



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:44 PM UTC

PDB ID : 6MWV / pdb\_00006mwv  
EMDB ID : EMD-9278  
Title : CryoEM structure of Chimeric Eastern Equine Encephalitis Virus with Fab of  
EEEV-58 Antibody  
Authors : Hasan, S.S.; Sun, C.; Kim, A.S.; Watanabe, Y.; Chen, C.L.; Klose, T.; Buda,  
G.; Crispin, M.; Diamond, M.S.; Klimstra, W.B.; Rossmann, M.G.  
Deposited on : 2018-10-30  
Resolution : 7.30 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:

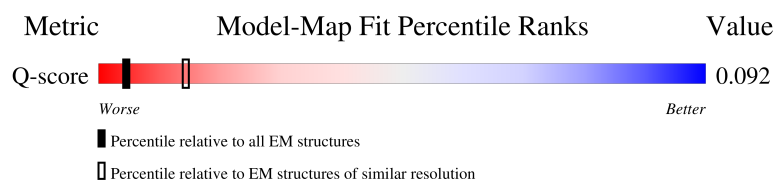
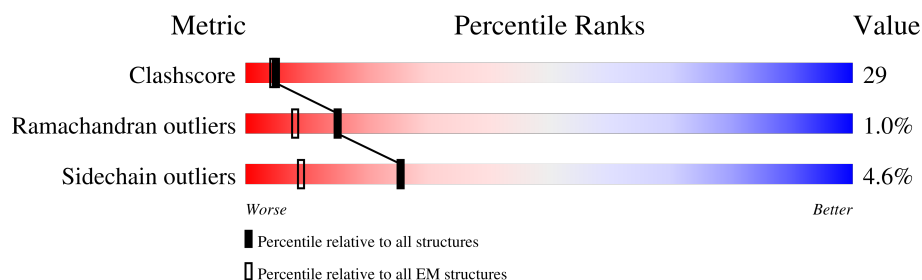
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 7.30 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.



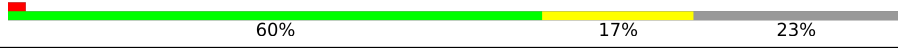
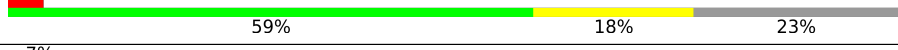
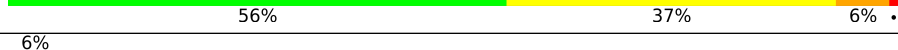
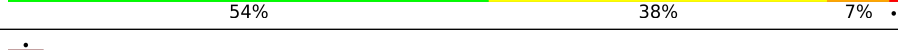
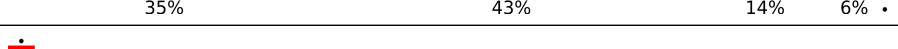
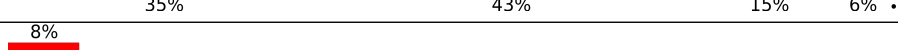
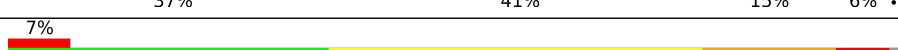
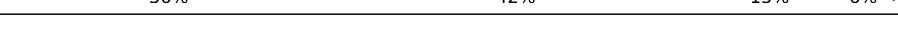
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 436 ( 6.80 - 7.80 )                                      |

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     | 441    |                  |
| 1   | E     | 441    |                  |
| 1   | I     | 441    |                  |
| 1   | M     | 441    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | B     | 420    |    |
| 2   | F     | 420    |    |
| 2   | J     | 420    |    |
| 2   | N     | 420    |    |
| 3   | C     | 218    |    |
| 3   | G     | 218    |    |
| 3   | K     | 218    |    |
| 3   | O     | 218    |    |
| 4   | D     | 214    |    |
| 4   | H     | 214    |    |
| 4   | L     | 214    |    |
| 4   | P     | 214    |  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35528 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 E1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 400      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3063  | 1940 | 511 | 592 | 20 |         |       |
| 1   | E     | 400      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3063  | 1940 | 511 | 592 | 20 |         |       |
| 1   | I     | 400      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3063  | 1940 | 511 | 592 | 20 |         |       |
| 1   | M     | 400      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3063  | 1940 | 511 | 592 | 20 |         |       |

- Molecule 2 is a protein called E2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 325      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2550  | 1601 | 471 | 462 | 16 |         |       |
| 2   | F     | 325      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2550  | 1601 | 471 | 462 | 16 |         |       |
| 2   | J     | 325      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2550  | 1601 | 471 | 462 | 16 |         |       |
| 2   | N     | 325      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2550  | 1601 | 471 | 462 | 16 |         |       |

- Molecule 3 is a protein called EEEV-58 antibody heavy chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1671  | 1066 | 272 | 326 | 7 |         |       |
| 3   | G     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1671  | 1066 | 272 | 326 | 7 |         |       |
| 3   | K     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1671  | 1066 | 272 | 326 | 7 |         |       |
| 3   | O     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1671  | 1066 | 272 | 326 | 7 |         |       |

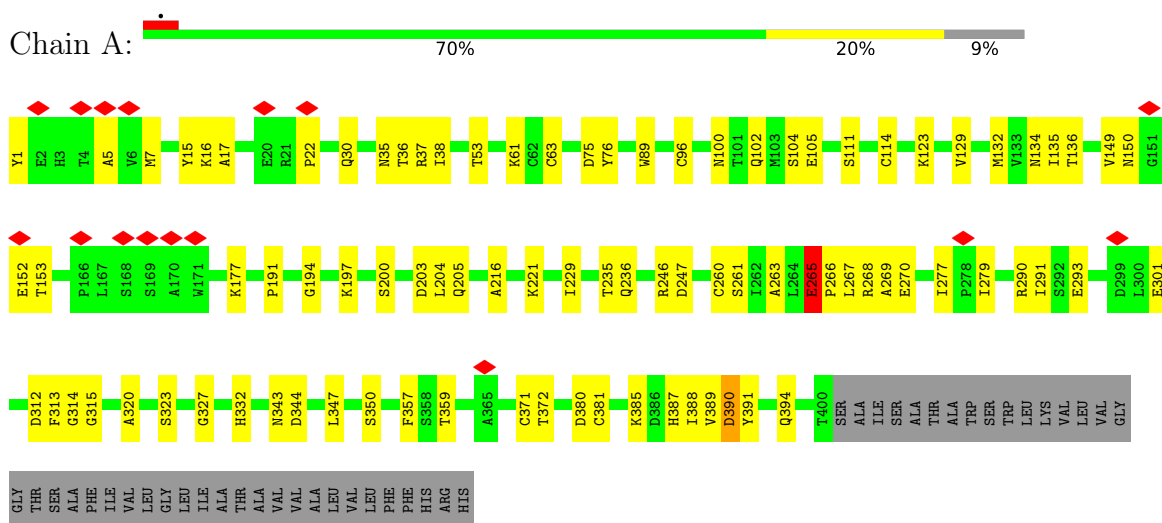
- Molecule 4 is a protein called EEEV-58 antibody light chain.

| Mol | Chain | Residues | Atoms         |          |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 4   | D     | 211      | Total<br>1598 | C<br>999 | N<br>270 | O<br>322 | S<br>7 | 0       | 0     |
| 4   | H     | 211      | Total<br>1598 | C<br>999 | N<br>270 | O<br>322 | S<br>7 | 0       | 0     |
| 4   | L     | 211      | Total<br>1598 | C<br>999 | N<br>270 | O<br>322 | S<br>7 | 0       | 0     |
| 4   | P     | 211      | Total<br>1598 | C<br>999 | N<br>270 | O<br>322 | S<br>7 | 0       | 0     |

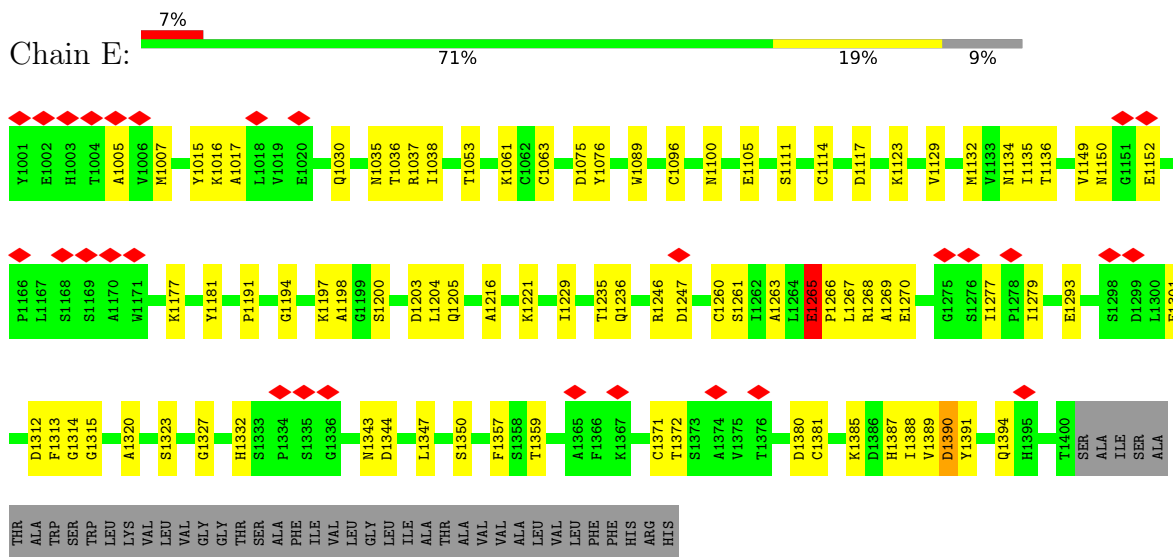
### 3 Residue-property plots

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: E1

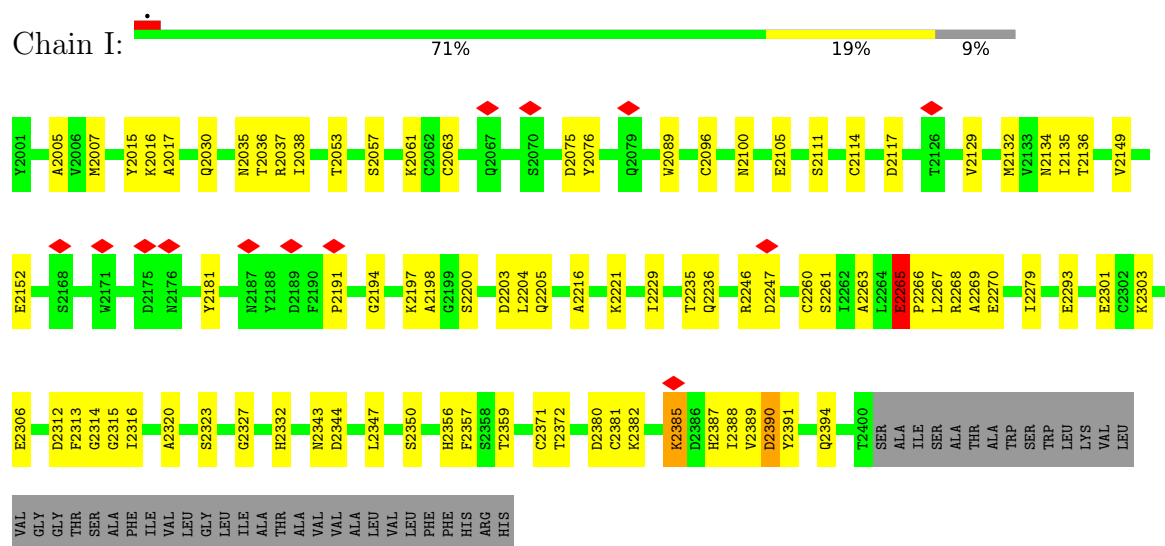


#### • Molecule 1: E1

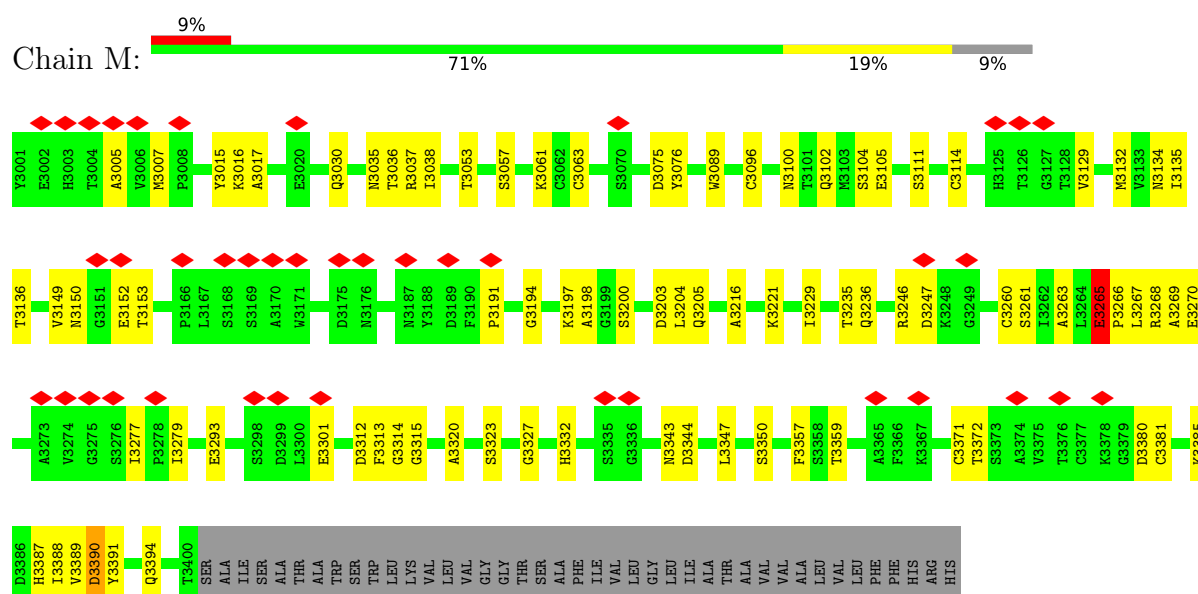


#### • Molecule 1: E1

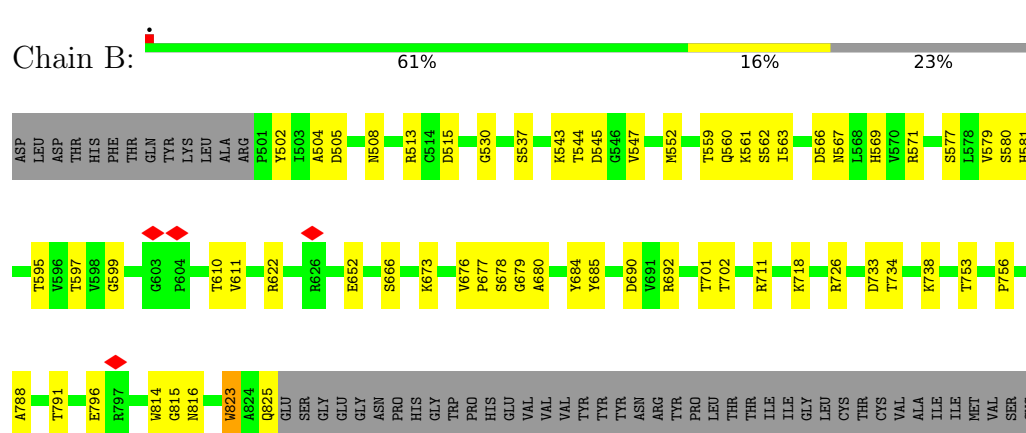
Chain I:



• Molecule 1: E1



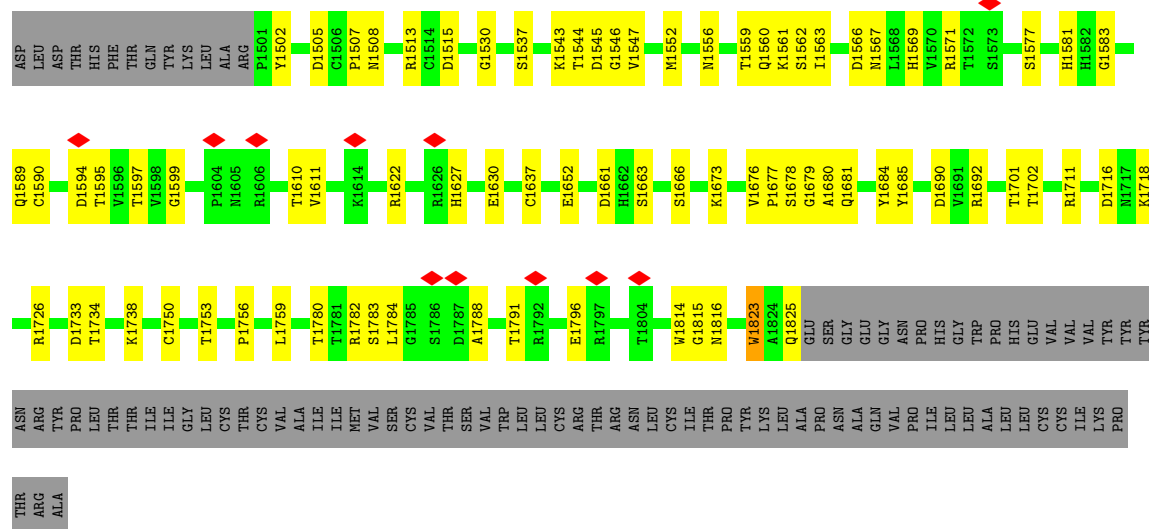
• Molecule 2: E2



LEU  
LEU  
CYS  
ARG  
THR  
THR  
PHE  
ARG  
ASN  
LEU  
CYS  
THR  
THR  
LEU  
PRO  
TYR  
LYS  
LEU  
ALA  
PRO  
ASN  
ALA  
GLN  
VAL  
PRO  
ILE  
LEU  
LEU  
ALA  
LEU  
CYS  
CYS  
ILE  
LYS  
PRO  
THR  
ARG  
ALA

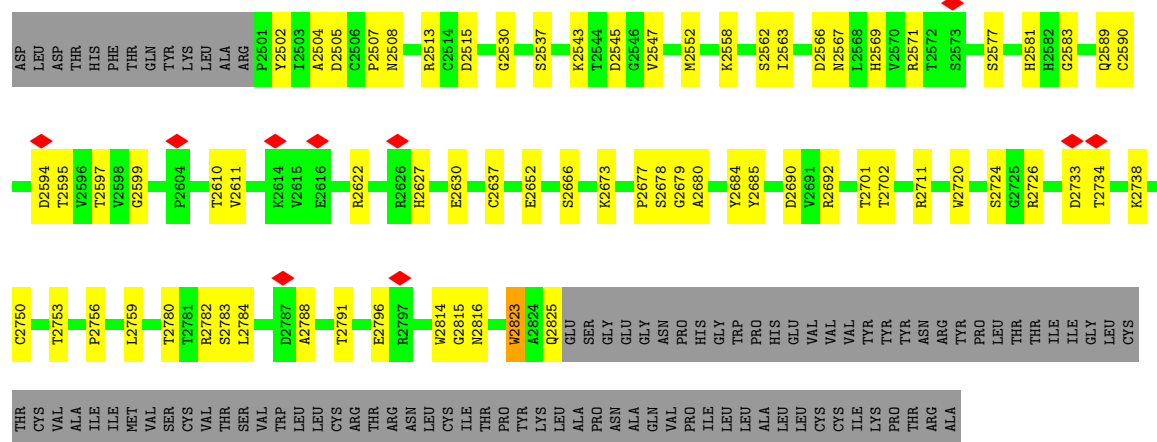
• Molecule 2: E2

Chain F:  59% 19% 23%



• Molecule 2: E2

Chain J:  60% 17% 23%

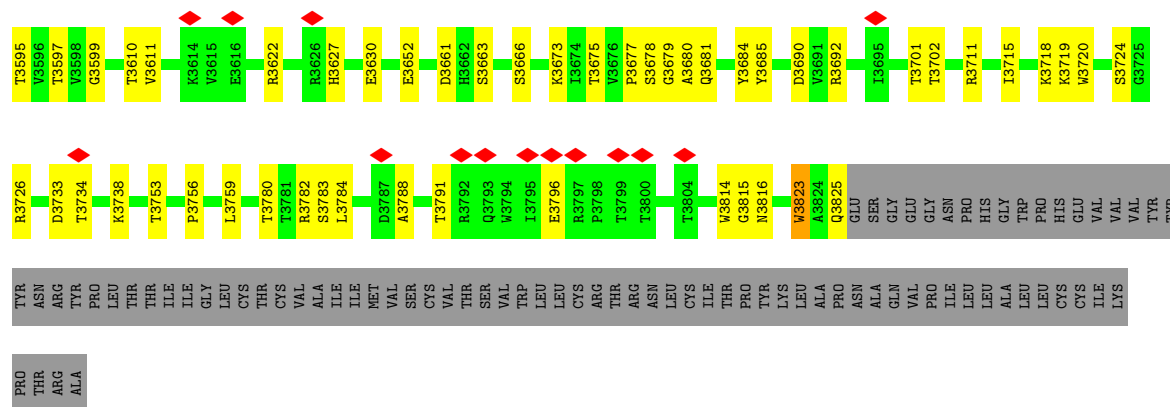


• Molecule 2: E2

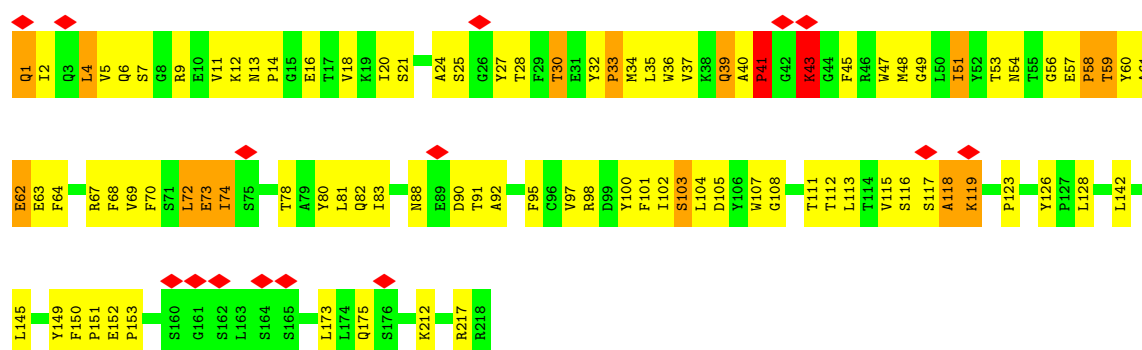
Chain N:  59% 18% 23%



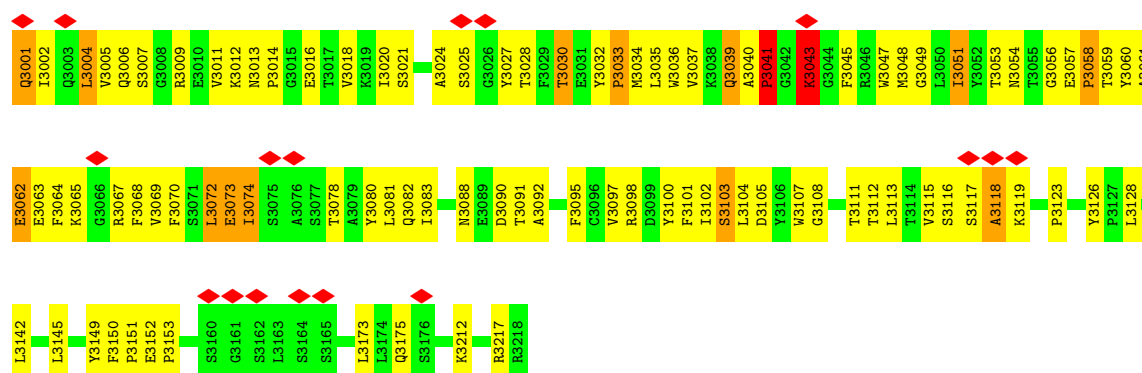




• Molecule 3: EEEV-58 antibody heavy chain

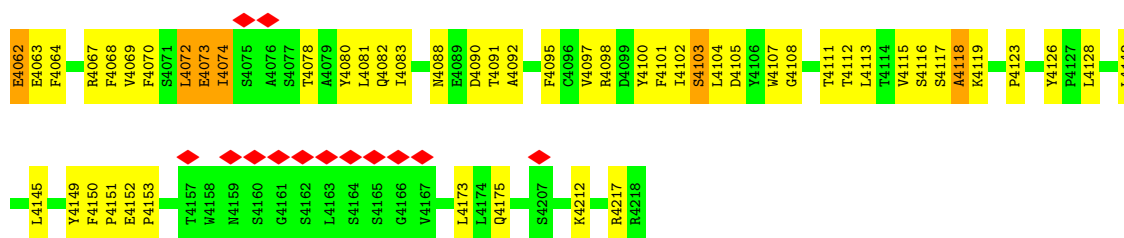


• Molecule 3: EEEV-58 antibody heavy chain



• Molecule 3: EEEV-58 antibody heavy chain

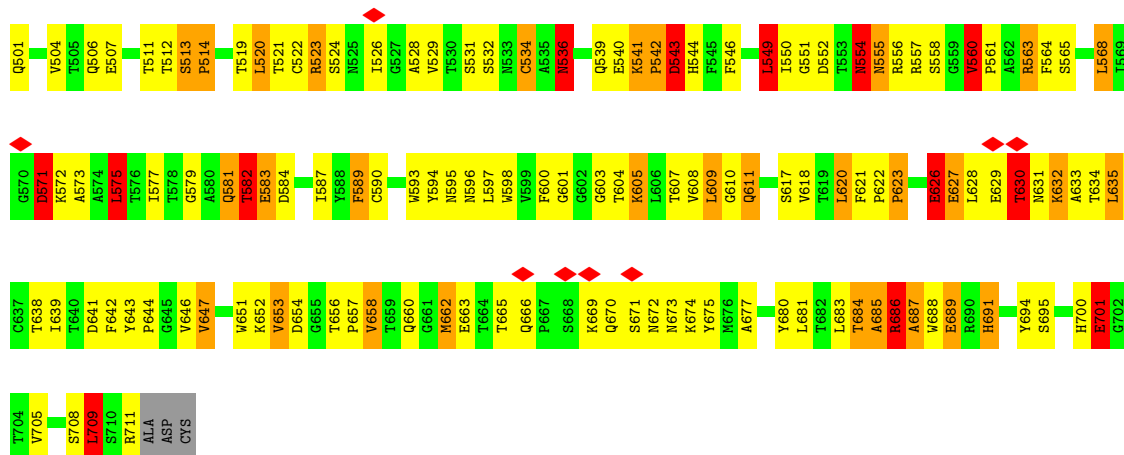




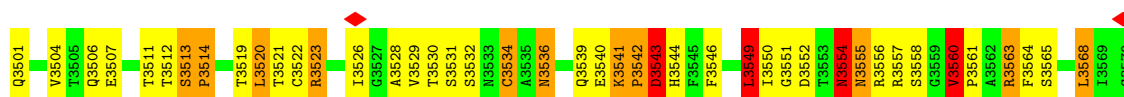
• Molecule 3: EEEV-58 antibody heavy chain

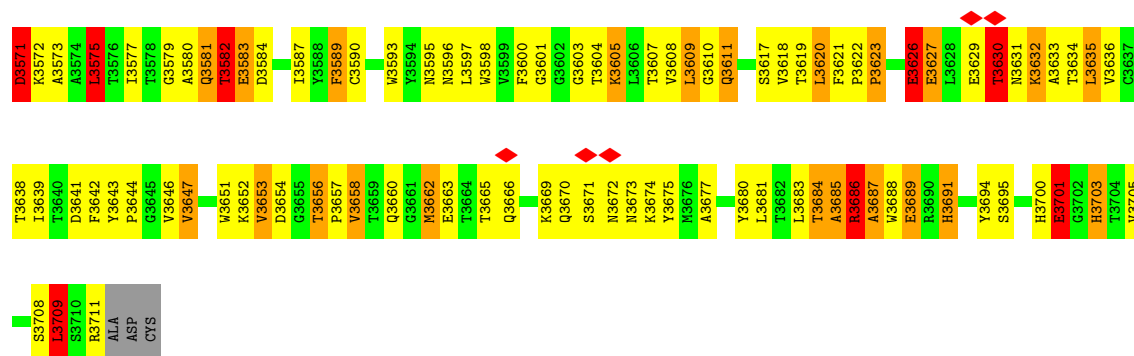


• Molecule 4: EEEV-58 antibody light chain

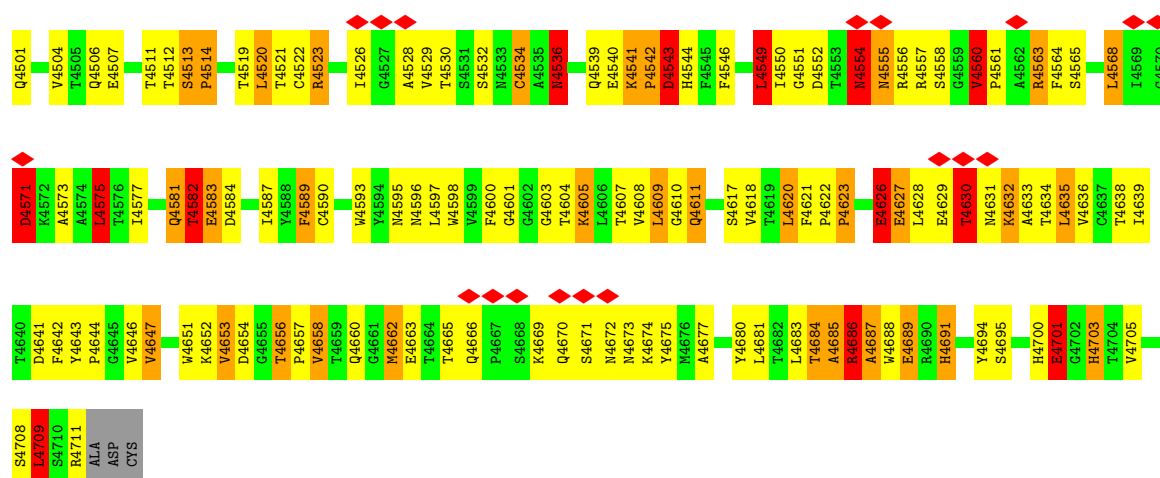


• Molecule 4: EEEV-58 antibody light chain

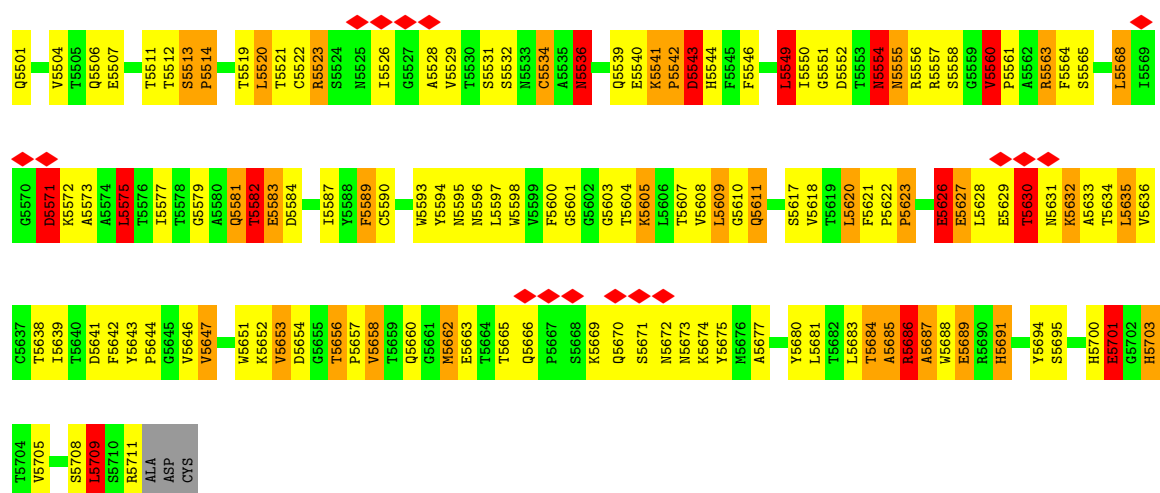




• Molecule 4: EEEV-58 antibody light chain



• Molecule 4: EEEV-58 antibody light chain



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 7335                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 31                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 7.238                                   | Depositor |
| Minimum map value                    | -8.327                                  | Depositor |
| Average map value                    | 0.069                                   | Depositor |
| Map value standard deviation         | 1.011                                   | Depositor |
| Recommended contour level            | 0.7                                     | Depositor |
| Map size (Å)                         | 907.2, 907.2, 907.2                     | wwPDB     |
| Map dimensions                       | 560, 560, 560                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.62, 1.62, 1.62                        | 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     | 0.44         | 0/3147          | 0.63        | 1/4294 (0.0%)    |
| 1   | E     | 0.44         | 0/3147          | 0.63        | 1/4294 (0.0%)    |
| 1   | I     | 0.44         | 0/3147          | 0.63        | 1/4294 (0.0%)    |
| 1   | M     | 0.44         | 0/3147          | 0.63        | 1/4294 (0.0%)    |
| 2   | B     | 0.43         | 0/2624          | 0.64        | 2/3571 (0.1%)    |
| 2   | F     | 0.43         | 0/2624          | 0.64        | 2/3571 (0.1%)    |
| 2   | J     | 0.43         | 0/2624          | 0.64        | 2/3571 (0.1%)    |
| 2   | N     | 0.43         | 0/2624          | 0.64        | 2/3571 (0.1%)    |
| 3   | C     | 0.84         | 5/1714 (0.3%)   | 1.15        | 12/2340 (0.5%)   |
| 3   | G     | 0.84         | 5/1714 (0.3%)   | 1.15        | 12/2340 (0.5%)   |
| 3   | K     | 0.84         | 5/1714 (0.3%)   | 1.15        | 12/2340 (0.5%)   |
| 3   | O     | 0.84         | 5/1714 (0.3%)   | 1.15        | 13/2340 (0.6%)   |
| 4   | D     | 1.18         | 4/1634 (0.2%)   | 1.94        | 57/2232 (2.6%)   |
| 4   | H     | 1.18         | 4/1634 (0.2%)   | 1.94        | 57/2232 (2.6%)   |
| 4   | L     | 1.18         | 4/1634 (0.2%)   | 1.94        | 56/2232 (2.5%)   |
| 4   | P     | 1.18         | 4/1634 (0.2%)   | 1.94        | 57/2232 (2.6%)   |
| All | All   | 0.71         | 36/36476 (0.1%) | 1.09        | 288/49748 (0.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| 1   | M     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (36) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | C     | 58   | PRO  | N-CD    | 17.50 | 1.72        | 1.47     |
| 3   | O     | 5058 | PRO  | N-CD    | 17.50 | 1.72        | 1.47     |
| 3   | G     | 3058 | PRO  | N-CD    | 17.47 | 1.72        | 1.47     |
| 3   | K     | 4058 | PRO  | N-CD    | 17.46 | 1.72        | 1.47     |
| 3   | G     | 3041 | PRO  | N-CD    | 14.07 | 1.67        | 1.47     |
| 3   | K     | 4041 | PRO  | N-CD    | 14.06 | 1.67        | 1.47     |
| 3   | C     | 41   | PRO  | N-CD    | 14.02 | 1.67        | 1.47     |
| 3   | O     | 5041 | PRO  | N-CD    | 14.01 | 1.67        | 1.47     |
| 4   | L     | 4514 | PRO  | N-CD    | 13.25 | 1.66        | 1.47     |
| 4   | H     | 3514 | PRO  | N-CD    | 13.21 | 1.66        | 1.47     |
| 4   | D     | 514  | PRO  | N-CD    | 13.21 | 1.66        | 1.47     |
| 4   | P     | 5514 | PRO  | N-CD    | 13.19 | 1.66        | 1.47     |
| 3   | O     | 5014 | PRO  | N-CD    | 9.55  | 1.61        | 1.47     |
| 3   | K     | 4014 | PRO  | N-CD    | 9.53  | 1.61        | 1.47     |
| 3   | G     | 3014 | PRO  | N-CD    | 9.51  | 1.61        | 1.47     |
| 3   | C     | 14   | PRO  | N-CD    | 9.46  | 1.60        | 1.47     |
| 4   | P     | 5544 | HIS  | CG-CD2  | 9.28  | 1.46        | 1.35     |
| 4   | L     | 4544 | HIS  | CG-CD2  | 9.28  | 1.46        | 1.35     |
| 4   | D     | 544  | HIS  | CG-CD2  | 9.26  | 1.46        | 1.35     |
| 4   | H     | 3544 | HIS  | CG-CD2  | 9.24  | 1.46        | 1.35     |
| 4   | D     | 542  | PRO  | N-CD    | 7.03  | 1.57        | 1.47     |
| 4   | P     | 5542 | PRO  | N-CD    | 7.00  | 1.57        | 1.47     |
| 4   | H     | 3542 | PRO  | N-CD    | 6.98  | 1.57        | 1.47     |
| 4   | L     | 4542 | PRO  | N-CD    | 6.97  | 1.57        | 1.47     |
| 3   | C     | 33   | PRO  | N-CD    | 6.25  | 1.56        | 1.47     |
| 3   | O     | 5033 | PRO  | N-CD    | 6.24  | 1.56        | 1.47     |
| 3   | G     | 3033 | PRO  | N-CD    | 6.23  | 1.56        | 1.47     |
| 3   | K     | 4033 | PRO  | N-CD    | 6.20  | 1.56        | 1.47     |
| 4   | P     | 5544 | HIS  | CD2-NE2 | -5.16 | 1.32        | 1.37     |
| 3   | G     | 3108 | GLY  | C-N     | 5.15  | 1.41        | 1.33     |
| 3   | C     | 108  | GLY  | C-N     | 5.13  | 1.41        | 1.33     |
| 4   | D     | 544  | HIS  | CD2-NE2 | -5.12 | 1.32        | 1.37     |
| 4   | H     | 3544 | HIS  | CD2-NE2 | -5.12 | 1.32        | 1.37     |
| 3   | K     | 4108 | GLY  | C-N     | 5.12  | 1.41        | 1.33     |
| 3   | O     | 5108 | GLY  | C-N     | 5.11  | 1.41        | 1.33     |
| 4   | L     | 4544 | HIS  | CD2-NE2 | -5.09 | 1.32        | 1.37     |

All (288) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | P     | 5701 | GLU  | CB-CG-CD | 12.70 | 134.18      | 112.60   |
| 4   | L     | 4701 | GLU  | CB-CG-CD | 12.69 | 134.17      | 112.60   |
| 4   | H     | 3701 | GLU  | CB-CG-CD | 12.68 | 134.16      | 112.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | D     | 701  | GLU  | CB-CG-CD | 12.65 | 134.10      | 112.60   |
| 4   | D     | 658  | VAL  | N-CA-C   | -8.97 | 100.07      | 110.21   |
| 4   | P     | 5658 | VAL  | N-CA-C   | -8.95 | 100.09      | 110.21   |
| 4   | L     | 4658 | VAL  | N-CA-C   | -8.95 | 100.10      | 110.21   |
| 4   | H     | 3658 | VAL  | N-CA-C   | -8.93 | 100.12      | 110.21   |
| 4   | P     | 5703 | HIS  | CA-CB-CG | -8.54 | 105.25      | 113.80   |
| 4   | L     | 4703 | HIS  | CA-CB-CG | -8.53 | 105.27      | 113.80   |
| 4   | H     | 3703 | HIS  | CA-CB-CG | -8.52 | 105.28      | 113.80   |
| 4   | D     | 703  | HIS  | CA-CB-CG | -8.48 | 105.32      | 113.80   |
| 4   | P     | 5575 | LEU  | CA-C-O   | -8.13 | 111.60      | 120.30   |
| 4   | D     | 575  | LEU  | CA-C-O   | -8.11 | 111.62      | 120.30   |
| 4   | L     | 4575 | LEU  | CA-C-O   | -8.11 | 111.63      | 120.30   |
| 4   | H     | 3575 | LEU  | CA-C-O   | -8.06 | 111.67      | 120.30   |
| 4   | L     | 4674 | LYS  | CA-C-O   | -7.84 | 111.68      | 121.88   |
| 4   | H     | 3674 | LYS  | CA-C-O   | -7.82 | 111.72      | 121.88   |
| 4   | P     | 5674 | LYS  | CA-C-O   | -7.80 | 111.74      | 121.88   |
| 4   | D     | 674  | LYS  | CA-C-O   | -7.78 | 111.77      | 121.88   |
| 4   | L     | 4658 | VAL  | CB-CA-C  | 7.77  | 120.15      | 111.45   |
| 4   | P     | 5658 | VAL  | CB-CA-C  | 7.76  | 120.14      | 111.45   |
| 4   | D     | 658  | VAL  | CB-CA-C  | 7.76  | 120.14      | 111.45   |
| 4   | H     | 3658 | VAL  | CB-CA-C  | 7.73  | 120.11      | 111.45   |
| 4   | L     | 4627 | GLU  | CB-CG-CD | 7.49  | 125.33      | 112.60   |
| 4   | P     | 5627 | GLU  | CB-CG-CD | 7.48  | 125.31      | 112.60   |
| 4   | H     | 3627 | GLU  | CB-CG-CD | 7.48  | 125.31      | 112.60   |
| 4   | D     | 627  | GLU  | CB-CG-CD | 7.44  | 125.25      | 112.60   |
| 4   | H     | 3589 | PHE  | CA-C-O   | -7.25 | 113.03      | 120.71   |
| 4   | L     | 4589 | PHE  | CA-C-O   | -7.24 | 113.04      | 120.71   |
| 4   | P     | 5589 | PHE  | CA-C-O   | -7.23 | 113.05      | 120.71   |
| 4   | D     | 589  | PHE  | CA-C-O   | -7.21 | 113.06      | 120.71   |
| 4   | L     | 4541 | LYS  | CA-C-O   | -6.96 | 113.66      | 120.97   |
| 4   | D     | 541  | LYS  | CA-C-O   | -6.96 | 113.66      | 120.97   |
| 4   | H     | 3541 | LYS  | CA-C-O   | -6.94 | 113.68      | 120.97   |
| 4   | P     | 5541 | LYS  | CA-C-O   | -6.93 | 113.69      | 120.97   |
| 4   | D     | 701  | GLU  | N-CA-CB  | 6.90  | 122.14      | 110.49   |
| 4   | P     | 5701 | GLU  | N-CA-CB  | 6.90  | 122.15      | 110.49   |
| 4   | H     | 3687 | ALA  | N-CA-C   | -6.88 | 103.79      | 111.28   |
| 4   | L     | 4701 | GLU  | N-CA-CB  | 6.87  | 122.09      | 110.49   |
| 4   | H     | 3701 | GLU  | N-CA-CB  | 6.86  | 122.09      | 110.49   |
| 4   | L     | 4687 | ALA  | N-CA-C   | -6.86 | 103.81      | 111.28   |
| 4   | D     | 687  | ALA  | N-CA-C   | -6.84 | 103.82      | 111.28   |
| 1   | E     | 1265 | GLU  | N-CA-C   | -6.84 | 94.68       | 109.81   |
| 4   | P     | 5687 | ALA  | N-CA-C   | -6.84 | 103.83      | 111.28   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 265  | GLU  | N-CA-C    | -6.83 | 94.72       | 109.81   |
| 1   | I     | 2265 | GLU  | N-CA-C    | -6.82 | 94.74       | 109.81   |
| 1   | M     | 3265 | GLU  | N-CA-C    | -6.82 | 94.74       | 109.81   |
| 4   | P     | 5634 | THR  | CA-CB-OG1 | -6.73 | 99.50       | 109.60   |
| 4   | D     | 634  | THR  | CA-CB-OG1 | -6.73 | 99.50       | 109.60   |
| 4   | H     | 3634 | THR  | CA-CB-OG1 | -6.73 | 99.51       | 109.60   |
| 4   | L     | 4634 | THR  | CA-CB-OG1 | -6.72 | 99.52       | 109.60   |
| 3   | O     | 5004 | LEU  | N-CA-C    | -6.66 | 97.56       | 108.41   |
| 3   | G     | 3004 | LEU  | N-CA-C    | -6.64 | 97.58       | 108.41   |
| 3   | C     | 4    | LEU  | N-CA-C    | -6.64 | 97.59       | 108.41   |
| 4   | D     | 686  | ARG  | N-CA-C    | 6.63  | 118.30      | 111.14   |
| 3   | K     | 4004 | LEU  | N-CA-C    | -6.62 | 97.61       | 108.41   |
| 4   | L     | 4686 | ARG  | N-CA-C    | 6.62  | 118.29      | 111.14   |
| 4   | H     | 3686 | ARG  | N-CA-C    | 6.62  | 118.29      | 111.14   |
| 4   | P     | 5686 | ARG  | N-CA-C    | 6.60  | 118.27      | 111.14   |
| 4   | H     | 3541 | LYS  | N-CA-C    | -6.53 | 101.84      | 110.40   |
| 3   | G     | 3043 | LYS  | N-CA-C    | 6.53  | 124.71      | 110.80   |
| 3   | O     | 5043 | LYS  | N-CA-C    | 6.52  | 124.70      | 110.80   |
| 3   | C     | 43   | LYS  | N-CA-C    | 6.52  | 124.68      | 110.80   |
| 4   | P     | 5541 | LYS  | N-CA-C    | -6.51 | 101.87      | 110.40   |
| 3   | K     | 4043 | LYS  | N-CA-C    | 6.51  | 124.67      | 110.80   |
| 4   | D     | 541  | LYS  | N-CA-C    | -6.51 | 101.88      | 110.40   |
| 3   | G     | 3030 | THR  | N-CA-C    | 6.50  | 120.47      | 112.54   |
| 3   | K     | 4030 | THR  | N-CA-C    | 6.47  | 120.44      | 112.54   |
| 4   | L     | 4541 | LYS  | N-CA-C    | -6.47 | 101.92      | 110.40   |
| 3   | O     | 5030 | THR  | N-CA-C    | 6.46  | 120.42      | 112.54   |
| 3   | C     | 30   | THR  | N-CA-C    | 6.44  | 120.39      | 112.54   |
| 4   | H     | 3582 | THR  | CA-C-O    | 6.40  | 127.33      | 120.10   |
| 4   | L     | 4582 | THR  | CA-C-O    | 6.38  | 127.31      | 120.10   |
| 4   | P     | 5582 | THR  | CA-C-O    | 6.37  | 127.30      | 120.10   |
| 4   | D     | 582  | THR  | CA-C-O    | 6.33  | 127.25      | 120.10   |
| 4   | D     | 560  | VAL  | N-CA-C    | -6.14 | 101.20      | 107.89   |
| 4   | H     | 3560 | VAL  | N-CA-C    | -6.13 | 101.21      | 107.89   |
| 4   | P     | 5560 | VAL  | N-CA-C    | -6.12 | 101.22      | 107.89   |
| 4   | L     | 4560 | VAL  | N-CA-C    | -6.11 | 101.23      | 107.89   |
| 4   | H     | 3677 | ALA  | O-C-N     | 6.10  | 129.50      | 123.46   |
| 4   | P     | 5635 | LEU  | CA-CB-CG  | 6.08  | 137.60      | 116.30   |
| 4   | H     | 3635 | LEU  | CA-CB-CG  | 6.08  | 137.59      | 116.30   |
| 4   | L     | 4635 | LEU  | CA-CB-CG  | 6.08  | 137.58      | 116.30   |
| 4   | D     | 635  | LEU  | CA-CB-CG  | 6.08  | 137.57      | 116.30   |
| 4   | D     | 677  | ALA  | O-C-N     | 6.08  | 129.47      | 123.46   |
| 4   | L     | 4677 | ALA  | O-C-N     | 6.05  | 129.45      | 123.46   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | P     | 5677 | ALA  | O-C-N    | 6.03  | 129.43      | 123.46   |
| 4   | L     | 4600 | PHE  | CA-C-O   | -5.98 | 114.23      | 121.28   |
| 4   | H     | 3600 | PHE  | CA-C-O   | -5.97 | 114.23      | 121.28   |
| 4   | D     | 600  | PHE  | CA-C-O   | -5.94 | 114.27      | 121.28   |
| 4   | D     | 536  | ASN  | CA-C-O   | -5.92 | 114.42      | 121.11   |
| 4   | P     | 5600 | PHE  | CA-C-O   | -5.92 | 114.29      | 121.28   |
| 4   | P     | 5685 | ALA  | CA-C-N   | 5.91  | 128.48      | 120.44   |
| 4   | P     | 5685 | ALA  | C-N-CA   | 5.91  | 128.48      | 120.44   |
| 4   | H     | 3685 | ALA  | CA-C-N   | 5.90  | 128.46      | 120.44   |
| 4   | H     | 3685 | ALA  | C-N-CA   | 5.90  | 128.46      | 120.44   |
| 4   | L     | 4685 | ALA  | CA-C-N   | 5.90  | 128.46      | 120.44   |
| 4   | L     | 4685 | ALA  | C-N-CA   | 5.90  | 128.46      | 120.44   |
| 4   | P     | 5536 | ASN  | CA-C-O   | -5.89 | 114.45      | 121.11   |
| 4   | H     | 3536 | ASN  | CA-C-O   | -5.87 | 114.47      | 121.11   |
| 4   | L     | 4536 | ASN  | CA-C-O   | -5.87 | 114.47      | 121.11   |
| 4   | D     | 685  | ALA  | CA-C-N   | 5.86  | 128.41      | 120.44   |
| 4   | D     | 685  | ALA  | C-N-CA   | 5.86  | 128.41      | 120.44   |
| 4   | D     | 511  | THR  | CA-C-O   | -5.83 | 114.07      | 120.36   |
| 4   | H     | 3554 | ASN  | CA-C-O   | -5.82 | 113.46      | 119.51   |
| 4   | P     | 5511 | THR  | CA-C-O   | -5.81 | 114.08      | 120.36   |
| 4   | H     | 3641 | ASP  | CA-C-O   | -5.81 | 114.80      | 121.54   |
| 4   | D     | 641  | ASP  | CA-C-O   | -5.80 | 114.81      | 121.54   |
| 3   | C     | 34   | MET  | N-CA-C   | 5.80  | 118.36      | 108.90   |
| 4   | L     | 4511 | THR  | CA-C-O   | -5.79 | 114.11      | 120.36   |
| 4   | L     | 4554 | ASN  | CA-C-O   | -5.78 | 113.50      | 119.51   |
| 4   | P     | 5554 | ASN  | CA-C-O   | -5.78 | 113.50      | 119.51   |
| 2   | F     | 1685 | TYR  | CA-CB-CG | 5.78  | 124.30      | 113.90   |
| 3   | G     | 3034 | MET  | N-CA-C   | 5.78  | 118.31      | 108.90   |
| 2   | B     | 685  | TYR  | CA-CB-CG | 5.77  | 124.29      | 113.90   |
| 4   | H     | 3511 | THR  | CA-C-O   | -5.77 | 114.12      | 120.36   |
| 4   | L     | 4641 | ASP  | CA-C-O   | -5.77 | 114.85      | 121.54   |
| 2   | N     | 3685 | TYR  | CA-CB-CG | 5.77  | 124.29      | 113.90   |
| 3   | K     | 4034 | MET  | N-CA-C   | 5.76  | 118.28      | 108.90   |
| 3   | O     | 5034 | MET  | N-CA-C   | 5.76  | 118.28      | 108.90   |
| 2   | J     | 2685 | TYR  | CA-CB-CG | 5.75  | 124.26      | 113.90   |
| 4   | D     | 554  | ASN  | CA-C-O   | -5.75 | 113.53      | 119.51   |
| 4   | P     | 5641 | ASP  | CA-C-O   | -5.75 | 114.87      | 121.54   |
| 4   | L     | 4611 | GLN  | CA-C-N   | -5.68 | 114.09      | 119.89   |
| 4   | L     | 4611 | GLN  | C-N-CA   | -5.68 | 114.09      | 119.89   |
| 3   | G     | 3039 | GLN  | N-CA-C   | -5.67 | 98.10       | 108.02   |
| 3   | K     | 4039 | GLN  | N-CA-C   | -5.66 | 98.11       | 108.02   |
| 3   | O     | 5039 | GLN  | N-CA-C   | -5.66 | 98.12       | 108.02   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 4   | P     | 5611 | GLN  | CA-C-N    | -5.65 | 114.14      | 119.90   |
| 4   | P     | 5611 | GLN  | C-N-CA    | -5.65 | 114.14      | 119.90   |
| 3   | C     | 39   | GLN  | N-CA-C    | -5.64 | 98.14       | 108.02   |
| 4   | H     | 3611 | GLN  | CA-C-N    | -5.64 | 114.15      | 119.90   |
| 4   | H     | 3611 | GLN  | C-N-CA    | -5.64 | 114.15      | 119.90   |
| 4   | D     | 611  | GLN  | CA-C-N    | -5.64 | 114.15      | 119.90   |
| 4   | D     | 611  | GLN  | C-N-CA    | -5.64 | 114.15      | 119.90   |
| 4   | H     | 3677 | ALA  | CA-C-O    | -5.64 | 114.90      | 121.10   |
| 4   | H     | 3647 | VAL  | N-CA-CB   | 5.62  | 120.72      | 112.35   |
| 4   | D     | 677  | ALA  | CA-C-O    | -5.62 | 114.92      | 121.10   |
| 4   | L     | 4677 | ALA  | CA-C-O    | -5.61 | 114.93      | 121.10   |
| 4   | P     | 5647 | VAL  | N-CA-CB   | 5.61  | 120.70      | 112.35   |
| 4   | L     | 4647 | VAL  | N-CA-CB   | 5.60  | 120.69      | 112.35   |
| 4   | P     | 5634 | THR  | CA-CB-CG2 | 5.60  | 120.01      | 110.50   |
| 4   | P     | 5677 | ALA  | CA-C-O    | -5.59 | 114.95      | 121.10   |
| 4   | D     | 647  | VAL  | N-CA-CB   | 5.58  | 120.66      | 112.35   |
| 4   | L     | 4634 | THR  | CA-CB-CG2 | 5.56  | 119.95      | 110.50   |
| 4   | D     | 634  | THR  | CA-CB-CG2 | 5.55  | 119.94      | 110.50   |
| 4   | L     | 4656 | THR  | CA-CB-OG1 | -5.55 | 101.28      | 109.60   |
| 4   | P     | 5656 | THR  | CA-CB-OG1 | -5.54 | 101.30      | 109.60   |
| 4   | D     | 656  | THR  | CA-CB-OG1 | -5.53 | 101.31      | 109.60   |
| 4   | H     | 3653 | VAL  | O-C-N     | 5.53  | 129.25      | 122.95   |
| 4   | H     | 3634 | THR  | CA-CB-CG2 | 5.53  | 119.90      | 110.50   |
| 4   | D     | 653  | VAL  | O-C-N     | 5.52  | 129.25      | 122.95   |
| 4   | H     | 3656 | THR  | CA-CB-OG1 | -5.52 | 101.32      | 109.60   |
| 4   | H     | 3563 | ARG  | N-CA-C    | -5.51 | 106.39      | 113.01   |
| 4   | L     | 4653 | VAL  | O-C-N     | 5.51  | 129.23      | 122.95   |
| 4   | L     | 4607 | THR  | CA-C-O    | -5.51 | 114.38      | 120.38   |
| 4   | H     | 3607 | THR  | CA-C-O    | -5.50 | 114.39      | 120.38   |
| 4   | P     | 5607 | THR  | CA-C-O    | -5.49 | 114.39      | 120.38   |
| 3   | G     | 3111 | THR  | N-CA-C    | -5.49 | 99.34       | 108.34   |
| 3   | O     | 5111 | THR  | N-CA-C    | -5.48 | 99.35       | 108.34   |
| 4   | L     | 4563 | ARG  | N-CA-C    | -5.48 | 106.44      | 113.01   |
| 3   | K     | 4111 | THR  | N-CA-C    | -5.48 | 99.36       | 108.34   |
| 4   | L     | 4701 | GLU  | CA-C-N    | 5.48  | 132.15      | 121.41   |
| 4   | L     | 4701 | GLU  | C-N-CA    | 5.48  | 132.15      | 121.41   |
| 4   | P     | 5563 | ARG  | N-CA-C    | -5.47 | 106.44      | 113.01   |
| 3   | C     | 111  | THR  | N-CA-C    | -5.47 | 99.37       | 108.34   |
| 4   | D     | 563  | ARG  | N-CA-C    | -5.47 | 106.44      | 113.01   |
| 4   | P     | 5701 | GLU  | CA-C-N    | 5.47  | 132.13      | 121.41   |
| 4   | P     | 5701 | GLU  | C-N-CA    | 5.47  | 132.13      | 121.41   |
| 4   | P     | 5653 | VAL  | O-C-N     | 5.47  | 129.19      | 122.95   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 4   | D     | 607  | THR  | CA-C-O    | -5.46 | 114.43      | 120.38   |
| 4   | P     | 5617 | SER  | O-C-N     | 5.46  | 130.01      | 123.13   |
| 4   | D     | 701  | GLU  | CA-C-N    | 5.46  | 132.10      | 121.41   |
| 4   | D     | 701  | GLU  | C-N-CA    | 5.46  | 132.10      | 121.41   |
| 4   | D     | 617  | SER  | O-C-N     | 5.46  | 130.00      | 123.13   |
| 4   | H     | 3701 | GLU  | CA-C-N    | 5.45  | 132.10      | 121.41   |
| 4   | H     | 3701 | GLU  | C-N-CA    | 5.45  | 132.10      | 121.41   |
| 4   | D     | 534  | CYS  | CA-C-O    | -5.44 | 115.67      | 122.03   |
| 4   | H     | 3534 | CYS  | CA-C-O    | -5.42 | 115.69      | 122.03   |
| 4   | L     | 4617 | SER  | O-C-N     | 5.42  | 129.96      | 123.13   |
| 4   | L     | 4534 | CYS  | CA-C-O    | -5.41 | 115.70      | 122.03   |
| 4   | P     | 5534 | CYS  | CA-C-O    | -5.40 | 115.71      | 122.03   |
| 4   | H     | 3617 | SER  | O-C-N     | 5.39  | 129.93      | 123.13   |
| 4   | H     | 3543 | ASP  | CA-C-O    | -5.39 | 112.81      | 120.51   |
| 4   | L     | 4529 | VAL  | CA-C-O    | -5.38 | 114.71      | 121.11   |
| 4   | H     | 3529 | VAL  | CA-C-O    | -5.38 | 114.71      | 121.11   |
| 4   | L     | 4543 | ASP  | CA-C-O    | -5.37 | 112.83      | 120.51   |
| 4   | D     | 543  | ASP  | CA-C-O    | -5.36 | 112.85      | 120.51   |
| 4   | P     | 5529 | VAL  | CA-C-O    | -5.35 | 114.74      | 121.11   |
| 4   | P     | 5543 | ASP  | CA-C-O    | -5.33 | 112.88      | 120.51   |
| 4   | D     | 529  | VAL  | CA-C-O    | -5.32 | 114.78      | 121.11   |
| 3   | G     | 3074 | ILE  | CA-C-O    | 5.24  | 127.33      | 120.78   |
| 4   | P     | 5646 | VAL  | CA-C-O    | -5.22 | 114.74      | 120.43   |
| 4   | L     | 4646 | VAL  | CA-C-O    | -5.22 | 114.74      | 120.43   |
| 4   | H     | 3675 | TYR  | O-C-N     | 5.21  | 130.08      | 122.94   |
| 4   | D     | 630  | THR  | CA-CB-CG2 | 5.21  | 119.35      | 110.50   |
| 4   | P     | 5630 | THR  | CA-CB-CG2 | 5.21  | 119.35      | 110.50   |
| 4   | H     | 3571 | ASP  | CA-C-N    | -5.20 | 113.78      | 122.21   |
| 4   | H     | 3571 | ASP  | C-N-CA    | -5.20 | 113.78      | 122.21   |
| 4   | P     | 5675 | TYR  | O-C-N     | 5.20  | 130.07      | 122.94   |
| 4   | H     | 3630 | THR  | CA-CB-CG2 | 5.20  | 119.34      | 110.50   |
| 3   | C     | 74   | ILE  | CA-C-O    | 5.20  | 127.27      | 120.78   |
| 3   | K     | 4074 | ILE  | CA-C-O    | 5.19  | 127.27      | 120.78   |
| 4   | H     | 3555 | ASN  | CA-C-O    | -5.19 | 114.80      | 120.36   |
| 4   | L     | 4630 | THR  | CA-CB-CG2 | 5.19  | 119.33      | 110.50   |
| 4   | P     | 5513 | SER  | O-C-N     | 5.19  | 126.60      | 121.57   |
| 4   | D     | 555  | ASN  | CA-C-O    | -5.19 | 114.81      | 120.36   |
| 4   | L     | 4571 | ASP  | CA-C-N    | -5.19 | 113.81      | 122.21   |
| 4   | L     | 4571 | ASP  | C-N-CA    | -5.19 | 113.81      | 122.21   |
| 4   | P     | 5555 | ASN  | CA-C-O    | -5.18 | 114.81      | 120.36   |
| 4   | D     | 646  | VAL  | CA-C-O    | -5.18 | 114.78      | 120.43   |
| 4   | H     | 3513 | SER  | O-C-N     | 5.18  | 126.59      | 121.57   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | L     | 4675 | TYR  | O-C-N   | 5.18  | 130.04      | 122.94   |
| 3   | G     | 3040 | ALA  | CA-C-N  | 5.18  | 126.31      | 119.84   |
| 3   | G     | 3040 | ALA  | C-N-CA  | 5.18  | 126.31      | 119.84   |
| 4   | P     | 5568 | LEU  | N-CA-C  | -5.18 | 100.46      | 108.90   |
| 4   | D     | 675  | TYR  | O-C-N   | 5.17  | 130.03      | 122.94   |
| 3   | O     | 5074 | ILE  | CA-C-O  | 5.17  | 127.25      | 120.78   |
| 3   | C     | 40   | ALA  | CA-C-N  | 5.17  | 126.30      | 119.84   |
| 3   | C     | 40   | ALA  | C-N-CA  | 5.17  | 126.30      | 119.84   |
| 4   | D     | 568  | LEU  | N-CA-C  | -5.17 | 100.48      | 108.90   |
| 4   | L     | 4555 | ASN  | CA-C-O  | -5.16 | 114.83      | 120.36   |
| 4   | P     | 5623 | PRO  | CA-C-O  | -5.16 | 115.45      | 121.34   |
| 4   | D     | 571  | ASP  | CA-C-N  | -5.16 | 113.85      | 122.21   |
| 4   | D     | 571  | ASP  | C-N-CA  | -5.16 | 113.85      | 122.21   |
| 3   | K     | 4040 | ALA  | CA-C-N  | 5.16  | 126.29      | 119.84   |
| 3   | K     | 4040 | ALA  | C-N-CA  | 5.16  | 126.29      | 119.84   |
| 4   | L     | 4513 | SER  | O-C-N   | 5.16  | 126.57      | 121.57   |
| 4   | P     | 5571 | ASP  | CA-C-N  | -5.16 | 113.86      | 122.21   |
| 4   | P     | 5571 | ASP  | C-N-CA  | -5.16 | 113.86      | 122.21   |
| 4   | H     | 3646 | VAL  | CA-C-O  | -5.15 | 114.82      | 120.43   |
| 4   | H     | 3568 | LEU  | N-CA-C  | -5.14 | 100.52      | 108.90   |
| 3   | C     | 56   | GLY  | O-C-N   | -5.14 | 116.44      | 122.50   |
| 4   | L     | 4568 | LEU  | N-CA-C  | -5.14 | 100.52      | 108.90   |
| 4   | H     | 3623 | PRO  | CA-C-O  | -5.14 | 115.48      | 121.34   |
| 4   | L     | 4623 | PRO  | CA-C-O  | -5.14 | 115.48      | 121.34   |
| 4   | D     | 513  | SER  | O-C-N   | 5.13  | 126.55      | 121.57   |
| 3   | O     | 5040 | ALA  | CA-C-N  | 5.13  | 126.26      | 119.84   |
| 3   | O     | 5040 | ALA  | C-N-CA  | 5.13  | 126.26      | 119.84   |
| 4   | D     | 623  | PRO  | CA-C-O  | -5.12 | 115.50      | 121.34   |
| 4   | H     | 3709 | LEU  | CB-CA-C | 5.12  | 118.93      | 109.71   |
| 4   | P     | 5549 | LEU  | CA-C-N  | 5.12  | 130.82      | 122.69   |
| 4   | P     | 5549 | LEU  | C-N-CA  | 5.12  | 130.82      | 122.69   |
| 4   | P     | 5709 | LEU  | CB-CA-C | 5.10  | 118.89      | 109.71   |
| 4   | D     | 709  | LEU  | CB-CA-C | 5.10  | 118.89      | 109.71   |
| 4   | L     | 4709 | LEU  | CB-CA-C | 5.10  | 118.89      | 109.71   |
| 3   | G     | 3001 | GLN  | CA-C-O  | -5.10 | 112.14      | 120.80   |
| 3   | K     | 4001 | GLN  | CA-C-O  | -5.10 | 112.14      | 120.80   |
| 3   | C     | 1    | GLN  | CA-C-O  | -5.09 | 112.15      | 120.80   |
| 4   | D     | 549  | LEU  | CA-C-N  | 5.09  | 130.78      | 122.69   |
| 4   | D     | 549  | LEU  | C-N-CA  | 5.09  | 130.78      | 122.69   |
| 3   | G     | 3056 | GLY  | O-C-N   | -5.09 | 116.50      | 122.50   |
| 3   | O     | 5001 | GLN  | CA-C-O  | -5.09 | 112.15      | 120.80   |
| 3   | K     | 4056 | GLY  | O-C-N   | -5.08 | 116.50      | 122.50   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 4   | L     | 4549 | LEU  | CA-C-N    | 5.08  | 130.78      | 122.69   |
| 4   | L     | 4549 | LEU  | C-N-CA    | 5.08  | 130.78      | 122.69   |
| 4   | D     | 623  | PRO  | N-CA-C    | -5.08 | 103.22      | 111.14   |
| 3   | C     | 59   | THR  | N-CA-C    | -5.08 | 101.42      | 109.59   |
| 2   | J     | 2823 | TRP  | CA-CB-CG  | 5.07  | 123.23      | 113.60   |
| 4   | P     | 5623 | PRO  | N-CA-C    | -5.07 | 103.23      | 111.14   |
| 3   | O     | 5056 | GLY  | O-C-N     | -5.07 | 116.52      | 122.50   |
| 4   | L     | 4623 | PRO  | N-CA-C    | -5.06 | 103.24      | 111.14   |
| 4   | D     | 560  | VAL  | O-C-N     | 5.06  | 125.96      | 121.41   |
| 2   | N     | 3823 | TRP  | CA-CB-CG  | 5.06  | 123.21      | 113.60   |
| 3   | G     | 3059 | THR  | N-CA-C    | -5.06 | 101.45      | 109.59   |
| 4   | H     | 3626 | GLU  | CB-CG-CD  | 5.05  | 121.19      | 112.60   |
| 4   | L     | 4647 | VAL  | CA-CB-CG1 | 5.05  | 118.98      | 110.40   |
| 2   | B     | 823  | TRP  | CA-CB-CG  | 5.05  | 123.19      | 113.60   |
| 4   | H     | 3623 | PRO  | N-CA-C    | -5.05 | 103.27      | 111.14   |
| 4   | H     | 3549 | LEU  | CA-C-N    | 5.04  | 130.70      | 122.69   |
| 4   | H     | 3549 | LEU  | C-N-CA    | 5.04  | 130.70      | 122.69   |
| 4   | H     | 3647 | VAL  | CA-CB-CG1 | 5.04  | 118.97      | 110.40   |
| 3   | O     | 5059 | THR  | N-CA-C    | -5.04 | 101.48      | 109.59   |
| 4   | P     | 5647 | VAL  | CA-CB-CG1 | 5.04  | 118.96      | 110.40   |
| 4   | D     | 647  | VAL  | CA-CB-CG1 | 5.03  | 118.96      | 110.40   |
| 3   | K     | 4059 | THR  | N-CA-C    | -5.03 | 101.49      | 109.59   |
| 4   | L     | 4560 | VAL  | O-C-N     | 5.03  | 125.94      | 121.41   |
| 4   | L     | 4626 | GLU  | CB-CG-CD  | 5.03  | 121.15      | 112.60   |
| 2   | F     | 1823 | TRP  | CA-CB-CG  | 5.03  | 123.16      | 113.60   |
| 4   | P     | 5626 | GLU  | CB-CG-CD  | 5.03  | 121.15      | 112.60   |
| 4   | D     | 626  | GLU  | CB-CG-CD  | 5.03  | 121.14      | 112.60   |
| 4   | H     | 3619 | THR  | O-C-N     | 5.01  | 129.47      | 123.36   |
| 4   | P     | 5560 | VAL  | O-C-N     | 5.01  | 125.92      | 121.41   |
| 4   | H     | 3560 | VAL  | O-C-N     | 5.00  | 125.92      | 121.41   |
| 4   | P     | 5579 | GLY  | N-CA-C    | -5.00 | 101.32      | 113.18   |
| 3   | O     | 5095 | PHE  | O-C-N     | -5.00 | 116.86      | 123.21   |
| 4   | D     | 579  | GLY  | N-CA-C    | -5.00 | 101.32      | 113.18   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 385  | LYS  | Peptide |
| 1   | E     | 1385 | LYS  | Peptide |
| 1   | I     | 2385 | LYS  | Peptide |
| 1   | M     | 3385 | LYS  | Peptide |

## 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     | 3063  | 0        | 2950     | 85      | 0            |
| 1   | E     | 3063  | 0        | 2947     | 66      | 0            |
| 1   | I     | 3063  | 0        | 2945     | 76      | 0            |
| 1   | M     | 3063  | 0        | 2947     | 58      | 0            |
| 2   | B     | 2550  | 0        | 2488     | 158     | 0            |
| 2   | F     | 2550  | 0        | 2490     | 131     | 0            |
| 2   | J     | 2550  | 0        | 2490     | 93      | 0            |
| 2   | N     | 2550  | 0        | 2487     | 148     | 0            |
| 3   | C     | 1671  | 0        | 1640     | 260     | 0            |
| 3   | G     | 1671  | 0        | 1638     | 231     | 0            |
| 3   | K     | 1671  | 0        | 1638     | 250     | 0            |
| 3   | O     | 1671  | 0        | 1634     | 267     | 0            |
| 4   | D     | 1598  | 0        | 1525     | 258     | 0            |
| 4   | H     | 1598  | 0        | 1524     | 245     | 0            |
| 4   | L     | 1598  | 0        | 1522     | 195     | 0            |
| 4   | P     | 1598  | 0        | 1524     | 215     | 0            |
| All | All   | 35528 | 0        | 34389    | 2055    | 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 29.

All (2055) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:5032:TYR:HE1 | 3:O:5100:TYR:CD1 | 1.00                     | 1.69              |
| 3:O:5118:ALA:HB3 | 3:O:5150:PHE:CE2 | 1.17                     | 1.69              |
| 2:B:543:LYS:HE2  | 4:D:534:CYS:SG   | 1.34                     | 1.67              |
| 3:G:3118:ALA:HB3 | 3:G:3150:PHE:CE2 | 1.17                     | 1.65              |
| 3:G:3032:TYR:HE1 | 3:G:3100:TYR:CD1 | 1.00                     | 1.64              |
| 3:C:32:TYR:HE1   | 3:C:100:TYR:CD1  | 1.00                     | 1.62              |
| 3:C:118:ALA:HB3  | 3:C:150:PHE:CE2  | 1.17                     | 1.62              |
| 3:O:5032:TYR:CE1 | 3:O:5100:TYR:CD1 | 1.86                     | 1.62              |
| 3:K:4032:TYR:CE1 | 3:K:4100:TYR:CD1 | 1.86                     | 1.62              |
| 3:K:4032:TYR:HE1 | 3:K:4100:TYR:CD1 | 1.00                     | 1.61              |
| 3:K:4118:ALA:HB3 | 3:K:4150:PHE:CE2 | 1.17                     | 1.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:563:ILE:HG23  | 4:D:532:SER:CB    | 1.21                     | 1.59              |
| 3:C:32:TYR:CE1    | 3:C:100:TYR:CD1   | 1.86                     | 1.58              |
| 3:G:3032:TYR:CE1  | 3:G:3100:TYR:CD1  | 1.86                     | 1.58              |
| 3:C:35:LEU:CD1    | 3:C:104:LEU:HD21  | 1.36                     | 1.55              |
| 3:K:4035:LEU:HD13 | 3:K:4104:LEU:CD2  | 1.36                     | 1.55              |
| 3:O:5035:LEU:CD1  | 3:O:5104:LEU:HD21 | 1.36                     | 1.55              |
| 3:C:45:PHE:CZ     | 4:D:546:PHE:CZ    | 1.96                     | 1.54              |
| 3:O:5045:PHE:CZ   | 4:P:5546:PHE:HZ   | 1.25                     | 1.53              |
| 3:K:4045:PHE:CZ   | 4:L:4546:PHE:HZ   | 1.25                     | 1.53              |
| 3:G:3045:PHE:CZ   | 4:H:3546:PHE:HZ   | 1.25                     | 1.53              |
| 3:C:35:LEU:HD13   | 3:C:104:LEU:CD2   | 1.36                     | 1.52              |
| 3:C:45:PHE:CZ     | 4:D:546:PHE:HZ    | 1.25                     | 1.52              |
| 3:G:3045:PHE:CZ   | 4:H:3546:PHE:CZ   | 1.96                     | 1.52              |
| 3:O:5045:PHE:CZ   | 4:P:5546:PHE:CZ   | 1.96                     | 1.52              |
| 3:K:4045:PHE:CZ   | 4:L:4546:PHE:CZ   | 1.96                     | 1.51              |
| 3:G:3035:LEU:HD13 | 3:G:3104:LEU:CD2  | 1.36                     | 1.51              |
| 3:G:3035:LEU:CD1  | 3:G:3104:LEU:HD21 | 1.36                     | 1.50              |
| 3:K:4035:LEU:CD1  | 3:K:4104:LEU:HD21 | 1.36                     | 1.49              |
| 2:B:563:ILE:HG22  | 4:D:532:SER:N     | 1.21                     | 1.49              |
| 3:O:5035:LEU:HD13 | 3:O:5104:LEU:CD2  | 1.36                     | 1.49              |
| 3:C:118:ALA:CB    | 3:C:150:PHE:CE2   | 1.92                     | 1.48              |
| 3:G:3118:ALA:CB   | 3:G:3150:PHE:CE2  | 1.92                     | 1.48              |
| 2:B:678:SER:HB2   | 4:D:597:LEU:CD2   | 1.43                     | 1.47              |
| 2:F:1546:GLY:N    | 3:G:3102:ILE:CD1  | 1.76                     | 1.47              |
| 3:K:4118:ALA:CB   | 3:K:4150:PHE:CE2  | 1.93                     | 1.47              |
| 3:O:5118:ALA:CB   | 3:O:5150:PHE:CE2  | 1.92                     | 1.46              |
| 2:N:3681:GLN:HB2  | 3:O:5065:LYS:CE   | 1.40                     | 1.45              |
| 3:C:58:PRO:CD     | 3:C:58:PRO:N      | 1.72                     | 1.45              |
| 3:O:5058:PRO:N    | 3:O:5058:PRO:CD   | 1.72                     | 1.44              |
| 2:N:3719:LYS:CD   | 3:O:5052:TYR:OH   | 1.66                     | 1.43              |
| 3:C:102:ILE:CB    | 4:D:552:ASP:HB2   | 1.49                     | 1.42              |
| 2:B:543:LYS:CE    | 4:D:534:CYS:SG    | 2.06                     | 1.42              |
| 2:J:2680:ALA:N    | 3:K:4062:GLU:HG3  | 1.17                     | 1.42              |
| 3:K:4102:ILE:CB   | 4:L:4552:ASP:HB2  | 1.49                     | 1.41              |
| 2:N:3680:ALA:C    | 3:O:5065:LYS:HD2  | 1.19                     | 1.41              |
| 2:F:1546:GLY:N    | 3:G:3102:ILE:HD11 | 1.08                     | 1.40              |
| 2:F:1544:THR:CG2  | 4:H:3534:CYS:SG   | 2.09                     | 1.40              |
| 3:G:3102:ILE:CB   | 4:H:3552:ASP:HB2  | 1.49                     | 1.40              |
| 2:B:562:SER:N     | 4:D:532:SER:HB2   | 1.36                     | 1.39              |
| 2:N:3680:ALA:C    | 3:O:5062:GLU:OE1  | 1.66                     | 1.38              |
| 3:K:4078:THR:HG21 | 3:K:4080:TYR:CZ   | 1.59                     | 1.37              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:O:5078:THR:HG21 | 3:O:5080:TYR:CZ  | 1.59                     | 1.37              |
| 3:G:3045:PHE:CE2  | 4:H:3546:PHE:CZ  | 2.14                     | 1.36              |
| 3:C:78:THR:HG21   | 3:C:80:TYR:CZ    | 1.59                     | 1.35              |
| 3:C:45:PHE:CE2    | 4:D:546:PHE:CZ   | 2.14                     | 1.35              |
| 3:O:5045:PHE:CE2  | 4:P:5546:PHE:CZ  | 2.14                     | 1.35              |
| 2:F:1562:SER:OG   | 4:H:3532:SER:CA  | 1.71                     | 1.35              |
| 2:B:563:ILE:CG2   | 4:D:532:SER:N    | 1.89                     | 1.35              |
| 3:K:4045:PHE:CE2  | 4:L:4546:PHE:CZ  | 2.14                     | 1.34              |
| 3:K:4058:PRO:CD   | 3:K:4058:PRO:N   | 1.72                     | 1.34              |
| 3:O:5032:TYR:OH   | 3:O:5100:TYR:CZ  | 1.69                     | 1.34              |
| 2:J:2720:TRP:CZ3  | 3:K:4057:GLU:OE2 | 1.80                     | 1.34              |
| 3:G:3078:THR:HG21 | 3:G:3080:TYR:CZ  | 1.59                     | 1.33              |
| 2:B:718:LYS:NZ    | 4:D:596:ASN:HB2  | 1.40                     | 1.33              |
| 2:B:547:VAL:HG22  | 3:C:102:ILE:CD1  | 1.54                     | 1.32              |
| 3:G:3032:TYR:OH   | 3:G:3100:TYR:CZ  | 1.68                     | 1.32              |
| 2:N:3680:ALA:C    | 3:O:5065:LYS:CD  | 1.98                     | 1.32              |
| 1:A:1:TYR:N       | 1:I:2385:LYS:CD  | 1.80                     | 1.31              |
| 2:N:3719:LYS:CG   | 3:O:5052:TYR:OH  | 1.78                     | 1.31              |
| 3:C:32:TYR:OH     | 3:C:100:TYR:CE1  | 1.84                     | 1.31              |
| 3:C:32:TYR:OH     | 3:C:100:TYR:CZ   | 1.69                     | 1.30              |
| 3:K:4032:TYR:OH   | 3:K:4100:TYR:CE1 | 1.84                     | 1.30              |
| 3:G:3032:TYR:OH   | 3:G:3100:TYR:CE1 | 1.84                     | 1.30              |
| 3:G:3002:ILE:CD1  | 3:G:3098:ARG:NH1 | 1.95                     | 1.29              |
| 3:C:2:ILE:CD1     | 3:C:98:ARG:NH1   | 1.95                     | 1.29              |
| 3:O:5002:ILE:CD1  | 3:O:5098:ARG:NH1 | 1.95                     | 1.29              |
| 3:O:5032:TYR:OH   | 3:O:5100:TYR:CE1 | 1.84                     | 1.29              |
| 2:N:3680:ALA:CA   | 3:O:5062:GLU:OE1 | 1.81                     | 1.29              |
| 2:B:678:SER:CB    | 4:D:597:LEU:HD22 | 1.63                     | 1.28              |
| 2:F:1560:GLN:N    | 4:H:3595:ASN:OD1 | 1.65                     | 1.28              |
| 3:K:4032:TYR:OH   | 3:K:4100:TYR:CZ  | 1.68                     | 1.27              |
| 2:B:718:LYS:HD2   | 3:C:59:THR:CG2   | 1.65                     | 1.27              |
| 3:G:3058:PRO:CD   | 3:G:3058:PRO:N   | 1.72                     | 1.27              |
| 3:K:4002:ILE:CD1  | 3:K:4098:ARG:NH1 | 1.95                     | 1.27              |
| 2:N:3719:LYS:HD2  | 3:O:5052:TYR:OH  | 1.13                     | 1.26              |
| 3:K:4032:TYR:CE1  | 3:K:4100:TYR:CG  | 2.24                     | 1.25              |
| 3:G:3102:ILE:HB   | 4:H:3552:ASP:CB  | 1.66                     | 1.25              |
| 3:O:5032:TYR:CE1  | 3:O:5100:TYR:CG  | 2.24                     | 1.25              |
| 3:O:5102:ILE:HB   | 4:P:5552:ASP:CB  | 1.66                     | 1.25              |
| 3:O:5102:ILE:CB   | 4:P:5552:ASP:HB2 | 1.49                     | 1.25              |
| 3:C:32:TYR:CE1    | 3:C:100:TYR:CG   | 2.24                     | 1.24              |
| 3:G:3032:TYR:CE1  | 3:G:3100:TYR:CG  | 2.24                     | 1.24              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:K:4102:ILE:HB   | 4:L:4552:ASP:CB  | 1.66                     | 1.23              |
| 3:C:102:ILE:HB    | 4:D:552:ASP:CB   | 1.66                     | 1.23              |
| 2:F:1546:GLY:H    | 3:G:3102:ILE:CD1 | 1.42                     | 1.23              |
| 2:B:563:ILE:CG2   | 4:D:532:SER:CB   | 2.17                     | 1.22              |
| 3:K:4021:SER:OG   | 3:K:4080:TYR:CE2 | 1.92                     | 1.22              |
| 2:N:3563:ILE:CG2  | 4:P:5532:SER:HA  | 1.68                     | 1.22              |
| 3:C:21:SER:OG     | 3:C:80:TYR:HE2   | 1.21                     | 1.22              |
| 1:A:1:TYR:H1      | 1:I:2385:LYS:CD  | 1.46                     | 1.21              |
| 2:B:545:ASP:OD1   | 3:C:102:ILE:HD13 | 1.34                     | 1.21              |
| 2:N:3680:ALA:O    | 3:O:5062:GLU:OE1 | 1.57                     | 1.21              |
| 3:G:3217:ARG:NH2  | 4:H:3622:PRO:HD2 | 1.55                     | 1.21              |
| 3:C:21:SER:OG     | 3:C:80:TYR:CE2   | 1.92                     | 1.21              |
| 3:O:5217:ARG:NH2  | 4:P:5622:PRO:HD2 | 1.55                     | 1.21              |
| 2:N:3563:ILE:HG21 | 4:P:5532:SER:N   | 1.53                     | 1.20              |
| 2:B:563:ILE:HG23  | 4:D:532:SER:OG   | 1.41                     | 1.20              |
| 3:G:3045:PHE:HZ   | 4:H:3546:PHE:CZ  | 1.43                     | 1.20              |
| 2:B:562:SER:O     | 4:D:532:SER:HA   | 1.03                     | 1.20              |
| 3:C:45:PHE:HZ     | 4:D:546:PHE:CZ   | 1.43                     | 1.20              |
| 2:N:3563:ILE:HG22 | 4:P:5531:SER:O   | 1.40                     | 1.20              |
| 3:G:3021:SER:OG   | 3:G:3080:TYR:CE2 | 1.92                     | 1.19              |
| 2:F:1676:VAL:H    | 4:H:3501:GLN:CD  | 1.49                     | 1.19              |
| 3:C:78:THR:CG2    | 3:C:80:TYR:CZ    | 2.26                     | 1.19              |
| 2:J:2680:ALA:N    | 3:K:4062:GLU:CG  | 2.04                     | 1.19              |
| 3:G:3078:THR:CG2  | 3:G:3080:TYR:CZ  | 2.26                     | 1.18              |
| 3:C:32:TYR:HE1    | 3:C:100:TYR:CG   | 1.61                     | 1.18              |
| 3:K:4078:THR:CG2  | 3:K:4080:TYR:CZ  | 2.26                     | 1.18              |
| 3:O:5078:THR:CG2  | 3:O:5080:TYR:CZ  | 2.26                     | 1.18              |
| 3:K:4045:PHE:HZ   | 4:L:4546:PHE:CZ  | 1.43                     | 1.18              |
| 3:C:217:ARG:NH2   | 4:D:622:PRO:HD2  | 1.55                     | 1.17              |
| 4:D:514:PRO:CG    | 4:D:609:LEU:O    | 1.93                     | 1.17              |
| 3:O:5032:TYR:HE1  | 3:O:5100:TYR:CG  | 1.61                     | 1.17              |
| 3:O:5102:ILE:HG22 | 4:P:5534:CYS:HB3 | 1.25                     | 1.17              |
| 4:H:3514:PRO:CG   | 4:H:3609:LEU:O   | 1.93                     | 1.17              |
| 3:K:4217:ARG:NH2  | 4:L:4622:PRO:HD2 | 1.55                     | 1.17              |
| 2:B:562:SER:O     | 4:D:532:SER:CA   | 1.94                     | 1.16              |
| 4:P:5514:PRO:CG   | 4:P:5609:LEU:O   | 1.93                     | 1.16              |
| 1:A:1:TYR:H1      | 1:I:2385:LYS:HD2 | 1.01                     | 1.16              |
| 4:H:3514:PRO:HG3  | 4:H:3609:LEU:O   | 1.45                     | 1.16              |
| 2:N:3681:GLN:CB   | 3:O:5065:LYS:CE  | 2.08                     | 1.16              |
| 2:N:3678:SER:OG   | 3:O:5061:ALA:HB2 | 1.41                     | 1.16              |
| 3:O:5021:SER:OG   | 3:O:5080:TYR:CE2 | 1.92                     | 1.15              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:563:ILE:CG2   | 4:D:532:SER:H     | 1.54                     | 1.15              |
| 2:N:3563:ILE:CG2  | 4:P:5532:SER:CA   | 2.25                     | 1.15              |
| 3:K:4102:ILE:HG22 | 4:L:4534:CYS:HB3  | 1.25                     | 1.15              |
| 1:A:1:TYR:N       | 1:I:2385:LYS:HD3  | 1.44                     | 1.15              |
| 4:D:514:PRO:HG3   | 4:D:609:LEU:O     | 1.45                     | 1.15              |
| 1:A:123:LYS:HE2   | 1:E:1150:ASN:HD22 | 1.06                     | 1.14              |
| 2:B:718:LYS:CE    | 4:D:596:ASN:HB2   | 1.76                     | 1.14              |
| 2:F:1680:ALA:O    | 3:G:3062:GLU:HG2  | 1.47                     | 1.14              |
| 2:B:560:GLN:HB2   | 4:D:595:ASN:HA    | 1.19                     | 1.14              |
| 2:B:563:ILE:HG23  | 4:D:532:SER:HB3   | 1.21                     | 1.14              |
| 2:J:2720:TRP:CH2  | 3:K:4057:GLU:OE2  | 1.98                     | 1.14              |
| 4:L:4514:PRO:CG   | 4:L:4609:LEU:O    | 1.93                     | 1.14              |
| 2:F:1545:ASP:HB2  | 3:G:3102:ILE:HA   | 1.17                     | 1.14              |
| 2:B:547:VAL:CG2   | 3:C:102:ILE:HD11  | 1.77                     | 1.14              |
| 3:G:3021:SER:OG   | 3:G:3080:TYR:HE2  | 1.21                     | 1.14              |
| 2:B:543:LYS:NZ    | 3:C:102:ILE:HG21  | 1.61                     | 1.13              |
| 3:G:3032:TYR:HE1  | 3:G:3100:TYR:CG   | 1.61                     | 1.13              |
| 1:A:150:ASN:HD22  | 1:E:1123:LYS:HE2  | 1.06                     | 1.13              |
| 2:F:1676:VAL:CG2  | 4:H:3501:GLN:HE21 | 1.62                     | 1.13              |
| 3:G:3002:ILE:HD11 | 3:G:3098:ARG:NH1  | 1.62                     | 1.13              |
| 3:O:5021:SER:OG   | 3:O:5080:TYR:HE2  | 1.21                     | 1.13              |
| 4:L:4514:PRO:HG3  | 4:L:4609:LEU:O    | 1.45                     | 1.12              |
| 2:B:718:LYS:CB    | 3:C:59:THR:HG23   | 1.78                     | 1.12              |
| 3:C:35:LEU:CD2    | 3:C:37:VAL:HG23   | 1.80                     | 1.12              |
| 2:J:2678:SER:OG   | 3:K:4062:GLU:N    | 1.83                     | 1.12              |
| 2:F:1678:SER:OG   | 4:H:3597:LEU:CD1  | 1.79                     | 1.11              |
| 3:G:3035:LEU:CD2  | 3:G:3037:VAL:HG23 | 1.80                     | 1.11              |
| 2:F:1544:THR:HG22 | 4:H:3534:CYS:SG   | 1.81                     | 1.11              |
| 3:K:4021:SER:OG   | 3:K:4080:TYR:HE2  | 1.21                     | 1.11              |
| 3:C:102:ILE:HG13  | 4:D:552:ASP:CG    | 1.75                     | 1.11              |
| 4:P:5514:PRO:HG3  | 4:P:5609:LEU:O    | 1.45                     | 1.11              |
| 2:F:1560:GLN:HG3  | 4:H:3595:ASN:OD1  | 1.49                     | 1.11              |
| 2:F:1678:SER:OG   | 4:H:3597:LEU:HD13 | 1.37                     | 1.10              |
| 3:G:3035:LEU:CD2  | 3:G:3037:VAL:CG2  | 2.29                     | 1.10              |
| 3:C:35:LEU:CD2    | 3:C:37:VAL:CG2    | 2.29                     | 1.10              |
| 3:G:3102:ILE:HG22 | 4:H:3534:CYS:HB3  | 1.25                     | 1.10              |
| 3:K:4035:LEU:CD2  | 3:K:4037:VAL:CG2  | 2.29                     | 1.10              |
| 2:N:3680:ALA:N    | 3:O:5062:GLU:OE1  | 1.83                     | 1.10              |
| 3:O:5035:LEU:CD2  | 3:O:5037:VAL:HG23 | 1.80                     | 1.10              |
| 3:K:4035:LEU:CD2  | 3:K:4037:VAL:HG23 | 1.80                     | 1.10              |
| 3:K:4102:ILE:HG13 | 4:L:4552:ASP:CG   | 1.76                     | 1.10              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:N:3563:ILE:CG2  | 4:P:5531:SER:C    | 2.23                     | 1.10              |
| 2:N:3563:ILE:HG23 | 4:P:5532:SER:HA   | 1.11                     | 1.10              |
| 3:O:5035:LEU:CD2  | 3:O:5037:VAL:CG2  | 2.29                     | 1.09              |
| 2:B:718:LYS:CD    | 3:C:59:THR:CG2    | 2.28                     | 1.09              |
| 3:C:102:ILE:HG22  | 4:D:534:CYS:HB3   | 1.25                     | 1.09              |
| 3:G:3102:ILE:HG13 | 4:H:3552:ASP:CG   | 1.76                     | 1.09              |
| 3:O:5045:PHE:HZ   | 4:P:5546:PHE:CZ   | 1.43                     | 1.08              |
| 3:G:3118:ALA:HB3  | 3:G:3150:PHE:CZ   | 1.88                     | 1.08              |
| 3:C:2:ILE:HD11    | 3:C:98:ARG:NH1    | 1.62                     | 1.08              |
| 2:N:3677:PRO:O    | 4:P:5597:LEU:HD22 | 1.52                     | 1.08              |
| 2:N:3678:SER:OG   | 3:O:5061:ALA:CB   | 1.91                     | 1.08              |
| 3:K:4032:TYR:HE1  | 3:K:4100:TYR:CG   | 1.61                     | 1.08              |
| 2:B:561:LYS:C     | 4:D:532:SER:HB2   | 1.79                     | 1.08              |
| 2:J:2562:SER:HG   | 4:L:4593:TRP:CD1  | 1.70                     | 1.08              |
| 3:K:4118:ALA:HB3  | 3:K:4150:PHE:CZ   | 1.88                     | 1.08              |
| 3:C:118:ALA:HB3   | 3:C:150:PHE:CZ    | 1.88                     | 1.07              |
| 2:B:718:LYS:CD    | 3:C:59:THR:HG21   | 1.82                     | 1.07              |
| 3:O:5118:ALA:HB3  | 3:O:5150:PHE:CZ   | 1.88                     | 1.07              |
| 2:B:545:ASP:OD1   | 3:C:102:ILE:CD1   | 2.02                     | 1.07              |
| 2:F:1545:ASP:CB   | 3:G:3102:ILE:HA   | 1.78                     | 1.06              |
| 3:K:4102:ILE:HG21 | 4:L:4552:ASP:OD1  | 1.55                     | 1.06              |
| 2:F:1718:LYS:CD   | 4:H:3596:ASN:O    | 2.03                     | 1.06              |
| 2:N:3681:GLN:HA   | 3:O:5065:LYS:HD3  | 1.37                     | 1.06              |
| 2:F:1560:GLN:H    | 4:H:3595:ASN:CG   | 1.60                     | 1.06              |
| 2:F:1676:VAL:CG2  | 4:H:3501:GLN:NE2  | 2.17                     | 1.06              |
| 2:J:2680:ALA:H    | 3:K:4062:GLU:CG   | 1.64                     | 1.06              |
| 2:B:563:ILE:HG23  | 4:D:532:SER:CA    | 1.83                     | 1.06              |
| 3:G:3102:ILE:HG21 | 4:H:3552:ASP:OD1  | 1.55                     | 1.06              |
| 3:K:4002:ILE:HD11 | 3:K:4098:ARG:HH12 | 1.12                     | 1.06              |
| 3:O:5039:GLN:NE2  | 3:O:5045:PHE:CE1  | 2.24                     | 1.06              |
| 3:C:39:GLN:NE2    | 3:C:45:PHE:CE1    | 2.24                     | 1.05              |
| 2:B:562:SER:N     | 4:D:532:SER:CB    | 2.19                     | 1.05              |
| 2:F:1677:PRO:CA   | 4:H:3501:GLN:HB2  | 1.85                     | 1.05              |
| 2:F:1677:PRO:HA   | 4:H:3501:GLN:HB2  | 1.11                     | 1.05              |
| 2:F:1676:VAL:HG22 | 4:H:3501:GLN:NE2  | 1.70                     | 1.05              |
| 3:C:2:ILE:HD11    | 3:C:98:ARG:HH12   | 1.12                     | 1.05              |
| 4:L:4514:PRO:HD3  | 4:L:4609:LEU:CB   | 1.87                     | 1.05              |
| 3:O:5102:ILE:HG21 | 4:P:5552:ASP:OD1  | 1.55                     | 1.05              |
| 4:H:3514:PRO:HD3  | 4:H:3609:LEU:CB   | 1.87                     | 1.04              |
| 3:K:4039:GLN:NE2  | 3:K:4045:PHE:CE1  | 2.24                     | 1.04              |
| 3:G:3039:GLN:NE2  | 3:G:3045:PHE:CE1  | 2.24                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:4002:ILE:HD11 | 3:K:4098:ARG:NH1  | 1.62                     | 1.04              |
| 3:K:4045:PHE:CE2  | 4:L:4546:PHE:CE1  | 2.46                     | 1.04              |
| 2:N:3559:THR:HG22 | 4:P:5594:TYR:O    | 1.24                     | 1.04              |
| 3:G:3045:PHE:CE2  | 4:H:3546:PHE:CE1  | 2.46                     | 1.04              |
| 2:F:1544:THR:HG23 | 4:H:3534:CYS:SG   | 1.95                     | 1.04              |
| 2:F:1562:SER:OG   | 4:H:3532:SER:HA   | 0.87                     | 1.04              |
| 2:N:3718:LYS:O    | 3:O:5052:TYR:HE2  | 1.40                     | 1.04              |
| 1:A:22:PRO:HB3    | 1:I:2382:LYS:CB   | 1.88                     | 1.04              |
| 4:P:5514:PRO:HD3  | 4:P:5609:LEU:CB   | 1.87                     | 1.04              |
| 2:F:1718:LYS:HD2  | 4:H:3596:ASN:O    | 1.55                     | 1.03              |
| 2:N:3563:ILE:HG21 | 4:P:5531:SER:C    | 1.83                     | 1.03              |
| 2:B:560:GLN:CB    | 4:D:595:ASN:HA    | 1.88                     | 1.03              |
| 3:C:102:ILE:HG21  | 4:D:552:ASP:OD1   | 1.55                     | 1.03              |
| 3:O:5045:PHE:CE2  | 4:P:5546:PHE:CE1  | 2.46                     | 1.03              |
| 3:C:45:PHE:CE2    | 4:D:546:PHE:CE1   | 2.46                     | 1.03              |
| 4:D:514:PRO:HD3   | 4:D:609:LEU:CB    | 1.87                     | 1.03              |
| 3:O:5002:ILE:HD11 | 3:O:5098:ARG:HH12 | 1.12                     | 1.03              |
| 2:N:3559:THR:CG2  | 4:P:5594:TYR:O    | 0.75                     | 1.03              |
| 3:C:102:ILE:CB    | 4:D:552:ASP:CB    | 2.30                     | 1.02              |
| 2:B:718:LYS:HE3   | 4:D:596:ASN:O     | 1.60                     | 1.02              |
| 2:F:1676:VAL:HG23 | 4:H:3501:GLN:HE21 | 1.18                     | 1.02              |
| 3:K:4102:ILE:CB   | 4:L:4552:ASP:CB   | 2.30                     | 1.02              |
| 2:N:3680:ALA:CA   | 3:O:5065:LYS:HD2  | 1.88                     | 1.02              |
| 2:J:2679:GLY:C    | 3:K:4062:GLU:HG3  | 1.84                     | 1.01              |
| 3:K:4045:PHE:CZ   | 4:L:4546:PHE:CE1  | 2.48                     | 1.01              |
| 2:B:562:SER:C     | 4:D:532:SER:HA    | 1.85                     | 1.01              |
| 3:G:3002:ILE:HD11 | 3:G:3098:ARG:HH12 | 1.12                     | 1.01              |
| 2:B:562:SER:C     | 4:D:532:SER:CB    | 2.33                     | 1.01              |
| 2:B:562:SER:C     | 4:D:532:SER:HB3   | 1.83                     | 1.01              |
| 3:G:3045:PHE:CZ   | 4:H:3546:PHE:CE1  | 2.48                     | 1.01              |
| 2:B:563:ILE:CG2   | 4:D:532:SER:OG    | 2.06                     | 1.01              |
| 3:C:45:PHE:CZ     | 4:D:546:PHE:CE1   | 2.48                     | 1.01              |
| 2:N:3563:ILE:HG21 | 4:P:5532:SER:CA   | 1.88                     | 1.01              |
| 2:N:3718:LYS:O    | 3:O:5052:TYR:CE2  | 2.14                     | 1.00              |
| 3:C:35:LEU:HD21   | 3:C:37:VAL:HG22   | 1.43                     | 1.00              |
| 1:A:152:GLU:OE2   | 1:E:1177:LYS:NZ   | 1.95                     | 1.00              |
| 2:N:3559:THR:HG23 | 4:P:5594:TYR:O    | 1.60                     | 1.00              |
| 3:O:5045:PHE:CZ   | 4:P:5546:PHE:CE1  | 2.48                     | 1.00              |
| 3:G:3035:LEU:HD21 | 3:G:3037:VAL:HG22 | 1.43                     | 1.00              |
| 2:N:3680:ALA:HB3  | 3:O:5062:GLU:OE2  | 1.61                     | 1.00              |
| 3:C:32:TYR:CZ     | 3:C:100:TYR:CE1   | 2.50                     | 0.99              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:5032:TYR:CZ   | 3:O:5100:TYR:CE1  | 2.50                     | 0.99              |
| 3:C:45:PHE:HE2    | 4:D:546:PHE:CZ    | 1.80                     | 0.99              |
| 3:O:5002:ILE:HD11 | 3:O:5098:ARG:NH1  | 1.62                     | 0.99              |
| 3:O:5035:LEU:HD21 | 3:O:5037:VAL:HG22 | 1.43                     | 0.99              |
| 2:N:3675:THR:HG21 | 4:P:5501:GLN:CD   | 1.87                     | 0.99              |
| 3:O:5011:VAL:HG11 | 3:O:5151:PRO:CB   | 1.93                     | 0.99              |
| 2:F:1676:VAL:N    | 4:H:3501:GLN:CD   | 2.15                     | 0.99              |
| 3:K:4035:LEU:HD21 | 3:K:4037:VAL:HG22 | 1.43                     | 0.99              |
| 1:A:150:ASN:ND2   | 1:E:1123:LYS:HE2  | 1.77                     | 0.99              |
| 3:C:97:VAL:HG11   | 3:C:104:LEU:HD23  | 1.46                     | 0.98              |
| 2:J:2562:SER:HG   | 4:L:4593:TRP:HD1  | 1.02                     | 0.98              |
| 1:A:123:LYS:HE2   | 1:E:1150:ASN:ND2  | 1.77                     | 0.98              |
| 1:A:177:LYS:NZ    | 1:E:1152:GLU:OE2  | 1.95                     | 0.98              |
| 4:H:3563:ARG:NH2  | 4:H:3584:ASP:OD1  | 1.96                     | 0.98              |
| 3:G:3097:VAL:HG11 | 3:G:3104:LEU:HD23 | 1.45                     | 0.98              |
| 2:N:3719:LYS:CG   | 3:O:5052:TYR:CZ   | 2.47                     | 0.98              |
| 3:C:11:VAL:HG11   | 3:C:151:PRO:CB    | 1.93                     | 0.98              |
| 2:N:3681:GLN:CA   | 3:O:5065:LYS:HD3  | 1.87                     | 0.98              |
| 3:O:5097:VAL:HG11 | 3:O:5104:LEU:HD23 | 1.45                     | 0.98              |
| 3:K:4011:VAL:HG11 | 3:K:4151:PRO:CB   | 1.93                     | 0.98              |
| 3:K:4032:TYR:CZ   | 3:K:4100:TYR:CE1  | 2.50                     | 0.98              |
| 3:G:3011:VAL:HG11 | 3:G:3151:PRO:CB   | 1.93                     | 0.98              |
| 3:G:3032:TYR:CZ   | 3:G:3100:TYR:CE1  | 2.50                     | 0.98              |
| 3:K:4102:ILE:CG2  | 4:L:4534:CYS:HB3  | 1.94                     | 0.98              |
| 2:F:1562:SER:O    | 4:H:3531:SER:OG   | 1.82                     | 0.97              |
| 3:G:3032:TYR:CE1  | 3:G:3100:TYR:CE1  | 2.52                     | 0.97              |
| 4:L:4563:ARG:NH2  | 4:L:4584:ASP:OD1  | 1.96                     | 0.97              |
| 4:D:563:ARG:NH2   | 4:D:584:ASP:OD1   | 1.96                     | 0.97              |
| 2:F:1545:ASP:C    | 3:G:3102:ILE:CD1  | 2.29                     | 0.97              |
| 3:G:3045:PHE:HE2  | 4:H:3546:PHE:CZ   | 1.80                     | 0.97              |
| 4:D:513:SER:OG    | 4:D:609:LEU:HD22  | 1.65                     | 0.97              |
| 2:B:563:ILE:HG22  | 4:D:531:SER:C     | 1.88                     | 0.97              |
| 2:F:1561:LYS:HA   | 4:H:3532:SER:OG   | 1.62                     | 0.97              |
| 4:P:5513:SER:OG   | 4:P:5609:LEU:HD22 | 1.65                     | 0.97              |
| 3:G:3217:ARG:HH21 | 4:H:3622:PRO:HD2  | 1.18                     | 0.97              |
| 4:L:4513:SER:OG   | 4:L:4609:LEU:HD22 | 1.65                     | 0.97              |
| 2:N:3560:GLN:N    | 4:P:5595:ASN:O    | 1.97                     | 0.97              |
| 4:P:5563:ARG:NH2  | 4:P:5584:ASP:OD1  | 1.96                     | 0.97              |
| 3:G:3102:ILE:CG2  | 4:H:3534:CYS:HB3  | 1.94                     | 0.97              |
| 4:H:3513:SER:OG   | 4:H:3609:LEU:HD22 | 1.65                     | 0.97              |
| 3:O:5045:PHE:HE2  | 4:P:5546:PHE:CZ   | 1.80                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:32:TYR:CE1    | 3:C:100:TYR:CE1   | 2.52                     | 0.96              |
| 2:J:2562:SER:OG   | 4:L:4593:TRP:HD1  | 1.48                     | 0.96              |
| 3:C:102:ILE:CG2   | 4:D:534:CYS:HB3   | 1.94                     | 0.96              |
| 2:B:718:LYS:NZ    | 4:D:596:ASN:CB    | 2.28                     | 0.96              |
| 3:O:5032:TYR:CE1  | 3:O:5100:TYR:CE1  | 2.52                     | 0.96              |
| 3:K:4032:TYR:CE1  | 3:K:4100:TYR:CE1  | 2.52                     | 0.96              |
| 3:K:4097:VAL:HG11 | 3:K:4104:LEU:HD23 | 1.46                     | 0.96              |
| 3:O:5011:VAL:HG21 | 3:O:5152:GLU:H    | 1.29                     | 0.96              |
| 3:O:5102:ILE:CG2  | 4:P:5534:CYS:HB3  | 1.94                     | 0.96              |
| 3:C:11:VAL:HG21   | 3:C:152:GLU:H     | 1.29                     | 0.96              |
| 2:F:1544:THR:HG1  | 4:H:3593:TRP:CD1  | 1.82                     | 0.95              |
| 3:G:3102:ILE:CB   | 4:H:3552:ASP:CB   | 2.30                     | 0.95              |
| 1:A:22:PRO:HB3    | 1:I:2382:LYS:HB3  | 1.46                     | 0.95              |
| 4:P:5631:ASN:HA   | 4:P:5685:ALA:HB2  | 1.47                     | 0.95              |
| 3:G:3102:ILE:HG23 | 4:H:3534:CYS:SG   | 2.07                     | 0.95              |
| 4:L:4631:ASN:HA   | 4:L:4685:ALA:HB2  | 1.47                     | 0.95              |
| 3:O:5035:LEU:HD22 | 3:O:5037:VAL:HG23 | 1.48                     | 0.95              |
| 2:B:563:ILE:N     | 4:D:532:SER:HB3   | 1.82                     | 0.95              |
| 2:N:3675:THR:HG21 | 4:P:5501:GLN:NE2  | 1.80                     | 0.95              |
| 3:K:4011:VAL:HG21 | 3:K:4152:GLU:H    | 1.29                     | 0.95              |
| 3:K:4035:LEU:HD22 | 3:K:4037:VAL:HG23 | 1.48                     | 0.95              |
| 3:O:5102:ILE:HG23 | 4:P:5534:CYS:SG   | 2.07                     | 0.94              |
| 2:J:2720:TRP:HZ3  | 3:K:4057:GLU:OE2  | 1.50                     | 0.94              |
| 4:D:631:ASN:HA    | 4:D:685:ALA:HB2   | 1.47                     | 0.94              |
| 2:N:3563:ILE:HG22 | 4:P:5531:SER:C    | 1.89                     | 0.94              |
| 2:N:3559:THR:HG22 | 4:P:5596:ASN:H    | 1.30                     | 0.94              |
| 3:O:5032:TYR:HE1  | 3:O:5100:TYR:HD1  | 1.13                     | 0.94              |
| 4:L:4694:TYR:HB2  | 4:L:4709:LEU:HD22 | 1.50                     | 0.94              |
| 3:G:3011:VAL:HG21 | 3:G:3152:GLU:H    | 1.29                     | 0.94              |
| 3:G:3032:TYR:CZ   | 3:G:3100:TYR:CD1  | 2.56                     | 0.94              |
| 2:F:1545:ASP:C    | 3:G:3102:ILE:HD13 | 1.89                     | 0.93              |
| 3:K:4032:TYR:CZ   | 3:K:4100:TYR:CD1  | 2.56                     | 0.93              |
| 3:K:4217:ARG:HH21 | 4:L:4622:PRO:HD2  | 1.18                     | 0.93              |
| 3:C:102:ILE:HG23  | 4:D:534:CYS:SG    | 2.07                     | 0.93              |
| 4:D:694:TYR:HB2   | 4:D:709:LEU:HD22  | 1.50                     | 0.93              |
| 3:O:5097:VAL:CG1  | 3:O:5104:LEU:HD23 | 1.98                     | 0.93              |
| 3:C:35:LEU:HD22   | 3:C:37:VAL:HG23   | 1.48                     | 0.93              |
| 3:K:4102:ILE:HG23 | 4:L:4534:CYS:SG   | 2.07                     | 0.93              |
| 3:O:5217:ARG:HH21 | 4:P:5622:PRO:HD2  | 1.19                     | 0.93              |
| 3:C:32:TYR:CZ     | 3:C:100:TYR:CD1   | 2.56                     | 0.93              |
| 2:B:543:LYS:NZ    | 4:D:534:CYS:SG    | 2.41                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:563:ILE:CG2   | 4:D:532:SER:CA    | 2.44                     | 0.93              |
| 3:K:4118:ALA:HB1  | 3:K:4150:PHE:CE2  | 2.03                     | 0.93              |
| 3:G:3097:VAL:CG1  | 3:G:3104:LEU:HD23 | 1.98                     | 0.92              |
| 3:G:3035:LEU:HD21 | 3:G:3037:VAL:CG2  | 1.98                     | 0.92              |
| 3:K:4097:VAL:CG1  | 3:K:4104:LEU:HD23 | 1.98                     | 0.92              |
| 3:O:5032:TYR:CZ   | 3:O:5100:TYR:CD1  | 2.56                     | 0.92              |
| 4:H:3631:ASN:HA   | 4:H:3685:ALA:HB2  | 1.47                     | 0.92              |
| 2:J:2678:SER:H    | 3:K:4062:GLU:HG2  | 1.31                     | 0.92              |
| 2:N:3563:ILE:CG2  | 4:P:5531:SER:O    | 2.16                     | 0.92              |
| 3:C:217:ARG:HH21  | 4:D:622:PRO:HD2   | 1.18                     | 0.92              |
| 2:B:543:LYS:HD3   | 3:C:102:ILE:HD12  | 1.52                     | 0.92              |
| 2:N:3681:GLN:CB   | 3:O:5065:LYS:HE2  | 1.82                     | 0.92              |
| 3:O:5078:THR:HG21 | 3:O:5080:TYR:OH   | 1.69                     | 0.92              |
| 3:C:78:THR:HG21   | 3:C:80:TYR:OH     | 1.69                     | 0.92              |
| 3:C:118:ALA:HB1   | 3:C:150:PHE:CE2   | 2.03                     | 0.92              |
| 3:G:3118:ALA:HB1  | 3:G:3150:PHE:CE2  | 2.03                     | 0.92              |
| 1:A:150:ASN:HD22  | 1:E:1123:LYS:CE   | 1.83                     | 0.92              |
| 3:K:4035:LEU:HD21 | 3:K:4037:VAL:CG2  | 1.98                     | 0.92              |
| 3:C:97:VAL:CG1    | 3:C:104:LEU:HD23  | 1.98                     | 0.91              |
| 2:B:718:LYS:HZ1   | 4:D:596:ASN:CB    | 1.83                     | 0.91              |
| 3:G:3035:LEU:HD22 | 3:G:3037:VAL:HG23 | 1.48                     | 0.91              |
| 3:G:3118:ALA:CB   | 3:G:3150:PHE:CZ   | 2.51                     | 0.91              |
| 4:P:5694:TYR:HB2  | 4:P:5709:LEU:HD22 | 1.50                     | 0.91              |
| 3:K:4032:TYR:HE1  | 3:K:4100:TYR:HD1  | 1.13                     | 0.91              |
| 2:B:547:VAL:CG2   | 3:C:102:ILE:CG1   | 2.49                     | 0.91              |
| 4:H:3694:TYR:HB2  | 4:H:3709:LEU:HD22 | 1.50                     | 0.91              |
| 3:C:11:VAL:HG11   | 3:C:151:PRO:HB3   | 1.53                     | 0.90              |
| 2:N:3719:LYS:HG2  | 3:O:5052:TYR:CZ   | 2.04                     | 0.90              |
| 3:G:3011:VAL:HG21 | 3:G:3152:GLU:N    | 1.87                     | 0.90              |
| 3:O:5011:VAL:HG11 | 3:O:5151:PRO:HB3  | 1.53                     | 0.90              |
| 3:K:4118:ALA:CB   | 3:K:4150:PHE:CZ   | 2.51                     | 0.90              |
| 2:B:718:LYS:HZ1   | 4:D:596:ASN:HB2   | 1.10                     | 0.90              |
| 3:C:11:VAL:HG21   | 3:C:152:GLU:N     | 1.87                     | 0.90              |
| 2:F:1562:SER:HG   | 4:H:3532:SER:HA   | 1.10                     | 0.90              |
| 2:J:2680:ALA:H    | 3:K:4062:GLU:HG3  | 1.09                     | 0.90              |
| 3:K:4045:PHE:HE2  | 4:L:4546:PHE:CZ   | 1.80                     | 0.90              |
| 4:L:4552:ASP:HB3  | 4:L:4555:ASN:ND2  | 1.87                     | 0.90              |
| 1:A:123:LYS:CE    | 1:E:1150:ASN:HD22 | 1.83                     | 0.90              |
| 2:B:562:SER:C     | 4:D:532:SER:CA    | 2.44                     | 0.90              |
| 3:G:3078:THR:HG21 | 3:G:3080:TYR:OH   | 1.69                     | 0.90              |
| 3:K:4011:VAL:HG21 | 3:K:4152:GLU:N    | 1.87                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:35:LEU:HD21   | 3:C:37:VAL:CG2    | 1.98                     | 0.89              |
| 3:G:3011:VAL:HG11 | 3:G:3151:PRO:HB3  | 1.53                     | 0.89              |
| 3:K:4078:THR:HG21 | 3:K:4080:TYR:OH   | 1.69                     | 0.89              |
| 2:N:3560:GLN:H    | 4:P:5595:ASN:C    | 1.66                     | 0.89              |
| 3:O:5118:ALA:HB1  | 3:O:5150:PHE:CE2  | 2.02                     | 0.89              |
| 4:P:5552:ASP:HB3  | 4:P:5555:ASN:ND2  | 1.87                     | 0.89              |
| 2:F:1546:GLY:N    | 3:G:3102:ILE:HD13 | 1.88                     | 0.89              |
| 2:B:718:LYS:HD2   | 3:C:59:THR:HG21   | 0.92                     | 0.89              |
| 2:B:718:LYS:HB2   | 3:C:59:THR:HG23   | 1.52                     | 0.89              |
| 3:C:173:LEU:HD12  | 4:D:665:THR:HG22  | 1.54                     | 0.89              |
| 4:D:552:ASP:HB3   | 4:D:555:ASN:ND2   | 1.87                     | 0.89              |
| 3:O:5011:VAL:HG21 | 3:O:5152:GLU:N    | 1.87                     | 0.89              |
| 3:O:5035:LEU:HD21 | 3:O:5037:VAL:CG2  | 1.98                     | 0.89              |
| 4:P:5554:ASN:C    | 4:P:5554:ASN:HD22 | 1.81                     | 0.89              |
| 2:B:547:VAL:HG22  | 3:C:102:ILE:CG1   | 2.02                     | 0.88              |
| 3:G:3032:TYR:HE1  | 3:G:3100:TYR:HD1  | 1.13                     | 0.88              |
| 4:D:694:TYR:HB2   | 4:D:709:LEU:CD2   | 2.03                     | 0.88              |
| 3:C:118:ALA:CB    | 3:C:150:PHE:CZ    | 2.51                     | 0.88              |
| 4:H:3552:ASP:HB3  | 4:H:3555:ASN:ND2  | 1.87                     | 0.88              |
| 4:P:5694:TYR:HB2  | 4:P:5709:LEU:CD2  | 2.03                     | 0.88              |
| 4:H:3694:TYR:HB2  | 4:H:3709:LEU:CD2  | 2.03                     | 0.88              |
| 2:F:1560:GLN:CG   | 4:H:3595:ASN:OD1  | 2.21                     | 0.88              |
| 3:G:3173:LEU:HD12 | 4:H:3665:THR:HG22 | 1.54                     | 0.88              |
| 4:H:3554:ASN:C    | 4:H:3554:ASN:HD22 | 1.81                     | 0.88              |
| 2:B:680:ALA:O     | 3:C:62:GLU:HG3    | 1.74                     | 0.88              |
| 3:K:4173:LEU:HD12 | 4:L:4665:THR:HG22 | 1.54                     | 0.88              |
| 3:K:4011:VAL:HG11 | 3:K:4151:PRO:HB3  | 1.53                     | 0.87              |
| 4:L:4694:TYR:HB2  | 4:L:4709:LEU:CD2  | 2.03                     | 0.87              |
| 3:C:32:TYR:HE1    | 3:C:100:TYR:HD1   | 1.13                     | 0.87              |
| 2:F:1546:GLY:CA   | 3:G:3102:ILE:HD11 | 2.04                     | 0.87              |
| 2:B:718:LYS:HB3   | 3:C:59:THR:HG23   | 1.56                     | 0.87              |
| 4:D:554:ASN:HD22  | 4:D:554:ASN:C     | 1.81                     | 0.87              |
| 3:G:3011:VAL:CB   | 3:G:3151:PRO:HB2  | 2.05                     | 0.87              |
| 2:N:3563:ILE:HG23 | 4:P:5532:SER:CA   | 1.93                     | 0.87              |
| 3:O:5118:ALA:CB   | 3:O:5150:PHE:CZ   | 2.51                     | 0.87              |
| 3:K:4011:VAL:CB   | 3:K:4151:PRO:HB2  | 2.05                     | 0.87              |
| 2:N:3719:LYS:HG3  | 3:O:5052:TYR:OH   | 1.71                     | 0.87              |
| 3:C:11:VAL:CB     | 3:C:151:PRO:HB2   | 2.05                     | 0.86              |
| 3:O:5173:LEU:HD12 | 4:P:5665:THR:HG22 | 1.54                     | 0.86              |
| 4:L:4554:ASN:HD22 | 4:L:4554:ASN:C    | 1.81                     | 0.86              |
| 3:G:3039:GLN:NE2  | 3:G:3045:PHE:CZ   | 2.44                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:5011:VAL:CB   | 3:O:5151:PRO:HB2  | 2.05                     | 0.86              |
| 3:O:5039:GLN:NE2  | 3:O:5045:PHE:CZ   | 2.44                     | 0.85              |
| 2:N:3681:GLN:HB2  | 3:O:5065:LYS:HE2  | 0.87                     | 0.85              |
| 3:C:70:PHE:HE1    | 3:C:81:LEU:HD13   | 1.40                     | 0.85              |
| 4:D:513:SER:HA    | 4:D:609:LEU:HB2   | 1.59                     | 0.85              |
| 3:K:4039:GLN:NE2  | 3:K:4045:PHE:CZ   | 2.44                     | 0.85              |
| 3:C:39:GLN:NE2    | 3:C:45:PHE:CZ     | 2.44                     | 0.85              |
| 3:G:3070:PHE:HE1  | 3:G:3081:LEU:HD13 | 1.40                     | 0.85              |
| 2:J:2562:SER:OG   | 4:L:4593:TRP:CD1  | 2.25                     | 0.85              |
| 2:N:3545:ASP:OD2  | 3:O:5102:ILE:N    | 2.09                     | 0.85              |
| 2:F:1718:LYS:CD   | 4:H:3596:ASN:C    | 2.29                     | 0.85              |
| 2:N:3559:THR:HG22 | 4:P:5596:ASN:N    | 1.90                     | 0.85              |
| 3:O:5070:PHE:HE1  | 3:O:5081:LEU:HD13 | 1.40                     | 0.85              |
| 2:B:562:SER:H     | 4:D:532:SER:HB2   | 1.42                     | 0.85              |
| 3:K:4070:PHE:HE1  | 3:K:4081:LEU:HD13 | 1.40                     | 0.84              |
| 2:B:561:LYS:C     | 4:D:532:SER:CB    | 2.50                     | 0.84              |
| 2:B:678:SER:CB    | 4:D:597:LEU:CD2   | 2.34                     | 0.84              |
| 3:C:35:LEU:HD22   | 3:C:37:VAL:CG2    | 2.05                     | 0.84              |
| 3:C:102:ILE:HG21  | 4:D:552:ASP:CG    | 2.03                     | 0.84              |
| 2:J:2680:ALA:HB2  | 3:K:4062:GLU:CD   | 2.02                     | 0.84              |
| 3:O:5175:GLN:HG3  | 4:P:5663:GLU:OE2  | 1.78                     | 0.84              |
| 1:A:1:TYR:H2      | 1:I:2385:LYS:CD   | 1.50                     | 0.84              |
| 3:C:175:GLN:HG3   | 4:D:663:GLU:OE2   | 1.78                     | 0.84              |
| 3:G:3078:THR:CG2  | 3:G:3080:TYR:CE1  | 2.61                     | 0.84              |
| 4:H:3513:SER:HA   | 4:H:3609:LEU:HB2  | 1.59                     | 0.84              |
| 2:N:3681:GLN:CA   | 3:O:5065:LYS:CD   | 2.37                     | 0.84              |
| 3:O:5091:THR:HG22 | 3:O:5115:VAL:H    | 1.43                     | 0.84              |
| 3:G:3091:THR:HG22 | 3:G:3115:VAL:H    | 1.43                     | 0.84              |
| 2:N:3560:GLN:HB2  | 4:P:5593:TRP:HE1  | 1.43                     | 0.84              |
| 3:K:4175:GLN:HG3  | 4:L:4663:GLU:OE2  | 1.78                     | 0.84              |
| 1:A:291:ILE:HG23  | 1:I:2316:ILE:HD13 | 1.58                     | 0.83              |
| 3:G:3037:VAL:HG21 | 3:G:3107:TRP:CH2  | 2.13                     | 0.83              |
| 2:N:3679:GLY:HA2  | 3:O:5062:GLU:O    | 1.40                     | 0.83              |
| 4:P:5582:THR:OG1  | 4:P:5610:GLY:HA3  | 1.78                     | 0.83              |
| 2:B:543:LYS:HD3   | 3:C:102:ILE:CD1   | 2.08                     | 0.83              |
| 3:C:11:VAL:HG11   | 3:C:151:PRO:HB2   | 1.60                     | 0.83              |
| 4:D:582:THR:OG1   | 4:D:610:GLY:HA3   | 1.78                     | 0.83              |
| 3:K:4037:VAL:HG21 | 3:K:4107:TRP:CH2  | 2.13                     | 0.83              |
| 3:C:91:THR:HG22   | 3:C:115:VAL:H     | 1.43                     | 0.83              |
| 3:G:3175:GLN:HG3  | 4:H:3663:GLU:OE2  | 1.78                     | 0.83              |
| 3:K:4011:VAL:HG11 | 3:K:4151:PRO:HB2  | 1.60                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:4078:THR:CG2  | 3:K:4080:TYR:CE1  | 2.61                     | 0.83              |
| 2:N:3560:GLN:O    | 4:P:5595:ASN:OD1  | 1.96                     | 0.83              |
| 3:C:78:THR:CG2    | 3:C:80:TYR:CE1    | 2.61                     | 0.83              |
| 3:G:3102:ILE:HG21 | 4:H:3552:ASP:CG   | 2.03                     | 0.83              |
| 4:L:4582:THR:OG1  | 4:L:4610:GLY:HA3  | 1.78                     | 0.83              |
| 2:N:3677:PRO:O    | 4:P:5597:LEU:CD2  | 2.25                     | 0.83              |
| 3:O:5078:THR:CG2  | 3:O:5080:TYR:CE1  | 2.61                     | 0.83              |
| 4:D:683:LEU:HD11  | 4:D:694:TYR:HE2   | 1.44                     | 0.83              |
| 4:H:3683:LEU:HD11 | 4:H:3694:TYR:HE2  | 1.44                     | 0.83              |
| 2:F:1543:LYS:CE   | 4:H:3531:SER:O    | 2.26                     | 0.83              |
| 4:L:4513:SER:HA   | 4:L:4609:LEU:HB2  | 1.59                     | 0.83              |
| 4:P:5513:SER:HA   | 4:P:5609:LEU:HB2  | 1.59                     | 0.83              |
| 3:G:3030:THR:HG23 | 3:G:3054:ASN:HD22 | 1.44                     | 0.82              |
| 3:O:5037:VAL:HG21 | 3:O:5107:TRP:CH2  | 2.13                     | 0.82              |
| 3:K:4102:ILE:HG21 | 4:L:4552:ASP:CG   | 2.03                     | 0.82              |
| 1:A:1:TYR:H2      | 1:I:2385:LYS:HD3  | 1.04                     | 0.82              |
| 4:L:4683:LEU:HD11 | 4:L:4694:TYR:HE2  | 1.44                     | 0.82              |
| 3:G:3098:ARG:NH2  | 3:G:3105:ASP:OD2  | 2.13                     | 0.82              |
| 3:K:4035:LEU:HD22 | 3:K:4037:VAL:CG2  | 2.05                     | 0.82              |
| 4:H:3582:THR:OG1  | 4:H:3610:GLY:HA3  | 1.78                     | 0.82              |
| 3:C:30:THR:HG23   | 3:C:54:ASN:HD22   | 1.44                     | 0.82              |
| 4:H:3653:VAL:HG23 | 4:H:3658:VAL:HG21 | 1.60                     | 0.82              |
| 3:K:4030:THR:HG23 | 3:K:4054:ASN:HD22 | 1.44                     | 0.82              |
| 3:C:37:VAL:HG21   | 3:C:107:TRP:CH2   | 2.13                     | 0.82              |
| 3:G:3011:VAL:HG11 | 3:G:3151:PRO:HB2  | 1.60                     | 0.82              |
| 3:O:5011:VAL:HG11 | 3:O:5151:PRO:HB2  | 1.60                     | 0.82              |
| 3:O:5102:ILE:HG22 | 3:O:5102:ILE:O    | 1.79                     | 0.82              |
| 4:P:5514:PRO:HD3  | 4:P:5609:LEU:HB2  | 1.62                     | 0.82              |
| 3:K:4102:ILE:HG13 | 4:L:4552:ASP:OD2  | 1.80                     | 0.82              |
| 3:O:5030:THR:HG23 | 3:O:5054:ASN:HD22 | 1.44                     | 0.82              |
| 3:C:102:ILE:HG22  | 3:C:102:ILE:O     | 1.79                     | 0.82              |
| 3:G:3102:ILE:HG22 | 3:G:3102:ILE:O    | 1.79                     | 0.82              |
| 3:K:4102:ILE:HG22 | 3:K:4102:ILE:O    | 1.78                     | 0.82              |
| 3:O:5078:THR:HG21 | 3:O:5080:TYR:CE2  | 2.14                     | 0.82              |
| 2:B:560:GLN:HB2   | 4:D:595:ASN:CA    | 2.07                     | 0.81              |
| 4:D:653:VAL:HG23  | 4:D:658:VAL:HG21  | 1.61                     | 0.81              |
| 3:G:3102:ILE:CG2  | 4:H:3534:CYS:SG   | 2.68                     | 0.81              |
| 4:P:5653:VAL:HG23 | 4:P:5658:VAL:HG21 | 1.60                     | 0.81              |
| 3:C:11:VAL:HG21   | 3:C:151:PRO:HB2   | 1.62                     | 0.81              |
| 3:K:4098:ARG:NH2  | 3:K:4105:ASP:OD2  | 2.13                     | 0.81              |
| 3:O:5102:ILE:CG2  | 4:P:5534:CYS:SG   | 2.68                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1563:ILE:HA   | 4:H:3531:SER:OG   | 1.81                     | 0.81              |
| 3:K:4102:ILE:CG2  | 4:L:4534:CYS:SG   | 2.68                     | 0.81              |
| 4:L:4653:VAL:HG23 | 4:L:4658:VAL:HG21 | 1.60                     | 0.81              |
| 3:O:5098:ARG:NH2  | 3:O:5105:ASP:OD2  | 2.13                     | 0.81              |
| 2:B:547:VAL:CG2   | 3:C:102:ILE:CD1   | 2.45                     | 0.81              |
| 3:K:4078:THR:HG21 | 3:K:4080:TYR:CE2  | 2.14                     | 0.81              |
| 3:C:102:ILE:CG2   | 4:D:534:CYS:SG    | 2.68                     | 0.81              |
| 3:O:5035:LEU:HD22 | 3:O:5037:VAL:CG2  | 2.05                     | 0.81              |
| 3:G:3102:ILE:HG13 | 4:H:3552:ASP:OD2  | 1.80                     | 0.81              |
| 3:G:3078:THR:HG21 | 3:G:3080:TYR:CE2  | 2.14                     | 0.81              |
| 3:C:98:ARG:NH2    | 3:C:105:ASP:OD2   | 2.13                     | 0.81              |
| 3:K:4091:THR:HG22 | 3:K:4115:VAL:H    | 1.43                     | 0.81              |
| 2:N:3680:ALA:HB3  | 3:O:5062:GLU:CD   | 2.06                     | 0.81              |
| 3:G:3011:VAL:HG21 | 3:G:3151:PRO:HB2  | 1.62                     | 0.80              |
| 3:K:4011:VAL:HG21 | 3:K:4151:PRO:HB2  | 1.62                     | 0.80              |
| 3:O:5011:VAL:HG21 | 3:O:5151:PRO:HB2  | 1.62                     | 0.80              |
| 3:O:5102:ILE:CG2  | 4:P:5552:ASP:HA   | 2.12                     | 0.80              |
| 3:C:78:THR:HG21   | 3:C:80:TYR:CE2    | 2.14                     | 0.80              |
| 2:B:547:VAL:HG21  | 3:C:102:ILE:HG13  | 1.61                     | 0.80              |
| 3:G:3102:ILE:CG2  | 4:H:3552:ASP:HA   | 2.12                     | 0.80              |
| 4:P:5683:LEU:HD11 | 4:P:5694:TYR:HE2  | 1.44                     | 0.80              |
| 2:B:679:GLY:O     | 3:C:62:GLU:OE1    | 1.90                     | 0.80              |
| 1:I:2389:VAL:O    | 2:J:2823:TRP:N    | 2.13                     | 0.80              |
| 3:C:102:ILE:CG1   | 4:D:552:ASP:HB2   | 2.12                     | 0.80              |
| 4:H:3514:PRO:HD3  | 4:H:3609:LEU:HB2  | 1.62                     | 0.80              |
| 3:G:3102:ILE:CG1  | 4:H:3552:ASP:HB2  | 2.12                     | 0.80              |
| 3:K:4102:ILE:CG2  | 4:L:4552:ASP:HA   | 2.12                     | 0.80              |
| 2:N:3563:ILE:CG2  | 4:P:5532:SER:N    | 2.28                     | 0.80              |
| 4:D:514:PRO:HD3   | 4:D:609:LEU:HB2   | 1.62                     | 0.80              |
| 3:G:3035:LEU:HD22 | 3:G:3037:VAL:CG2  | 2.05                     | 0.80              |
| 3:K:4102:ILE:CG2  | 4:L:4534:CYS:CB   | 2.60                     | 0.80              |
| 3:C:102:ILE:HG13  | 4:D:552:ASP:OD2   | 1.80                     | 0.79              |
| 3:C:102:ILE:CG2   | 4:D:552:ASP:HA    | 2.12                     | 0.79              |
| 3:O:5102:ILE:CG2  | 4:P:5534:CYS:CB   | 2.60                     | 0.79              |
| 3:C:102:ILE:CG2   | 4:D:534:CYS:CB    | 2.60                     | 0.79              |
| 3:O:5102:ILE:CB   | 4:P:5552:ASP:CB   | 2.30                     | 0.79              |
| 1:E:1389:VAL:O    | 2:F:1823:TRP:N    | 2.13                     | 0.79              |
| 3:O:5020:ILE:HD11 | 3:O:5113:LEU:HD11 | 1.65                     | 0.79              |
| 3:K:4102:ILE:CG1  | 4:L:4552:ASP:HB2  | 2.12                     | 0.79              |
| 3:K:4102:ILE:CG1  | 4:L:4552:ASP:CG   | 2.56                     | 0.79              |
| 2:N:3680:ALA:O    | 3:O:5065:LYS:HD2  | 1.79                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:389:VAL:O     | 2:B:823:TRP:N     | 2.13                     | 0.79              |
| 3:G:3002:ILE:HD12 | 3:G:3098:ARG:NH1  | 1.98                     | 0.79              |
| 4:L:4514:PRO:HD3  | 4:L:4609:LEU:HB2  | 1.62                     | 0.79              |
| 2:B:547:VAL:HG22  | 3:C:102:ILE:HD11  | 0.81                     | 0.79              |
| 1:M:3389:VAL:O    | 2:N:3823:TRP:N    | 2.13                     | 0.79              |
| 4:P:5542:PRO:O    | 4:P:5543:ASP:HB2  | 1.83                     | 0.79              |
| 3:O:5002:ILE:HD12 | 3:O:5098:ARG:NH1  | 1.98                     | 0.78              |
| 3:G:3020:ILE:HD11 | 3:G:3113:LEU:HD11 | 1.65                     | 0.78              |
| 3:G:3102:ILE:CG2  | 4:H:3534:CYS:CB   | 2.60                     | 0.78              |
| 4:H:3695:SER:HB2  | 4:H:3708:SER:OG   | 1.83                     | 0.78              |
| 3:K:4020:ILE:HD11 | 3:K:4113:LEU:HD11 | 1.65                     | 0.78              |
| 3:C:20:ILE:HD11   | 3:C:113:LEU:HD11  | 1.65                     | 0.78              |
| 2:F:1680:ALA:O    | 3:G:3062:GLU:CG   | 2.29                     | 0.78              |
| 3:G:3102:ILE:CG2  | 4:H:3552:ASP:CB   | 2.62                     | 0.78              |
| 4:L:4695:SER:HB2  | 4:L:4708:SER:OG   | 1.83                     | 0.78              |
| 3:O:5102:ILE:CG2  | 4:P:5552:ASP:CB   | 2.62                     | 0.78              |
| 4:P:5695:SER:HB2  | 4:P:5708:SER:OG   | 1.83                     | 0.78              |
| 3:G:3048:MET:HG2  | 3:G:3064:PHE:CZ   | 2.19                     | 0.78              |
| 4:H:3519:THR:C    | 4:H:3520:LEU:HD23 | 2.09                     | 0.78              |
| 2:B:718:LYS:CD    | 3:C:59:THR:HG23   | 2.11                     | 0.78              |
| 3:C:48:MET:HG2    | 3:C:64:PHE:CZ     | 2.19                     | 0.78              |
| 2:F:1544:THR:HG21 | 4:H:3534:CYS:SG   | 2.22                     | 0.78              |
| 3:G:3102:ILE:CG1  | 4:H:3552:ASP:CG   | 2.56                     | 0.78              |
| 4:H:3520:LEU:HD23 | 4:H:3520:LEU:N    | 1.99                     | 0.78              |
| 3:K:4048:MET:HG2  | 3:K:4064:PHE:CZ   | 2.19                     | 0.78              |
| 3:K:4102:ILE:CG2  | 4:L:4552:ASP:CB   | 2.62                     | 0.78              |
| 4:L:4519:THR:C    | 4:L:4520:LEU:HD23 | 2.09                     | 0.78              |
| 4:P:5519:THR:C    | 4:P:5520:LEU:HD23 | 2.09                     | 0.78              |
| 4:P:5520:LEU:N    | 4:P:5520:LEU:HD23 | 1.99                     | 0.78              |
| 2:B:543:LYS:NZ    | 3:C:102:ILE:CG2   | 2.43                     | 0.78              |
| 2:F:1677:PRO:HA   | 4:H:3501:GLN:CB   | 1.96                     | 0.78              |
| 4:D:542:PRO:O     | 4:D:543:ASP:HB2   | 1.83                     | 0.78              |
| 2:F:1676:VAL:H    | 4:H:3501:GLN:NE2  | 1.81                     | 0.78              |
| 4:H:3542:PRO:O    | 4:H:3543:ASP:HB2  | 1.83                     | 0.78              |
| 3:G:3011:VAL:CG1  | 3:G:3151:PRO:HB2  | 2.14                     | 0.78              |
| 3:O:5070:PHE:CE1  | 3:O:5081:LEU:HD13 | 2.19                     | 0.78              |
| 2:B:559:THR:OG1   | 4:D:595:ASN:ND2   | 2.01                     | 0.77              |
| 3:C:102:ILE:CG1   | 4:D:552:ASP:CG    | 2.56                     | 0.77              |
| 4:D:519:THR:C     | 4:D:520:LEU:HD23  | 2.09                     | 0.77              |
| 4:D:695:SER:HB2   | 4:D:708:SER:OG    | 1.83                     | 0.77              |
| 3:O:5011:VAL:CG1  | 3:O:5151:PRO:HB2  | 2.14                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:5048:MET:HG2  | 3:O:5064:PHE:CZ   | 2.19                     | 0.77              |
| 2:B:561:LYS:HG2   | 4:D:532:SER:OG    | 1.83                     | 0.77              |
| 2:F:1545:ASP:HB2  | 3:G:3102:ILE:CA   | 2.08                     | 0.77              |
| 3:K:4070:PHE:CE1  | 3:K:4081:LEU:HD13 | 2.19                     | 0.77              |
| 4:L:4520:LEU:HD23 | 4:L:4520:LEU:N    | 1.99                     | 0.77              |
| 4:L:4542:PRO:O    | 4:L:4543:ASP:HB2  | 1.83                     | 0.77              |
| 3:C:78:THR:HG22   | 3:C:80:TYR:CE1    | 2.20                     | 0.77              |
| 2:F:1562:SER:OG   | 4:H:3532:SER:CB   | 2.32                     | 0.77              |
| 3:K:4002:ILE:HD12 | 3:K:4098:ARG:NH1  | 1.98                     | 0.77              |
| 4:L:4685:ALA:O    | 4:L:4688:TRP:HB3  | 1.85                     | 0.77              |
| 3:C:70:PHE:CE1    | 3:C:81:LEU:HD13   | 2.19                     | 0.77              |
| 3:O:5078:THR:HG22 | 3:O:5080:TYR:CE1  | 2.20                     | 0.77              |
| 4:P:5685:ALA:O    | 4:P:5688:TRP:HB3  | 1.85                     | 0.77              |
| 2:F:1560:GLN:N    | 4:H:3595:ASN:CG   | 2.19                     | 0.77              |
| 3:G:3070:PHE:CE1  | 3:G:3081:LEU:HD13 | 2.19                     | 0.77              |
| 3:K:4011:VAL:CG1  | 3:K:4151:PRO:HB2  | 2.14                     | 0.77              |
| 3:O:5045:PHE:CE1  | 4:P:5589:PHE:CE2  | 2.73                     | 0.77              |
| 3:C:11:VAL:CG1    | 3:C:151:PRO:HB2   | 2.14                     | 0.77              |
| 2:J:2756:PRO:O    | 2:J:2814:TRP:NE1  | 2.18                     | 0.77              |
| 3:C:102:ILE:CG2   | 4:D:552:ASP:CB    | 2.62                     | 0.76              |
| 4:H:3514:PRO:HD3  | 4:H:3609:LEU:CA   | 2.15                     | 0.76              |
| 2:N:3684:TYR:OH   | 2:N:3701:THR:OG1  | 2.03                     | 0.76              |
| 4:D:520:LEU:HD23  | 4:D:520:LEU:N     | 1.99                     | 0.76              |
| 3:K:4021:SER:OG   | 3:K:4080:TYR:CD2  | 2.37                     | 0.76              |
| 4:H:3514:PRO:CD   | 4:H:3609:LEU:O    | 2.34                     | 0.76              |
| 3:K:4045:PHE:CE1  | 4:L:4589:PHE:CE2  | 2.73                     | 0.76              |
| 3:K:4078:THR:HG22 | 3:K:4080:TYR:CE1  | 2.20                     | 0.76              |
| 2:B:692:ARG:O     | 2:B:711:ARG:NH2   | 2.19                     | 0.76              |
| 3:C:45:PHE:CE1    | 4:D:589:PHE:CE2   | 2.73                     | 0.76              |
| 2:F:1692:ARG:O    | 2:F:1711:ARG:NH2  | 2.19                     | 0.76              |
| 4:H:3685:ALA:O    | 4:H:3688:TRP:HB3  | 1.85                     | 0.76              |
| 4:L:4514:PRO:HD3  | 4:L:4609:LEU:CA   | 2.15                     | 0.76              |
| 3:K:4011:VAL:CG2  | 3:K:4151:PRO:HB2  | 2.16                     | 0.76              |
| 2:B:545:ASP:CG    | 3:C:102:ILE:HD13  | 2.09                     | 0.76              |
| 3:O:5021:SER:CB   | 3:O:5080:TYR:CE2  | 2.69                     | 0.76              |
| 3:C:11:VAL:CG2    | 3:C:151:PRO:HB2   | 2.16                     | 0.76              |
| 3:G:3021:SER:CB   | 3:G:3080:TYR:CE2  | 2.69                     | 0.76              |
| 2:J:2595:THR:OG1  | 2:J:2611:VAL:O    | 2.04                     | 0.76              |
| 2:J:2678:SER:CB   | 3:K:4062:GLU:H    | 1.96                     | 0.76              |
| 1:A:291:ILE:HG23  | 1:I:2316:ILE:CD1  | 2.16                     | 0.76              |
| 3:G:3045:PHE:CE1  | 4:H:3589:PHE:CE2  | 2.73                     | 0.76              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:P:5514:PRO:HD3  | 4:P:5609:LEU:CA  | 2.15                     | 0.76              |
| 2:B:684:TYR:OH    | 2:B:701:THR:OG1  | 2.03                     | 0.76              |
| 2:B:756:PRO:O     | 2:B:814:TRP:NE1  | 2.18                     | 0.76              |
| 2:N:3692:ARG:O    | 2:N:3711:ARG:NH2 | 2.19                     | 0.76              |
| 3:O:5011:VAL:CG2  | 3:O:5151:PRO:HB2 | 2.16                     | 0.76              |
| 4:L:4514:PRO:CD   | 4:L:4609:LEU:O   | 2.34                     | 0.75              |
| 4:D:514:PRO:HD3   | 4:D:609:LEU:CA   | 2.15                     | 0.75              |
| 4:L:4631:ASN:CA   | 4:L:4685:ALA:HB2 | 2.17                     | 0.75              |
| 2:N:3753:THR:OG1  | 2:N:3816:ASN:ND2 | 2.20                     | 0.75              |
| 3:O:5217:ARG:NH2  | 4:P:5622:PRO:CD  | 2.45                     | 0.75              |
| 2:J:2753:THR:OG1  | 2:J:2816:ASN:ND2 | 2.20                     | 0.75              |
| 2:N:3756:PRO:O    | 2:N:3814:TRP:NE1 | 2.19                     | 0.75              |
| 2:F:1595:THR:OG1  | 2:F:1611:VAL:O   | 2.04                     | 0.75              |
| 3:G:3078:THR:HG22 | 3:G:3080:TYR:CE1 | 2.20                     | 0.75              |
| 3:K:4097:VAL:HG11 | 3:K:4104:LEU:CD2 | 2.16                     | 0.75              |
| 4:P:5514:PRO:CD   | 4:P:5609:LEU:O   | 2.34                     | 0.75              |
| 4:H:3631:ASN:CA   | 4:H:3685:ALA:HB2 | 2.17                     | 0.75              |
| 4:D:514:PRO:CD    | 4:D:609:LEU:O    | 2.34                     | 0.75              |
| 2:F:1756:PRO:O    | 2:F:1814:TRP:NE1 | 2.18                     | 0.75              |
| 3:G:3097:VAL:HG11 | 3:G:3104:LEU:CD2 | 2.16                     | 0.75              |
| 4:H:3514:PRO:CD   | 4:H:3609:LEU:CB  | 2.65                     | 0.75              |
| 3:K:4021:SER:CB   | 3:K:4080:TYR:CE2 | 2.69                     | 0.75              |
| 3:G:3102:ILE:HG21 | 4:H:3552:ASP:HA  | 1.68                     | 0.75              |
| 2:J:2692:ARG:O    | 2:J:2711:ARG:NH2 | 2.19                     | 0.75              |
| 3:G:3011:VAL:CG2  | 3:G:3151:PRO:HB2 | 2.16                     | 0.75              |
| 4:L:4514:PRO:CD   | 4:L:4609:LEU:CB  | 2.65                     | 0.75              |
| 2:N:3595:THR:OG1  | 2:N:3611:VAL:O   | 2.04                     | 0.75              |
| 2:N:3715:ILE:O    | 3:O:5065:LYS:NZ  | 2.19                     | 0.75              |
| 2:F:1561:LYS:CA   | 4:H:3532:SER:OG  | 2.35                     | 0.75              |
| 2:F:1680:ALA:C    | 3:G:3062:GLU:HG2 | 2.12                     | 0.75              |
| 2:B:595:THR:OG1   | 2:B:611:VAL:O    | 2.04                     | 0.74              |
| 3:C:21:SER:CB     | 3:C:80:TYR:CE2   | 2.69                     | 0.74              |
| 4:D:631:ASN:CA    | 4:D:685:ALA:HB2  | 2.17                     | 0.74              |
| 2:F:1753:THR:OG1  | 2:F:1816:ASN:ND2 | 2.20                     | 0.74              |
| 3:O:5097:VAL:HG11 | 3:O:5104:LEU:CD2 | 2.16                     | 0.74              |
| 3:K:4102:ILE:HG21 | 4:L:4552:ASP:HA  | 1.69                     | 0.74              |
| 2:B:718:LYS:HB2   | 3:C:59:THR:CG2   | 2.17                     | 0.74              |
| 3:C:2:ILE:HD13    | 3:C:98:ARG:NH1   | 2.00                     | 0.74              |
| 3:C:97:VAL:CG2    | 3:C:107:TRP:CE3  | 2.70                     | 0.74              |
| 3:C:102:ILE:HG21  | 4:D:552:ASP:HA   | 1.69                     | 0.74              |
| 3:C:118:ALA:CB    | 3:C:150:PHE:HE2  | 1.65                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:685:ALA:O     | 4:D:688:TRP:HB3   | 1.85                     | 0.74              |
| 3:O:5024:ALA:HB1  | 3:O:5027:TYR:CE1  | 2.22                     | 0.74              |
| 3:O:5097:VAL:HG21 | 3:O:5107:TRP:CE3  | 2.23                     | 0.74              |
| 2:B:753:THR:OG1   | 2:B:816:ASN:ND2   | 2.20                     | 0.74              |
| 3:C:97:VAL:HG11   | 3:C:104:LEU:CD2   | 2.16                     | 0.74              |
| 3:O:5102:ILE:HG21 | 4:P:5552:ASP:HA   | 1.69                     | 0.74              |
| 4:P:5631:ASN:CA   | 4:P:5685:ALA:HB2  | 2.17                     | 0.74              |
| 1:A:30:GLN:OE1    | 1:A:136:THR:OG1   | 2.06                     | 0.74              |
| 1:E:1030:GLN:OE1  | 1:E:1136:THR:OG1  | 2.06                     | 0.74              |
| 3:G:3024:ALA:HB1  | 3:G:3027:TYR:CE1  | 2.22                     | 0.74              |
| 3:O:5002:ILE:HD13 | 3:O:5098:ARG:NH1  | 2.00                     | 0.74              |
| 2:F:1560:GLN:CB   | 4:H:3595:ASN:OD1  | 2.35                     | 0.74              |
| 3:G:3217:ARG:NH2  | 4:H:3622:PRO:CD   | 2.45                     | 0.74              |
| 3:C:2:ILE:HD12    | 3:C:98:ARG:NH1    | 1.98                     | 0.74              |
| 4:H:3552:ASP:HB3  | 4:H:3555:ASN:HD22 | 1.51                     | 0.74              |
| 4:L:4552:ASP:HB3  | 4:L:4555:ASN:HD22 | 1.51                     | 0.74              |
| 4:D:514:PRO:CD    | 4:D:609:LEU:CB    | 2.65                     | 0.74              |
| 1:M:3030:GLN:OE1  | 1:M:3136:THR:OG1  | 2.06                     | 0.74              |
| 2:N:3563:ILE:HG12 | 4:P:5532:SER:HB3  | 1.68                     | 0.74              |
| 2:N:3680:ALA:CB   | 3:O:5062:GLU:OE1  | 2.36                     | 0.74              |
| 3:G:3039:GLN:CD   | 3:G:3045:PHE:CZ   | 2.66                     | 0.74              |
| 3:K:4126:TYR:CE2  | 4:L:4627:GLU:HG3  | 2.23                     | 0.73              |
| 3:O:5039:GLN:CD   | 3:O:5045:PHE:CZ   | 2.66                     | 0.73              |
| 3:O:5097:VAL:CG2  | 3:O:5107:TRP:CE3  | 2.70                     | 0.73              |
| 2:F:1684:TYR:OH   | 2:F:1701:THR:OG1  | 2.03                     | 0.73              |
| 3:C:97:VAL:HG21   | 3:C:107:TRP:CE3   | 2.23                     | 0.73              |
| 3:G:3097:VAL:CG2  | 3:G:3107:TRP:CE3  | 2.70                     | 0.73              |
| 3:K:4039:GLN:CD   | 3:K:4045:PHE:CZ   | 2.66                     | 0.73              |
| 3:C:24:ALA:HB1    | 3:C:27:TYR:CE1    | 2.22                     | 0.73              |
| 3:K:4097:VAL:CG2  | 3:K:4107:TRP:CE3  | 2.70                     | 0.73              |
| 3:O:5021:SER:OG   | 3:O:5080:TYR:CD2  | 2.37                     | 0.73              |
| 3:C:126:TYR:CE2   | 4:D:627:GLU:HG3   | 2.23                     | 0.73              |
| 4:P:5514:PRO:CD   | 4:P:5609:LEU:CB   | 2.65                     | 0.73              |
| 3:C:39:GLN:CD     | 3:C:45:PHE:CZ     | 2.66                     | 0.73              |
| 3:G:3011:VAL:CG1  | 3:G:3151:PRO:CB   | 2.67                     | 0.73              |
| 3:K:4024:ALA:HB1  | 3:K:4027:TYR:CE1  | 2.22                     | 0.73              |
| 3:G:3002:ILE:HD13 | 3:G:3098:ARG:NH1  | 2.00                     | 0.73              |
| 3:G:3097:VAL:HG21 | 3:G:3107:TRP:CE3  | 2.23                     | 0.73              |
| 3:K:4097:VAL:HG21 | 3:K:4107:TRP:CE3  | 2.23                     | 0.73              |
| 3:O:5126:TYR:CE2  | 4:P:5627:GLU:HG3  | 2.23                     | 0.73              |
| 3:G:3126:TYR:CE2  | 4:H:3627:GLU:HG3  | 2.23                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:N:3719:LYS:CG   | 3:O:5052:TYR:CE2  | 2.71                     | 0.73              |
| 3:O:5102:ILE:HG21 | 4:P:5552:ASP:CG   | 2.03                     | 0.73              |
| 2:B:561:LYS:CG    | 4:D:532:SER:OG    | 2.37                     | 0.72              |
| 1:I:2030:GLN:OE1  | 1:I:2136:THR:OG1  | 2.06                     | 0.72              |
| 3:K:4011:VAL:CG1  | 3:K:4151:PRO:CB   | 2.67                     | 0.72              |
| 2:J:2545:ASP:OD2  | 4:L:4598:TRP:HZ2  | 1.71                     | 0.72              |
| 3:O:5011:VAL:CG1  | 3:O:5151:PRO:CB   | 2.67                     | 0.72              |
| 2:B:547:VAL:HG21  | 3:C:102:ILE:CG1   | 2.16                     | 0.72              |
| 2:N:3677:PRO:C    | 4:P:5597:LEU:CD2  | 2.62                     | 0.72              |
| 4:P:5552:ASP:HB3  | 4:P:5555:ASN:HD22 | 1.51                     | 0.72              |
| 4:D:552:ASP:HB3   | 4:D:555:ASN:HD22  | 1.51                     | 0.72              |
| 2:B:547:VAL:CG2   | 3:C:102:ILE:HG13  | 2.19                     | 0.72              |
| 2:B:622:ARG:NH2   | 2:B:815:GLY:O     | 2.23                     | 0.72              |
| 2:F:1622:ARG:NH2  | 2:F:1815:GLY:O    | 2.23                     | 0.72              |
| 2:N:3622:ARG:NH2  | 2:N:3815:GLY:O    | 2.23                     | 0.72              |
| 1:A:291:ILE:HG12  | 1:I:2306:GLU:HB2  | 1.71                     | 0.72              |
| 2:N:3677:PRO:C    | 4:P:5597:LEU:HD22 | 2.15                     | 0.72              |
| 2:J:2622:ARG:NH2  | 2:J:2815:GLY:O    | 2.23                     | 0.72              |
| 1:A:22:PRO:CB     | 1:I:2382:LYS:HB3  | 2.18                     | 0.72              |
| 2:N:3680:ALA:N    | 3:O:5062:GLU:HA   | 1.97                     | 0.72              |
| 3:O:5078:THR:HG22 | 3:O:5080:TYR:CZ   | 2.25                     | 0.71              |
| 3:C:102:ILE:HG22  | 4:D:534:CYS:CB    | 2.13                     | 0.71              |
| 2:F:1783:SER:OG   | 2:F:1788:ALA:O    | 2.06                     | 0.71              |
| 1:E:1076:TYR:OH   | 1:E:1105:GLU:OE1  | 2.08                     | 0.71              |
| 3:K:4102:ILE:HB   | 4:L:4552:ASP:HB2  | 0.75                     | 0.71              |
| 2:B:563:ILE:HG22  | 4:D:532:SER:H     | 1.08                     | 0.71              |
| 2:J:2684:TYR:OH   | 2:J:2701:THR:OG1  | 2.04                     | 0.71              |
| 1:A:290:ARG:HH22  | 1:I:2356:HIS:CE1  | 2.08                     | 0.71              |
| 2:B:678:SER:HB2   | 4:D:597:LEU:HD22  | 0.75                     | 0.71              |
| 3:C:78:THR:HG22   | 3:C:80:TYR:CZ     | 2.25                     | 0.71              |
| 3:C:102:ILE:CG2   | 4:D:552:ASP:CA    | 2.69                     | 0.71              |
| 3:K:4002:ILE:HD12 | 3:K:4098:ARG:CZ   | 2.21                     | 0.71              |
| 3:K:4002:ILE:HD13 | 3:K:4098:ARG:NH1  | 2.00                     | 0.71              |
| 3:K:4118:ALA:CB   | 3:K:4150:PHE:HE2  | 1.65                     | 0.71              |
| 2:B:718:LYS:CB    | 3:C:59:THR:CG2    | 2.65                     | 0.71              |
| 1:M:3076:TYR:OH   | 1:M:3105:GLU:OE1  | 2.08                     | 0.71              |
| 1:A:76:TYR:OH     | 1:A:105:GLU:OE1   | 2.08                     | 0.70              |
| 2:B:560:GLN:HG3   | 4:D:595:ASN:O     | 1.91                     | 0.70              |
| 4:D:593:TRP:CH2   | 4:D:596:ASN:C     | 2.70                     | 0.70              |
| 3:O:5102:ILE:HB   | 4:P:5552:ASP:HB2  | 0.75                     | 0.70              |
| 3:G:3102:ILE:CG2  | 4:H:3552:ASP:CA   | 2.69                     | 0.70              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:11:VAL:CG1    | 3:C:151:PRO:CB   | 2.67                     | 0.70              |
| 2:J:2680:ALA:CA   | 3:K:4062:GLU:HG3 | 2.19                     | 0.70              |
| 3:K:4102:ILE:CG2  | 4:L:4552:ASP:CA  | 2.69                     | 0.70              |
| 2:N:3783:SER:OG   | 2:N:3788:ALA:O   | 2.06                     | 0.70              |
| 3:O:5102:ILE:CG2  | 4:P:5552:ASP:CA  | 2.69                     | 0.70              |
| 3:C:2:ILE:HD12    | 3:C:98:ARG:CZ    | 2.21                     | 0.70              |
| 3:G:3102:ILE:HB   | 4:H:3552:ASP:HB2 | 0.75                     | 0.70              |
| 4:P:5542:PRO:HB3  | 4:P:5669:LYS:HD3 | 1.74                     | 0.70              |
| 3:G:3002:ILE:HD12 | 3:G:3098:ARG:CZ  | 2.21                     | 0.70              |
| 4:H:3593:TRP:CH2  | 4:H:3596:ASN:C   | 2.70                     | 0.70              |
| 2:B:547:VAL:HG21  | 4:D:552:ASP:OD2  | 1.91                     | 0.70              |
| 4:P:5557:ARG:HD2  | 4:P:5558:SER:O   | 1.92                     | 0.70              |
| 2:N:3719:LYS:HG2  | 3:O:5052:TYR:CE2 | 2.27                     | 0.70              |
| 3:O:5002:ILE:HD12 | 3:O:5098:ARG:CZ  | 2.21                     | 0.70              |
| 4:D:557:ARG:HD2   | 4:D:558:SER:O    | 1.92                     | 0.69              |
| 4:L:4593:TRP:CH2  | 4:L:4596:ASN:C   | 2.70                     | 0.69              |
| 3:C:21:SER:OG     | 3:C:80:TYR:CD2   | 2.37                     | 0.69              |
| 3:K:4217:ARG:NH2  | 4:L:4622:PRO:CD  | 2.45                     | 0.69              |
| 4:P:5593:TRP:CH2  | 4:P:5596:ASN:C   | 2.70                     | 0.69              |
| 1:A:111:SER:N     | 1:A:114:CYS:SG   | 2.66                     | 0.69              |
| 2:F:1560:GLN:CA   | 4:H:3595:ASN:OD1 | 2.40                     | 0.69              |
| 4:H:3542:PRO:HB3  | 4:H:3669:LYS:HD3 | 1.73                     | 0.69              |
| 1:I:2076:TYR:OH   | 1:I:2105:GLU:OE1 | 2.08                     | 0.69              |
| 3:K:4060:TYR:OH   | 3:K:4069:VAL:HA  | 1.92                     | 0.69              |
| 2:B:563:ILE:CG2   | 4:D:532:SER:HB3  | 2.01                     | 0.69              |
| 3:K:4030:THR:HG23 | 3:K:4054:ASN:ND2 | 2.07                     | 0.69              |
| 4:L:4557:ARG:HD2  | 4:L:4558:SER:O   | 1.92                     | 0.69              |
| 1:M:3111:SER:N    | 1:M:3114:CYS:SG  | 2.66                     | 0.69              |
| 1:E:1111:SER:N    | 1:E:1114:CYS:SG  | 2.65                     | 0.69              |
| 3:O:5060:TYR:OH   | 3:O:5069:VAL:HA  | 1.92                     | 0.69              |
| 3:G:3060:TYR:OH   | 3:G:3069:VAL:HA  | 1.92                     | 0.69              |
| 4:L:4542:PRO:HB3  | 4:L:4669:LYS:HD3 | 1.74                     | 0.69              |
| 1:M:3359:THR:O    | 1:M:3394:GLN:NE2 | 2.26                     | 0.69              |
| 2:B:552:MET:N     | 2:B:563:ILE:O    | 2.26                     | 0.69              |
| 3:C:30:THR:HG23   | 3:C:54:ASN:ND2   | 2.07                     | 0.69              |
| 3:G:3030:THR:HG23 | 3:G:3054:ASN:ND2 | 2.07                     | 0.69              |
| 4:H:3557:ARG:HD2  | 4:H:3558:SER:O   | 1.92                     | 0.69              |
| 2:J:2678:SER:N    | 3:K:4062:GLU:HG2 | 2.06                     | 0.69              |
| 3:C:60:TYR:OH     | 3:C:69:VAL:HA    | 1.92                     | 0.69              |
| 3:C:217:ARG:NH2   | 4:D:622:PRO:CD   | 2.45                     | 0.69              |
| 3:C:2:ILE:CD1     | 3:C:98:ARG:CZ    | 2.70                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:542:PRO:HB3   | 4:D:669:LYS:HD3   | 1.73                     | 0.69              |
| 3:O:5002:ILE:CD1  | 3:O:5098:ARG:CZ   | 2.70                     | 0.69              |
| 3:O:5030:THR:HG23 | 3:O:5054:ASN:ND2  | 2.07                     | 0.68              |
| 1:A:359:THR:O     | 1:A:394:GLN:NE2   | 2.26                     | 0.68              |
| 2:F:1716:ASP:OD2  | 4:H:3596:ASN:ND2  | 2.26                     | 0.68              |
| 2:N:3719:LYS:HG3  | 3:O:5052:TYR:CE2  | 2.28                     | 0.68              |
| 3:C:102:ILE:HB    | 4:D:552:ASP:HB2   | 0.75                     | 0.68              |
| 1:E:1359:THR:O    | 1:E:1394:GLN:NE2  | 2.26                     | 0.68              |
| 3:G:3002:ILE:CD1  | 3:G:3098:ARG:CZ   | 2.70                     | 0.68              |
| 1:I:2391:TYR:OH   | 2:J:2784:LEU:HD11 | 1.94                     | 0.68              |
| 1:I:2111:SER:N    | 1:I:2114:CYS:SG   | 2.66                     | 0.68              |
| 2:B:783:SER:OG    | 2:B:788:ALA:O     | 2.06                     | 0.68              |
| 1:I:2359:THR:O    | 1:I:2394:GLN:NE2  | 2.26                     | 0.68              |
| 2:N:3552:MET:N    | 2:N:3563:ILE:O    | 2.26                     | 0.68              |
| 3:G:3102:ILE:HG21 | 4:H:3552:ASP:CB   | 2.23                     | 0.68              |
| 2:J:2552:MET:N    | 2:J:2563:ILE:O    | 2.26                     | 0.68              |
| 2:J:2783:SER:OG   | 2:J:2788:ALA:O    | 2.06                     | 0.68              |
| 1:A:391:TYR:OH    | 2:B:784:LEU:HD11  | 1.94                     | 0.68              |
| 1:E:1391:TYR:OH   | 2:F:1784:LEU:HD11 | 1.94                     | 0.68              |
| 2:N:3719:LYS:HG3  | 3:O:5052:TYR:CZ   | 2.28                     | 0.67              |
| 3:C:128:LEU:HB3   | 4:D:621:PHE:CD2   | 2.30                     | 0.67              |
| 3:K:4102:ILE:HG21 | 4:L:4552:ASP:CB   | 2.23                     | 0.67              |
| 2:B:680:ALA:O     | 3:C:62:GLU:CG     | 2.35                     | 0.67              |
| 3:G:3128:LEU:HB3  | 4:H:3621:PHE:CD2  | 2.30                     | 0.67              |
| 2:F:1552:MET:N    | 2:F:1563:ILE:O    | 2.26                     | 0.67              |
| 3:O:5118:ALA:CB   | 3:O:5150:PHE:HE2  | 1.65                     | 0.67              |
| 3:O:5128:LEU:HB3  | 4:P:5621:PHE:CD2  | 2.30                     | 0.67              |
| 2:F:1547:VAL:CG2  | 4:H:3552:ASP:OD2  | 2.43                     | 0.67              |
| 3:C:102:ILE:HG21  | 4:D:552:ASP:CB    | 2.23                     | 0.67              |
| 4:H:3683:LEU:HD11 | 4:H:3694:TYR:CE2  | 2.29                     | 0.67              |
| 2:J:2680:ALA:H    | 3:K:4062:GLU:HG2  | 1.55                     | 0.67              |
| 3:O:5102:ILE:HG21 | 4:P:5552:ASP:CB   | 2.23                     | 0.67              |
| 1:A:22:PRO:HB3    | 1:I:2382:LYS:HB2  | 1.73                     | 0.66              |
| 1:M:3391:TYR:OH   | 2:N:3784:LEU:HD11 | 1.94                     | 0.66              |
| 3:O:5102:ILE:HG22 | 4:P:5534:CYS:CB   | 2.13                     | 0.66              |
| 3:C:73:GLU:OE1    | 3:C:80:TYR:CZ     | 2.49                     | 0.66              |
| 4:D:672:ASN:O     | 4:D:673:ASN:HB2   | 1.95                     | 0.66              |
| 3:C:102:ILE:CG1   | 4:D:552:ASP:CB    | 2.73                     | 0.66              |
| 2:B:678:SER:HB2   | 4:D:597:LEU:HD23  | 1.69                     | 0.66              |
| 3:G:3073:GLU:OE1  | 3:G:3080:TYR:CZ   | 2.49                     | 0.66              |
| 2:B:718:LYS:HD3   | 3:C:59:THR:CG2    | 2.23                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:P:5672:ASN:O    | 4:P:5673:ASN:HB2  | 1.95                     | 0.66              |
| 2:B:718:LYS:CE    | 4:D:596:ASN:CB    | 2.66                     | 0.66              |
| 2:F:1543:LYS:HE2  | 4:H:3531:SER:O    | 1.95                     | 0.66              |
| 2:N:3680:ALA:N    | 3:O:5062:GLU:CD   | 2.54                     | 0.66              |
| 3:O:5041:PRO:HD3  | 3:O:5092:ALA:HA   | 1.77                     | 0.66              |
| 3:O:5073:GLU:OE1  | 3:O:5080:TYR:CZ   | 2.49                     | 0.66              |
| 3:K:4128:LEU:HB3  | 4:L:4621:PHE:CD2  | 2.30                     | 0.66              |
| 4:P:5506:GLN:CD   | 4:P:5590:CYS:SG   | 2.79                     | 0.66              |
| 3:C:41:PRO:HD3    | 3:C:92:ALA:HA     | 1.77                     | 0.66              |
| 4:H:3506:GLN:CD   | 4:H:3590:CYS:SG   | 2.79                     | 0.66              |
| 3:O:5006:GLN:HE22 | 3:O:5095:PHE:HA   | 1.62                     | 0.65              |
| 3:C:6:GLN:HE22    | 3:C:95:PHE:HA     | 1.62                     | 0.65              |
| 3:K:4041:PRO:HD3  | 3:K:4092:ALA:HA   | 1.77                     | 0.65              |
| 4:P:5683:LEU:HD11 | 4:P:5694:TYR:CE2  | 2.29                     | 0.65              |
| 3:G:3118:ALA:CB   | 3:G:3150:PHE:HE2  | 1.65                     | 0.65              |
| 4:P:5652:LYS:HG2  | 4:P:5657:PRO:HA   | 1.79                     | 0.65              |
| 3:G:3021:SER:OG   | 3:G:3080:TYR:CD2  | 2.37                     | 0.65              |
| 3:G:3041:PRO:HD3  | 3:G:3092:ALA:HA   | 1.77                     | 0.65              |
| 3:K:4073:GLU:OE1  | 3:K:4080:TYR:CZ   | 2.49                     | 0.65              |
| 4:L:4610:GLY:O    | 4:L:4611:GLN:HG3  | 1.97                     | 0.65              |
| 2:N:3680:ALA:O    | 3:O:5065:LYS:CD   | 2.42                     | 0.65              |
| 3:G:3006:GLN:HE22 | 3:G:3095:PHE:HA   | 1.62                     | 0.65              |
| 4:L:4672:ASN:O    | 4:L:4673:ASN:HB2  | 1.95                     | 0.65              |
| 4:H:3652:LYS:HG2  | 4:H:3657:PRO:HA   | 1.79                     | 0.65              |
| 4:P:5610:GLY:O    | 4:P:5611:GLN:HG3  | 1.97                     | 0.65              |
| 4:D:506:GLN:CD    | 4:D:590:CYS:SG    | 2.79                     | 0.64              |
| 3:K:4102:ILE:CG1  | 4:L:4552:ASP:CB   | 2.73                     | 0.64              |
| 2:B:559:THR:HG1   | 4:D:595:ASN:ND2   | 1.92                     | 0.64              |
| 2:F:1545:ASP:CB   | 3:G:3102:ILE:CA   | 2.60                     | 0.64              |
| 4:H:3564:PHE:CE1  | 4:H:3577:ILE:HG12 | 2.33                     | 0.64              |
| 4:L:4506:GLN:CD   | 4:L:4590:CYS:SG   | 2.79                     | 0.64              |
| 3:O:5073:GLU:OE1  | 3:O:5080:TYR:CE1  | 2.51                     | 0.64              |
| 3:K:4073:GLU:OE1  | 3:K:4080:TYR:CE1  | 2.50                     | 0.64              |
| 2:N:3720:TRP:CE2  | 3:O:5057:GLU:OE2  | 2.50                     | 0.64              |
| 4:H:3672:ASN:O    | 4:H:3673:ASN:HB2  | 1.95                     | 0.64              |
| 2:J:2678:SER:OG   | 3:K:4062:GLU:CA   | 2.45                     | 0.64              |
| 4:L:4581:GLN:HB3  | 4:L:4583:GLU:HG2  | 1.80                     | 0.64              |
| 4:L:4631:ASN:HA   | 4:L:4685:ALA:CB   | 2.25                     | 0.64              |
| 3:C:73:GLU:OE1    | 3:C:80:TYR:CE1    | 2.50                     | 0.64              |
| 2:F:1677:PRO:CA   | 4:H:3501:GLN:CB   | 2.56                     | 0.64              |
| 3:G:3073:GLU:OE1  | 3:G:3080:TYR:CE1  | 2.51                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:4002:ILE:CD1  | 3:K:4098:ARG:CZ   | 2.70                     | 0.64              |
| 4:L:4652:LYS:HG2  | 4:L:4657:PRO:HA   | 1.79                     | 0.64              |
| 4:D:564:PHE:CE1   | 4:D:577:ILE:HG12  | 2.33                     | 0.64              |
| 3:K:4030:THR:CG2  | 3:K:4030:THR:O    | 2.46                     | 0.64              |
| 4:L:4554:ASN:C    | 4:L:4554:ASN:ND2  | 2.54                     | 0.64              |
| 1:A:123:LYS:CE    | 1:E:1150:ASN:ND2  | 2.52                     | 0.64              |
| 4:D:652:LYS:HG2   | 4:D:657:PRO:HA    | 1.79                     | 0.64              |
| 4:D:610:GLY:O     | 4:D:611:GLN:HG3   | 1.97                     | 0.63              |
| 4:D:683:LEU:HD11  | 4:D:694:TYR:CE2   | 2.29                     | 0.63              |
| 4:P:5581:GLN:HB3  | 4:P:5583:GLU:HG2  | 1.80                     | 0.63              |
| 3:C:30:THR:O      | 3:C:30:THR:CG2    | 2.46                     | 0.63              |
| 4:D:513:SER:OG    | 4:D:609:LEU:CD2   | 2.44                     | 0.63              |
| 4:H:3513:SER:OG   | 4:H:3609:LEU:CD2  | 2.44                     | 0.63              |
| 4:H:3568:LEU:HD23 | 4:H:3573:ALA:HA   | 1.80                     | 0.63              |
| 3:K:4006:GLN:HE22 | 3:K:4095:PHE:HA   | 1.62                     | 0.63              |
| 4:P:5568:LEU:HD23 | 4:P:5573:ALA:HA   | 1.80                     | 0.63              |
| 4:D:568:LEU:HD23  | 4:D:573:ALA:HA    | 1.80                     | 0.63              |
| 3:G:3030:THR:CG2  | 3:G:3030:THR:O    | 2.46                     | 0.63              |
| 4:L:4647:VAL:HG12 | 4:L:4700:HIS:HB2  | 1.81                     | 0.63              |
| 1:A:150:ASN:ND2   | 1:E:1123:LYS:CE   | 2.52                     | 0.63              |
| 4:H:3647:VAL:HG12 | 4:H:3700:HIS:HB2  | 1.81                     | 0.63              |
| 4:L:4564:PHE:CE1  | 4:L:4577:ILE:HG12 | 2.33                     | 0.63              |
| 4:D:514:PRO:HD3   | 4:D:609:LEU:C     | 2.23                     | 0.63              |
| 4:L:4683:LEU:HD11 | 4:L:4694:TYR:CE2  | 2.29                     | 0.63              |
| 2:B:560:GLN:CG    | 4:D:595:ASN:HA    | 2.29                     | 0.63              |
| 1:A:291:ILE:CG2   | 1:I:2316:ILE:HD13 | 2.28                     | 0.63              |
| 3:G:3072:LEU:HD13 | 3:G:3074:ILE:HG13 | 1.81                     | 0.63              |
| 4:H:3610:GLY:O    | 4:H:3611:GLN:HG3  | 1.97                     | 0.63              |
| 4:P:5647:VAL:HG12 | 4:P:5700:HIS:HB2  | 1.81                     | 0.63              |
| 4:D:581:GLN:HB3   | 4:D:583:GLU:HG2   | 1.80                     | 0.62              |
| 4:L:4514:PRO:HD3  | 4:L:4609:LEU:HB3  | 1.79                     | 0.62              |
| 4:P:5561:PRO:HG2  | 4:P:5563:ARG:NH1  | 2.14                     | 0.62              |
| 3:G:3035:LEU:HG   | 3:G:3047:TRP:CD1  | 2.35                     | 0.62              |
| 4:H:3561:PRO:HG2  | 4:H:3563:ARG:NH1  | 2.14                     | 0.62              |
| 4:L:4568:LEU:HD23 | 4:L:4573:ALA:HA   | 1.80                     | 0.62              |
| 3:O:5030:THR:O    | 3:O:5030:THR:CG2  | 2.46                     | 0.62              |
| 3:O:5035:LEU:HG   | 3:O:5047:TRP:CD1  | 2.34                     | 0.62              |
| 4:P:5514:PRO:HD3  | 4:P:5609:LEU:C    | 2.23                     | 0.62              |
| 4:D:514:PRO:HD3   | 4:D:609:LEU:HB3   | 1.79                     | 0.62              |
| 4:D:631:ASN:HA    | 4:D:685:ALA:CB    | 2.25                     | 0.62              |
| 4:H:3514:PRO:HD3  | 4:H:3609:LEU:HB3  | 1.79                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:P:5564:PHE:CE1  | 4:P:5577:ILE:HG12 | 2.33                     | 0.62              |
| 4:H:3514:PRO:HD3  | 4:H:3609:LEU:O    | 2.00                     | 0.62              |
| 2:B:544:THR:HG21  | 4:D:593:TRP:CD1   | 2.34                     | 0.62              |
| 2:B:562:SER:CA    | 4:D:532:SER:CB    | 2.77                     | 0.62              |
| 4:H:3514:PRO:HD3  | 4:H:3609:LEU:C    | 2.23                     | 0.62              |
| 2:J:2545:ASP:OD2  | 4:L:4598:TRP:CZ2  | 2.53                     | 0.62              |
| 3:K:4072:LEU:HD13 | 3:K:4074:ILE:HG13 | 1.81                     | 0.62              |
| 2:F:1718:LYS:HE2  | 4:H:3595:ASN:O    | 1.98                     | 0.62              |
| 4:L:4514:PRO:HD3  | 4:L:4609:LEU:C    | 2.23                     | 0.62              |
| 4:L:4561:PRO:HG2  | 4:L:4563:ARG:NH1  | 2.14                     | 0.62              |
| 4:H:3581:GLN:HB3  | 4:H:3583:GLU:HG2  | 1.80                     | 0.62              |
| 3:K:4078:THR:HG22 | 3:K:4080:TYR:CZ   | 2.25                     | 0.62              |
| 4:P:5513:SER:OG   | 4:P:5609:LEU:CD2  | 2.44                     | 0.62              |
| 2:B:676:VAL:O     | 4:D:501:GLN:NE2   | 2.33                     | 0.62              |
| 3:O:5072:LEU:HD13 | 3:O:5074:ILE:HG13 | 1.81                     | 0.62              |
| 1:A:53:THR:OG1    | 1:A:236:GLN:OE1   | 2.18                     | 0.62              |
| 2:F:1718:LYS:HD2  | 4:H:3596:ASN:C    | 2.14                     | 0.62              |
| 3:C:72:LEU:HD13   | 3:C:74:ILE:HG13   | 1.81                     | 0.61              |
| 2:B:505:ASP:O     | 2:B:726:ARG:NH1   | 2.32                     | 0.61              |
| 3:C:9:ARG:HG2     | 3:C:112:THR:H     | 1.66                     | 0.61              |
| 3:K:4035:LEU:HG   | 3:K:4047:TRP:CD1  | 2.34                     | 0.61              |
| 3:O:5011:VAL:HG23 | 3:O:5152:GLU:O    | 2.00                     | 0.61              |
| 2:B:560:GLN:CB    | 4:D:595:ASN:CA    | 2.64                     | 0.61              |
| 4:P:5631:ASN:C    | 4:P:5685:ALA:HB2  | 2.25                     | 0.61              |
| 4:D:514:PRO:HD3   | 4:D:609:LEU:O     | 2.00                     | 0.61              |
| 4:D:647:VAL:HG12  | 4:D:700:HIS:HB2   | 1.80                     | 0.61              |
| 4:H:3513:SER:HG   | 4:H:3609:LEU:HD22 | 1.63                     | 0.61              |
| 3:K:4032:TYR:CE1  | 3:K:4100:TYR:HD1  | 1.97                     | 0.61              |
| 4:L:4514:PRO:HD3  | 4:L:4609:LEU:O    | 2.00                     | 0.61              |
| 2:N:3505:ASP:O    | 2:N:3726:ARG:NH1  | 2.32                     | 0.61              |
| 4:P:5631:ASN:HA   | 4:P:5685:ALA:CB   | 2.25                     | 0.61              |
| 2:B:718:LYS:CE    | 4:D:596:ASN:O     | 2.44                     | 0.61              |
| 4:D:561:PRO:HG2   | 4:D:563:ARG:NH1   | 2.14                     | 0.61              |
| 4:D:631:ASN:C     | 4:D:685:ALA:HB2   | 2.25                     | 0.61              |
| 2:F:1505:ASP:O    | 2:F:1726:ARG:NH1  | 2.32                     | 0.61              |
| 4:H:3662:MET:HA   | 4:H:3680:TYR:O    | 2.01                     | 0.61              |
| 2:B:676:VAL:HB    | 3:C:62:GLU:HG2    | 1.82                     | 0.61              |
| 3:G:3011:VAL:HG23 | 3:G:3152:GLU:O    | 2.00                     | 0.61              |
| 3:G:3102:ILE:CG1  | 4:H:3552:ASP:CB   | 2.73                     | 0.61              |
| 4:H:3514:PRO:CD   | 4:H:3609:LEU:HB3  | 2.31                     | 0.61              |
| 4:H:3631:ASN:C    | 4:H:3685:ALA:HB2  | 2.25                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:J:2678:SER:CB   | 3:K:4062:GLU:N    | 2.55                     | 0.61              |
| 1:E:1198:ALA:HB3  | 2:J:2759:LEU:HD11 | 1.81                     | 0.61              |
| 1:I:2198:ALA:HB3  | 2:N:3759:LEU:HD11 | 1.81                     | 0.61              |
| 4:L:4662:MET:HA   | 4:L:4680:TYR:O    | 2.01                     | 0.61              |
| 4:D:554:ASN:C     | 4:D:554:ASN:ND2   | 2.54                     | 0.61              |
| 2:N:3680:ALA:C    | 3:O:5065:LYS:HD3  | 2.16                     | 0.61              |
| 3:O:5102:ILE:HG21 | 4:P:5552:ASP:CA   | 2.31                     | 0.61              |
| 3:G:3118:ALA:HB1  | 3:G:3150:PHE:CD2  | 2.36                     | 0.61              |
| 4:L:4631:ASN:C    | 4:L:4685:ALA:HB2  | 2.25                     | 0.61              |
| 4:P:5514:PRO:CD   | 4:P:5609:LEU:HB3  | 2.31                     | 0.61              |
| 3:C:11:VAL:HG23   | 3:C:152:GLU:O     | 2.00                     | 0.61              |
| 4:D:662:MET:HA    | 4:D:680:TYR:O     | 2.01                     | 0.61              |
| 2:J:2505:ASP:O    | 2:J:2726:ARG:NH1  | 2.32                     | 0.61              |
| 3:K:4118:ALA:HB1  | 3:K:4150:PHE:CD2  | 2.36                     | 0.61              |
| 3:C:35:LEU:HG     | 3:C:47:TRP:CD1    | 2.34                     | 0.60              |
| 4:D:514:PRO:CD    | 4:D:609:LEU:HB3   | 2.31                     | 0.60              |
| 2:F:1581:HIS:NE2  | 2:F:1583:GLY:O    | 2.34                     | 0.60              |
| 3:K:4011:VAL:HG23 | 3:K:4152:GLU:O    | 2.00                     | 0.60              |
| 3:O:5009:ARG:HG2  | 3:O:5112:THR:H    | 1.65                     | 0.60              |
| 1:E:1053:THR:OG1  | 1:E:1236:GLN:OE1  | 2.18                     | 0.60              |
| 3:G:3097:VAL:HG21 | 3:G:3107:TRP:CZ3  | 2.36                     | 0.60              |
| 4:H:3514:PRO:CD   | 4:H:3609:LEU:HB2  | 2.31                     | 0.60              |
| 1:I:2053:THR:OG1  | 1:I:2236:GLN:OE1  | 2.18                     | 0.60              |
| 2:J:2679:GLY:HA3  | 3:K:4062:GLU:O    | 2.01                     | 0.60              |
| 4:L:4513:SER:OG   | 4:L:4609:LEU:CD2  | 2.44                     | 0.60              |
| 4:L:4514:PRO:CD   | 4:L:4609:LEU:HB3  | 2.31                     | 0.60              |
| 1:M:3053:THR:OG1  | 1:M:3236:GLN:OE1  | 2.18                     | 0.60              |
| 2:F:1543:LYS:HE3  | 4:H:3531:SER:O    | 2.02                     | 0.60              |
| 2:J:2558:LYS:NZ   | 4:L:4501:GLN:HG3  | 2.16                     | 0.60              |
| 4:P:5514:PRO:HD3  | 4:P:5609:LEU:O    | 2.00                     | 0.60              |
| 2:B:545:ASP:OD1   | 3:C:102:ILE:HD12  | 2.00                     | 0.60              |
| 2:B:560:GLN:O     | 4:D:595:ASN:ND2   | 2.27                     | 0.60              |
| 2:F:1759:LEU:HD11 | 1:M:3198:ALA:HB3  | 1.81                     | 0.60              |
| 3:G:3009:ARG:HG2  | 3:G:3112:THR:H    | 1.66                     | 0.60              |
| 3:G:3145:LEU:HD13 | 4:H:3680:TYR:HE2  | 1.67                     | 0.60              |
| 3:C:102:ILE:CG2   | 4:D:552:ASP:CG    | 2.75                     | 0.60              |
| 3:O:5097:VAL:HG21 | 3:O:5107:TRP:CZ3  | 2.36                     | 0.60              |
| 2:J:2678:SER:H    | 3:K:4062:GLU:CG   | 2.01                     | 0.60              |
| 2:N:3675:THR:CG2  | 4:P:5501:GLN:NE2  | 2.62                     | 0.60              |
| 4:D:686:ARG:HH11  | 4:D:686:ARG:HG3   | 1.67                     | 0.60              |
| 2:F:1678:SER:O    | 4:H:3597:LEU:HD22 | 1.95                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:4145:LEU:HD13 | 4:L:4680:TYR:HE2  | 1.67                     | 0.60              |
| 3:C:145:LEU:HD13  | 4:D:680:TYR:HE2   | 1.67                     | 0.60              |
| 3:K:4009:ARG:HG2  | 3:K:4112:THR:H    | 1.66                     | 0.60              |
| 4:L:4514:PRO:CD   | 4:L:4609:LEU:HB2  | 2.31                     | 0.60              |
| 3:K:4021:SER:HA   | 3:K:4080:TYR:CD2  | 2.37                     | 0.60              |
| 4:L:4686:ARG:HH11 | 4:L:4686:ARG:HG3  | 1.67                     | 0.60              |
| 3:O:5009:ARG:O    | 3:O:5153:PRO:HD3  | 2.02                     | 0.60              |
| 4:P:5541:LYS:HE2  | 4:P:5583:GLU:O    | 2.02                     | 0.60              |
| 3:G:3021:SER:HA   | 3:G:3080:TYR:CD2  | 2.37                     | 0.59              |
| 2:F:1676:VAL:HG23 | 4:H:3501:GLN:NE2  | 1.95                     | 0.59              |
| 2:F:1677:PRO:C    | 4:H:3501:GLN:CB   | 2.75                     | 0.59              |
| 2:J:2581:HIS:NE2  | 2:J:2583:GLY:O    | 2.34                     | 0.59              |
| 3:K:4009:ARG:O    | 3:K:4153:PRO:HD3  | 2.02                     | 0.59              |
| 3:K:4102:ILE:CG2  | 4:L:4552:ASP:CG   | 2.75                     | 0.59              |
| 3:O:5118:ALA:HB3  | 3:O:5150:PHE:HE2  | 0.78                     | 0.59              |
| 2:J:2678:SER:HG   | 3:K:4062:GLU:H    | 1.47                     | 0.59              |
| 4:L:4541:LYS:HE2  | 4:L:4583:GLU:O    | 2.02                     | 0.59              |
| 4:P:5662:MET:HA   | 4:P:5680:TYR:O    | 2.01                     | 0.59              |
| 3:C:9:ARG:O       | 3:C:153:PRO:HD3   | 2.02                     | 0.59              |
| 4:H:3541:LYS:HE2  | 4:H:3583:GLU:O    | 2.02                     | 0.59              |
| 2:J:2558:LYS:CE   | 4:L:4501:GLN:HG3  | 2.33                     | 0.59              |
| 2:B:581:HIS:NE2   | 2:B:583:GLY:O     | 2.34                     | 0.59              |
| 2:F:1546:GLY:H    | 3:G:3102:ILE:HD11 | 0.63                     | 0.59              |
| 2:N:3720:TRP:HZ3  | 3:O:5055:THR:HG21 | 1.68                     | 0.59              |
| 4:D:514:PRO:CD    | 4:D:609:LEU:HB2   | 2.31                     | 0.59              |
| 3:G:3009:ARG:O    | 3:G:3153:PRO:HD3  | 2.02                     | 0.59              |
| 3:G:3102:ILE:HG21 | 4:H:3552:ASP:CA   | 2.31                     | 0.59              |
| 3:K:4102:ILE:HG21 | 4:L:4552:ASP:CA   | 2.31                     | 0.59              |
| 3:O:5021:SER:HA   | 3:O:5080:TYR:CD2  | 2.37                     | 0.59              |
| 4:P:5528:ALA:HA   | 4:P:5571:ASP:HB2  | 1.85                     | 0.59              |
| 2:F:1680:ALA:C    | 3:G:3062:GLU:CG   | 2.65                     | 0.59              |
| 3:G:3102:ILE:CG2  | 4:H:3552:ASP:CG   | 2.75                     | 0.59              |
| 1:M:3197:LYS:O    | 1:M:3200:SER:OG   | 2.18                     | 0.59              |
| 3:O:5118:ALA:CB   | 3:O:5150:PHE:CD2  | 2.77                     | 0.59              |
| 3:O:5145:LEU:HD13 | 4:P:5680:TYR:HE2  | 1.66                     | 0.59              |
| 3:G:3073:GLU:CD   | 3:G:3080:TYR:CE1  | 2.80                     | 0.59              |
| 4:H:3528:ALA:HA   | 4:H:3571:ASP:HB2  | 1.85                     | 0.59              |
| 4:H:3631:ASN:HA   | 4:H:3685:ALA:CB   | 2.25                     | 0.59              |
| 3:K:4073:GLU:CD   | 3:K:4080:TYR:CE1  | 2.80                     | 0.59              |
| 2:N:3559:THR:O    | 4:P:5595:ASN:OD1  | 1.98                     | 0.59              |
| 3:C:97:VAL:HG21   | 3:C:107:TRP:CZ3   | 2.36                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:4097:VAL:HG21 | 3:K:4107:TRP:CZ3  | 2.36                     | 0.59              |
| 1:M:3057:SER:OG   | 2:N:3724:SER:O    | 2.16                     | 0.59              |
| 3:O:5102:ILE:CG2  | 3:O:5102:ILE:O    | 2.51                     | 0.59              |
| 4:D:541:LYS:HE2   | 4:D:583:GLU:O     | 2.02                     | 0.59              |
| 2:N:3581:HIS:NE2  | 2:N:3583:GLY:O    | 2.34                     | 0.59              |
| 1:A:291:ILE:HG21  | 1:I:2306:GLU:HB3  | 1.84                     | 0.58              |
| 3:C:21:SER:HA     | 3:C:80:TYR:CD2    | 2.37                     | 0.58              |
| 3:C:73:GLU:CD     | 3:C:80:TYR:CE1    | 2.80                     | 0.58              |
| 4:D:700:HIS:O     | 4:D:701:GLU:C     | 2.46                     | 0.58              |
| 3:G:3118:ALA:HB3  | 3:G:3150:PHE:HE2  | 0.78                     | 0.58              |
| 4:L:4528:ALA:HA   | 4:L:4571:ASP:HB2  | 1.84                     | 0.58              |
| 1:M:3038:ILE:HD12 | 1:M:3269:ALA:HB3  | 1.85                     | 0.58              |
| 2:N:3559:THR:CG2  | 4:P:5596:ASN:H    | 2.05                     | 0.58              |
| 4:P:5686:ARG:HG3  | 4:P:5686:ARG:HH11 | 1.67                     | 0.58              |
| 4:D:689:GLU:HA    | 4:D:711:ARG:NH2   | 2.18                     | 0.58              |
| 3:G:3118:ALA:CB   | 3:G:3150:PHE:CD2  | 2.77                     | 0.58              |
| 3:O:5118:ALA:HB1  | 3:O:5150:PHE:CD2  | 2.36                     | 0.58              |
| 3:O:5073:GLU:CD   | 3:O:5080:TYR:CE1  | 2.80                     | 0.58              |
| 1:A:291:ILE:HG12  | 1:I:2306:GLU:CB   | 2.32                     | 0.58              |
| 4:H:3686:ARG:HG3  | 4:H:3686:ARG:HH11 | 1.67                     | 0.58              |
| 3:O:5032:TYR:CE1  | 3:O:5100:TYR:HD1  | 1.97                     | 0.58              |
| 3:C:118:ALA:HB1   | 3:C:150:PHE:CD2   | 2.36                     | 0.58              |
| 4:L:4689:GLU:HA   | 4:L:4711:ARG:NH2  | 2.18                     | 0.58              |
| 4:P:5514:PRO:CD   | 4:P:5609:LEU:HB2  | 2.31                     | 0.58              |
| 2:F:1569:HIS:N    | 2:F:1599:GLY:O    | 2.37                     | 0.58              |
| 4:P:5689:GLU:HA   | 4:P:5711:ARG:NH2  | 2.18                     | 0.58              |
| 3:C:45:PHE:HE1    | 4:D:589:PHE:CE2   | 2.22                     | 0.58              |
| 4:D:528:ALA:HA    | 4:D:571:ASP:HB2   | 1.84                     | 0.58              |
| 4:H:3700:HIS:O    | 4:H:3701:GLU:C    | 2.46                     | 0.58              |
| 4:P:5514:PRO:HD3  | 4:P:5609:LEU:HB3  | 1.79                     | 0.58              |
| 1:E:1038:ILE:HD12 | 1:E:1269:ALA:HB3  | 1.85                     | 0.58              |
| 4:H:3689:GLU:HA   | 4:H:3711:ARG:NH2  | 2.18                     | 0.58              |
| 2:J:2562:SER:N    | 4:L:4595:ASN:OD1  | 2.33                     | 0.58              |
| 1:A:38:ILE:HD12   | 1:A:269:ALA:HB3   | 1.85                     | 0.58              |
| 2:B:718:LYS:HE2   | 4:D:596:ASN:HB2   | 1.80                     | 0.58              |
| 3:C:102:ILE:CG2   | 3:C:102:ILE:O     | 2.51                     | 0.58              |
| 2:F:1547:VAL:HG22 | 4:H:3552:ASP:OD2  | 2.03                     | 0.58              |
| 4:D:688:TRP:CZ2   | 4:D:711:ARG:HG3   | 2.39                     | 0.58              |
| 1:E:1387:HIS:CD2  | 2:F:1825:GLN:HE21 | 2.22                     | 0.58              |
| 1:M:3387:HIS:CD2  | 2:N:3825:GLN:HE21 | 2.22                     | 0.58              |
| 3:G:3145:LEU:CD1  | 4:H:3680:TYR:HE2  | 2.17                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:3688:TRP:CZ2  | 4:H:3711:ARG:HG3  | 2.39                     | 0.57              |
| 4:L:4700:HIS:O    | 4:L:4701:GLU:C    | 2.46                     | 0.57              |
| 2:N:3559:THR:HG21 | 4:P:5594:TYR:CB   | 2.32                     | 0.57              |
| 3:G:3102:ILE:CB   | 4:H:3552:ASP:CG   | 2.77                     | 0.57              |
| 4:P:5688:TRP:CZ2  | 4:P:5711:ARG:HG3  | 2.39                     | 0.57              |
| 2:B:569:HIS:N     | 2:B:599:GLY:O     | 2.37                     | 0.57              |
| 3:K:4102:ILE:HG13 | 4:L:4552:ASP:CB   | 2.34                     | 0.57              |
| 4:L:4688:TRP:CZ2  | 4:L:4711:ARG:HG3  | 2.39                     | 0.57              |
| 4:P:5611:GLN:HG3  | 4:P:5611:GLN:O    | 2.04                     | 0.57              |
| 1:A:197:LYS:O     | 1:A:200:SER:OG    | 2.18                     | 0.57              |
| 4:D:611:GLN:HG3   | 4:D:611:GLN:O     | 2.05                     | 0.57              |
| 2:F:1676:VAL:N    | 4:H:3501:GLN:OE1  | 2.31                     | 0.57              |
| 3:O:5145:LEU:CD1  | 4:P:5680:TYR:HE2  | 2.17                     | 0.57              |
| 4:H:3611:GLN:HG3  | 4:H:3611:GLN:O    | 2.05                     | 0.57              |
| 1:M:3391:TYR:CZ   | 2:N:3784:LEU:HD11 | 2.40                     | 0.57              |
| 3:C:145:LEU:CD1   | 4:D:680:TYR:HE2   | 2.17                     | 0.57              |
| 3:K:4102:ILE:CB   | 4:L:4552:ASP:CG   | 2.77                     | 0.57              |
| 1:A:391:TYR:CZ    | 2:B:784:LEU:HD11  | 2.40                     | 0.57              |
| 1:I:2391:TYR:CZ   | 2:J:2784:LEU:HD11 | 2.39                     | 0.57              |
| 3:K:4037:VAL:HG21 | 3:K:4107:TRP:HH2  | 1.70                     | 0.57              |
| 3:C:102:ILE:CB    | 4:D:552:ASP:CG    | 2.78                     | 0.57              |
| 2:F:1577:SER:O    | 2:F:1589:GLN:N    | 2.37                     | 0.57              |
| 2:N:3680:ALA:CB   | 3:O:5062:GLU:CD   | 2.78                     | 0.57              |
| 4:P:5700:HIS:O    | 4:P:5701:GLU:C    | 2.46                     | 0.57              |
| 1:A:387:HIS:CD2   | 2:B:825:GLN:HE21  | 2.22                     | 0.57              |
| 3:C:61:ALA:HB3    | 3:C:64:PHE:HD2    | 1.70                     | 0.57              |
| 2:N:3530:GLY:O    | 2:N:3590:CYS:N    | 2.38                     | 0.57              |
| 2:N:3577:SER:O    | 2:N:3589:GLN:N    | 2.37                     | 0.57              |
| 1:E:1391:TYR:CZ   | 2:F:1784:LEU:HD11 | 2.40                     | 0.56              |
| 2:B:678:SER:OG    | 3:C:61:ALA:HB1    | 2.04                     | 0.56              |
| 3:C:117:SER:O     | 3:C:118:ALA:HB2   | 2.05                     | 0.56              |
| 4:D:684:THR:O     | 4:D:685:ALA:C     | 2.48                     | 0.56              |
| 3:G:3078:THR:CG2  | 3:G:3080:TYR:CE2  | 2.84                     | 0.56              |
| 1:I:2038:ILE:HD12 | 1:I:2269:ALA:HB3  | 1.85                     | 0.56              |
| 3:K:4100:TYR:CE2  | 3:K:4101:PHE:CZ   | 2.93                     | 0.56              |
| 3:O:5078:THR:CG2  | 3:O:5080:TYR:CE2  | 2.84                     | 0.56              |
| 3:C:100:TYR:CE2   | 3:C:101:PHE:CZ    | 2.93                     | 0.56              |
| 2:F:1530:GLY:O    | 2:F:1590:CYS:N    | 2.38                     | 0.56              |
| 2:F:1547:VAL:HG21 | 4:H:3552:ASP:OD2  | 2.05                     | 0.56              |
| 3:G:3035:LEU:HD23 | 3:G:3037:VAL:HG23 | 1.82                     | 0.56              |
| 3:K:4061:ALA:HB3  | 3:K:4064:PHE:HD2  | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:4117:SER:O    | 3:K:4118:ALA:HB2  | 2.05                     | 0.56              |
| 4:L:4557:ARG:HE   | 4:L:4560:VAL:HG23 | 1.70                     | 0.56              |
| 3:O:5061:ALA:HB3  | 3:O:5064:PHE:HD2  | 1.70                     | 0.56              |
| 3:C:11:VAL:HB     | 3:C:151:PRO:HB2   | 1.87                     | 0.56              |
| 3:G:3030:THR:CG2  | 3:G:3054:ASN:HD22 | 2.17                     | 0.56              |
| 3:C:102:ILE:HG21  | 4:D:552:ASP:CA    | 2.31                     | 0.56              |
| 4:L:4611:GLN:HG3  | 4:L:4611:GLN:O    | 2.05                     | 0.56              |
| 3:O:5117:SER:O    | 3:O:5118:ALA:HB2  | 2.05                     | 0.56              |
| 1:I:2057:SER:OG   | 2:J:2724:SER:O    | 2.16                     | 0.56              |
| 2:N:3720:TRP:CZ3  | 3:O:5055:THR:HG21 | 2.40                     | 0.56              |
| 3:G:3061:ALA:HB3  | 3:G:3064:PHE:HD2  | 1.70                     | 0.56              |
| 3:K:4118:ALA:HB3  | 3:K:4150:PHE:HE2  | 0.78                     | 0.56              |
| 3:O:5045:PHE:CE1  | 4:P:5589:PHE:CZ   | 2.94                     | 0.56              |
| 2:B:563:ILE:HG21  | 4:D:532:SER:OG    | 1.99                     | 0.56              |
| 3:G:3078:THR:HG22 | 3:G:3080:TYR:CZ   | 2.25                     | 0.56              |
| 3:G:3117:SER:O    | 3:G:3118:ALA:HB2  | 2.05                     | 0.56              |
| 2:J:2547:VAL:HG11 | 3:K:4102:ILE:N    | 2.20                     | 0.56              |
| 3:K:4126:TYR:CZ   | 4:L:4627:GLU:HG3  | 2.41                     | 0.56              |
| 3:K:4145:LEU:CD1  | 4:L:4680:TYR:HE2  | 2.18                     | 0.56              |
| 2:F:1677:PRO:C    | 4:H:3501:GLN:HG2  | 2.30                     | 0.56              |
| 1:I:2387:HIS:CD2  | 2:J:2825:GLN:HE21 | 2.22                     | 0.56              |
| 3:K:4045:PHE:CE1  | 4:L:4589:PHE:CZ   | 2.94                     | 0.56              |
| 3:O:5021:SER:CB   | 3:O:5080:TYR:HE2  | 2.13                     | 0.56              |
| 1:A:194:GLY:N     | 1:A:205:GLN:OE1   | 2.39                     | 0.55              |
| 1:A:221:LYS:O     | 1:A:235:THR:OG1   | 2.19                     | 0.55              |
| 3:C:45:PHE:CE1    | 4:D:589:PHE:CZ    | 2.94                     | 0.55              |
| 4:D:557:ARG:HE    | 4:D:560:VAL:HG23  | 1.70                     | 0.55              |
| 4:H:3620:LEU:HD23 | 4:H:3636:VAL:O    | 2.06                     | 0.55              |
| 2:J:2530:GLY:O    | 2:J:2590:CYS:N    | 2.38                     | 0.55              |
| 2:N:3569:HIS:N    | 2:N:3599:GLY:O    | 2.37                     | 0.55              |
| 1:A:291:ILE:CG2   | 1:I:2316:ILE:CD1  | 2.84                     | 0.55              |
| 3:C:32:TYR:CE1    | 3:C:100:TYR:HD1   | 1.97                     | 0.55              |
| 4:D:620:LEU:HD23  | 4:D:636:VAL:O     | 2.06                     | 0.55              |
| 3:G:3100:TYR:CE2  | 3:G:3101:PHE:CZ   | 2.93                     | 0.55              |
| 3:O:5100:TYR:CE2  | 3:O:5101:PHE:CZ   | 2.93                     | 0.55              |
| 4:P:5689:GLU:HA   | 4:P:5711:ARG:HH21 | 1.72                     | 0.55              |
| 4:L:4684:THR:O    | 4:L:4685:ALA:C    | 2.48                     | 0.55              |
| 4:P:5620:LEU:HD23 | 4:P:5636:VAL:O    | 2.06                     | 0.55              |
| 3:C:126:TYR:CZ    | 4:D:627:GLU:HG3   | 2.41                     | 0.55              |
| 4:D:653:VAL:CG2   | 4:D:658:VAL:HG21  | 2.35                     | 0.55              |
| 4:H:3557:ARG:HE   | 4:H:3560:VAL:HG23 | 1.70                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:L:4620:LEU:HD21 | 4:L:4651:TRP:HH2  | 1.72                     | 0.55              |
| 1:M:3194:GLY:N    | 1:M:3205:GLN:OE1  | 2.39                     | 0.55              |
| 2:N:3559:THR:HG21 | 4:P:5594:TYR:HB3  | 1.87                     | 0.55              |
| 3:G:3045:PHE:CE1  | 4:H:3589:PHE:CZ   | 2.94                     | 0.55              |
| 2:J:2507:PRO:HB3  | 2:N:3630:GLU:HB2  | 1.89                     | 0.55              |
| 4:L:4620:LEU:HD23 | 4:L:4636:VAL:O    | 2.06                     | 0.55              |
| 3:O:5030:THR:CG2  | 3:O:5054:ASN:HD22 | 2.17                     | 0.55              |
| 3:O:5126:TYR:CZ   | 4:P:5627:GLU:HG3  | 2.41                     | 0.55              |
| 1:E:1194:GLY:N    | 1:E:1205:GLN:OE1  | 2.39                     | 0.55              |
| 2:J:2569:HIS:N    | 2:J:2599:GLY:O    | 2.37                     | 0.55              |
| 3:O:5045:PHE:HE1  | 4:P:5589:PHE:CE2  | 2.22                     | 0.55              |
| 4:P:5653:VAL:CG2  | 4:P:5658:VAL:HG21 | 2.35                     | 0.55              |
| 2:B:530:GLY:O     | 2:B:590:CYS:N     | 2.38                     | 0.55              |
| 3:C:45:PHE:HZ     | 4:D:546:PHE:HZ    | 0.62                     | 0.55              |
| 4:D:524:SER:OG    | 4:D:594:TYR:OH    | 2.23                     | 0.55              |
| 2:F:1508:ASN:OD1  | 2:F:1610:THR:OG1  | 2.11                     | 0.55              |
| 3:G:3102:ILE:CG2  | 3:G:3102:ILE:O    | 2.51                     | 0.55              |
| 4:H:3620:LEU:HD21 | 4:H:3651:TRP:HH2  | 1.72                     | 0.55              |
| 2:J:2502:TYR:N    | 2:J:2537:SER:O    | 2.40                     | 0.55              |
| 2:J:2577:SER:O    | 2:J:2589:GLN:N    | 2.37                     | 0.55              |
| 2:J:2720:TRP:HH2  | 3:K:4057:GLU:OE2  | 1.83                     | 0.55              |
| 3:K:4032:TYR:CZ   | 3:K:4100:TYR:CZ   | 2.84                     | 0.55              |
| 2:N:3508:ASN:OD1  | 2:N:3610:THR:OG1  | 2.11                     | 0.55              |
| 4:D:620:LEU:HD21  | 4:D:651:TRP:HH2   | 1.72                     | 0.55              |
| 3:G:3045:PHE:HE1  | 4:H:3589:PHE:CE2  | 2.22                     | 0.55              |
| 3:G:3126:TYR:CZ   | 4:H:3627:GLU:HG3  | 2.41                     | 0.55              |
| 4:H:3689:GLU:HA   | 4:H:3711:ARG:HH21 | 1.72                     | 0.55              |
| 4:D:689:GLU:HA    | 4:D:711:ARG:HE    | 1.72                     | 0.55              |
| 1:I:2194:GLY:N    | 1:I:2205:GLN:OE1  | 2.39                     | 0.55              |
| 4:P:5689:GLU:HA   | 4:P:5711:ARG:HE   | 1.72                     | 0.55              |
| 2:B:502:TYR:N     | 2:B:537:SER:O     | 2.40                     | 0.54              |
| 3:K:4045:PHE:HE1  | 4:L:4589:PHE:CE2  | 2.22                     | 0.54              |
| 2:B:718:LYS:CG    | 3:C:59:THR:HG23   | 2.35                     | 0.54              |
| 4:H:3684:THR:O    | 4:H:3685:ALA:C    | 2.48                     | 0.54              |
| 4:H:3689:GLU:HA   | 4:H:3711:ARG:HE   | 1.72                     | 0.54              |
| 2:N:3718:LYS:O    | 3:O:5052:TYR:CD2  | 2.58                     | 0.54              |
| 3:O:5102:ILE:HG22 | 4:P:5552:ASP:HA   | 1.89                     | 0.54              |
| 4:P:5620:LEU:HD21 | 4:P:5651:TRP:HH2  | 1.72                     | 0.54              |
| 2:F:1594:ASP:OD2  | 2:J:2627:HIS:HB2  | 2.08                     | 0.54              |
| 2:F:1718:LYS:HD3  | 4:H:3596:ASN:O    | 1.99                     | 0.54              |
| 3:K:4032:TYR:CE1  | 3:K:4100:TYR:CB   | 2.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:P:5684:THR:O    | 4:P:5685:ALA:C    | 2.48                     | 0.54              |
| 4:D:689:GLU:HA    | 4:D:711:ARG:HH21  | 1.72                     | 0.54              |
| 3:K:4078:THR:CG2  | 3:K:4080:TYR:CE2  | 2.84                     | 0.54              |
| 3:O:5035:LEU:HD23 | 3:O:5037:VAL:HG23 | 1.82                     | 0.54              |
| 2:B:652:GLU:OE2   | 2:B:738:LYS:NZ    | 2.41                     | 0.54              |
| 3:C:118:ALA:HB3   | 3:C:150:PHE:HE2   | 0.78                     | 0.54              |
| 4:D:565:SER:O     | 4:D:575:LEU:HD23  | 2.07                     | 0.54              |
| 2:F:1677:PRO:HD2  | 2:F:1680:ALA:HB3  | 1.90                     | 0.54              |
| 3:K:4045:PHE:HZ   | 4:L:4546:PHE:HZ   | 0.62                     | 0.54              |
| 4:L:4565:SER:O    | 4:L:4575:LEU:HD23 | 2.07                     | 0.54              |
| 2:F:1630:GLU:HB2  | 2:N:3507:PRO:HB3  | 1.89                     | 0.54              |
| 3:G:3011:VAL:HB   | 3:G:3151:PRO:HB2  | 1.87                     | 0.54              |
| 4:H:3565:SER:O    | 4:H:3575:LEU:HD23 | 2.07                     | 0.54              |
| 1:M:3371:CYS:O    | 1:M:3372:THR:OG1  | 2.25                     | 0.54              |
| 2:N:3502:TYR:N    | 2:N:3537:SER:O    | 2.40                     | 0.54              |
| 2:N:3652:GLU:OE2  | 2:N:3738:LYS:NZ   | 2.41                     | 0.54              |
| 4:P:5557:ARG:HE   | 4:P:5560:VAL:HG23 | 1.70                     | 0.54              |
| 4:P:5565:SER:O    | 4:P:5575:LEU:HD23 | 2.07                     | 0.54              |
| 4:D:654:ASP:OD2   | 4:D:691:HIS:HB3   | 2.08                     | 0.54              |
| 3:G:3002:ILE:CD1  | 3:G:3098:ARG:HH12 | 1.83                     | 0.54              |
| 1:E:1061:LYS:NZ   | 1:E:1063:CYS:O    | 2.41                     | 0.54              |
| 2:F:1502:TYR:N    | 2:F:1537:SER:O    | 2.40                     | 0.54              |
| 3:G:3011:VAL:CG2  | 3:G:3152:GLU:HB2  | 2.38                     | 0.54              |
| 2:J:2652:GLU:OE2  | 2:J:2738:LYS:NZ   | 2.41                     | 0.54              |
| 4:L:4689:GLU:HA   | 4:L:4711:ARG:NE   | 2.23                     | 0.54              |
| 3:O:5011:VAL:CG2  | 3:O:5152:GLU:HB2  | 2.38                     | 0.54              |
| 1:E:1221:LYS:O    | 1:E:1235:THR:OG1  | 2.19                     | 0.54              |
| 3:K:4011:VAL:CG2  | 3:K:4152:GLU:HB2  | 2.38                     | 0.54              |
| 3:K:4035:LEU:HD23 | 3:K:4037:VAL:HG23 | 1.82                     | 0.54              |
| 4:L:4653:VAL:CG2  | 4:L:4658:VAL:HG21 | 2.35                     | 0.54              |
| 1:M:3061:LYS:NZ   | 1:M:3063:CYS:O    | 2.41                     | 0.54              |
| 3:C:11:VAL:CG2    | 3:C:152:GLU:HB2   | 2.38                     | 0.53              |
| 2:B:543:LYS:HB2   | 3:C:102:ILE:HD12  | 1.90                     | 0.53              |
| 2:B:678:SER:N     | 3:C:62:GLU:HB2    | 2.17                     | 0.53              |
| 2:B:690:ASP:OD2   | 2:B:702:THR:N     | 2.41                     | 0.53              |
| 2:F:1627:HIS:HB2  | 2:N:3594:ASP:OD2  | 2.08                     | 0.53              |
| 3:O:5032:TYR:CE1  | 3:O:5100:TYR:CB   | 2.89                     | 0.53              |
| 3:O:5032:TYR:CZ   | 3:O:5100:TYR:CZ   | 2.84                     | 0.53              |
| 1:A:61:LYS:NZ     | 1:A:63:CYS:O      | 2.41                     | 0.53              |
| 2:F:1652:GLU:OE2  | 2:F:1738:LYS:NZ   | 2.41                     | 0.53              |
| 4:H:3689:GLU:HA   | 4:H:3711:ARG:NE   | 2.23                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:2061:LYS:NZ   | 1:I:2063:CYS:O    | 2.41                     | 0.53              |
| 3:K:4039:GLN:CD   | 3:K:4045:PHE:CE1  | 2.87                     | 0.53              |
| 4:P:5654:ASP:OD2  | 4:P:5691:HIS:HB3  | 2.08                     | 0.53              |
| 1:I:2197:LYS:O    | 1:I:2200:SER:OG   | 2.18                     | 0.53              |
| 2:J:2690:ASP:OD2  | 2:J:2702:THR:N    | 2.42                     | 0.53              |
| 4:P:5683:LEU:HD22 | 4:P:5687:ALA:HB1  | 1.91                     | 0.53              |
| 4:P:5689:GLU:HA   | 4:P:5711:ARG:NE   | 2.23                     | 0.53              |
| 3:G:3128:LEU:HB3  | 4:H:3621:PHE:CG   | 2.44                     | 0.53              |
| 2:J:2594:ASP:OD2  | 2:N:3627:HIS:HB2  | 2.08                     | 0.53              |
| 3:K:4033:PRO:HA   | 3:K:4053:THR:HG23 | 1.91                     | 0.53              |
| 2:N:3679:GLY:HA3  | 3:O:5064:PHE:H    | 1.73                     | 0.53              |
| 4:D:689:GLU:HA    | 4:D:711:ARG:NE    | 2.23                     | 0.53              |
| 3:G:3102:ILE:HG22 | 4:H:3552:ASP:HA   | 1.89                     | 0.53              |
| 4:H:3654:ASP:OD2  | 4:H:3691:HIS:HB3  | 2.08                     | 0.53              |
| 4:L:4654:ASP:OD2  | 4:L:4691:HIS:HB3  | 2.08                     | 0.53              |
| 4:L:4689:GLU:HA   | 4:L:4711:ARG:HH21 | 1.72                     | 0.53              |
| 4:L:4689:GLU:HA   | 4:L:4711:ARG:HE   | 1.71                     | 0.53              |
| 3:C:21:SER:CB     | 3:C:80:TYR:HE2    | 2.13                     | 0.53              |
| 3:K:4030:THR:CG2  | 3:K:4054:ASN:HD22 | 2.17                     | 0.53              |
| 4:L:4683:LEU:HD22 | 4:L:4687:ALA:HB1  | 1.91                     | 0.53              |
| 3:O:5037:VAL:HG21 | 3:O:5107:TRP:HH2  | 1.70                     | 0.53              |
| 3:O:5128:LEU:HB3  | 4:P:5621:PHE:CG   | 2.44                     | 0.53              |
| 3:C:32:TYR:CE1    | 3:C:100:TYR:CB    | 2.89                     | 0.53              |
| 3:C:128:LEU:HB3   | 4:D:621:PHE:CG    | 2.44                     | 0.53              |
| 4:D:504:VAL:CG1   | 4:D:522:CYS:SG    | 2.97                     | 0.53              |
| 1:E:1035:ASN:OD1  | 1:E:1036:THR:N    | 2.42                     | 0.53              |
| 3:G:3217:ARG:HH21 | 4:H:3622:PRO:CD   | 2.08                     | 0.53              |
| 4:H:3504:VAL:CG1  | 4:H:3522:CYS:SG   | 2.97                     | 0.53              |
| 1:I:2221:LYS:O    | 1:I:2235:THR:OG1  | 2.19                     | 0.53              |
| 4:P:5554:ASN:C    | 4:P:5554:ASN:ND2  | 2.54                     | 0.53              |
| 1:A:343:ASN:OD1   | 1:A:344:ASP:N     | 2.42                     | 0.53              |
| 3:C:33:PRO:HA     | 3:C:53:THR:HG23   | 1.91                     | 0.53              |
| 4:D:507:GLU:OE2   | 4:D:521:THR:OG1   | 2.23                     | 0.53              |
| 4:D:653:VAL:HG23  | 4:D:658:VAL:CG2   | 2.35                     | 0.53              |
| 2:F:1690:ASP:OD2  | 2:F:1702:THR:N    | 2.41                     | 0.53              |
| 3:G:3033:PRO:HA   | 3:G:3053:THR:HG23 | 1.91                     | 0.53              |
| 3:G:3045:PHE:HZ   | 4:H:3546:PHE:HZ   | 0.62                     | 0.53              |
| 4:H:3653:VAL:CG2  | 4:H:3658:VAL:HG21 | 2.35                     | 0.53              |
| 4:H:3683:LEU:HD22 | 4:H:3687:ALA:HB1  | 1.91                     | 0.53              |
| 2:J:2558:LYS:HZ1  | 4:L:4501:GLN:HG3  | 1.73                     | 0.53              |
| 4:L:4504:VAL:CG1  | 4:L:4522:CYS:SG   | 2.97                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:L:4653:VAL:HG23 | 4:L:4658:VAL:CG2  | 2.35                     | 0.53              |
| 3:G:3033:PRO:HB2  | 3:G:3051:ILE:O    | 2.09                     | 0.53              |
| 3:O:5033:PRO:HA   | 3:O:5053:THR:HG23 | 1.91                     | 0.53              |
| 4:P:5504:VAL:CG1  | 4:P:5522:CYS:SG   | 2.97                     | 0.53              |
| 4:P:5653:VAL:HG23 | 4:P:5658:VAL:CG2  | 2.35                     | 0.53              |
| 1:E:1005:ALA:N    | 1:E:1279:ILE:O    | 2.42                     | 0.52              |
| 4:H:3630:THR:HG22 | 4:H:3632:LYS:HB2  | 1.91                     | 0.52              |
| 3:K:4030:THR:O    | 3:K:4030:THR:HG22 | 2.09                     | 0.52              |
| 4:L:4514:PRO:HG2  | 4:L:4609:LEU:O    | 2.03                     | 0.52              |
| 4:D:683:LEU:HD22  | 4:D:687:ALA:HB1   | 1.91                     | 0.52              |
| 2:F:1507:PRO:HB3  | 2:J:2630:GLU:HB2  | 1.89                     | 0.52              |
| 1:I:2035:ASN:OD1  | 1:I:2036:THR:N    | 2.42                     | 0.52              |
| 1:I:2343:ASN:OD1  | 1:I:2344:ASP:N    | 2.42                     | 0.52              |
| 1:M:3035:ASN:OD1  | 1:M:3036:THR:N    | 2.42                     | 0.52              |
| 1:M:3260:CYS:H    | 2:N:3782:ARG:HH22 | 1.58                     | 0.52              |
| 1:A:35:ASN:OD1    | 1:A:36:THR:N      | 2.42                     | 0.52              |
| 3:C:37:VAL:HG21   | 3:C:107:TRP:HH2   | 1.70                     | 0.52              |
| 1:E:1343:ASN:OD1  | 1:E:1344:ASP:N    | 2.42                     | 0.52              |
| 3:O:5011:VAL:HB   | 3:O:5151:PRO:HB2  | 1.87                     | 0.52              |
| 3:O:5033:PRO:HB2  | 3:O:5051:ILE:O    | 2.09                     | 0.52              |
| 3:K:4102:ILE:CG2  | 3:K:4102:ILE:O    | 2.51                     | 0.52              |
| 2:N:3690:ASP:OD2  | 2:N:3702:THR:N    | 2.42                     | 0.52              |
| 4:P:5514:PRO:HG2  | 4:P:5609:LEU:O    | 2.03                     | 0.52              |
| 2:B:577:SER:O     | 2:B:589:GLN:N     | 2.37                     | 0.52              |
| 3:C:33:PRO:HB2    | 3:C:51:ILE:O      | 2.09                     | 0.52              |
| 4:H:3653:VAL:HG23 | 4:H:3658:VAL:CG2  | 2.35                     | 0.52              |
| 1:I:2005:ALA:N    | 1:I:2279:ILE:O    | 2.42                     | 0.52              |
| 2:J:2547:VAL:HG21 | 3:K:4102:ILE:CG2  | 2.37                     | 0.52              |
| 3:K:4102:ILE:HG22 | 4:L:4552:ASP:HA   | 1.89                     | 0.52              |
| 1:M:3315:GLY:O    | 1:M:3357:PHE:N    | 2.42                     | 0.52              |
| 1:M:3343:ASN:OD1  | 1:M:3344:ASP:N    | 2.42                     | 0.52              |
| 2:B:543:LYS:CD    | 3:C:102:ILE:HD12  | 2.32                     | 0.52              |
| 2:J:2677:PRO:HD2  | 2:J:2680:ALA:HB3  | 1.90                     | 0.52              |
| 3:G:3032:TYR:CE1  | 3:G:3100:TYR:CB   | 2.89                     | 0.52              |
| 3:G:3102:ILE:HG13 | 4:H:3552:ASP:CB   | 2.34                     | 0.52              |
| 3:O:5212:LYS:CE   | 4:P:5626:GLU:OE1  | 2.58                     | 0.52              |
| 3:C:24:ALA:HB1    | 3:C:27:TYR:HE1    | 1.75                     | 0.52              |
| 2:F:1679:GLY:HA3  | 3:G:3062:GLU:N    | 2.25                     | 0.52              |
| 3:K:4128:LEU:HB3  | 4:L:4621:PHE:CG   | 2.44                     | 0.52              |
| 1:M:3005:ALA:N    | 1:M:3279:ILE:O    | 2.42                     | 0.52              |
| 2:B:544:THR:OG1   | 4:D:593:TRP:CE2   | 2.62                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:560:GLN:HG3   | 4:D:595:ASN:CA    | 2.39                     | 0.52              |
| 2:B:677:PRO:HD2   | 2:B:680:ALA:HB3   | 1.90                     | 0.52              |
| 3:C:30:THR:O      | 3:C:30:THR:HG22   | 2.09                     | 0.52              |
| 3:O:5030:THR:O    | 3:O:5030:THR:HG22 | 2.09                     | 0.52              |
| 3:C:78:THR:CG2    | 3:C:80:TYR:CE2    | 2.84                     | 0.52              |
| 3:C:212:LYS:CE    | 4:D:626:GLU:OE1   | 2.58                     | 0.52              |
| 3:G:3107:TRP:HB2  | 4:H:3546:PHE:CB   | 2.40                     | 0.52              |
| 3:K:4107:TRP:HB2  | 4:L:4546:PHE:CB   | 2.40                     | 0.52              |
| 3:K:4212:LYS:CE   | 4:L:4626:GLU:OE1  | 2.58                     | 0.52              |
| 2:J:2733:ASP:OD1  | 2:J:2734:THR:N    | 2.44                     | 0.51              |
| 2:N:3561:LYS:HE2  | 4:P:5532:SER:OG   | 2.09                     | 0.51              |
| 3:O:5035:LEU:HD23 | 3:O:5036:TRP:N    | 2.25                     | 0.51              |
| 4:D:630:THR:HG22  | 4:D:632:LYS:HB2   | 1.91                     | 0.51              |
| 3:G:3030:THR:O    | 3:G:3030:THR:HG22 | 2.09                     | 0.51              |
| 3:G:3212:LYS:CE   | 4:H:3626:GLU:OE1  | 2.58                     | 0.51              |
| 4:H:3542:PRO:HB2  | 4:H:3669:LYS:HB2  | 1.92                     | 0.51              |
| 3:O:5097:VAL:CG2  | 3:O:5107:TRP:CD2  | 2.93                     | 0.51              |
| 4:P:5507:GLU:OE2  | 4:P:5521:THR:OG1  | 2.23                     | 0.51              |
| 3:C:39:GLN:CD     | 3:C:45:PHE:CE1    | 2.87                     | 0.51              |
| 4:D:542:PRO:HB2   | 4:D:669:LYS:HB2   | 1.92                     | 0.51              |
| 1:E:1260:CYS:H    | 2:F:1782:ARG:HH22 | 1.58                     | 0.51              |
| 3:G:3097:VAL:CG2  | 3:G:3107:TRP:CD2  | 2.93                     | 0.51              |
| 2:J:2562:SER:O    | 4:L:4532:SER:CB   | 1.85                     | 0.51              |
| 3:K:4033:PRO:HB2  | 3:K:4051:ILE:O    | 2.09                     | 0.51              |
| 3:C:107:TRP:HB2   | 4:D:546:PHE:CB    | 2.40                     | 0.51              |
| 3:G:3035:LEU:HD23 | 3:G:3036:TRP:N    | 2.25                     | 0.51              |
| 4:H:3520:LEU:N    | 4:H:3520:LEU:CD2  | 2.70                     | 0.51              |
| 2:N:3733:ASP:OD1  | 2:N:3734:THR:N    | 2.44                     | 0.51              |
| 1:A:5:ALA:N       | 1:A:279:ILE:O     | 2.42                     | 0.51              |
| 1:A:389:VAL:HG12  | 1:A:390:ASP:H     | 1.76                     | 0.51              |
| 2:B:561:LYS:HG3   | 4:D:532:SER:OG    | 2.10                     | 0.51              |
| 2:B:718:LYS:HE3   | 4:D:596:ASN:C     | 2.35                     | 0.51              |
| 1:E:1315:GLY:O    | 1:E:1357:PHE:N    | 2.42                     | 0.51              |
| 1:I:2260:CYS:H    | 2:J:2782:ARG:HH22 | 1.58                     | 0.51              |
| 2:J:2569:HIS:O    | 2:J:2599:GLY:N    | 2.44                     | 0.51              |
| 1:A:315:GLY:O     | 1:A:357:PHE:N     | 2.42                     | 0.51              |
| 2:J:2508:ASN:OD1  | 2:J:2610:THR:OG1  | 2.11                     | 0.51              |
| 3:K:4011:VAL:HB   | 3:K:4151:PRO:HB2  | 1.87                     | 0.51              |
| 4:P:5630:THR:HG22 | 4:P:5632:LYS:HB2  | 1.92                     | 0.51              |
| 3:C:97:VAL:CG2    | 3:C:107:TRP:CD2   | 2.93                     | 0.51              |
| 1:E:1117:ASP:OD1  | 1:E:1181:TYR:OH   | 2.20                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1676:VAL:N    | 4:H:3501:GLN:NE2  | 2.51                     | 0.51              |
| 2:J:2680:ALA:HB2  | 3:K:4062:GLU:CG   | 2.41                     | 0.51              |
| 4:L:4549:LEU:HD12 | 4:L:4560:VAL:HG21 | 1.93                     | 0.51              |
| 4:L:4630:THR:HG22 | 4:L:4632:LYS:HB2  | 1.91                     | 0.51              |
| 2:F:1569:HIS:O    | 2:F:1599:GLY:N    | 2.44                     | 0.51              |
| 3:G:3037:VAL:HG21 | 3:G:3107:TRP:HH2  | 1.70                     | 0.51              |
| 3:K:4035:LEU:HD23 | 3:K:4036:TRP:N    | 2.25                     | 0.51              |
| 4:L:4589:PHE:CE1  | 4:L:4603:GLY:HA3  | 2.46                     | 0.51              |
| 2:N:3680:ALA:HA   | 3:O:5065:LYS:HD2  | 1.89                     | 0.51              |
| 3:O:5032:TYR:CD1  | 3:O:5100:TYR:HB2  | 2.46                     | 0.51              |
| 3:C:35:LEU:HD23   | 3:C:36:TRP:N      | 2.25                     | 0.51              |
| 1:E:1389:VAL:HG12 | 1:E:1390:ASP:H    | 1.76                     | 0.51              |
| 2:F:1733:ASP:OD1  | 2:F:1734:THR:N    | 2.44                     | 0.51              |
| 2:J:2680:ALA:CA   | 3:K:4062:GLU:CG   | 2.81                     | 0.51              |
| 3:K:4097:VAL:CG2  | 3:K:4107:TRP:CD2  | 2.93                     | 0.51              |
| 4:P:5549:LEU:HD12 | 4:P:5560:VAL:HG21 | 1.93                     | 0.51              |
| 4:L:4507:GLU:OE2  | 4:L:4521:THR:OG1  | 2.23                     | 0.50              |
| 1:A:260:CYS:H     | 2:B:782:ARG:HH22  | 1.58                     | 0.50              |
| 4:H:3507:GLU:O    | 4:H:3604:THR:OG1  | 2.27                     | 0.50              |
| 1:I:2203:ASP:OD1  | 1:I:2204:LEU:N    | 2.43                     | 0.50              |
| 1:M:3389:VAL:HG12 | 1:M:3390:ASP:H    | 1.76                     | 0.50              |
| 2:N:3569:HIS:O    | 2:N:3599:GLY:N    | 2.44                     | 0.50              |
| 2:B:508:ASN:OD1   | 2:B:610:THR:OG1   | 2.11                     | 0.50              |
| 2:B:560:GLN:CG    | 4:D:595:ASN:CA    | 2.90                     | 0.50              |
| 2:B:733:ASP:OD1   | 2:B:734:THR:N     | 2.44                     | 0.50              |
| 1:E:1203:ASP:OD1  | 1:E:1204:LEU:N    | 2.43                     | 0.50              |
| 3:G:3032:TYR:CD1  | 3:G:3100:TYR:HB2  | 2.46                     | 0.50              |
| 1:I:2389:VAL:HG12 | 1:I:2390:ASP:H    | 1.76                     | 0.50              |
| 3:K:4032:TYR:CD1  | 3:K:4100:TYR:HB2  | 2.46                     | 0.50              |
| 1:M:3203:ASP:OD1  | 1:M:3204:LEU:N    | 2.43                     | 0.50              |
| 3:O:5107:TRP:HB2  | 4:P:5546:PHE:CB   | 2.40                     | 0.50              |
| 2:B:678:SER:H     | 3:C:62:GLU:HB2    | 1.76                     | 0.50              |
| 3:C:13:ASN:OD1    | 3:C:116:SER:O     | 2.29                     | 0.50              |
| 1:I:2315:GLY:O    | 1:I:2357:PHE:N    | 2.42                     | 0.50              |
| 1:A:15:TYR:O      | 1:A:17:ALA:N      | 2.44                     | 0.50              |
| 1:A:388:ILE:HD12  | 1:A:388:ILE:O     | 2.12                     | 0.50              |
| 3:C:30:THR:CG2    | 3:C:54:ASN:HD22   | 2.17                     | 0.50              |
| 3:C:32:TYR:CD1    | 3:C:100:TYR:HB2   | 2.46                     | 0.50              |
| 4:D:643:TYR:HA    | 4:D:644:PRO:C     | 2.36                     | 0.50              |
| 3:G:3013:ASN:OD1  | 3:G:3116:SER:O    | 2.29                     | 0.50              |
| 4:H:3643:TYR:HA   | 4:H:3644:PRO:C    | 2.36                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:5102:ILE:HB   | 4:P:5552:ASP:CA   | 2.40                     | 0.50              |
| 4:P:5589:PHE:CE1  | 4:P:5603:GLY:HA3  | 2.46                     | 0.50              |
| 3:C:102:ILE:HG22  | 4:D:552:ASP:HA    | 1.89                     | 0.50              |
| 4:H:3589:PHE:CE1  | 4:H:3603:GLY:HA3  | 2.46                     | 0.50              |
| 1:M:3015:TYR:O    | 1:M:3017:ALA:N    | 2.44                     | 0.50              |
| 2:B:563:ILE:CB    | 4:D:532:SER:HB3   | 2.41                     | 0.50              |
| 2:B:569:HIS:O     | 2:B:599:GLY:N     | 2.44                     | 0.50              |
| 3:C:118:ALA:CB    | 3:C:150:PHE:CD2   | 2.77                     | 0.50              |
| 4:D:589:PHE:CE1   | 4:D:603:GLY:HA3   | 2.46                     | 0.50              |
| 4:P:5549:LEU:HD12 | 4:P:5560:VAL:CG2  | 2.42                     | 0.50              |
| 4:L:4542:PRO:HB2  | 4:L:4669:LYS:HB2  | 1.92                     | 0.50              |
| 1:M:3221:LYS:O    | 1:M:3235:THR:OG1  | 2.19                     | 0.50              |
| 4:P:5520:LEU:N    | 4:P:5520:LEU:CD2  | 2.70                     | 0.50              |
| 4:P:5542:PRO:HB2  | 4:P:5669:LYS:HB2  | 1.92                     | 0.50              |
| 4:P:5643:TYR:HA   | 4:P:5644:PRO:C    | 2.36                     | 0.50              |
| 4:D:549:LEU:HD12  | 4:D:560:VAL:HG21  | 1.93                     | 0.50              |
| 1:I:2388:ILE:HD12 | 1:I:2388:ILE:O    | 2.12                     | 0.50              |
| 2:B:678:SER:CB    | 4:D:597:LEU:HD23  | 2.34                     | 0.49              |
| 1:I:2007:MET:SD   | 1:I:2279:ILE:HD12 | 2.52                     | 0.49              |
| 4:L:4549:LEU:HD12 | 4:L:4560:VAL:CG2  | 2.42                     | 0.49              |
| 3:O:5217:ARG:HH21 | 4:P:5622:PRO:CD   | 2.08                     | 0.49              |
| 1:E:1388:ILE:HD12 | 1:E:1388:ILE:O    | 2.12                     | 0.49              |
| 4:H:3542:PRO:HB3  | 4:H:3669:LYS:CD   | 2.42                     | 0.49              |
| 1:I:2015:TYR:O    | 1:I:2017:ALA:N    | 2.44                     | 0.49              |
| 1:A:22:PRO:CB     | 1:I:2382:LYS:CB   | 2.76                     | 0.49              |
| 3:C:2:ILE:HA      | 3:C:25:SER:O      | 2.13                     | 0.49              |
| 3:G:3002:ILE:HA   | 3:G:3025:SER:O    | 2.13                     | 0.49              |
| 3:G:3102:ILE:HB   | 4:H:3552:ASP:CA   | 2.40                     | 0.49              |
| 3:K:4013:ASN:OD1  | 3:K:4116:SER:O    | 2.29                     | 0.49              |
| 4:L:4643:TYR:HA   | 4:L:4644:PRO:C    | 2.36                     | 0.49              |
| 2:B:544:THR:CB    | 4:D:593:TRP:NE1   | 2.75                     | 0.49              |
| 2:B:718:LYS:HZ2   | 4:D:596:ASN:HB2   | 1.61                     | 0.49              |
| 3:C:35:LEU:HD23   | 3:C:37:VAL:HG23   | 1.82                     | 0.49              |
| 3:K:4035:LEU:CD2  | 3:K:4037:VAL:HG22 | 2.12                     | 0.49              |
| 2:N:3780:THR:OG1  | 2:N:3791:THR:O    | 2.30                     | 0.49              |
| 4:D:549:LEU:HD12  | 4:D:560:VAL:CG2   | 2.42                     | 0.49              |
| 1:M:3301:GLU:O    | 1:M:3320:ALA:N    | 2.43                     | 0.49              |
| 3:O:5013:ASN:OD1  | 3:O:5116:SER:O    | 2.29                     | 0.49              |
| 1:A:203:ASP:OD1   | 1:A:204:LEU:N     | 2.43                     | 0.49              |
| 4:D:506:GLN:OE1   | 4:D:601:GLY:HA3   | 2.13                     | 0.49              |
| 2:F:1796:GLU:N    | 2:F:1796:GLU:OE1  | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:3048:MET:HG2  | 3:G:3064:PHE:CE1  | 2.48                     | 0.49              |
| 4:H:3549:LEU:HD12 | 4:H:3560:VAL:HG21 | 1.93                     | 0.49              |
| 3:O:5048:MET:HG2  | 3:O:5064:PHE:CE1  | 2.48                     | 0.49              |
| 1:A:89:TRP:N      | 2:B:515:ASP:OD2   | 2.46                     | 0.49              |
| 4:D:512:THR:HG22  | 4:D:608:VAL:HG22  | 1.95                     | 0.49              |
| 3:K:4024:ALA:HB1  | 3:K:4027:TYR:HE1  | 1.75                     | 0.49              |
| 1:M:3388:ILE:HD12 | 1:M:3388:ILE:O    | 2.12                     | 0.49              |
| 2:N:3559:THR:C    | 4:P:5595:ASN:O    | 2.44                     | 0.49              |
| 2:N:3560:GLN:O    | 4:P:5595:ASN:HA   | 2.13                     | 0.49              |
| 1:A:265:GLU:OE1   | 1:A:268:ARG:NH2   | 2.46                     | 0.49              |
| 1:A:301:GLU:O     | 1:A:320:ALA:N     | 2.43                     | 0.49              |
| 3:C:11:VAL:CB     | 3:C:151:PRO:CB    | 2.86                     | 0.49              |
| 1:E:1197:LYS:O    | 1:E:1200:SER:OG   | 2.18                     | 0.49              |
| 4:H:3506:GLN:OE1  | 4:H:3601:GLY:HA3  | 2.13                     | 0.49              |
| 3:O:5002:ILE:HA   | 3:O:5025:SER:O    | 2.13                     | 0.49              |
| 3:O:5045:PHE:HZ   | 4:P:5546:PHE:HZ   | 0.62                     | 0.49              |
| 4:P:5506:GLN:OE1  | 4:P:5601:GLY:HA3  | 2.13                     | 0.49              |
| 2:B:544:THR:HG21  | 4:D:593:TRP:CG    | 2.48                     | 0.49              |
| 3:C:48:MET:HG2    | 3:C:64:PHE:CE1    | 2.48                     | 0.49              |
| 2:F:1562:SER:O    | 4:H:3531:SER:C    | 2.56                     | 0.49              |
| 3:G:3039:GLN:CD   | 3:G:3045:PHE:CE1  | 2.86                     | 0.49              |
| 4:H:3512:THR:HG22 | 4:H:3608:VAL:HG22 | 1.95                     | 0.49              |
| 4:L:4512:THR:HG22 | 4:L:4608:VAL:HG22 | 1.95                     | 0.49              |
| 2:N:3677:PRO:N    | 3:O:5062:GLU:HB2  | 2.07                     | 0.49              |
| 4:P:5597:LEU:C    | 4:P:5597:LEU:HD12 | 2.38                     | 0.49              |
| 1:E:1015:TYR:O    | 1:E:1017:ALA:N    | 2.44                     | 0.48              |
| 4:H:3549:LEU:HD12 | 4:H:3560:VAL:CG2  | 2.42                     | 0.48              |
| 1:I:2265:GLU:OE1  | 1:I:2268:ARG:NH2  | 2.46                     | 0.48              |
| 2:N:3678:SER:OG   | 3:O:5047:TRP:CZ3  | 2.64                     | 0.48              |
| 4:P:5512:THR:HG22 | 4:P:5608:VAL:HG22 | 1.95                     | 0.48              |
| 1:E:1007:MET:SD   | 1:E:1279:ILE:HD12 | 2.52                     | 0.48              |
| 3:G:3018:VAL:O    | 3:G:3082:GLN:HA   | 2.14                     | 0.48              |
| 1:I:2117:ASP:OD1  | 1:I:2181:TYR:OH   | 2.20                     | 0.48              |
| 3:K:4048:MET:HG2  | 3:K:4064:PHE:CE1  | 2.48                     | 0.48              |
| 1:M:3007:MET:SD   | 1:M:3279:ILE:HD12 | 2.52                     | 0.48              |
| 1:A:7:MET:SD      | 1:A:279:ILE:HD12  | 2.52                     | 0.48              |
| 1:E:1265:GLU:OE1  | 1:E:1268:ARG:NH2  | 2.46                     | 0.48              |
| 2:F:1563:ILE:CG2  | 4:H:3530:THR:HB   | 2.43                     | 0.48              |
| 1:I:2301:GLU:OE1  | 1:I:2303:LYS:NZ   | 2.40                     | 0.48              |
| 1:M:3037:ARG:HH12 | 1:M:3132:MET:HG3  | 1.79                     | 0.48              |
| 2:N:3560:GLN:C    | 4:P:5595:ASN:OD1  | 2.54                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1679:GLY:HA3  | 3:G:3062:GLU:H    | 1.77                     | 0.48              |
| 2:J:2796:GLU:OE1  | 2:J:2796:GLU:N    | 2.46                     | 0.48              |
| 1:M:3268:ARG:NE   | 1:M:3270:GLU:OE2  | 2.47                     | 0.48              |
| 1:A:371:CYS:O     | 1:A:372:THR:OG1   | 2.25                     | 0.48              |
| 1:E:1096:CYS:O    | 1:E:1100:ASN:ND2  | 2.46                     | 0.48              |
| 1:I:2089:TRP:N    | 2:J:2515:ASP:OD2  | 2.46                     | 0.48              |
| 3:K:4057:GLU:C    | 3:K:4058:PRO:CD   | 2.74                     | 0.48              |
| 4:L:4506:GLN:OE1  | 4:L:4601:GLY:HA3  | 2.13                     | 0.48              |
| 1:M:3265:GLU:OE1  | 1:M:3268:ARG:NH2  | 2.46                     | 0.48              |
| 2:N:3796:GLU:OE1  | 2:N:3796:GLU:N    | 2.45                     | 0.48              |
| 2:B:796:GLU:OE1   | 2:B:796:GLU:N     | 2.46                     | 0.48              |
| 4:D:507:GLU:O     | 4:D:604:THR:OG1   | 2.27                     | 0.48              |
| 2:F:1543:LYS:HE3  | 4:H:3531:SER:HB2  | 1.94                     | 0.48              |
| 1:I:2037:ARG:HH12 | 1:I:2132:MET:HG3  | 1.79                     | 0.48              |
| 1:I:2268:ARG:NE   | 1:I:2270:GLU:OE2  | 2.47                     | 0.48              |
| 3:K:4002:ILE:HA   | 3:K:4025:SER:O    | 2.13                     | 0.48              |
| 3:K:4097:VAL:HG22 | 3:K:4107:TRP:CE3  | 2.49                     | 0.48              |
| 4:L:4507:GLU:O    | 4:L:4604:THR:OG1  | 2.27                     | 0.48              |
| 1:M:3260:CYS:H    | 2:N:3782:ARG:NH2  | 2.11                     | 0.48              |
| 2:N:3678:SER:CB   | 3:O:5047:TRP:CZ3  | 2.97                     | 0.48              |
| 4:D:597:LEU:C     | 4:D:597:LEU:HD12  | 2.38                     | 0.48              |
| 1:E:1268:ARG:NE   | 1:E:1270:GLU:OE2  | 2.47                     | 0.48              |
| 4:H:3514:PRO:HG2  | 4:H:3609:LEU:O    | 2.03                     | 0.48              |
| 4:H:3597:LEU:HD12 | 4:H:3597:LEU:C    | 2.38                     | 0.48              |
| 3:K:4104:LEU:N    | 4:L:4536:ASN:OD1  | 2.43                     | 0.48              |
| 1:M:3129:VAL:HG22 | 1:M:3149:VAL:HG11 | 1.96                     | 0.48              |
| 2:N:3679:GLY:CA   | 3:O:5064:PHE:H    | 2.26                     | 0.48              |
| 3:O:5035:LEU:HG   | 3:O:5047:TRP:NE1  | 2.29                     | 0.48              |
| 1:A:37:ARG:HH12   | 1:A:132:MET:HG3   | 1.79                     | 0.48              |
| 3:C:18:VAL:O      | 3:C:82:GLN:HA     | 2.14                     | 0.48              |
| 3:C:35:LEU:HB3    | 3:C:97:VAL:HB     | 1.95                     | 0.48              |
| 3:C:217:ARG:HH21  | 4:D:622:PRO:CD    | 2.08                     | 0.48              |
| 1:E:1260:CYS:H    | 2:F:1782:ARG:NH2  | 2.11                     | 0.48              |
| 4:L:4597:LEU:C    | 4:L:4597:LEU:HD12 | 2.38                     | 0.48              |
| 4:L:4662:MET:HE3  | 4:L:4662:MET:HB2  | 1.59                     | 0.48              |
| 3:O:5018:VAL:O    | 3:O:5082:GLN:HA   | 2.14                     | 0.48              |
| 3:O:5035:LEU:HB3  | 3:O:5097:VAL:HB   | 1.95                     | 0.48              |
| 1:A:268:ARG:NE    | 1:A:270:GLU:OE2   | 2.47                     | 0.47              |
| 3:C:2:ILE:CD1     | 3:C:98:ARG:HH11   | 2.15                     | 0.47              |
| 3:C:102:ILE:HB    | 4:D:552:ASP:CA    | 2.40                     | 0.47              |
| 4:D:703:HIS:ND1   | 4:D:703:HIS:N     | 2.62                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:P:5542:PRO:HB3  | 4:P:5669:LYS:CD   | 2.42                     | 0.47              |
| 1:A:391:TYR:CE2   | 2:B:784:LEU:HD11  | 2.49                     | 0.47              |
| 2:F:1718:LYS:HE2  | 4:H:3595:ASN:C    | 2.20                     | 0.47              |
| 3:K:4018:VAL:O    | 3:K:4082:GLN:HA   | 2.14                     | 0.47              |
| 1:M:3391:TYR:CE2  | 2:N:3784:LEU:HD11 | 2.49                     | 0.47              |
| 2:N:3561:LYS:CE   | 4:P:5532:SER:OG   | 2.41                     | 0.47              |
| 4:P:5689:GLU:HA   | 4:P:5711:ARG:CZ   | 2.44                     | 0.47              |
| 4:D:689:GLU:HA    | 4:D:711:ARG:CZ    | 2.44                     | 0.47              |
| 1:E:1089:TRP:N    | 2:F:1515:ASP:OD2  | 2.46                     | 0.47              |
| 3:G:3021:SER:HG   | 3:G:3080:TYR:HE2  | 0.56                     | 0.47              |
| 1:I:2312:ASP:OD1  | 1:I:2313:PHE:N    | 2.48                     | 0.47              |
| 2:J:2563:ILE:HG22 | 4:L:4532:SER:CA   | 2.31                     | 0.47              |
| 1:M:3312:ASP:OD1  | 1:M:3313:PHE:N    | 2.48                     | 0.47              |
| 3:O:5097:VAL:HG21 | 3:O:5107:TRP:CD2  | 2.49                     | 0.47              |
| 1:A:129:VAL:HG22  | 1:A:149:VAL:HG11  | 1.96                     | 0.47              |
| 1:A:390:ASP:O     | 2:B:823:TRP:HB3   | 2.14                     | 0.47              |
| 1:I:2260:CYS:H    | 2:J:2782:ARG:NH2  | 2.12                     | 0.47              |
| 3:C:11:VAL:CG2    | 3:C:152:GLU:N     | 2.70                     | 0.47              |
| 3:C:103:SER:HA    | 4:D:598:TRP:CH2   | 2.50                     | 0.47              |
| 3:G:3097:VAL:HG22 | 3:G:3107:TRP:CE3  | 2.49                     | 0.47              |
| 1:I:2323:SER:N    | 1:I:2350:SER:OG   | 2.47                     | 0.47              |
| 3:K:4035:LEU:HB3  | 3:K:4097:VAL:HB   | 1.95                     | 0.47              |
| 3:K:4102:ILE:HG22 | 4:L:4534:CYS:CB   | 2.13                     | 0.47              |
| 3:K:4107:TRP:CB   | 4:L:4546:PHE:HB2  | 2.45                     | 0.47              |
| 1:M:3096:CYS:O    | 1:M:3100:ASN:ND2  | 2.46                     | 0.47              |
| 4:P:5703:HIS:N    | 4:P:5703:HIS:ND1  | 2.62                     | 0.47              |
| 2:B:780:THR:OG1   | 2:B:791:THR:O     | 2.30                     | 0.47              |
| 3:C:107:TRP:CB    | 4:D:546:PHE:HB2   | 2.45                     | 0.47              |
| 1:E:1323:SER:N    | 1:E:1350:SER:OG   | 2.47                     | 0.47              |
| 4:H:3689:GLU:HA   | 4:H:3711:ARG:CZ   | 2.44                     | 0.47              |
| 1:M:3323:SER:N    | 1:M:3350:SER:OG   | 2.47                     | 0.47              |
| 3:O:5107:TRP:CB   | 4:P:5546:PHE:HB2  | 2.45                     | 0.47              |
| 1:A:260:CYS:H     | 2:B:782:ARG:NH2   | 2.11                     | 0.47              |
| 1:A:312:ASP:OD1   | 1:A:313:PHE:N     | 2.48                     | 0.47              |
| 1:E:1229:ILE:HG21 | 2:F:1513:ARG:HE   | 1.80                     | 0.47              |
| 1:E:1371:CYS:O    | 1:E:1372:THR:OG1  | 2.25                     | 0.47              |
| 3:G:3057:GLU:C    | 3:G:3058:PRO:CD   | 2.74                     | 0.47              |
| 4:H:3703:HIS:ND1  | 4:H:3703:HIS:N    | 2.62                     | 0.47              |
| 1:I:2391:TYR:CE2  | 2:J:2784:LEU:HD11 | 2.49                     | 0.47              |
| 2:J:2558:LYS:HE3  | 4:L:4501:GLN:HG3  | 1.97                     | 0.47              |
| 3:K:4035:LEU:HG   | 3:K:4047:TRP:NE1  | 2.29                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:4097:VAL:HG21 | 3:K:4107:TRP:CD2  | 2.50                     | 0.47              |
| 3:K:4103:SER:HA   | 4:L:4598:TRP:CH2  | 2.50                     | 0.47              |
| 4:L:4703:HIS:ND1  | 4:L:4703:HIS:N    | 2.62                     | 0.47              |
| 3:O:5011:VAL:CG2  | 3:O:5152:GLU:N    | 2.70                     | 0.47              |
| 1:A:246:ARG:NH1   | 1:A:247:ASP:OD2   | 2.48                     | 0.47              |
| 3:C:78:THR:CG2    | 3:C:80:TYR:OH     | 2.48                     | 0.47              |
| 3:G:3035:LEU:HG   | 3:G:3047:TRP:NE1  | 2.29                     | 0.47              |
| 3:G:3035:LEU:HB3  | 3:G:3097:VAL:HB   | 1.95                     | 0.47              |
| 1:E:1246:ARG:NH1  | 1:E:1247:ASP:OD2  | 2.48                     | 0.47              |
| 3:G:3097:VAL:HG21 | 3:G:3107:TRP:CD2  | 2.49                     | 0.47              |
| 2:J:2547:VAL:HG11 | 3:K:4102:ILE:CA   | 2.43                     | 0.47              |
| 4:L:4689:GLU:HA   | 4:L:4711:ARG:CZ   | 2.44                     | 0.47              |
| 1:M:3229:ILE:HG21 | 2:N:3513:ARG:HE   | 1.80                     | 0.47              |
| 1:A:323:SER:N     | 1:A:350:SER:OG    | 2.47                     | 0.47              |
| 3:C:12:LYS:HD2    | 3:C:16:GLU:OE1    | 2.16                     | 0.47              |
| 4:D:524:SER:HG    | 4:D:594:TYR:HH    | 1.52                     | 0.47              |
| 1:E:1037:ARG:HH12 | 1:E:1132:MET:HG3  | 1.79                     | 0.47              |
| 1:E:1312:ASP:OD1  | 1:E:1313:PHE:N    | 2.48                     | 0.47              |
| 4:H:3549:LEU:HA   | 4:H:3560:VAL:HG21 | 1.97                     | 0.47              |
| 4:H:3662:MET:HE3  | 4:H:3662:MET:HB2  | 1.59                     | 0.47              |
| 1:I:2016:LYS:O    | 1:I:2332:HIS:ND1  | 2.48                     | 0.47              |
| 1:I:2229:ILE:HG21 | 2:J:2513:ARG:HE   | 1.80                     | 0.47              |
| 1:I:2390:ASP:O    | 2:J:2823:TRP:HB3  | 2.14                     | 0.47              |
| 1:M:3016:LYS:O    | 1:M:3332:HIS:ND1  | 2.48                     | 0.47              |
| 4:P:5549:LEU:HA   | 4:P:5560:VAL:HG21 | 1.97                     | 0.47              |
| 3:G:3107:TRP:CB   | 4:H:3546:PHE:HB2  | 2.45                     | 0.46              |
| 1:M:3246:ARG:NH1  | 1:M:3247:ASP:OD2  | 2.48                     | 0.46              |
| 1:M:3390:ASP:O    | 2:N:3823:TRP:HB3  | 2.14                     | 0.46              |
| 1:A:16:LYS:O      | 1:A:332:HIS:ND1   | 2.48                     | 0.46              |
| 1:A:229:ILE:HG21  | 2:B:513:ARG:HE    | 1.80                     | 0.46              |
| 1:E:1391:TYR:CE2  | 2:F:1784:LEU:HD11 | 2.49                     | 0.46              |
| 3:G:3048:MET:HE1  | 3:G:3081:LEU:HD21 | 1.97                     | 0.46              |
| 2:J:2780:THR:OG1  | 2:J:2791:THR:O    | 2.30                     | 0.46              |
| 3:O:5047:TRP:NE1  | 3:O:5049:GLY:O    | 2.49                     | 0.46              |
| 3:G:3035:LEU:HD23 | 3:G:3035:LEU:C    | 2.40                     | 0.46              |
| 3:G:3103:SER:HA   | 4:H:3598:TRP:CH2  | 2.50                     | 0.46              |
| 3:K:4047:TRP:NE1  | 3:K:4049:GLY:O    | 2.49                     | 0.46              |
| 2:N:3558:LYS:O    | 4:P:5596:ASN:HB3  | 2.16                     | 0.46              |
| 3:C:35:LEU:HG     | 3:C:47:TRP:NE1    | 2.29                     | 0.46              |
| 3:G:3012:LYS:HD2  | 3:G:3016:GLU:OE1  | 2.16                     | 0.46              |
| 3:G:3097:VAL:HG22 | 3:G:3107:TRP:CD2  | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:2129:VAL:HG22 | 1:I:2149:VAL:HG11 | 1.96                     | 0.46              |
| 3:O:5024:ALA:HB1  | 3:O:5027:TYR:HE1  | 1.75                     | 0.46              |
| 1:E:1016:LYS:O    | 1:E:1332:HIS:ND1  | 2.48                     | 0.46              |
| 1:E:1390:ASP:O    | 2:F:1823:TRP:HB3  | 2.14                     | 0.46              |
| 1:I:2246:ARG:NH1  | 1:I:2247:ASP:OD2  | 2.48                     | 0.46              |
| 3:K:4072:LEU:HD13 | 3:K:4074:ILE:CG1  | 2.46                     | 0.46              |
| 2:N:3661:ASP:OD1  | 2:N:3663:SER:OG   | 2.28                     | 0.46              |
| 3:C:48:MET:HE1    | 3:C:81:LEU:HD21   | 1.97                     | 0.46              |
| 3:C:97:VAL:CG1    | 3:C:104:LEU:HB3   | 2.46                     | 0.46              |
| 2:N:3680:ALA:N    | 3:O:5062:GLU:CA   | 2.71                     | 0.46              |
| 3:C:97:VAL:HG22   | 3:C:107:TRP:CD2   | 2.51                     | 0.46              |
| 4:D:557:ARG:CD    | 4:D:558:SER:O     | 2.62                     | 0.46              |
| 1:E:1129:VAL:HG22 | 1:E:1149:VAL:HG11 | 1.96                     | 0.46              |
| 3:G:3097:VAL:CG1  | 3:G:3104:LEU:HB3  | 2.46                     | 0.46              |
| 2:N:3680:ALA:CA   | 3:O:5062:GLU:CD   | 2.79                     | 0.46              |
| 3:O:5103:SER:HA   | 4:P:5598:TRP:CH2  | 2.50                     | 0.46              |
| 2:F:1544:THR:OG1  | 4:H:3593:TRP:CD1  | 2.58                     | 0.46              |
| 3:O:5011:VAL:CB   | 3:O:5151:PRO:CB   | 2.86                     | 0.46              |
| 3:O:5072:LEU:HD13 | 3:O:5074:ILE:CG1  | 2.46                     | 0.46              |
| 3:C:35:LEU:HD23   | 3:C:35:LEU:C      | 2.40                     | 0.46              |
| 1:E:1301:GLU:O    | 1:E:1320:ALA:N    | 2.43                     | 0.46              |
| 2:J:2678:SER:HB3  | 3:K:4062:GLU:HB2  | 0.75                     | 0.46              |
| 3:O:5033:PRO:CB   | 3:O:5051:ILE:O    | 2.64                     | 0.46              |
| 3:C:21:SER:HG     | 3:C:80:TYR:HE2    | 0.51                     | 0.46              |
| 3:C:33:PRO:CB     | 3:C:51:ILE:O      | 2.64                     | 0.46              |
| 3:G:3011:VAL:CG2  | 3:G:3152:GLU:N    | 2.70                     | 0.46              |
| 1:I:2371:CYS:O    | 1:I:2372:THR:OG1  | 2.25                     | 0.46              |
| 2:J:2680:ALA:CB   | 3:K:4062:GLU:CD   | 2.82                     | 0.46              |
| 3:K:4217:ARG:HH21 | 4:L:4622:PRO:CD   | 2.08                     | 0.46              |
| 1:M:3263:ALA:HB3  | 1:M:3268:ARG:HE   | 1.81                     | 0.46              |
| 3:O:5035:LEU:CD2  | 3:O:5037:VAL:HG22 | 2.12                     | 0.46              |
| 3:O:5045:PHE:HE1  | 4:P:5589:PHE:CZ   | 2.33                     | 0.46              |
| 3:C:30:THR:CG2    | 3:C:54:ASN:ND2    | 2.78                     | 0.45              |
| 3:C:97:VAL:HG21   | 3:C:107:TRP:CD2   | 2.49                     | 0.45              |
| 3:G:3047:TRP:NE1  | 3:G:3049:GLY:O    | 2.49                     | 0.45              |
| 3:K:4030:THR:CG2  | 3:K:4054:ASN:ND2  | 2.78                     | 0.45              |
| 3:K:4045:PHE:HE1  | 4:L:4589:PHE:CZ   | 2.33                     | 0.45              |
| 3:K:4067:ARG:HH22 | 3:K:4090:ASP:CG   | 2.24                     | 0.45              |
| 3:O:5048:MET:HE1  | 3:O:5081:LEU:HD21 | 1.97                     | 0.45              |
| 3:O:5097:VAL:CG1  | 3:O:5104:LEU:HB3  | 2.46                     | 0.45              |
| 3:C:45:PHE:HE1    | 4:D:589:PHE:CZ    | 2.33                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:47:TRP:NE1    | 3:C:49:GLY:O      | 2.49                     | 0.45              |
| 3:G:3002:ILE:CD1  | 3:G:3098:ARG:HH11 | 2.15                     | 0.45              |
| 3:K:4035:LEU:HD23 | 3:K:4035:LEU:C    | 2.40                     | 0.45              |
| 3:K:4097:VAL:CG1  | 3:K:4104:LEU:HB3  | 2.46                     | 0.45              |
| 3:O:5035:LEU:HD23 | 3:O:5035:LEU:C    | 2.40                     | 0.45              |
| 1:A:261:SER:O     | 1:A:270:GLU:N     | 2.50                     | 0.45              |
| 3:C:72:LEU:HD13   | 3:C:74:ILE:CG1    | 2.46                     | 0.45              |
| 4:D:549:LEU:HA    | 4:D:560:VAL:HG21  | 1.97                     | 0.45              |
| 1:E:1391:TYR:CZ   | 2:F:1784:LEU:CD1  | 2.99                     | 0.45              |
| 3:G:3011:VAL:CB   | 3:G:3151:PRO:CB   | 2.86                     | 0.45              |
| 3:G:3045:PHE:HE1  | 4:H:3589:PHE:CZ   | 2.33                     | 0.45              |
| 1:I:2261:SER:O    | 1:I:2270:GLU:N    | 2.50                     | 0.45              |
| 3:K:4048:MET:HE1  | 3:K:4081:LEU:HD21 | 1.97                     | 0.45              |
| 4:L:4549:LEU:HA   | 4:L:4560:VAL:HG21 | 1.97                     | 0.45              |
| 4:P:5653:VAL:H    | 4:P:5658:VAL:HG23 | 1.81                     | 0.45              |
| 2:B:560:GLN:CG    | 4:D:595:ASN:O     | 2.64                     | 0.45              |
| 2:B:566:ASP:OD1   | 2:B:567:ASN:N     | 2.50                     | 0.45              |
| 2:B:718:LYS:HZ2   | 4:D:596:ASN:CG    | 2.25                     | 0.45              |
| 2:F:1677:PRO:C    | 4:H:3501:GLN:CG   | 2.85                     | 0.45              |
| 3:G:3024:ALA:HB1  | 3:G:3027:TYR:HE1  | 1.75                     | 0.45              |
| 1:I:2096:CYS:O    | 1:I:2100:ASN:ND2  | 2.46                     | 0.45              |
| 1:I:2391:TYR:CZ   | 2:J:2784:LEU:CD1  | 2.99                     | 0.45              |
| 3:K:4033:PRO:CB   | 3:K:4051:ILE:O    | 2.64                     | 0.45              |
| 3:K:4047:TRP:CZ2  | 3:K:4049:GLY:HA2  | 2.52                     | 0.45              |
| 3:K:4097:VAL:HG22 | 3:K:4107:TRP:CD2  | 2.51                     | 0.45              |
| 1:M:3261:SER:O    | 1:M:3270:GLU:N    | 2.50                     | 0.45              |
| 1:M:3391:TYR:CZ   | 2:N:3784:LEU:CD1  | 2.99                     | 0.45              |
| 2:N:3680:ALA:HB3  | 3:O:5062:GLU:OE1  | 2.05                     | 0.45              |
| 3:O:5097:VAL:HG22 | 3:O:5107:TRP:CD2  | 2.51                     | 0.45              |
| 4:D:653:VAL:H     | 4:D:658:VAL:HG23  | 1.81                     | 0.45              |
| 3:G:3032:TYR:CE1  | 3:G:3100:TYR:HD1  | 1.97                     | 0.45              |
| 4:H:3653:VAL:H    | 4:H:3658:VAL:HG23 | 1.81                     | 0.45              |
| 3:K:4012:LYS:HD2  | 3:K:4016:GLU:OE1  | 2.16                     | 0.45              |
| 3:K:4102:ILE:HB   | 4:L:4552:ASP:CA   | 2.40                     | 0.45              |
| 4:L:4669:LYS:HB3  | 4:L:4669:LYS:HE2  | 1.73                     | 0.45              |
| 3:G:3107:TRP:CB   | 4:H:3546:PHE:CB   | 2.95                     | 0.45              |
| 1:I:2263:ALA:HB3  | 1:I:2268:ARG:HE   | 1.81                     | 0.45              |
| 3:O:5047:TRP:CZ2  | 3:O:5049:GLY:HA2  | 2.52                     | 0.45              |
| 3:O:5104:LEU:N    | 4:P:5536:ASN:OD1  | 2.43                     | 0.45              |
| 1:A:96:CYS:O      | 1:A:100:ASN:ND2   | 2.46                     | 0.45              |
| 4:D:563:ARG:CZ    | 4:D:564:PHE:HE2   | 2.30                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1263:ALA:HB3  | 1:E:1268:ARG:HE   | 1.81                     | 0.45              |
| 2:F:1566:ASP:OD1  | 2:F:1567:ASN:N    | 2.50                     | 0.45              |
| 3:G:3033:PRO:CB   | 3:G:3051:ILE:O    | 2.64                     | 0.45              |
| 3:G:3047:TRP:CZ2  | 3:G:3049:GLY:HA2  | 2.52                     | 0.45              |
| 4:H:3507:GLU:OE2  | 4:H:3521:THR:OG1  | 2.23                     | 0.45              |
| 1:I:2301:GLU:O    | 1:I:2320:ALA:N    | 2.43                     | 0.45              |
| 2:J:2680:ALA:CB   | 3:K:4062:GLU:CG   | 2.94                     | 0.45              |
| 4:L:4653:VAL:H    | 4:L:4658:VAL:HG23 | 1.81                     | 0.45              |
| 1:M:3089:TRP:N    | 2:N:3515:ASP:OD2  | 2.46                     | 0.45              |
| 2:N:3563:ILE:CG2  | 4:P:5532:SER:CB   | 2.92                     | 0.45              |
| 3:O:5012:LYS:HD2  | 3:O:5016:GLU:OE1  | 2.16                     | 0.45              |
| 3:O:5102:ILE:O    | 4:P:5534:CYS:HB3  | 2.17                     | 0.45              |
| 1:E:1380:ASP:OD1  | 1:E:1381:CYS:N    | 2.50                     | 0.45              |
| 2:F:1780:THR:OG1  | 2:F:1791:THR:O    | 2.30                     | 0.45              |
| 3:K:4103:SER:OG   | 4:L:4551:GLY:HA3  | 2.17                     | 0.45              |
| 4:L:4563:ARG:CZ   | 4:L:4564:PHE:HE2  | 2.30                     | 0.45              |
| 1:A:327:GLY:O     | 1:A:347:LEU:N     | 2.50                     | 0.45              |
| 1:A:391:TYR:CZ    | 2:B:784:LEU:CD1   | 2.99                     | 0.45              |
| 3:C:103:SER:OG    | 4:D:551:GLY:HA3   | 2.17                     | 0.45              |
| 4:P:5557:ARG:HD2  | 4:P:5558:SER:N    | 2.32                     | 0.45              |
| 4:P:5563:ARG:CZ   | 4:P:5564:PHE:HE2  | 2.30                     | 0.45              |
| 1:E:1261:SER:O    | 1:E:1270:GLU:N    | 2.50                     | 0.44              |
| 2:F:1661:ASP:OD1  | 2:F:1663:SER:OG   | 2.28                     | 0.44              |
| 3:G:3012:LYS:O    | 3:G:3115:VAL:HA   | 2.17                     | 0.44              |
| 3:G:3067:ARG:HH22 | 3:G:3090:ASP:CG   | 2.24                     | 0.44              |
| 4:H:3669:LYS:HB3  | 4:H:3669:LYS:HE2  | 1.73                     | 0.44              |
| 2:J:2547:VAL:CG1  | 3:K:4102:ILE:N    | 2.79                     | 0.44              |
| 2:N:3563:ILE:HG21 | 4:P:5532:SER:CB   | 2.45                     | 0.44              |
| 3:O:5012:LYS:O    | 3:O:5115:VAL:HA   | 2.17                     | 0.44              |
| 2:B:544:THR:HB    | 4:D:593:TRP:NE1   | 2.31                     | 0.44              |
| 3:C:47:TRP:CZ2    | 3:C:49:GLY:HA2    | 2.52                     | 0.44              |
| 4:D:514:PRO:HG2   | 4:D:609:LEU:O     | 2.03                     | 0.44              |
| 4:H:3557:ARG:HD2  | 4:H:3558:SER:N    | 2.32                     | 0.44              |
| 1:I:2380:ASP:OD1  | 1:I:2381:CYS:N    | 2.50                     | 0.44              |
| 2:J:2566:ASP:OD1  | 2:J:2567:ASN:N    | 2.50                     | 0.44              |
| 3:K:4078:THR:CG2  | 3:K:4080:TYR:OH   | 2.48                     | 0.44              |
| 3:O:5039:GLN:CD   | 3:O:5045:PHE:CE1  | 2.87                     | 0.44              |
| 4:P:5523:ARG:HG3  | 4:P:5523:ARG:NH1  | 2.32                     | 0.44              |
| 2:B:571:ARG:HG3   | 2:B:597:THR:OG1   | 2.18                     | 0.44              |
| 1:E:1327:GLY:O    | 1:E:1347:LEU:N    | 2.50                     | 0.44              |
| 3:G:3072:LEU:HD13 | 3:G:3074:ILE:CG1  | 2.46                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:3563:ARG:CZ   | 4:H:3564:PHE:HE2  | 2.30                     | 0.44              |
| 4:H:3638:THR:C    | 4:H:3639:ILE:HG13 | 2.42                     | 0.44              |
| 3:K:4032:TYR:CZ   | 3:K:4100:TYR:CG   | 2.96                     | 0.44              |
| 2:N:3679:GLY:CA   | 3:O:5065:LYS:H    | 2.31                     | 0.44              |
| 3:O:5067:ARG:HH22 | 3:O:5090:ASP:CG   | 2.24                     | 0.44              |
| 3:C:107:TRP:CB    | 4:D:546:PHE:CB    | 2.95                     | 0.44              |
| 4:D:582:THR:HG1   | 4:D:610:GLY:HA3   | 1.79                     | 0.44              |
| 2:F:1543:LYS:NZ   | 4:H:3531:SER:HB2  | 2.31                     | 0.44              |
| 3:K:4100:TYR:CD2  | 3:K:4101:PHE:CE2  | 3.06                     | 0.44              |
| 2:N:3566:ASP:OD1  | 2:N:3567:ASN:N    | 2.50                     | 0.44              |
| 1:A:263:ALA:HB3   | 1:A:268:ARG:HE    | 1.81                     | 0.44              |
| 3:C:67:ARG:HH22   | 3:C:90:ASP:CG     | 2.24                     | 0.44              |
| 2:F:1563:ILE:HG21 | 4:H:3530:THR:HB   | 2.00                     | 0.44              |
| 3:G:3102:ILE:O    | 4:H:3534:CYS:HB3  | 2.17                     | 0.44              |
| 3:K:4102:ILE:O    | 4:L:4534:CYS:HB3  | 2.17                     | 0.44              |
| 3:O:5103:SER:OG   | 4:P:5551:GLY:HA3  | 2.17                     | 0.44              |
| 4:P:5539:GLN:NE2  | 4:P:5541:LYS:HE3  | 2.33                     | 0.44              |
| 4:P:5638:THR:C    | 4:P:5639:ILE:HG13 | 2.42                     | 0.44              |
| 4:D:539:GLN:NE2   | 4:D:541:LYS:HE3   | 2.33                     | 0.44              |
| 4:D:557:ARG:HD2   | 4:D:558:SER:N     | 2.32                     | 0.44              |
| 4:D:683:LEU:HD22  | 4:D:687:ALA:CB    | 2.48                     | 0.44              |
| 1:E:1312:ASP:O    | 1:E:1314:GLY:N    | 2.50                     | 0.44              |
| 2:F:1681:GLN:OE1  | 3:G:3065:LYS:NZ   | 2.49                     | 0.44              |
| 4:H:3539:GLN:NE2  | 4:H:3541:LYS:HE3  | 2.33                     | 0.44              |
| 4:L:4539:GLN:NE2  | 4:L:4541:LYS:HE3  | 2.32                     | 0.44              |
| 2:N:3719:LYS:HG3  | 3:O:5052:TYR:HE2  | 1.80                     | 0.44              |
| 3:O:5097:VAL:HG22 | 3:O:5107:TRP:CE3  | 2.49                     | 0.44              |
| 4:P:5557:ARG:CD   | 4:P:5558:SER:O    | 2.63                     | 0.44              |
| 2:B:560:GLN:HG3   | 4:D:595:ASN:HB3   | 2.00                     | 0.44              |
| 3:C:57:GLU:C      | 3:C:58:PRO:CD     | 2.74                     | 0.44              |
| 3:G:3100:TYR:CD2  | 3:G:3101:PHE:CE2  | 3.06                     | 0.44              |
| 3:G:3123:PRO:HB3  | 3:G:3149:TYR:HB3  | 2.00                     | 0.44              |
| 4:H:3554:ASN:C    | 4:H:3554:ASN:ND2  | 2.54                     | 0.44              |
| 2:J:2571:ARG:HG3  | 2:J:2597:THR:OG1  | 2.17                     | 0.44              |
| 4:L:4557:ARG:HD2  | 4:L:4558:SER:N    | 2.32                     | 0.44              |
| 2:N:3720:TRP:CZ2  | 3:O:5057:GLU:OE2  | 2.53                     | 0.44              |
| 3:O:5100:TYR:CD2  | 3:O:5101:PHE:CE2  | 3.06                     | 0.44              |
| 3:C:102:ILE:O     | 4:D:534:CYS:HB3   | 2.17                     | 0.44              |
| 4:D:523:ARG:NH1   | 4:D:523:ARG:HG3   | 2.32                     | 0.44              |
| 2:F:1571:ARG:HG3  | 2:F:1597:THR:OG1  | 2.18                     | 0.44              |
| 4:H:3557:ARG:CD   | 4:H:3558:SER:O    | 2.63                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:4012:LYS:O    | 3:K:4115:VAL:HA   | 2.17                     | 0.44              |
| 1:A:380:ASP:OD1   | 1:A:381:CYS:N     | 2.50                     | 0.44              |
| 4:D:542:PRO:HB3   | 4:D:669:LYS:CD    | 2.42                     | 0.44              |
| 1:M:3380:ASP:OD1  | 1:M:3381:CYS:N    | 2.50                     | 0.44              |
| 2:N:3677:PRO:C    | 4:P:5597:LEU:HD23 | 2.42                     | 0.44              |
| 3:O:5123:PRO:HB3  | 3:O:5149:TYR:HB3  | 2.00                     | 0.44              |
| 3:O:5150:PHE:HA   | 3:O:5151:PRO:HA   | 1.84                     | 0.44              |
| 4:P:5556:ARG:HD3  | 4:P:5560:VAL:HG12 | 2.00                     | 0.44              |
| 3:C:12:LYS:O      | 3:C:115:VAL:HA    | 2.17                     | 0.43              |
| 3:C:100:TYR:CD2   | 3:C:101:PHE:CE2   | 3.06                     | 0.43              |
| 4:D:556:ARG:HD3   | 4:D:560:VAL:HG12  | 2.00                     | 0.43              |
| 2:F:1556:ASN:O    | 2:F:1559:THR:OG1  | 2.30                     | 0.43              |
| 3:G:3078:THR:CG2  | 3:G:3080:TYR:OH   | 2.48                     | 0.43              |
| 3:K:4002:ILE:CD1  | 3:K:4098:ARG:HH12 | 1.83                     | 0.43              |
| 4:L:4556:ARG:HD3  | 4:L:4560:VAL:HG12 | 2.00                     | 0.43              |
| 2:N:3677:PRO:N    | 3:O:5062:GLU:CG   | 2.74                     | 0.43              |
| 3:C:32:TYR:CZ     | 3:C:100:TYR:CG    | 2.96                     | 0.43              |
| 4:D:669:LYS:HB3   | 4:D:669:LYS:HE2   | 1.73                     | 0.43              |
| 3:G:3103:SER:OG   | 4:H:3551:GLY:HA3  | 2.17                     | 0.43              |
| 4:H:3582:THR:HG1  | 4:H:3610:GLY:HA3  | 1.81                     | 0.43              |
| 1:I:2152:GLU:OE1  | 1:I:2152:GLU:N    | 2.52                     | 0.43              |
| 2:J:2563:ILE:HG21 | 4:L:4530:THR:OG1  | 2.18                     | 0.43              |
| 4:L:4557:ARG:CD   | 4:L:4558:SER:O    | 2.62                     | 0.43              |
| 3:O:5107:TRP:CB   | 4:P:5546:PHE:CB   | 2.95                     | 0.43              |
| 4:P:5582:THR:HG1  | 4:P:5610:GLY:HA3  | 1.75                     | 0.43              |
| 4:D:638:THR:C     | 4:D:639:ILE:HG13  | 2.43                     | 0.43              |
| 4:D:662:MET:HB2   | 4:D:662:MET:HE3   | 1.59                     | 0.43              |
| 1:I:2312:ASP:O    | 1:I:2314:GLY:N    | 2.51                     | 0.43              |
| 4:L:4523:ARG:NH1  | 4:L:4523:ARG:HG3  | 2.32                     | 0.43              |
| 1:M:3327:GLY:O    | 1:M:3347:LEU:N    | 2.50                     | 0.43              |
| 1:A:312:ASP:O     | 1:A:314:GLY:N     | 2.51                     | 0.43              |
| 3:C:2:ILE:HD13    | 3:C:98:ARG:HH11   | 1.80                     | 0.43              |
| 4:D:689:GLU:O     | 4:D:689:GLU:HG3   | 2.18                     | 0.43              |
| 4:H:3689:GLU:O    | 4:H:3689:GLU:HG3  | 2.18                     | 0.43              |
| 1:M:3007:MET:O    | 1:M:3277:ILE:N    | 2.48                     | 0.43              |
| 2:N:3571:ARG:HG3  | 2:N:3597:THR:OG1  | 2.18                     | 0.43              |
| 4:P:5656:THR:HA   | 4:P:5657:PRO:HD2  | 1.62                     | 0.43              |
| 4:P:5689:GLU:O    | 4:P:5689:GLU:HG3  | 2.18                     | 0.43              |
| 3:C:107:TRP:HB2   | 4:D:546:PHE:HB2   | 2.01                     | 0.43              |
| 3:G:3078:THR:HB   | 3:G:3080:TYR:CE1  | 2.54                     | 0.43              |
| 3:G:3173:LEU:HD12 | 4:H:3665:THR:CG2  | 2.39                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:4107:TRP:CB   | 4:L:4546:PHE:CB   | 2.95                     | 0.43              |
| 4:L:4514:PRO:CD   | 4:L:4609:LEU:C    | 2.89                     | 0.43              |
| 4:L:4638:THR:C    | 4:L:4639:ILE:HG13 | 2.43                     | 0.43              |
| 1:M:3152:GLU:N    | 1:M:3152:GLU:OE1  | 2.52                     | 0.43              |
| 2:N:3680:ALA:H    | 3:O:5062:GLU:CD   | 2.23                     | 0.43              |
| 2:B:563:ILE:HG22  | 4:D:531:SER:CA    | 2.46                     | 0.43              |
| 3:G:3107:TRP:HB2  | 4:H:3546:PHE:HB2  | 2.01                     | 0.43              |
| 4:H:3542:PRO:CB   | 4:H:3669:LYS:CD   | 2.95                     | 0.43              |
| 4:H:3623:PRO:CG   | 4:H:3633:ALA:HB1  | 2.49                     | 0.43              |
| 3:K:4078:THR:HB   | 3:K:4080:TYR:CE1  | 2.54                     | 0.43              |
| 3:K:4123:PRO:HB3  | 3:K:4149:TYR:HB3  | 2.00                     | 0.43              |
| 3:K:4150:PHE:HA   | 3:K:4151:PRO:HA   | 1.84                     | 0.43              |
| 3:C:68:PHE:CD1    | 3:C:83:ILE:HG12   | 2.54                     | 0.43              |
| 3:C:97:VAL:HG22   | 3:C:107:TRP:CE3   | 2.49                     | 0.43              |
| 3:K:4039:GLN:OE1  | 3:K:4045:PHE:CZ   | 2.72                     | 0.43              |
| 1:M:3150:ASN:CG   | 1:M:3153:THR:HG1  | 2.20                     | 0.43              |
| 4:P:5507:GLU:O    | 4:P:5604:THR:OG1  | 2.27                     | 0.43              |
| 1:A:152:GLU:OE1   | 1:A:152:GLU:N     | 2.52                     | 0.43              |
| 4:D:520:LEU:N     | 4:D:520:LEU:CD2   | 2.70                     | 0.43              |
| 4:D:623:PRO:CG    | 4:D:633:ALA:HB1   | 2.49                     | 0.43              |
| 4:H:3639:ILE:HG22 | 4:H:3642:PHE:CD2  | 2.54                     | 0.43              |
| 1:M:3312:ASP:O    | 1:M:3314:GLY:N    | 2.51                     | 0.43              |
| 3:O:5173:LEU:HD12 | 4:P:5665:THR:CG2  | 2.39                     | 0.43              |
| 1:A:7:MET:O       | 1:A:277:ILE:N     | 2.48                     | 0.43              |
| 3:C:78:THR:HB     | 3:C:80:TYR:CE1    | 2.54                     | 0.43              |
| 4:L:4561:PRO:CG   | 4:L:4563:ARG:NH1  | 2.82                     | 0.43              |
| 2:B:560:GLN:HG3   | 4:D:595:ASN:C     | 2.44                     | 0.43              |
| 2:B:666:SER:N     | 2:B:673:LYS:O     | 2.52                     | 0.43              |
| 4:H:3656:THR:HA   | 4:H:3657:PRO:HD2  | 1.62                     | 0.43              |
| 3:K:4011:VAL:CG2  | 3:K:4152:GLU:N    | 2.70                     | 0.43              |
| 3:K:4068:PHE:CD1  | 3:K:4083:ILE:HG12 | 2.54                     | 0.43              |
| 4:L:4623:PRO:CG   | 4:L:4633:ALA:HB1  | 2.49                     | 0.43              |
| 4:L:4683:LEU:HD22 | 4:L:4687:ALA:CB   | 2.48                     | 0.43              |
| 1:M:3102:GLN:NE2  | 1:M:3104:SER:OG   | 2.47                     | 0.43              |
| 4:H:3523:ARG:HG3  | 4:H:3523:ARG:NH1  | 2.32                     | 0.42              |
| 3:K:4107:TRP:HB2  | 4:L:4546:PHE:HB2  | 2.01                     | 0.42              |
| 4:L:4639:ILE:HG22 | 4:L:4642:PHE:CD2  | 2.54                     | 0.42              |
| 4:P:5526:ILE:O    | 4:P:5526:ILE:HG22 | 2.19                     | 0.42              |
| 3:C:37:VAL:HB     | 3:C:107:TRP:HZ3   | 1.84                     | 0.42              |
| 4:D:542:PRO:CB    | 4:D:669:LYS:CD    | 2.95                     | 0.42              |
| 3:G:3039:GLN:OE1  | 3:G:3045:PHE:CZ   | 2.72                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:3540:GLU:HB2  | 4:H:3546:PHE:CE1  | 2.54                     | 0.42              |
| 4:H:3683:LEU:HD22 | 4:H:3687:ALA:CB   | 2.48                     | 0.42              |
| 3:K:4088:ASN:O    | 3:K:4091:THR:HG23 | 2.19                     | 0.42              |
| 4:L:4582:THR:HG1  | 4:L:4610:GLY:HA3  | 1.78                     | 0.42              |
| 3:O:5078:THR:HB   | 3:O:5080:TYR:CE1  | 2.54                     | 0.42              |
| 3:O:5088:ASN:O    | 3:O:5091:THR:HG23 | 2.19                     | 0.42              |
| 4:P:5540:GLU:HB2  | 4:P:5546:PHE:CE1  | 2.54                     | 0.42              |
| 4:P:5683:LEU:HD22 | 4:P:5687:ALA:CB   | 2.48                     | 0.42              |
| 3:K:4013:ASN:CG   | 3:K:4117:SER:HA   | 2.45                     | 0.42              |
| 3:O:5037:VAL:HB   | 3:O:5107:TRP:HZ3  | 1.84                     | 0.42              |
| 4:P:5639:ILE:HG22 | 4:P:5642:PHE:CD2  | 2.54                     | 0.42              |
| 1:A:150:ASN:CG    | 1:A:153:THR:HG1   | 2.24                     | 0.42              |
| 2:B:563:ILE:CA    | 4:D:532:SER:HB3   | 2.49                     | 0.42              |
| 3:C:13:ASN:CG     | 3:C:117:SER:HA    | 2.45                     | 0.42              |
| 2:N:3666:SER:N    | 2:N:3673:LYS:O    | 2.52                     | 0.42              |
| 3:O:5013:ASN:CG   | 3:O:5117:SER:HA   | 2.45                     | 0.42              |
| 3:O:5030:THR:CG2  | 3:O:5054:ASN:ND2  | 2.78                     | 0.42              |
| 3:O:5039:GLN:OE1  | 3:O:5045:PHE:CZ   | 2.72                     | 0.42              |
| 3:O:5068:PHE:CD1  | 3:O:5083:ILE:HG12 | 2.54                     | 0.42              |
| 2:B:559:THR:HB    | 4:D:594:TYR:C     | 2.45                     | 0.42              |
| 3:C:88:ASN:O      | 3:C:91:THR:HG23   | 2.19                     | 0.42              |
| 3:C:123:PRO:HB3   | 3:C:149:TYR:HB3   | 2.00                     | 0.42              |
| 4:L:4520:LEU:N    | 4:L:4520:LEU:CD2  | 2.70                     | 0.42              |
| 4:D:639:ILE:HG22  | 4:D:642:PHE:CD2   | 2.54                     | 0.42              |
| 3:G:3013:ASN:CG   | 3:G:3117:SER:HA   | 2.45                     | 0.42              |
| 3:G:3175:GLN:CG   | 4:H:3663:GLU:OE2  | 2.60                     | 0.42              |
| 2:N:3505:ASP:OD2  | 2:N:3513:ARG:NH2  | 2.53                     | 0.42              |
| 4:D:540:GLU:HB2   | 4:D:546:PHE:CE1   | 2.54                     | 0.42              |
| 1:E:1152:GLU:OE1  | 1:E:1152:GLU:N    | 2.51                     | 0.42              |
| 2:F:1630:GLU:HB2  | 2:N:3507:PRO:CB   | 2.49                     | 0.42              |
| 2:F:1666:SER:N    | 2:F:1673:LYS:O    | 2.52                     | 0.42              |
| 3:G:3004:LEU:HD23 | 3:G:3024:ALA:HA   | 2.02                     | 0.42              |
| 3:G:3021:SER:CB   | 3:G:3080:TYR:HE2  | 2.13                     | 0.42              |
| 3:G:3037:VAL:HB   | 3:G:3107:TRP:HZ3  | 1.84                     | 0.42              |
| 3:G:3068:PHE:CD1  | 3:G:3083:ILE:HG12 | 2.54                     | 0.42              |
| 4:H:3686:ARG:H    | 4:H:3686:ARG:HG2  | 1.64                     | 0.42              |
| 4:L:4689:GLU:O    | 4:L:4689:GLU:HG3  | 2.18                     | 0.42              |
| 4:P:5623:PRO:CG   | 4:P:5633:ALA:HB1  | 2.49                     | 0.42              |
| 4:D:587:ILE:HG12  | 4:D:605:LYS:HG3   | 2.02                     | 0.42              |
| 4:H:3556:ARG:HD3  | 4:H:3560:VAL:HG12 | 2.00                     | 0.42              |
| 1:M:3075:ASP:HB2  | 1:M:3216:ALA:HB3  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:104:LEU:N     | 4:D:536:ASN:OD1   | 2.43                     | 0.42              |
| 3:C:150:PHE:HA    | 3:C:151:PRO:HA    | 1.84                     | 0.42              |
| 2:F:1678:SER:HB2  | 4:H:3597:LEU:HD11 | 1.36                     | 0.42              |
| 4:H:3504:VAL:HG13 | 4:H:3522:CYS:SG   | 2.60                     | 0.42              |
| 1:I:2075:ASP:HB2  | 1:I:2216:ALA:HB3  | 2.02                     | 0.42              |
| 2:J:2666:SER:N    | 2:J:2673:LYS:O    | 2.52                     | 0.42              |
| 1:M:3038:ILE:HG23 | 1:M:3129:VAL:HG12 | 2.02                     | 0.42              |
| 3:O:5170:PHE:HA   | 3:O:5171:PRO:HD3  | 1.95                     | 0.42              |
| 4:P:5587:ILE:HG12 | 4:P:5605:LYS:HG3  | 2.02                     | 0.42              |
| 1:A:75:ASP:HB2    | 1:A:216:ALA:HB3   | 2.02                     | 0.42              |
| 3:C:39:GLN:OE1    | 3:C:45:PHE:CZ     | 2.72                     | 0.42              |
| 4:D:683:LEU:CD1   | 4:D:694:TYR:CE2   | 3.02                     | 0.42              |
| 3:K:4004:LEU:HD23 | 3:K:4024:ALA:HA   | 2.01                     | 0.42              |
| 4:L:4587:ILE:HG12 | 4:L:4605:LYS:HG3  | 2.02                     | 0.42              |
| 4:L:4593:TRP:CZ3  | 4:L:4597:LEU:CA   | 3.03                     | 0.42              |
| 3:O:5011:VAL:CG2  | 3:O:5152:GLU:O    | 2.68                     | 0.42              |
| 3:C:107:TRP:CG    | 4:D:546:PHE:HB3   | 2.55                     | 0.41              |
| 4:H:3526:ILE:O    | 4:H:3526:ILE:HG22 | 2.19                     | 0.41              |
| 4:H:3593:TRP:CZ3  | 4:H:3597:LEU:CA   | 3.03                     | 0.41              |
| 3:K:4037:VAL:HB   | 3:K:4107:TRP:HZ3  | 1.84                     | 0.41              |
| 3:K:4107:TRP:CG   | 4:L:4546:PHE:HB3  | 2.55                     | 0.41              |
| 4:L:4504:VAL:HG13 | 4:L:4522:CYS:SG   | 2.60                     | 0.41              |
| 4:P:5504:VAL:HG13 | 4:P:5522:CYS:SG   | 2.60                     | 0.41              |
| 4:P:5549:LEU:HD12 | 4:P:5549:LEU:HA   | 1.85                     | 0.41              |
| 4:P:5575:LEU:HD23 | 4:P:5575:LEU:HA   | 1.87                     | 0.41              |
| 4:P:5593:TRP:CZ3  | 4:P:5597:LEU:CA   | 3.03                     | 0.41              |
| 4:D:561:PRO:CG    | 4:D:563:ARG:NH1   | 2.82                     | 0.41              |
| 1:E:1075:ASP:HB2  | 1:E:1216:ALA:HB3  | 2.02                     | 0.41              |
| 2:F:1507:PRO:CB   | 2:J:2630:GLU:HB2  | 2.49                     | 0.41              |
| 3:G:3088:ASN:O    | 3:G:3091:THR:HG23 | 2.19                     | 0.41              |
| 4:H:3609:LEU:HD12 | 4:H:3609:LEU:HA   | 1.86                     | 0.41              |
| 3:K:4100:TYR:HE2  | 3:K:4101:PHE:CZ   | 2.38                     | 0.41              |
| 3:C:18:VAL:HG11   | 3:C:113:LEU:HD13  | 2.02                     | 0.41              |
| 2:F:1505:ASP:OD2  | 2:F:1513:ARG:NH2  | 2.53                     | 0.41              |
| 1:I:2038:ILE:HG23 | 1:I:2129:VAL:HG12 | 2.02                     | 0.41              |
| 2:J:2505:ASP:OD2  | 2:J:2513:ARG:NH2  | 2.53                     | 0.41              |
| 3:K:4067:ARG:NH2  | 3:K:4090:ASP:OD2  | 2.52                     | 0.41              |
| 2:N:3677:PRO:CB   | 4:P:5597:LEU:HD23 | 2.49                     | 0.41              |
| 3:O:5107:TRP:CG   | 4:P:5546:PHE:HB3  | 2.55                     | 0.41              |
| 4:P:5514:PRO:CD   | 4:P:5609:LEU:C    | 2.89                     | 0.41              |
| 2:B:505:ASP:OD2   | 2:B:513:ARG:NH2   | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1391:TYR:CE2  | 2:F:1784:LEU:CD1  | 3.04                     | 0.41              |
| 3:G:3018:VAL:HG11 | 3:G:3113:LEU:HD13 | 2.02                     | 0.41              |
| 4:H:3689:GLU:CA   | 4:H:3711:ARG:HH21 | 2.33                     | 0.41              |
| 2:J:2637:CYS:SG   | 2:J:2750:CYS:N    | 2.93                     | 0.41              |
| 4:L:4540:GLU:HB2  | 4:L:4546:PHE:CE1  | 2.55                     | 0.41              |
| 1:M:3391:TYR:CE2  | 2:N:3784:LEU:CD1  | 3.04                     | 0.41              |
| 3:O:5107:TRP:HB2  | 4:P:5546:PHE:HB2  | 2.01                     | 0.41              |
| 2:B:678:SER:OG    | 3:C:61:ALA:CB     | 2.69                     | 0.41              |
| 1:E:1134:ASN:OD1  | 1:E:1135:ILE:N    | 2.54                     | 0.41              |
| 4:H:3587:ILE:HG12 | 4:H:3605:LYS:HG3  | 2.02                     | 0.41              |
| 1:I:2293:GLU:OE1  | 1:I:2293:GLU:N    | 2.54                     | 0.41              |
| 2:J:2543:LYS:HE3  | 4:L:4532:SER:C    | 2.46                     | 0.41              |
| 4:L:4656:THR:HA   | 4:L:4657:PRO:HD2  | 1.62                     | 0.41              |
| 4:L:4683:LEU:CD1  | 4:L:4694:TYR:CE2  | 3.02                     | 0.41              |
| 4:L:4689:GLU:CA   | 4:L:4711:ARG:HH21 | 2.33                     | 0.41              |
| 4:P:5521:THR:HG21 | 4:P:5572:LYS:HE2  | 2.03                     | 0.41              |
| 1:A:134:ASN:OD1   | 1:A:135:ILE:N     | 2.54                     | 0.41              |
| 2:B:677:PRO:HA    | 4:D:501:GLN:HG2   | 2.03                     | 0.41              |
| 3:C:32:TYR:CZ     | 3:C:100:TYR:CZ    | 2.84                     | 0.41              |
| 4:D:521:THR:HG21  | 4:D:572:LYS:HE2   | 2.03                     | 0.41              |
| 4:D:526:ILE:O     | 4:D:526:ILE:HG22  | 2.19                     | 0.41              |
| 4:D:556:ARG:HD3   | 4:D:560:VAL:O     | 2.20                     | 0.41              |
| 1:E:1007:MET:O    | 1:E:1277:ILE:N    | 2.48                     | 0.41              |
| 1:E:1293:GLU:OE1  | 1:E:1293:GLU:N    | 2.54                     | 0.41              |
| 2:F:1637:CYS:SG   | 2:F:1750:CYS:N    | 2.93                     | 0.41              |
| 4:H:3561:PRO:CG   | 4:H:3563:ARG:NH1  | 2.82                     | 0.41              |
| 3:K:4118:ALA:CB   | 3:K:4150:PHE:CD2  | 2.77                     | 0.41              |
| 1:A:293:GLU:N     | 1:A:293:GLU:OE1   | 2.54                     | 0.41              |
| 1:A:391:TYR:CE2   | 2:B:784:LEU:CD1   | 3.04                     | 0.41              |
| 2:B:544:THR:OG1   | 4:D:593:TRP:NE1   | 2.54                     | 0.41              |
| 3:C:4:LEU:HD23    | 3:C:24:ALA:HA     | 2.01                     | 0.41              |
| 2:F:1543:LYS:CE   | 4:H:3531:SER:HB2  | 2.50                     | 0.41              |
| 2:F:1545:ASP:CG   | 4:H:3534:CYS:SG   | 3.04                     | 0.41              |
| 3:G:3030:THR:CG2  | 3:G:3054:ASN:ND2  | 2.78                     | 0.41              |
| 4:H:3581:GLN:C    | 4:H:3608:VAL:HG11 | 2.46                     | 0.41              |
| 4:L:4556:ARG:HD3  | 4:L:4560:VAL:O    | 2.21                     | 0.41              |
| 3:O:5078:THR:CG2  | 3:O:5080:TYR:OH   | 2.48                     | 0.41              |
| 4:L:4526:ILE:O    | 4:L:4526:ILE:HG22 | 2.19                     | 0.41              |
| 4:L:4542:PRO:HB3  | 4:L:4669:LYS:CD   | 2.42                     | 0.41              |
| 4:L:4542:PRO:CB   | 4:L:4669:LYS:CD   | 2.95                     | 0.41              |
| 4:L:4581:GLN:C    | 4:L:4608:VAL:HG11 | 2.46                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:5004:LEU:HD23 | 3:O:5024:ALA:HA   | 2.02                     | 0.41              |
| 3:O:5032:TYR:CZ   | 3:O:5100:TYR:CG   | 2.96                     | 0.41              |
| 4:P:5556:ARG:HD3  | 4:P:5560:VAL:O    | 2.20                     | 0.41              |
| 4:P:5689:GLU:CA   | 4:P:5711:ARG:NH2  | 2.83                     | 0.41              |
| 2:B:502:TYR:HE2   | 2:B:504:ALA:HB2   | 1.86                     | 0.41              |
| 3:C:102:ILE:HG13  | 4:D:552:ASP:CB    | 2.34                     | 0.41              |
| 3:C:173:LEU:HD12  | 4:D:665:THR:CG2   | 2.39                     | 0.41              |
| 4:D:581:GLN:C     | 4:D:608:VAL:HG11  | 2.46                     | 0.41              |
| 4:D:593:TRP:CZ3   | 4:D:597:LEU:CA    | 3.03                     | 0.41              |
| 2:F:1563:ILE:HG22 | 4:H:3531:SER:OG   | 2.21                     | 0.41              |
| 3:G:3011:VAL:CG2  | 3:G:3152:GLU:O    | 2.68                     | 0.41              |
| 4:H:3521:THR:HG21 | 4:H:3572:LYS:HE2  | 2.03                     | 0.41              |
| 4:H:3556:ARG:HD3  | 4:H:3560:VAL:O    | 2.20                     | 0.41              |
| 1:I:2134:ASN:OD1  | 1:I:2135:ILE:N    | 2.54                     | 0.41              |
| 1:I:2391:TYR:CE2  | 2:J:2784:LEU:CD1  | 3.04                     | 0.41              |
| 3:K:4018:VAL:HG11 | 3:K:4113:LEU:HD13 | 2.02                     | 0.41              |
| 1:M:3134:ASN:OD1  | 1:M:3135:ILE:N    | 2.54                     | 0.41              |
| 2:N:3502:TYR:HE2  | 2:N:3504:ALA:HB2  | 1.86                     | 0.41              |
| 2:N:3718:LYS:C    | 3:O:5052:TYR:HE2  | 2.20                     | 0.41              |
| 4:P:5581:GLN:C    | 4:P:5608:VAL:HG11 | 2.46                     | 0.41              |
| 4:P:5662:MET:HB2  | 4:P:5662:MET:HE3  | 1.59                     | 0.41              |
| 4:P:5669:LYS:HE2  | 4:P:5669:LYS:HB3  | 1.73                     | 0.41              |
| 1:A:102:GLN:NE2   | 1:A:104:SER:OG    | 2.47                     | 0.41              |
| 3:C:97:VAL:HG11   | 3:C:104:LEU:HB3   | 2.03                     | 0.41              |
| 1:E:1265:GLU:O    | 1:E:1267:LEU:N    | 2.54                     | 0.41              |
| 4:L:4689:GLU:OE2  | 4:L:4711:ARG:NH2  | 2.54                     | 0.41              |
| 3:O:5067:ARG:NH2  | 3:O:5090:ASP:OD2  | 2.52                     | 0.41              |
| 4:P:5689:GLU:CA   | 4:P:5711:ARG:HH21 | 2.33                     | 0.41              |
| 2:B:718:LYS:HB2   | 3:C:59:THR:OG1    | 2.21                     | 0.40              |
| 3:C:11:VAL:CG2    | 3:C:152:GLU:O     | 2.68                     | 0.40              |
| 3:C:91:THR:O      | 3:C:92:ALA:HB2    | 2.21                     | 0.40              |
| 4:H:3561:PRO:HG2  | 4:H:3563:ARG:HH12 | 1.85                     | 0.40              |
| 2:J:2502:TYR:HE2  | 2:J:2504:ALA:HB2  | 1.86                     | 0.40              |
| 4:L:4628:LEU:HD23 | 4:L:4628:LEU:HA   | 1.89                     | 0.40              |
| 1:M:3265:GLU:O    | 1:M:3267:LEU:N    | 2.54                     | 0.40              |
| 3:O:5018:VAL:HG11 | 3:O:5113:LEU:HD13 | 2.02                     | 0.40              |
| 1:A:38:ILE:HG23   | 1:A:129:VAL:HG12  | 2.02                     | 0.40              |
| 3:C:119:LYS:O     | 3:C:150:PHE:HD2   | 2.04                     | 0.40              |
| 4:D:556:ARG:C     | 4:D:557:ARG:O     | 2.62                     | 0.40              |
| 4:D:628:LEU:HD23  | 4:D:628:LEU:HA    | 1.89                     | 0.40              |
| 2:J:2680:ALA:HB2  | 3:K:4062:GLU:OE2  | 2.17                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:4011:VAL:CG2  | 3:K:4152:GLU:O    | 2.68                     | 0.40              |
| 3:K:4032:TYR:OH   | 3:K:4100:TYR:CE2  | 2.36                     | 0.40              |
| 3:O:5091:THR:O    | 3:O:5092:ALA:HB2  | 2.21                     | 0.40              |
| 4:P:5542:PRO:CB   | 4:P:5669:LYS:CD   | 2.95                     | 0.40              |
| 4:P:5628:LEU:HD23 | 4:P:5628:LEU:HA   | 1.89                     | 0.40              |
| 4:P:5689:GLU:OE2  | 4:P:5711:ARG:NH2  | 2.54                     | 0.40              |
| 3:C:35:LEU:CD2    | 3:C:37:VAL:HG22   | 2.12                     | 0.40              |
| 4:D:504:VAL:HG13  | 4:D:522:CYS:SG    | 2.60                     | 0.40              |
| 1:E:1038:ILE:HG23 | 1:E:1129:VAL:HG12 | 2.02                     | 0.40              |
| 3:G:3078:THR:CB   | 3:G:3080:TYR:CE1  | 3.04                     | 0.40              |
| 4:H:3686:ARG:HG3  | 4:H:3686:ARG:NH1  | 2.36                     | 0.40              |
| 4:H:3689:GLU:CA   | 4:H:3711:ARG:NH2  | 2.83                     | 0.40              |
| 1:I:2265:GLU:O    | 1:I:2267:LEU:N    | 2.54                     | 0.40              |
| 3:K:4011:VAL:HB   | 3:K:4151:PRO:CB   | 2.51                     | 0.40              |
| 3:K:4078:THR:CB   | 3:K:4080:TYR:CE1  | 3.04                     | 0.40              |
| 3:K:4091:THR:O    | 3:K:4092:ALA:HB2  | 2.21                     | 0.40              |
| 4:L:4549:LEU:HD12 | 4:L:4549:LEU:HA   | 1.85                     | 0.40              |
| 4:L:4686:ARG:H    | 4:L:4686:ARG:HG2  | 1.64                     | 0.40              |
| 1:M:3293:GLU:OE1  | 1:M:3293:GLU:N    | 2.54                     | 0.40              |
| 3:O:5057:GLU:C    | 3:O:5058:PRO:CD   | 2.74                     | 0.40              |
| 3:O:5119:LYS:O    | 3:O:5150:PHE:HD2  | 2.04                     | 0.40              |
| 1:A:265:GLU:O     | 1:A:267:LEU:N     | 2.54                     | 0.40              |
| 2:B:579:VAL:O     | 2:B:580:SER:OG    | 2.33                     | 0.40              |
| 3:C:100:TYR:HE2   | 3:C:101:PHE:CZ    | 2.38                     | 0.40              |
| 4:D:514:PRO:HD2   | 4:D:609:LEU:HB3   | 2.03                     | 0.40              |
| 4:H:3579:GLY:O    | 4:H:3580:ALA:C    | 2.64                     | 0.40              |
| 3:K:4021:SER:CB   | 3:K:4080:TYR:HE2  | 2.13                     | 0.40              |
| 3:K:4032:TYR:CE1  | 3:K:4100:TYR:HB2  | 2.56                     | 0.40              |
| 3:C:57:GLU:HA     | 3:C:58:PRO:CD     | 2.52                     | 0.40              |
| 4:D:689:GLU:CA    | 4:D:711:ARG:NH2   | 2.83                     | 0.40              |
| 3:G:3032:TYR:CE1  | 3:G:3100:TYR:HB2  | 2.56                     | 0.40              |
| 3:G:3107:TRP:CG   | 4:H:3546:PHE:HB3  | 2.55                     | 0.40              |
| 1:I:2327:GLY:O    | 1:I:2347:LEU:N    | 2.50                     | 0.40              |
| 3:K:4021:SER:CA   | 3:K:4080:TYR:CD2  | 3.05                     | 0.40              |
| 4:L:4689:GLU:CA   | 4:L:4711:ARG:NH2  | 2.84                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 398/441 (90%)   | 322 (81%)  | 72 (18%)  | 4 (1%)   | 12          | 48  |
| 1   | E     | 398/441 (90%)   | 322 (81%)  | 72 (18%)  | 4 (1%)   | 12          | 48  |
| 1   | I     | 398/441 (90%)   | 322 (81%)  | 72 (18%)  | 4 (1%)   | 12          | 48  |
| 1   | M     | 398/441 (90%)   | 322 (81%)  | 72 (18%)  | 4 (1%)   | 12          | 48  |
| 2   | B     | 323/420 (77%)   | 258 (80%)  | 65 (20%)  | 0        | 100         | 100 |
| 2   | F     | 323/420 (77%)   | 259 (80%)  | 64 (20%)  | 0        | 100         | 100 |
| 2   | J     | 323/420 (77%)   | 259 (80%)  | 64 (20%)  | 0        | 100         | 100 |
| 2   | N     | 323/420 (77%)   | 259 (80%)  | 64 (20%)  | 0        | 100         | 100 |
| 3   | C     | 216/218 (99%)   | 196 (91%)  | 15 (7%)   | 5 (2%)   | 5           | 28  |
| 3   | G     | 216/218 (99%)   | 196 (91%)  | 15 (7%)   | 5 (2%)   | 5           | 28  |
| 3   | K     | 216/218 (99%)   | 196 (91%)  | 15 (7%)   | 5 (2%)   | 5           | 28  |
| 3   | O     | 216/218 (99%)   | 196 (91%)  | 15 (7%)   | 5 (2%)   | 5           | 28  |
| 4   | D     | 209/214 (98%)   | 188 (90%)  | 19 (9%)   | 2 (1%)   | 12          | 48  |
| 4   | H     | 209/214 (98%)   | 188 (90%)  | 19 (9%)   | 2 (1%)   | 12          | 48  |
| 4   | L     | 209/214 (98%)   | 188 (90%)  | 19 (9%)   | 2 (1%)   | 12          | 48  |
| 4   | P     | 209/214 (98%)   | 188 (90%)  | 19 (9%)   | 2 (1%)   | 12          | 48  |
| All | All   | 4584/5172 (89%) | 3859 (84%) | 681 (15%) | 44 (1%)  | 15          | 48  |

All (44) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 390  | ASP  |
| 3   | C     | 43   | LYS  |
| 4   | D     | 543  | ASP  |
| 1   | E     | 1390 | ASP  |
| 3   | G     | 3043 | LYS  |
| 4   | H     | 3543 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | I     | 2390 | ASP  |
| 3   | K     | 4043 | LYS  |
| 4   | L     | 4543 | ASP  |
| 1   | M     | 3390 | ASP  |
| 3   | O     | 5043 | LYS  |
| 4   | P     | 5543 | ASP  |
| 3   | C     | 103  | SER  |
| 3   | G     | 3103 | SER  |
| 3   | K     | 4103 | SER  |
| 3   | O     | 5103 | SER  |
| 3   | C     | 41   | PRO  |
| 4   | D     | 701  | GLU  |
| 3   | G     | 3041 | PRO  |
| 4   | H     | 3701 | GLU  |
| 3   | K     | 4041 | PRO  |
| 4   | L     | 4701 | GLU  |
| 3   | O     | 5041 | PRO  |
| 4   | P     | 5701 | GLU  |
| 1   | A     | 265  | GLU  |
| 1   | A     | 266  | PRO  |
| 3   | C     | 118  | ALA  |
| 1   | E     | 1265 | GLU  |
| 1   | E     | 1266 | PRO  |
| 3   | G     | 3118 | ALA  |
| 1   | I     | 2265 | GLU  |
| 1   | I     | 2266 | PRO  |
| 3   | K     | 4118 | ALA  |
| 1   | M     | 3265 | GLU  |
| 1   | M     | 3266 | PRO  |
| 3   | O     | 5118 | ALA  |
| 3   | C     | 119  | LYS  |
| 3   | G     | 3119 | LYS  |
| 3   | K     | 4119 | LYS  |
| 3   | O     | 5119 | LYS  |
| 1   | A     | 191  | PRO  |
| 1   | E     | 1191 | PRO  |
| 1   | I     | 2191 | PRO  |
| 1   | M     | 3191 | PRO  |

### 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     | 339/370 (92%)   | 339 (100%) | 0        | 100         | 100 |
| 1   | E     | 339/370 (92%)   | 339 (100%) | 0        | 100         | 100 |
| 1   | I     | 339/370 (92%)   | 339 (100%) | 0        | 100         | 100 |
| 1   | M     | 339/370 (92%)   | 339 (100%) | 0        | 100         | 100 |
| 2   | B     | 282/367 (77%)   | 282 (100%) | 0        | 100         | 100 |
| 2   | F     | 282/367 (77%)   | 282 (100%) | 0        | 100         | 100 |
| 2   | J     | 282/367 (77%)   | 282 (100%) | 0        | 100         | 100 |
| 2   | N     | 282/367 (77%)   | 282 (100%) | 0        | 100         | 100 |
| 3   | C     | 188/188 (100%)  | 176 (94%)  | 12 (6%)  | 16          | 37  |
| 3   | G     | 188/188 (100%)  | 176 (94%)  | 12 (6%)  | 16          | 37  |
| 3   | K     | 188/188 (100%)  | 176 (94%)  | 12 (6%)  | 16          | 37  |
| 3   | O     | 188/188 (100%)  | 176 (94%)  | 12 (6%)  | 16          | 37  |
| 4   | D     | 178/183 (97%)   | 145 (82%)  | 33 (18%) | 1           | 8   |
| 4   | H     | 178/183 (97%)   | 145 (82%)  | 33 (18%) | 1           | 8   |
| 4   | L     | 178/183 (97%)   | 145 (82%)  | 33 (18%) | 1           | 8   |
| 4   | P     | 178/183 (97%)   | 145 (82%)  | 33 (18%) | 1           | 8   |
| All | All   | 3948/4432 (89%) | 3768 (95%) | 180 (5%) | 25          | 45  |

All (180) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 1   | GLN  |
| 3   | C     | 5   | VAL  |
| 3   | C     | 7   | SER  |
| 3   | C     | 28  | THR  |
| 3   | C     | 41  | PRO  |
| 3   | C     | 43  | LYS  |
| 3   | C     | 51  | ILE  |
| 3   | C     | 62  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | C     | 63   | GLU  |
| 3   | C     | 72   | LEU  |
| 3   | C     | 73   | GLU  |
| 3   | C     | 142  | LEU  |
| 4   | D     | 520  | LEU  |
| 4   | D     | 523  | ARG  |
| 4   | D     | 536  | ASN  |
| 4   | D     | 549  | LEU  |
| 4   | D     | 550  | ILE  |
| 4   | D     | 554  | ASN  |
| 4   | D     | 560  | VAL  |
| 4   | D     | 571  | ASP  |
| 4   | D     | 575  | LEU  |
| 4   | D     | 581  | GLN  |
| 4   | D     | 582  | THR  |
| 4   | D     | 583  | GLU  |
| 4   | D     | 605  | LYS  |
| 4   | D     | 609  | LEU  |
| 4   | D     | 618  | VAL  |
| 4   | D     | 620  | LEU  |
| 4   | D     | 626  | GLU  |
| 4   | D     | 629  | GLU  |
| 4   | D     | 630  | THR  |
| 4   | D     | 632  | LYS  |
| 4   | D     | 635  | LEU  |
| 4   | D     | 660  | GLN  |
| 4   | D     | 662  | MET  |
| 4   | D     | 666  | GLN  |
| 4   | D     | 670  | GLN  |
| 4   | D     | 671  | SER  |
| 4   | D     | 681  | LEU  |
| 4   | D     | 684  | THR  |
| 4   | D     | 686  | ARG  |
| 4   | D     | 689  | GLU  |
| 4   | D     | 691  | HIS  |
| 4   | D     | 705  | VAL  |
| 4   | D     | 709  | LEU  |
| 3   | G     | 3001 | GLN  |
| 3   | G     | 3005 | VAL  |
| 3   | G     | 3007 | SER  |
| 3   | G     | 3028 | THR  |
| 3   | G     | 3041 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | G     | 3043 | LYS  |
| 3   | G     | 3051 | ILE  |
| 3   | G     | 3062 | GLU  |
| 3   | G     | 3063 | GLU  |
| 3   | G     | 3072 | LEU  |
| 3   | G     | 3073 | GLU  |
| 3   | G     | 3142 | LEU  |
| 4   | H     | 3520 | LEU  |
| 4   | H     | 3523 | ARG  |
| 4   | H     | 3536 | ASN  |
| 4   | H     | 3549 | LEU  |
| 4   | H     | 3550 | ILE  |
| 4   | H     | 3554 | ASN  |
| 4   | H     | 3560 | VAL  |
| 4   | H     | 3571 | ASP  |
| 4   | H     | 3575 | LEU  |
| 4   | H     | 3581 | GLN  |
| 4   | H     | 3582 | THR  |
| 4   | H     | 3583 | GLU  |
| 4   | H     | 3605 | LYS  |
| 4   | H     | 3609 | LEU  |
| 4   | H     | 3618 | VAL  |
| 4   | H     | 3620 | LEU  |
| 4   | H     | 3626 | GLU  |
| 4   | H     | 3629 | GLU  |
| 4   | H     | 3630 | THR  |
| 4   | H     | 3632 | LYS  |
| 4   | H     | 3635 | LEU  |
| 4   | H     | 3660 | GLN  |
| 4   | H     | 3662 | MET  |
| 4   | H     | 3666 | GLN  |
| 4   | H     | 3670 | GLN  |
| 4   | H     | 3671 | SER  |
| 4   | H     | 3681 | LEU  |
| 4   | H     | 3684 | THR  |
| 4   | H     | 3686 | ARG  |
| 4   | H     | 3689 | GLU  |
| 4   | H     | 3691 | HIS  |
| 4   | H     | 3705 | VAL  |
| 4   | H     | 3709 | LEU  |
| 3   | K     | 4001 | GLN  |
| 3   | K     | 4005 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | K     | 4007 | SER  |
| 3   | K     | 4028 | THR  |
| 3   | K     | 4041 | PRO  |
| 3   | K     | 4043 | LYS  |
| 3   | K     | 4051 | ILE  |
| 3   | K     | 4062 | GLU  |
| 3   | K     | 4063 | GLU  |
| 3   | K     | 4072 | LEU  |
| 3   | K     | 4073 | GLU  |
| 3   | K     | 4142 | LEU  |
| 4   | L     | 4520 | LEU  |
| 4   | L     | 4523 | ARG  |
| 4   | L     | 4536 | ASN  |
| 4   | L     | 4549 | LEU  |
| 4   | L     | 4550 | ILE  |
| 4   | L     | 4554 | ASN  |
| 4   | L     | 4560 | VAL  |
| 4   | L     | 4571 | ASP  |
| 4   | L     | 4575 | LEU  |
| 4   | L     | 4581 | GLN  |
| 4   | L     | 4582 | THR  |
| 4   | L     | 4583 | GLU  |
| 4   | L     | 4605 | LYS  |
| 4   | L     | 4609 | LEU  |
| 4   | L     | 4618 | VAL  |
| 4   | L     | 4620 | LEU  |
| 4   | L     | 4626 | GLU  |
| 4   | L     | 4629 | GLU  |
| 4   | L     | 4630 | THR  |
| 4   | L     | 4632 | LYS  |
| 4   | L     | 4635 | LEU  |
| 4   | L     | 4660 | GLN  |
| 4   | L     | 4662 | MET  |
| 4   | L     | 4666 | GLN  |
| 4   | L     | 4670 | GLN  |
| 4   | L     | 4671 | SER  |
| 4   | L     | 4681 | LEU  |
| 4   | L     | 4684 | THR  |
| 4   | L     | 4686 | ARG  |
| 4   | L     | 4689 | GLU  |
| 4   | L     | 4691 | HIS  |
| 4   | L     | 4705 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L     | 4709 | LEU  |
| 3   | O     | 5001 | GLN  |
| 3   | O     | 5005 | VAL  |
| 3   | O     | 5007 | SER  |
| 3   | O     | 5028 | THR  |
| 3   | O     | 5041 | PRO  |
| 3   | O     | 5043 | LYS  |
| 3   | O     | 5051 | ILE  |
| 3   | O     | 5062 | GLU  |
| 3   | O     | 5063 | GLU  |
| 3   | O     | 5072 | LEU  |
| 3   | O     | 5073 | GLU  |
| 3   | O     | 5142 | LEU  |
| 4   | P     | 5520 | LEU  |
| 4   | P     | 5523 | ARG  |
| 4   | P     | 5536 | ASN  |
| 4   | P     | 5549 | LEU  |
| 4   | P     | 5550 | ILE  |
| 4   | P     | 5554 | ASN  |
| 4   | P     | 5560 | VAL  |
| 4   | P     | 5571 | ASP  |
| 4   | P     | 5575 | LEU  |
| 4   | P     | 5581 | GLN  |
| 4   | P     | 5582 | THR  |
| 4   | P     | 5583 | GLU  |
| 4   | P     | 5605 | LYS  |
| 4   | P     | 5609 | LEU  |
| 4   | P     | 5618 | VAL  |
| 4   | P     | 5620 | LEU  |
| 4   | P     | 5626 | GLU  |
| 4   | P     | 5629 | GLU  |
| 4   | P     | 5630 | THR  |
| 4   | P     | 5632 | LYS  |
| 4   | P     | 5635 | LEU  |
| 4   | P     | 5660 | GLN  |
| 4   | P     | 5662 | MET  |
| 4   | P     | 5666 | GLN  |
| 4   | P     | 5670 | GLN  |
| 4   | P     | 5671 | SER  |
| 4   | P     | 5681 | LEU  |
| 4   | P     | 5684 | THR  |
| 4   | P     | 5686 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | P     | 5689 | GLU  |
| 4   | P     | 5691 | HIS  |
| 4   | P     | 5705 | VAL  |
| 4   | P     | 5709 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 77   | GLN  |
| 1   | A     | 102  | GLN  |
| 1   | A     | 183  | HIS  |
| 1   | A     | 328  | ASN  |
| 1   | A     | 387  | HIS  |
| 1   | A     | 394  | GLN  |
| 2   | B     | 528  | HIS  |
| 2   | B     | 638  | ASN  |
| 2   | B     | 662  | HIS  |
| 2   | B     | 825  | GLN  |
| 3   | C     | 6    | GLN  |
| 3   | C     | 54   | ASN  |
| 3   | C     | 82   | GLN  |
| 3   | C     | 84   | ASN  |
| 3   | C     | 109  | GLN  |
| 3   | C     | 168  | HIS  |
| 4   | D     | 554  | ASN  |
| 4   | D     | 555  | ASN  |
| 4   | D     | 673  | ASN  |
| 1   | E     | 1102 | GLN  |
| 1   | E     | 1183 | HIS  |
| 1   | E     | 1387 | HIS  |
| 1   | E     | 1394 | GLN  |
| 2   | F     | 1528 | HIS  |
| 2   | F     | 1638 | ASN  |
| 2   | F     | 1642 | HIS  |
| 2   | F     | 1825 | GLN  |
| 3   | G     | 3003 | GLN  |
| 3   | G     | 3006 | GLN  |
| 3   | G     | 3054 | ASN  |
| 3   | G     | 3082 | GLN  |
| 3   | G     | 3084 | ASN  |
| 3   | G     | 3109 | GLN  |
| 3   | G     | 3168 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | H     | 3501 | GLN  |
| 4   | H     | 3554 | ASN  |
| 4   | H     | 3555 | ASN  |
| 4   | H     | 3596 | ASN  |
| 4   | H     | 3673 | ASN  |
| 1   | I     | 2102 | GLN  |
| 1   | I     | 2183 | HIS  |
| 1   | I     | 2328 | ASN  |
| 1   | I     | 2356 | HIS  |
| 1   | I     | 2387 | HIS  |
| 1   | I     | 2394 | GLN  |
| 2   | J     | 2528 | HIS  |
| 2   | J     | 2638 | ASN  |
| 2   | J     | 2642 | HIS  |
| 2   | J     | 2662 | HIS  |
| 2   | J     | 2825 | GLN  |
| 3   | K     | 4003 | GLN  |
| 3   | K     | 4006 | GLN  |
| 3   | K     | 4054 | ASN  |
| 3   | K     | 4082 | GLN  |
| 3   | K     | 4084 | ASN  |
| 3   | K     | 4109 | GLN  |
| 3   | K     | 4168 | HIS  |
| 4   | L     | 4554 | ASN  |
| 4   | L     | 4555 | ASN  |
| 4   | L     | 4581 | GLN  |
| 4   | L     | 4673 | ASN  |
| 1   | M     | 3102 | GLN  |
| 1   | M     | 3183 | HIS  |
| 1   | M     | 3328 | ASN  |
| 1   | M     | 3387 | HIS  |
| 1   | M     | 3394 | GLN  |
| 2   | N     | 3528 | HIS  |
| 2   | N     | 3638 | ASN  |
| 2   | N     | 3662 | HIS  |
| 2   | N     | 3825 | GLN  |
| 3   | O     | 5003 | GLN  |
| 3   | O     | 5006 | GLN  |
| 3   | O     | 5054 | ASN  |
| 3   | O     | 5082 | GLN  |
| 3   | O     | 5084 | ASN  |
| 3   | O     | 5085 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | O     | 5109 | GLN  |
| 3   | O     | 5168 | HIS  |
| 4   | P     | 5501 | GLN  |
| 4   | P     | 5554 | ASN  |
| 4   | P     | 5555 | ASN  |
| 4   | P     | 5673 | ASN  |

### 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.

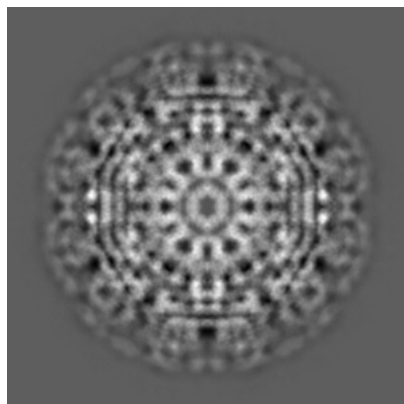
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9278. These allow visual inspection of the internal detail of the map and identification of artifacts.

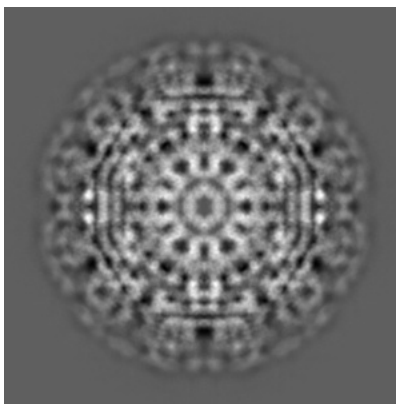
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

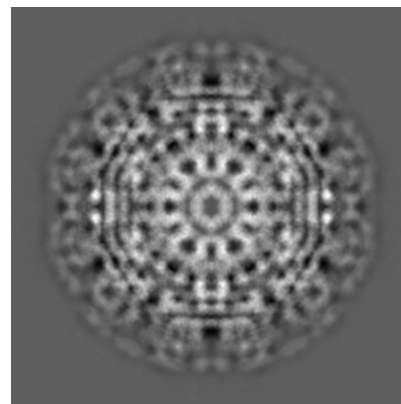
#### 6.1.1 Primary map



X

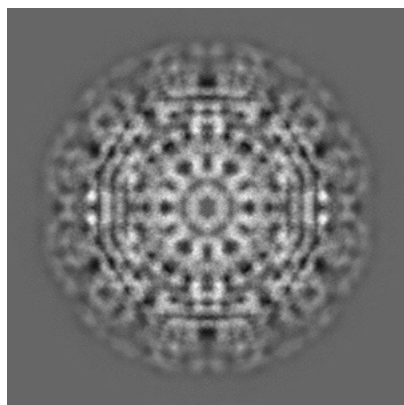


Y

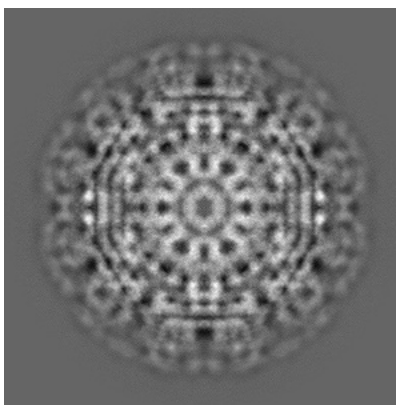


Z

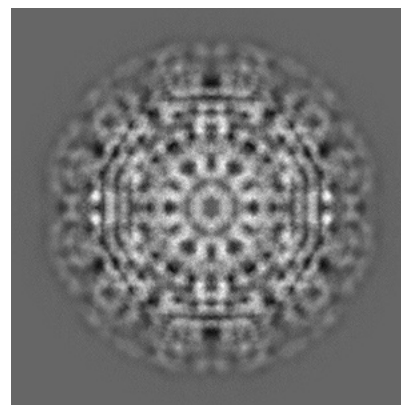
#### 6.1.2 Raw map



X



Y



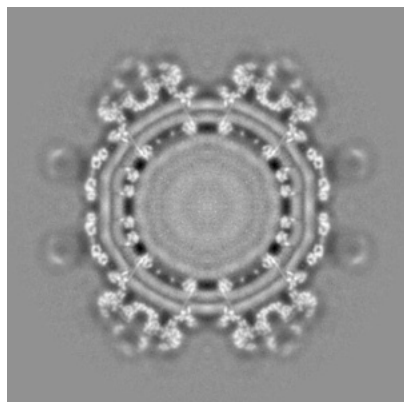
Z

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

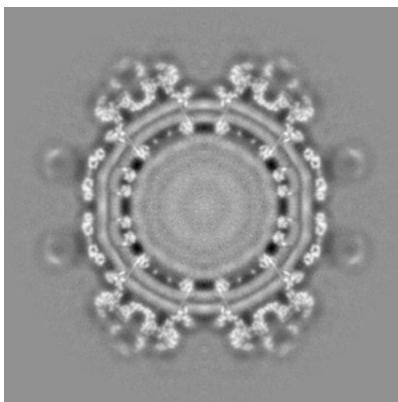


## 6.2 Central slices [i](#)

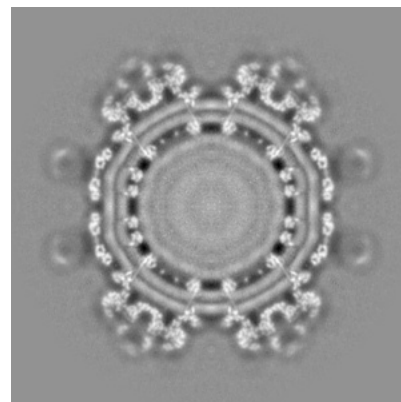
### 6.2.1 Primary map



X Index: 280

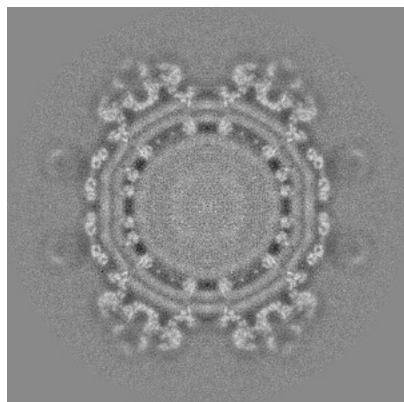


Y Index: 280

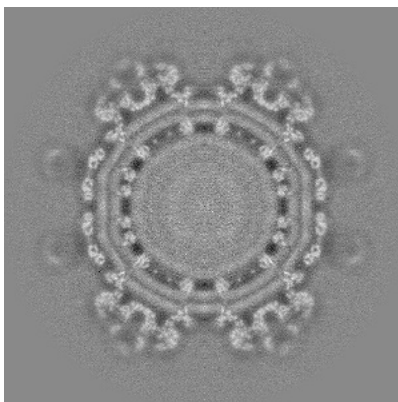


Z Index: 280

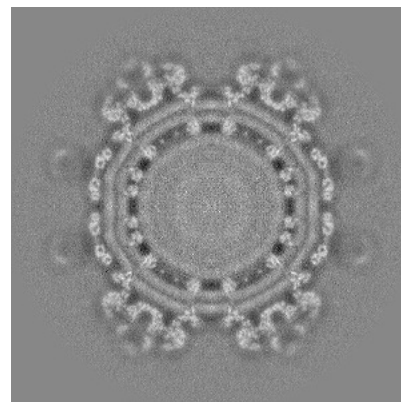
### 6.2.2 Raw map



X Index: 280



Y Index: 280

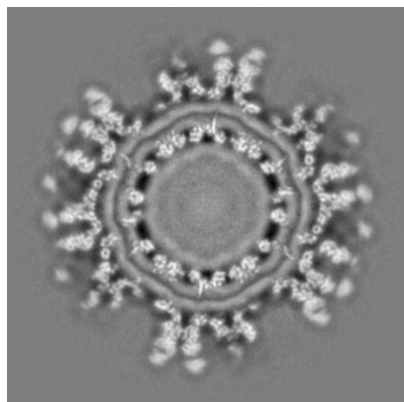


Z Index: 280

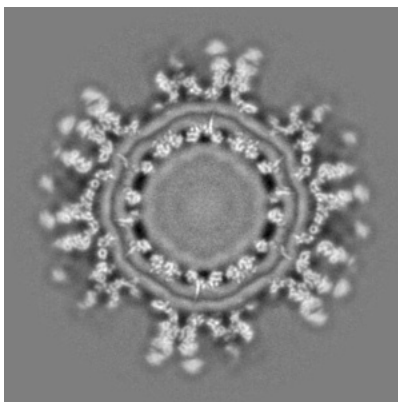
The images above show central slices of the map in three orthogonal directions.

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

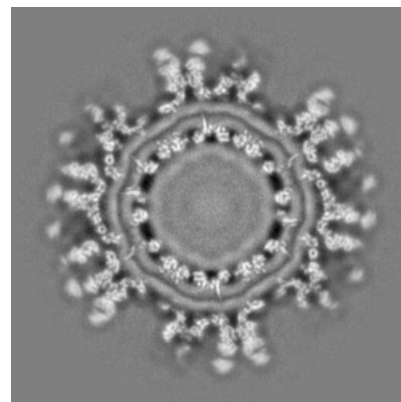
### 6.3.1 Primary map



X Index: 228

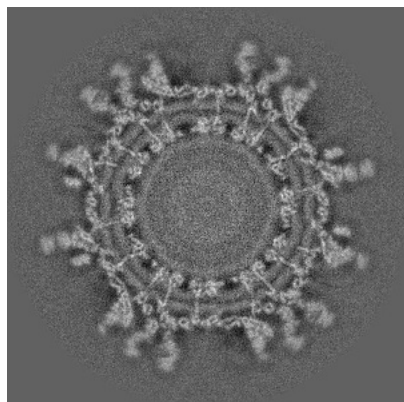


Y Index: 228

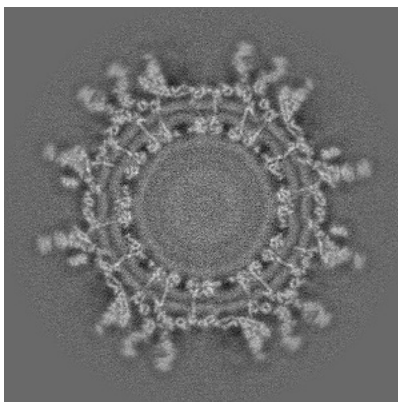


Z Index: 332

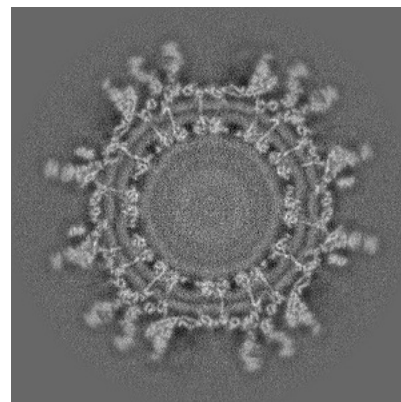
### 6.3.2 Raw map



X Index: 262



Y Index: 262

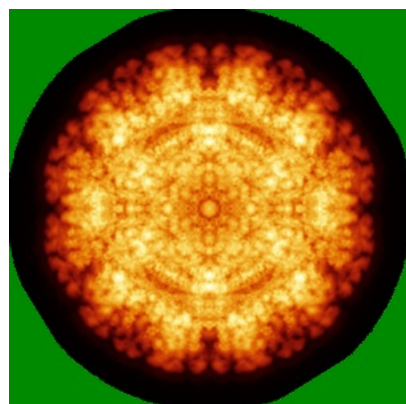


Z Index: 298

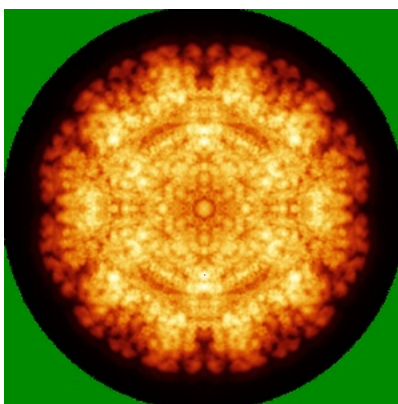
The images above show the largest variance slices of the map in three orthogonal directions.

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

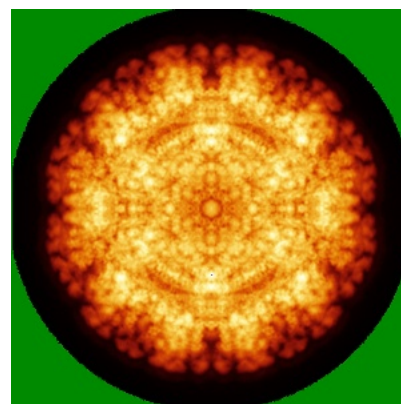
### 6.4.1 Primary map



X

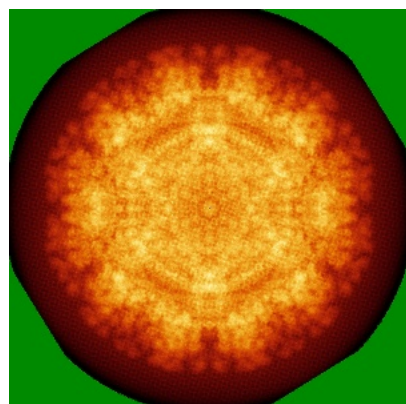


Y

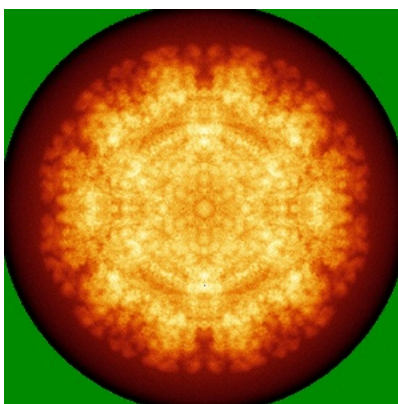


Z

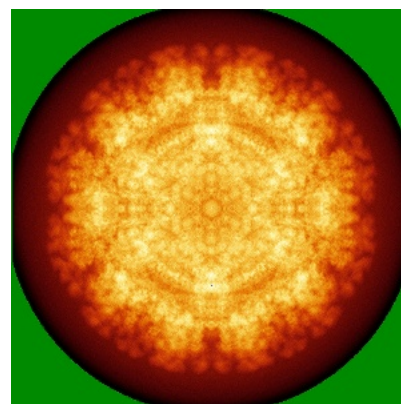
### 6.4.2 Raw map



X



Y

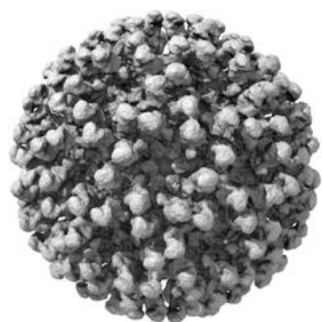


Z

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](#)

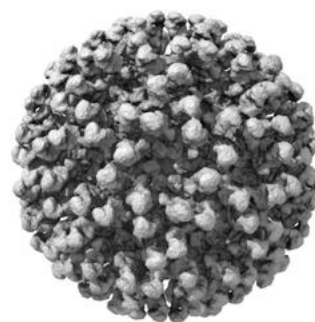
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

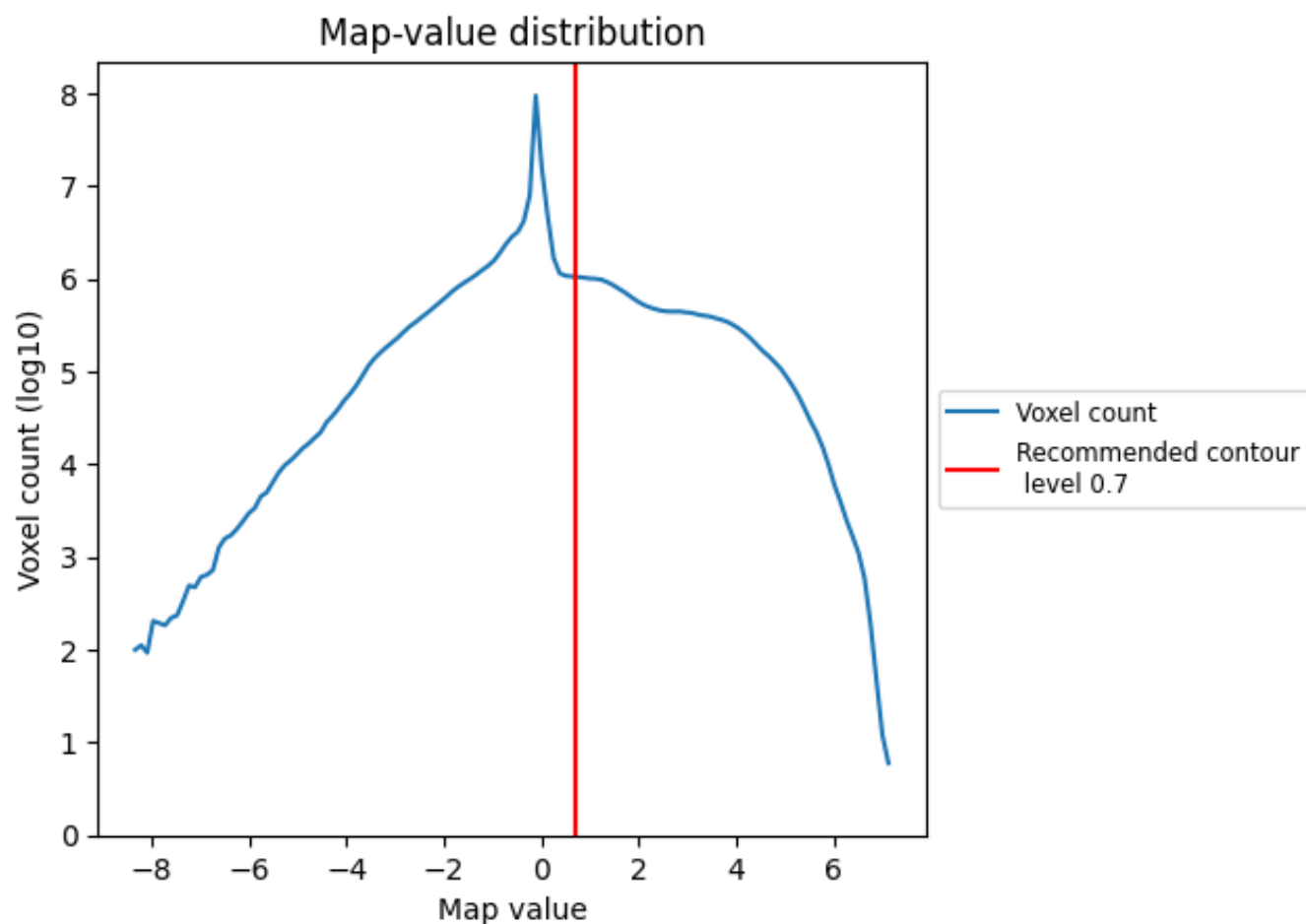
## 6.6 Mask visualisation [i](#)

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.

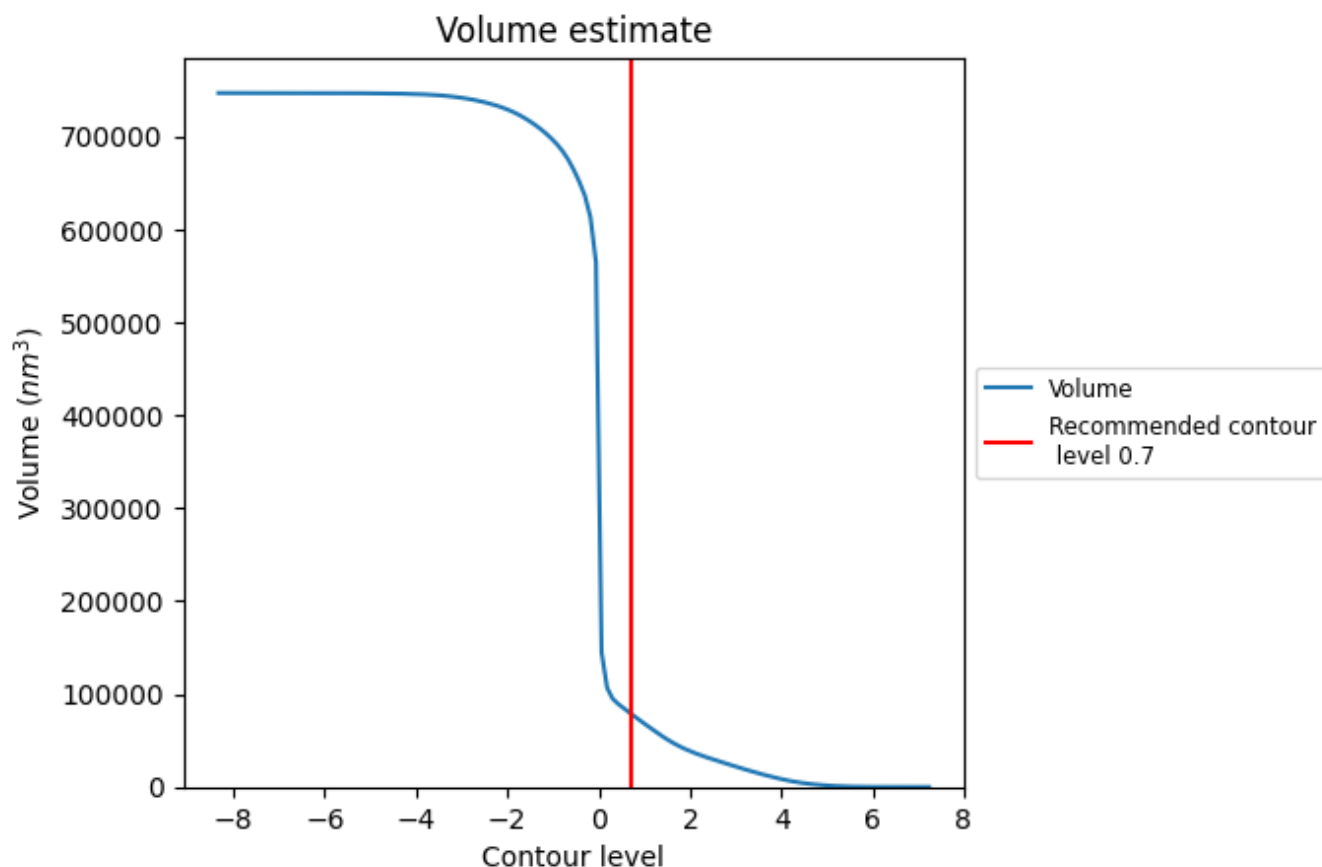
### 7.1 Map-value distribution [i](#)



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.



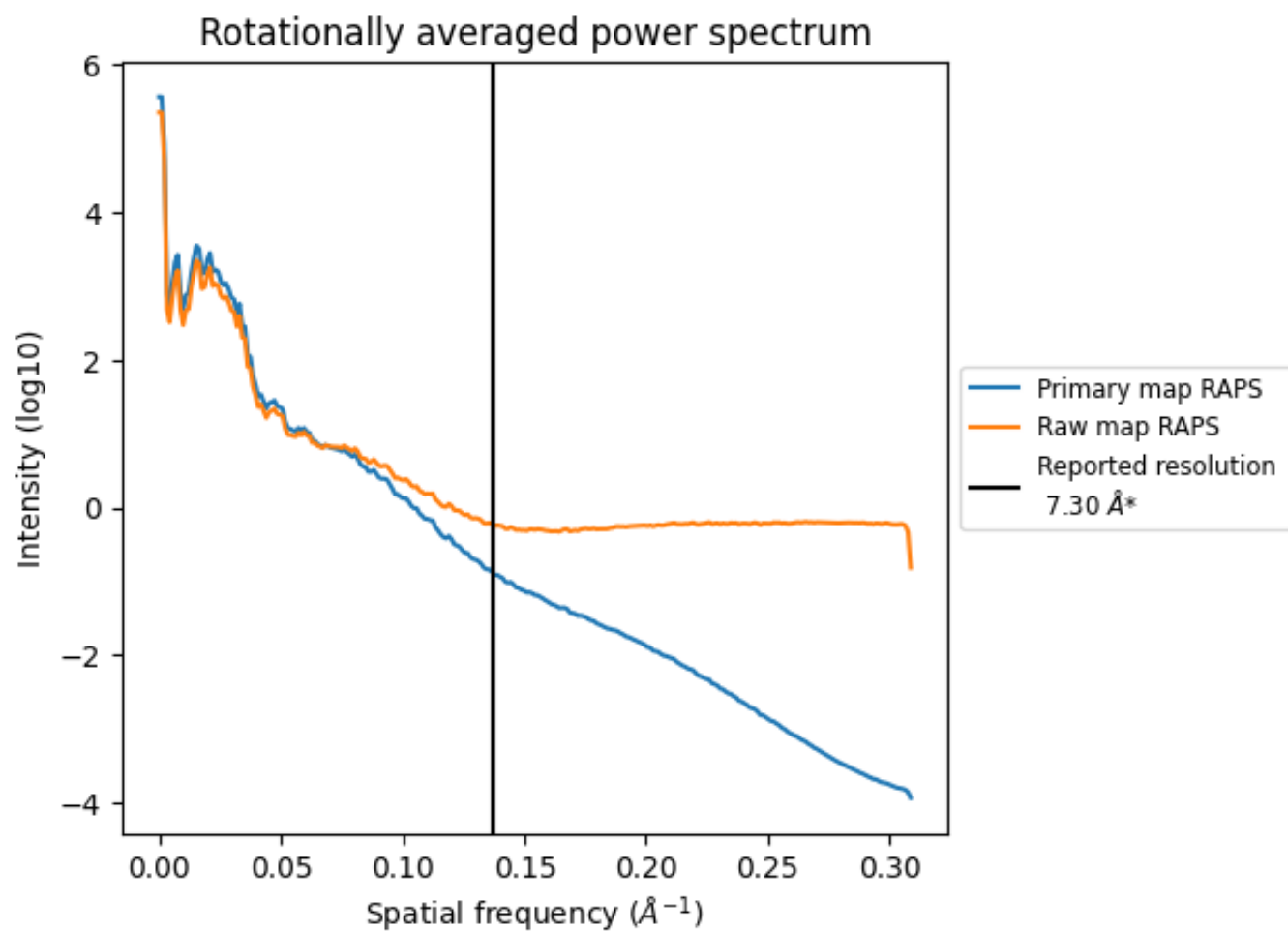
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79048  $\text{nm}^3$ ; this corresponds to an approximate mass of 71406 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 ⓘ



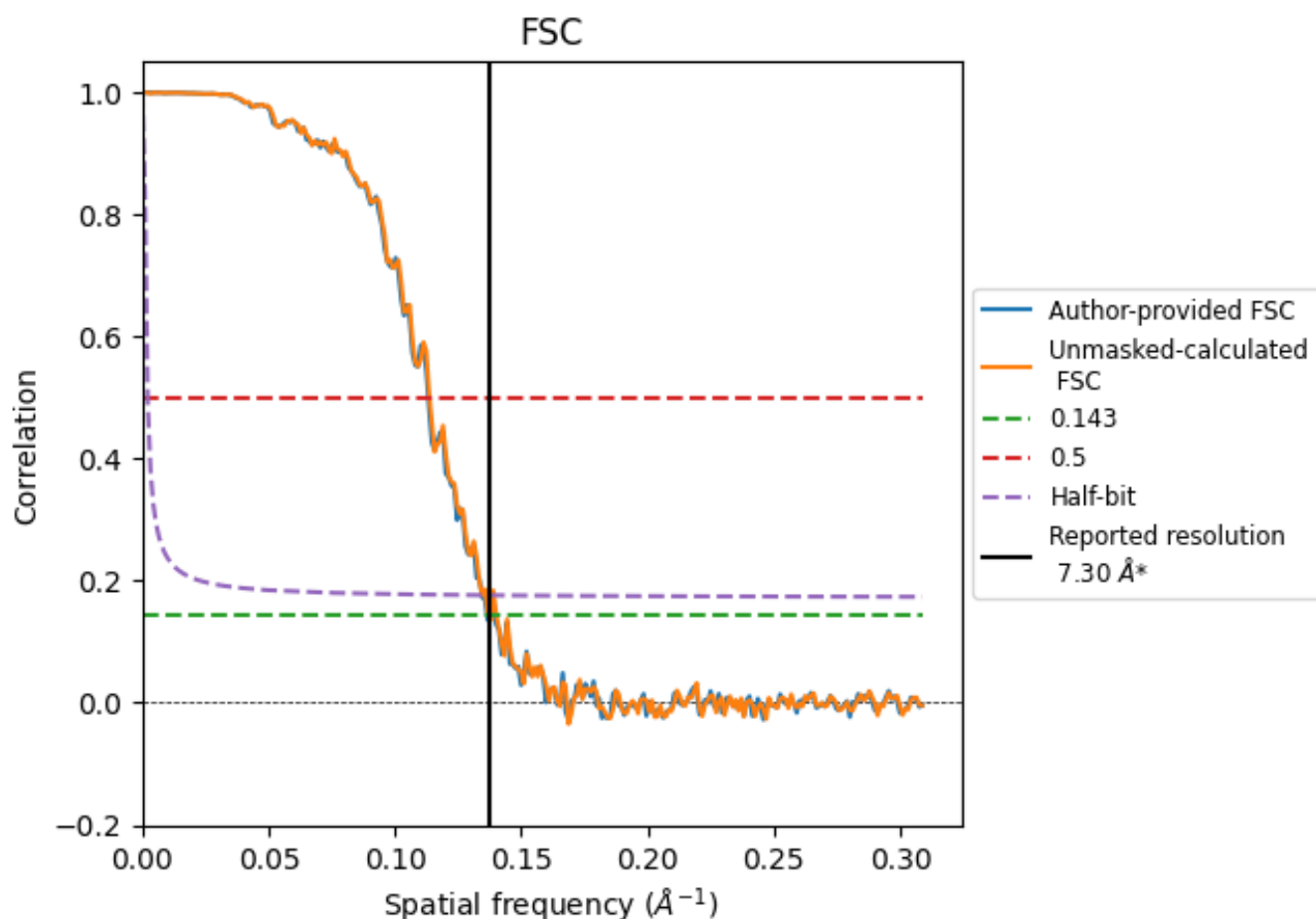
\*Reported resolution corresponds to spatial frequency of 0.137 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.137 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 7.30                               | -    | -        |
| Author-provided FSC curve | 7.33                               | 8.83 | 7.44     |
| Unmasked-calculated*      | 7.29                               | 8.80 | 7.36     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

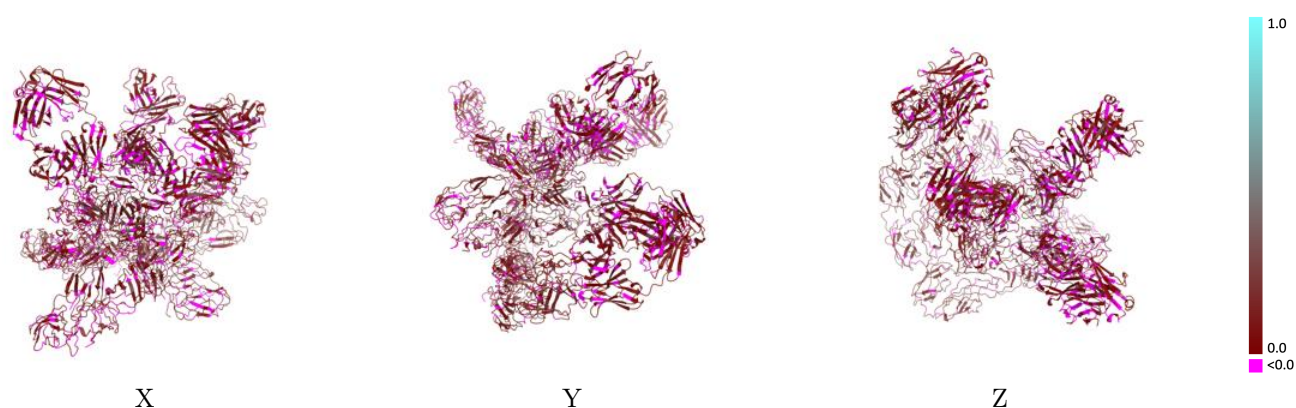
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9278 and PDB model 6MWV. Per-residue inclusion information can be found in section 3 on page 6.

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

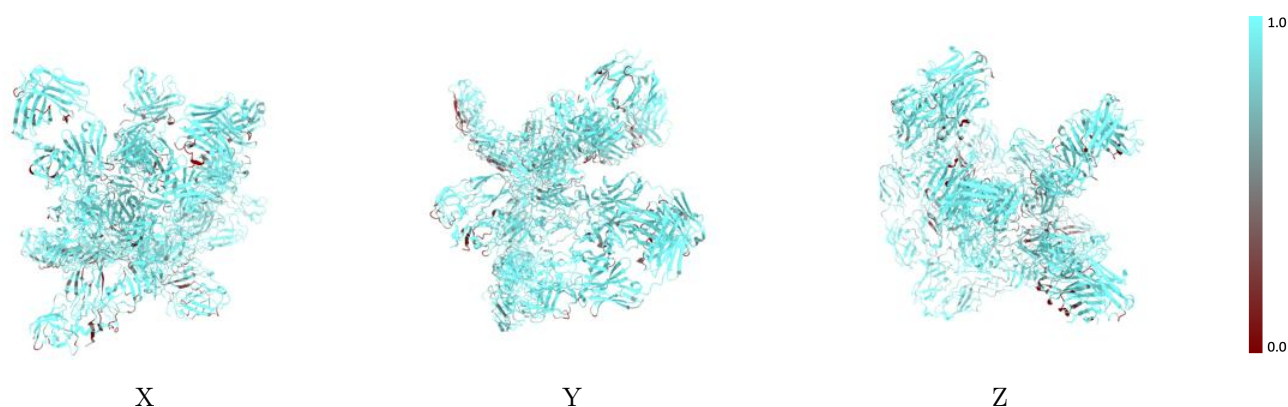
This section was not generated.

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



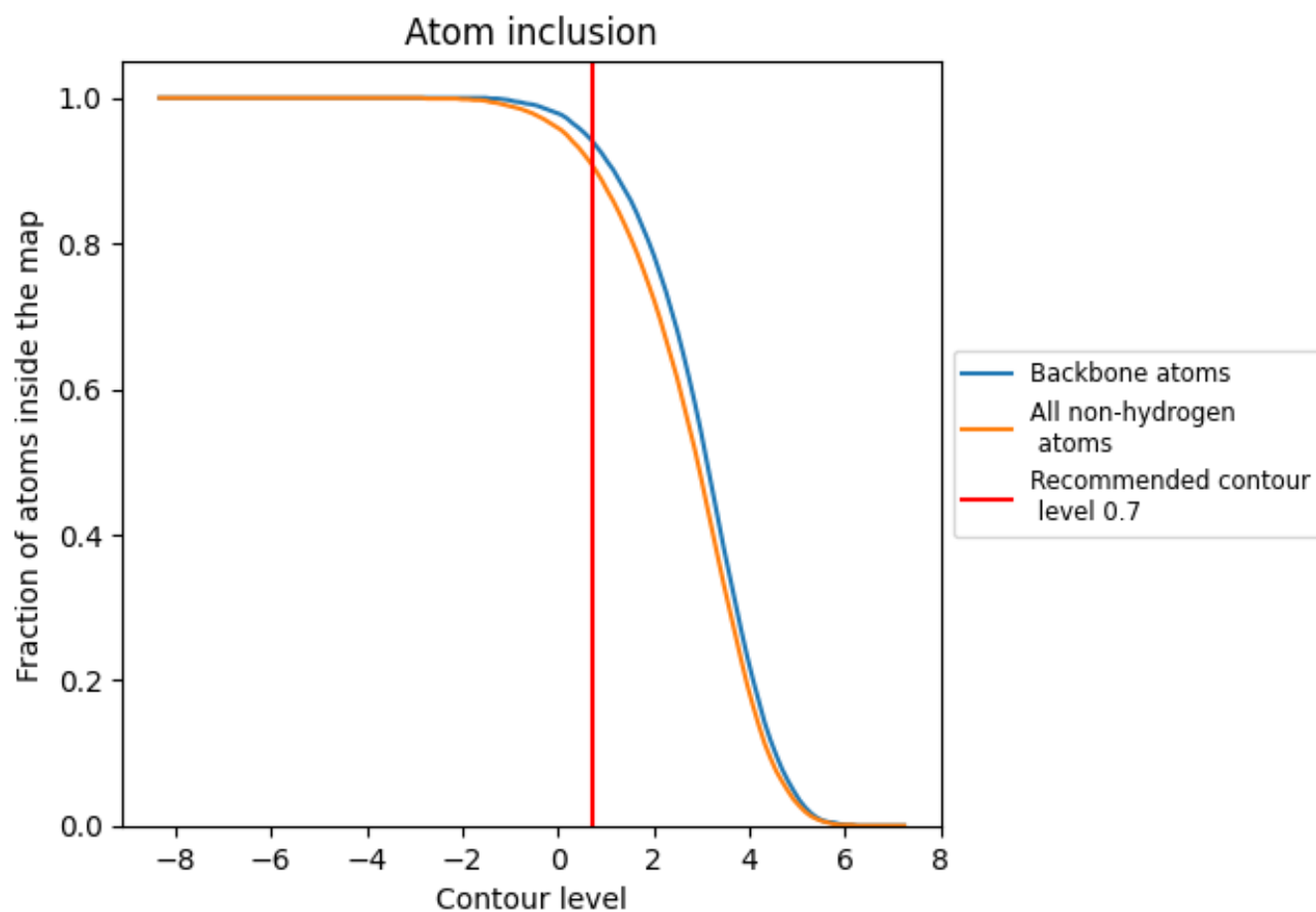
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.7) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9090   |  0.0920   |
| A     |  0.9200   |  0.1260   |
| B     |  0.9250   |  0.1360   |
| C     |  0.9300   |  0.0710   |
| D     |  0.9330   |  0.0740   |
| E     |  0.8810   |  0.1080   |
| F     |  0.9210   |  0.1170   |
| G     |  0.9170   |  0.0700   |
| H     |  0.9450   |  0.0640   |
| I     |  0.9210   |  0.1200   |
| J     |  0.9160   |  0.0900   |
| K     |  0.8870   |  0.0600   |
| L     |  0.9100   |  0.0580   |
| M     |  0.8650   |  0.0880   |
| N     |  0.8850  |  0.0780  |
| O     |  0.9090 |  0.0600 |
| P     |  0.9100 |  0.0630 |

