0.56              |
| 1:C:8:LEU:HD21   | 1:C:219:LEU:O    | 2.06                     | 0.56              |
| 1:C:115:ARG:NH2  | 1:D:476:ILE:N    | 2.53                     | 0.56              |
| 1:C:467:LYS:HD3  | 1:D:460:ASP:HB3  | 1.88                     | 0.56              |
| 1:D:329:PHE:CE2  | 1:E:332:LEU:CD2  | 2.88                     | 0.56              |
| 1:E:30:ARG:HH12  | 1:E:266:ARG:NH2  | 2.04                     | 0.56              |
| 1:H:294:SER:HB2  | 1:I:285:ALA:CB   | 2.36                     | 0.56              |
| 1:L:8:LEU:HD21   | 1:L:219:LEU:O    | 2.06                     | 0.56              |
| 1:L:30:ARG:HH12  | 1:L:266:ARG:NH2  | 2.04                     | 0.56              |
| 1:G:17:TYR:HB2   | 1:G:180:VAL:HG11 | 1.88                     | 0.56              |
| 1:I:8:LEU:HD21   | 1:I:219:LEU:O    | 2.06                     | 0.56              |
| 1:I:17:TYR:HB2   | 1:I:180:VAL:HG11 | 1.88                     | 0.56              |
| 1:I:30:ARG:HH12  | 1:I:266:ARG:NH2  | 2.04                     | 0.56              |
| 1:B:122:GLU:HG2  | 1:C:427:SER:CB   | 2.36                     | 0.55              |
| 1:D:112:MET:HG2  | 1:E:97:LEU:HD21  | 1.88                     | 0.55              |
| 1:D:126:TYR:HE1  | 1:D:158:MET:H    | 1.53                     | 0.55              |
| 1:E:8:LEU:HD21   | 1:E:219:LEU:O    | 2.06                     | 0.55              |
| 1:H:30:ARG:HH12  | 1:H:266:ARG:NH2  | 2.04                     | 0.55              |
| 1:A:30:ARG:HH12  | 1:A:266:ARG:NH2  | 2.04                     | 0.55              |
| 1:F:30:ARG:HH12  | 1:F:266:ARG:NH2  | 2.04                     | 0.55              |
| 1:F:442:LEU:HB3  | 1:G:470:ILE:CD1  | 2.35                     | 0.55              |
| 1:G:30:ARG:HH12  | 1:G:266:ARG:NH2  | 2.04                     | 0.55              |
| 1:A:186:ALA:HB2  | 1:B:171:ASP:CB   | 2.37                     | 0.55              |
| 1:C:126:TYR:HE1  | 1:C:158:MET:H    | 1.53                     | 0.55              |
| 1:D:30:ARG:HH12  | 1:D:266:ARG:NH2  | 2.04                     | 0.55              |
| 1:F:122:GLU:HG2  | 1:G:427:SER:CB   | 2.36                     | 0.55              |
| 1:F:126:TYR:HE1  | 1:F:158:MET:H    | 1.53                     | 0.55              |
| 1:K:228:ARG:HD2  | 1:K:244:TYR:HE2  | 1.69                     | 0.55              |
| 1:A:8:LEU:HD21   | 1:A:219:LEU:O    | 2.06                     | 0.55              |
| 1:A:473:ALA:HB2  | 1:L:439:LEU:HB2  | 1.85                     | 0.55              |
| 1:D:80:MET:SD    | 1:E:431:GLU:HA   | 2.47                     | 0.55              |
| 1:G:126:TYR:HE1  | 1:G:158:MET:H    | 1.53                     | 0.55              |
| 1:I:126:TYR:HE1  | 1:I:158:MET:H    | 1.53                     | 0.55              |
| 1:I:367:GLU:HB3  | 1:J:376:TYR:CE1  | 2.41                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:372:GLU:C    | 1:I:374:ILE:N    | 2.60                     | 0.55              |
| 1:J:17:TYR:HB2   | 1:J:180:VAL:HG11 | 1.88                     | 0.55              |
| 1:A:126:TYR:HE1  | 1:A:158:MET:H    | 1.53                     | 0.55              |
| 1:B:17:TYR:HB2   | 1:B:180:VAL:HG11 | 1.88                     | 0.55              |
| 1:D:413:GLN:H    | 1:E:93:ALA:HB3   | 1.72                     | 0.55              |
| 1:F:17:TYR:HB2   | 1:F:180:VAL:HG11 | 1.88                     | 0.55              |
| 1:K:30:ARG:HH12  | 1:K:266:ARG:NH2  | 2.04                     | 0.55              |
| 1:A:430:LEU:HD23 | 1:L:80:MET:HE3   | 1.89                     | 0.55              |
| 1:B:126:TYR:HE1  | 1:B:158:MET:H    | 1.53                     | 0.55              |
| 1:L:126:TYR:HE1  | 1:L:158:MET:H    | 1.53                     | 0.55              |
| 1:J:30:ARG:HH12  | 1:J:266:ARG:NH2  | 2.04                     | 0.55              |
| 1:A:17:TYR:HB2   | 1:A:180:VAL:HG11 | 1.88                     | 0.55              |
| 1:A:133:ALA:HB1  | 1:A:143:VAL:HG11 | 1.89                     | 0.55              |
| 1:C:17:TYR:HB2   | 1:C:180:VAL:HG11 | 1.88                     | 0.55              |
| 1:G:8:LEU:HD21   | 1:G:219:LEU:O    | 2.06                     | 0.55              |
| 1:L:133:ALA:HB1  | 1:L:143:VAL:HG11 | 1.89                     | 0.55              |
| 1:A:93:ALA:HB1   | 1:L:413:GLN:HB2  | 1.83                     | 0.55              |
| 1:B:372:GLU:C    | 1:B:374:ILE:N    | 2.60                     | 0.55              |
| 1:F:115:ARG:NH2  | 1:G:475:GLY:C    | 2.65                     | 0.55              |
| 1:G:442:LEU:HB3  | 1:H:470:ILE:HD11 | 1.89                     | 0.55              |
| 1:H:122:GLU:HG2  | 1:I:427:SER:CB   | 2.36                     | 0.55              |
| 1:A:93:ALA:HB3   | 1:L:413:GLN:H    | 1.72                     | 0.55              |
| 1:A:271:GLU:OE1  | 1:L:41:SER:HB3   | 2.07                     | 0.55              |
| 1:A:431:GLU:HA   | 1:L:80:MET:SD    | 2.47                     | 0.55              |
| 1:B:41:SER:HB3   | 1:C:271:GLU:OE1  | 2.06                     | 0.55              |
| 1:B:133:ALA:HB1  | 1:B:143:VAL:HG11 | 1.89                     | 0.55              |
| 1:E:17:TYR:HB2   | 1:E:180:VAL:HG11 | 1.88                     | 0.55              |
| 1:E:439:LEU:CD1  | 1:F:473:ALA:CB   | 2.84                     | 0.55              |
| 1:K:17:TYR:HB2   | 1:K:180:VAL:HG11 | 1.88                     | 0.55              |
| 1:K:133:ALA:HB1  | 1:K:143:VAL:HG11 | 1.89                     | 0.55              |
| 1:E:126:TYR:HE1  | 1:E:158:MET:H    | 1.53                     | 0.54              |
| 1:F:413:GLN:H    | 1:G:93:ALA:HB3   | 1.72                     | 0.54              |
| 1:F:439:LEU:HD12 | 1:G:473:ALA:HB3  | 1.89                     | 0.54              |
| 1:H:442:LEU:HB3  | 1:I:470:ILE:CD1  | 2.34                     | 0.54              |
| 1:J:133:ALA:HB1  | 1:J:143:VAL:HG11 | 1.89                     | 0.54              |
| 1:K:129:THR:HG21 | 1:K:158:MET:O    | 2.07                     | 0.54              |
| 1:K:439:LEU:CD1  | 1:L:473:ALA:CB   | 2.85                     | 0.54              |
| 1:B:30:ARG:HH12  | 1:B:266:ARG:NH2  | 2.04                     | 0.54              |
| 1:C:30:ARG:HH12  | 1:C:266:ARG:NH2  | 2.04                     | 0.54              |
| 1:D:17:TYR:HB2   | 1:D:180:VAL:HG11 | 1.88                     | 0.54              |
| 1:F:108:GLU:HB3  | 1:F:112:MET:HE3  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:108:GLU:HB3  | 1:G:112:MET:HE3  | 1.90                     | 0.54              |
| 1:H:17:TYR:HB2   | 1:H:180:VAL:HG11 | 1.88                     | 0.54              |
| 1:J:8:LEU:HD21   | 1:J:219:LEU:O    | 2.06                     | 0.54              |
| 1:L:17:TYR:HB2   | 1:L:180:VAL:HG11 | 1.88                     | 0.54              |
| 1:A:129:THR:HG21 | 1:A:158:MET:O    | 2.07                     | 0.54              |
| 1:H:41:SER:HB3   | 1:I:271:GLU:OE1  | 2.06                     | 0.54              |
| 1:H:108:GLU:HB3  | 1:H:112:MET:HE3  | 1.90                     | 0.54              |
| 1:I:115:ARG:NH2  | 1:J:476:ILE:N    | 2.56                     | 0.54              |
| 1:I:108:GLU:HB3  | 1:I:112:MET:HE3  | 1.90                     | 0.54              |
| 1:J:129:THR:HG21 | 1:J:158:MET:O    | 2.07                     | 0.54              |
| 1:L:108:GLU:HB3  | 1:L:112:MET:HE3  | 1.90                     | 0.54              |
| 1:B:108:GLU:HB3  | 1:B:112:MET:HE3  | 1.90                     | 0.54              |
| 1:E:108:GLU:HB3  | 1:E:112:MET:HE3  | 1.90                     | 0.54              |
| 1:E:186:ALA:HB2  | 1:F:171:ASP:CB   | 2.36                     | 0.54              |
| 1:I:129:THR:HG21 | 1:I:158:MET:O    | 2.07                     | 0.54              |
| 1:J:108:GLU:HB3  | 1:J:112:MET:HE3  | 1.90                     | 0.54              |
| 1:K:108:GLU:HB3  | 1:K:112:MET:HE3  | 1.90                     | 0.54              |
| 1:L:17:TYR:CZ    | 1:L:182:ARG:HG3  | 2.43                     | 0.54              |
| 1:A:332:LEU:CD2  | 1:L:329:PHE:CE2  | 2.91                     | 0.54              |
| 1:C:133:ALA:HB1  | 1:C:143:VAL:HG11 | 1.89                     | 0.54              |
| 1:C:186:ALA:HB2  | 1:D:171:ASP:CB   | 2.37                     | 0.54              |
| 1:D:41:SER:HB3   | 1:E:271:GLU:OE1  | 2.06                     | 0.54              |
| 1:F:413:GLN:CB   | 1:G:93:ALA:HB1   | 2.37                     | 0.54              |
| 1:K:17:TYR:CZ    | 1:K:182:ARG:HG3  | 2.43                     | 0.54              |
| 1:A:17:TYR:CZ    | 1:A:182:ARG:HG3  | 2.43                     | 0.54              |
| 1:A:108:GLU:HB3  | 1:A:112:MET:HE3  | 1.90                     | 0.54              |
| 1:C:108:GLU:HB3  | 1:C:112:MET:HE3  | 1.90                     | 0.54              |
| 1:H:372:GLU:C    | 1:H:374:ILE:N    | 2.60                     | 0.54              |
| 1:I:133:ALA:HB1  | 1:I:143:VAL:HG11 | 1.89                     | 0.54              |
| 1:A:97:LEU:HD21  | 1:L:112:MET:HG2  | 1.89                     | 0.54              |
| 1:E:372:GLU:C    | 1:E:374:ILE:N    | 2.60                     | 0.54              |
| 1:J:17:TYR:CZ    | 1:J:182:ARG:HG3  | 2.43                     | 0.54              |
| 1:J:115:ARG:NH2  | 1:K:475:GLY:C    | 2.66                     | 0.54              |
| 1:B:17:TYR:CZ    | 1:B:182:ARG:HG3  | 2.43                     | 0.54              |
| 1:C:17:TYR:CZ    | 1:C:182:ARG:HG3  | 2.43                     | 0.54              |
| 1:E:329:PHE:CE2  | 1:F:332:LEU:HD22 | 2.43                     | 0.54              |
| 1:F:129:THR:HG21 | 1:F:158:MET:O    | 2.07                     | 0.54              |
| 1:I:122:GLU:HG2  | 1:J:427:SER:CB   | 2.38                     | 0.54              |
| 1:D:108:GLU:HB3  | 1:D:112:MET:HE3  | 1.90                     | 0.54              |
| 1:G:467:LYS:HD3  | 1:H:460:ASP:HB3  | 1.90                     | 0.54              |
| 1:H:133:ALA:HB1  | 1:H:143:VAL:HG11 | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:439:LEU:HD12 | 1:K:473:ALA:HB3  | 1.89                     | 0.54              |
| 1:D:17:TYR:CZ    | 1:D:182:ARG:HG3  | 2.43                     | 0.53              |
| 1:D:413:GLN:CB   | 1:E:93:ALA:HB3   | 2.31                     | 0.53              |
| 1:I:17:TYR:CZ    | 1:I:182:ARG:HG3  | 2.43                     | 0.53              |
| 1:B:129:THR:HG21 | 1:B:158:MET:O    | 2.07                     | 0.53              |
| 1:E:17:TYR:CZ    | 1:E:182:ARG:HG3  | 2.43                     | 0.53              |
| 1:F:133:ALA:HB1  | 1:F:143:VAL:HG11 | 1.89                     | 0.53              |
| 1:H:129:THR:HG21 | 1:H:158:MET:O    | 2.07                     | 0.53              |
| 1:I:122:GLU:HG2  | 1:J:427:SER:OG   | 2.08                     | 0.53              |
| 1:A:467:LYS:HD3  | 1:B:460:ASP:HB3  | 1.91                     | 0.53              |
| 1:C:439:LEU:CD1  | 1:D:473:ALA:HB3  | 2.38                     | 0.53              |
| 1:D:129:THR:HG21 | 1:D:158:MET:O    | 2.07                     | 0.53              |
| 1:B:80:MET:SD    | 1:C:431:GLU:HA   | 2.48                     | 0.53              |
| 1:B:413:GLN:H    | 1:C:93:ALA:HB3   | 1.73                     | 0.53              |
| 1:C:367:GLU:HB3  | 1:D:376:TYR:CE1  | 2.43                     | 0.53              |
| 1:C:442:LEU:HB3  | 1:D:470:ILE:HD11 | 1.89                     | 0.53              |
| 1:E:129:THR:HG21 | 1:E:158:MET:O    | 2.07                     | 0.53              |
| 1:G:133:ALA:HB1  | 1:G:143:VAL:HG11 | 1.89                     | 0.53              |
| 1:H:413:GLN:H    | 1:I:93:ALA:HB3   | 1.74                     | 0.53              |
| 1:K:413:GLN:HB2  | 1:L:93:ALA:HB1   | 1.89                     | 0.53              |
| 1:D:133:ALA:HB1  | 1:D:143:VAL:HG11 | 1.89                     | 0.53              |
| 1:D:413:GLN:CB   | 1:E:93:ALA:CB    | 2.79                     | 0.53              |
| 1:E:133:ALA:HB1  | 1:E:143:VAL:HG11 | 1.89                     | 0.53              |
| 1:H:17:TYR:CZ    | 1:H:182:ARG:HG3  | 2.43                     | 0.53              |
| 1:L:129:THR:HG21 | 1:L:158:MET:O    | 2.07                     | 0.53              |
| 1:C:108:GLU:O    | 1:C:112:MET:HG3  | 2.09                     | 0.53              |
| 1:C:129:THR:HG21 | 1:C:158:MET:O    | 2.07                     | 0.53              |
| 1:F:17:TYR:CZ    | 1:F:182:ARG:HG3  | 2.43                     | 0.53              |
| 1:G:17:TYR:CZ    | 1:G:182:ARG:HG3  | 2.43                     | 0.53              |
| 1:B:413:GLN:CB   | 1:C:93:ALA:HB1   | 2.39                     | 0.53              |
| 1:D:108:GLU:O    | 1:D:112:MET:HG3  | 2.09                     | 0.53              |
| 1:A:442:LEU:HB3  | 1:B:470:ILE:HD11 | 1.90                     | 0.53              |
| 1:D:80:MET:HE3   | 1:E:430:LEU:HD23 | 1.90                     | 0.53              |
| 1:A:108:GLU:O    | 1:A:112:MET:HG3  | 2.09                     | 0.53              |
| 1:H:311:LEU:HD11 | 1:I:299:LEU:HD21 | 1.91                     | 0.53              |
| 1:F:112:MET:SD   | 1:F:415:PRO:HB3  | 2.49                     | 0.53              |
| 1:K:367:GLU:HB3  | 1:L:376:TYR:CE1  | 2.44                     | 0.53              |
| 1:D:112:MET:SD   | 1:D:415:PRO:HB3  | 2.49                     | 0.52              |
| 1:E:108:GLU:O    | 1:E:112:MET:HG3  | 2.09                     | 0.52              |
| 1:E:122:GLU:HG2  | 1:F:427:SER:CB   | 2.39                     | 0.52              |
| 1:H:80:MET:SD    | 1:I:431:GLU:HA   | 2.49                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:413:GLN:CB   | 1:I:93:ALA:HB1   | 2.39                     | 0.52              |
| 1:I:112:MET:HG2  | 1:J:97:LEU:CD2   | 2.39                     | 0.52              |
| 1:J:439:LEU:HB2  | 1:K:473:ALA:HB2  | 1.87                     | 0.52              |
| 1:L:108:GLU:O    | 1:L:112:MET:HG3  | 2.09                     | 0.52              |
| 1:A:367:GLU:HB3  | 1:B:376:TYR:CE1  | 2.45                     | 0.52              |
| 1:K:108:GLU:O    | 1:K:112:MET:HG3  | 2.09                     | 0.52              |
| 1:B:108:GLU:O    | 1:B:112:MET:HG3  | 2.09                     | 0.52              |
| 1:C:112:MET:SD   | 1:C:415:PRO:HB3  | 2.49                     | 0.52              |
| 1:E:367:GLU:HB3  | 1:F:376:TYR:CE1  | 2.44                     | 0.52              |
| 1:G:129:THR:HG21 | 1:G:158:MET:O    | 2.07                     | 0.52              |
| 1:G:367:GLU:HB3  | 1:H:376:TYR:CE1  | 2.44                     | 0.52              |
| 1:H:115:ARG:NH2  | 1:I:475:GLY:C    | 2.68                     | 0.52              |
| 1:K:112:MET:SD   | 1:K:415:PRO:HB3  | 2.49                     | 0.52              |
| 1:K:323:ARG:HG3  | 1:L:301:ASN:HD22 | 1.73                     | 0.52              |
| 1:B:115:ARG:NH2  | 1:C:475:GLY:C    | 2.67                     | 0.52              |
| 1:J:80:MET:SD    | 1:K:431:GLU:HA   | 2.49                     | 0.52              |
| 1:D:363:GLN:HB3  | 1:D:376:TYR:HE2  | 1.75                     | 0.52              |
| 1:G:186:ALA:HB2  | 1:H:171:ASP:CB   | 2.38                     | 0.52              |
| 1:H:329:PHE:CE2  | 1:I:332:LEU:CD2  | 2.93                     | 0.52              |
| 1:J:108:GLU:O    | 1:J:112:MET:HG3  | 2.09                     | 0.52              |
| 1:J:112:MET:SD   | 1:J:415:PRO:HB3  | 2.49                     | 0.52              |
| 1:K:442:LEU:HB3  | 1:L:470:ILE:HD11 | 1.90                     | 0.52              |
| 1:D:44:PRO:HB3   | 1:D:54:TYR:OH    | 2.10                     | 0.52              |
| 1:E:112:MET:SD   | 1:E:415:PRO:HB3  | 2.49                     | 0.52              |
| 1:F:80:MET:SD    | 1:G:431:GLU:HA   | 2.50                     | 0.52              |
| 1:F:142:ASN:HD21 | 1:F:255:ARG:HG2  | 1.75                     | 0.52              |
| 1:F:329:PHE:CE2  | 1:G:332:LEU:CD2  | 2.92                     | 0.52              |
| 1:G:44:PRO:HB3   | 1:G:54:TYR:OH    | 2.10                     | 0.52              |
| 1:H:44:PRO:HB3   | 1:H:54:TYR:OH    | 2.10                     | 0.52              |
| 1:H:363:GLN:HB3  | 1:H:376:TYR:HE2  | 1.75                     | 0.52              |
| 1:I:44:PRO:HB3   | 1:I:54:TYR:OH    | 2.10                     | 0.52              |
| 1:L:363:GLN:HB3  | 1:L:376:TYR:HE2  | 1.75                     | 0.52              |
| 1:E:142:ASN:HD21 | 1:E:255:ARG:HG2  | 1.75                     | 0.52              |
| 1:F:44:PRO:HB3   | 1:F:54:TYR:OH    | 2.10                     | 0.52              |
| 1:K:122:GLU:HG2  | 1:L:427:SER:HB3  | 1.92                     | 0.52              |
| 1:K:363:GLN:HB3  | 1:K:376:TYR:HE2  | 1.75                     | 0.52              |
| 1:E:122:GLU:HG2  | 1:F:427:SER:HB3  | 1.90                     | 0.52              |
| 1:E:363:GLN:HB3  | 1:E:376:TYR:HE2  | 1.75                     | 0.52              |
| 1:H:142:ASN:HD21 | 1:H:255:ARG:HG2  | 1.75                     | 0.52              |
| 1:A:363:GLN:HB3  | 1:A:376:TYR:HE2  | 1.75                     | 0.52              |
| 1:G:112:MET:SD   | 1:G:415:PRO:HB3  | 2.49                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:142:ASN:HD21 | 1:G:255:ARG:HG2  | 1.75                     | 0.52              |
| 1:G:329:PHE:CE2  | 1:H:332:LEU:HD23 | 2.44                     | 0.52              |
| 1:F:108:GLU:O    | 1:F:112:MET:HG3  | 2.09                     | 0.52              |
| 1:F:115:ARG:HH22 | 1:G:475:GLY:C    | 2.18                     | 0.52              |
| 1:F:311:LEU:HD11 | 1:G:299:LEU:HD21 | 1.91                     | 0.52              |
| 1:F:363:GLN:HB3  | 1:F:376:TYR:HE2  | 1.75                     | 0.52              |
| 1:G:363:GLN:HB3  | 1:G:376:TYR:HE2  | 1.75                     | 0.52              |
| 1:H:112:MET:SD   | 1:H:415:PRO:HB3  | 2.49                     | 0.52              |
| 1:I:112:MET:SD   | 1:I:415:PRO:HB3  | 2.49                     | 0.52              |
| 1:A:369:VAL:HG12 | 1:A:370:THR:H    | 1.76                     | 0.51              |
| 1:D:142:ASN:HD21 | 1:D:255:ARG:HG2  | 1.75                     | 0.51              |
| 1:G:112:MET:HG2  | 1:H:97:LEU:CD2   | 2.40                     | 0.51              |
| 1:H:108:GLU:O    | 1:H:112:MET:HG3  | 2.09                     | 0.51              |
| 1:I:122:GLU:HG2  | 1:J:427:SER:HB3  | 1.91                     | 0.51              |
| 1:K:44:PRO:HB3   | 1:K:54:TYR:OH    | 2.10                     | 0.51              |
| 1:L:112:MET:SD   | 1:L:415:PRO:HB3  | 2.49                     | 0.51              |
| 1:A:112:MET:SD   | 1:A:415:PRO:HB3  | 2.49                     | 0.51              |
| 1:C:363:GLN:HB3  | 1:C:376:TYR:HE2  | 1.75                     | 0.51              |
| 1:G:323:ARG:HG3  | 1:H:301:ASN:HD22 | 1.74                     | 0.51              |
| 1:C:369:VAL:HG12 | 1:C:370:THR:H    | 1.76                     | 0.51              |
| 1:D:372:GLU:C    | 1:D:374:ILE:N    | 2.60                     | 0.51              |
| 1:I:363:GLN:HB3  | 1:I:376:TYR:HE2  | 1.75                     | 0.51              |
| 1:C:44:PRO:HB3   | 1:C:54:TYR:OH    | 2.10                     | 0.51              |
| 1:F:115:ARG:HH21 | 1:G:476:ILE:N    | 2.09                     | 0.51              |
| 1:G:108:GLU:O    | 1:G:112:MET:HG3  | 2.09                     | 0.51              |
| 1:J:115:ARG:HH21 | 1:K:476:ILE:N    | 2.07                     | 0.51              |
| 1:J:413:GLN:CB   | 1:K:93:ALA:HB1   | 2.39                     | 0.51              |
| 1:K:329:PHE:CE2  | 1:L:332:LEU:HD22 | 2.44                     | 0.51              |
| 1:K:369:VAL:HG12 | 1:K:370:THR:H    | 1.76                     | 0.51              |
| 1:A:142:ASN:HD21 | 1:A:255:ARG:HG2  | 1.75                     | 0.51              |
| 1:B:112:MET:SD   | 1:B:415:PRO:HB3  | 2.49                     | 0.51              |
| 1:B:311:LEU:HD11 | 1:C:299:LEU:HD21 | 1.93                     | 0.51              |
| 1:B:329:PHE:CE2  | 1:C:332:LEU:CD2  | 2.93                     | 0.51              |
| 1:F:369:VAL:HG12 | 1:F:370:THR:H    | 1.75                     | 0.51              |
| 1:G:439:LEU:CD1  | 1:H:473:ALA:HB3  | 2.40                     | 0.51              |
| 1:I:108:GLU:O    | 1:I:112:MET:HG3  | 2.09                     | 0.51              |
| 1:I:369:VAL:HG12 | 1:I:370:THR:H    | 1.75                     | 0.51              |
| 1:A:329:PHE:CE2  | 1:B:332:LEU:HD23 | 2.45                     | 0.51              |
| 1:B:44:PRO:HB3   | 1:B:54:TYR:OH    | 2.10                     | 0.51              |
| 1:C:142:ASN:HD21 | 1:C:255:ARG:HG2  | 1.75                     | 0.51              |
| 1:D:112:MET:HG2  | 1:E:97:LEU:CD2   | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:369:VAL:HG12 | 1:E:370:THR:H    | 1.76                     | 0.51              |
| 1:J:369:VAL:HG12 | 1:J:370:THR:H    | 1.76                     | 0.51              |
| 1:D:122:GLU:HG2  | 1:E:427:SER:OG   | 2.10                     | 0.51              |
| 1:D:369:VAL:HG12 | 1:D:370:THR:H    | 1.76                     | 0.51              |
| 1:E:112:MET:HG2  | 1:F:97:LEU:CD2   | 2.39                     | 0.51              |
| 1:G:122:GLU:HG2  | 1:H:427:SER:CB   | 2.41                     | 0.51              |
| 1:I:142:ASN:HD21 | 1:I:255:ARG:HG2  | 1.75                     | 0.51              |
| 1:J:363:GLN:HB3  | 1:J:376:TYR:HE2  | 1.75                     | 0.51              |
| 1:A:44:PRO:HB3   | 1:A:54:TYR:OH    | 2.10                     | 0.51              |
| 1:E:122:GLU:HG2  | 1:F:427:SER:OG   | 2.11                     | 0.51              |
| 1:J:112:MET:HG2  | 1:K:97:LEU:HD21  | 1.91                     | 0.51              |
| 1:A:427:SER:OG   | 1:L:122:GLU:HG2  | 2.10                     | 0.51              |
| 1:B:142:ASN:HD21 | 1:B:255:ARG:HG2  | 1.75                     | 0.51              |
| 1:B:369:VAL:HG12 | 1:B:370:THR:H    | 1.76                     | 0.51              |
| 1:C:122:GLU:HG2  | 1:D:427:SER:HB3  | 1.93                     | 0.51              |
| 1:H:369:VAL:HG12 | 1:H:370:THR:H    | 1.76                     | 0.51              |
| 1:K:80:MET:HE3   | 1:L:430:LEU:HD23 | 1.92                     | 0.51              |
| 1:B:363:GLN:HB3  | 1:B:376:TYR:HE2  | 1.75                     | 0.51              |
| 1:C:122:GLU:HG2  | 1:D:427:SER:OG   | 2.11                     | 0.51              |
| 1:E:44:PRO:HB3   | 1:E:54:TYR:OH    | 2.10                     | 0.51              |
| 1:J:142:ASN:HD21 | 1:J:255:ARG:HG2  | 1.75                     | 0.51              |
| 1:I:67:ASN:ND2   | 1:J:386:GLY:HA2  | 2.26                     | 0.50              |
| 1:J:413:GLN:CB   | 1:K:93:ALA:HB3   | 2.30                     | 0.50              |
| 1:K:122:GLU:HG2  | 1:L:427:SER:CB   | 2.41                     | 0.50              |
| 1:K:165:SER:O    | 1:K:165:SER:OG   | 2.30                     | 0.50              |
| 1:A:357:MET:HB2  | 1:A:385:LEU:HD21 | 1.94                     | 0.50              |
| 1:B:340:VAL:O    | 1:B:344:VAL:HG12 | 2.12                     | 0.50              |
| 1:B:357:MET:HB2  | 1:B:385:LEU:HD21 | 1.94                     | 0.50              |
| 1:H:357:MET:HB2  | 1:H:385:LEU:HD21 | 1.94                     | 0.50              |
| 1:I:357:MET:HB2  | 1:I:385:LEU:HD21 | 1.94                     | 0.50              |
| 1:J:44:PRO:HB3   | 1:J:54:TYR:OH    | 2.10                     | 0.50              |
| 1:L:44:PRO:HB3   | 1:L:54:TYR:OH    | 2.10                     | 0.50              |
| 1:E:340:VAL:O    | 1:E:344:VAL:HG12 | 2.12                     | 0.50              |
| 1:I:340:VAL:O    | 1:I:344:VAL:HG12 | 2.12                     | 0.50              |
| 1:I:439:LEU:CD1  | 1:J:473:ALA:HB3  | 2.36                     | 0.50              |
| 1:J:115:ARG:HH22 | 1:K:475:GLY:C    | 2.19                     | 0.50              |
| 1:L:357:MET:HB2  | 1:L:385:LEU:HD21 | 1.94                     | 0.50              |
| 1:A:122:GLU:HG2  | 1:B:427:SER:HB3  | 1.94                     | 0.50              |
| 1:G:369:VAL:HG12 | 1:G:370:THR:H    | 1.76                     | 0.50              |
| 1:H:340:VAL:O    | 1:H:344:VAL:HG12 | 2.12                     | 0.50              |
| 1:J:357:MET:HB2  | 1:J:385:LEU:HD21 | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:340:VAL:O    | 1:L:344:VAL:HG12 | 2.12                     | 0.50              |
| 1:C:357:MET:HB2  | 1:C:385:LEU:HD21 | 1.94                     | 0.50              |
| 1:G:122:GLU:HG2  | 1:H:427:SER:OG   | 2.11                     | 0.50              |
| 1:K:340:VAL:O    | 1:K:344:VAL:HG12 | 2.12                     | 0.50              |
| 1:A:340:VAL:O    | 1:A:344:VAL:HG12 | 2.12                     | 0.50              |
| 1:C:122:GLU:HG2  | 1:D:427:SER:CB   | 2.41                     | 0.50              |
| 1:C:329:PHE:CE2  | 1:D:332:LEU:HD23 | 2.46                     | 0.50              |
| 1:D:115:ARG:NH2  | 1:E:475:GLY:C    | 2.70                     | 0.50              |
| 1:F:340:VAL:O    | 1:F:344:VAL:HG12 | 2.12                     | 0.50              |
| 1:G:357:MET:HB2  | 1:G:385:LEU:HD21 | 1.94                     | 0.50              |
| 1:K:142:ASN:HD21 | 1:K:255:ARG:HG2  | 1.75                     | 0.50              |
| 1:L:142:ASN:HD21 | 1:L:255:ARG:HG2  | 1.75                     | 0.50              |
| 1:A:323:ARG:HG3  | 1:B:301:ASN:HD22 | 1.74                     | 0.50              |
| 1:D:126:TYR:HE1  | 1:D:158:MET:N    | 2.10                     | 0.50              |
| 1:K:357:MET:HB2  | 1:K:385:LEU:HD21 | 1.94                     | 0.50              |
| 1:L:126:TYR:HE1  | 1:L:158:MET:N    | 2.10                     | 0.50              |
| 1:L:369:VAL:HG12 | 1:L:370:THR:H    | 1.76                     | 0.50              |
| 1:A:126:TYR:HE1  | 1:A:158:MET:N    | 2.10                     | 0.50              |
| 1:A:299:LEU:HD21 | 1:L:311:LEU:HD11 | 1.93                     | 0.50              |
| 1:B:126:TYR:HE1  | 1:B:158:MET:N    | 2.10                     | 0.50              |
| 1:B:439:LEU:HB2  | 1:C:473:ALA:HB2  | 1.90                     | 0.50              |
| 1:C:126:TYR:HE1  | 1:C:158:MET:N    | 2.10                     | 0.50              |
| 1:C:340:VAL:O    | 1:C:344:VAL:HG12 | 2.12                     | 0.50              |
| 1:D:165:SER:O    | 1:D:165:SER:OG   | 2.30                     | 0.50              |
| 1:F:126:TYR:HE1  | 1:F:158:MET:N    | 2.10                     | 0.50              |
| 1:H:439:LEU:HB2  | 1:I:473:ALA:HB2  | 1.89                     | 0.50              |
| 1:I:186:ALA:HB2  | 1:J:171:ASP:CB   | 2.39                     | 0.50              |
| 1:K:126:TYR:HE1  | 1:K:158:MET:N    | 2.10                     | 0.50              |
| 1:A:93:ALA:HB3   | 1:L:413:GLN:CB   | 2.30                     | 0.50              |
| 1:D:340:VAL:O    | 1:D:344:VAL:HG12 | 2.12                     | 0.50              |
| 1:E:126:TYR:HE1  | 1:E:158:MET:N    | 2.10                     | 0.50              |
| 1:E:413:GLN:HB2  | 1:F:93:ALA:HB1   | 1.92                     | 0.50              |
| 1:F:357:MET:HB2  | 1:F:385:LEU:HD21 | 1.94                     | 0.50              |
| 1:H:126:TYR:HE1  | 1:H:158:MET:N    | 2.10                     | 0.50              |
| 1:J:126:TYR:HE1  | 1:J:158:MET:N    | 2.10                     | 0.50              |
| 1:A:97:LEU:CD2   | 1:L:112:MET:HG2  | 2.41                     | 0.49              |
| 1:A:475:GLY:C    | 1:L:115:ARG:NH2  | 2.70                     | 0.49              |
| 1:C:112:MET:HG2  | 1:D:97:LEU:CD2   | 2.41                     | 0.49              |
| 1:D:357:MET:HB2  | 1:D:385:LEU:HD21 | 1.94                     | 0.49              |
| 1:G:126:TYR:HE1  | 1:G:158:MET:N    | 2.10                     | 0.49              |
| 1:H:115:ARG:HH22 | 1:I:475:GLY:C    | 2.20                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:80:MET:SD    | 1:J:431:GLU:HA   | 2.52                     | 0.49              |
| 1:I:126:TYR:HE1  | 1:I:158:MET:N    | 2.10                     | 0.49              |
| 1:A:122:GLU:HG2  | 1:B:427:SER:CB   | 2.42                     | 0.49              |
| 1:G:67:ASN:ND2   | 1:H:386:GLY:HA2  | 2.27                     | 0.49              |
| 1:A:439:LEU:CD1  | 1:B:473:ALA:HB3  | 2.41                     | 0.49              |
| 1:D:327:ILE:HD12 | 1:E:330:LEU:CD1  | 2.42                     | 0.49              |
| 1:J:172:ALA:HA   | 1:J:261:GLY:HA2  | 1.95                     | 0.49              |
| 1:I:172:ALA:HA   | 1:I:261:GLY:HA2  | 1.95                     | 0.49              |
| 1:I:329:PHE:CE2  | 1:J:332:LEU:HD23 | 2.47                     | 0.49              |
| 1:J:112:MET:HG2  | 1:K:97:LEU:CD2   | 2.42                     | 0.49              |
| 1:J:340:VAL:O    | 1:J:344:VAL:HG12 | 2.12                     | 0.49              |
| 1:K:172:ALA:HA   | 1:K:261:GLY:HA2  | 1.95                     | 0.49              |
| 1:A:93:ALA:HB1   | 1:L:413:GLN:CB   | 2.42                     | 0.49              |
| 1:B:61:VAL:HG22  | 1:B:64:ARG:HH22  | 1.78                     | 0.49              |
| 1:B:112:MET:HG2  | 1:C:97:LEU:HD21  | 1.94                     | 0.49              |
| 1:E:357:MET:HB2  | 1:E:385:LEU:HD21 | 1.94                     | 0.49              |
| 1:E:467:LYS:HD3  | 1:F:460:ASP:HB3  | 1.93                     | 0.49              |
| 1:J:311:LEU:HD11 | 1:K:299:LEU:HD21 | 1.94                     | 0.49              |
| 1:K:467:LYS:HD3  | 1:L:460:ASP:HB3  | 1.94                     | 0.49              |
| 1:B:115:ARG:HH22 | 1:C:475:GLY:C    | 2.20                     | 0.49              |
| 1:B:115:ARG:HH21 | 1:C:476:ILE:N    | 2.10                     | 0.49              |
| 1:I:61:VAL:HG22  | 1:I:64:ARG:HH22  | 1.78                     | 0.49              |
| 1:J:327:ILE:HD12 | 1:K:330:LEU:CD1  | 2.42                     | 0.49              |
| 1:A:97:LEU:HD21  | 1:L:112:MET:SD   | 2.53                     | 0.49              |
| 1:A:122:GLU:HG2  | 1:B:427:SER:OG   | 2.12                     | 0.49              |
| 1:D:311:LEU:HD11 | 1:E:299:LEU:HD21 | 1.95                     | 0.49              |
| 1:G:340:VAL:O    | 1:G:344:VAL:HG12 | 2.12                     | 0.49              |
| 1:D:112:MET:SD   | 1:E:97:LEU:HD21  | 2.53                     | 0.49              |
| 1:H:112:MET:HG2  | 1:I:97:LEU:HD21  | 1.93                     | 0.49              |
| 1:J:203:GLY:O    | 1:J:205:LYS:HG2  | 2.13                     | 0.49              |
| 1:K:61:VAL:HG22  | 1:K:64:ARG:HH22  | 1.78                     | 0.49              |
| 1:L:172:ALA:HA   | 1:L:261:GLY:HA2  | 1.95                     | 0.49              |
| 1:G:165:SER:O    | 1:G:165:SER:OG   | 2.30                     | 0.49              |
| 1:H:172:ALA:HA   | 1:H:261:GLY:HA2  | 1.95                     | 0.49              |
| 1:J:122:GLU:HG2  | 1:K:427:SER:OG   | 2.12                     | 0.49              |
| 1:L:61:VAL:HG22  | 1:L:64:ARG:HH22  | 1.78                     | 0.49              |
| 1:A:112:MET:HG2  | 1:B:97:LEU:CD2   | 2.41                     | 0.49              |
| 1:E:67:ASN:ND2   | 1:F:386:GLY:HA2  | 2.28                     | 0.49              |
| 1:G:122:GLU:HG2  | 1:H:427:SER:HB3  | 1.94                     | 0.49              |
| 1:D:392:LEU:HD12 | 1:D:392:LEU:HA   | 1.61                     | 0.48              |
| 1:E:413:GLN:H    | 1:F:93:ALA:HB3   | 1.78                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:112:MET:HG2  | 1:G:97:LEU:HD21  | 1.95                     | 0.48              |
| 1:G:61:VAL:HG22  | 1:G:64:ARG:HH22  | 1.78                     | 0.48              |
| 1:D:172:ALA:HA   | 1:D:261:GLY:HA2  | 1.95                     | 0.48              |
| 1:E:61:VAL:HG22  | 1:E:64:ARG:HH22  | 1.78                     | 0.48              |
| 1:E:80:MET:HE3   | 1:F:430:LEU:HD23 | 1.95                     | 0.48              |
| 1:F:439:LEU:HB2  | 1:G:473:ALA:HB2  | 1.91                     | 0.48              |
| 1:G:158:MET:HE3  | 1:G:158:MET:HB3  | 1.60                     | 0.48              |
| 1:A:67:ASN:ND2   | 1:B:386:GLY:HA2  | 2.28                     | 0.48              |
| 1:A:172:ALA:HA   | 1:A:261:GLY:HA2  | 1.95                     | 0.48              |
| 1:A:203:GLY:O    | 1:A:205:LYS:HG2  | 2.13                     | 0.48              |
| 1:A:351:ARG:O    | 1:A:352:LEU:C    | 2.56                     | 0.48              |
| 1:B:351:ARG:O    | 1:B:352:LEU:C    | 2.56                     | 0.48              |
| 1:D:61:VAL:HG22  | 1:D:64:ARG:HH22  | 1.78                     | 0.48              |
| 1:F:203:GLY:O    | 1:F:205:LYS:HG2  | 2.13                     | 0.48              |
| 1:H:115:ARG:HH21 | 1:I:476:ILE:N    | 2.11                     | 0.48              |
| 1:J:329:PHE:CE2  | 1:K:332:LEU:HD22 | 2.49                     | 0.48              |
| 1:A:461:ILE:HG12 | 1:L:449:TRP:CH2  | 2.48                     | 0.48              |
| 1:C:61:VAL:HG22  | 1:C:64:ARG:HH22  | 1.78                     | 0.48              |
| 1:C:67:ASN:ND2   | 1:D:386:GLY:HA2  | 2.28                     | 0.48              |
| 1:C:172:ALA:HA   | 1:C:261:GLY:HA2  | 1.95                     | 0.48              |
| 1:C:351:ARG:O    | 1:C:352:LEU:C    | 2.56                     | 0.48              |
| 1:D:449:TRP:CH2  | 1:E:461:ILE:HG12 | 2.48                     | 0.48              |
| 1:F:61:VAL:HG22  | 1:F:64:ARG:HH22  | 1.78                     | 0.48              |
| 1:K:115:ARG:HH22 | 1:L:475:GLY:C    | 2.20                     | 0.48              |
| 1:L:203:GLY:O    | 1:L:205:LYS:HG2  | 2.13                     | 0.48              |
| 1:E:172:ALA:HA   | 1:E:261:GLY:HA2  | 1.95                     | 0.48              |
| 1:E:203:GLY:O    | 1:E:205:LYS:HG2  | 2.13                     | 0.48              |
| 1:B:122:GLU:HG2  | 1:C:427:SER:OG   | 2.13                     | 0.48              |
| 1:C:203:GLY:O    | 1:C:205:LYS:HG2  | 2.13                     | 0.48              |
| 1:E:323:ARG:HG3  | 1:F:301:ASN:HD22 | 1.76                     | 0.48              |
| 1:G:319:PHE:CD2  | 1:H:298:GLY:HA3  | 2.48                     | 0.48              |
| 1:H:61:VAL:HG22  | 1:H:64:ARG:HH22  | 1.78                     | 0.48              |
| 1:J:76:ALA:HA    | 1:J:374:ILE:HD11 | 1.96                     | 0.48              |
| 1:K:76:ALA:HA    | 1:K:374:ILE:HD11 | 1.96                     | 0.48              |
| 1:A:115:ARG:HH22 | 1:B:475:GLY:C    | 2.22                     | 0.48              |
| 1:A:413:GLN:HB2  | 1:B:93:ALA:HB1   | 1.91                     | 0.48              |
| 1:E:319:PHE:CD2  | 1:F:298:GLY:HA3  | 2.49                     | 0.48              |
| 1:H:203:GLY:O    | 1:H:205:LYS:HG2  | 2.13                     | 0.48              |
| 1:J:351:ARG:O    | 1:J:352:LEU:C    | 2.56                     | 0.48              |
| 1:K:203:GLY:O    | 1:K:205:LYS:HG2  | 2.13                     | 0.48              |
| 1:L:76:ALA:HA    | 1:L:374:ILE:HD11 | 1.96                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:298:GLY:HA3  | 1:L:319:PHE:CD2  | 2.49                     | 0.48              |
| 1:D:413:GLN:CB   | 1:E:93:ALA:HB1   | 2.42                     | 0.48              |
| 1:H:122:GLU:HG2  | 1:I:427:SER:OG   | 2.13                     | 0.48              |
| 1:I:76:ALA:HA    | 1:I:374:ILE:HD11 | 1.96                     | 0.48              |
| 1:K:112:MET:HG2  | 1:L:97:LEU:CD2   | 2.43                     | 0.48              |
| 1:K:122:GLU:HG2  | 1:L:427:SER:OG   | 2.13                     | 0.48              |
| 1:A:76:ALA:HA    | 1:A:374:ILE:HD11 | 1.96                     | 0.48              |
| 1:B:172:ALA:HA   | 1:B:261:GLY:HA2  | 1.95                     | 0.48              |
| 1:D:329:PHE:CE2  | 1:E:332:LEU:HD22 | 2.48                     | 0.48              |
| 1:D:351:ARG:O    | 1:D:352:LEU:C    | 2.56                     | 0.48              |
| 1:E:80:MET:SD    | 1:F:431:GLU:HA   | 2.54                     | 0.48              |
| 1:I:203:GLY:O    | 1:I:205:LYS:HG2  | 2.13                     | 0.48              |
| 1:B:203:GLY:O    | 1:B:205:LYS:HG2  | 2.13                     | 0.48              |
| 1:C:80:MET:HE3   | 1:D:430:LEU:HD23 | 1.95                     | 0.48              |
| 1:E:115:ARG:HH22 | 1:F:475:GLY:C    | 2.22                     | 0.47              |
| 1:H:76:ALA:HA    | 1:H:374:ILE:HD11 | 1.96                     | 0.47              |
| 1:H:165:SER:O    | 1:H:165:SER:OG   | 2.29                     | 0.47              |
| 1:A:61:VAL:HG22  | 1:A:64:ARG:HH22  | 1.78                     | 0.47              |
| 1:A:469:ARG:HA   | 1:A:469:ARG:HD2  | 1.67                     | 0.47              |
| 1:B:76:ALA:HA    | 1:B:374:ILE:HD11 | 1.96                     | 0.47              |
| 1:F:172:ALA:HA   | 1:F:261:GLY:HA2  | 1.94                     | 0.47              |
| 1:G:203:GLY:O    | 1:G:205:LYS:HG2  | 2.13                     | 0.47              |
| 1:J:61:VAL:HG22  | 1:J:64:ARG:HH22  | 1.78                     | 0.47              |
| 1:K:351:ARG:O    | 1:K:352:LEU:C    | 2.56                     | 0.47              |
| 1:D:203:GLY:O    | 1:D:205:LYS:HG2  | 2.13                     | 0.47              |
| 1:F:122:GLU:HG2  | 1:G:427:SER:OG   | 2.14                     | 0.47              |
| 1:A:476:ILE:N    | 1:L:115:ARG:HH21 | 2.11                     | 0.47              |
| 1:C:323:ARG:HG3  | 1:D:301:ASN:HD22 | 1.74                     | 0.47              |
| 1:D:115:ARG:HH21 | 1:E:476:ILE:N    | 2.11                     | 0.47              |
| 1:E:351:ARG:O    | 1:E:352:LEU:C    | 2.56                     | 0.47              |
| 1:G:172:ALA:HA   | 1:G:261:GLY:HA2  | 1.95                     | 0.47              |
| 1:A:330:LEU:CD1  | 1:L:327:ILE:HD12 | 2.44                     | 0.47              |
| 1:C:76:ALA:HA    | 1:C:374:ILE:HD11 | 1.96                     | 0.47              |
| 1:E:108:GLU:C    | 1:E:112:MET:HE3  | 2.40                     | 0.47              |
| 1:F:108:GLU:C    | 1:F:112:MET:HE3  | 2.40                     | 0.47              |
| 1:J:112:MET:SD   | 1:K:97:LEU:HD21  | 2.55                     | 0.47              |
| 1:A:319:PHE:CD2  | 1:B:298:GLY:HA3  | 2.49                     | 0.47              |
| 1:D:319:PHE:CD2  | 1:E:298:GLY:HA3  | 2.49                     | 0.47              |
| 1:G:76:ALA:HA    | 1:G:374:ILE:HD11 | 1.96                     | 0.47              |
| 1:J:258:ARG:HE   | 1:J:258:ARG:HB2  | 1.45                     | 0.47              |
| 1:K:108:GLU:C    | 1:K:112:MET:HE3  | 2.40                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:108:GLU:C    | 1:B:112:MET:HE3  | 2.40                     | 0.47              |
| 1:D:76:ALA:HA    | 1:D:374:ILE:HD11 | 1.96                     | 0.47              |
| 1:D:464:ALA:O    | 1:E:460:ASP:OD2  | 2.33                     | 0.47              |
| 1:E:329:PHE:CE2  | 1:F:332:LEU:HD23 | 2.50                     | 0.47              |
| 1:F:76:ALA:HA    | 1:F:374:ILE:HD11 | 1.96                     | 0.47              |
| 1:H:80:MET:HE2   | 1:H:80:MET:HB2   | 1.49                     | 0.47              |
| 1:H:108:GLU:C    | 1:H:112:MET:HE3  | 2.40                     | 0.47              |
| 1:I:108:GLU:C    | 1:I:112:MET:HE3  | 2.40                     | 0.47              |
| 1:J:319:PHE:CD2  | 1:K:298:GLY:HA3  | 2.50                     | 0.47              |
| 1:A:80:MET:HE3   | 1:B:430:LEU:HD23 | 1.96                     | 0.47              |
| 1:D:115:ARG:HH22 | 1:E:475:GLY:C    | 2.23                     | 0.47              |
| 1:E:76:ALA:HA    | 1:E:374:ILE:HD11 | 1.96                     | 0.47              |
| 1:E:170:ARG:H    | 1:E:263:SER:HB3  | 1.80                     | 0.47              |
| 1:I:170:ARG:H    | 1:I:263:SER:HB3  | 1.80                     | 0.47              |
| 1:K:392:LEU:HD12 | 1:K:392:LEU:HA   | 1.61                     | 0.47              |
| 1:B:418:PRO:HB2  | 1:B:420:GLU:OE1  | 2.15                     | 0.47              |
| 1:C:108:GLU:C    | 1:C:112:MET:HE3  | 2.40                     | 0.47              |
| 1:D:170:ARG:H    | 1:D:263:SER:HB3  | 1.80                     | 0.47              |
| 1:E:439:LEU:CD1  | 1:F:473:ALA:HB3  | 2.42                     | 0.47              |
| 1:H:112:MET:HG2  | 1:I:97:LEU:CD2   | 2.45                     | 0.47              |
| 1:I:158:MET:HB3  | 1:I:158:MET:HE3  | 1.59                     | 0.47              |
| 1:J:108:GLU:C    | 1:J:112:MET:HE3  | 2.40                     | 0.47              |
| 1:J:413:GLN:H    | 1:K:93:ALA:CB    | 2.28                     | 0.47              |
| 1:K:80:MET:HE2   | 1:K:80:MET:HB2   | 1.49                     | 0.47              |
| 1:K:418:PRO:HB2  | 1:K:420:GLU:OE1  | 2.15                     | 0.47              |
| 1:L:108:GLU:C    | 1:L:112:MET:HE3  | 2.40                     | 0.47              |
| 1:B:433:ILE:HD12 | 1:B:433:ILE:HA   | 1.83                     | 0.47              |
| 1:C:80:MET:SD    | 1:D:431:GLU:HA   | 2.54                     | 0.47              |
| 1:C:158:MET:HE3  | 1:C:158:MET:HB3  | 1.59                     | 0.47              |
| 1:G:108:GLU:C    | 1:G:112:MET:HE3  | 2.40                     | 0.47              |
| 1:G:115:ARG:HH22 | 1:H:475:GLY:C    | 2.23                     | 0.47              |
| 1:J:449:TRP:CH2  | 1:K:461:ILE:HG12 | 2.49                     | 0.47              |
| 1:K:329:PHE:CE2  | 1:L:332:LEU:HD23 | 2.49                     | 0.47              |
| 1:A:413:GLN:H    | 1:B:93:ALA:HB3   | 1.80                     | 0.46              |
| 1:C:180:VAL:HA   | 1:C:215:THR:O    | 2.15                     | 0.46              |
| 1:E:180:VAL:HA   | 1:E:215:THR:O    | 2.15                     | 0.46              |
| 1:F:59:GLN:CA    | 1:G:351:ARG:HH22 | 2.25                     | 0.46              |
| 1:G:413:GLN:HB2  | 1:H:93:ALA:HB1   | 1.92                     | 0.46              |
| 1:G:413:GLN:H    | 1:H:93:ALA:HB3   | 1.80                     | 0.46              |
| 1:J:170:ARG:H    | 1:J:263:SER:HB3  | 1.80                     | 0.46              |
| 1:K:413:GLN:H    | 1:L:93:ALA:HB3   | 1.79                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:332:LEU:HD22 | 1:L:329:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:418:PRO:HB2  | 1:A:420:GLU:OE1  | 2.16                     | 0.46              |
| 1:E:165:SER:O    | 1:E:165:SER:OG   | 2.29                     | 0.46              |
| 1:F:469:ARG:HA   | 1:F:469:ARG:HD2  | 1.67                     | 0.46              |
| 1:G:180:VAL:HA   | 1:G:215:THR:O    | 2.15                     | 0.46              |
| 1:H:170:ARG:H    | 1:H:263:SER:HB3  | 1.80                     | 0.46              |
| 1:J:469:ARG:HD2  | 1:J:469:ARG:HA   | 1.67                     | 0.46              |
| 1:L:418:PRO:HB2  | 1:L:420:GLU:OE1  | 2.15                     | 0.46              |
| 1:A:170:ARG:H    | 1:A:263:SER:HB3  | 1.80                     | 0.46              |
| 1:B:112:MET:SD   | 1:C:97:LEU:HD21  | 2.56                     | 0.46              |
| 1:D:67:ASN:ND2   | 1:E:386:GLY:HA2  | 2.31                     | 0.46              |
| 1:D:108:GLU:C    | 1:D:112:MET:HE3  | 2.40                     | 0.46              |
| 1:D:180:VAL:HA   | 1:D:215:THR:O    | 2.15                     | 0.46              |
| 1:E:418:PRO:HB2  | 1:E:420:GLU:OE1  | 2.15                     | 0.46              |
| 1:F:430:LEU:O    | 1:F:433:ILE:HG22 | 2.16                     | 0.46              |
| 1:I:319:PHE:CD2  | 1:J:298:GLY:HA3  | 2.49                     | 0.46              |
| 1:J:381:LEU:HD23 | 1:J:381:LEU:HA   | 1.71                     | 0.46              |
| 1:K:170:ARG:H    | 1:K:263:SER:HB3  | 1.80                     | 0.46              |
| 1:L:180:VAL:HA   | 1:L:215:THR:O    | 2.15                     | 0.46              |
| 1:A:180:VAL:HA   | 1:A:215:THR:O    | 2.15                     | 0.46              |
| 1:A:460:ASP:OD2  | 1:L:464:ALA:O    | 2.34                     | 0.46              |
| 1:A:473:ALA:CB   | 1:L:439:LEU:HD12 | 2.45                     | 0.46              |
| 1:B:25:ALA:O     | 1:B:29:THR:HG23  | 2.16                     | 0.46              |
| 1:B:170:ARG:H    | 1:B:263:SER:HB3  | 1.80                     | 0.46              |
| 1:C:413:GLN:HB2  | 1:D:93:ALA:HB1   | 1.94                     | 0.46              |
| 1:C:418:PRO:HB2  | 1:C:420:GLU:OE1  | 2.15                     | 0.46              |
| 1:G:430:LEU:O    | 1:G:433:ILE:HG22 | 2.16                     | 0.46              |
| 1:I:80:MET:CE    | 1:J:431:GLU:OE1  | 2.58                     | 0.46              |
| 1:J:322:GLY:O    | 1:K:300:VAL:O    | 2.33                     | 0.46              |
| 1:K:67:ASN:ND2   | 1:L:386:GLY:HA2  | 2.31                     | 0.46              |
| 1:K:180:VAL:HA   | 1:K:215:THR:O    | 2.15                     | 0.46              |
| 1:L:351:ARG:O    | 1:L:352:LEU:C    | 2.56                     | 0.46              |
| 1:A:108:GLU:C    | 1:A:112:MET:HE3  | 2.40                     | 0.46              |
| 1:D:430:LEU:O    | 1:D:433:ILE:HG22 | 2.16                     | 0.46              |
| 1:D:433:ILE:HD12 | 1:D:433:ILE:HA   | 1.83                     | 0.46              |
| 1:G:25:ALA:O     | 1:G:29:THR:HG23  | 2.16                     | 0.46              |
| 1:H:327:ILE:HD12 | 1:I:330:LEU:CD1  | 2.46                     | 0.46              |
| 1:H:418:PRO:HB2  | 1:H:420:GLU:OE1  | 2.15                     | 0.46              |
| 1:I:25:ALA:O     | 1:I:29:THR:HG23  | 2.16                     | 0.46              |
| 1:I:431:GLU:H    | 1:I:431:GLU:HG2  | 1.22                     | 0.46              |
| 1:K:413:GLN:CB   | 1:L:93:ALA:CB    | 2.88                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:475:GLY:C    | 1:L:115:ARG:HH22 | 2.22                     | 0.46              |
| 1:D:25:ALA:O     | 1:D:29:THR:HG23  | 2.16                     | 0.46              |
| 1:D:418:PRO:HB2  | 1:D:420:GLU:OE1  | 2.15                     | 0.46              |
| 1:F:112:MET:HG2  | 1:G:97:LEU:CD2   | 2.46                     | 0.46              |
| 1:F:351:ARG:O    | 1:F:352:LEU:C    | 2.56                     | 0.46              |
| 1:F:392:LEU:HD12 | 1:F:392:LEU:HA   | 1.61                     | 0.46              |
| 1:H:258:ARG:HE   | 1:H:258:ARG:HB2  | 1.45                     | 0.46              |
| 1:I:180:VAL:HA   | 1:I:215:THR:O    | 2.15                     | 0.46              |
| 1:K:110:LEU:O    | 1:K:114:GLU:N    | 2.46                     | 0.46              |
| 1:K:146:TYR:O    | 1:K:148:PRO:HD3  | 2.16                     | 0.46              |
| 1:L:146:TYR:O    | 1:L:148:PRO:HD3  | 2.16                     | 0.46              |
| 1:A:146:TYR:O    | 1:A:148:PRO:HD3  | 2.16                     | 0.46              |
| 1:B:165:SER:O    | 1:B:165:SER:OG   | 2.29                     | 0.46              |
| 1:D:431:GLU:H    | 1:D:431:GLU:HG2  | 1.22                     | 0.46              |
| 1:E:367:GLU:HG2  | 1:F:376:TYR:CE1  | 2.49                     | 0.46              |
| 1:F:322:GLY:O    | 1:G:300:VAL:O    | 2.33                     | 0.46              |
| 1:I:430:LEU:O    | 1:I:433:ILE:HG22 | 2.16                     | 0.46              |
| 1:J:418:PRO:HB2  | 1:J:420:GLU:OE1  | 2.16                     | 0.46              |
| 1:J:426:ILE:H    | 1:J:426:ILE:HG13 | 1.59                     | 0.46              |
| 1:A:80:MET:SD    | 1:B:431:GLU:HA   | 2.56                     | 0.46              |
| 1:B:322:GLY:O    | 1:C:300:VAL:O    | 2.34                     | 0.46              |
| 1:E:369:VAL:HB   | 1:F:375:ARG:HG2  | 1.98                     | 0.46              |
| 1:E:381:LEU:HD23 | 1:E:381:LEU:HA   | 1.71                     | 0.46              |
| 1:F:327:ILE:HD12 | 1:G:330:LEU:CD1  | 2.46                     | 0.46              |
| 1:G:170:ARG:H    | 1:G:263:SER:HB3  | 1.80                     | 0.46              |
| 1:H:227:LEU:HD23 | 1:H:227:LEU:HA   | 1.83                     | 0.46              |
| 1:H:322:GLY:O    | 1:I:300:VAL:O    | 2.34                     | 0.46              |
| 1:J:180:VAL:HA   | 1:J:215:THR:O    | 2.15                     | 0.46              |
| 1:J:413:GLN:O    | 1:K:93:ALA:HB1   | 2.16                     | 0.46              |
| 1:K:115:ARG:NH2  | 1:L:475:GLY:C    | 2.74                     | 0.46              |
| 1:L:25:ALA:O     | 1:L:29:THR:HG23  | 2.16                     | 0.46              |
| 1:A:386:GLY:HA2  | 1:L:67:ASN:ND2   | 2.31                     | 0.46              |
| 1:D:442:LEU:CB   | 1:E:470:ILE:HD11 | 2.41                     | 0.46              |
| 1:F:146:TYR:O    | 1:F:148:PRO:HD3  | 2.16                     | 0.46              |
| 1:F:180:VAL:HA   | 1:F:215:THR:O    | 2.15                     | 0.46              |
| 1:G:146:TYR:O    | 1:G:148:PRO:HD3  | 2.16                     | 0.46              |
| 1:H:146:TYR:O    | 1:H:148:PRO:HD3  | 2.16                     | 0.46              |
| 1:H:430:LEU:O    | 1:H:433:ILE:HG22 | 2.16                     | 0.46              |
| 1:J:146:TYR:O    | 1:J:148:PRO:HD3  | 2.16                     | 0.46              |
| 1:B:146:TYR:O    | 1:B:148:PRO:HD3  | 2.16                     | 0.46              |
| 1:E:25:ALA:O     | 1:E:29:THR:HG23  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:80:MET:HE2   | 1:E:80:MET:HB2   | 1.49                     | 0.46              |
| 1:E:430:LEU:O    | 1:E:433:ILE:HG22 | 2.16                     | 0.46              |
| 1:F:158:MET:HB3  | 1:F:158:MET:HE3  | 1.60                     | 0.46              |
| 1:F:418:PRO:HB2  | 1:F:420:GLU:OE1  | 2.16                     | 0.46              |
| 1:H:112:MET:SD   | 1:I:97:LEU:HD21  | 2.56                     | 0.46              |
| 1:I:146:TYR:O    | 1:I:148:PRO:HD3  | 2.16                     | 0.46              |
| 1:I:351:ARG:O    | 1:I:352:LEU:C    | 2.56                     | 0.46              |
| 1:I:469:ARG:HD2  | 1:I:469:ARG:HA   | 1.67                     | 0.46              |
| 1:K:25:ALA:O     | 1:K:29:THR:HG23  | 2.16                     | 0.46              |
| 1:K:80:MET:SD    | 1:L:431:GLU:HA   | 2.56                     | 0.46              |
| 1:B:112:MET:HG2  | 1:C:97:LEU:CD2   | 2.45                     | 0.45              |
| 1:B:180:VAL:HA   | 1:B:215:THR:O    | 2.15                     | 0.45              |
| 1:D:146:TYR:O    | 1:D:148:PRO:HD3  | 2.16                     | 0.45              |
| 1:D:413:GLN:O    | 1:E:93:ALA:HB1   | 2.15                     | 0.45              |
| 1:E:392:LEU:HD12 | 1:E:392:LEU:HA   | 1.61                     | 0.45              |
| 1:F:170:ARG:H    | 1:F:263:SER:HB3  | 1.80                     | 0.45              |
| 1:G:80:MET:HE1   | 1:H:431:GLU:OE2  | 2.16                     | 0.45              |
| 1:H:319:PHE:CD2  | 1:I:298:GLY:HA3  | 2.51                     | 0.45              |
| 1:I:165:SER:O    | 1:I:165:SER:OG   | 2.30                     | 0.45              |
| 1:J:25:ALA:O     | 1:J:29:THR:HG23  | 2.16                     | 0.45              |
| 1:K:386:GLY:C    | 1:K:388:VAL:H    | 2.24                     | 0.45              |
| 1:L:431:GLU:H    | 1:L:431:GLU:HG2  | 1.22                     | 0.45              |
| 1:C:430:LEU:O    | 1:C:433:ILE:HG22 | 2.16                     | 0.45              |
| 1:D:322:GLY:O    | 1:E:300:VAL:O    | 2.34                     | 0.45              |
| 1:D:442:LEU:CB   | 1:E:470:ILE:CD1  | 2.93                     | 0.45              |
| 1:F:25:ALA:O     | 1:F:29:THR:HG23  | 2.16                     | 0.45              |
| 1:F:381:LEU:HD23 | 1:F:381:LEU:HA   | 1.71                     | 0.45              |
| 1:G:418:PRO:HB2  | 1:G:420:GLU:OE1  | 2.15                     | 0.45              |
| 1:H:25:ALA:O     | 1:H:29:THR:HG23  | 2.16                     | 0.45              |
| 1:H:351:ARG:O    | 1:H:352:LEU:C    | 2.56                     | 0.45              |
| 1:H:386:GLY:C    | 1:H:388:VAL:H    | 2.25                     | 0.45              |
| 1:I:418:PRO:HB2  | 1:I:420:GLU:OE1  | 2.15                     | 0.45              |
| 1:K:430:LEU:O    | 1:K:433:ILE:HG22 | 2.16                     | 0.45              |
| 1:L:170:ARG:H    | 1:L:263:SER:HB3  | 1.80                     | 0.45              |
| 1:A:93:ALA:HB1   | 1:L:413:GLN:O    | 2.15                     | 0.45              |
| 1:A:431:GLU:H    | 1:A:431:GLU:HG2  | 1.22                     | 0.45              |
| 1:C:319:PHE:CD2  | 1:D:298:GLY:HA3  | 2.51                     | 0.45              |
| 1:C:392:LEU:HD12 | 1:C:392:LEU:HA   | 1.61                     | 0.45              |
| 1:D:413:GLN:O    | 1:E:93:ALA:CB    | 2.64                     | 0.45              |
| 1:D:439:LEU:HD12 | 1:E:473:ALA:CB   | 2.46                     | 0.45              |
| 1:E:146:TYR:O    | 1:E:148:PRO:HD3  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:413:GLN:H    | 1:G:93:ALA:CB    | 2.29                     | 0.45              |
| 1:G:392:LEU:HA   | 1:G:392:LEU:HD12 | 1.61                     | 0.45              |
| 1:G:469:ARG:HA   | 1:G:469:ARG:HD2  | 1.67                     | 0.45              |
| 1:I:80:MET:CE    | 1:J:431:GLU:CD   | 2.75                     | 0.45              |
| 1:A:80:MET:HE2   | 1:A:80:MET:HB2   | 1.49                     | 0.45              |
| 1:A:93:ALA:CB    | 1:L:413:GLN:O    | 2.64                     | 0.45              |
| 1:A:386:GLY:C    | 1:A:388:VAL:H    | 2.24                     | 0.45              |
| 1:B:439:LEU:HD12 | 1:C:473:ALA:CB   | 2.46                     | 0.45              |
| 1:C:146:TYR:O    | 1:C:148:PRO:HD3  | 2.16                     | 0.45              |
| 1:E:227:LEU:HD23 | 1:E:227:LEU:HA   | 1.83                     | 0.45              |
| 1:F:112:MET:SD   | 1:G:97:LEU:HD21  | 2.56                     | 0.45              |
| 1:F:412:GLN:HB3  | 1:F:413:GLN:H    | 1.57                     | 0.45              |
| 1:G:80:MET:SD    | 1:H:431:GLU:HA   | 2.55                     | 0.45              |
| 1:I:381:LEU:HD23 | 1:I:381:LEU:HA   | 1.71                     | 0.45              |
| 1:K:372:GLU:C    | 1:K:374:ILE:H    | 2.25                     | 0.45              |
| 1:C:170:ARG:H    | 1:C:263:SER:HB3  | 1.80                     | 0.45              |
| 1:C:412:GLN:HB3  | 1:C:413:GLN:H    | 1.57                     | 0.45              |
| 1:G:80:MET:HE3   | 1:H:430:LEU:HD23 | 1.97                     | 0.45              |
| 1:I:367:GLU:HG2  | 1:J:376:TYR:CE1  | 2.49                     | 0.45              |
| 1:J:413:GLN:O    | 1:K:93:ALA:CB    | 2.65                     | 0.45              |
| 1:K:319:PHE:CD2  | 1:L:298:GLY:HA3  | 2.51                     | 0.45              |
| 1:A:430:LEU:O    | 1:A:433:ILE:HG22 | 2.16                     | 0.45              |
| 1:B:374:ILE:HD12 | 1:B:374:ILE:HA   | 1.82                     | 0.45              |
| 1:B:386:GLY:C    | 1:B:388:VAL:H    | 2.24                     | 0.45              |
| 1:B:430:LEU:O    | 1:B:433:ILE:HG22 | 2.16                     | 0.45              |
| 1:D:327:ILE:HD12 | 1:E:330:LEU:HD12 | 1.99                     | 0.45              |
| 1:D:374:ILE:HD12 | 1:D:374:ILE:HA   | 1.82                     | 0.45              |
| 1:F:227:LEU:HD23 | 1:F:227:LEU:HA   | 1.83                     | 0.45              |
| 1:I:80:MET:HE3   | 1:J:430:LEU:HD23 | 1.96                     | 0.45              |
| 1:K:158:MET:HB3  | 1:K:158:MET:HE3  | 1.59                     | 0.45              |
| 1:L:372:GLU:C    | 1:L:374:ILE:H    | 2.25                     | 0.45              |
| 1:B:413:GLN:O    | 1:C:93:ALA:CB    | 2.65                     | 0.45              |
| 1:D:227:LEU:HD23 | 1:D:227:LEU:HA   | 1.83                     | 0.45              |
| 1:F:431:GLU:H    | 1:F:431:GLU:HG2  | 1.22                     | 0.45              |
| 1:A:158:MET:HE3  | 1:A:158:MET:HB3  | 1.60                     | 0.45              |
| 1:G:367:GLU:HG2  | 1:H:376:TYR:CE1  | 2.51                     | 0.45              |
| 1:G:369:VAL:HB   | 1:H:375:ARG:HG2  | 1.99                     | 0.45              |
| 1:G:386:GLY:C    | 1:G:388:VAL:H    | 2.25                     | 0.45              |
| 1:H:180:VAL:HA   | 1:H:215:THR:O    | 2.15                     | 0.45              |
| 1:J:110:LEU:O    | 1:J:114:GLU:N    | 2.46                     | 0.45              |
| 1:J:386:GLY:C    | 1:J:388:VAL:H    | 2.25                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:442:LEU:CB   | 1:K:470:ILE:CD1  | 2.95                     | 0.45              |
| 1:L:430:LEU:O    | 1:L:433:ILE:HG22 | 2.16                     | 0.45              |
| 1:A:396:LEU:HD23 | 1:A:396:LEU:HA   | 1.82                     | 0.45              |
| 1:B:431:GLU:H    | 1:B:431:GLU:HG2  | 1.22                     | 0.45              |
| 1:C:25:ALA:O     | 1:C:29:THR:HG23  | 2.16                     | 0.45              |
| 1:C:115:ARG:HH22 | 1:D:475:GLY:C    | 2.25                     | 0.45              |
| 1:G:351:ARG:O    | 1:G:352:LEU:C    | 2.56                     | 0.45              |
| 1:H:158:MET:HE3  | 1:H:158:MET:HB3  | 1.60                     | 0.45              |
| 1:H:311:LEU:HD13 | 1:H:311:LEU:HA   | 1.84                     | 0.45              |
| 1:H:439:LEU:HD12 | 1:I:473:ALA:CB   | 2.45                     | 0.45              |
| 1:A:25:ALA:O     | 1:A:29:THR:HG23  | 2.16                     | 0.45              |
| 1:A:311:LEU:HA   | 1:A:311:LEU:HD13 | 1.84                     | 0.45              |
| 1:C:80:MET:HE1   | 1:D:431:GLU:OE2  | 2.16                     | 0.45              |
| 1:C:433:ILE:HD12 | 1:C:433:ILE:HA   | 1.83                     | 0.45              |
| 1:A:392:LEU:HD12 | 1:A:392:LEU:HA   | 1.61                     | 0.44              |
| 1:F:413:GLN:O    | 1:G:93:ALA:HB1   | 2.17                     | 0.44              |
| 1:I:369:VAL:HB   | 1:J:375:ARG:HG2  | 1.99                     | 0.44              |
| 1:A:206:LYS:H    | 1:A:206:LYS:HG2  | 1.52                     | 0.44              |
| 1:A:322:GLY:O    | 1:B:300:VAL:O    | 2.35                     | 0.44              |
| 1:B:128:VAL:O    | 1:B:132:GLU:HG2  | 2.18                     | 0.44              |
| 1:C:416:GLU:H    | 1:C:416:GLU:HG2  | 1.65                     | 0.44              |
| 1:E:386:GLY:C    | 1:E:388:VAL:H    | 2.25                     | 0.44              |
| 1:J:372:GLU:C    | 1:J:374:ILE:H    | 2.25                     | 0.44              |
| 1:A:372:GLU:C    | 1:A:374:ILE:H    | 2.25                     | 0.44              |
| 1:B:206:LYS:H    | 1:B:206:LYS:HG2  | 1.52                     | 0.44              |
| 1:D:413:GLN:H    | 1:E:93:ALA:CB    | 2.31                     | 0.44              |
| 1:D:474:ILE:H    | 1:D:474:ILE:HG12 | 1.67                     | 0.44              |
| 1:E:115:ARG:NH2  | 1:F:475:GLY:C    | 2.76                     | 0.44              |
| 1:J:430:LEU:O    | 1:J:433:ILE:HG22 | 2.16                     | 0.44              |
| 1:A:467:LYS:CB   | 1:B:460:ASP:OD2  | 2.64                     | 0.44              |
| 1:F:165:SER:O    | 1:F:165:SER:OG   | 2.30                     | 0.44              |
| 1:B:327:ILE:HD12 | 1:C:330:LEU:CD1  | 2.47                     | 0.44              |
| 1:D:128:VAL:O    | 1:D:132:GLU:HG2  | 2.18                     | 0.44              |
| 1:F:319:PHE:CD2  | 1:G:298:GLY:HA3  | 2.52                     | 0.44              |
| 1:F:413:GLN:O    | 1:G:93:ALA:CB    | 2.65                     | 0.44              |
| 1:F:439:LEU:HD12 | 1:G:473:ALA:CB   | 2.47                     | 0.44              |
| 1:G:416:GLU:H    | 1:G:416:GLU:HG2  | 1.65                     | 0.44              |
| 1:H:388:VAL:O    | 1:H:389:TYR:C    | 2.59                     | 0.44              |
| 1:I:372:GLU:C    | 1:I:374:ILE:H    | 2.25                     | 0.44              |
| 1:I:467:LYS:CB   | 1:J:460:ASP:OD2  | 2.60                     | 0.44              |
| 1:L:128:VAL:O    | 1:L:132:GLU:HG2  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:431:GLU:OE1  | 1:L:80:MET:CE    | 2.60                     | 0.44              |
| 1:B:319:PHE:CD2  | 1:C:298:GLY:HA3  | 2.52                     | 0.44              |
| 1:D:381:LEU:HD23 | 1:D:381:LEU:HA   | 1.72                     | 0.44              |
| 1:H:413:GLN:O    | 1:I:93:ALA:CB    | 2.66                     | 0.44              |
| 1:I:227:LEU:HD23 | 1:I:227:LEU:HA   | 1.83                     | 0.44              |
| 1:J:67:ASN:ND2   | 1:K:386:GLY:HA2  | 2.33                     | 0.44              |
| 1:J:327:ILE:HD12 | 1:K:330:LEU:HD12 | 1.99                     | 0.44              |
| 1:B:449:TRP:CH2  | 1:C:461:ILE:HG12 | 2.53                     | 0.44              |
| 1:C:227:LEU:HD23 | 1:C:227:LEU:HA   | 1.83                     | 0.44              |
| 1:D:369:VAL:HB   | 1:E:375:ARG:CG   | 2.48                     | 0.44              |
| 1:E:388:VAL:O    | 1:E:389:TYR:C    | 2.59                     | 0.44              |
| 1:F:388:VAL:O    | 1:F:389:TYR:C    | 2.59                     | 0.44              |
| 1:G:372:GLU:C    | 1:G:374:ILE:H    | 2.25                     | 0.44              |
| 1:K:396:LEU:HD23 | 1:K:396:LEU:HA   | 1.82                     | 0.44              |
| 1:A:93:ALA:CB    | 1:L:413:GLN:H    | 2.31                     | 0.44              |
| 1:A:227:LEU:HD23 | 1:A:227:LEU:HA   | 1.83                     | 0.44              |
| 1:C:80:MET:HE2   | 1:C:80:MET:HB2   | 1.49                     | 0.44              |
| 1:C:258:ARG:HE   | 1:C:258:ARG:HB2  | 1.45                     | 0.44              |
| 1:D:258:ARG:HE   | 1:D:258:ARG:HB2  | 1.45                     | 0.44              |
| 1:G:322:GLY:O    | 1:H:300:VAL:O    | 2.35                     | 0.44              |
| 1:H:372:GLU:C    | 1:H:374:ILE:H    | 2.25                     | 0.44              |
| 1:J:186:ALA:CB   | 1:K:171:ASP:HB3  | 2.47                     | 0.44              |
| 1:K:369:VAL:HB   | 1:L:375:ARG:HG2  | 1.99                     | 0.44              |
| 1:B:426:ILE:H    | 1:B:426:ILE:HG13 | 1.59                     | 0.44              |
| 1:C:322:GLY:O    | 1:D:300:VAL:O    | 2.35                     | 0.44              |
| 1:D:388:VAL:O    | 1:D:389:TYR:C    | 2.59                     | 0.44              |
| 1:E:469:ARG:HD2  | 1:E:469:ARG:HA   | 1.67                     | 0.44              |
| 1:H:59:GLN:CA    | 1:I:351:ARG:HH22 | 2.27                     | 0.44              |
| 1:H:449:TRP:CH2  | 1:I:461:ILE:HG12 | 2.52                     | 0.44              |
| 1:J:329:PHE:CE2  | 1:K:332:LEU:HD23 | 2.53                     | 0.44              |
| 1:K:128:VAL:O    | 1:K:132:GLU:HG2  | 2.18                     | 0.44              |
| 1:A:470:ILE:CD1  | 1:L:442:LEU:CB   | 2.95                     | 0.43              |
| 1:D:329:PHE:CE2  | 1:E:332:LEU:HD23 | 2.53                     | 0.43              |
| 1:D:386:GLY:C    | 1:D:388:VAL:H    | 2.25                     | 0.43              |
| 1:F:314:ALA:HB1  | 1:F:318:ASP:HB3  | 2.00                     | 0.43              |
| 1:G:227:LEU:HD23 | 1:G:227:LEU:HA   | 1.83                     | 0.43              |
| 1:I:80:MET:HE2   | 1:I:80:MET:HB2   | 1.49                     | 0.43              |
| 1:I:413:GLN:H    | 1:J:93:ALA:HB3   | 1.83                     | 0.43              |
| 1:J:464:ALA:O    | 1:K:460:ASP:OD2  | 2.36                     | 0.43              |
| 1:L:206:LYS:H    | 1:L:206:LYS:HG2  | 1.52                     | 0.43              |
| 1:F:372:GLU:C    | 1:F:374:ILE:H    | 2.25                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:329:PHE:CE2  | 1:I:332:LEU:HD22 | 2.53                     | 0.43              |
| 1:J:128:VAL:O    | 1:J:132:GLU:HG2  | 2.18                     | 0.43              |
| 1:K:322:GLY:O    | 1:L:300:VAL:O    | 2.36                     | 0.43              |
| 1:A:115:ARG:NH2  | 1:B:475:GLY:C    | 2.76                     | 0.43              |
| 1:A:128:VAL:O    | 1:A:132:GLU:HG2  | 2.18                     | 0.43              |
| 1:B:258:ARG:HE   | 1:B:258:ARG:HB2  | 1.45                     | 0.43              |
| 1:B:413:GLN:O    | 1:C:93:ALA:HB1   | 2.18                     | 0.43              |
| 1:B:464:ALA:O    | 1:C:460:ASP:OD2  | 2.36                     | 0.43              |
| 1:D:167:VAL:HG23 | 1:D:264:TYR:OH   | 2.19                     | 0.43              |
| 1:D:335:GLN:HE22 | 1:E:336:ALA:HB1  | 1.83                     | 0.43              |
| 1:D:416:GLU:H    | 1:D:416:GLU:HG2  | 1.65                     | 0.43              |
| 1:F:128:VAL:O    | 1:F:132:GLU:HG2  | 2.18                     | 0.43              |
| 1:F:416:GLU:H    | 1:F:416:GLU:HG2  | 1.65                     | 0.43              |
| 1:G:433:ILE:HD12 | 1:G:433:ILE:HA   | 1.83                     | 0.43              |
| 1:J:335:GLN:HE22 | 1:K:336:ALA:HB1  | 1.82                     | 0.43              |
| 1:K:372:GLU:O    | 1:K:373:GLU:C    | 2.61                     | 0.43              |
| 1:B:80:MET:CE    | 1:C:431:GLU:OE1  | 2.59                     | 0.43              |
| 1:B:413:GLN:H    | 1:C:93:ALA:CB    | 2.31                     | 0.43              |
| 1:E:314:ALA:HB1  | 1:E:318:ASP:HB3  | 2.00                     | 0.43              |
| 1:E:372:GLU:O    | 1:E:373:GLU:C    | 2.61                     | 0.43              |
| 1:G:314:ALA:HB1  | 1:G:318:ASP:HB3  | 2.00                     | 0.43              |
| 1:H:186:ALA:CB   | 1:I:171:ASP:HB3  | 2.46                     | 0.43              |
| 1:L:372:GLU:O    | 1:L:373:GLU:C    | 2.61                     | 0.43              |
| 1:A:330:LEU:HD12 | 1:L:327:ILE:HD12 | 2.00                     | 0.43              |
| 1:A:372:GLU:O    | 1:A:373:GLU:C    | 2.61                     | 0.43              |
| 1:G:24:ARG:O     | 1:G:25:ALA:C     | 2.62                     | 0.43              |
| 1:G:128:VAL:O    | 1:G:132:GLU:HG2  | 2.18                     | 0.43              |
| 1:G:374:ILE:HD12 | 1:G:374:ILE:HA   | 1.82                     | 0.43              |
| 1:H:8:LEU:HD23   | 1:H:8:LEU:H      | 1.83                     | 0.43              |
| 1:H:128:VAL:O    | 1:H:132:GLU:HG2  | 2.18                     | 0.43              |
| 1:H:417:LEU:HA   | 1:H:418:PRO:HD3  | 1.90                     | 0.43              |
| 1:J:59:GLN:CA    | 1:K:351:ARG:HH22 | 2.25                     | 0.43              |
| 1:K:80:MET:CE    | 1:L:431:GLU:OE1  | 2.61                     | 0.43              |
| 1:K:408:LEU:HD23 | 1:K:408:LEU:HA   | 1.86                     | 0.43              |
| 1:L:314:ALA:HB1  | 1:L:318:ASP:HB3  | 2.00                     | 0.43              |
| 1:L:386:GLY:C    | 1:L:388:VAL:H    | 2.24                     | 0.43              |
| 1:L:461:ILE:HD12 | 1:L:461:ILE:HA   | 1.95                     | 0.43              |
| 1:B:372:GLU:C    | 1:B:374:ILE:H    | 2.25                     | 0.43              |
| 1:C:388:VAL:O    | 1:C:389:TYR:C    | 2.59                     | 0.43              |
| 1:D:314:ALA:HB1  | 1:D:318:ASP:HB3  | 2.00                     | 0.43              |
| 1:H:413:GLN:H    | 1:I:93:ALA:CB    | 2.31                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:8:LEU:H      | 1:J:8:LEU:HD23   | 1.83                     | 0.43              |
| 1:K:8:LEU:HD23   | 1:K:8:LEU:H      | 1.83                     | 0.43              |
| 1:K:381:LEU:HD23 | 1:K:381:LEU:HA   | 1.72                     | 0.43              |
| 1:K:426:ILE:H    | 1:K:426:ILE:HG13 | 1.59                     | 0.43              |
| 1:K:474:ILE:H    | 1:K:474:ILE:HG12 | 1.66                     | 0.43              |
| 1:L:412:GLN:HB3  | 1:L:413:GLN:H    | 1.57                     | 0.43              |
| 1:A:314:ALA:HB1  | 1:A:318:ASP:HB3  | 2.00                     | 0.43              |
| 1:A:461:ILE:HD12 | 1:A:461:ILE:HA   | 1.95                     | 0.43              |
| 1:B:167:VAL:HG23 | 1:B:264:TYR:OH   | 2.19                     | 0.43              |
| 1:B:440:ASP:O    | 1:B:443:GLU:HG3  | 2.19                     | 0.43              |
| 1:B:461:ILE:HD12 | 1:B:461:ILE:HA   | 1.95                     | 0.43              |
| 1:C:413:GLN:H    | 1:D:93:ALA:HB3   | 1.83                     | 0.43              |
| 1:D:434:GLY:O    | 1:D:435:ARG:HD2  | 2.19                     | 0.43              |
| 1:E:412:GLN:HB3  | 1:E:413:GLN:H    | 1.57                     | 0.43              |
| 1:F:24:ARG:O     | 1:F:25:ALA:C     | 2.62                     | 0.43              |
| 1:F:27:TYR:CZ    | 1:F:264:TYR:HB2  | 2.54                     | 0.43              |
| 1:F:329:PHE:CE2  | 1:G:332:LEU:HD22 | 2.53                     | 0.43              |
| 1:F:449:TRP:CH2  | 1:G:461:ILE:HG12 | 2.53                     | 0.43              |
| 1:G:27:TYR:CZ    | 1:G:264:TYR:HB2  | 2.54                     | 0.43              |
| 1:G:396:LEU:HD23 | 1:G:396:LEU:HA   | 1.82                     | 0.43              |
| 1:H:71:SER:OG    | 1:I:383:ASP:OD1  | 2.29                     | 0.43              |
| 1:K:367:GLU:HG2  | 1:L:376:TYR:CE1  | 2.50                     | 0.43              |
| 1:L:440:ASP:O    | 1:L:443:GLU:HG3  | 2.19                     | 0.43              |
| 1:A:220:ASP:HB3  | 1:A:223:SER:O    | 2.19                     | 0.43              |
| 1:B:434:GLY:O    | 1:B:435:ARG:HD2  | 2.19                     | 0.43              |
| 1:C:128:VAL:O    | 1:C:132:GLU:HG2  | 2.18                     | 0.43              |
| 1:C:220:ASP:HB3  | 1:C:223:SER:O    | 2.19                     | 0.43              |
| 1:D:158:MET:HE3  | 1:D:158:MET:HB3  | 1.59                     | 0.43              |
| 1:D:372:GLU:O    | 1:D:373:GLU:C    | 2.61                     | 0.43              |
| 1:E:8:LEU:HD23   | 1:E:8:LEU:H      | 1.83                     | 0.43              |
| 1:F:80:MET:CE    | 1:G:431:GLU:OE1  | 2.60                     | 0.43              |
| 1:F:440:ASP:O    | 1:F:443:GLU:HG3  | 2.19                     | 0.43              |
| 1:G:115:ARG:NH2  | 1:H:475:GLY:C    | 2.77                     | 0.43              |
| 1:G:167:VAL:HG23 | 1:G:264:TYR:OH   | 2.19                     | 0.43              |
| 1:H:24:ARG:O     | 1:H:25:ALA:C     | 2.62                     | 0.43              |
| 1:H:67:ASN:ND2   | 1:I:386:GLY:HA2  | 2.34                     | 0.43              |
| 1:H:220:ASP:HB3  | 1:H:223:SER:O    | 2.19                     | 0.43              |
| 1:I:110:LEU:O    | 1:I:114:GLU:N    | 2.46                     | 0.43              |
| 1:J:372:GLU:O    | 1:J:373:GLU:C    | 2.61                     | 0.43              |
| 1:K:314:ALA:HB1  | 1:K:318:ASP:HB3  | 2.00                     | 0.43              |
| 1:L:8:LEU:HD23   | 1:L:8:LEU:H      | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:165:SER:O    | 1:A:165:SER:OG   | 2.30                     | 0.43              |
| 1:A:369:VAL:HB   | 1:B:375:ARG:HG2  | 2.00                     | 0.43              |
| 1:B:372:GLU:O    | 1:B:373:GLU:C    | 2.61                     | 0.43              |
| 1:C:206:LYS:H    | 1:C:206:LYS:HG2  | 1.52                     | 0.43              |
| 1:E:416:GLU:H    | 1:E:416:GLU:HG2  | 1.65                     | 0.43              |
| 1:F:167:VAL:HG23 | 1:F:264:TYR:OH   | 2.19                     | 0.43              |
| 1:F:335:GLN:HE22 | 1:G:336:ALA:HB1  | 1.84                     | 0.43              |
| 1:H:27:TYR:CZ    | 1:H:264:TYR:HB2  | 2.54                     | 0.43              |
| 1:H:413:GLN:O    | 1:I:93:ALA:HB1   | 2.18                     | 0.43              |
| 1:I:128:VAL:O    | 1:I:132:GLU:HG2  | 2.18                     | 0.43              |
| 1:J:412:GLN:HB3  | 1:J:413:GLN:H    | 1.57                     | 0.43              |
| 1:A:8:LEU:HD23   | 1:A:8:LEU:H      | 1.83                     | 0.43              |
| 1:A:412:GLN:HB3  | 1:A:413:GLN:H    | 1.57                     | 0.43              |
| 1:B:24:ARG:O     | 1:B:25:ALA:C     | 2.62                     | 0.43              |
| 1:B:27:TYR:CZ    | 1:B:264:TYR:HB2  | 2.54                     | 0.43              |
| 1:B:227:LEU:HD23 | 1:B:227:LEU:HA   | 1.83                     | 0.43              |
| 1:C:27:TYR:CZ    | 1:C:264:TYR:HB2  | 2.54                     | 0.43              |
| 1:C:367:GLU:HG2  | 1:D:376:TYR:CE1  | 2.51                     | 0.43              |
| 1:C:369:VAL:HB   | 1:D:375:ARG:HG2  | 2.00                     | 0.43              |
| 1:C:372:GLU:O    | 1:C:373:GLU:C    | 2.62                     | 0.43              |
| 1:C:413:GLN:CB   | 1:D:93:ALA:CB    | 2.92                     | 0.43              |
| 1:D:220:ASP:HB3  | 1:D:223:SER:O    | 2.19                     | 0.43              |
| 1:E:27:TYR:CZ    | 1:E:264:TYR:HB2  | 2.54                     | 0.43              |
| 1:E:128:VAL:O    | 1:E:132:GLU:HG2  | 2.18                     | 0.43              |
| 1:F:434:GLY:O    | 1:F:435:ARG:HD2  | 2.19                     | 0.43              |
| 1:H:314:ALA:HB1  | 1:H:318:ASP:HB3  | 2.00                     | 0.43              |
| 1:I:8:LEU:HD23   | 1:I:8:LEU:H      | 1.83                     | 0.43              |
| 1:I:386:GLY:C    | 1:I:388:VAL:H    | 2.25                     | 0.43              |
| 1:J:311:LEU:HD13 | 1:J:311:LEU:HA   | 1.84                     | 0.43              |
| 1:B:329:PHE:CE2  | 1:C:332:LEU:HD22 | 2.54                     | 0.42              |
| 1:B:396:LEU:HD23 | 1:B:396:LEU:HA   | 1.82                     | 0.42              |
| 1:C:167:VAL:HG23 | 1:C:264:TYR:OH   | 2.19                     | 0.42              |
| 1:C:467:LYS:CB   | 1:D:460:ASP:OD2  | 2.61                     | 0.42              |
| 1:C:474:ILE:H    | 1:C:474:ILE:HG12 | 1.66                     | 0.42              |
| 1:D:8:LEU:HD23   | 1:D:8:LEU:H      | 1.83                     | 0.42              |
| 1:D:27:TYR:CZ    | 1:D:264:TYR:HB2  | 2.54                     | 0.42              |
| 1:E:372:GLU:C    | 1:E:374:ILE:H    | 2.25                     | 0.42              |
| 1:G:381:LEU:HD23 | 1:G:381:LEU:HA   | 1.71                     | 0.42              |
| 1:I:220:ASP:HB3  | 1:I:223:SER:O    | 2.19                     | 0.42              |
| 1:J:314:ALA:HB1  | 1:J:318:ASP:HB3  | 2.00                     | 0.42              |
| 1:J:374:ILE:HD12 | 1:J:374:ILE:HA   | 1.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:388:VAL:O    | 1:J:389:TYR:C    | 2.59                     | 0.42              |
| 1:K:440:ASP:O    | 1:K:443:GLU:HG3  | 2.19                     | 0.42              |
| 1:A:375:ARG:CG   | 1:L:369:VAL:HB   | 2.49                     | 0.42              |
| 1:E:167:VAL:HG23 | 1:E:264:TYR:OH   | 2.19                     | 0.42              |
| 1:E:440:ASP:O    | 1:E:443:GLU:HG3  | 2.19                     | 0.42              |
| 1:F:8:LEU:HD23   | 1:F:8:LEU:H      | 1.83                     | 0.42              |
| 1:G:388:VAL:O    | 1:G:389:TYR:C    | 2.59                     | 0.42              |
| 1:A:27:TYR:CZ    | 1:A:264:TYR:HB2  | 2.54                     | 0.42              |
| 1:B:67:ASN:ND2   | 1:C:386:GLY:HA2  | 2.33                     | 0.42              |
| 1:C:186:ALA:CB   | 1:D:171:ASP:HB3  | 2.47                     | 0.42              |
| 1:C:314:ALA:HB1  | 1:C:318:ASP:HB3  | 2.00                     | 0.42              |
| 1:E:112:MET:CG   | 1:F:97:LEU:HD21  | 2.50                     | 0.42              |
| 1:F:80:MET:HB2   | 1:F:80:MET:HE2   | 1.49                     | 0.42              |
| 1:I:24:ARG:O     | 1:I:25:ALA:C     | 2.62                     | 0.42              |
| 1:I:27:TYR:CZ    | 1:I:264:TYR:HB2  | 2.54                     | 0.42              |
| 1:L:24:ARG:O     | 1:L:25:ALA:C     | 2.62                     | 0.42              |
| 1:B:314:ALA:HB1  | 1:B:318:ASP:HB3  | 2.00                     | 0.42              |
| 1:B:335:GLN:HE22 | 1:C:336:ALA:HB1  | 1.85                     | 0.42              |
| 1:C:8:LEU:HD23   | 1:C:8:LEU:H      | 1.83                     | 0.42              |
| 1:E:434:GLY:O    | 1:E:435:ARG:HD2  | 2.19                     | 0.42              |
| 1:F:327:ILE:HD12 | 1:G:330:LEU:HD12 | 2.02                     | 0.42              |
| 1:G:220:ASP:HB3  | 1:G:223:SER:O    | 2.19                     | 0.42              |
| 1:G:440:ASP:O    | 1:G:443:GLU:HG3  | 2.19                     | 0.42              |
| 1:H:434:GLY:O    | 1:H:435:ARG:HD2  | 2.19                     | 0.42              |
| 1:I:434:GLY:O    | 1:I:435:ARG:HD2  | 2.19                     | 0.42              |
| 1:K:220:ASP:HB3  | 1:K:223:SER:O    | 2.19                     | 0.42              |
| 1:K:240:SER:O    | 1:K:241:ASP:C    | 2.63                     | 0.42              |
| 1:L:392:LEU:HD12 | 1:L:392:LEU:HA   | 1.61                     | 0.42              |
| 1:A:167:VAL:HG23 | 1:A:264:TYR:OH   | 2.19                     | 0.42              |
| 1:A:434:GLY:O    | 1:A:435:ARG:HD2  | 2.19                     | 0.42              |
| 1:C:440:ASP:O    | 1:C:443:GLU:HG3  | 2.19                     | 0.42              |
| 1:E:80:MET:HE1   | 1:F:431:GLU:OE2  | 2.19                     | 0.42              |
| 1:F:220:ASP:HB3  | 1:F:223:SER:O    | 2.19                     | 0.42              |
| 1:I:80:MET:HE1   | 1:J:431:GLU:OE2  | 2.15                     | 0.42              |
| 1:I:112:MET:CG   | 1:J:97:LEU:HD21  | 2.48                     | 0.42              |
| 1:J:167:VAL:HG23 | 1:J:264:TYR:OH   | 2.19                     | 0.42              |
| 1:J:227:LEU:HD23 | 1:J:227:LEU:HA   | 1.83                     | 0.42              |
| 1:A:80:MET:HE1   | 1:B:431:GLU:OE2  | 2.17                     | 0.42              |
| 1:B:8:LEU:HD23   | 1:B:8:LEU:H      | 1.83                     | 0.42              |
| 1:B:186:ALA:CB   | 1:C:171:ASP:HB3  | 2.47                     | 0.42              |
| 1:B:220:ASP:HB3  | 1:B:223:SER:O    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:434:GLY:O    | 1:C:435:ARG:HD2  | 2.19                     | 0.42              |
| 1:D:80:MET:HE2   | 1:D:80:MET:HB2   | 1.49                     | 0.42              |
| 1:E:110:LEU:O    | 1:E:114:GLU:N    | 2.46                     | 0.42              |
| 1:E:220:ASP:HB3  | 1:E:223:SER:O    | 2.19                     | 0.42              |
| 1:E:467:LYS:CB   | 1:F:460:ASP:OD2  | 2.65                     | 0.42              |
| 1:F:381:LEU:HD22 | 1:F:385:LEU:HG   | 2.02                     | 0.42              |
| 1:G:8:LEU:H      | 1:G:8:LEU:HD23   | 1.83                     | 0.42              |
| 1:G:381:LEU:HD22 | 1:G:385:LEU:HG   | 2.02                     | 0.42              |
| 1:G:467:LYS:CB   | 1:H:460:ASP:OD2  | 2.63                     | 0.42              |
| 1:H:80:MET:CE    | 1:I:431:GLU:OE1  | 2.59                     | 0.42              |
| 1:I:167:VAL:HG23 | 1:I:264:TYR:OH   | 2.19                     | 0.42              |
| 1:I:314:ALA:HB1  | 1:I:318:ASP:HB3  | 2.00                     | 0.42              |
| 1:I:322:GLY:O    | 1:J:300:VAL:O    | 2.37                     | 0.42              |
| 1:I:381:LEU:HD22 | 1:I:385:LEU:HG   | 2.02                     | 0.42              |
| 1:J:165:SER:O    | 1:J:165:SER:OG   | 2.29                     | 0.42              |
| 1:J:452:LEU:O    | 1:J:456:ARG:NH1  | 2.53                     | 0.42              |
| 1:L:27:TYR:CZ    | 1:L:264:TYR:HB2  | 2.54                     | 0.42              |
| 1:L:434:GLY:O    | 1:L:435:ARG:HD2  | 2.19                     | 0.42              |
| 1:B:388:VAL:O    | 1:B:389:TYR:C    | 2.59                     | 0.42              |
| 1:B:392:LEU:HA   | 1:B:392:LEU:HD12 | 1.61                     | 0.42              |
| 1:C:386:GLY:C    | 1:C:388:VAL:H    | 2.25                     | 0.42              |
| 1:D:469:ARG:HA   | 1:D:469:ARG:HD2  | 1.67                     | 0.42              |
| 1:E:381:LEU:HD22 | 1:E:385:LEU:HG   | 2.02                     | 0.42              |
| 1:G:434:GLY:O    | 1:G:435:ARG:HD2  | 2.19                     | 0.42              |
| 1:H:256:MET:HB3  | 1:H:266:ARG:O    | 2.20                     | 0.42              |
| 1:H:327:ILE:HD12 | 1:I:330:LEU:HD12 | 2.02                     | 0.42              |
| 1:H:381:LEU:HD22 | 1:H:385:LEU:HG   | 2.02                     | 0.42              |
| 1:H:440:ASP:O    | 1:H:443:GLU:HG3  | 2.19                     | 0.42              |
| 1:I:440:ASP:O    | 1:I:443:GLU:HG3  | 2.19                     | 0.42              |
| 1:J:440:ASP:O    | 1:J:443:GLU:HG3  | 2.19                     | 0.42              |
| 1:K:388:VAL:O    | 1:K:389:TYR:C    | 2.59                     | 0.42              |
| 1:K:452:LEU:O    | 1:K:456:ARG:NH1  | 2.53                     | 0.42              |
| 1:L:388:VAL:O    | 1:L:389:TYR:C    | 2.59                     | 0.42              |
| 1:A:440:ASP:O    | 1:A:443:GLU:HG3  | 2.19                     | 0.42              |
| 1:B:474:ILE:H    | 1:B:474:ILE:HG12 | 1.67                     | 0.42              |
| 1:C:372:GLU:C    | 1:C:374:ILE:H    | 2.25                     | 0.42              |
| 1:C:381:LEU:HD23 | 1:C:381:LEU:HA   | 1.71                     | 0.42              |
| 1:D:372:GLU:C    | 1:D:374:ILE:H    | 2.25                     | 0.42              |
| 1:E:126:TYR:CE1  | 1:E:158:MET:N    | 2.88                     | 0.42              |
| 1:E:258:ARG:HE   | 1:E:258:ARG:HB2  | 1.45                     | 0.42              |
| 1:E:413:GLN:CB   | 1:F:93:ALA:CB    | 2.89                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:186:ALA:CB   | 1:G:171:ASP:HB3  | 2.45                     | 0.42              |
| 1:F:464:ALA:O    | 1:G:460:ASP:OD2  | 2.37                     | 0.42              |
| 1:I:372:GLU:O    | 1:I:373:GLU:C    | 2.61                     | 0.42              |
| 1:I:392:LEU:HD12 | 1:I:392:LEU:HA   | 1.61                     | 0.42              |
| 1:J:24:ARG:O     | 1:J:25:ALA:C     | 2.62                     | 0.42              |
| 1:J:240:SER:O    | 1:J:241:ASP:C    | 2.63                     | 0.42              |
| 1:J:256:MET:HB3  | 1:J:266:ARG:O    | 2.20                     | 0.42              |
| 1:J:396:LEU:HD23 | 1:J:396:LEU:HA   | 1.82                     | 0.42              |
| 1:J:434:GLY:O    | 1:J:435:ARG:HD2  | 2.19                     | 0.42              |
| 1:K:167:VAL:HG23 | 1:K:264:TYR:OH   | 2.19                     | 0.42              |
| 1:L:256:MET:HB3  | 1:L:266:ARG:O    | 2.20                     | 0.42              |
| 1:A:300:VAL:O    | 1:L:322:GLY:O    | 2.36                     | 0.42              |
| 1:A:474:ILE:H    | 1:A:474:ILE:HG12 | 1.67                     | 0.42              |
| 1:D:367:GLU:CG   | 1:E:376:TYR:CE1  | 3.01                     | 0.42              |
| 1:D:440:ASP:O    | 1:D:443:GLU:HG3  | 2.19                     | 0.42              |
| 1:G:352:LEU:HD13 | 1:G:352:LEU:HA   | 1.90                     | 0.42              |
| 1:I:452:LEU:O    | 1:I:456:ARG:NH1  | 2.53                     | 0.42              |
| 1:J:27:TYR:CZ    | 1:J:264:TYR:HB2  | 2.54                     | 0.42              |
| 1:J:381:LEU:HD22 | 1:J:385:LEU:HG   | 2.02                     | 0.42              |
| 1:K:206:LYS:H    | 1:K:206:LYS:HG2  | 1.52                     | 0.42              |
| 1:L:94:LYS:HE3   | 1:L:94:LYS:HB3   | 1.93                     | 0.42              |
| 1:L:220:ASP:HB3  | 1:L:223:SER:O    | 2.19                     | 0.42              |
| 1:L:452:LEU:O    | 1:L:456:ARG:NH1  | 2.53                     | 0.42              |
| 1:B:95:GLN:HE21  | 1:B:95:GLN:HB2   | 1.73                     | 0.42              |
| 1:D:24:ARG:O     | 1:D:25:ALA:C     | 2.62                     | 0.42              |
| 1:E:186:ALA:CB   | 1:F:171:ASP:HB3  | 2.47                     | 0.42              |
| 1:E:256:MET:HB3  | 1:E:266:ARG:O    | 2.20                     | 0.42              |
| 1:F:367:GLU:CG   | 1:G:376:TYR:CE1  | 3.02                     | 0.42              |
| 1:F:386:GLY:C    | 1:F:388:VAL:H    | 2.25                     | 0.42              |
| 1:H:167:VAL:HG23 | 1:H:264:TYR:OH   | 2.19                     | 0.42              |
| 1:H:452:LEU:O    | 1:H:456:ARG:NH1  | 2.53                     | 0.42              |
| 1:L:167:VAL:HG23 | 1:L:264:TYR:OH   | 2.19                     | 0.42              |
| 1:A:431:GLU:CD   | 1:L:80:MET:CE    | 2.81                     | 0.41              |
| 1:B:59:GLN:CA    | 1:C:351:ARG:HH22 | 2.27                     | 0.41              |
| 1:B:256:MET:HB3  | 1:B:266:ARG:O    | 2.20                     | 0.41              |
| 1:D:112:MET:CG   | 1:E:97:LEU:HD21  | 2.50                     | 0.41              |
| 1:E:443:GLU:OE2  | 1:E:444:ARG:HG3  | 2.20                     | 0.41              |
| 1:F:126:TYR:CE1  | 1:F:158:MET:N    | 2.88                     | 0.41              |
| 1:F:256:MET:HB3  | 1:F:266:ARG:O    | 2.20                     | 0.41              |
| 1:F:413:GLN:N    | 1:G:93:ALA:HB3   | 2.35                     | 0.41              |
| 1:H:110:LEU:O    | 1:H:114:GLU:N    | 2.46                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:367:GLU:CG   | 1:I:376:TYR:CE1  | 3.02                     | 0.41              |
| 1:H:392:LEU:HD12 | 1:H:392:LEU:HA   | 1.61                     | 0.41              |
| 1:I:442:LEU:HB3  | 1:J:470:ILE:CD1  | 2.49                     | 0.41              |
| 1:I:474:ILE:H    | 1:I:474:ILE:HG12 | 1.67                     | 0.41              |
| 1:J:94:LYS:HE3   | 1:J:94:LYS:HB3   | 1.93                     | 0.41              |
| 1:J:220:ASP:HB3  | 1:J:223:SER:O    | 2.19                     | 0.41              |
| 1:L:158:MET:HB3  | 1:L:158:MET:HE3  | 1.59                     | 0.41              |
| 1:A:244:TYR:HA   | 1:A:245:PRO:HD3  | 1.95                     | 0.41              |
| 1:A:452:LEU:O    | 1:A:456:ARG:NH1  | 2.53                     | 0.41              |
| 1:C:256:MET:HB3  | 1:C:266:ARG:O    | 2.20                     | 0.41              |
| 1:D:381:LEU:HD22 | 1:D:385:LEU:HG   | 2.02                     | 0.41              |
| 1:H:464:ALA:O    | 1:I:460:ASP:OD2  | 2.36                     | 0.41              |
| 1:I:311:LEU:HA   | 1:I:311:LEU:HD13 | 1.84                     | 0.41              |
| 1:I:412:GLN:HB3  | 1:I:413:GLN:H    | 1.57                     | 0.41              |
| 1:I:443:GLU:OE2  | 1:I:444:ARG:HG3  | 2.21                     | 0.41              |
| 1:J:376:TYR:C    | 1:J:378:ALA:N    | 2.78                     | 0.41              |
| 1:K:24:ARG:O     | 1:K:25:ALA:C     | 2.62                     | 0.41              |
| 1:K:27:TYR:CZ    | 1:K:264:TYR:HB2  | 2.54                     | 0.41              |
| 1:A:94:LYS:HE3   | 1:A:94:LYS:HB3   | 1.93                     | 0.41              |
| 1:A:381:LEU:HD23 | 1:A:381:LEU:HA   | 1.71                     | 0.41              |
| 1:B:56:THR:HG21  | 1:C:274:GLY:H    | 1.85                     | 0.41              |
| 1:B:469:ARG:HD2  | 1:B:469:ARG:HA   | 1.67                     | 0.41              |
| 1:D:256:MET:HB3  | 1:D:266:ARG:O    | 2.20                     | 0.41              |
| 1:E:95:GLN:HE21  | 1:E:95:GLN:HB2   | 1.72                     | 0.41              |
| 1:E:413:GLN:O    | 1:F:93:ALA:HB1   | 2.20                     | 0.41              |
| 1:F:443:GLU:OE2  | 1:F:444:ARG:HG3  | 2.20                     | 0.41              |
| 1:I:396:LEU:HD23 | 1:I:396:LEU:HA   | 1.82                     | 0.41              |
| 1:K:381:LEU:HD22 | 1:K:385:LEU:HG   | 2.02                     | 0.41              |
| 1:K:434:GLY:O    | 1:K:435:ARG:HD2  | 2.19                     | 0.41              |
| 1:L:227:LEU:HD23 | 1:L:227:LEU:HA   | 1.83                     | 0.41              |
| 1:L:376:TYR:C    | 1:L:378:ALA:N    | 2.78                     | 0.41              |
| 1:A:258:ARG:HE   | 1:A:258:ARG:HB2  | 1.45                     | 0.41              |
| 1:G:121:ILE:HD12 | 1:G:121:ILE:HA   | 1.87                     | 0.41              |
| 1:G:443:GLU:OE2  | 1:G:444:ARG:HG3  | 2.20                     | 0.41              |
| 1:H:381:LEU:HA   | 1:H:381:LEU:HD23 | 1.72                     | 0.41              |
| 1:J:392:LEU:HA   | 1:J:392:LEU:HD12 | 1.61                     | 0.41              |
| 1:J:443:GLU:OE2  | 1:J:444:ARG:HG3  | 2.20                     | 0.41              |
| 1:K:227:LEU:HD23 | 1:K:227:LEU:HA   | 1.83                     | 0.41              |
| 1:K:443:GLU:OE2  | 1:K:444:ARG:HG3  | 2.20                     | 0.41              |
| 1:L:469:ARG:HA   | 1:L:469:ARG:HD2  | 1.67                     | 0.41              |
| 1:C:426:ILE:H    | 1:C:426:ILE:HG13 | 1.59                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:452:LEU:O    | 1:C:456:ARG:NH1  | 2.53                     | 0.41              |
| 1:D:240:SER:O    | 1:D:241:ASP:C    | 2.63                     | 0.41              |
| 1:D:311:LEU:HA   | 1:D:311:LEU:HD13 | 1.84                     | 0.41              |
| 1:D:443:GLU:OE2  | 1:D:444:ARG:HG3  | 2.20                     | 0.41              |
| 1:F:67:ASN:ND2   | 1:G:386:GLY:HA2  | 2.35                     | 0.41              |
| 1:F:396:LEU:HA   | 1:F:396:LEU:HD23 | 1.82                     | 0.41              |
| 1:G:452:LEU:O    | 1:G:456:ARG:NH1  | 2.53                     | 0.41              |
| 1:I:413:GLN:HB2  | 1:J:93:ALA:HB1   | 1.97                     | 0.41              |
| 1:L:381:LEU:HD23 | 1:L:381:LEU:HA   | 1.71                     | 0.41              |
| 1:A:24:ARG:O     | 1:A:25:ALA:C     | 2.62                     | 0.41              |
| 1:A:367:GLU:HG2  | 1:B:376:TYR:CE1  | 2.51                     | 0.41              |
| 1:A:381:LEU:HD22 | 1:A:385:LEU:HG   | 2.02                     | 0.41              |
| 1:A:388:VAL:O    | 1:A:389:TYR:C    | 2.59                     | 0.41              |
| 1:B:408:LEU:HA   | 1:B:408:LEU:HD23 | 1.87                     | 0.41              |
| 1:B:452:LEU:O    | 1:B:456:ARG:NH1  | 2.53                     | 0.41              |
| 1:E:452:LEU:O    | 1:E:456:ARG:NH1  | 2.53                     | 0.41              |
| 1:L:474:ILE:H    | 1:L:474:ILE:HG12 | 1.67                     | 0.41              |
| 1:B:367:GLU:CG   | 1:C:376:TYR:CE1  | 3.01                     | 0.41              |
| 1:C:240:SER:O    | 1:C:241:ASP:C    | 2.63                     | 0.41              |
| 1:D:59:GLN:CA    | 1:E:351:ARG:HH22 | 2.27                     | 0.41              |
| 1:E:112:MET:SD   | 1:F:97:LEU:HD21  | 2.61                     | 0.41              |
| 1:F:452:LEU:O    | 1:F:456:ARG:NH1  | 2.53                     | 0.41              |
| 1:G:256:MET:HB3  | 1:G:266:ARG:O    | 2.20                     | 0.41              |
| 1:H:95:GLN:HE21  | 1:H:95:GLN:HB2   | 1.72                     | 0.41              |
| 1:H:442:LEU:CB   | 1:I:470:ILE:CD1  | 2.99                     | 0.41              |
| 1:I:240:SER:O    | 1:I:241:ASP:C    | 2.63                     | 0.41              |
| 1:J:439:LEU:HD12 | 1:K:473:ALA:CB   | 2.49                     | 0.41              |
| 1:K:430:LEU:O    | 1:K:431:GLU:C    | 2.63                     | 0.41              |
| 1:L:381:LEU:HD22 | 1:L:385:LEU:HG   | 2.02                     | 0.41              |
| 1:A:171:ASP:HB3  | 1:L:186:ALA:CB   | 2.49                     | 0.41              |
| 1:B:240:SER:O    | 1:B:241:ASP:C    | 2.63                     | 0.41              |
| 1:B:352:LEU:HD13 | 1:B:352:LEU:HA   | 1.89                     | 0.41              |
| 1:B:381:LEU:HD22 | 1:B:385:LEU:HG   | 2.02                     | 0.41              |
| 1:D:206:LYS:H    | 1:D:206:LYS:HG2  | 1.52                     | 0.41              |
| 1:D:352:LEU:HD13 | 1:D:352:LEU:HA   | 1.90                     | 0.41              |
| 1:D:413:GLN:N    | 1:E:93:ALA:HB3   | 2.36                     | 0.41              |
| 1:E:240:SER:O    | 1:E:241:ASP:C    | 2.63                     | 0.41              |
| 1:G:290:SER:HB3  | 1:H:344:VAL:HG11 | 2.02                     | 0.41              |
| 1:H:372:GLU:O    | 1:H:373:GLU:C    | 2.61                     | 0.41              |
| 1:H:408:LEU:HD23 | 1:H:408:LEU:HA   | 1.86                     | 0.41              |
| 1:I:256:MET:HB3  | 1:I:266:ARG:O    | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:95:GLN:HE21  | 1:L:95:GLN:HB2   | 1.73                     | 0.41              |
| 1:B:130:LEU:HD12 | 1:B:130:LEU:HA   | 1.96                     | 0.41              |
| 1:B:412:GLN:HB3  | 1:B:413:GLN:H    | 1.57                     | 0.41              |
| 1:C:24:ARG:O     | 1:C:25:ALA:C     | 2.62                     | 0.41              |
| 1:C:115:ARG:NH2  | 1:D:475:GLY:C    | 2.79                     | 0.41              |
| 1:C:381:LEU:HD22 | 1:C:385:LEU:HG   | 2.02                     | 0.41              |
| 1:D:452:LEU:O    | 1:D:456:ARG:NH1  | 2.53                     | 0.41              |
| 1:E:322:GLY:O    | 1:F:300:VAL:O    | 2.39                     | 0.41              |
| 1:E:413:GLN:O    | 1:F:93:ALA:CB    | 2.69                     | 0.41              |
| 1:H:335:GLN:HE22 | 1:I:336:ALA:HB1  | 1.85                     | 0.41              |
| 1:H:443:GLU:OE2  | 1:H:444:ARG:HG3  | 2.20                     | 0.41              |
| 1:I:56:THR:HG21  | 1:J:274:GLY:H    | 1.86                     | 0.41              |
| 1:J:431:GLU:H    | 1:J:431:GLU:HG2  | 1.22                     | 0.41              |
| 1:K:256:MET:HB3  | 1:K:266:ARG:O    | 2.20                     | 0.41              |
| 1:K:413:GLN:CB   | 1:L:93:ALA:HB1   | 2.51                     | 0.41              |
| 1:L:443:GLU:OE2  | 1:L:444:ARG:HG3  | 2.20                     | 0.41              |
| 1:A:97:LEU:HD21  | 1:L:112:MET:CG   | 2.51                     | 0.41              |
| 1:A:256:MET:HB3  | 1:A:266:ARG:O    | 2.20                     | 0.41              |
| 1:B:327:ILE:HD12 | 1:C:330:LEU:HD12 | 2.03                     | 0.41              |
| 1:C:311:LEU:HD13 | 1:C:311:LEU:HA   | 1.84                     | 0.41              |
| 1:C:461:ILE:HD12 | 1:C:461:ILE:HA   | 1.95                     | 0.41              |
| 1:E:474:ILE:H    | 1:E:474:ILE:HG12 | 1.67                     | 0.41              |
| 1:F:56:THR:HG21  | 1:G:274:GLY:H    | 1.86                     | 0.41              |
| 1:H:196:LYS:HE3  | 1:H:196:LYS:HB3  | 1.91                     | 0.41              |
| 1:H:396:LEU:HD23 | 1:H:396:LEU:HA   | 1.82                     | 0.41              |
| 1:I:453:ALA:N    | 1:I:454:PRO:HD2  | 2.36                     | 0.41              |
| 1:K:386:GLY:C    | 1:K:388:VAL:N    | 2.78                     | 0.41              |
| 1:B:386:GLY:C    | 1:B:388:VAL:N    | 2.78                     | 0.40              |
| 1:C:396:LEU:HD23 | 1:C:396:LEU:HA   | 1.82                     | 0.40              |
| 1:E:196:LYS:HE3  | 1:E:196:LYS:HB3  | 1.91                     | 0.40              |
| 1:F:240:SER:O    | 1:F:241:ASP:C    | 2.63                     | 0.40              |
| 1:G:80:MET:CE    | 1:H:431:GLU:OE1  | 2.62                     | 0.40              |
| 1:G:112:MET:CG   | 1:H:97:LEU:HD21  | 2.51                     | 0.40              |
| 1:H:453:ALA:N    | 1:H:454:PRO:HD2  | 2.36                     | 0.40              |
| 1:I:388:VAL:O    | 1:I:389:TYR:C    | 2.59                     | 0.40              |
| 1:I:467:LYS:CD   | 1:J:460:ASP:HB3  | 2.49                     | 0.40              |
| 1:J:453:ALA:N    | 1:J:454:PRO:HD2  | 2.36                     | 0.40              |
| 1:K:94:LYS:HE3   | 1:K:94:LYS:HB3   | 1.93                     | 0.40              |
| 1:L:80:MET:HE2   | 1:L:80:MET:HB2   | 1.49                     | 0.40              |
| 1:L:386:GLY:C    | 1:L:388:VAL:N    | 2.78                     | 0.40              |
| 1:A:470:ILE:HD11 | 1:L:442:LEU:CB   | 2.44                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:430:LEU:O    | 1:B:431:GLU:C    | 2.63                     | 0.40              |
| 1:B:442:LEU:CB   | 1:C:470:ILE:CD1  | 2.98                     | 0.40              |
| 1:B:443:GLU:OE2  | 1:B:444:ARG:HG3  | 2.20                     | 0.40              |
| 1:F:112:MET:SD   | 1:F:415:PRO:CB   | 3.10                     | 0.40              |
| 1:I:115:ARG:HH22 | 1:J:475:GLY:C    | 2.28                     | 0.40              |
| 1:J:408:LEU:HD23 | 1:J:408:LEU:HA   | 1.86                     | 0.40              |
| 1:L:426:ILE:H    | 1:L:426:ILE:HG13 | 1.59                     | 0.40              |
| 1:C:442:LEU:HB3  | 1:D:470:ILE:CD1  | 2.51                     | 0.40              |
| 1:D:95:GLN:HE21  | 1:D:95:GLN:HB2   | 1.73                     | 0.40              |
| 1:D:112:MET:SD   | 1:D:415:PRO:CB   | 3.10                     | 0.40              |
| 1:G:240:SER:O    | 1:G:241:ASP:C    | 2.63                     | 0.40              |
| 1:G:453:ALA:N    | 1:G:454:PRO:HD2  | 2.36                     | 0.40              |
| 1:H:56:THR:HG21  | 1:I:274:GLY:H    | 1.87                     | 0.40              |
| 1:I:293:SER:HG   | 1:J:337:ASP:HB3  | 1.84                     | 0.40              |
| 1:I:323:ARG:HG3  | 1:J:301:ASN:HD22 | 1.75                     | 0.40              |
| 1:J:73:LEU:HG    | 1:J:134:LEU:HD11 | 2.03                     | 0.40              |
| 1:K:73:LEU:HG    | 1:K:134:LEU:HD11 | 2.03                     | 0.40              |
| 1:L:417:LEU:HA   | 1:L:418:PRO:HD3  | 1.90                     | 0.40              |
| 1:A:186:ALA:CB   | 1:B:171:ASP:HB3  | 2.47                     | 0.40              |
| 1:F:442:LEU:CB   | 1:G:470:ILE:CD1  | 2.99                     | 0.40              |
| 1:G:110:LEU:O    | 1:G:114:GLU:N    | 2.46                     | 0.40              |
| 1:G:112:MET:SD   | 1:G:415:PRO:CB   | 3.10                     | 0.40              |
| 1:G:376:TYR:C    | 1:G:378:ALA:N    | 2.78                     | 0.40              |
| 1:H:433:ILE:HD12 | 1:H:433:ILE:HA   | 1.83                     | 0.40              |
| 1:I:112:MET:SD   | 1:I:415:PRO:CB   | 3.10                     | 0.40              |
| 1:I:186:ALA:O    | 1:I:187:PHE:C    | 2.65                     | 0.40              |
| 1:I:430:LEU:O    | 1:I:431:GLU:C    | 2.63                     | 0.40              |
| 1:L:112:MET:SD   | 1:L:415:PRO:CB   | 3.10                     | 0.40              |
| 1:A:59:GLN:OE1   | 1:A:61:VAL:N     | 2.55                     | 0.40              |
| 1:A:386:GLY:C    | 1:A:388:VAL:N    | 2.78                     | 0.40              |
| 1:A:417:LEU:HA   | 1:A:418:PRO:HD3  | 1.90                     | 0.40              |
| 1:A:443:GLU:OE2  | 1:A:444:ARG:HG3  | 2.21                     | 0.40              |
| 1:B:158:MET:HB3  | 1:B:158:MET:HE3  | 1.59                     | 0.40              |
| 1:C:112:MET:SD   | 1:C:415:PRO:CB   | 3.10                     | 0.40              |
| 1:D:453:ALA:N    | 1:D:454:PRO:HD2  | 2.36                     | 0.40              |
| 1:E:442:LEU:HB3  | 1:F:470:ILE:CD1  | 2.50                     | 0.40              |
| 1:F:59:GLN:OE1   | 1:F:61:VAL:N     | 2.55                     | 0.40              |
| 1:F:329:PHE:CE2  | 1:G:332:LEU:HD23 | 2.56                     | 0.40              |
| 1:G:282:LEU:HD12 | 1:G:282:LEU:HA   | 1.95                     | 0.40              |
| 1:H:376:TYR:C    | 1:H:378:ALA:N    | 2.78                     | 0.40              |
| 1:I:112:MET:SD   | 1:J:97:LEU:HD21  | 2.61                     | 0.40              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:J:386:GLY:C   | 1:J:388:VAL:N  | 2.79                     | 0.40              |
| 1:K:412:GLN:HB3 | 1:K:413:GLN:H  | 1.57                     | 0.40              |
| 1:K:469:ARG:HD2 | 1:K:469:ARG:HA | 1.67                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | B     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | C     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | D     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | E     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | F     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | G     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | H     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | I     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | J     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | K     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| 1   | L     | 465/536 (87%)   | 436 (94%)  | 28 (6%)  | 1 (0%)   | 43          | 77 |
| All | All   | 5580/6432 (87%) | 5232 (94%) | 336 (6%) | 12 (0%)  | 44          | 77 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 388 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 388 | VAL  |
| 1   | C     | 388 | VAL  |
| 1   | D     | 388 | VAL  |
| 1   | H     | 388 | VAL  |
| 1   | E     | 388 | VAL  |
| 1   | F     | 388 | VAL  |
| 1   | G     | 388 | VAL  |
| 1   | I     | 388 | VAL  |
| 1   | J     | 388 | VAL  |
| 1   | K     | 388 | VAL  |
| 1   | L     | 388 | 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     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | B     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | C     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | D     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | E     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | F     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | G     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | H     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | I     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | J     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | K     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| 1   | L     | 396/442 (90%)   | 330 (83%)  | 66 (17%)  | 2           | 12 |
| All | All   | 4752/5304 (90%) | 3960 (83%) | 792 (17%) | 4           | 12 |

All (792) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | THR  |
| 1   | A     | 15  | SER  |
| 1   | A     | 34  | CYS  |
| 1   | A     | 38  | THR  |
| 1   | A     | 52  | THR  |
| 1   | A     | 56  | THR  |
| 1   | A     | 75  | LEU  |
| 1   | A     | 86  | LEU  |
| 1   | A     | 88  | ILE  |
| 1   | A     | 95  | GLN  |
| 1   | A     | 96  | LEU  |
| 1   | A     | 106 | VAL  |
| 1   | A     | 108 | GLU  |
| 1   | A     | 116 | ILE  |
| 1   | A     | 121 | ILE  |
| 1   | A     | 124 | ASN  |
| 1   | A     | 129 | THR  |
| 1   | A     | 130 | LEU  |
| 1   | A     | 138 | VAL  |
| 1   | A     | 139 | VAL  |
| 1   | A     | 147 | LEU  |
| 1   | A     | 158 | MET  |
| 1   | A     | 160 | LEU  |
| 1   | A     | 164 | SER  |
| 1   | A     | 165 | SER  |
| 1   | A     | 179 | MET  |
| 1   | A     | 193 | ASP  |
| 1   | A     | 206 | LYS  |
| 1   | A     | 210 | THR  |
| 1   | A     | 217 | ILE  |
| 1   | A     | 221 | GLU  |
| 1   | A     | 223 | SER  |
| 1   | A     | 227 | LEU  |
| 1   | A     | 237 | VAL  |
| 1   | A     | 238 | GLN  |
| 1   | A     | 243 | THR  |
| 1   | A     | 256 | MET  |
| 1   | A     | 259 | LEU  |
| 1   | A     | 263 | SER  |
| 1   | A     | 275 | ASP  |
| 1   | A     | 282 | LEU  |
| 1   | A     | 286 | ILE  |
| 1   | A     | 297 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 307 | GLN  |
| 1   | A     | 311 | LEU  |
| 1   | A     | 313 | LYS  |
| 1   | A     | 321 | THR  |
| 1   | A     | 326 | ASP  |
| 1   | A     | 351 | ARG  |
| 1   | A     | 352 | LEU  |
| 1   | A     | 353 | SER  |
| 1   | A     | 357 | MET  |
| 1   | A     | 368 | ARG  |
| 1   | A     | 369 | VAL  |
| 1   | A     | 389 | TYR  |
| 1   | A     | 397 | GLN  |
| 1   | A     | 399 | PRO  |
| 1   | A     | 403 | VAL  |
| 1   | A     | 412 | GLN  |
| 1   | A     | 416 | GLU  |
| 1   | A     | 417 | LEU  |
| 1   | A     | 422 | VAL  |
| 1   | A     | 431 | GLU  |
| 1   | A     | 446 | VAL  |
| 1   | A     | 452 | LEU  |
| 1   | A     | 474 | ILE  |
| 1   | B     | 6   | THR  |
| 1   | B     | 15  | SER  |
| 1   | B     | 34  | CYS  |
| 1   | B     | 38  | THR  |
| 1   | B     | 52  | THR  |
| 1   | B     | 56  | THR  |
| 1   | B     | 75  | LEU  |
| 1   | B     | 86  | LEU  |
| 1   | B     | 88  | ILE  |
| 1   | B     | 95  | GLN  |
| 1   | B     | 96  | LEU  |
| 1   | B     | 106 | VAL  |
| 1   | B     | 108 | GLU  |
| 1   | B     | 116 | ILE  |
| 1   | B     | 121 | ILE  |
| 1   | B     | 124 | ASN  |
| 1   | B     | 129 | THR  |
| 1   | B     | 130 | LEU  |
| 1   | B     | 138 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 139 | VAL  |
| 1   | B     | 147 | LEU  |
| 1   | B     | 158 | MET  |
| 1   | B     | 160 | LEU  |
| 1   | B     | 164 | SER  |
| 1   | B     | 165 | SER  |
| 1   | B     | 179 | MET  |
| 1   | B     | 193 | ASP  |
| 1   | B     | 206 | LYS  |
| 1   | B     | 210 | THR  |
| 1   | B     | 217 | ILE  |
| 1   | B     | 221 | GLU  |
| 1   | B     | 223 | SER  |
| 1   | B     | 227 | LEU  |
| 1   | B     | 237 | VAL  |
| 1   | B     | 238 | GLN  |
| 1   | B     | 243 | THR  |
| 1   | B     | 256 | MET  |
| 1   | B     | 259 | LEU  |
| 1   | B     | 263 | SER  |
| 1   | B     | 275 | ASP  |
| 1   | B     | 282 | LEU  |
| 1   | B     | 286 | ILE  |
| 1   | B     | 297 | ILE  |
| 1   | B     | 307 | GLN  |
| 1   | B     | 311 | LEU  |
| 1   | B     | 313 | LYS  |
| 1   | B     | 321 | THR  |
| 1   | B     | 326 | ASP  |
| 1   | B     | 351 | ARG  |
| 1   | B     | 352 | LEU  |
| 1   | B     | 353 | SER  |
| 1   | B     | 357 | MET  |
| 1   | B     | 368 | ARG  |
| 1   | B     | 369 | VAL  |
| 1   | B     | 389 | TYR  |
| 1   | B     | 397 | GLN  |
| 1   | B     | 399 | PRO  |
| 1   | B     | 403 | VAL  |
| 1   | B     | 412 | GLN  |
| 1   | B     | 416 | GLU  |
| 1   | B     | 417 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 422 | VAL  |
| 1   | B     | 431 | GLU  |
| 1   | B     | 446 | VAL  |
| 1   | B     | 452 | LEU  |
| 1   | B     | 474 | ILE  |
| 1   | C     | 6   | THR  |
| 1   | C     | 15  | SER  |
| 1   | C     | 34  | CYS  |
| 1   | C     | 38  | THR  |
| 1   | C     | 52  | THR  |
| 1   | C     | 56  | THR  |
| 1   | C     | 75  | LEU  |
| 1   | C     | 86  | LEU  |
| 1   | C     | 88  | ILE  |
| 1   | C     | 95  | GLN  |
| 1   | C     | 96  | LEU  |
| 1   | C     | 106 | VAL  |
| 1   | C     | 108 | GLU  |
| 1   | C     | 116 | ILE  |
| 1   | C     | 121 | ILE  |
| 1   | C     | 124 | ASN  |
| 1   | C     | 129 | THR  |
| 1   | C     | 130 | LEU  |
| 1   | C     | 138 | VAL  |
| 1   | C     | 139 | VAL  |
| 1   | C     | 147 | LEU  |
| 1   | C     | 158 | MET  |
| 1   | C     | 160 | LEU  |
| 1   | C     | 164 | SER  |
| 1   | C     | 165 | SER  |
| 1   | C     | 179 | MET  |
| 1   | C     | 193 | ASP  |
| 1   | C     | 206 | LYS  |
| 1   | C     | 210 | THR  |
| 1   | C     | 217 | ILE  |
| 1   | C     | 221 | GLU  |
| 1   | C     | 223 | SER  |
| 1   | C     | 227 | LEU  |
| 1   | C     | 237 | VAL  |
| 1   | C     | 238 | GLN  |
| 1   | C     | 243 | THR  |
| 1   | C     | 256 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 259 | LEU  |
| 1   | C     | 263 | SER  |
| 1   | C     | 275 | ASP  |
| 1   | C     | 282 | LEU  |
| 1   | C     | 286 | ILE  |
| 1   | C     | 297 | ILE  |
| 1   | C     | 307 | GLN  |
| 1   | C     | 311 | LEU  |
| 1   | C     | 313 | LYS  |
| 1   | C     | 321 | THR  |
| 1   | C     | 326 | ASP  |
| 1   | C     | 351 | ARG  |
| 1   | C     | 352 | LEU  |
| 1   | C     | 353 | SER  |
| 1   | C     | 357 | MET  |
| 1   | C     | 368 | ARG  |
| 1   | C     | 369 | VAL  |
| 1   | C     | 389 | TYR  |
| 1   | C     | 397 | GLN  |
| 1   | C     | 399 | PRO  |
| 1   | C     | 403 | VAL  |
| 1   | C     | 412 | GLN  |
| 1   | C     | 416 | GLU  |
| 1   | C     | 417 | LEU  |
| 1   | C     | 422 | VAL  |
| 1   | C     | 431 | GLU  |
| 1   | C     | 446 | VAL  |
| 1   | C     | 452 | LEU  |
| 1   | C     | 474 | ILE  |
| 1   | D     | 6   | THR  |
| 1   | D     | 15  | SER  |
| 1   | D     | 34  | CYS  |
| 1   | D     | 38  | THR  |
| 1   | D     | 52  | THR  |
| 1   | D     | 56  | THR  |
| 1   | D     | 75  | LEU  |
| 1   | D     | 86  | LEU  |
| 1   | D     | 88  | ILE  |
| 1   | D     | 95  | GLN  |
| 1   | D     | 96  | LEU  |
| 1   | D     | 106 | VAL  |
| 1   | D     | 108 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 116 | ILE  |
| 1   | D     | 121 | ILE  |
| 1   | D     | 124 | ASN  |
| 1   | D     | 129 | THR  |
| 1   | D     | 130 | LEU  |
| 1   | D     | 138 | VAL  |
| 1   | D     | 139 | VAL  |
| 1   | D     | 147 | LEU  |
| 1   | D     | 158 | MET  |
| 1   | D     | 160 | LEU  |
| 1   | D     | 164 | SER  |
| 1   | D     | 165 | SER  |
| 1   | D     | 179 | MET  |
| 1   | D     | 193 | ASP  |
| 1   | D     | 206 | LYS  |
| 1   | D     | 210 | THR  |
| 1   | D     | 217 | ILE  |
| 1   | D     | 221 | GLU  |
| 1   | D     | 223 | SER  |
| 1   | D     | 227 | LEU  |
| 1   | D     | 237 | VAL  |
| 1   | D     | 238 | GLN  |
| 1   | D     | 243 | THR  |
| 1   | D     | 256 | MET  |
| 1   | D     | 259 | LEU  |
| 1   | D     | 263 | SER  |
| 1   | D     | 275 | ASP  |
| 1   | D     | 282 | LEU  |
| 1   | D     | 286 | ILE  |
| 1   | D     | 297 | ILE  |
| 1   | D     | 307 | GLN  |
| 1   | D     | 311 | LEU  |
| 1   | D     | 313 | LYS  |
| 1   | D     | 321 | THR  |
| 1   | D     | 326 | ASP  |
| 1   | D     | 351 | ARG  |
| 1   | D     | 352 | LEU  |
| 1   | D     | 353 | SER  |
| 1   | D     | 357 | MET  |
| 1   | D     | 368 | ARG  |
| 1   | D     | 369 | VAL  |
| 1   | D     | 389 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 397 | GLN  |
| 1   | D     | 399 | PRO  |
| 1   | D     | 403 | VAL  |
| 1   | D     | 412 | GLN  |
| 1   | D     | 416 | GLU  |
| 1   | D     | 417 | LEU  |
| 1   | D     | 422 | VAL  |
| 1   | D     | 431 | GLU  |
| 1   | D     | 446 | VAL  |
| 1   | D     | 452 | LEU  |
| 1   | D     | 474 | ILE  |
| 1   | E     | 6   | THR  |
| 1   | E     | 15  | SER  |
| 1   | E     | 34  | CYS  |
| 1   | E     | 38  | THR  |
| 1   | E     | 52  | THR  |
| 1   | E     | 56  | THR  |
| 1   | E     | 75  | LEU  |
| 1   | E     | 86  | LEU  |
| 1   | E     | 88  | ILE  |
| 1   | E     | 95  | GLN  |
| 1   | E     | 96  | LEU  |
| 1   | E     | 106 | VAL  |
| 1   | E     | 108 | GLU  |
| 1   | E     | 116 | ILE  |
| 1   | E     | 121 | ILE  |
| 1   | E     | 124 | ASN  |
| 1   | E     | 129 | THR  |
| 1   | E     | 130 | LEU  |
| 1   | E     | 138 | VAL  |
| 1   | E     | 139 | VAL  |
| 1   | E     | 147 | LEU  |
| 1   | E     | 158 | MET  |
| 1   | E     | 160 | LEU  |
| 1   | E     | 164 | SER  |
| 1   | E     | 165 | SER  |
| 1   | E     | 179 | MET  |
| 1   | E     | 193 | ASP  |
| 1   | E     | 206 | LYS  |
| 1   | E     | 210 | THR  |
| 1   | E     | 217 | ILE  |
| 1   | E     | 221 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 223 | SER  |
| 1   | E     | 227 | LEU  |
| 1   | E     | 237 | VAL  |
| 1   | E     | 238 | GLN  |
| 1   | E     | 243 | THR  |
| 1   | E     | 256 | MET  |
| 1   | E     | 259 | LEU  |
| 1   | E     | 263 | SER  |
| 1   | E     | 275 | ASP  |
| 1   | E     | 282 | LEU  |
| 1   | E     | 286 | ILE  |
| 1   | E     | 297 | ILE  |
| 1   | E     | 307 | GLN  |
| 1   | E     | 311 | LEU  |
| 1   | E     | 313 | LYS  |
| 1   | E     | 321 | THR  |
| 1   | E     | 326 | ASP  |
| 1   | E     | 351 | ARG  |
| 1   | E     | 352 | LEU  |
| 1   | E     | 353 | SER  |
| 1   | E     | 357 | MET  |
| 1   | E     | 368 | ARG  |
| 1   | E     | 369 | VAL  |
| 1   | E     | 389 | TYR  |
| 1   | E     | 397 | GLN  |
| 1   | E     | 399 | PRO  |
| 1   | E     | 403 | VAL  |
| 1   | E     | 412 | GLN  |
| 1   | E     | 416 | GLU  |
| 1   | E     | 417 | LEU  |
| 1   | E     | 422 | VAL  |
| 1   | E     | 431 | GLU  |
| 1   | E     | 446 | VAL  |
| 1   | E     | 452 | LEU  |
| 1   | E     | 474 | ILE  |
| 1   | F     | 6   | THR  |
| 1   | F     | 15  | SER  |
| 1   | F     | 34  | CYS  |
| 1   | F     | 38  | THR  |
| 1   | F     | 52  | THR  |
| 1   | F     | 56  | THR  |
| 1   | F     | 75  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 86  | LEU  |
| 1   | F     | 88  | ILE  |
| 1   | F     | 95  | GLN  |
| 1   | F     | 96  | LEU  |
| 1   | F     | 106 | VAL  |
| 1   | F     | 108 | GLU  |
| 1   | F     | 116 | ILE  |
| 1   | F     | 121 | ILE  |
| 1   | F     | 124 | ASN  |
| 1   | F     | 129 | THR  |
| 1   | F     | 130 | LEU  |
| 1   | F     | 138 | VAL  |
| 1   | F     | 139 | VAL  |
| 1   | F     | 147 | LEU  |
| 1   | F     | 158 | MET  |
| 1   | F     | 160 | LEU  |
| 1   | F     | 164 | SER  |
| 1   | F     | 165 | SER  |
| 1   | F     | 179 | MET  |
| 1   | F     | 193 | ASP  |
| 1   | F     | 206 | LYS  |
| 1   | F     | 210 | THR  |
| 1   | F     | 217 | ILE  |
| 1   | F     | 221 | GLU  |
| 1   | F     | 223 | SER  |
| 1   | F     | 227 | LEU  |
| 1   | F     | 237 | VAL  |
| 1   | F     | 238 | GLN  |
| 1   | F     | 243 | THR  |
| 1   | F     | 256 | MET  |
| 1   | F     | 259 | LEU  |
| 1   | F     | 263 | SER  |
| 1   | F     | 275 | ASP  |
| 1   | F     | 282 | LEU  |
| 1   | F     | 286 | ILE  |
| 1   | F     | 297 | ILE  |
| 1   | F     | 307 | GLN  |
| 1   | F     | 311 | LEU  |
| 1   | F     | 313 | LYS  |
| 1   | F     | 321 | THR  |
| 1   | F     | 326 | ASP  |
| 1   | F     | 351 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 352 | LEU  |
| 1   | F     | 353 | SER  |
| 1   | F     | 357 | MET  |
| 1   | F     | 368 | ARG  |
| 1   | F     | 369 | VAL  |
| 1   | F     | 389 | TYR  |
| 1   | F     | 397 | GLN  |
| 1   | F     | 399 | PRO  |
| 1   | F     | 403 | VAL  |
| 1   | F     | 412 | GLN  |
| 1   | F     | 416 | GLU  |
| 1   | F     | 417 | LEU  |
| 1   | F     | 422 | VAL  |
| 1   | F     | 431 | GLU  |
| 1   | F     | 446 | VAL  |
| 1   | F     | 452 | LEU  |
| 1   | F     | 474 | ILE  |
| 1   | G     | 6   | THR  |
| 1   | G     | 15  | SER  |
| 1   | G     | 34  | CYS  |
| 1   | G     | 38  | THR  |
| 1   | G     | 52  | THR  |
| 1   | G     | 56  | THR  |
| 1   | G     | 75  | LEU  |
| 1   | G     | 86  | LEU  |
| 1   | G     | 88  | ILE  |
| 1   | G     | 95  | GLN  |
| 1   | G     | 96  | LEU  |
| 1   | G     | 106 | VAL  |
| 1   | G     | 108 | GLU  |
| 1   | G     | 116 | ILE  |
| 1   | G     | 121 | ILE  |
| 1   | G     | 124 | ASN  |
| 1   | G     | 129 | THR  |
| 1   | G     | 130 | LEU  |
| 1   | G     | 138 | VAL  |
| 1   | G     | 139 | VAL  |
| 1   | G     | 147 | LEU  |
| 1   | G     | 158 | MET  |
| 1   | G     | 160 | LEU  |
| 1   | G     | 164 | SER  |
| 1   | G     | 165 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 179 | MET  |
| 1   | G     | 193 | ASP  |
| 1   | G     | 206 | LYS  |
| 1   | G     | 210 | THR  |
| 1   | G     | 217 | ILE  |
| 1   | G     | 221 | GLU  |
| 1   | G     | 223 | SER  |
| 1   | G     | 227 | LEU  |
| 1   | G     | 237 | VAL  |
| 1   | G     | 238 | GLN  |
| 1   | G     | 243 | THR  |
| 1   | G     | 256 | MET  |
| 1   | G     | 259 | LEU  |
| 1   | G     | 263 | SER  |
| 1   | G     | 275 | ASP  |
| 1   | G     | 282 | LEU  |
| 1   | G     | 286 | ILE  |
| 1   | G     | 297 | ILE  |
| 1   | G     | 307 | GLN  |
| 1   | G     | 311 | LEU  |
| 1   | G     | 313 | LYS  |
| 1   | G     | 321 | THR  |
| 1   | G     | 326 | ASP  |
| 1   | G     | 351 | ARG  |
| 1   | G     | 352 | LEU  |
| 1   | G     | 353 | SER  |
| 1   | G     | 357 | MET  |
| 1   | G     | 368 | ARG  |
| 1   | G     | 369 | VAL  |
| 1   | G     | 389 | TYR  |
| 1   | G     | 397 | GLN  |
| 1   | G     | 399 | PRO  |
| 1   | G     | 403 | VAL  |
| 1   | G     | 412 | GLN  |
| 1   | G     | 416 | GLU  |
| 1   | G     | 417 | LEU  |
| 1   | G     | 422 | VAL  |
| 1   | G     | 431 | GLU  |
| 1   | G     | 446 | VAL  |
| 1   | G     | 452 | LEU  |
| 1   | G     | 474 | ILE  |
| 1   | H     | 6   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 15  | SER  |
| 1   | H     | 34  | CYS  |
| 1   | H     | 38  | THR  |
| 1   | H     | 52  | THR  |
| 1   | H     | 56  | THR  |
| 1   | H     | 75  | LEU  |
| 1   | H     | 86  | LEU  |
| 1   | H     | 88  | ILE  |
| 1   | H     | 95  | GLN  |
| 1   | H     | 96  | LEU  |
| 1   | H     | 106 | VAL  |
| 1   | H     | 108 | GLU  |
| 1   | H     | 116 | ILE  |
| 1   | H     | 121 | ILE  |
| 1   | H     | 124 | ASN  |
| 1   | H     | 129 | THR  |
| 1   | H     | 130 | LEU  |
| 1   | H     | 138 | VAL  |
| 1   | H     | 139 | VAL  |
| 1   | H     | 147 | LEU  |
| 1   | H     | 158 | MET  |
| 1   | H     | 160 | LEU  |
| 1   | H     | 164 | SER  |
| 1   | H     | 165 | SER  |
| 1   | H     | 179 | MET  |
| 1   | H     | 193 | ASP  |
| 1   | H     | 206 | LYS  |
| 1   | H     | 210 | THR  |
| 1   | H     | 217 | ILE  |
| 1   | H     | 221 | GLU  |
| 1   | H     | 223 | SER  |
| 1   | H     | 227 | LEU  |
| 1   | H     | 237 | VAL  |
| 1   | H     | 238 | GLN  |
| 1   | H     | 243 | THR  |
| 1   | H     | 256 | MET  |
| 1   | H     | 259 | LEU  |
| 1   | H     | 263 | SER  |
| 1   | H     | 275 | ASP  |
| 1   | H     | 282 | LEU  |
| 1   | H     | 286 | ILE  |
| 1   | H     | 297 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 307 | GLN  |
| 1   | H     | 311 | LEU  |
| 1   | H     | 313 | LYS  |
| 1   | H     | 321 | THR  |
| 1   | H     | 326 | ASP  |
| 1   | H     | 351 | ARG  |
| 1   | H     | 352 | LEU  |
| 1   | H     | 353 | SER  |
| 1   | H     | 357 | MET  |
| 1   | H     | 368 | ARG  |
| 1   | H     | 369 | VAL  |
| 1   | H     | 389 | TYR  |
| 1   | H     | 397 | GLN  |
| 1   | H     | 399 | PRO  |
| 1   | H     | 403 | VAL  |
| 1   | H     | 412 | GLN  |
| 1   | H     | 416 | GLU  |
| 1   | H     | 417 | LEU  |
| 1   | H     | 422 | VAL  |
| 1   | H     | 431 | GLU  |
| 1   | H     | 446 | VAL  |
| 1   | H     | 452 | LEU  |
| 1   | H     | 474 | ILE  |
| 1   | I     | 6   | THR  |
| 1   | I     | 15  | SER  |
| 1   | I     | 34  | CYS  |
| 1   | I     | 38  | THR  |
| 1   | I     | 52  | THR  |
| 1   | I     | 56  | THR  |
| 1   | I     | 75  | LEU  |
| 1   | I     | 86  | LEU  |
| 1   | I     | 88  | ILE  |
| 1   | I     | 95  | GLN  |
| 1   | I     | 96  | LEU  |
| 1   | I     | 106 | VAL  |
| 1   | I     | 108 | GLU  |
| 1   | I     | 116 | ILE  |
| 1   | I     | 121 | ILE  |
| 1   | I     | 124 | ASN  |
| 1   | I     | 129 | THR  |
| 1   | I     | 130 | LEU  |
| 1   | I     | 138 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 139 | VAL  |
| 1   | I     | 147 | LEU  |
| 1   | I     | 158 | MET  |
| 1   | I     | 160 | LEU  |
| 1   | I     | 164 | SER  |
| 1   | I     | 165 | SER  |
| 1   | I     | 179 | MET  |
| 1   | I     | 193 | ASP  |
| 1   | I     | 206 | LYS  |
| 1   | I     | 210 | THR  |
| 1   | I     | 217 | ILE  |
| 1   | I     | 221 | GLU  |
| 1   | I     | 223 | SER  |
| 1   | I     | 227 | LEU  |
| 1   | I     | 237 | VAL  |
| 1   | I     | 238 | GLN  |
| 1   | I     | 243 | THR  |
| 1   | I     | 256 | MET  |
| 1   | I     | 259 | LEU  |
| 1   | I     | 263 | SER  |
| 1   | I     | 275 | ASP  |
| 1   | I     | 282 | LEU  |
| 1   | I     | 286 | ILE  |
| 1   | I     | 297 | ILE  |
| 1   | I     | 307 | GLN  |
| 1   | I     | 311 | LEU  |
| 1   | I     | 313 | LYS  |
| 1   | I     | 321 | THR  |
| 1   | I     | 326 | ASP  |
| 1   | I     | 351 | ARG  |
| 1   | I     | 352 | LEU  |
| 1   | I     | 353 | SER  |
| 1   | I     | 357 | MET  |
| 1   | I     | 368 | ARG  |
| 1   | I     | 369 | VAL  |
| 1   | I     | 389 | TYR  |
| 1   | I     | 397 | GLN  |
| 1   | I     | 399 | PRO  |
| 1   | I     | 403 | VAL  |
| 1   | I     | 412 | GLN  |
| 1   | I     | 416 | GLU  |
| 1   | I     | 417 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 422 | VAL  |
| 1   | I     | 431 | GLU  |
| 1   | I     | 446 | VAL  |
| 1   | I     | 452 | LEU  |
| 1   | I     | 474 | ILE  |
| 1   | J     | 6   | THR  |
| 1   | J     | 15  | SER  |
| 1   | J     | 34  | CYS  |
| 1   | J     | 38  | THR  |
| 1   | J     | 52  | THR  |
| 1   | J     | 56  | THR  |
| 1   | J     | 75  | LEU  |
| 1   | J     | 86  | LEU  |
| 1   | J     | 88  | ILE  |
| 1   | J     | 95  | GLN  |
| 1   | J     | 96  | LEU  |
| 1   | J     | 106 | VAL  |
| 1   | J     | 108 | GLU  |
| 1   | J     | 116 | ILE  |
| 1   | J     | 121 | ILE  |
| 1   | J     | 124 | ASN  |
| 1   | J     | 129 | THR  |
| 1   | J     | 130 | LEU  |
| 1   | J     | 138 | VAL  |
| 1   | J     | 139 | VAL  |
| 1   | J     | 147 | LEU  |
| 1   | J     | 158 | MET  |
| 1   | J     | 160 | LEU  |
| 1   | J     | 164 | SER  |
| 1   | J     | 165 | SER  |
| 1   | J     | 179 | MET  |
| 1   | J     | 193 | ASP  |
| 1   | J     | 206 | LYS  |
| 1   | J     | 210 | THR  |
| 1   | J     | 217 | ILE  |
| 1   | J     | 221 | GLU  |
| 1   | J     | 223 | SER  |
| 1   | J     | 227 | LEU  |
| 1   | J     | 237 | VAL  |
| 1   | J     | 238 | GLN  |
| 1   | J     | 243 | THR  |
| 1   | J     | 256 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 259 | LEU  |
| 1   | J     | 263 | SER  |
| 1   | J     | 275 | ASP  |
| 1   | J     | 282 | LEU  |
| 1   | J     | 286 | ILE  |
| 1   | J     | 297 | ILE  |
| 1   | J     | 307 | GLN  |
| 1   | J     | 311 | LEU  |
| 1   | J     | 313 | LYS  |
| 1   | J     | 321 | THR  |
| 1   | J     | 326 | ASP  |
| 1   | J     | 351 | ARG  |
| 1   | J     | 352 | LEU  |
| 1   | J     | 353 | SER  |
| 1   | J     | 357 | MET  |
| 1   | J     | 368 | ARG  |
| 1   | J     | 369 | VAL  |
| 1   | J     | 389 | TYR  |
| 1   | J     | 397 | GLN  |
| 1   | J     | 399 | PRO  |
| 1   | J     | 403 | VAL  |
| 1   | J     | 412 | GLN  |
| 1   | J     | 416 | GLU  |
| 1   | J     | 417 | LEU  |
| 1   | J     | 422 | VAL  |
| 1   | J     | 431 | GLU  |
| 1   | J     | 446 | VAL  |
| 1   | J     | 452 | LEU  |
| 1   | J     | 474 | ILE  |
| 1   | K     | 6   | THR  |
| 1   | K     | 15  | SER  |
| 1   | K     | 34  | CYS  |
| 1   | K     | 38  | THR  |
| 1   | K     | 52  | THR  |
| 1   | K     | 56  | THR  |
| 1   | K     | 75  | LEU  |
| 1   | K     | 86  | LEU  |
| 1   | K     | 88  | ILE  |
| 1   | K     | 95  | GLN  |
| 1   | K     | 96  | LEU  |
| 1   | K     | 106 | VAL  |
| 1   | K     | 108 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 116 | ILE  |
| 1   | K     | 121 | ILE  |
| 1   | K     | 124 | ASN  |
| 1   | K     | 129 | THR  |
| 1   | K     | 130 | LEU  |
| 1   | K     | 138 | VAL  |
| 1   | K     | 139 | VAL  |
| 1   | K     | 147 | LEU  |
| 1   | K     | 158 | MET  |
| 1   | K     | 160 | LEU  |
| 1   | K     | 164 | SER  |
| 1   | K     | 165 | SER  |
| 1   | K     | 179 | MET  |
| 1   | K     | 193 | ASP  |
| 1   | K     | 206 | LYS  |
| 1   | K     | 210 | THR  |
| 1   | K     | 217 | ILE  |
| 1   | K     | 221 | GLU  |
| 1   | K     | 223 | SER  |
| 1   | K     | 227 | LEU  |
| 1   | K     | 237 | VAL  |
| 1   | K     | 238 | GLN  |
| 1   | K     | 243 | THR  |
| 1   | K     | 256 | MET  |
| 1   | K     | 259 | LEU  |
| 1   | K     | 263 | SER  |
| 1   | K     | 275 | ASP  |
| 1   | K     | 282 | LEU  |
| 1   | K     | 286 | ILE  |
| 1   | K     | 297 | ILE  |
| 1   | K     | 307 | GLN  |
| 1   | K     | 311 | LEU  |
| 1   | K     | 313 | LYS  |
| 1   | K     | 321 | THR  |
| 1   | K     | 326 | ASP  |
| 1   | K     | 351 | ARG  |
| 1   | K     | 352 | LEU  |
| 1   | K     | 353 | SER  |
| 1   | K     | 357 | MET  |
| 1   | K     | 368 | ARG  |
| 1   | K     | 369 | VAL  |
| 1   | K     | 389 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 397 | GLN  |
| 1   | K     | 399 | PRO  |
| 1   | K     | 403 | VAL  |
| 1   | K     | 412 | GLN  |
| 1   | K     | 416 | GLU  |
| 1   | K     | 417 | LEU  |
| 1   | K     | 422 | VAL  |
| 1   | K     | 431 | GLU  |
| 1   | K     | 446 | VAL  |
| 1   | K     | 452 | LEU  |
| 1   | K     | 474 | ILE  |
| 1   | L     | 6   | THR  |
| 1   | L     | 15  | SER  |
| 1   | L     | 34  | CYS  |
| 1   | L     | 38  | THR  |
| 1   | L     | 52  | THR  |
| 1   | L     | 56  | THR  |
| 1   | L     | 75  | LEU  |
| 1   | L     | 86  | LEU  |
| 1   | L     | 88  | ILE  |
| 1   | L     | 95  | GLN  |
| 1   | L     | 96  | LEU  |
| 1   | L     | 106 | VAL  |
| 1   | L     | 108 | GLU  |
| 1   | L     | 116 | ILE  |
| 1   | L     | 121 | ILE  |
| 1   | L     | 124 | ASN  |
| 1   | L     | 129 | THR  |
| 1   | L     | 130 | LEU  |
| 1   | L     | 138 | VAL  |
| 1   | L     | 139 | VAL  |
| 1   | L     | 147 | LEU  |
| 1   | L     | 158 | MET  |
| 1   | L     | 160 | LEU  |
| 1   | L     | 164 | SER  |
| 1   | L     | 165 | SER  |
| 1   | L     | 179 | MET  |
| 1   | L     | 193 | ASP  |
| 1   | L     | 206 | LYS  |
| 1   | L     | 210 | THR  |
| 1   | L     | 217 | ILE  |
| 1   | L     | 221 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 223 | SER  |
| 1   | L     | 227 | LEU  |
| 1   | L     | 237 | VAL  |
| 1   | L     | 238 | GLN  |
| 1   | L     | 243 | THR  |
| 1   | L     | 256 | MET  |
| 1   | L     | 259 | LEU  |
| 1   | L     | 263 | SER  |
| 1   | L     | 275 | ASP  |
| 1   | L     | 282 | LEU  |
| 1   | L     | 286 | ILE  |
| 1   | L     | 297 | ILE  |
| 1   | L     | 307 | GLN  |
| 1   | L     | 311 | LEU  |
| 1   | L     | 313 | LYS  |
| 1   | L     | 321 | THR  |
| 1   | L     | 326 | ASP  |
| 1   | L     | 351 | ARG  |
| 1   | L     | 352 | LEU  |
| 1   | L     | 353 | SER  |
| 1   | L     | 357 | MET  |
| 1   | L     | 368 | ARG  |
| 1   | L     | 369 | VAL  |
| 1   | L     | 389 | TYR  |
| 1   | L     | 397 | GLN  |
| 1   | L     | 399 | PRO  |
| 1   | L     | 403 | VAL  |
| 1   | L     | 412 | GLN  |
| 1   | L     | 416 | GLU  |
| 1   | L     | 417 | LEU  |
| 1   | L     | 422 | VAL  |
| 1   | L     | 431 | GLU  |
| 1   | L     | 446 | VAL  |
| 1   | L     | 452 | LEU  |
| 1   | L     | 474 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 55  | GLN  |
| 1   | A     | 95  | GLN  |
| 1   | A     | 156 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 397 | GLN  |
| 1   | B     | 55  | GLN  |
| 1   | B     | 95  | GLN  |
| 1   | B     | 156 | ASN  |
| 1   | B     | 335 | GLN  |
| 1   | B     | 397 | GLN  |
| 1   | C     | 55  | GLN  |
| 1   | C     | 95  | GLN  |
| 1   | C     | 156 | ASN  |
| 1   | C     | 397 | GLN  |
| 1   | D     | 55  | GLN  |
| 1   | D     | 95  | GLN  |
| 1   | D     | 156 | ASN  |
| 1   | D     | 335 | GLN  |
| 1   | D     | 397 | GLN  |
| 1   | E     | 55  | GLN  |
| 1   | E     | 95  | GLN  |
| 1   | E     | 156 | ASN  |
| 1   | E     | 397 | GLN  |
| 1   | F     | 55  | GLN  |
| 1   | F     | 95  | GLN  |
| 1   | F     | 156 | ASN  |
| 1   | F     | 335 | GLN  |
| 1   | F     | 397 | GLN  |
| 1   | G     | 55  | GLN  |
| 1   | G     | 95  | GLN  |
| 1   | G     | 156 | ASN  |
| 1   | G     | 397 | GLN  |
| 1   | H     | 55  | GLN  |
| 1   | H     | 95  | GLN  |
| 1   | H     | 156 | ASN  |
| 1   | H     | 335 | GLN  |
| 1   | H     | 397 | GLN  |
| 1   | I     | 55  | GLN  |
| 1   | I     | 95  | GLN  |
| 1   | I     | 156 | ASN  |
| 1   | I     | 397 | GLN  |
| 1   | J     | 55  | GLN  |
| 1   | J     | 95  | GLN  |
| 1   | J     | 156 | ASN  |
| 1   | J     | 397 | GLN  |
| 1   | K     | 55  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 95  | GLN  |
| 1   | K     | 156 | ASN  |
| 1   | K     | 397 | GLN  |
| 1   | L     | 55  | GLN  |
| 1   | L     | 95  | GLN  |
| 1   | L     | 156 | ASN  |
| 1   | L     | 397 | 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.

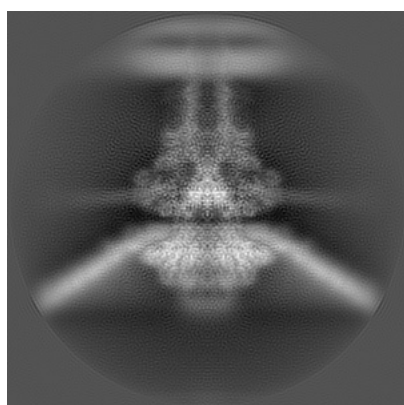
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31321. These allow visual inspection of the internal detail of the map and identification of artifacts.

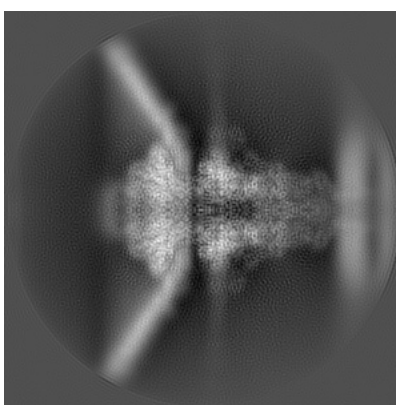
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

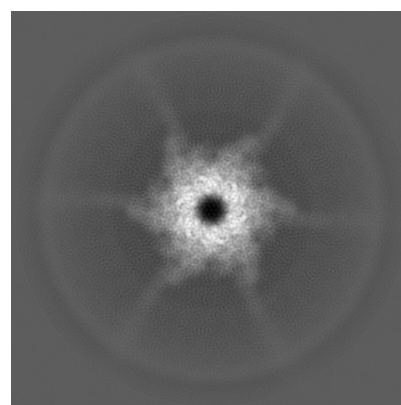
#### 6.1.1 Primary map



X



Y

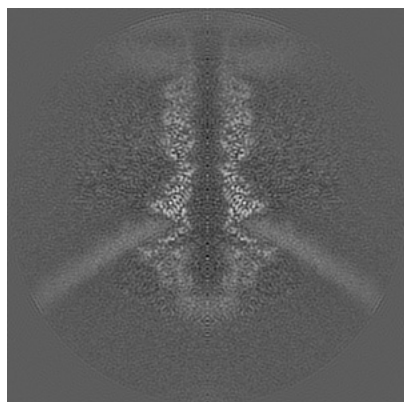


Z

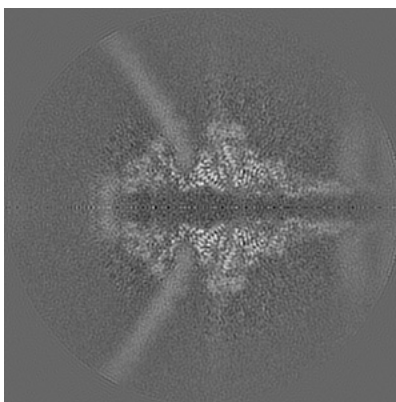
The images above show the map projected in three orthogonal directions.

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

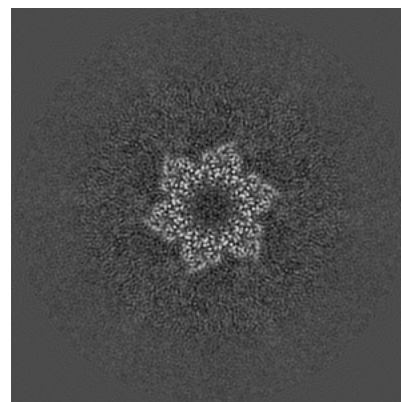
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

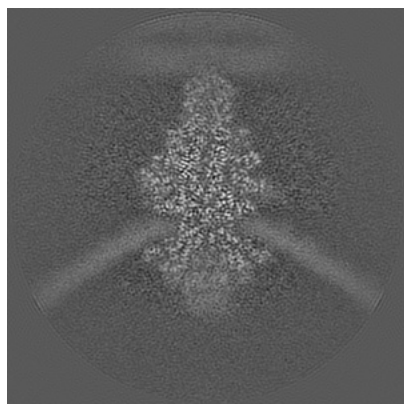


Z Index: 200

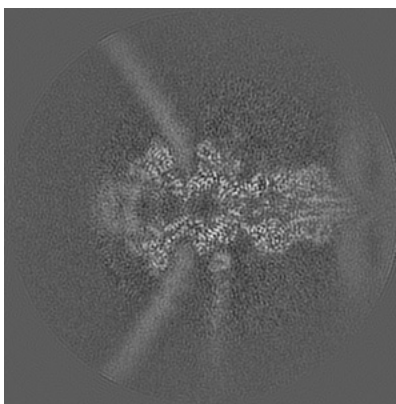
The images above show central slices of the map in three orthogonal directions.

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

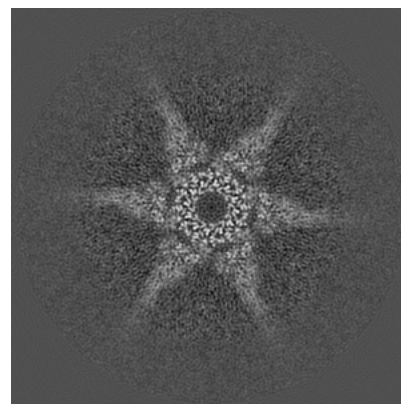
### 6.3.1 Primary map



X Index: 177



Y Index: 216

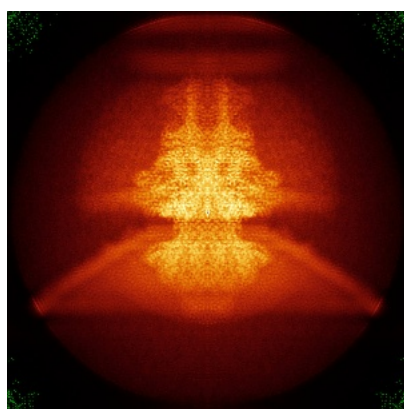


Z Index: 217

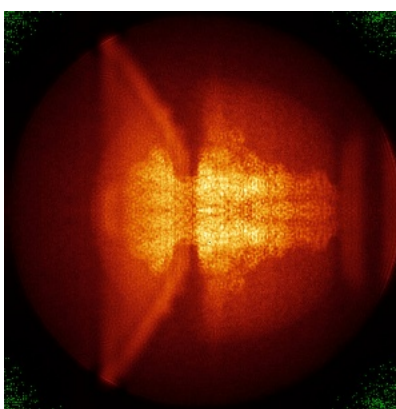
The images above show the largest variance slices of the map in three orthogonal directions.

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

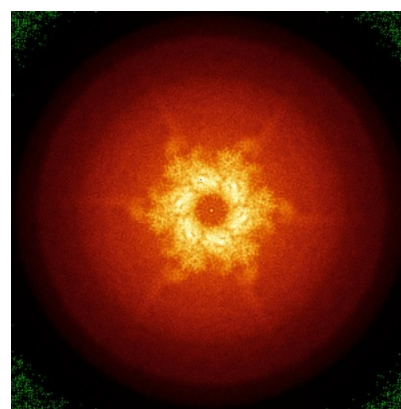
### 6.4.1 Primary map



X



Y

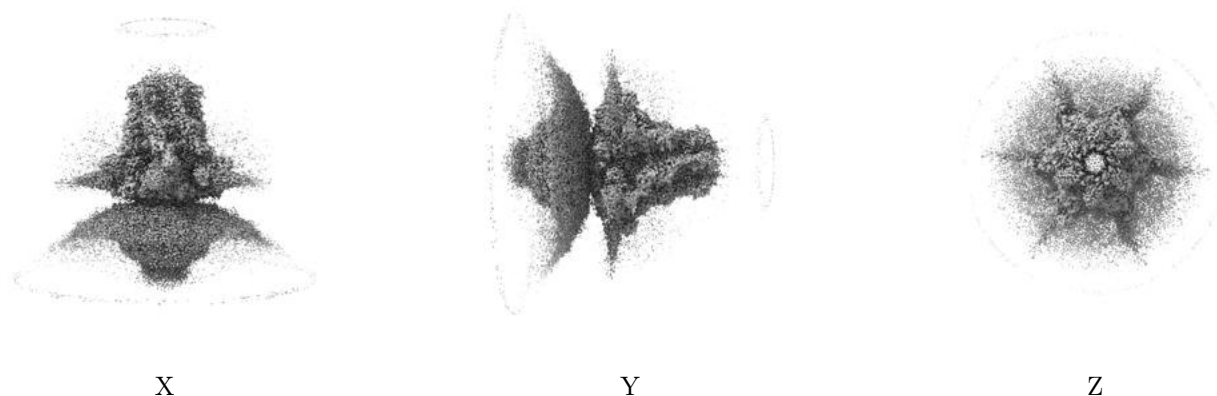


Z

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 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

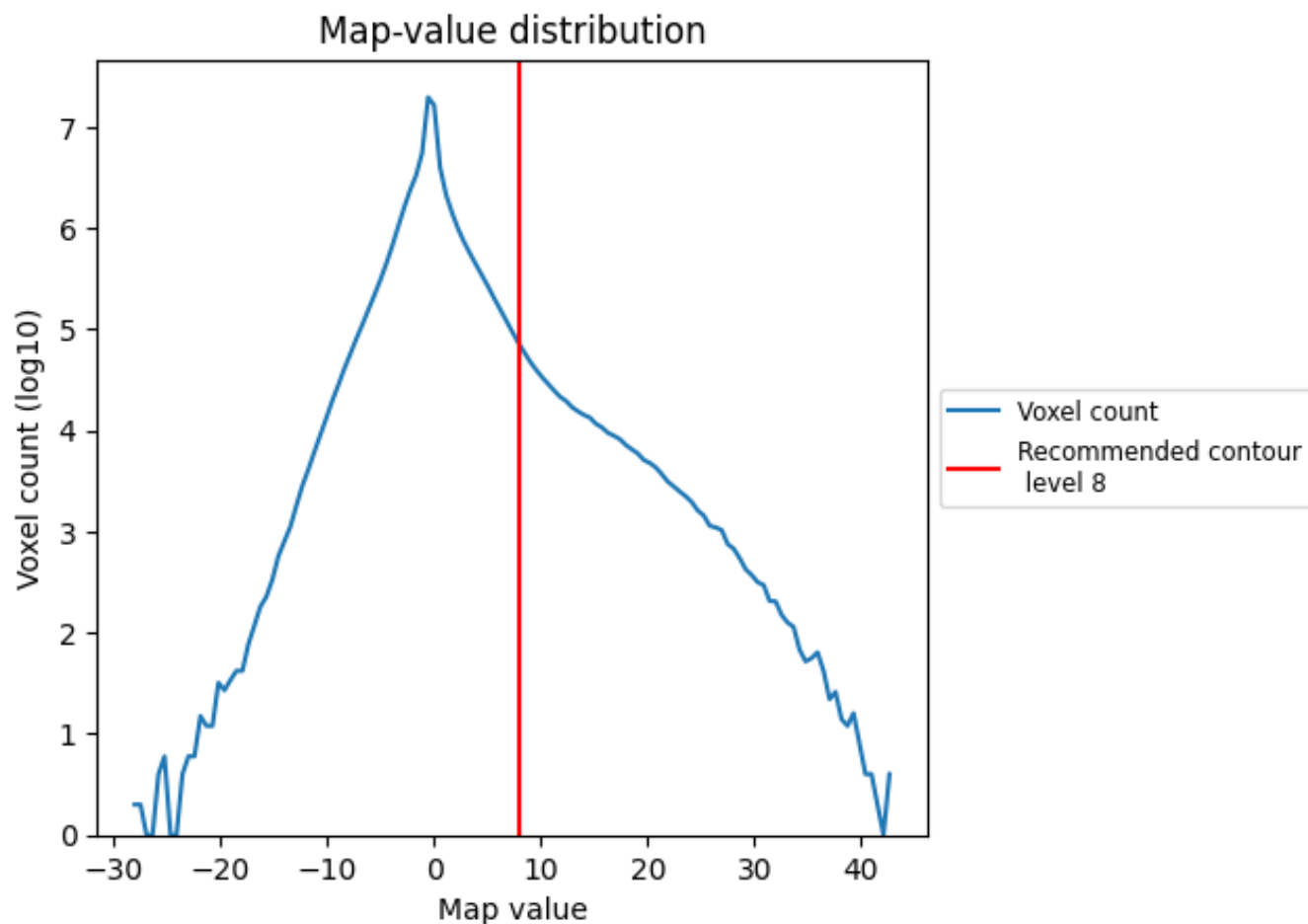
## 6.6 Mask visualisation [i](#)

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.

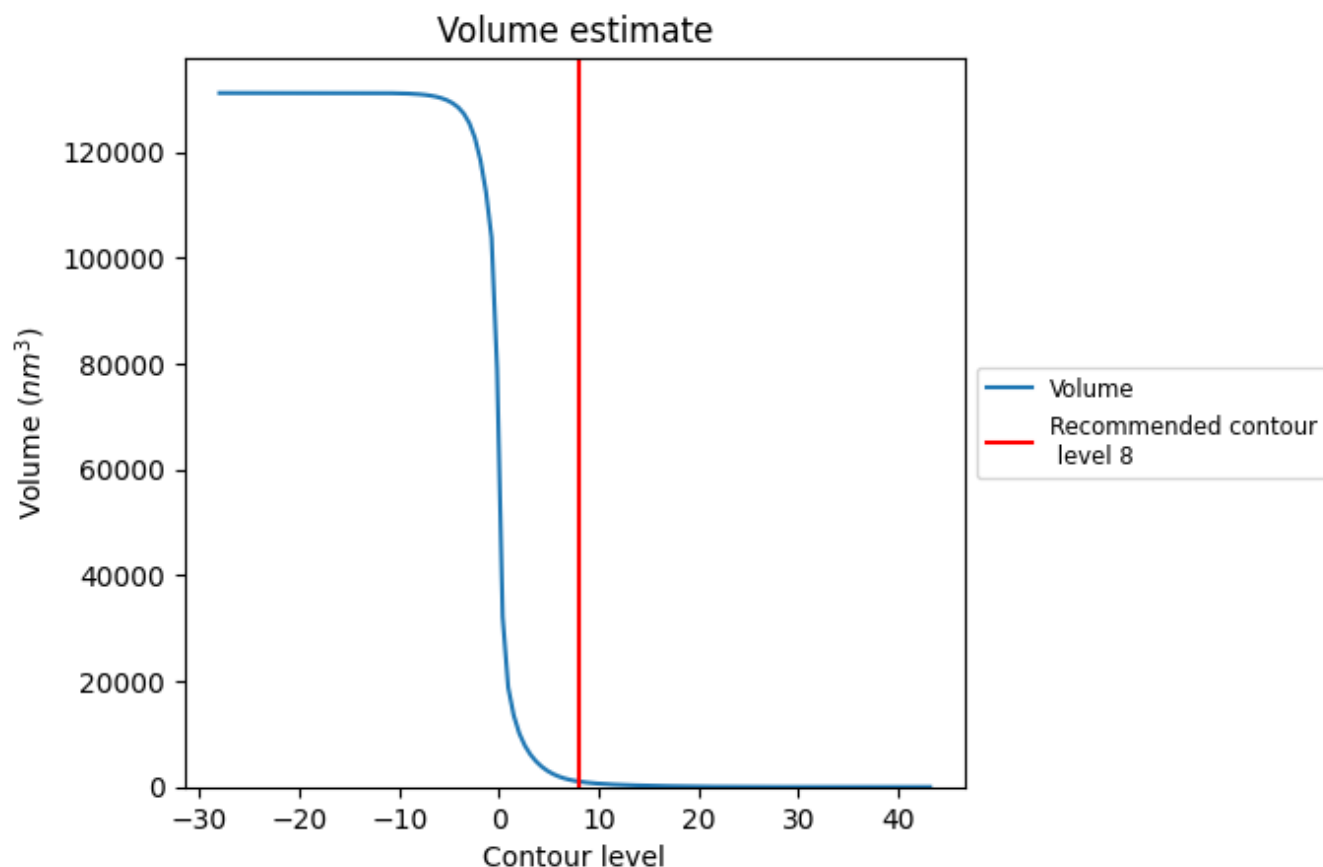
### 7.1 Map-value distribution [i](#)



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.



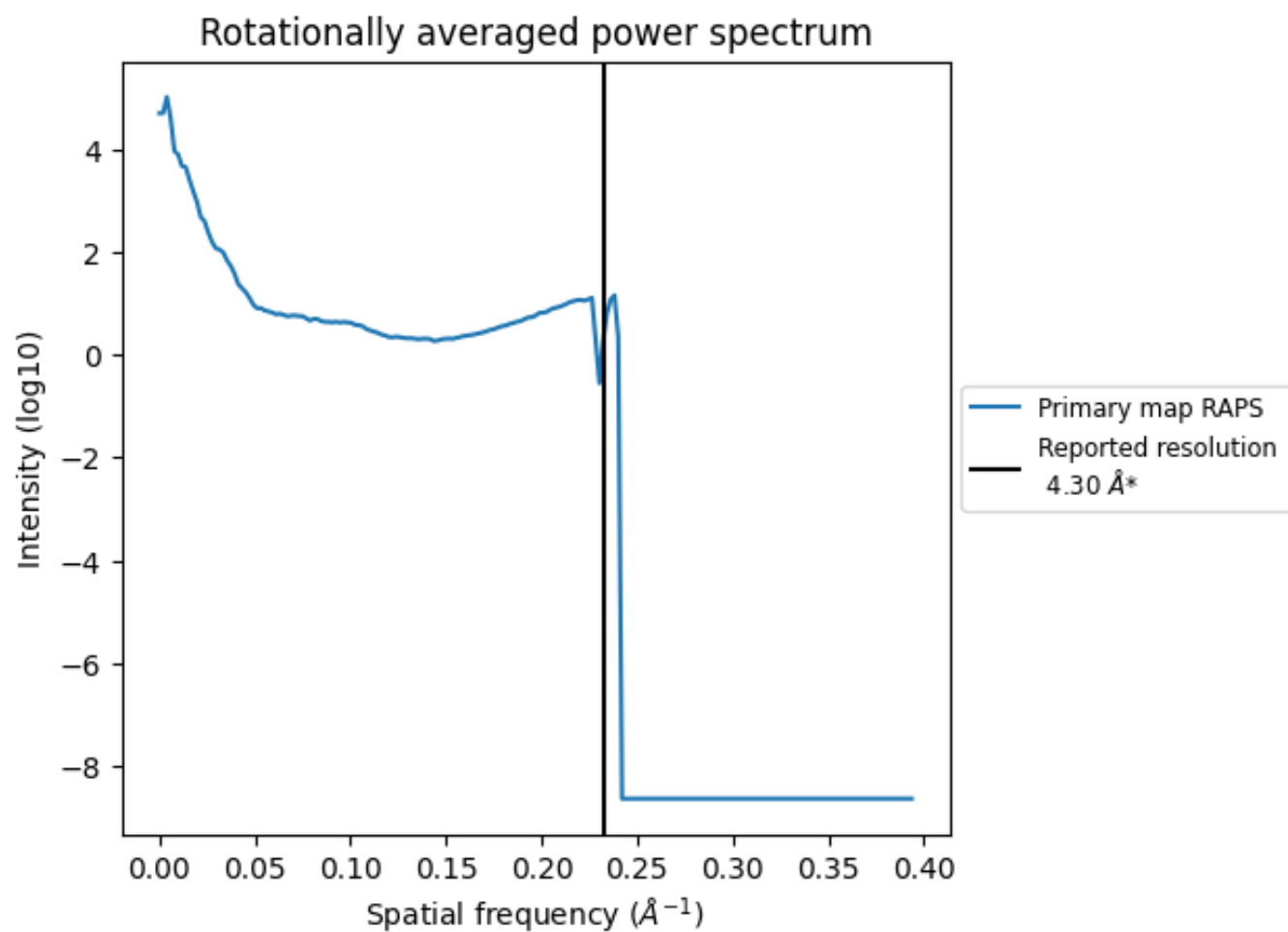
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1038  $\text{nm}^3$ ; this corresponds to an approximate mass of 938 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 0.233 Å<sup>-1</sup>

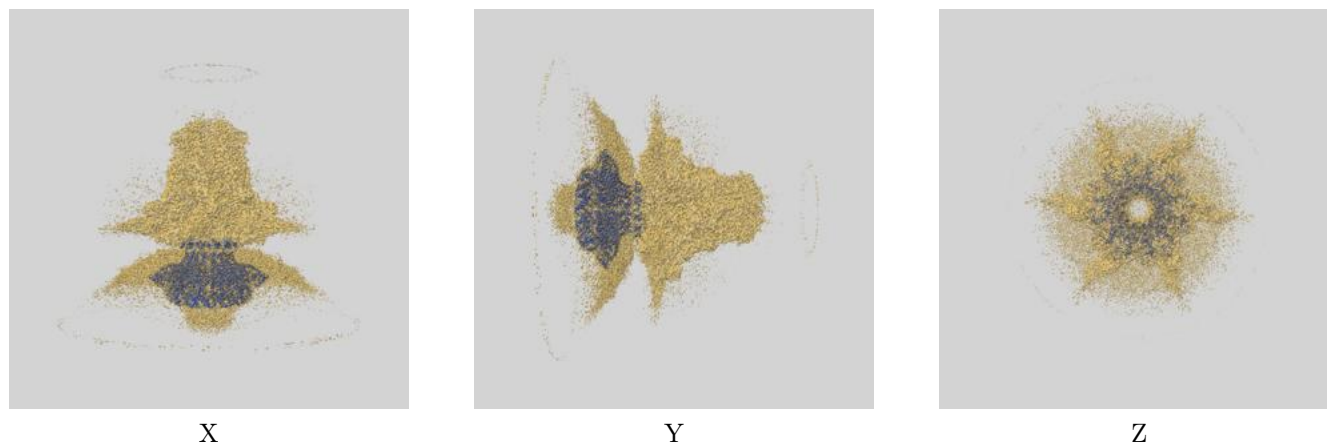
## 8 Fourier-Shell correlation ⓘ

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

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

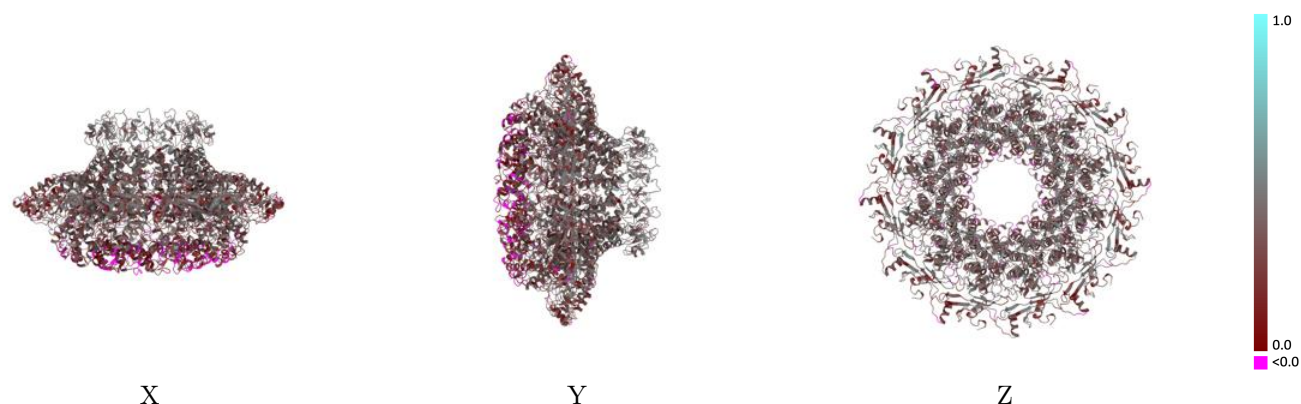
This section contains information regarding the fit between EMDB map EMD-31321 and PDB model 7EY6. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



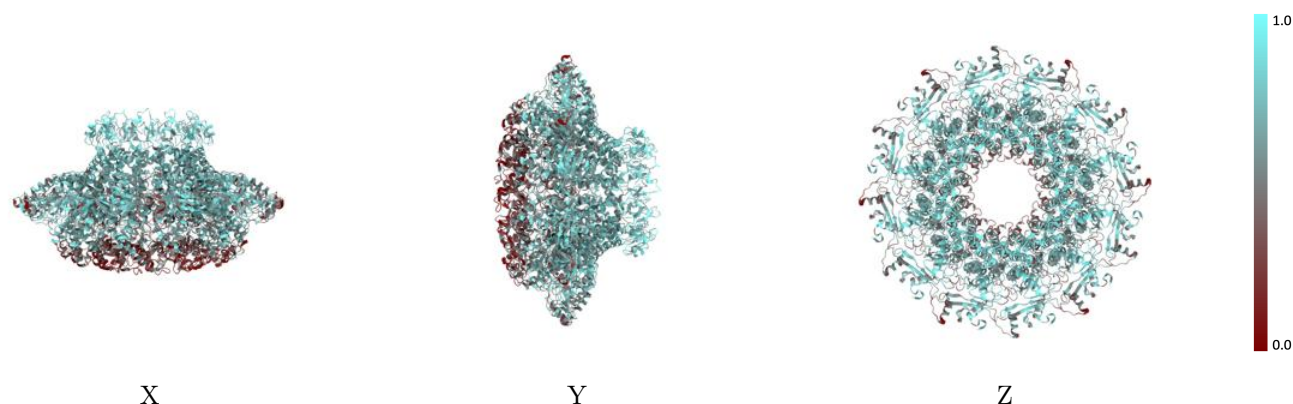
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



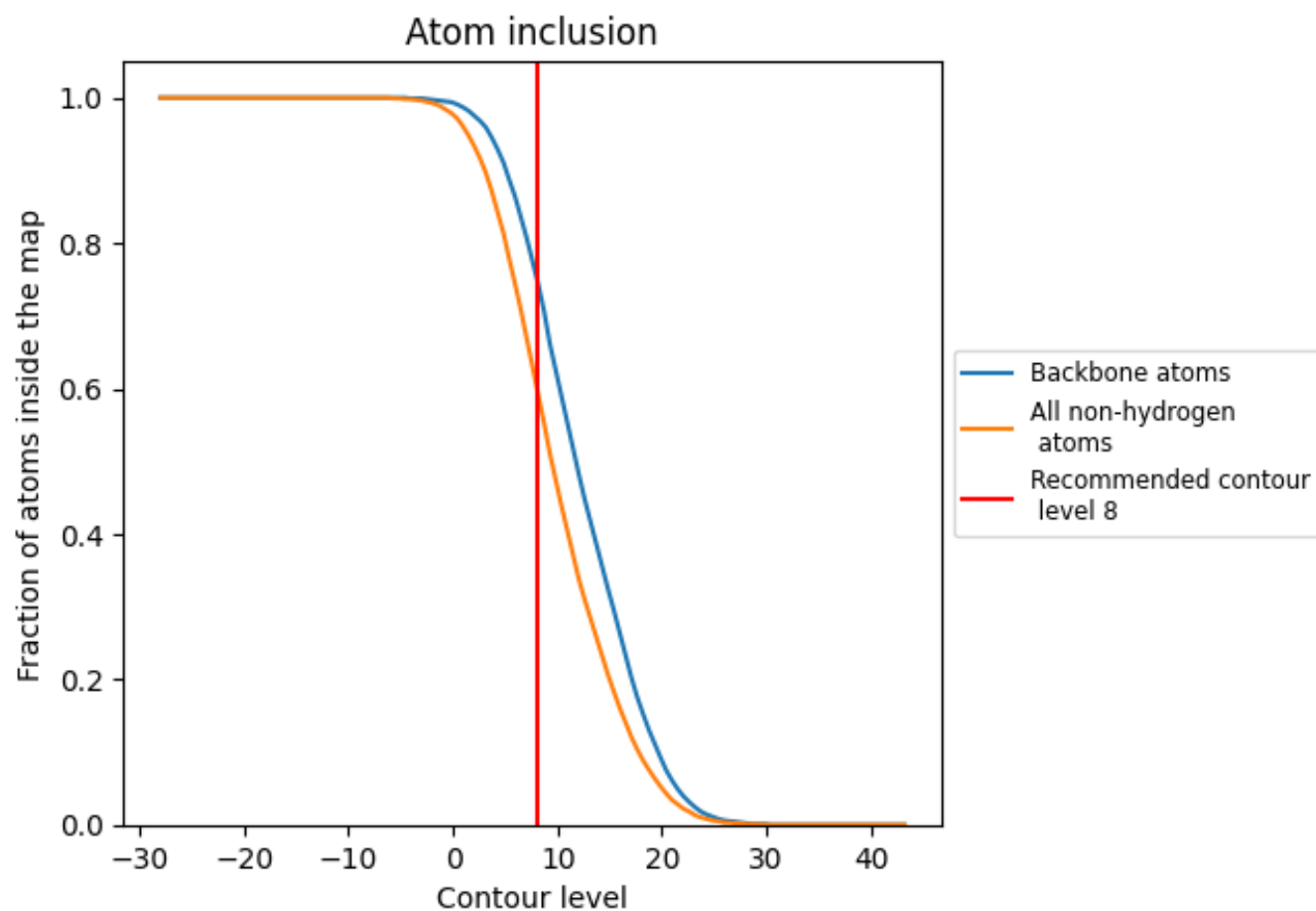
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 60% 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 (8) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6020 | <div></div> 0.3220 |
| A     | <div></div> 0.5880 | <div></div> 0.3050 |
| B     | <div></div> 0.6180 | <div></div> 0.3400 |
| C     | <div></div> 0.5860 | <div></div> 0.3040 |
| D     | <div></div> 0.6170 | <div></div> 0.3380 |
| E     | <div></div> 0.5880 | <div></div> 0.3060 |
| F     | <div></div> 0.6180 | <div></div> 0.3390 |
| G     | <div></div> 0.5870 | <div></div> 0.3050 |
| H     | <div></div> 0.6190 | <div></div> 0.3390 |
| I     | <div></div> 0.5860 | <div></div> 0.3050 |
| J     | <div></div> 0.6180 | <div></div> 0.3390 |
| K     | <div></div> 0.5870 | <div></div> 0.3050 |
| L     | <div></div> 0.6170 | <div></div> 0.3380 |

1.0

0.0

<0.0