



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 12:55 PM UTC

PDB ID : 8YGP / pdb\_00008ygp  
EMDB ID : EMD-39259  
Title : The tetramer Structure of DSR2-SPR with NAD  
Authors : Gao, X.; Zhu, H.; Cui, S.  
Deposited on : 2024-02-26  
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

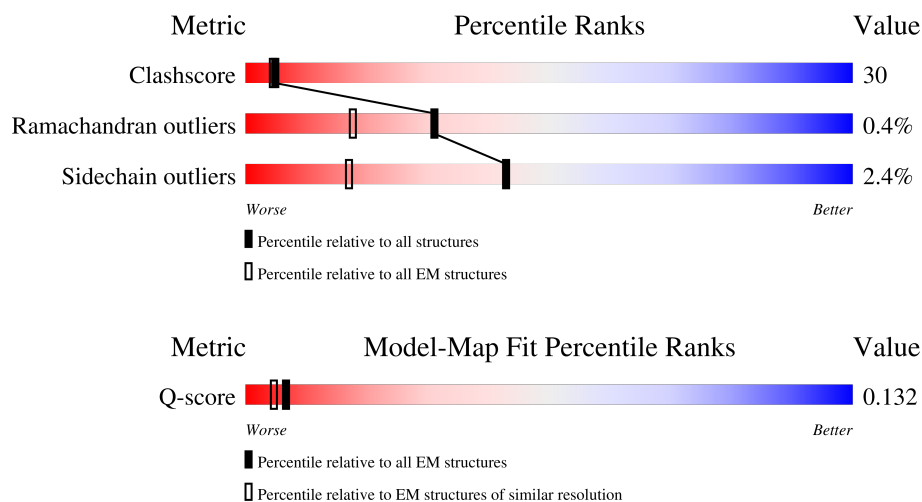
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.40 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                       | 3132 ( 3.91 - 4.90 )                                     |

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     | 1005   | <div> <div>22%</div> <div>51%</div> <div>43%</div> <div>...</div> </div> |
| 1   | B     | 1005   | <div> <div>26%</div> <div>54%</div> <div>41%</div> <div>...</div> </div> |
| 1   | E     | 1005   | <div> <div>47%</div> <div>49%</div> <div>..</div> </div>                 |
| 1   | F     | 1005   | <div> <div>6%</div> <div>45%</div> <div>48%</div> <div>...</div> </div>  |

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| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 2   | C     | 264    | <div><div><div>40%</div><div>36%</div><div>19%</div><div>43%</div></div></div> |
| 2   | D     | 264    | <div><div><div>36%</div><div>31%</div><div>26%</div><div>43%</div></div></div> |
| 2   | G     | 264    | <div><div><div>14%</div><div>29%</div><div>25%</div><div>43%</div></div></div> |
| 2   | H     | 264    | <div><div><div>18%</div><div>28%</div><div>26%</div><div>43%</div></div></div> |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 37524 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 SIR2-like domain-containing protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 983      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8183  | 5292 | 1322 | 1538 | 31 |         |       |
| 1   | B     | 983      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8183  | 5292 | 1322 | 1538 | 31 |         |       |
| 1   | E     | 983      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8183  | 5292 | 1322 | 1538 | 31 |         |       |
| 1   | F     | 983      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8183  | 5292 | 1322 | 1538 | 31 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 171     | ALA      | HIS    | engineered mutation | UNP D4G637 |
| B     | 171     | ALA      | HIS    | engineered mutation | UNP D4G637 |
| E     | 171     | ALA      | HIS    | engineered mutation | UNP D4G637 |
| F     | 171     | ALA      | HIS    | engineered mutation | UNP D4G637 |

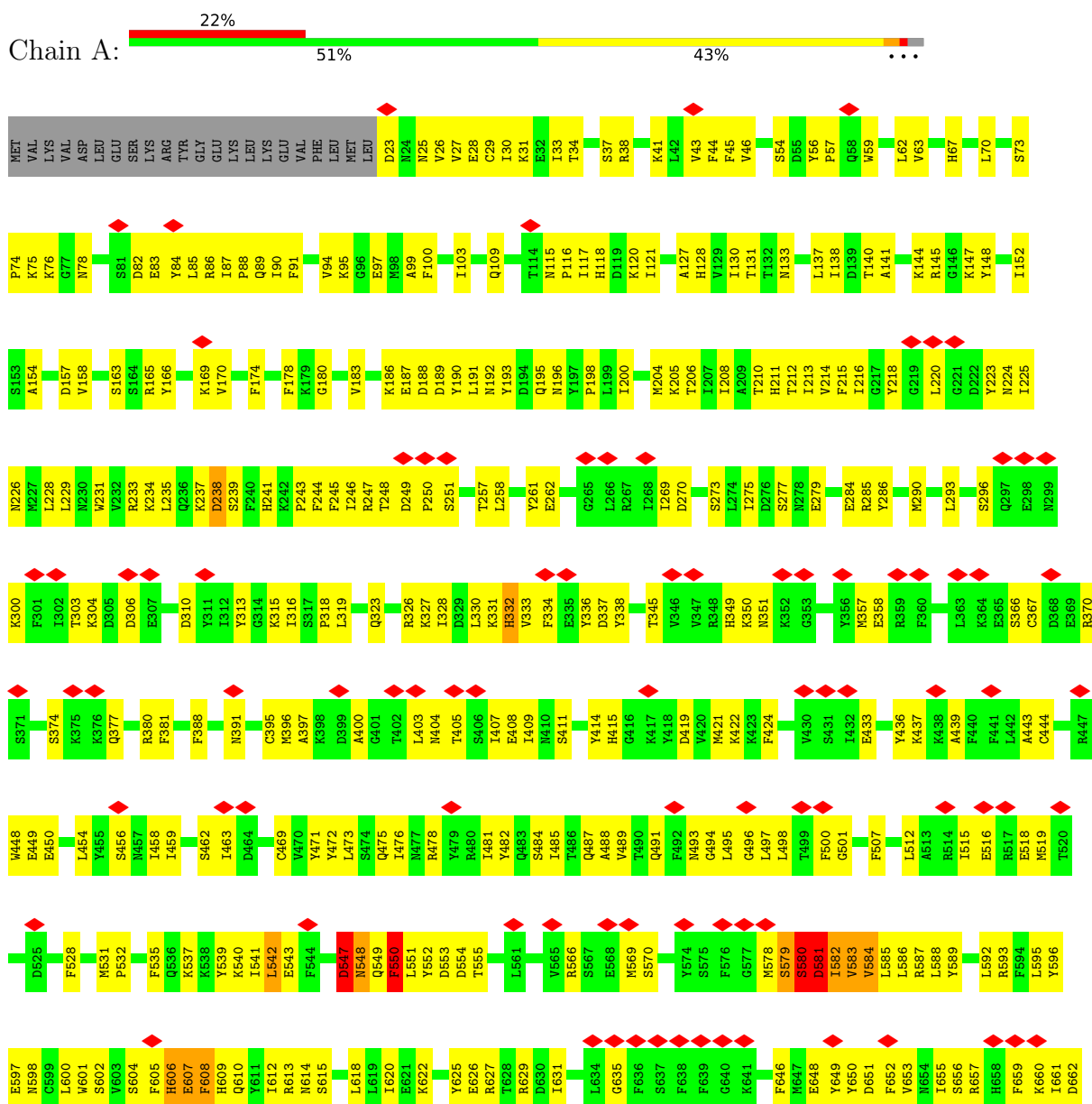
- Molecule 2 is a protein called SPR.

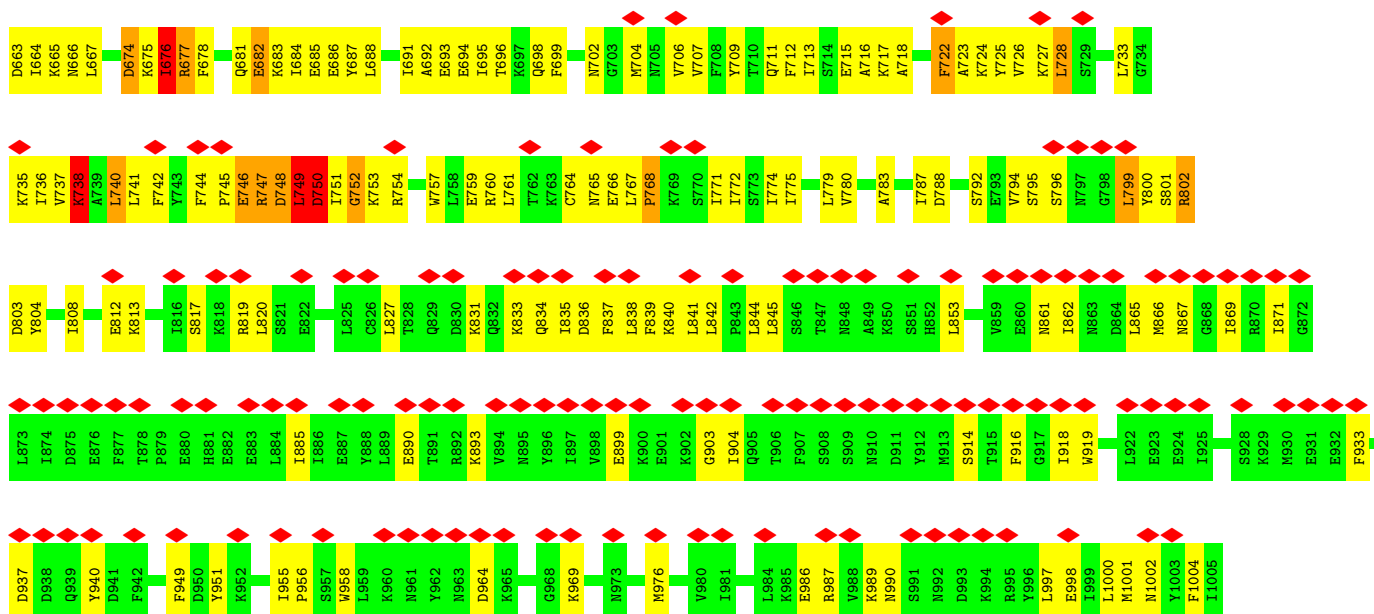
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | C     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 758 | 189 | 247 | 4 |         |       |
| 2   | D     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 758 | 189 | 247 | 4 |         |       |
| 2   | G     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 758 | 189 | 247 | 4 |         |       |
| 2   | H     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 758 | 189 | 247 | 4 |         |       |

### 3 Residue-property plots

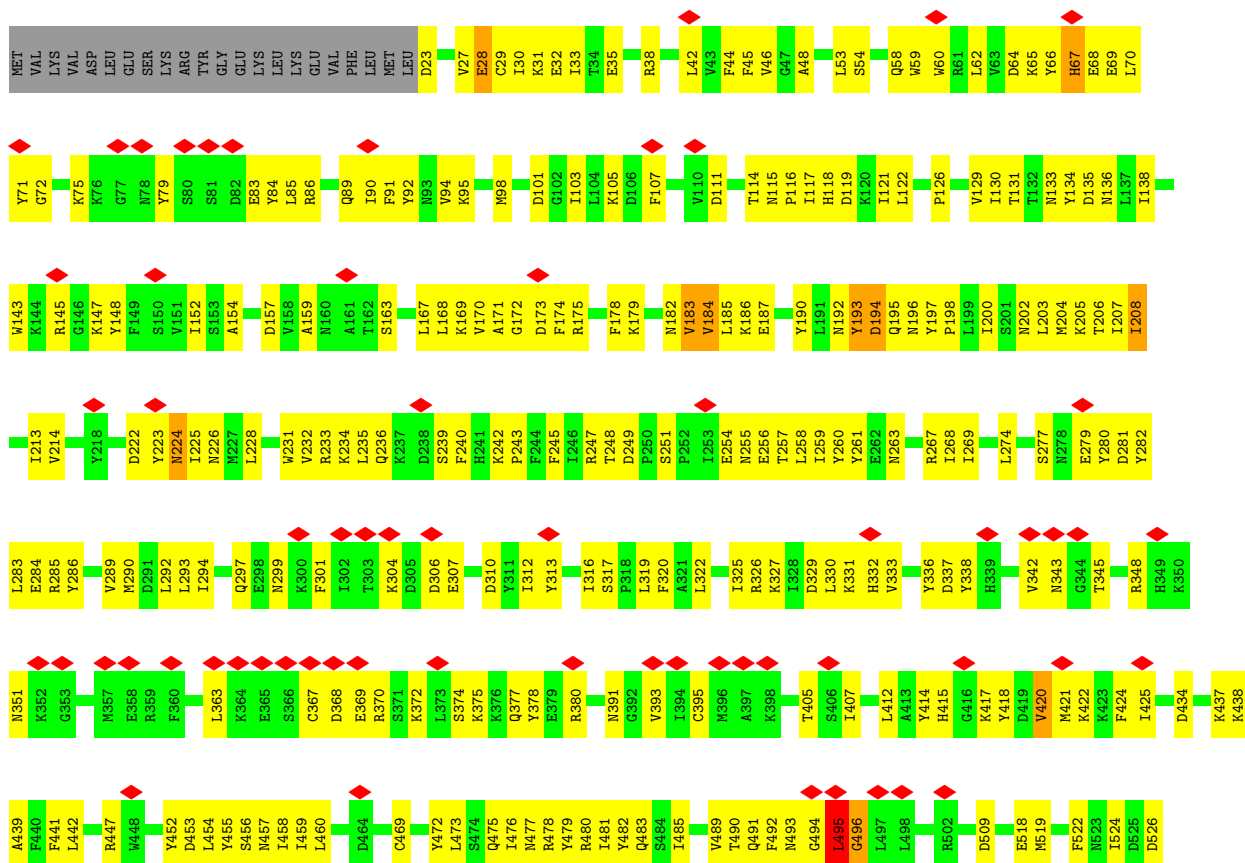
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

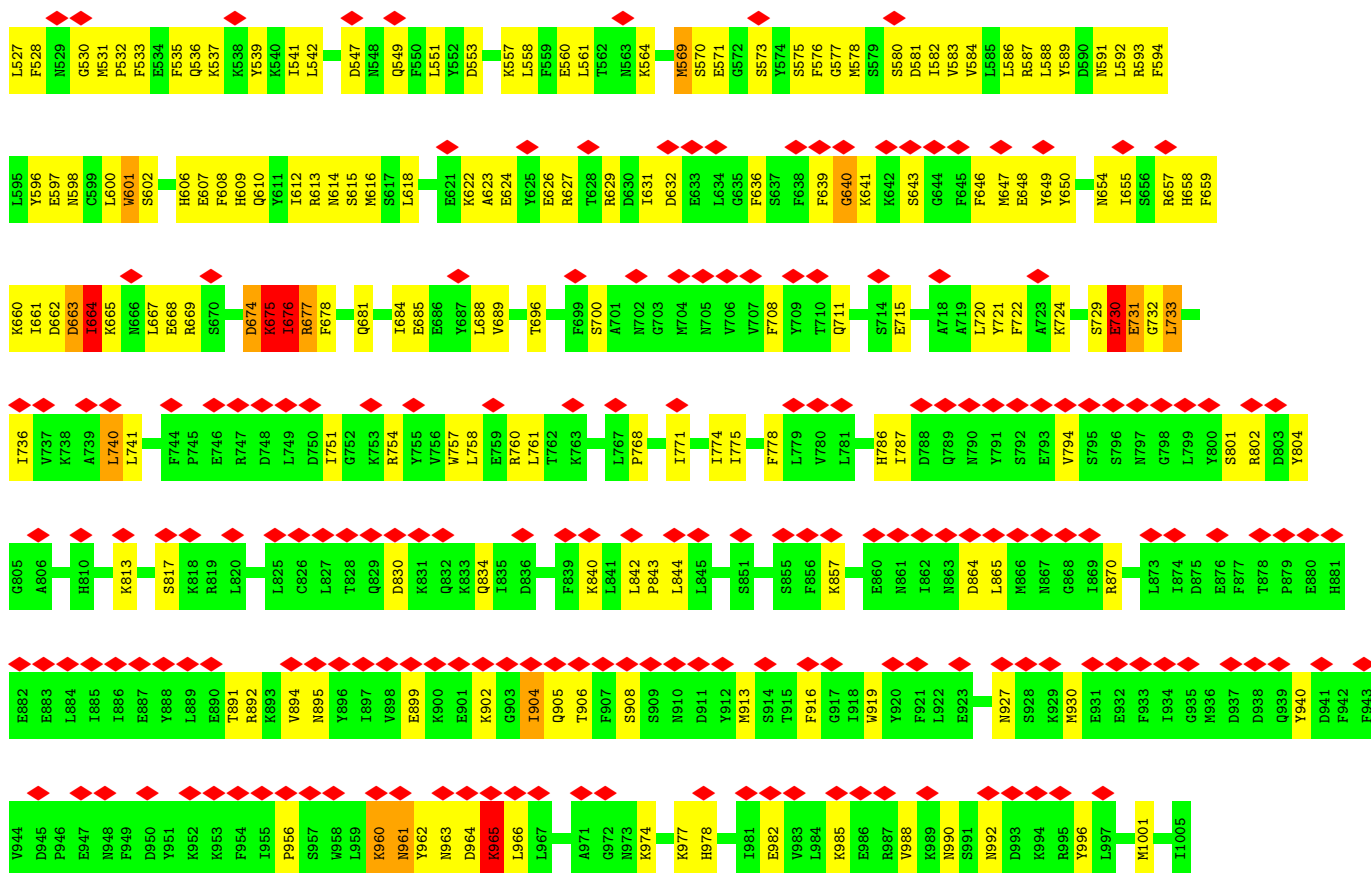
- Molecule 1: SIR2-like domain-containing protein





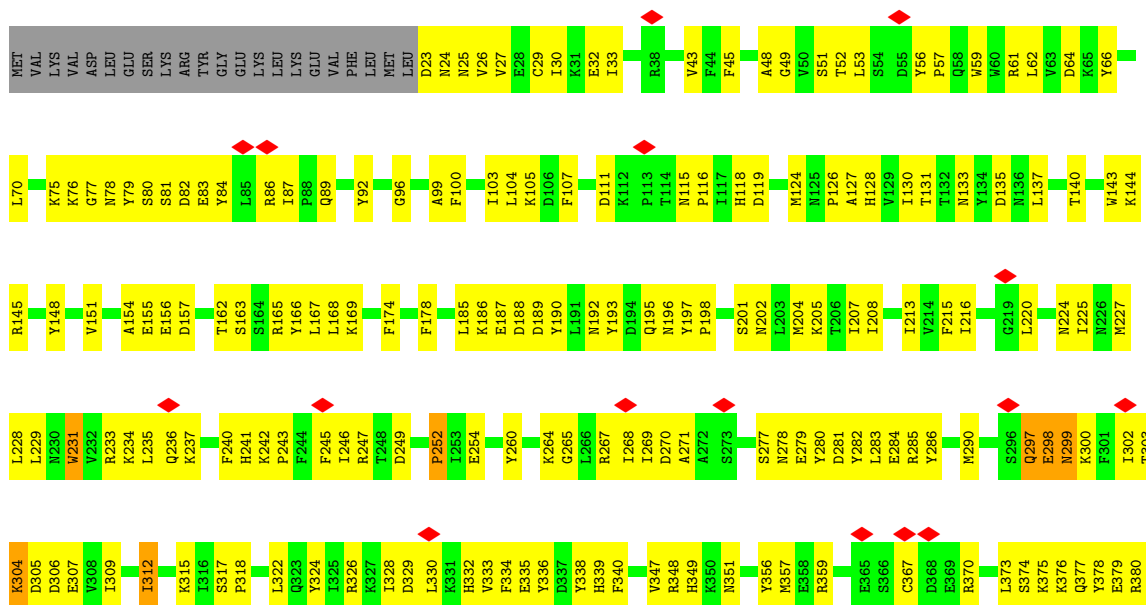
• Molecule 1: SIR2-like domain-containing protein

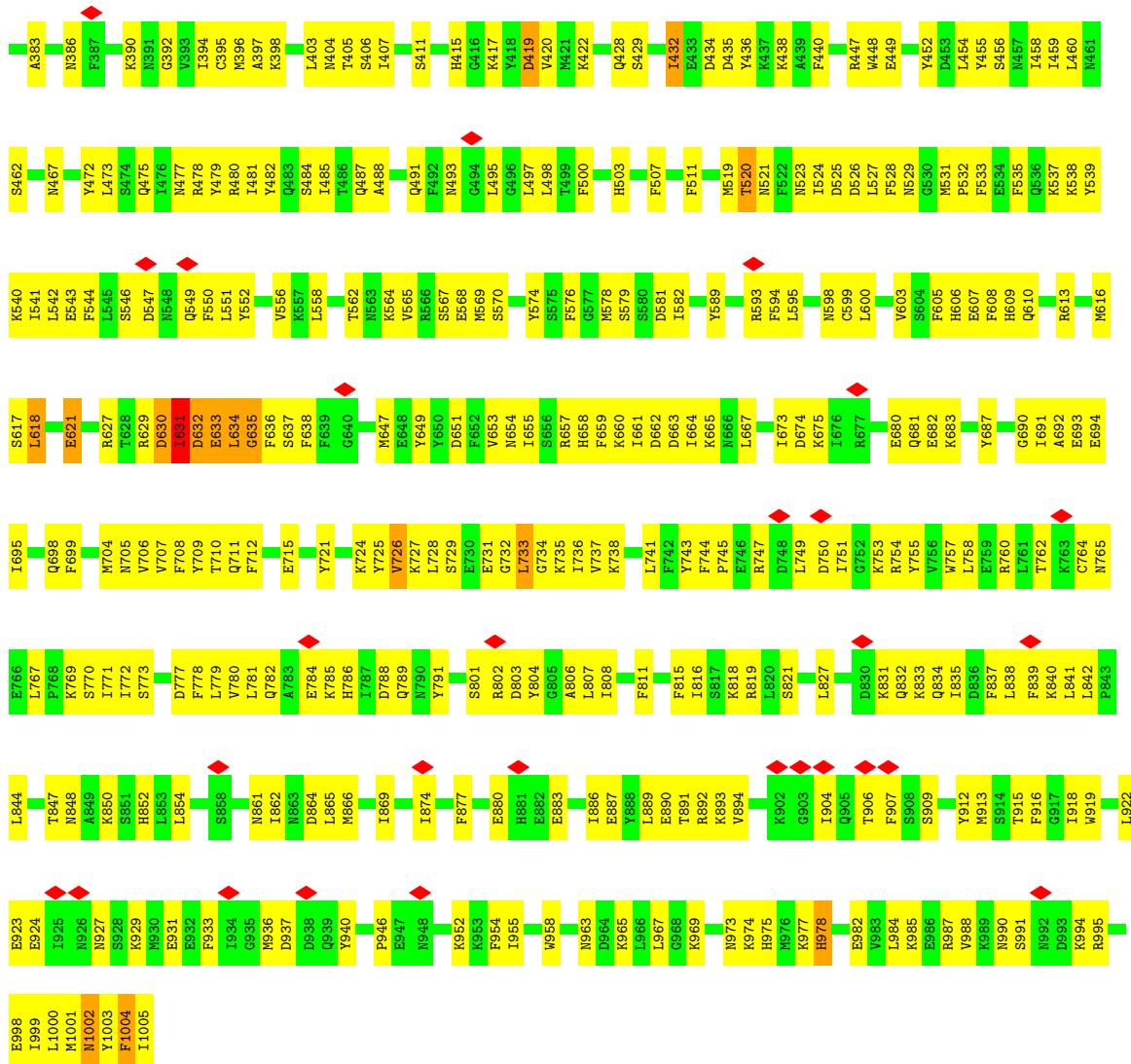




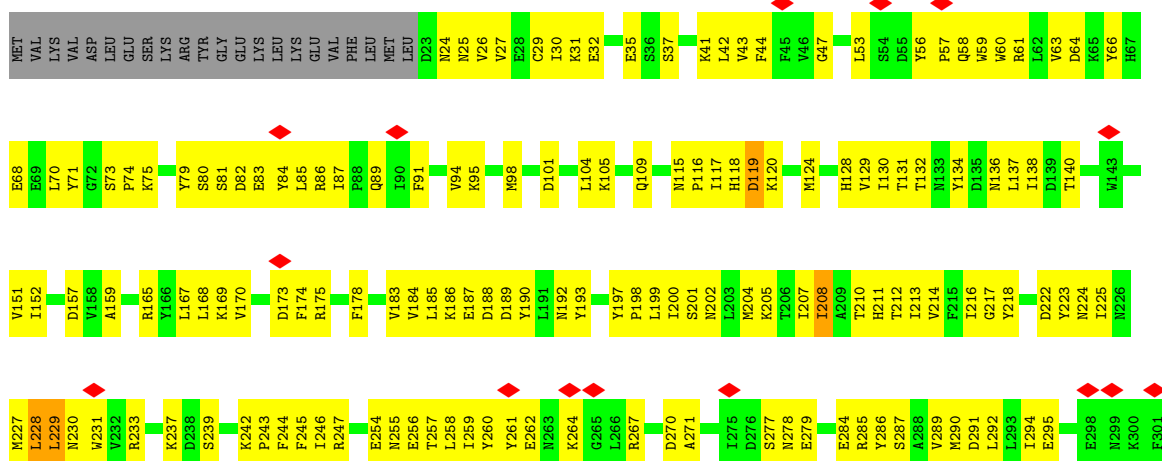
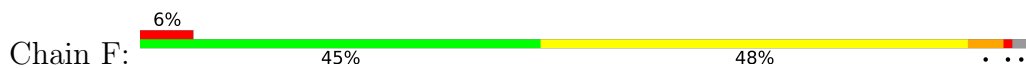
• Molecule 1: SIR2-like domain-containing protein

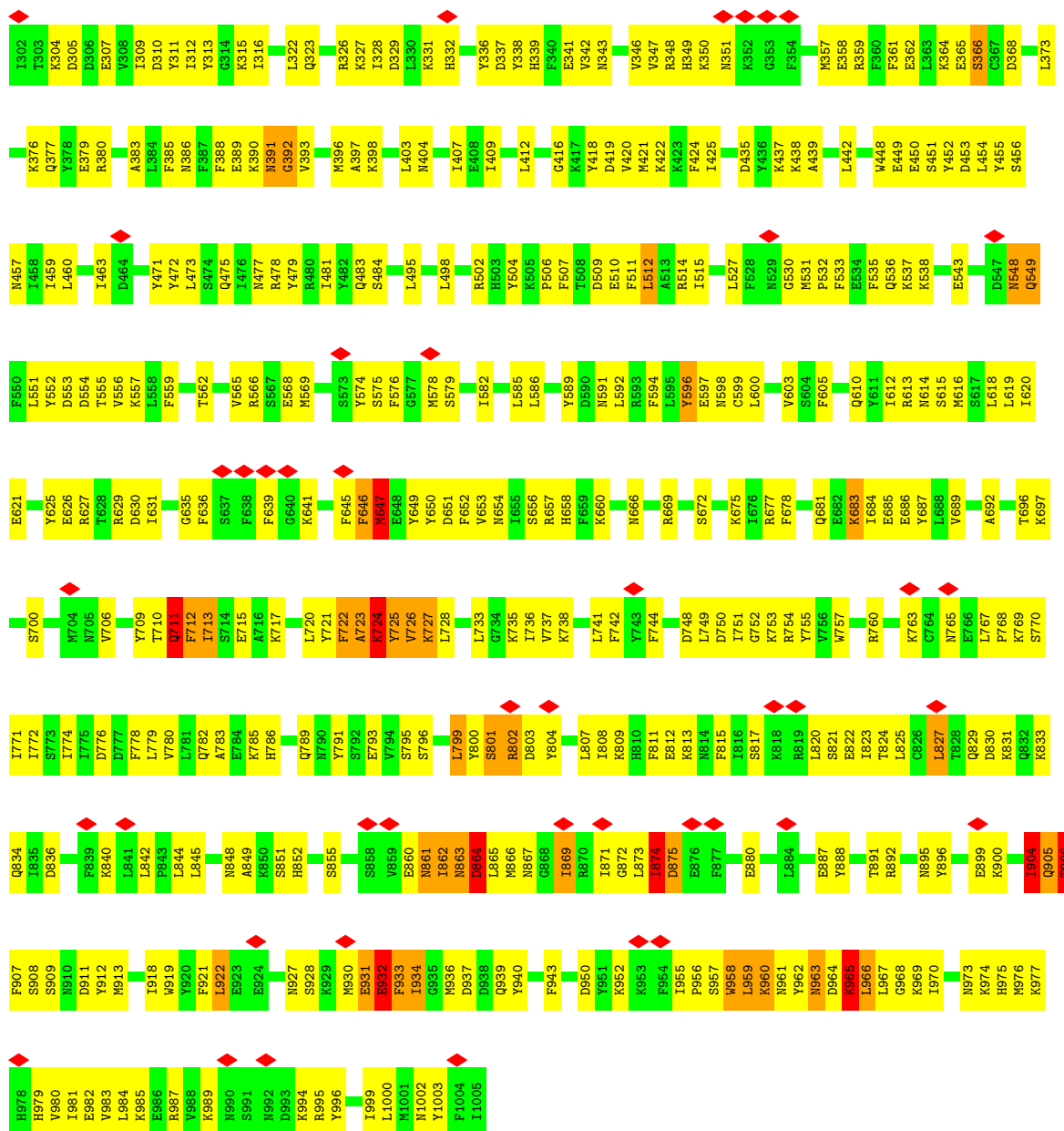
Chain E: 47% 49%



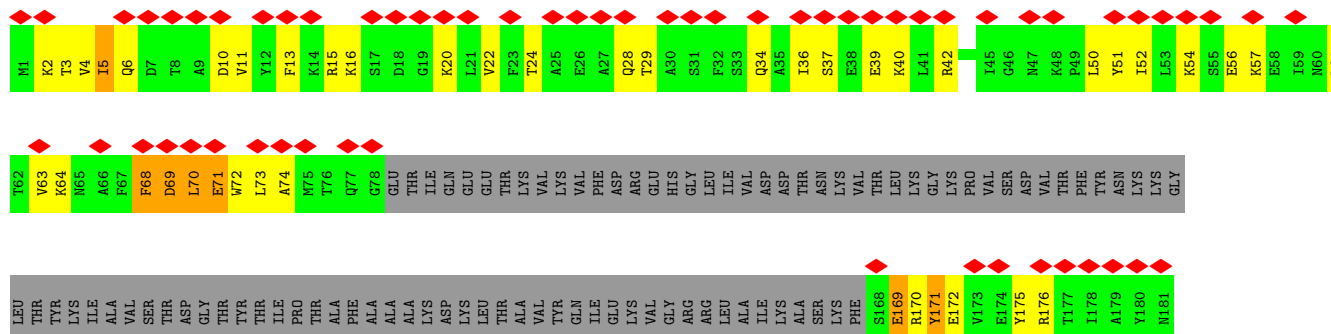
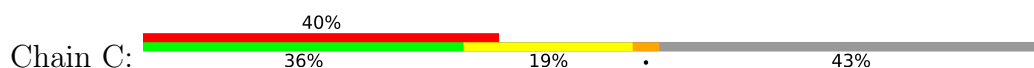


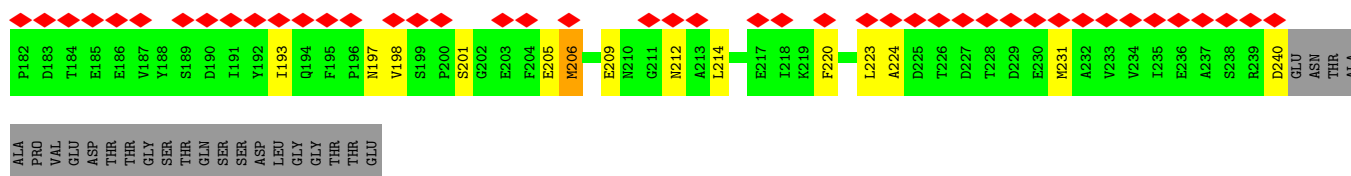
• Molecule 1: SIR2-like domain-containing protein



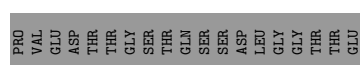
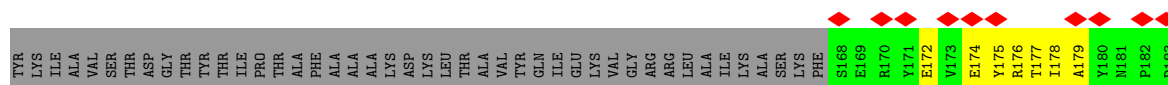
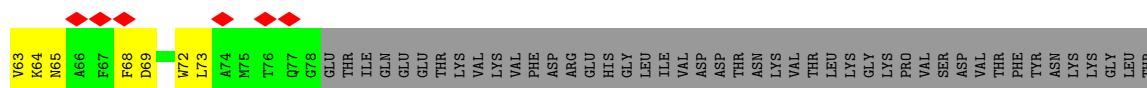
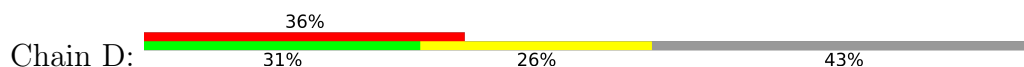


## • Molecule 2: SPR

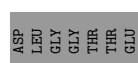
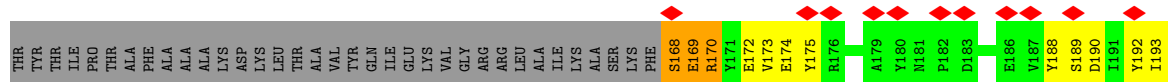
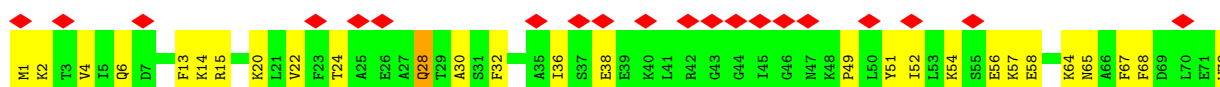
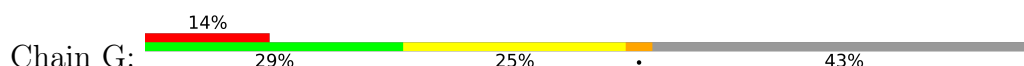




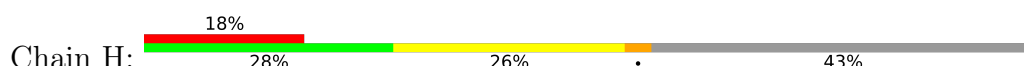
• Molecule 2: SPR



• Molecule 2: SPR



• Molecule 2: SPR





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 49893                                   | 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 ( $e^-/\text{\AA}^2$ ) | 66                                      | Depositor |
| Minimum defocus (nm)                 | 1800                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 2.187                                   | Depositor |
| Minimum map value                    | -0.025                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.025                                   | Depositor |
| Recommended contour level            | 0.03                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 381.8, 381.8, 381.8                     | wwPDB     |
| Map dimensions                       | 460, 460, 460                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.83, 0.83, 0.83                        | 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     | 0.37         | 9/8374 (0.1%)   | 0.78        | 33/11280 (0.3%)  |
| 1   | B     | 0.24         | 0/8374          | 0.80        | 34/11280 (0.3%)  |
| 1   | E     | 0.27         | 1/8374 (0.0%)   | 0.67        | 13/11280 (0.1%)  |
| 1   | F     | 0.37         | 3/8374 (0.0%)   | 0.88        | 42/11280 (0.4%)  |
| 2   | C     | 0.29         | 0/1218          | 0.80        | 4/1645 (0.2%)    |
| 2   | D     | 0.15         | 0/1218          | 0.45        | 0/1645           |
| 2   | G     | 0.45         | 0/1218          | 0.75        | 5/1645 (0.3%)    |
| 2   | H     | 0.38         | 0/1218          | 1.23        | 11/1645 (0.7%)   |
| All | All   | 0.32         | 13/38368 (0.0%) | 0.80        | 142/51700 (0.3%) |

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                   |
| 2   | H     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | A     | 580 | SER  | C-O   | -11.02 | 1.10        | 1.23     |
| 1   | A     | 582 | ILE  | N-CA  | -7.17  | 1.38        | 1.46     |
| 1   | A     | 584 | VAL  | N-CA  | -6.32  | 1.39        | 1.46     |
| 1   | A     | 607 | GLU  | CA-C  | -6.31  | 1.45        | 1.52     |
| 1   | F     | 961 | ASN  | CA-C  | -6.25  | 1.44        | 1.52     |
| 1   | A     | 550 | PHE  | CA-C  | -6.07  | 1.45        | 1.52     |
| 1   | A     | 583 | VAL  | CA-C  | -6.04  | 1.45        | 1.52     |
| 1   | A     | 608 | PHE  | CA-C  | -5.64  | 1.45        | 1.52     |
| 1   | F     | 864 | ASP  | CA-C  | -5.61  | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | E     | 631 | ILE  | N-CA  | 5.54  | 1.52        | 1.46     |
| 1   | A     | 582 | ILE  | C-O   | -5.21 | 1.18        | 1.24     |
| 1   | A     | 583 | VAL  | N-CA  | -5.11 | 1.41        | 1.46     |
| 1   | F     | 711 | GLN  | N-CA  | -5.02 | 1.39        | 1.46     |

All (142) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | B     | 601 | TRP  | N-CA-C  | 30.70  | 149.99      | 112.54   |
| 1   | E     | 630 | ASP  | N-CA-C  | -28.52 | 72.89       | 110.53   |
| 1   | B     | 182 | ASN  | N-CA-C  | 23.94  | 137.06      | 110.97   |
| 1   | F     | 392 | GLY  | N-CA-C  | 23.47  | 144.41      | 115.31   |
| 2   | H     | 230 | GLU  | N-CA-C  | 23.36  | 142.73      | 111.90   |
| 1   | B     | 676 | ILE  | N-CA-C  | -21.30 | 82.54       | 108.53   |
| 1   | B     | 676 | ILE  | CB-CA-C | 20.94  | 141.48      | 110.91   |
| 2   | H     | 230 | GLU  | CB-CA-C | -20.53 | 79.43       | 111.66   |
| 1   | B     | 194 | ASP  | N-CA-C  | -18.69 | 93.31       | 114.62   |
| 2   | H     | 24  | THR  | CB-CA-C | -18.46 | 74.12       | 109.37   |
| 1   | A     | 579 | SER  | N-CA-C  | -18.20 | 87.86       | 110.61   |
| 1   | F     | 802 | ARG  | N-CA-C  | -17.92 | 91.20       | 114.31   |
| 2   | C     | 171 | TYR  | N-CA-C  | -17.79 | 83.62       | 110.30   |
| 1   | A     | 738 | LYS  | N-CA-CB | -17.70 | 86.14       | 110.56   |
| 1   | A     | 737 | VAL  | N-CA-C  | 17.64  | 146.04      | 109.34   |
| 1   | F     | 964 | ASP  | N-CA-C  | 16.97  | 146.95      | 110.80   |
| 1   | F     | 964 | ASP  | N-CA-CB | -16.40 | 82.78       | 110.49   |
| 1   | F     | 391 | ASN  | N-CA-C  | -16.37 | 86.06       | 109.31   |
| 1   | F     | 549 | GLN  | N-CA-C  | -15.61 | 91.75       | 114.39   |
| 1   | F     | 366 | SER  | N-CA-C  | -15.58 | 86.69       | 109.59   |
| 1   | B     | 663 | ASP  | N-CA-C  | 15.47  | 143.74      | 110.80   |
| 1   | F     | 801 | SER  | N-CA-C  | -14.89 | 85.72       | 109.39   |
| 1   | A     | 737 | VAL  | CB-CA-C | -14.52 | 87.47       | 111.29   |
| 1   | A     | 723 | ALA  | N-CA-C  | -14.02 | 95.76       | 113.43   |
| 1   | B     | 731 | GLU  | N-CA-C  | -13.98 | 81.02       | 110.80   |
| 1   | F     | 647 | MET  | N-CA-CB | -13.90 | 87.97       | 110.63   |
| 1   | A     | 581 | ASP  | N-CA-C  | -13.87 | 96.68       | 113.19   |
| 1   | A     | 750 | ASP  | N-CA-C  | 13.75  | 131.67      | 110.36   |
| 1   | A     | 749 | LEU  | N-CA-C  | -13.09 | 85.16       | 107.80   |
| 1   | A     | 606 | HIS  | N-CA-C  | 12.91  | 127.89      | 111.24   |
| 1   | A     | 608 | PHE  | N-CA-C  | -12.78 | 95.86       | 111.33   |
| 1   | F     | 646 | PHE  | CB-CA-C | -12.48 | 89.21       | 109.80   |
| 1   | B     | 193 | TYR  | N-CA-C  | 12.47  | 137.36      | 110.80   |
| 1   | A     | 582 | ILE  | N-CA-C  | -12.38 | 97.99       | 110.62   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 547 | ASP  | N-CA-C  | -12.22 | 92.33       | 108.34   |
| 1   | F     | 875 | ASP  | N-CA-CB | -11.87 | 92.84       | 109.94   |
| 1   | B     | 602 | SER  | N-CA-CB | -11.85 | 90.91       | 110.22   |
| 1   | F     | 647 | MET  | N-CA-C  | 11.60  | 128.85      | 110.17   |
| 1   | F     | 724 | LYS  | N-CA-C  | -11.01 | 94.98       | 110.50   |
| 1   | A     | 550 | PHE  | N-CA-C  | -10.98 | 98.84       | 111.03   |
| 2   | H     | 231 | MET  | N-CA-CB | -10.63 | 92.53       | 110.49   |
| 1   | E     | 632 | ASP  | N-CA-C  | 10.62  | 121.96      | 107.73   |
| 1   | A     | 747 | ARG  | N-CA-C  | -10.46 | 88.53       | 110.80   |
| 1   | E     | 252 | PRO  | CA-N-CD | -10.44 | 97.38       | 112.00   |
| 1   | A     | 722 | PHE  | CB-CA-C | -10.38 | 96.12       | 111.91   |
| 1   | F     | 961 | ASN  | N-CA-C  | -10.31 | 92.13       | 108.63   |
| 1   | F     | 875 | ASP  | N-CA-C  | 10.26  | 123.88      | 109.31   |
| 1   | F     | 904 | ILE  | N-CA-C  | -10.19 | 93.28       | 107.75   |
| 1   | B     | 664 | ILE  | N-CA-CB | -10.04 | 94.67       | 111.23   |
| 1   | F     | 722 | PHE  | CB-CA-C | -10.00 | 95.09       | 111.50   |
| 1   | B     | 601 | TRP  | CB-CA-C | -9.93  | 89.55       | 110.31   |
| 2   | C     | 68  | PHE  | N-CA-C  | -9.93  | 94.36       | 109.94   |
| 1   | A     | 752 | GLY  | N-CA-C  | -9.89  | 100.67      | 112.64   |
| 1   | B     | 183 | VAL  | N-CA-C  | -9.83  | 88.89       | 109.34   |
| 1   | B     | 733 | LEU  | N-CA-C  | 9.66   | 121.57      | 111.14   |
| 1   | B     | 663 | ASP  | CB-CA-C | -9.64  | 91.24       | 110.42   |
| 1   | F     | 830 | ASP  | N-CA-C  | 9.63   | 131.31      | 110.80   |
| 1   | F     | 963 | ASN  | N-CA-C  | -9.59  | 94.83       | 109.79   |
| 1   | B     | 183 | VAL  | N-CA-CB | 9.49   | 126.89      | 111.23   |
| 1   | B     | 194 | ASP  | N-CA-CB | 9.41   | 126.04      | 111.18   |
| 1   | B     | 677 | ARG  | N-CA-C  | 9.35   | 124.31      | 108.23   |
| 2   | H     | 24  | THR  | CA-C-N  | 9.29   | 136.81      | 121.39   |
| 2   | H     | 24  | THR  | C-N-CA  | 9.29   | 136.81      | 121.39   |
| 1   | A     | 799 | LEU  | N-CA-C  | -9.28  | 98.69       | 110.19   |
| 1   | F     | 906 | THR  | N-CA-C  | 9.27   | 124.40      | 113.18   |
| 1   | F     | 229 | LEU  | N-CA-C  | -9.13  | 99.88       | 112.12   |
| 2   | C     | 171 | TYR  | CB-CA-C | 8.91   | 122.44      | 110.06   |
| 1   | E     | 305 | ASP  | N-CA-C  | 8.90   | 122.64      | 111.69   |
| 1   | A     | 543 | GLU  | N-CA-CB | 8.85   | 125.45      | 110.49   |
| 1   | E     | 520 | THR  | N-CA-C  | -8.73  | 95.05       | 108.31   |
| 1   | F     | 366 | SER  | CB-CA-C | 8.44   | 122.91      | 110.26   |
| 1   | A     | 607 | GLU  | N-CA-C  | -8.25  | 101.08      | 112.30   |
| 1   | F     | 960 | LYS  | N-CA-C  | -8.24  | 102.23      | 111.71   |
| 1   | B     | 664 | ILE  | N-CA-C  | -8.09  | 92.51       | 109.34   |
| 1   | A     | 542 | LEU  | CB-CA-C | -8.08  | 98.98       | 112.00   |
| 1   | F     | 933 | PHE  | N-CA-C  | 7.94   | 120.64      | 111.11   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | F     | 228 | LEU  | CB-CA-C  | -7.70 | 98.68       | 111.23   |
| 1   | E     | 631 | ILE  | N-CA-C   | 7.54  | 119.20      | 108.42   |
| 1   | A     | 543 | GLU  | N-CA-C   | -7.39 | 95.06       | 110.80   |
| 2   | G     | 207 | SER  | N-CA-C   | 7.29  | 121.22      | 111.30   |
| 1   | E     | 621 | GLU  | N-CA-C   | 7.12  | 118.94      | 111.03   |
| 1   | F     | 965 | LYS  | N-CA-C   | -7.07 | 105.20      | 114.31   |
| 1   | A     | 746 | GLU  | N-CA-C   | 7.05  | 123.93      | 114.12   |
| 1   | B     | 730 | GLU  | CB-CA-C  | -7.01 | 96.47       | 110.42   |
| 1   | A     | 583 | VAL  | N-CA-C   | -6.97 | 102.98      | 110.23   |
| 1   | B     | 675 | LYS  | N-CA-C   | 6.94  | 119.26      | 110.24   |
| 1   | B     | 962 | TYR  | N-CA-C   | 6.78  | 118.10      | 108.74   |
| 2   | H     | 24  | THR  | N-CA-C   | 6.71  | 120.34      | 109.40   |
| 1   | B     | 492 | PHE  | N-CA-C   | -6.71 | 104.57      | 112.89   |
| 1   | F     | 549 | GLN  | N-CA-CB  | 6.71  | 119.83      | 110.98   |
| 1   | F     | 966 | LEU  | N-CA-C   | -6.69 | 103.19      | 111.75   |
| 1   | A     | 550 | PHE  | CA-C-N   | -6.67 | 111.25      | 120.38   |
| 1   | A     | 550 | PHE  | C-N-CA   | -6.67 | 111.25      | 120.38   |
| 1   | E     | 693 | GLU  | CA-CB-CG | 6.66  | 127.42      | 114.10   |
| 1   | B     | 730 | GLU  | N-CA-C   | -6.62 | 96.71       | 110.80   |
| 1   | F     | 548 | ASN  | CB-CA-C  | -6.62 | 101.25      | 111.83   |
| 1   | F     | 799 | LEU  | N-CA-C   | 6.56  | 120.14      | 111.28   |
| 1   | E     | 521 | ASN  | N-CA-CB  | -6.47 | 100.02      | 110.69   |
| 1   | B     | 787 | ILE  | N-CA-C   | -6.46 | 107.57      | 113.71   |
| 1   | B     | 182 | ASN  | CB-CA-C  | -6.40 | 101.11      | 110.96   |
| 2   | H     | 171 | TYR  | CB-CA-C  | 6.39  | 123.13      | 110.42   |
| 2   | H     | 170 | ARG  | N-CA-C   | -6.35 | 97.28       | 110.80   |
| 1   | B     | 963 | ASN  | N-CA-C   | -6.27 | 103.68      | 113.02   |
| 1   | A     | 682 | GLU  | N-CA-C   | 6.11  | 118.44      | 111.11   |
| 1   | A     | 748 | ASP  | N-CA-C   | 6.00  | 118.04      | 110.24   |
| 1   | A     | 738 | LYS  | N-CA-C   | -5.96 | 106.25      | 112.93   |
| 1   | A     | 548 | ASN  | N-CA-CB  | -5.96 | 102.67      | 110.59   |
| 1   | F     | 861 | ASN  | N-CA-C   | -5.89 | 101.58      | 110.24   |
| 1   | A     | 580 | SER  | O-C-N    | -5.89 | 116.33      | 123.10   |
| 1   | F     | 723 | ALA  | N-CA-C   | -5.86 | 98.32       | 110.80   |
| 1   | F     | 959 | LEU  | N-CA-C   | -5.78 | 106.23      | 113.28   |
| 1   | F     | 603 | VAL  | N-CA-C   | 5.74  | 117.16      | 110.62   |
| 1   | F     | 712 | PHE  | N-CA-C   | -5.71 | 104.07      | 113.50   |
| 1   | B     | 569 | MET  | CB-CG-SD | 5.71  | 129.84      | 112.70   |
| 1   | F     | 712 | PHE  | N-CA-CB  | 5.68  | 122.38      | 111.07   |
| 2   | H     | 227 | ASP  | N-CA-C   | 5.68  | 117.16      | 110.97   |
| 1   | F     | 932 | GLU  | N-CA-C   | 5.67  | 117.32      | 111.03   |
| 1   | F     | 864 | ASP  | N-CA-C   | -5.62 | 98.84       | 110.80   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 495 | LEU  | CA-C-N  | -5.61 | 113.75      | 119.98   |
| 1   | B     | 495 | LEU  | C-N-CA  | -5.61 | 113.75      | 119.98   |
| 1   | A     | 722 | PHE  | N-CA-C  | -5.59 | 102.04      | 110.70   |
| 1   | F     | 722 | PHE  | N-CA-C  | -5.55 | 98.47       | 108.58   |
| 1   | B     | 674 | ASP  | N-CA-C  | -5.55 | 99.99       | 108.76   |
| 2   | G     | 170 | ARG  | N-CA-C  | 5.55  | 117.70      | 110.43   |
| 1   | F     | 711 | GLN  | N-CA-C  | 5.53  | 122.57      | 110.80   |
| 1   | B     | 965 | LYS  | N-CA-C  | -5.53 | 105.64      | 112.38   |
| 1   | F     | 867 | ASN  | N-CA-C  | 5.50  | 119.96      | 112.04   |
| 2   | C     | 206 | MET  | CB-CA-C | -5.50 | 104.13      | 111.88   |
| 1   | E     | 693 | GLU  | CA-C-N  | -5.48 | 111.98      | 120.31   |
| 1   | E     | 693 | GLU  | C-N-CA  | -5.48 | 111.98      | 120.31   |
| 2   | G     | 169 | GLU  | N-CA-C  | -5.47 | 103.86      | 111.30   |
| 1   | B     | 183 | VAL  | CB-CA-C | -5.42 | 102.40      | 111.29   |
| 2   | G     | 233 | VAL  | N-CA-C  | -5.37 | 100.92      | 108.27   |
| 1   | E     | 521 | ASN  | N-CA-C  | 5.28  | 118.31      | 107.69   |
| 2   | H     | 231 | MET  | N-CA-C  | -5.22 | 99.69       | 110.80   |
| 2   | G     | 237 | ALA  | CB-CA-C | -5.18 | 107.93      | 114.40   |
| 1   | A     | 677 | ARG  | N-CA-C  | -5.15 | 98.17       | 107.75   |
| 1   | A     | 580 | SER  | CB-CA-C | 5.06  | 118.06      | 109.50   |
| 1   | E     | 635 | GLY  | N-CA-C  | -5.06 | 101.18      | 113.18   |
| 1   | F     | 802 | ARG  | N-CA-CB | -5.04 | 104.19      | 110.90   |
| 1   | B     | 496 | GLY  | N-CA-C  | 5.04  | 118.78      | 112.73   |
| 1   | B     | 640 | GLY  | N-CA-C  | -5.01 | 101.31      | 113.18   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 580 | SER  | Mainchain |
| 1   | E     | 297 | GLN  | Peptide   |
| 2   | H     | 24  | THR  | 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     | 8183  | 0        | 8010     | 503     | 0            |
| 1   | B     | 8183  | 0        | 8010     | 426     | 0            |
| 1   | E     | 8183  | 0        | 8010     | 517     | 0            |
| 1   | F     | 8183  | 0        | 8010     | 569     | 0            |
| 2   | C     | 1198  | 0        | 1159     | 67      | 0            |
| 2   | D     | 1198  | 0        | 1159     | 76      | 0            |
| 2   | G     | 1198  | 0        | 1159     | 101     | 0            |
| 2   | H     | 1198  | 0        | 1159     | 111     | 0            |
| All | All   | 37524 | 0        | 36676    | 2201    | 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 30.

All (2201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:134:TYR:CD2 | 1:B:183:VAL:HG13 | 1.48                     | 1.45              |
| 1:B:601:TRP:CD2 | 1:B:601:TRP:O    | 1.72                     | 1.39              |
| 1:B:134:TYR:CD2 | 1:B:183:VAL:CG1  | 2.09                     | 1.34              |
| 1:B:134:TYR:CE2 | 1:B:183:VAL:HG13 | 1.81                     | 1.14              |
| 1:E:519:MET:SD  | 1:E:520:THR:O    | 2.04                     | 1.14              |
| 1:B:601:TRP:O   | 1:B:601:TRP:CE3  | 2.01                     | 1.14              |
| 1:A:405:THR:H   | 2:C:4:VAL:HB     | 1.16                     | 1.10              |
| 2:H:23:PHE:H    | 2:H:69:ASP:HB2   | 1.18                     | 1.09              |
| 1:B:601:TRP:O   | 1:B:601:TRP:CG   | 2.06                     | 1.09              |
| 1:A:582:ILE:HA  | 1:A:585:LEU:HG   | 1.35                     | 1.08              |
| 2:H:24:THR:O    | 2:H:65:ASN:ND2   | 1.89                     | 1.06              |
| 1:F:963:ASN:O   | 1:F:967:LEU:HD21 | 1.56                     | 1.03              |
| 2:H:13:PHE:HB3  | 2:H:171:TYR:HE2  | 1.23                     | 1.00              |
| 1:B:193:TYR:O   | 1:B:193:TYR:HD1  | 1.45                     | 0.98              |
| 1:B:134:TYR:CD2 | 1:B:183:VAL:HG11 | 1.97                     | 0.97              |
| 1:F:908:SER:HA  | 2:G:231:MET:HB3  | 1.45                     | 0.97              |
| 1:A:403:LEU:H   | 2:C:6:GLN:HE22   | 1.15                     | 0.94              |
| 1:B:134:TYR:HD2 | 1:B:183:VAL:HG13 | 1.22                     | 0.92              |
| 1:B:610:GLN:O   | 1:B:614:ASN:ND2  | 2.03                     | 0.92              |
| 1:F:801:SER:O   | 1:F:840:LYS:HE3  | 1.70                     | 0.91              |
| 1:E:531:MET:HE3 | 1:E:532:PRO:HD2  | 1.52                     | 0.91              |
| 1:A:549:GLN:CA  | 1:A:552:TYR:HB2  | 2.01                     | 0.90              |
| 1:F:652:PHE:CZ  | 1:F:722:PHE:O    | 2.25                     | 0.90              |
| 1:A:547:ASP:O   | 1:A:550:PHE:CE1  | 2.25                     | 0.90              |
| 1:B:193:TYR:O   | 1:B:193:TYR:CD1  | 2.26                     | 0.89              |
| 1:A:247:ARG:NH2 | 1:A:251:SER:O    | 2.04                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:963:ASN:O    | 1:F:967:LEU:CD2  | 2.20                     | 0.88              |
| 1:E:1001:MET:HE3 | 1:F:985:LYS:HZ2  | 1.39                     | 0.88              |
| 1:B:134:TYR:HD2  | 1:B:183:VAL:CG1  | 1.71                     | 0.87              |
| 1:A:547:ASP:O    | 1:A:550:PHE:HE1  | 1.57                     | 0.87              |
| 2:H:230:GLU:O    | 2:H:231:MET:HE2  | 1.73                     | 0.87              |
| 2:C:16:LYS:HG3   | 2:C:170:ARG:HB2  | 1.57                     | 0.87              |
| 1:E:629:ARG:CD   | 1:E:630:ASP:O    | 2.24                     | 0.86              |
| 1:E:749:LEU:HG   | 1:E:753:LYS:HD3  | 1.57                     | 0.86              |
| 1:F:223:TYR:O    | 1:F:227:MET:HB3  | 1.77                     | 0.85              |
| 1:A:582:ILE:HA   | 1:A:585:LEU:CG   | 2.06                     | 0.85              |
| 1:B:58:GLN:HG3   | 1:B:60:TRP:H     | 1.41                     | 0.84              |
| 1:F:809:LYS:HZ3  | 1:F:815:PHE:H    | 1.25                     | 0.84              |
| 1:A:713:ILE:HG21 | 1:A:717:LYS:HB2  | 1.57                     | 0.84              |
| 1:E:698:GLN:HG2  | 1:E:712:PHE:HE2  | 1.42                     | 0.84              |
| 1:B:193:TYR:CD1  | 1:B:193:TYR:C    | 2.55                     | 0.84              |
| 1:F:222:ASP:H    | 1:F:225:ILE:HG22 | 1.42                     | 0.84              |
| 1:F:652:PHE:HZ   | 1:F:722:PHE:O    | 1.60                     | 0.83              |
| 2:G:28:GLN:HB3   | 2:G:64:LYS:HD3   | 1.59                     | 0.83              |
| 1:A:549:GLN:HA   | 1:A:552:TYR:HB2  | 1.60                     | 0.83              |
| 1:B:576:PHE:HA   | 1:B:639:PHE:HB3  | 1.58                     | 0.82              |
| 1:F:331:LYS:HZ1  | 1:F:338:TYR:H    | 1.26                     | 0.82              |
| 1:F:376:LYS:HZ1  | 1:F:380:ARG:HD3  | 1.44                     | 0.82              |
| 1:A:682:GLU:O    | 1:A:686:GLU:HG2  | 1.80                     | 0.82              |
| 1:E:629:ARG:HG3  | 1:E:631:ILE:HB   | 1.59                     | 0.82              |
| 1:B:472:TYR:HE2  | 1:B:542:LEU:HG   | 1.42                     | 0.82              |
| 1:A:580:SER:HB2  | 1:A:582:ILE:HG23 | 1.60                     | 0.82              |
| 1:F:962:TYR:HD1  | 1:F:967:LEU:HD22 | 1.45                     | 0.82              |
| 1:A:646:PHE:HB3  | 1:A:677:ARG:HE   | 1.43                     | 0.81              |
| 1:A:580:SER:C    | 1:A:582:ILE:N    | 2.28                     | 0.81              |
| 1:E:242:LYS:NZ   | 1:E:265:GLY:O    | 2.13                     | 0.81              |
| 1:B:612:ILE:HG21 | 1:B:654:ASN:HB3  | 1.62                     | 0.81              |
| 1:A:489:VAL:O    | 1:A:493:ASN:ND2  | 2.13                     | 0.80              |
| 2:H:64:LYS:HG2   | 2:H:217:GLU:HB3  | 1.61                     | 0.80              |
| 1:F:974:LYS:HA   | 1:F:977:LYS:HE3  | 1.64                     | 0.79              |
| 1:F:338:TYR:HA   | 1:F:348:ARG:HA   | 1.62                     | 0.79              |
| 1:B:213:ILE:HB   | 1:B:243:PRO:HB3  | 1.63                     | 0.79              |
| 1:F:310:ASP:HA   | 1:F:380:ARG:HH12 | 1.46                     | 0.79              |
| 1:A:357:MET:HE3  | 1:A:357:MET:H    | 1.48                     | 0.79              |
| 2:H:22:VAL:CG1   | 2:H:171:TYR:OH   | 2.30                     | 0.79              |
| 2:H:23:PHE:HE1   | 2:H:66:ALA:HB2   | 1.46                     | 0.79              |
| 1:F:800:TYR:C    | 1:F:802:ARG:H    | 1.89                     | 0.79              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:800:TYR:O    | 1:F:802:ARG:N     | 2.14                     | 0.79              |
| 1:E:987:ARG:NH1  | 1:F:630:ASP:OD2   | 2.16                     | 0.79              |
| 1:A:405:THR:N    | 2:C:4:VAL:HB      | 1.98                     | 0.78              |
| 1:E:837:PHE:HA   | 1:E:840:LYS:HB3   | 1.65                     | 0.78              |
| 1:B:569:MET:HE3  | 1:B:570:SER:H     | 1.46                     | 0.78              |
| 1:F:553:ASP:OD1  | 1:F:554:ASP:N     | 2.17                     | 0.77              |
| 1:A:580:SER:C    | 1:A:582:ILE:H     | 1.89                     | 0.77              |
| 1:A:316:ILE:HG23 | 1:A:319:LEU:HD22  | 1.66                     | 0.77              |
| 1:A:582:ILE:CA   | 1:A:585:LEU:HG    | 2.14                     | 0.77              |
| 1:E:647:MET:SD   | 1:E:647:MET:N     | 2.58                     | 0.77              |
| 1:B:152:ILE:HG23 | 1:B:157:ASP:HB2   | 1.66                     | 0.77              |
| 1:B:661:ILE:HG13 | 1:B:663:ASP:H     | 1.49                     | 0.77              |
| 2:D:26:GLU:O     | 2:D:65:ASN:ND2    | 2.18                     | 0.77              |
| 1:F:985:LYS:O    | 1:F:989:LYS:HB3   | 1.85                     | 0.77              |
| 1:A:86:ARG:NH2   | 1:E:260:TYR:OH    | 2.18                     | 0.76              |
| 1:F:909:SER:H    | 2:G:231:MET:CB    | 1.98                     | 0.76              |
| 1:A:582:ILE:HG13 | 1:A:583:VAL:N     | 2.01                     | 0.76              |
| 1:F:247:ARG:HB3  | 1:F:271:ALA:H     | 1.51                     | 0.75              |
| 1:F:984:LEU:HB3  | 1:F:1000:LEU:HD12 | 1.66                     | 0.75              |
| 2:G:20:LYS:HG2   | 2:G:72:TRP:CZ3    | 2.21                     | 0.75              |
| 1:E:487:GLN:NE2  | 2:H:207:SER:H     | 1.85                     | 0.75              |
| 1:E:605:PHE:HA   | 2:H:207:SER:HB2   | 1.67                     | 0.75              |
| 1:A:771:ILE:HG12 | 1:A:775:ILE:HD11  | 1.67                     | 0.75              |
| 1:F:551:LEU:O    | 1:F:555:THR:OG1   | 2.05                     | 0.75              |
| 1:F:801:SER:C    | 1:F:840:LYS:HE3   | 2.11                     | 0.75              |
| 1:F:869:ILE:HD11 | 1:F:874:ILE:O     | 1.87                     | 0.75              |
| 1:A:586:LEU:HA   | 1:A:589:TYR:HD2   | 1.52                     | 0.74              |
| 1:E:487:GLN:HE22 | 2:H:207:SER:H     | 1.33                     | 0.74              |
| 1:F:357:MET:HE3  | 1:F:357:MET:H     | 1.49                     | 0.74              |
| 2:H:21:LEU:O     | 2:H:69:ASP:HB3    | 1.87                     | 0.74              |
| 1:A:678:PHE:HB2  | 1:A:726:VAL:HA    | 1.68                     | 0.74              |
| 1:F:85:LEU:O     | 1:F:89:GLN:NE2    | 2.20                     | 0.74              |
| 1:F:41:LYS:HG2   | 1:F:211:HIS:HD2   | 1.52                     | 0.74              |
| 1:E:543:GLU:O    | 1:E:546:SER:OG    | 2.05                     | 0.74              |
| 1:E:706:VAL:HA   | 1:E:709:TYR:HB3   | 1.70                     | 0.74              |
| 2:G:14:LYS:O     | 2:G:172:GLU:N     | 2.20                     | 0.74              |
| 1:F:711:GLN:O    | 1:F:712:PHE:CD1   | 2.41                     | 0.74              |
| 1:E:788:ASP:OD1  | 1:E:789:GLN:N     | 2.21                     | 0.73              |
| 1:B:233:ARG:NH1  | 1:B:263:ASN:O     | 2.21                     | 0.73              |
| 2:D:45:ILE:HG23  | 2:D:47:ASN:H      | 1.52                     | 0.73              |
| 1:E:30:ILE:HA    | 1:E:33:ILE:HD12   | 1.69                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:713:ILE:HG13 | 1:A:716:ALA:HB3  | 1.71                     | 0.73              |
| 1:F:342:VAL:HG21 | 1:F:586:LEU:HB3  | 1.71                     | 0.73              |
| 1:F:909:SER:H    | 2:G:231:MET:HB2  | 1.52                     | 0.73              |
| 1:E:967:LEU:HD22 | 1:E:1004:PHE:HE1 | 1.52                     | 0.73              |
| 1:F:1002:ASN:OD1 | 1:F:1003:TYR:N   | 2.21                     | 0.73              |
| 1:B:640:GLY:O    | 1:B:641:LYS:HG3  | 1.89                     | 0.72              |
| 1:B:584:VAL:O    | 1:B:588:LEU:HB2  | 1.89                     | 0.72              |
| 2:C:212:ASN:ND2  | 2:C:214:LEU:O    | 2.22                     | 0.72              |
| 1:A:331:LYS:HB2  | 1:A:541:ILE:HG12 | 1.72                     | 0.72              |
| 1:A:570:SER:O    | 1:B:669:ARG:NH2  | 2.23                     | 0.72              |
| 1:B:457:ASN:HA   | 1:B:460:LEU:HD12 | 1.71                     | 0.72              |
| 1:A:759:GLU:HG3  | 2:D:41:LEU:HB3   | 1.72                     | 0.72              |
| 1:E:578:MET:H    | 1:E:578:MET:HE3  | 1.54                     | 0.72              |
| 1:E:487:GLN:NE2  | 2:H:205:GLU:OE2  | 2.22                     | 0.72              |
| 1:F:341:GLU:OE1  | 1:F:343:ASN:ND2  | 2.22                     | 0.72              |
| 1:A:548:ASN:HB2  | 2:D:210:ASN:HD21 | 1.53                     | 0.72              |
| 1:F:970:ILE:O    | 1:F:973:ASN:ND2  | 2.23                     | 0.72              |
| 1:B:685:GLU:OE1  | 1:B:732:GLY:N    | 2.22                     | 0.72              |
| 1:E:304:LYS:HZ3  | 1:E:307:GLU:HB2  | 1.55                     | 0.72              |
| 1:B:172:GLY:O    | 1:B:183:VAL:HG22 | 1.89                     | 0.71              |
| 1:B:593:ARG:HA   | 1:B:596:TYR:HB2  | 1.72                     | 0.71              |
| 1:A:606:HIS:HD2  | 2:D:208:LEU:HB3  | 1.55                     | 0.71              |
| 1:A:751:ILE:HA   | 1:A:754:ARG:CG   | 2.19                     | 0.71              |
| 1:A:753:LYS:HB3  | 1:A:757:TRP:CZ3  | 2.25                     | 0.71              |
| 2:C:2:LYS:HD2    | 2:C:3:THR:HG22   | 1.72                     | 0.71              |
| 1:F:574:TYR:N    | 2:H:32:PHE:O     | 2.20                     | 0.71              |
| 1:F:887:GLU:OE2  | 1:F:891:THR:OG1  | 2.09                     | 0.71              |
| 2:G:14:LYS:HA    | 2:G:20:LYS:HB3   | 1.72                     | 0.71              |
| 1:A:332:HIS:HA   | 1:A:336:TYR:H    | 1.54                     | 0.71              |
| 1:B:327:LYS:HA   | 1:B:327:LYS:HE3  | 1.72                     | 0.71              |
| 1:B:661:ILE:O    | 1:B:665:LYS:HB3  | 1.90                     | 0.71              |
| 1:E:674:ASP:OD1  | 1:E:725:TYR:OH   | 2.05                     | 0.71              |
| 2:H:190:ASP:H    | 2:H:237:ALA:HB3  | 1.55                     | 0.71              |
| 1:F:453:ASP:O    | 1:F:456:SER:OG   | 2.06                     | 0.71              |
| 1:F:800:TYR:C    | 1:F:802:ARG:N    | 2.41                     | 0.71              |
| 2:G:15:ARG:HG2   | 2:G:20:LYS:HG3   | 1.73                     | 0.71              |
| 1:F:41:LYS:HZ2   | 1:F:211:HIS:HA   | 1.56                     | 0.71              |
| 2:H:13:PHE:HB3   | 2:H:171:TYR:CE2  | 2.16                     | 0.71              |
| 1:E:151:VAL:HA   | 1:E:167:LEU:HB3  | 1.71                     | 0.71              |
| 1:F:575:SER:HA   | 2:H:31:SER:HA    | 1.72                     | 0.70              |
| 1:B:145:ARG:HG3  | 1:B:147:LYS:HE2  | 1.72                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:588:LEU:HD21 | 1:B:615:SER:HB2  | 1.73                     | 0.70              |
| 2:D:30:ALA:HA    | 2:D:63:VAL:HG12  | 1.73                     | 0.70              |
| 1:E:370:ARG:NH1  | 1:E:370:ARG:O    | 2.25                     | 0.70              |
| 1:A:842:LEU:HD12 | 1:A:845:LEU:HD12 | 1.72                     | 0.70              |
| 1:E:473:LEU:HD22 | 1:E:600:LEU:HD21 | 1.73                     | 0.70              |
| 1:E:631:ILE:HG13 | 1:E:632:ASP:N    | 2.06                     | 0.70              |
| 1:F:339:HIS:N    | 1:F:347:VAL:O    | 2.24                     | 0.70              |
| 1:F:471:TYR:O    | 1:F:475:GLN:NE2  | 2.24                     | 0.70              |
| 1:F:842:LEU:HA   | 1:F:845:LEU:HD12 | 1.73                     | 0.70              |
| 1:B:477:ASN:O    | 1:B:481:ILE:HG12 | 1.91                     | 0.70              |
| 1:A:482:TYR:HE2  | 1:A:519:MET:HB2  | 1.57                     | 0.70              |
| 1:B:405:THR:O    | 2:D:1:MET:N      | 2.25                     | 0.70              |
| 1:F:614:ASN:OD1  | 1:F:615:SER:N    | 2.24                     | 0.70              |
| 2:H:24:THR:O     | 2:H:24:THR:OG1   | 1.94                     | 0.70              |
| 1:B:729:SER:HB3  | 1:B:731:GLU:CD   | 2.16                     | 0.70              |
| 1:F:960:LYS:HZ1  | 1:F:999:ILE:HG13 | 1.56                     | 0.70              |
| 1:A:154:ALA:N    | 1:A:157:ASP:OD2  | 2.24                     | 0.70              |
| 1:E:704:MET:HA   | 1:E:704:MET:HE2  | 1.74                     | 0.70              |
| 2:G:168:SER:N    | 2:G:170:ARG:HE   | 1.88                     | 0.70              |
| 1:B:575:SER:HB2  | 1:B:578:MET:HG2  | 1.73                     | 0.69              |
| 1:E:277:SER:OG   | 1:E:285:ARG:NH2  | 2.25                     | 0.69              |
| 2:H:23:PHE:H     | 2:H:69:ASP:CB    | 2.02                     | 0.69              |
| 1:A:549:GLN:O    | 1:A:553:ASP:N    | 2.26                     | 0.69              |
| 1:E:909:SER:HB3  | 2:H:231:MET:HE3  | 1.73                     | 0.69              |
| 2:C:15:ARG:HD2   | 2:C:169:GLU:HB2  | 1.73                     | 0.69              |
| 1:B:343:ASN:HA   | 1:B:586:LEU:HG   | 1.73                     | 0.69              |
| 2:H:179:ALA:HB2  | 2:H:191:ILE:HD11 | 1.73                     | 0.69              |
| 1:A:627:ARG:O    | 1:B:990:ASN:ND2  | 2.26                     | 0.69              |
| 1:E:195:GLN:O    | 1:F:237:LYS:NZ   | 2.21                     | 0.69              |
| 1:B:551:LEU:HD13 | 1:B:607:GLU:HB2  | 1.75                     | 0.69              |
| 1:E:967:LEU:HD22 | 1:E:1004:PHE:CE1 | 2.28                     | 0.69              |
| 1:A:551:LEU:O    | 1:A:555:THR:OG1  | 2.09                     | 0.69              |
| 1:E:728:LEU:HD13 | 1:E:765:ASN:HB3  | 1.75                     | 0.69              |
| 1:E:751:ILE:O    | 1:E:804:TYR:OH   | 2.09                     | 0.69              |
| 1:F:261:TYR:HA   | 1:F:264:LYS:HG2  | 1.75                     | 0.68              |
| 1:E:309:ILE:H    | 1:E:309:ILE:HD12 | 1.57                     | 0.68              |
| 2:H:72:TRP:HA    | 2:H:72:TRP:CE3   | 2.29                     | 0.68              |
| 1:A:74:PRO:O     | 1:A:76:LYS:NZ    | 2.26                     | 0.68              |
| 1:E:395:CYS:SG   | 1:E:396:MET:N    | 2.67                     | 0.68              |
| 1:A:659:PHE:CD2  | 1:A:664:ILE:HD11 | 2.29                     | 0.68              |
| 1:A:676:ILE:HG23 | 1:A:677:ARG:N    | 2.08                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:831:LYS:HB3  | 1:A:834:GLN:HB3  | 1.76                     | 0.68              |
| 1:B:561:LEU:HA   | 1:B:564:LYS:HB2  | 1.75                     | 0.68              |
| 1:E:236:GLN:HB3  | 1:E:240:PHE:HB2  | 1.74                     | 0.68              |
| 1:A:746:GLU:O    | 1:A:748:ASP:N    | 2.27                     | 0.68              |
| 1:E:662:ASP:OD1  | 1:E:663:ASP:N    | 2.27                     | 0.68              |
| 1:F:711:GLN:O    | 1:F:712:PHE:HD1  | 1.76                     | 0.68              |
| 1:F:869:ILE:CD1  | 1:F:874:ILE:O    | 2.41                     | 0.68              |
| 1:A:86:ARG:HD2   | 1:A:187:GLU:HG3  | 1.76                     | 0.68              |
| 1:F:437:LYS:NZ   | 1:F:599:CYS:SG   | 2.62                     | 0.68              |
| 1:A:681:GLN:O    | 1:A:685:GLU:HB2  | 1.94                     | 0.68              |
| 1:A:622:LYS:O    | 1:A:626:GLU:HB2  | 1.94                     | 0.68              |
| 1:B:115:ASN:H    | 1:B:118:HIS:CD2  | 2.12                     | 0.68              |
| 1:B:184:VAL:C    | 1:B:185:LEU:HD22 | 2.19                     | 0.68              |
| 1:E:252:PRO:HD2  | 1:E:252:PRO:O    | 1.94                     | 0.67              |
| 1:E:493:ASN:HA   | 1:E:503:HIS:HE1  | 1.58                     | 0.67              |
| 2:C:61:LEU:HB2   | 2:C:220:PHE:HB2  | 1.75                     | 0.67              |
| 1:A:235:LEU:HD22 | 1:B:195:GLN:HA   | 1.76                     | 0.67              |
| 1:A:707:VAL:O    | 1:A:711:GLN:NE2  | 2.27                     | 0.67              |
| 1:A:606:HIS:CD2  | 2:D:208:LEU:HB3  | 2.29                     | 0.67              |
| 1:B:646:PHE:HB3  | 1:B:677:ARG:NH1  | 2.09                     | 0.67              |
| 1:B:724:LYS:HD2  | 1:B:761:LEU:HA   | 1.75                     | 0.67              |
| 1:E:915:THR:HA   | 1:E:918:ILE:HG22 | 1.75                     | 0.67              |
| 1:A:296:SER:HA   | 1:A:300:LYS:HD2  | 1.77                     | 0.67              |
| 1:B:587:ARG:O    | 1:B:591:ASN:ND2  | 2.27                     | 0.67              |
| 2:G:175:TYR:HB2  | 2:G:193:ILE:HB   | 1.77                     | 0.67              |
| 2:C:170:ARG:HA   | 2:C:170:ARG:CZ   | 2.23                     | 0.67              |
| 1:E:231:TRP:HA   | 1:E:234:LYS:HB2  | 1.77                     | 0.67              |
| 1:E:247:ARG:HD3  | 1:E:249:ASP:H    | 1.58                     | 0.67              |
| 1:E:616:MET:HG2  | 1:E:659:PHE:CZ   | 2.30                     | 0.67              |
| 1:E:629:ARG:HD3  | 1:E:630:ASP:O    | 1.93                     | 0.67              |
| 1:F:279:GLU:O    | 1:F:285:ARG:NH1  | 2.25                     | 0.67              |
| 1:A:607:GLU:C    | 1:A:609:HIS:N    | 2.41                     | 0.67              |
| 1:A:802:ARG:HB2  | 1:A:840:LYS:HB3  | 1.74                     | 0.67              |
| 1:A:582:ILE:O    | 1:A:583:VAL:C    | 2.36                     | 0.67              |
| 1:A:699:PHE:HB2  | 1:A:704:MET:HG3  | 1.76                     | 0.67              |
| 1:B:118:HIS:HA   | 1:B:121:ILE:HG22 | 1.77                     | 0.67              |
| 1:B:724:LYS:HZ2  | 1:B:760:ARG:HB3  | 1.58                     | 0.67              |
| 2:C:16:LYS:CG    | 2:C:170:ARG:HB2  | 2.25                     | 0.67              |
| 1:E:567:SER:OG   | 1:E:568:GLU:OE1  | 2.10                     | 0.67              |
| 1:E:605:PHE:O    | 1:E:609:HIS:ND1  | 2.24                     | 0.67              |
| 1:F:304:LYS:HB2  | 1:F:307:GLU:HB2  | 1.77                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:849:ALA:HA   | 1:F:852:HIS:HE1  | 1.59                     | 0.67              |
| 2:D:31:SER:N     | 2:D:62:THR:O     | 2.28                     | 0.67              |
| 1:F:228:LEU:HD12 | 1:F:228:LEU:O    | 1.94                     | 0.67              |
| 1:F:892:ARG:HA   | 1:F:895:ASN:HD22 | 1.59                     | 0.67              |
| 1:A:463:ILE:HD13 | 1:B:143:TRP:HB3  | 1.76                     | 0.66              |
| 1:E:937:ASP:OD1  | 1:E:940:TYR:N    | 2.22                     | 0.66              |
| 1:A:580:SER:C    | 1:A:583:VAL:H    | 2.02                     | 0.66              |
| 1:A:582:ILE:O    | 1:A:586:LEU:N    | 2.23                     | 0.66              |
| 1:B:593:ARG:O    | 1:B:597:GLU:N    | 2.28                     | 0.66              |
| 1:E:302:ILE:HG23 | 1:E:307:GLU:HB3  | 1.77                     | 0.66              |
| 1:E:374:SER:HB2  | 1:E:377:GLN:HG2  | 1.77                     | 0.66              |
| 1:A:501:GLY:HA3  | 1:A:747:ARG:HH22 | 1.60                     | 0.66              |
| 1:A:751:ILE:HG23 | 1:A:799:LEU:HD22 | 1.75                     | 0.66              |
| 1:B:482:TYR:HA   | 1:B:485:ILE:HD12 | 1.78                     | 0.66              |
| 1:B:571:GLU:OE1  | 1:B:571:GLU:N    | 2.29                     | 0.66              |
| 2:C:70:LEU:HA    | 2:C:73:LEU:HB3   | 1.76                     | 0.66              |
| 2:D:28:GLN:OE1   | 2:D:28:GLN:N     | 2.27                     | 0.66              |
| 1:E:570:SER:O    | 1:F:669:ARG:NH2  | 2.28                     | 0.66              |
| 1:E:982:GLU:OE1  | 1:E:985:LYS:NZ   | 2.23                     | 0.66              |
| 2:H:169:GLU:O    | 2:H:170:ARG:C    | 2.38                     | 0.66              |
| 1:A:549:GLN:HB2  | 1:A:552:TYR:HB2  | 1.78                     | 0.66              |
| 1:A:780:VAL:HG11 | 1:A:819:ARG:HB2  | 1.78                     | 0.66              |
| 2:H:45:ILE:HG23  | 2:H:47:ASN:H     | 1.61                     | 0.66              |
| 1:A:676:ILE:HG23 | 1:A:677:ARG:H    | 1.61                     | 0.66              |
| 1:F:605:PHE:HD2  | 2:G:209:GLU:HB2  | 1.60                     | 0.66              |
| 1:A:75:LYS:NZ    | 1:A:78:ASN:O     | 2.28                     | 0.66              |
| 1:A:407:ILE:HB   | 2:C:2:LYS:HZ1    | 1.60                     | 0.66              |
| 1:F:753:LYS:HE2  | 1:F:757:TRP:CE2  | 2.30                     | 0.66              |
| 1:B:242:LYS:O    | 1:B:267:ARG:NH2  | 2.29                     | 0.66              |
| 2:H:54:LYS:NZ    | 2:H:56:GLU:OE2   | 2.29                     | 0.66              |
| 1:E:404:ASN:HA   | 2:G:4:VAL:HG11   | 1.77                     | 0.66              |
| 1:F:452:TYR:HE1  | 1:F:514:ARG:HH21 | 1.42                     | 0.66              |
| 1:F:869:ILE:HG12 | 1:F:919:TRP:HZ2  | 1.60                     | 0.66              |
| 1:E:80:SER:HA    | 1:E:84:TYR:HB2   | 1.78                     | 0.65              |
| 1:F:783:ALA:HA   | 1:F:786:HIS:CD2  | 2.32                     | 0.65              |
| 1:A:581:ASP:O    | 1:A:584:VAL:HB   | 1.96                     | 0.65              |
| 1:A:433:GLU:OE1  | 1:A:437:LYS:NZ   | 2.30                     | 0.65              |
| 1:A:648:GLU:HB3  | 1:A:651:ASP:HB2  | 1.79                     | 0.65              |
| 2:C:22:VAL:HG12  | 2:C:69:ASP:OD1   | 1.97                     | 0.65              |
| 1:F:930:MET:SD   | 1:F:931:GLU:N    | 2.70                     | 0.65              |
| 1:A:405:THR:HB   | 2:C:4:VAL:HG21   | 1.77                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:549:GLN:CB   | 1:A:552:TYR:HB2  | 2.27                     | 0.65              |
| 1:A:698:GLN:O    | 1:A:702:ASN:N    | 2.24                     | 0.65              |
| 1:B:569:MET:CE   | 1:B:570:SER:H    | 2.10                     | 0.65              |
| 1:F:331:LYS:HZ1  | 1:F:337:ASP:H    | 1.45                     | 0.65              |
| 1:F:717:LYS:NZ   | 1:F:748:ASP:O    | 2.23                     | 0.65              |
| 2:H:21:LEU:C     | 2:H:69:ASP:HB3   | 2.22                     | 0.65              |
| 1:B:578:MET:HA   | 1:B:582:ILE:HG13 | 1.79                     | 0.65              |
| 1:E:519:MET:O    | 1:E:520:THR:C    | 2.39                     | 0.65              |
| 1:F:173:ASP:OD2  | 1:F:175:ARG:NE   | 2.28                     | 0.65              |
| 2:H:11:VAL:HG13  | 2:H:175:TYR:HE1  | 1.61                     | 0.65              |
| 1:E:755:TYR:CE2  | 1:E:803:ASP:HB3  | 2.31                     | 0.65              |
| 2:H:22:VAL:HG13  | 2:H:171:TYR:OH   | 1.97                     | 0.65              |
| 1:A:46:VAL:HG23  | 1:A:216:ILE:HD11 | 1.78                     | 0.65              |
| 1:E:589:TYR:OH   | 1:E:651:ASP:OD1  | 2.12                     | 0.65              |
| 1:E:606:HIS:NE2  | 2:H:205:GLU:O    | 2.30                     | 0.65              |
| 1:F:25:ASN:OD1   | 1:F:26:VAL:N     | 2.30                     | 0.65              |
| 1:F:91:PHE:HA    | 1:F:94:VAL:HG12  | 1.80                     | 0.65              |
| 2:C:16:LYS:O     | 2:C:169:GLU:HG2  | 1.98                     | 0.64              |
| 1:E:205:LYS:HZ3  | 1:F:199:LEU:HD23 | 1.63                     | 0.64              |
| 1:F:913:MET:HE3  | 1:F:913:MET:H    | 1.63                     | 0.64              |
| 2:H:14:LYS:HB3   | 2:H:172:GLU:HG2  | 1.79                     | 0.64              |
| 1:B:184:VAL:O    | 1:B:185:LEU:HD22 | 1.96                     | 0.64              |
| 2:D:22:VAL:HB    | 2:D:72:TRP:HB2   | 1.78                     | 0.64              |
| 1:E:127:ALA:O    | 1:E:128:HIS:ND1  | 2.30                     | 0.64              |
| 1:E:711:GLN:NE2  | 1:E:715:GLU:OE2  | 2.30                     | 0.64              |
| 1:A:82:ASP:OD1   | 1:A:83:GLU:N     | 2.30                     | 0.64              |
| 1:A:235:LEU:HD11 | 1:B:198:PRO:HG3  | 1.77                     | 0.64              |
| 1:E:29:CYS:SG    | 1:E:267:ARG:NH2  | 2.68                     | 0.64              |
| 1:E:75:LYS:HG2   | 1:E:77:GLY:H     | 1.62                     | 0.64              |
| 2:G:73:LEU:O     | 2:G:77:GLN:HB3   | 1.97                     | 0.64              |
| 1:A:63:VAL:HG21  | 1:A:84:TYR:HD1   | 1.63                     | 0.64              |
| 1:A:812:GLU:CD   | 1:A:813:LYS:H    | 2.05                     | 0.64              |
| 1:B:624:GLU:HB3  | 1:B:627:ARG:HH21 | 1.61                     | 0.64              |
| 1:F:70:LEU:HD21  | 1:F:95:LYS:HE2   | 1.79                     | 0.64              |
| 1:F:331:LYS:NZ   | 1:F:338:TYR:H    | 1.93                     | 0.64              |
| 2:H:32:PHE:HE1   | 2:H:59:ILE:HG23  | 1.61                     | 0.64              |
| 1:B:613:ARG:HA   | 1:B:659:PHE:CZ   | 2.32                     | 0.64              |
| 1:E:440:PHE:CD2  | 1:E:599:CYS:HA   | 2.33                     | 0.64              |
| 1:F:396:MET:SD   | 1:F:398:LYS:N    | 2.67                     | 0.64              |
| 1:F:404:ASN:O    | 2:H:1:MET:N      | 2.24                     | 0.64              |
| 1:F:495:LEU:HA   | 1:F:498:LEU:HD23 | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:189:ASP:O    | 1:A:193:TYR:N    | 2.31                     | 0.64              |
| 1:B:455:TYR:O    | 1:B:459:ILE:HG12 | 1.97                     | 0.64              |
| 1:E:189:ASP:O    | 1:E:193:TYR:N    | 2.30                     | 0.64              |
| 1:F:721:TYR:O    | 1:F:723:ALA:N    | 2.30                     | 0.64              |
| 1:F:849:ALA:HA   | 1:F:852:HIS:CE1  | 2.32                     | 0.64              |
| 1:E:82:ASP:OD1   | 1:E:83:GLU:N     | 2.31                     | 0.64              |
| 1:E:616:MET:HG2  | 1:E:659:PHE:HZ   | 1.63                     | 0.64              |
| 1:F:869:ILE:HA   | 1:F:874:ILE:H    | 1.63                     | 0.64              |
| 1:A:223:TYR:O    | 1:A:226:ASN:N    | 2.29                     | 0.64              |
| 1:A:659:PHE:HB3  | 1:A:718:ALA:HB3  | 1.79                     | 0.64              |
| 1:B:609:HIS:HA   | 1:B:658:HIS:HB3  | 1.80                     | 0.64              |
| 1:B:626:GLU:HA   | 1:B:629:ARG:HE   | 1.63                     | 0.64              |
| 2:G:14:LYS:N     | 2:G:172:GLU:O    | 2.29                     | 0.64              |
| 1:B:648:GLU:HB3  | 2:D:2:LYS:HZ1    | 1.62                     | 0.63              |
| 2:G:15:ARG:HA    | 2:G:170:ARG:O    | 1.97                     | 0.63              |
| 1:A:411:SER:HB3  | 1:A:414:TYR:HB3  | 1.79                     | 0.63              |
| 1:A:473:LEU:HD12 | 1:A:600:LEU:HD21 | 1.79                     | 0.63              |
| 1:F:724:LYS:HB3  | 1:F:760:ARG:O    | 1.99                     | 0.63              |
| 1:A:607:GLU:O    | 1:A:608:PHE:C    | 2.39                     | 0.63              |
| 2:G:65:ASN:CG    | 2:G:67:PHE:H     | 2.05                     | 0.63              |
| 2:C:22:VAL:HG21  | 2:C:171:TYR:HE1  | 1.63                     | 0.63              |
| 1:E:241:HIS:NE2  | 1:F:159:ALA:O    | 2.27                     | 0.63              |
| 1:E:488:ALA:HA   | 1:E:491:GLN:HE21 | 1.63                     | 0.63              |
| 1:F:339:HIS:HD2  | 1:F:349:HIS:HB3  | 1.63                     | 0.63              |
| 1:F:975:HIS:ND1  | 1:F:976:MET:SD   | 2.70                     | 0.63              |
| 1:A:583:VAL:O    | 1:A:586:LEU:HD12 | 1.98                     | 0.63              |
| 1:E:190:TYR:OH   | 1:E:224:ASN:OD1  | 2.15                     | 0.63              |
| 1:E:277:SER:OG   | 1:E:278:ASN:N    | 2.30                     | 0.63              |
| 1:F:709:TYR:CD1  | 1:F:713:ILE:HG13 | 2.33                     | 0.63              |
| 1:A:334:PHE:O    | 1:A:337:ASP:HB2  | 1.97                     | 0.63              |
| 1:F:939:GLN:HG2  | 1:F:943:PHE:CZ   | 2.33                     | 0.63              |
| 2:G:194:GLN:NE2  | 2:G:195:PHE:O    | 2.32                     | 0.63              |
| 1:A:614:ASN:OD1  | 1:A:615:SER:N    | 2.31                     | 0.63              |
| 1:F:960:LYS:HD3  | 1:F:996:TYR:CE2  | 2.33                     | 0.63              |
| 1:E:78:ASN:HB2   | 1:E:81:SER:HB3   | 1.81                     | 0.63              |
| 1:F:722:PHE:HA   | 1:F:724:LYS:HE2  | 1.79                     | 0.63              |
| 1:E:544:PHE:CZ   | 1:E:550:PHE:HB2  | 2.33                     | 0.63              |
| 1:A:83:GLU:HA    | 1:A:86:ARG:HB2   | 1.80                     | 0.62              |
| 1:B:29:CYS:O     | 1:B:33:ILE:HG12  | 1.98                     | 0.62              |
| 1:E:396:MET:SD   | 1:E:397:ALA:N    | 2.72                     | 0.62              |
| 1:E:606:HIS:HB3  | 1:E:610:GLN:NE2  | 2.14                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:780:VAL:HG11 | 1:F:820:LEU:HB3  | 1.81                     | 0.62              |
| 2:G:189:SER:HB3  | 2:G:238:SER:HB3  | 1.81                     | 0.62              |
| 1:A:458:ILE:O    | 1:A:462:SER:OG   | 2.15                     | 0.62              |
| 1:A:728:LEU:HG   | 1:A:764:CYS:SG   | 2.38                     | 0.62              |
| 1:A:802:ARG:HD2  | 1:A:840:LYS:HG2  | 1.80                     | 0.62              |
| 1:B:247:ARG:HE   | 1:B:248:THR:H    | 1.45                     | 0.62              |
| 1:E:680:GLU:O    | 1:E:680:GLU:OE2  | 2.15                     | 0.62              |
| 1:F:960:LYS:HD2  | 1:F:962:TYR:CE2  | 2.34                     | 0.62              |
| 2:C:170:ARG:O    | 2:C:172:GLU:N    | 2.32                     | 0.62              |
| 1:E:674:ASP:HA   | 1:E:725:TYR:CE1  | 2.35                     | 0.62              |
| 2:H:35:ALA:O     | 2:H:58:GLU:N     | 2.33                     | 0.62              |
| 1:E:419:ASP:OD1  | 1:E:419:ASP:N    | 2.31                     | 0.62              |
| 1:E:375:LYS:HA   | 1:E:378:TYR:HD1  | 1.64                     | 0.62              |
| 1:E:481:ILE:O    | 1:E:485:ILE:HG12 | 2.00                     | 0.62              |
| 1:F:326:ARG:NH1  | 1:F:591:ASN:OD1  | 2.28                     | 0.62              |
| 1:F:860:GLU:O    | 1:F:861:ASN:C    | 2.43                     | 0.62              |
| 1:F:861:ASN:O    | 1:F:862:ILE:C    | 2.43                     | 0.62              |
| 2:D:22:VAL:HG23  | 2:D:69:ASP:HB2   | 1.80                     | 0.62              |
| 1:A:41:LYS:HD2   | 1:A:211:HIS:HA   | 1.82                     | 0.62              |
| 1:B:90:ILE:HG12  | 1:F:260:TYR:HD2  | 1.65                     | 0.62              |
| 2:C:22:VAL:HG21  | 2:C:171:TYR:CE1  | 2.35                     | 0.62              |
| 1:E:731:GLU:HA   | 1:E:734:GLY:HA2  | 1.82                     | 0.62              |
| 1:E:984:LEU:O    | 1:E:988:VAL:HG23 | 2.00                     | 0.62              |
| 1:A:651:ASP:O    | 1:A:655:ILE:HG12 | 1.99                     | 0.62              |
| 1:B:490:THR:HA   | 1:B:493:ASN:HB2  | 1.82                     | 0.62              |
| 1:E:581:ASP:OD1  | 1:E:582:ILE:N    | 2.33                     | 0.62              |
| 1:A:717:LYS:NZ   | 1:A:749:LEU:HB3  | 2.15                     | 0.62              |
| 1:B:476:ILE:O    | 1:B:480:ARG:HG2  | 1.99                     | 0.62              |
| 1:B:899:GLU:HA   | 1:B:904:ILE:HD12 | 1.82                     | 0.62              |
| 1:F:979:HIS:HD1  | 1:F:980:VAL:HG23 | 1.64                     | 0.62              |
| 1:F:724:LYS:HD2  | 1:F:725:TYR:CE1  | 2.35                     | 0.62              |
| 1:A:662:ASP:HA   | 1:A:665:LYS:HE2  | 1.80                     | 0.61              |
| 1:B:223:TYR:HA   | 1:B:226:ASN:ND2  | 2.15                     | 0.61              |
| 1:F:627:ARG:NH1  | 1:F:672:SER:OG   | 2.31                     | 0.61              |
| 2:G:192:TYR:HB2  | 2:G:235:ILE:HB   | 1.80                     | 0.61              |
| 1:B:348:ARG:NH1  | 1:B:351:ASN:O    | 2.33                     | 0.61              |
| 1:E:370:ARG:NH1  | 1:E:373:LEU:HD22 | 2.15                     | 0.61              |
| 1:E:724:LYS:NZ   | 1:E:760:ARG:O    | 2.30                     | 0.61              |
| 1:E:558:LEU:O    | 1:E:562:THR:HG23 | 2.00                     | 0.61              |
| 1:F:228:LEU:O    | 1:F:228:LEU:CG   | 2.49                     | 0.61              |
| 1:F:509:ASP:HA   | 1:F:512:LEU:HD12 | 1.81                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:683:LYS:HA   | 1:F:686:GLU:OE2  | 2.00                     | 0.61              |
| 1:A:586:LEU:HA   | 1:A:589:TYR:CD2  | 2.35                     | 0.61              |
| 1:A:956:PRO:O    | 1:A:987:ARG:NH1  | 2.34                     | 0.61              |
| 1:F:627:ARG:HH21 | 1:F:675:LYS:HZ2  | 1.48                     | 0.61              |
| 1:F:995:ARG:O    | 1:F:999:ILE:HG12 | 2.01                     | 0.61              |
| 1:A:67:HIS:ND1   | 1:A:73:SER:O     | 2.34                     | 0.61              |
| 1:A:147:LYS:HD3  | 1:B:530:GLY:HA3  | 1.82                     | 0.61              |
| 1:B:646:PHE:HB3  | 1:B:677:ARG:HH12 | 1.66                     | 0.61              |
| 1:E:140:THR:O    | 1:E:144:LYS:HE2  | 2.01                     | 0.61              |
| 1:E:208:ILE:HA   | 1:E:213:ILE:HG13 | 1.82                     | 0.61              |
| 1:F:686:GLU:HA   | 1:F:689:VAL:HG22 | 1.81                     | 0.61              |
| 1:A:660:LYS:HG3  | 1:A:661:ILE:H    | 1.66                     | 0.61              |
| 1:B:724:LYS:NZ   | 1:B:760:ARG:HB3  | 2.16                     | 0.61              |
| 1:E:758:LEU:HD11 | 1:E:807:LEU:HD22 | 1.81                     | 0.61              |
| 1:F:116:PRO:O    | 1:F:120:LYS:NZ   | 2.32                     | 0.61              |
| 1:F:956:PRO:HG3  | 1:F:987:ARG:HD2  | 1.82                     | 0.61              |
| 2:G:72:TRP:O     | 2:G:76:THR:HB    | 2.00                     | 0.61              |
| 1:A:475:GLN:OE1  | 1:A:478:ARG:NH1  | 2.29                     | 0.61              |
| 1:A:528:PHE:HE2  | 1:A:542:LEU:O    | 1.83                     | 0.61              |
| 2:D:61:LEU:O     | 2:D:220:PHE:N    | 2.32                     | 0.61              |
| 1:F:86:ARG:HG3   | 1:F:87:ILE:HD12  | 1.83                     | 0.61              |
| 1:F:286:TYR:O    | 1:F:290:MET:HG2  | 2.00                     | 0.61              |
| 1:F:439:ALA:HB2  | 1:F:454:LEU:HD22 | 1.83                     | 0.61              |
| 1:F:936:MET:N    | 1:F:936:MET:SD   | 2.74                     | 0.61              |
| 1:B:472:TYR:CE2  | 1:B:542:LEU:HG   | 2.32                     | 0.61              |
| 2:D:203:GLU:OE1  | 2:D:203:GLU:N    | 2.26                     | 0.61              |
| 1:E:848:ASN:OD1  | 1:E:852:HIS:NE2  | 2.33                     | 0.61              |
| 2:H:196:PRO:HG3  | 2:H:230:GLU:HA   | 1.82                     | 0.61              |
| 1:A:34:THR:O     | 1:A:37:SER:OG    | 2.14                     | 0.61              |
| 1:A:578:MET:HE1  | 1:A:586:LEU:HD21 | 1.82                     | 0.61              |
| 1:B:609:HIS:NE2  | 1:B:660:LYS:HG2  | 2.16                     | 0.61              |
| 1:E:904:ILE:HG12 | 2:H:235:ILE:HG23 | 1.81                     | 0.61              |
| 1:F:294:ILE:O    | 1:F:295:GLU:HG2  | 2.01                     | 0.61              |
| 1:B:154:ALA:N    | 1:B:157:ASP:OD2  | 2.30                     | 0.60              |
| 1:E:912:TYR:O    | 1:E:915:THR:OG1  | 2.15                     | 0.60              |
| 1:F:962:TYR:CD1  | 1:F:967:LEU:HD22 | 2.31                     | 0.60              |
| 1:A:94:VAL:HG13  | 1:A:95:LYS:HD3   | 1.81                     | 0.60              |
| 1:A:238:ASP:OD1  | 1:A:238:ASP:N    | 2.32                     | 0.60              |
| 1:B:452:TYR:HA   | 1:B:455:TYR:CD2  | 2.36                     | 0.60              |
| 1:B:688:LEU:HD21 | 1:B:736:ILE:HD11 | 1.83                     | 0.60              |
| 2:D:196:PRO:HG2  | 2:D:230:GLU:HA   | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:56:TYR:CZ    | 1:E:135:ASP:HB3  | 2.36                     | 0.60              |
| 1:F:504:TYR:HE2  | 1:F:706:VAL:HG21 | 1.67                     | 0.60              |
| 1:F:960:LYS:O    | 1:F:962:TYR:N    | 2.33                     | 0.60              |
| 1:A:751:ILE:HG13 | 1:A:754:ARG:HB2  | 1.83                     | 0.60              |
| 1:A:808:ILE:HG13 | 1:A:844:LEU:HD11 | 1.83                     | 0.60              |
| 1:B:42:LEU:HD12  | 1:B:44:PHE:HE1   | 1.67                     | 0.60              |
| 1:B:663:ASP:O    | 1:B:667:LEU:HB2  | 2.01                     | 0.60              |
| 1:E:375:LYS:HA   | 1:E:378:TYR:CD1  | 2.35                     | 0.60              |
| 1:E:922:LEU:HD22 | 1:E:969:LYS:HE2  | 1.81                     | 0.60              |
| 1:F:357:MET:SD   | 1:F:358:GLU:N    | 2.74                     | 0.60              |
| 2:G:38:GLU:HA    | 2:G:54:LYS:HZ1   | 1.65                     | 0.60              |
| 1:A:685:GLU:OE2  | 1:A:728:LEU:HA   | 2.01                     | 0.60              |
| 1:B:647:MET:SD   | 1:B:647:MET:N    | 2.75                     | 0.60              |
| 1:F:407:ILE:H    | 2:H:2:LYS:HB3    | 1.65                     | 0.60              |
| 1:B:130:ILE:HD13 | 1:B:168:LEU:HB3  | 1.82                     | 0.60              |
| 1:B:175:ARG:NH1  | 1:B:175:ARG:O    | 2.34                     | 0.60              |
| 1:F:895:ASN:O    | 1:F:899:GLU:HB2  | 2.02                     | 0.60              |
| 1:F:228:LEU:O    | 1:F:228:LEU:HG   | 2.01                     | 0.60              |
| 1:F:530:GLY:C    | 1:F:531:MET:HE2  | 2.26                     | 0.60              |
| 1:F:987:ARG:HA   | 1:F:987:ARG:CZ   | 2.32                     | 0.60              |
| 1:B:375:LYS:HA   | 1:B:378:TYR:HB2  | 1.84                     | 0.60              |
| 1:E:192:ASN:O    | 1:E:196:ASN:N    | 2.31                     | 0.60              |
| 2:G:168:SER:O    | 2:G:169:GLU:C    | 2.43                     | 0.60              |
| 1:B:794:VAL:HG22 | 2:C:223:LEU:HD12 | 1.84                     | 0.60              |
| 1:E:683:LYS:HA   | 1:E:683:LYS:HE3  | 1.84                     | 0.60              |
| 1:E:698:GLN:HG2  | 1:E:712:PHE:CE2  | 2.32                     | 0.60              |
| 1:F:134:TYR:OH   | 1:F:184:VAL:O    | 2.20                     | 0.60              |
| 1:A:374:SER:OG   | 1:A:377:GLN:OE1  | 2.19                     | 0.59              |
| 1:A:491:GLN:OE1  | 1:A:491:GLN:N    | 2.31                     | 0.59              |
| 1:E:565:VAL:O    | 1:E:569:MET:HG2  | 2.01                     | 0.59              |
| 1:E:245:PHE:HD2  | 1:E:268:ILE:HG23 | 1.66                     | 0.59              |
| 1:A:25:ASN:HA    | 1:A:28:GLU:OE2   | 2.01                     | 0.59              |
| 1:A:531:MET:HE3  | 1:A:532:PRO:HD2  | 1.84                     | 0.59              |
| 1:F:233:ARG:NE   | 1:F:264:LYS:HA   | 2.17                     | 0.59              |
| 2:G:188:TYR:CD2  | 2:G:238:SER:HB2  | 2.37                     | 0.59              |
| 1:A:239:SER:O    | 1:A:239:SER:OG   | 2.19                     | 0.59              |
| 1:B:414:TYR:OH   | 1:B:650:TYR:O    | 2.20                     | 0.59              |
| 1:E:242:LYS:HZ2  | 1:E:265:GLY:C    | 2.05                     | 0.59              |
| 2:H:22:VAL:HG12  | 2:H:171:TYR:OH   | 2.03                     | 0.59              |
| 1:A:495:LEU:HD13 | 2:D:218:ILE:HD12 | 1.84                     | 0.59              |
| 1:B:116:PRO:HA   | 1:B:119:ASP:OD2  | 2.01                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:801:SER:HB3  | 1:E:840:LYS:HZ3  | 1.67                     | 0.59              |
| 1:F:796:SER:OG   | 2:G:222:ALA:O    | 2.20                     | 0.59              |
| 1:F:809:LYS:HB2  | 1:F:844:LEU:HD11 | 1.84                     | 0.59              |
| 1:E:632:ASP:CG   | 1:E:633:GLU:H    | 2.11                     | 0.59              |
| 1:E:990:ASN:HA   | 1:F:994:LYS:HE3  | 1.85                     | 0.59              |
| 1:E:1001:MET:O   | 1:E:1002:ASN:HB2 | 2.02                     | 0.59              |
| 1:F:86:ARG:NH1   | 1:F:87:ILE:HA    | 2.17                     | 0.59              |
| 2:G:13:PHE:N     | 2:G:22:VAL:O     | 2.36                     | 0.59              |
| 2:H:62:THR:OG1   | 2:H:218:ILE:O    | 2.16                     | 0.59              |
| 1:B:659:PHE:HB3  | 1:B:662:ASP:HA   | 1.83                     | 0.59              |
| 1:E:281:ASP:O    | 1:E:285:ARG:NH2  | 2.36                     | 0.59              |
| 1:E:526:ASP:CG   | 1:E:529:ASN:H    | 2.11                     | 0.59              |
| 1:E:680:GLU:OE1  | 1:E:683:LYS:N    | 2.32                     | 0.59              |
| 1:F:222:ASP:H    | 1:F:225:ILE:CG2  | 2.13                     | 0.59              |
| 1:A:404:ASN:HA   | 2:C:4:VAL:O      | 2.02                     | 0.59              |
| 1:E:629:ARG:HD2  | 1:E:630:ASP:O    | 2.03                     | 0.59              |
| 1:F:170:VAL:HA   | 1:F:200:ILE:HD11 | 1.84                     | 0.59              |
| 2:G:14:LYS:HA    | 2:G:20:LYS:HE3   | 1.84                     | 0.59              |
| 1:E:978:HIS:O    | 1:E:982:GLU:HG2  | 2.02                     | 0.59              |
| 1:F:891:THR:O    | 1:F:895:ASN:ND2  | 2.36                     | 0.59              |
| 1:A:213:ILE:HB   | 1:A:243:PRO:HB3  | 1.84                     | 0.59              |
| 1:A:548:ASN:CB   | 2:D:210:ASN:HD21 | 2.16                     | 0.59              |
| 1:B:442:LEU:HB3  | 1:B:447:ARG:HH12 | 1.68                     | 0.59              |
| 1:B:964:ASP:HB2  | 1:B:965:LYS:NZ   | 2.18                     | 0.59              |
| 1:E:815:PHE:CG   | 1:E:815:PHE:O    | 2.56                     | 0.59              |
| 1:F:81:SER:OG    | 1:F:82:ASP:N     | 2.35                     | 0.59              |
| 2:H:60:ASN:HA    | 2:H:219:LYS:HZ3  | 1.68                     | 0.59              |
| 1:A:275:ILE:HG23 | 1:A:285:ARG:HH12 | 1.66                     | 0.58              |
| 1:F:962:TYR:CE2  | 1:F:999:ILE:HG21 | 2.38                     | 0.58              |
| 1:A:610:GLN:HA   | 1:A:613:ARG:HB3  | 1.85                     | 0.58              |
| 1:A:794:VAL:HA   | 2:D:225:ASP:HA   | 1.85                     | 0.58              |
| 1:B:46:VAL:HG11  | 1:B:138:ILE:HG21 | 1.84                     | 0.58              |
| 1:B:247:ARG:HE   | 1:B:248:THR:N    | 2.01                     | 0.58              |
| 2:C:28:GLN:HB3   | 2:C:64:LYS:HD2   | 1.85                     | 0.58              |
| 1:F:817:SER:HB3  | 1:F:821:SER:HB3  | 1.85                     | 0.58              |
| 1:A:54:SER:OG    | 1:A:115:ASN:ND2  | 2.30                     | 0.58              |
| 1:A:367:CYS:SG   | 1:A:370:ARG:NH2  | 2.77                     | 0.58              |
| 1:A:449:GLU:HG3  | 1:A:507:PHE:HE1  | 1.69                     | 0.58              |
| 1:B:118:HIS:O    | 1:B:122:LEU:HG   | 2.03                     | 0.58              |
| 1:B:134:TYR:CG   | 1:B:183:VAL:HG11 | 2.38                     | 0.58              |
| 1:F:836:ASP:OD1  | 1:F:836:ASP:N    | 2.32                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:254:GLU:O    | 1:B:257:THR:OG1  | 2.19                     | 0.58              |
| 1:B:407:ILE:HG12 | 2:D:2:LYS:HB3    | 1.85                     | 0.58              |
| 2:D:190:ASP:H    | 2:D:237:ALA:HB3  | 1.69                     | 0.58              |
| 1:F:53:LEU:HB3   | 1:F:115:ASN:HD22 | 1.68                     | 0.58              |
| 1:F:776:ASP:O    | 1:F:780:VAL:HG22 | 2.04                     | 0.58              |
| 2:H:171:TYR:C    | 2:H:172:GLU:OE1  | 2.47                     | 0.58              |
| 1:A:1000:LEU:HA  | 1:A:1004:PHE:HB2 | 1.85                     | 0.58              |
| 1:E:242:LYS:HG3  | 1:E:267:ARG:HD3  | 1.85                     | 0.58              |
| 1:F:311:TYR:O    | 1:F:315:LYS:HG2  | 2.03                     | 0.58              |
| 1:F:706:VAL:O    | 1:F:710:THR:HG23 | 2.04                     | 0.58              |
| 1:F:852:HIS:O    | 1:F:855:SER:OG   | 2.22                     | 0.58              |
| 2:G:4:VAL:O      | 2:G:6:GLN:HG3    | 2.02                     | 0.58              |
| 1:A:631:ILE:HD12 | 1:A:635:GLY:HA3  | 1.84                     | 0.58              |
| 1:A:779:LEU:HD11 | 1:A:844:LEU:HD22 | 1.86                     | 0.58              |
| 1:B:297:GLN:HE21 | 1:B:301:PHE:HZ   | 1.51                     | 0.58              |
| 1:B:964:ASP:CG   | 1:B:966:LEU:HB2  | 2.28                     | 0.58              |
| 1:E:396:MET:HE1  | 1:E:398:LYS:NZ   | 2.19                     | 0.58              |
| 1:E:629:ARG:C    | 1:E:630:ASP:O    | 2.20                     | 0.58              |
| 1:E:893:LYS:NZ   | 1:E:933:PHE:HA   | 2.19                     | 0.58              |
| 1:F:812:GLU:OE1  | 1:F:813:LYS:N    | 2.34                     | 0.58              |
| 1:A:606:HIS:O    | 1:A:609:HIS:CD2  | 2.57                     | 0.58              |
| 1:E:549:GLN:HA   | 1:E:552:TYR:HD2  | 1.69                     | 0.58              |
| 1:F:228:LEU:HA   | 1:F:231:TRP:HE3  | 1.67                     | 0.58              |
| 1:E:32:GLU:OE1   | 1:E:267:ARG:NH2  | 2.36                     | 0.58              |
| 1:F:548:ASN:HB3  | 2:G:209:GLU:OE2  | 2.02                     | 0.58              |
| 2:D:175:TYR:HB2  | 2:D:193:ILE:HB   | 1.85                     | 0.58              |
| 1:E:782:GLN:HA   | 1:E:785:LYS:HB2  | 1.86                     | 0.58              |
| 1:A:141:ALA:HA   | 1:A:144:LYS:HZ2  | 1.69                     | 0.57              |
| 1:A:783:ALA:HB1  | 1:A:838:LEU:HD12 | 1.86                     | 0.57              |
| 2:C:69:ASP:OD1   | 2:C:69:ASP:N     | 2.37                     | 0.57              |
| 1:E:48:ALA:O     | 1:E:51:SER:OG    | 2.22                     | 0.57              |
| 1:E:277:SER:OG   | 1:E:284:GLU:OE2  | 2.16                     | 0.57              |
| 1:E:279:GLU:HG2  | 1:E:280:TYR:H    | 1.68                     | 0.57              |
| 1:E:661:ILE:HG13 | 1:E:665:LYS:HZ3  | 1.68                     | 0.57              |
| 1:E:744:PHE:HB3  | 1:E:749:LEU:HD22 | 1.86                     | 0.57              |
| 1:F:277:SER:OG   | 1:F:278:ASN:N    | 2.36                     | 0.57              |
| 1:F:908:SER:CA   | 2:G:231:MET:HB3  | 2.27                     | 0.57              |
| 1:A:26:VAL:O     | 1:A:30:ILE:HG22  | 2.03                     | 0.57              |
| 1:A:148:TYR:HB3  | 1:B:532:PRO:HD3  | 1.85                     | 0.57              |
| 1:B:131:THR:OG1  | 1:B:133:ASN:OD1  | 2.20                     | 0.57              |
| 1:B:927:ASN:HB3  | 1:B:930:MET:HE1  | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:403:LEU:H    | 2:H:6:GLN:HB2    | 1.68                     | 0.57              |
| 1:F:737:VAL:HG21 | 1:F:771:ILE:HD12 | 1.86                     | 0.57              |
| 1:F:822:GLU:HA   | 1:F:825:LEU:HG   | 1.85                     | 0.57              |
| 1:F:869:ILE:HD12 | 1:F:874:ILE:N    | 2.19                     | 0.57              |
| 1:A:29:CYS:O     | 1:A:33:ILE:HG12  | 2.04                     | 0.57              |
| 1:B:325:ILE:HG21 | 1:B:330:LEU:HD13 | 1.85                     | 0.57              |
| 1:B:479:TYR:CE2  | 1:B:524:ILE:HD13 | 2.39                     | 0.57              |
| 1:E:691:ILE:HA   | 1:E:694:GLU:OE2  | 2.05                     | 0.57              |
| 1:F:24:ASN:OD1   | 1:F:25:ASN:N     | 2.38                     | 0.57              |
| 1:F:582:ILE:HA   | 1:F:585:LEU:HD23 | 1.86                     | 0.57              |
| 1:F:875:ASP:OD2  | 2:G:49:PRO:HD2   | 2.04                     | 0.57              |
| 1:A:780:VAL:HG22 | 1:A:820:LEU:HD22 | 1.85                     | 0.57              |
| 2:D:32:PHE:HD1   | 2:D:61:LEU:HD13  | 1.70                     | 0.57              |
| 1:E:126:PRO:O    | 1:E:165:ARG:NH2  | 2.37                     | 0.57              |
| 1:E:927:ASN:HD21 | 1:E:929:LYS:HD3  | 1.69                     | 0.57              |
| 1:F:419:ASP:OD1  | 1:F:420:VAL:N    | 2.38                     | 0.57              |
| 2:G:36:ILE:HG23  | 2:G:54:LYS:HD2   | 1.86                     | 0.57              |
| 1:A:450:GLU:OE1  | 1:A:450:GLU:N    | 2.38                     | 0.57              |
| 1:B:105:LYS:HA   | 1:B:178:PHE:HD2  | 1.69                     | 0.57              |
| 2:D:1:MET:HE2    | 2:D:1:MET:H1     | 1.69                     | 0.57              |
| 1:E:186:LYS:HD2  | 1:E:188:ASP:H    | 1.69                     | 0.57              |
| 1:E:242:LYS:HE2  | 1:E:242:LYS:HA   | 1.86                     | 0.57              |
| 1:E:373:LEU:HD23 | 1:E:378:TYR:CD2  | 2.40                     | 0.57              |
| 1:F:309:ILE:HA   | 1:F:312:ILE:HG12 | 1.87                     | 0.57              |
| 1:B:187:GLU:HA   | 1:B:190:TYR:CD1  | 2.39                     | 0.57              |
| 1:E:526:ASP:CG   | 1:E:528:PHE:H    | 2.11                     | 0.57              |
| 1:F:652:PHE:CE2  | 1:F:726:VAL:HG11 | 2.40                     | 0.57              |
| 1:A:498:LEU:HD11 | 2:D:23:PHE:HE1   | 1.70                     | 0.57              |
| 1:B:179:LYS:HD3  | 1:B:179:LYS:N    | 2.19                     | 0.57              |
| 1:B:259:ILE:O    | 1:B:263:ASN:ND2  | 2.38                     | 0.57              |
| 1:B:576:PHE:CE1  | 1:B:641:LYS:HB2  | 2.39                     | 0.57              |
| 1:B:593:ARG:HG3  | 1:B:597:GLU:HB3  | 1.86                     | 0.57              |
| 2:D:41:LEU:HD11  | 2:D:54:LYS:HE2   | 1.85                     | 0.57              |
| 1:F:472:TYR:HD1  | 1:F:473:LEU:HD12 | 1.70                     | 0.57              |
| 1:A:290:MET:O    | 1:A:293:LEU:HG   | 2.05                     | 0.57              |
| 1:B:312:ILE:O    | 1:B:316:ILE:HG22 | 2.04                     | 0.57              |
| 1:E:32:GLU:OE2   | 1:E:267:ARG:NH1  | 2.35                     | 0.57              |
| 1:F:801:SER:HB3  | 1:F:840:LYS:HZ1  | 1.69                     | 0.57              |
| 1:A:86:ARG:HH12  | 1:A:89:GLN:HB3   | 1.68                     | 0.57              |
| 1:A:192:ASN:OD1  | 1:A:196:ASN:ND2  | 2.36                     | 0.57              |
| 1:A:497:LEU:HD21 | 2:D:73:LEU:HD12  | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:475:GLN:HA   | 1:E:478:ARG:HH12 | 1.70                     | 0.57              |
| 1:E:762:THR:HG22 | 1:E:767:LEU:HD21 | 1.87                     | 0.57              |
| 1:F:188:ASP:OD1  | 1:F:189:ASP:N    | 2.38                     | 0.57              |
| 1:F:373:LEU:HB3  | 1:F:377:GLN:HB2  | 1.87                     | 0.57              |
| 1:A:407:ILE:HB   | 2:C:2:LYS:NZ     | 2.19                     | 0.57              |
| 1:A:717:LYS:HG3  | 1:A:757:TRP:CH2  | 2.40                     | 0.57              |
| 1:F:627:ARG:HH21 | 1:F:675:LYS:NZ   | 2.02                     | 0.57              |
| 1:F:753:LYS:HE2  | 1:F:757:TRP:NE1  | 2.20                     | 0.57              |
| 1:F:768:PRO:HD2  | 1:F:771:ILE:HG12 | 1.86                     | 0.57              |
| 1:A:663:ASP:HA   | 1:A:666:ASN:OD1  | 2.05                     | 0.56              |
| 1:A:771:ILE:O    | 1:A:775:ILE:HD12 | 2.05                     | 0.56              |
| 1:E:755:TYR:HE2  | 1:E:803:ASP:HB3  | 1.70                     | 0.56              |
| 1:E:807:LEU:HD12 | 1:E:808:ILE:H    | 1.70                     | 0.56              |
| 1:E:827:LEU:HB3  | 1:E:831:LYS:HD3  | 1.86                     | 0.56              |
| 1:F:119:ASP:HB2  | 1:F:120:LYS:NZ   | 2.19                     | 0.56              |
| 1:F:815:PHE:CZ   | 1:F:817:SER:HA   | 2.39                     | 0.56              |
| 1:F:957:SER:HA   | 1:F:960:LYS:HB3  | 1.86                     | 0.56              |
| 1:B:740:LEU:HD11 | 1:B:757:TRP:HE3  | 1.69                     | 0.56              |
| 2:C:3:THR:OG1    | 2:C:5:ILE:HD11   | 2.05                     | 0.56              |
| 2:C:224:ALA:HB2  | 2:C:231:MET:HE3  | 1.87                     | 0.56              |
| 1:F:247:ARG:NH1  | 1:F:270:ASP:OD1  | 2.34                     | 0.56              |
| 1:A:367:CYS:HA   | 1:A:370:ARG:HE   | 1.69                     | 0.56              |
| 1:A:549:GLN:HA   | 1:A:552:TYR:CB   | 2.33                     | 0.56              |
| 1:A:580:SER:CB   | 1:A:582:ILE:HG12 | 2.35                     | 0.56              |
| 1:A:613:ARG:HD3  | 1:A:663:ASP:HB3  | 1.86                     | 0.56              |
| 1:B:439:ALA:HB2  | 1:B:454:LEU:HD22 | 1.86                     | 0.56              |
| 2:D:179:ALA:O    | 2:D:189:SER:OG   | 2.24                     | 0.56              |
| 1:E:475:GLN:HA   | 1:E:478:ARG:NH1  | 2.20                     | 0.56              |
| 1:E:551:LEU:HG   | 1:E:607:GLU:HG2  | 1.87                     | 0.56              |
| 1:E:681:GLN:NE2  | 1:E:682:GLU:OE1  | 2.38                     | 0.56              |
| 1:F:755:TYR:CE2  | 1:F:803:ASP:HB3  | 2.41                     | 0.56              |
| 1:F:863:ASN:HD21 | 1:F:865:LEU:HB2  | 1.71                     | 0.56              |
| 1:E:405:THR:O    | 2:G:1:MET:N      | 2.38                     | 0.56              |
| 1:E:680:GLU:CD   | 1:E:683:LYS:H    | 2.12                     | 0.56              |
| 1:B:412:LEU:HD21 | 1:B:420:VAL:HG23 | 1.86                     | 0.56              |
| 1:B:685:GLU:OE1  | 1:B:731:GLU:HB2  | 2.06                     | 0.56              |
| 1:B:740:LEU:HD22 | 1:B:758:LEU:HD21 | 1.87                     | 0.56              |
| 1:E:216:ILE:HD13 | 1:E:246:ILE:HD13 | 1.86                     | 0.56              |
| 1:E:729:SER:OG   | 1:E:732:GLY:N    | 2.37                     | 0.56              |
| 1:F:390:LYS:C    | 1:F:391:ASN:O    | 2.36                     | 0.56              |
| 1:A:500:PHE:HA   | 1:A:747:ARG:HG3  | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:475:GLN:HB3  | 1:B:527:LEU:HD11 | 1.88                     | 0.56              |
| 1:E:174:PHE:HB3  | 1:E:178:PHE:CD1  | 2.41                     | 0.56              |
| 1:F:559:PHE:O    | 1:F:562:THR:OG1  | 2.19                     | 0.56              |
| 1:F:966:LEU:O    | 1:F:970:ILE:HG12 | 2.05                     | 0.56              |
| 1:A:802:ARG:CB   | 1:A:840:LYS:HB3  | 2.36                     | 0.56              |
| 1:E:89:GLN:HE21  | 1:E:187:GLU:HG3  | 1.71                     | 0.56              |
| 1:F:75:LYS:NZ    | 1:F:83:GLU:HB3   | 2.20                     | 0.56              |
| 1:F:592:LEU:O    | 1:F:596:TYR:HB2  | 2.06                     | 0.56              |
| 1:F:822:GLU:OE1  | 1:F:822:GLU:N    | 2.34                     | 0.56              |
| 1:A:491:GLN:O    | 1:A:496:GLY:N    | 2.38                     | 0.56              |
| 1:A:800:TYR:HD1  | 2:D:226:THR:HG23 | 1.71                     | 0.56              |
| 2:C:40:LYS:NZ    | 2:C:42:ARG:O     | 2.38                     | 0.56              |
| 1:F:27:VAL:O     | 1:F:31:LYS:HG2   | 2.05                     | 0.56              |
| 1:F:386:ASN:O    | 1:F:390:LYS:HB3  | 2.06                     | 0.56              |
| 1:F:442:LEU:HD12 | 1:F:451:SER:HA   | 1.87                     | 0.56              |
| 2:H:197:ASN:OD1  | 2:H:198:VAL:N    | 2.39                     | 0.56              |
| 1:E:1000:LEU:HA  | 1:E:1004:PHE:CE2 | 2.40                     | 0.56              |
| 1:F:532:PRO:O    | 1:F:536:GLN:NE2  | 2.29                     | 0.56              |
| 1:F:722:PHE:HA   | 1:F:724:LYS:CE   | 2.35                     | 0.56              |
| 1:A:70:LEU:HD21  | 1:A:91:PHE:HA    | 1.87                     | 0.56              |
| 1:E:616:MET:SD   | 1:E:617:SER:N    | 2.79                     | 0.56              |
| 1:F:47:GLY:N     | 1:F:216:ILE:O    | 2.38                     | 0.56              |
| 1:F:242:LYS:HE3  | 1:F:267:ARG:HG2  | 1.88                     | 0.56              |
| 2:H:68:PHE:HD1   | 2:H:70:LEU:H     | 1.53                     | 0.56              |
| 1:A:580:SER:O    | 1:A:583:VAL:HB   | 2.07                     | 0.55              |
| 1:A:768:PRO:O    | 1:A:772:ILE:N    | 2.33                     | 0.55              |
| 1:F:189:ASP:O    | 1:F:193:TYR:N    | 2.39                     | 0.55              |
| 1:E:807:LEU:HD12 | 1:E:808:ILE:N    | 2.21                     | 0.55              |
| 1:F:727:LYS:HE3  | 1:F:765:ASN:HB3  | 1.88                     | 0.55              |
| 1:A:56:TYR:HD1   | 1:A:57:PRO:HD2   | 1.72                     | 0.55              |
| 1:E:452:TYR:HA   | 1:E:455:TYR:CD2  | 2.42                     | 0.55              |
| 1:E:931:GLU:OE1  | 1:E:931:GLU:N    | 2.39                     | 0.55              |
| 1:A:117:ILE:HA   | 1:A:120:LYS:HD2  | 1.88                     | 0.55              |
| 1:A:817:SER:OG   | 1:A:844:LEU:O    | 2.18                     | 0.55              |
| 1:B:407:ILE:HB   | 2:D:2:LYS:HG2    | 1.89                     | 0.55              |
| 1:E:680:GLU:O    | 1:E:680:GLU:CD   | 2.50                     | 0.55              |
| 1:F:610:GLN:OE1  | 1:F:613:ARG:NH2  | 2.39                     | 0.55              |
| 1:A:327:LYS:HA   | 1:A:330:LEU:HG   | 1.88                     | 0.55              |
| 1:A:752:GLY:HA2  | 1:A:799:LEU:HD13 | 1.87                     | 0.55              |
| 1:E:53:LEU:HD11  | 1:E:286:TYR:CE2  | 2.41                     | 0.55              |
| 1:F:741:LEU:HB3  | 1:F:778:PHE:CD2  | 2.42                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:760:ARG:HA   | 1:F:763:LYS:HG3  | 1.87                     | 0.55              |
| 1:F:906:THR:O    | 2:G:232:ALA:HB3  | 2.06                     | 0.55              |
| 1:A:475:GLN:HA   | 1:A:478:ARG:NH1  | 2.22                     | 0.55              |
| 1:B:659:PHE:HD2  | 1:B:662:ASP:HA   | 1.71                     | 0.55              |
| 2:C:42:ARG:HD3   | 2:C:52:ILE:HD13  | 1.88                     | 0.55              |
| 2:C:52:ILE:HD11  | 2:C:54:LYS:HG2   | 1.87                     | 0.55              |
| 1:F:89:GLN:CD    | 1:F:187:GLU:HG2  | 2.31                     | 0.55              |
| 1:F:189:ASP:OD1  | 1:F:190:TYR:N    | 2.39                     | 0.55              |
| 1:F:620:ILE:HA   | 1:F:645:PHE:HE2  | 1.71                     | 0.55              |
| 1:F:922:LEU:HA   | 1:F:969:LYS:HZ3  | 1.71                     | 0.55              |
| 1:A:247:ARG:HB2  | 1:A:270:ASP:HA   | 1.89                     | 0.55              |
| 1:B:135:ASP:O    | 1:B:169:LYS:NZ   | 2.40                     | 0.55              |
| 1:B:721:TYR:OH   | 1:B:760:ARG:NH2  | 2.39                     | 0.55              |
| 1:E:284:GLU:HG2  | 1:E:285:ARG:N    | 2.21                     | 0.55              |
| 1:E:304:LYS:HD2  | 1:E:307:GLU:H    | 1.72                     | 0.55              |
| 1:F:285:ARG:O    | 1:F:289:VAL:HG22 | 2.06                     | 0.55              |
| 1:F:366:SER:OG   | 1:F:368:ASP:OD1  | 2.25                     | 0.55              |
| 1:F:376:LYS:HZ1  | 1:F:380:ARG:CD   | 2.18                     | 0.55              |
| 2:G:65:ASN:OD1   | 2:G:67:PHE:N     | 2.35                     | 0.55              |
| 2:H:15:ARG:HD3   | 2:H:20:LYS:HD3   | 1.88                     | 0.55              |
| 1:F:802:ARG:HB2  | 1:F:840:LYS:HA   | 1.89                     | 0.55              |
| 1:F:904:ILE:HG22 | 2:G:235:ILE:H    | 1.70                     | 0.55              |
| 1:A:70:LEU:HD23  | 1:A:95:LYS:HE3   | 1.89                     | 0.55              |
| 1:A:316:ILE:HA   | 1:A:319:LEU:HD13 | 1.89                     | 0.55              |
| 1:A:532:PRO:HB3  | 1:B:148:TYR:CZ   | 2.42                     | 0.55              |
| 1:B:236:GLN:NE2  | 1:B:239:SER:O    | 2.40                     | 0.55              |
| 1:B:282:TYR:H    | 1:B:285:ARG:CZ   | 2.20                     | 0.55              |
| 1:B:481:ILE:O    | 1:B:485:ILE:HG13 | 2.07                     | 0.55              |
| 2:C:175:TYR:N    | 2:C:193:ILE:O    | 2.40                     | 0.55              |
| 1:E:145:ARG:O    | 1:E:145:ARG:NE   | 2.40                     | 0.55              |
| 1:F:132:THR:HA   | 1:F:170:VAL:HG12 | 1.88                     | 0.55              |
| 2:G:24:THR:HB    | 2:G:65:ASN:HD22  | 1.72                     | 0.55              |
| 1:A:583:VAL:O    | 1:A:587:ARG:HG3  | 2.06                     | 0.55              |
| 1:B:307:GLU:HA   | 1:B:310:ASP:HB2  | 1.89                     | 0.55              |
| 1:B:434:ASP:O    | 1:B:438:LYS:HG3  | 2.06                     | 0.55              |
| 1:E:396:MET:SD   | 1:E:398:LYS:HD2  | 2.47                     | 0.55              |
| 1:F:228:LEU:O    | 1:F:228:LEU:CD1  | 2.55                     | 0.55              |
| 1:A:116:PRO:HB2  | 1:A:120:LYS:HE3  | 1.89                     | 0.54              |
| 1:A:454:LEU:O    | 1:A:458:ILE:HD12 | 2.06                     | 0.54              |
| 1:A:750:ASP:OD2  | 1:A:751:ILE:HG22 | 2.06                     | 0.54              |
| 1:B:581:ASP:CG   | 1:B:622:LYS:HD3  | 2.32                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:406:SER:OG   | 1:E:407:ILE:N    | 2.40                     | 0.54              |
| 1:E:916:PHE:HA   | 1:E:919:TRP:CZ3  | 2.42                     | 0.54              |
| 1:F:696:THR:O    | 1:F:700:SER:CB   | 2.54                     | 0.54              |
| 1:A:59:TRP:HZ3   | 1:A:62:LEU:HD23  | 1.72                     | 0.54              |
| 1:A:547:ASP:HB2  | 1:A:549:GLN:OE1  | 2.08                     | 0.54              |
| 1:A:580:SER:HB2  | 1:A:582:ILE:CG2  | 2.36                     | 0.54              |
| 1:A:580:SER:HB2  | 1:A:582:ILE:HG12 | 1.88                     | 0.54              |
| 1:E:801:SER:H    | 1:E:840:LYS:HZ1  | 1.55                     | 0.54              |
| 1:F:259:ILE:O    | 1:F:262:GLU:HG3  | 2.07                     | 0.54              |
| 1:F:812:GLU:CD   | 1:F:813:LYS:H    | 2.14                     | 0.54              |
| 1:F:862:ILE:HD13 | 1:F:862:ILE:H    | 1.72                     | 0.54              |
| 1:A:152:ILE:HG23 | 1:A:157:ASP:HB2  | 1.89                     | 0.54              |
| 1:A:270:ASP:O    | 1:A:273:SER:OG   | 2.24                     | 0.54              |
| 1:A:535:PHE:HE1  | 1:A:542:LEU:HD23 | 1.72                     | 0.54              |
| 1:B:304:LYS:HB3  | 1:B:307:GLU:HB2  | 1.88                     | 0.54              |
| 1:E:690:GLY:O    | 1:E:694:GLU:HG3  | 2.07                     | 0.54              |
| 1:F:278:ASN:O    | 1:F:285:ARG:NH2  | 2.40                     | 0.54              |
| 1:F:291:ASP:HA   | 1:F:294:ILE:HD12 | 1.90                     | 0.54              |
| 2:G:214:LEU:O    | 2:G:216:PRO:HD3  | 2.07                     | 0.54              |
| 2:H:177:THR:O    | 2:H:191:ILE:N    | 2.30                     | 0.54              |
| 1:F:225:ILE:HD12 | 1:F:229:LEU:HD21 | 1.90                     | 0.54              |
| 1:F:294:ILE:HG22 | 1:F:295:GLU:H    | 1.73                     | 0.54              |
| 1:F:424:PHE:O    | 1:F:438:LYS:NZ   | 2.38                     | 0.54              |
| 2:G:205:GLU:O    | 2:G:206:MET:C    | 2.46                     | 0.54              |
| 1:B:319:LEU:HB2  | 1:B:322:LEU:HD13 | 1.88                     | 0.54              |
| 1:B:741:LEU:HD11 | 1:B:775:ILE:HG22 | 1.90                     | 0.54              |
| 1:E:205:LYS:HD3  | 1:E:231:TRP:CH2  | 2.42                     | 0.54              |
| 1:F:793:GLU:OE1  | 1:F:799:LEU:HB3  | 2.07                     | 0.54              |
| 1:F:937:ASP:OD1  | 1:F:940:TYR:N    | 2.39                     | 0.54              |
| 1:B:224:ASN:O    | 1:B:228:LEU:HG   | 2.07                     | 0.54              |
| 1:B:990:ASN:HB3  | 1:B:992:ASN:HD22 | 1.72                     | 0.54              |
| 1:F:44:PHE:HZ    | 1:F:124:MET:HG3  | 1.72                     | 0.54              |
| 1:F:327:LYS:HD3  | 1:F:392:GLY:HA3  | 1.90                     | 0.54              |
| 1:B:786:HIS:O    | 1:B:834:GLN:NE2  | 2.41                     | 0.54              |
| 1:E:655:ILE:HG23 | 1:E:659:PHE:HE2  | 1.72                     | 0.54              |
| 1:F:57:PRO:HA    | 1:F:61:ARG:NH2   | 2.22                     | 0.54              |
| 1:A:95:LYS:HD3   | 1:A:95:LYS:N     | 2.23                     | 0.54              |
| 1:A:223:TYR:HB3  | 1:A:225:ILE:HG13 | 1.90                     | 0.54              |
| 1:E:500:PHE:HA   | 1:E:747:ARG:CZ   | 2.37                     | 0.54              |
| 1:E:729:SER:N    | 1:E:732:GLY:HA3  | 2.23                     | 0.54              |
| 1:F:931:GLU:H    | 1:F:931:GLU:CD   | 2.15                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:53:LEU:HD13  | 1:B:117:ILE:HG13 | 1.90                     | 0.54              |
| 1:F:230:ASN:N    | 1:F:230:ASN:OD1  | 2.40                     | 0.54              |
| 1:A:366:SER:O    | 1:A:370:ARG:NE   | 2.41                     | 0.54              |
| 1:A:652:PHE:CZ   | 1:A:687:TYR:HB3  | 2.43                     | 0.54              |
| 1:A:989:LYS:HD2  | 1:B:1001:MET:SD  | 2.48                     | 0.54              |
| 1:B:768:PRO:HD2  | 1:B:771:ILE:HD13 | 1.90                     | 0.54              |
| 1:B:974:LYS:HA   | 1:B:977:LYS:HD3  | 1.90                     | 0.54              |
| 2:D:34:GLN:HA    | 2:D:59:ILE:HD13  | 1.90                     | 0.54              |
| 1:E:918:ILE:HG23 | 2:H:51:TYR:CD2   | 2.42                     | 0.54              |
| 1:F:118:HIS:NE2  | 1:F:138:ILE:HA   | 2.23                     | 0.54              |
| 1:F:213:ILE:HB   | 1:F:243:PRO:HB3  | 1.89                     | 0.54              |
| 1:F:311:TYR:CZ   | 1:F:315:LYS:HE2  | 2.43                     | 0.54              |
| 1:B:494:GLY:O    | 1:B:496:GLY:N    | 2.41                     | 0.53              |
| 1:F:615:SER:HA   | 1:F:618:LEU:HD13 | 1.90                     | 0.53              |
| 1:F:651:ASP:HA   | 1:F:654:ASN:HD21 | 1.71                     | 0.53              |
| 1:F:681:GLN:HA   | 1:F:684:ILE:HD11 | 1.91                     | 0.53              |
| 1:F:861:ASN:OD1  | 1:F:862:ILE:HG12 | 2.08                     | 0.53              |
| 1:A:751:ILE:HA   | 1:A:754:ARG:HG2  | 1.90                     | 0.53              |
| 1:A:869:ILE:HG12 | 2:D:50:LEU:HD13  | 1.90                     | 0.53              |
| 1:A:976:MET:SD   | 1:A:976:MET:N    | 2.81                     | 0.53              |
| 2:C:39:GLU:HG2   | 2:C:40:LYS:H     | 1.74                     | 0.53              |
| 1:E:312:ILE:HD11 | 1:E:356:TYR:CD2  | 2.43                     | 0.53              |
| 1:E:579:SER:H    | 1:E:582:ILE:HD11 | 1.72                     | 0.53              |
| 1:F:553:ASP:O    | 1:F:557:LYS:NZ   | 2.42                     | 0.53              |
| 2:H:171:TYR:O    | 2:H:196:PRO:O    | 2.25                     | 0.53              |
| 1:A:275:ILE:HG23 | 1:A:285:ARG:NH1  | 2.24                     | 0.53              |
| 1:A:607:GLU:O    | 1:A:610:GLN:N    | 2.41                     | 0.53              |
| 1:A:652:PHE:HZ   | 1:A:687:TYR:HB3  | 1.74                     | 0.53              |
| 1:B:594:PHE:O    | 1:B:598:ASN:ND2  | 2.41                     | 0.53              |
| 1:E:57:PRO:HB3   | 1:E:107:PHE:HE1  | 1.73                     | 0.53              |
| 1:E:270:ASP:OD1  | 1:E:271:ALA:N    | 2.41                     | 0.53              |
| 1:F:358:GLU:HA   | 1:F:361:PHE:CE1  | 2.43                     | 0.53              |
| 1:F:479:TYR:O    | 1:F:483:GLN:NE2  | 2.41                     | 0.53              |
| 1:F:509:ASP:OD1  | 1:F:510:GLU:N    | 2.42                     | 0.53              |
| 1:A:99:ALA:O     | 1:A:103:ILE:HG13 | 2.08                     | 0.53              |
| 1:A:303:THR:OG1  | 1:A:304:LYS:N    | 2.42                     | 0.53              |
| 1:A:388:PHE:HA   | 1:A:391:ASN:ND2  | 2.23                     | 0.53              |
| 1:A:582:ILE:HA   | 1:A:585:LEU:CD1  | 2.38                     | 0.53              |
| 1:B:65:LYS:HE2   | 1:B:103:ILE:HG23 | 1.90                     | 0.53              |
| 2:H:60:ASN:HA    | 2:H:219:LYS:NZ   | 2.22                     | 0.53              |
| 1:A:550:PHE:O    | 1:A:551:LEU:C    | 2.45                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:695:ILE:O    | 1:A:698:GLN:HB2  | 2.08                     | 0.53              |
| 1:B:231:TRP:O    | 1:B:235:LEU:HG   | 2.09                     | 0.53              |
| 1:B:616:MET:HA   | 1:B:616:MET:HE3  | 1.91                     | 0.53              |
| 1:E:326:ARG:HH21 | 1:E:594:PHE:HE2  | 1.56                     | 0.53              |
| 1:F:187:GLU:HA   | 1:F:190:TYR:HD2  | 1.73                     | 0.53              |
| 1:A:403:LEU:N    | 2:C:6:GLN:HE22   | 1.97                     | 0.53              |
| 1:A:800:TYR:CD1  | 2:D:226:THR:HG23 | 2.43                     | 0.53              |
| 1:B:491:GLN:HG3  | 2:C:206:MET:HE3  | 1.91                     | 0.53              |
| 1:F:89:GLN:HA    | 1:F:186:LYS:HE2  | 1.89                     | 0.53              |
| 1:F:720:LEU:HB2  | 1:F:757:TRP:HZ3  | 1.73                     | 0.53              |
| 1:E:606:HIS:O    | 1:E:609:HIS:N    | 2.42                     | 0.53              |
| 1:E:687:TYR:CZ   | 1:E:691:ILE:HD11 | 2.43                     | 0.53              |
| 1:E:724:LYS:HZ2  | 1:E:764:CYS:HB2  | 1.73                     | 0.53              |
| 1:F:41:LYS:HG2   | 1:F:211:HIS:CD2  | 2.39                     | 0.53              |
| 1:F:965:LYS:C    | 1:F:967:LEU:N    | 2.61                     | 0.53              |
| 1:A:41:LYS:O     | 1:A:212:THR:N    | 2.39                     | 0.53              |
| 1:A:800:TYR:O    | 1:A:802:ARG:N    | 2.38                     | 0.53              |
| 1:E:755:TYR:CD1  | 1:E:807:LEU:HD23 | 2.44                     | 0.53              |
| 1:F:976:MET:HB3  | 1:F:979:HIS:CE1  | 2.44                     | 0.53              |
| 1:E:595:LEU:HG   | 1:E:603:VAL:HG12 | 1.91                     | 0.53              |
| 1:F:646:PHE:HD1  | 1:F:677:ARG:HB3  | 1.74                     | 0.53              |
| 2:H:58:GLU:O     | 2:H:59:ILE:HD13  | 2.08                     | 0.53              |
| 1:A:188:ASP:O    | 1:A:192:ASN:N    | 2.40                     | 0.53              |
| 1:A:736:ILE:HG21 | 1:A:761:LEU:HD22 | 1.90                     | 0.53              |
| 1:A:738:LYS:O    | 1:A:741:LEU:HD22 | 2.09                     | 0.53              |
| 2:D:14:LYS:HG3   | 2:D:172:GLU:HB3  | 1.91                     | 0.53              |
| 2:D:174:GLU:HG2  | 2:D:194:GLN:HB3  | 1.90                     | 0.53              |
| 1:E:459:ILE:HD11 | 1:E:478:ARG:HH11 | 1.74                     | 0.53              |
| 1:E:699:PHE:HD2  | 1:E:743:TYR:HB3  | 1.73                     | 0.53              |
| 1:E:841:LEU:HD23 | 1:E:844:LEU:HD12 | 1.91                     | 0.53              |
| 1:F:576:PHE:HB2  | 2:H:30:ALA:HB3   | 1.91                     | 0.53              |
| 1:F:957:SER:CA   | 1:F:960:LYS:HB3  | 2.39                     | 0.53              |
| 1:A:128:HIS:CE1  | 1:A:166:TYR:H    | 2.26                     | 0.52              |
| 2:D:60:ASN:ND2   | 2:D:221:GLU:OE2  | 2.41                     | 0.52              |
| 1:F:44:PHE:CZ    | 1:F:124:MET:HG3  | 2.44                     | 0.52              |
| 2:H:71:GLU:O     | 2:H:72:TRP:HB2   | 2.08                     | 0.52              |
| 1:A:403:LEU:H    | 2:C:6:GLN:NE2    | 1.96                     | 0.52              |
| 1:B:631:ILE:HB   | 1:B:636:PHE:HD1  | 1.74                     | 0.52              |
| 1:F:89:GLN:CD    | 1:F:89:GLN:H     | 2.17                     | 0.52              |
| 1:F:627:ARG:NH2  | 1:F:675:LYS:HZ2  | 2.06                     | 0.52              |
| 1:F:905:GLN:C    | 2:G:234:VAL:HB   | 2.34                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:15:ARG:HD2   | 2:H:72:TRP:HE1   | 1.74                     | 0.52              |
| 1:A:583:VAL:O    | 1:A:584:VAL:C    | 2.49                     | 0.52              |
| 1:B:38:ARG:HA    | 1:B:38:ARG:NE    | 2.25                     | 0.52              |
| 1:E:99:ALA:O     | 1:E:103:ILE:HG12 | 2.10                     | 0.52              |
| 1:E:324:TYR:HA   | 1:E:390:LYS:HZ3  | 1.74                     | 0.52              |
| 1:E:455:TYR:HA   | 1:E:458:ILE:HG12 | 1.90                     | 0.52              |
| 1:E:755:TYR:CZ   | 1:E:807:LEU:HB3  | 2.45                     | 0.52              |
| 1:F:105:LYS:HA   | 1:F:178:PHE:HD2  | 1.73                     | 0.52              |
| 1:F:422:LYS:O    | 1:F:425:ILE:HG22 | 2.09                     | 0.52              |
| 2:G:197:ASN:HB2  | 2:G:230:GLU:CD   | 2.34                     | 0.52              |
| 2:H:14:LYS:HZ1   | 2:H:21:LEU:HD13  | 1.75                     | 0.52              |
| 2:H:21:LEU:HB3   | 2:H:69:ASP:OD2   | 2.09                     | 0.52              |
| 1:B:282:TYR:H    | 1:B:285:ARG:NH2  | 2.07                     | 0.52              |
| 1:E:245:PHE:O    | 1:E:269:ILE:N    | 2.41                     | 0.52              |
| 1:F:960:LYS:HA   | 1:F:962:TYR:CE2  | 2.45                     | 0.52              |
| 1:A:128:HIS:HE1  | 1:A:165:ARG:HA   | 1.75                     | 0.52              |
| 1:B:105:LYS:HD2  | 1:B:178:PHE:CD2  | 2.44                     | 0.52              |
| 1:B:205:LYS:NZ   | 1:B:232:VAL:HG22 | 2.25                     | 0.52              |
| 1:B:577:GLY:HA2  | 2:D:5:ILE:HG22   | 1.90                     | 0.52              |
| 2:C:16:LYS:HE3   | 2:C:172:GLU:HG2  | 1.91                     | 0.52              |
| 1:E:79:TYR:HA    | 1:E:83:GLU:CD    | 2.35                     | 0.52              |
| 1:E:201:SER:HA   | 1:E:204:MET:HG2  | 1.90                     | 0.52              |
| 1:E:540:LYS:HG3  | 1:E:541:ILE:N    | 2.25                     | 0.52              |
| 1:F:733:LEU:HD12 | 1:F:771:ILE:HD11 | 1.91                     | 0.52              |
| 1:F:801:SER:H    | 1:F:840:LYS:NZ   | 2.06                     | 0.52              |
| 1:A:205:LYS:HB2  | 1:B:202:ASN:HD21 | 1.75                     | 0.52              |
| 1:A:548:ASN:HA   | 1:A:550:PHE:CE1  | 2.44                     | 0.52              |
| 1:A:779:LEU:HD13 | 1:A:841:LEU:HD22 | 1.90                     | 0.52              |
| 1:B:842:LEU:HG   | 1:B:843:PRO:HD3  | 1.91                     | 0.52              |
| 2:C:13:PHE:HZ    | 2:C:63:VAL:HG21  | 1.73                     | 0.52              |
| 1:F:386:ASN:O    | 1:F:390:LYS:CB   | 2.57                     | 0.52              |
| 1:F:646:PHE:CD1  | 1:F:677:ARG:HB3  | 2.45                     | 0.52              |
| 1:A:469:CYS:HB2  | 1:A:539:TYR:CE2  | 2.45                     | 0.52              |
| 1:A:606:HIS:O    | 1:A:609:HIS:HD2  | 1.92                     | 0.52              |
| 1:B:134:TYR:CE2  | 1:B:183:VAL:CG1  | 2.67                     | 0.52              |
| 1:B:640:GLY:O    | 1:B:641:LYS:CG   | 2.58                     | 0.52              |
| 1:E:967:LEU:HD13 | 1:E:1003:TYR:HE2 | 1.75                     | 0.52              |
| 1:A:488:ALA:HA   | 1:A:491:GLN:HE22 | 1.73                     | 0.52              |
| 1:A:893:LYS:HD2  | 1:A:933:PHE:HE1  | 1.75                     | 0.52              |
| 1:B:274:LEU:HD13 | 1:B:292:LEU:HG   | 1.91                     | 0.52              |
| 1:B:573:SER:HA   | 2:D:31:SER:HA    | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:50:LEU:HD23  | 2:D:51:TYR:H     | 1.75                     | 0.52              |
| 1:E:533:PHE:O    | 1:E:537:LYS:HG2  | 2.09                     | 0.52              |
| 1:E:657:ARG:HB3  | 1:E:658:HIS:ND1  | 2.25                     | 0.52              |
| 1:B:475:GLN:HG3  | 1:B:478:ARG:HH12 | 1.75                     | 0.52              |
| 1:E:26:VAL:O     | 1:E:30:ILE:HG12  | 2.09                     | 0.52              |
| 1:E:376:LYS:HD2  | 1:E:380:ARG:HE   | 1.75                     | 0.52              |
| 1:E:564:LYS:O    | 1:E:567:SER:OG   | 2.27                     | 0.52              |
| 1:E:692:ALA:HB2  | 1:E:736:ILE:HG22 | 1.91                     | 0.52              |
| 1:E:735:LYS:HA   | 1:E:738:LYS:HZ3  | 1.75                     | 0.52              |
| 1:E:779:LEU:O    | 1:E:782:GLN:HG3  | 2.10                     | 0.52              |
| 1:F:598:ASN:CG   | 1:F:600:LEU:HD13 | 2.34                     | 0.52              |
| 1:F:896:TYR:HB2  | 1:F:933:PHE:HE1  | 1.75                     | 0.52              |
| 1:F:906:THR:CG2  | 2:G:233:VAL:HA   | 2.40                     | 0.52              |
| 1:A:548:ASN:HD22 | 2:D:209:GLU:HB2  | 1.74                     | 0.52              |
| 1:E:610:GLN:HB3  | 1:E:613:ARG:NH2  | 2.25                     | 0.52              |
| 1:A:751:ILE:HG23 | 1:A:799:LEU:CD2  | 2.40                     | 0.51              |
| 1:B:322:LEU:H    | 1:B:322:LEU:HD12 | 1.75                     | 0.51              |
| 2:C:34:GLN:HG2   | 2:C:57:LYS:HZ1   | 1.75                     | 0.51              |
| 2:D:10:ASP:HA    | 2:D:26:GLU:HA    | 1.91                     | 0.51              |
| 1:E:66:TYR:O     | 1:E:70:LEU:HD12  | 2.09                     | 0.51              |
| 1:E:629:ARG:NH1  | 1:E:631:ILE:HD12 | 2.25                     | 0.51              |
| 1:F:741:LEU:HB3  | 1:F:778:PHE:HD2  | 1.75                     | 0.51              |
| 1:A:585:LEU:O    | 1:A:588:LEU:HB2  | 2.10                     | 0.51              |
| 1:A:625:TYR:HA   | 1:B:992:ASN:ND2  | 2.25                     | 0.51              |
| 1:B:531:MET:HE3  | 1:B:535:PHE:HB3  | 1.92                     | 0.51              |
| 2:D:225:ASP:H    | 2:D:230:GLU:HG3  | 1.75                     | 0.51              |
| 1:E:815:PHE:HZ   | 1:E:844:LEU:HB3  | 1.75                     | 0.51              |
| 1:F:921:PHE:HE2  | 1:F:970:ILE:HA   | 1.74                     | 0.51              |
| 1:A:357:MET:SD   | 1:A:358:GLU:N    | 2.84                     | 0.51              |
| 1:A:443:ALA:O    | 1:A:448:TRP:NE1  | 2.39                     | 0.51              |
| 1:A:549:GLN:C    | 1:A:552:TYR:HB2  | 2.34                     | 0.51              |
| 1:B:472:TYR:CE1  | 1:B:476:ILE:HD11 | 2.46                     | 0.51              |
| 1:E:398:LYS:HD2  | 1:E:398:LYS:H    | 1.76                     | 0.51              |
| 1:E:411:SER:O    | 1:E:415:HIS:ND1  | 2.41                     | 0.51              |
| 1:E:479:TYR:CD2  | 1:E:524:ILE:HG12 | 2.44                     | 0.51              |
| 1:F:201:SER:O    | 1:F:204:MET:HE3  | 2.10                     | 0.51              |
| 2:H:35:ALA:HB3   | 2:H:58:GLU:HB3   | 1.91                     | 0.51              |
| 1:A:549:GLN:HG3  | 1:B:549:GLN:HE22 | 1.76                     | 0.51              |
| 1:B:48:ALA:HA    | 1:B:133:ASN:HD22 | 1.74                     | 0.51              |
| 1:B:135:ASP:HA   | 1:B:174:PHE:HE2  | 1.74                     | 0.51              |
| 1:B:472:TYR:HA   | 1:B:475:GLN:HE21 | 1.75                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:612:ILE:HG22 | 1:B:659:PHE:HE1  | 1.76                     | 0.51              |
| 2:D:1:MET:N      | 2:D:1:MET:HE2    | 2.25                     | 0.51              |
| 1:E:770:SER:O    | 1:E:773:SER:OG   | 2.26                     | 0.51              |
| 1:A:601:TRP:O    | 1:A:604:SER:OG   | 2.28                     | 0.51              |
| 1:E:403:LEU:O    | 2:G:6:GLN:NE2    | 2.44                     | 0.51              |
| 1:E:456:SER:O    | 1:E:460:LEU:HD23 | 2.10                     | 0.51              |
| 1:E:556:VAL:HG11 | 1:F:552:TYR:HE2  | 1.74                     | 0.51              |
| 1:E:633:GLU:C    | 1:E:635:GLY:N    | 2.65                     | 0.51              |
| 1:F:331:LYS:NZ   | 1:F:337:ASP:H    | 2.08                     | 0.51              |
| 1:F:438:LYS:O    | 1:F:442:LEU:HG   | 2.11                     | 0.51              |
| 1:F:657:ARG:HA   | 1:F:715:GLU:CD   | 2.35                     | 0.51              |
| 1:F:861:ASN:C    | 1:F:863:ASN:N    | 2.68                     | 0.51              |
| 2:G:72:TRP:O     | 2:G:76:THR:CB    | 2.57                     | 0.51              |
| 1:A:117:ILE:HG13 | 1:A:120:LYS:HZ3  | 1.75                     | 0.51              |
| 1:A:528:PHE:CE2  | 1:A:542:LEU:O    | 2.62                     | 0.51              |
| 1:B:64:ASP:O     | 1:B:68:GLU:HG2   | 2.10                     | 0.51              |
| 1:B:66:TYR:CE1   | 1:B:103:ILE:HG21 | 2.46                     | 0.51              |
| 1:B:802:ARG:HB3  | 1:B:840:LYS:HB3  | 1.93                     | 0.51              |
| 1:B:985:LYS:HA   | 1:B:988:VAL:HG22 | 1.92                     | 0.51              |
| 1:F:202:ASN:HA   | 1:F:205:LYS:HZ2  | 1.75                     | 0.51              |
| 1:A:250:PRO:HB3  | 1:A:279:GLU:HA   | 1.91                     | 0.51              |
| 1:A:620:ILE:HG13 | 1:A:667:LEU:HD21 | 1.93                     | 0.51              |
| 1:A:986:GLU:OE2  | 1:A:990:ASN:ND2  | 2.42                     | 0.51              |
| 1:B:614:ASN:O    | 1:B:618:LEU:HD22 | 2.11                     | 0.51              |
| 1:E:202:ASN:CG   | 1:F:205:LYS:HE2  | 2.36                     | 0.51              |
| 1:B:90:ILE:HG12  | 1:F:260:TYR:CD2  | 2.45                     | 0.51              |
| 1:B:919:TRP:HZ3  | 2:C:50:LEU:HG    | 1.75                     | 0.51              |
| 1:E:155:GLU:HG2  | 1:E:197:TYR:HD1  | 1.75                     | 0.51              |
| 1:E:396:MET:HE1  | 1:E:398:LYS:HZ2  | 1.74                     | 0.51              |
| 1:F:242:LYS:HG2  | 1:F:267:ARG:CZ   | 2.40                     | 0.51              |
| 1:F:457:ASN:O    | 1:F:460:LEU:HG   | 2.11                     | 0.51              |
| 1:F:610:GLN:HA   | 1:F:613:ARG:NH2  | 2.26                     | 0.51              |
| 1:A:241:HIS:NE2  | 1:B:159:ALA:HB1  | 2.26                     | 0.51              |
| 1:A:803:ASP:OD1  | 1:A:803:ASP:N    | 2.41                     | 0.51              |
| 1:B:255:ASN:HA   | 1:B:258:LEU:HG   | 1.93                     | 0.51              |
| 1:E:174:PHE:HB3  | 1:E:178:PHE:CE1  | 2.46                     | 0.51              |
| 1:E:333:VAL:HG23 | 1:E:541:ILE:HG13 | 1.92                     | 0.51              |
| 1:E:422:LYS:HE2  | 1:E:422:LYS:HA   | 1.93                     | 0.51              |
| 1:E:436:TYR:OH   | 1:E:599:CYS:O    | 2.29                     | 0.51              |
| 1:E:834:GLN:O    | 1:E:838:LEU:N    | 2.40                     | 0.51              |
| 1:F:129:VAL:HB   | 1:F:167:LEU:HG   | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:254:GLU:O    | 1:F:257:THR:OG1  | 2.27                     | 0.51              |
| 1:F:477:ASN:O    | 1:F:481:ILE:HG22 | 2.10                     | 0.51              |
| 2:G:189:SER:CB   | 2:G:238:SER:HB3  | 2.40                     | 0.51              |
| 1:A:436:TYR:OH   | 1:A:598:ASN:O    | 2.18                     | 0.51              |
| 1:A:459:ILE:HG13 | 1:A:471:TYR:CE2  | 2.46                     | 0.51              |
| 1:B:491:GLN:O    | 1:B:495:LEU:HB2  | 2.10                     | 0.51              |
| 2:D:176:ARG:NH1  | 2:D:178:ILE:HG13 | 2.26                     | 0.51              |
| 1:E:487:GLN:HE22 | 2:H:207:SER:N    | 2.06                     | 0.51              |
| 1:E:497:LEU:HB3  | 1:E:503:HIS:ND1  | 2.25                     | 0.51              |
| 1:F:66:TYR:HB3   | 1:F:87:ILE:HG12  | 1.93                     | 0.51              |
| 1:F:98:MET:HA    | 1:F:98:MET:HE3   | 1.93                     | 0.51              |
| 2:H:23:PHE:O     | 2:H:69:ASP:HB2   | 2.11                     | 0.51              |
| 1:A:337:ASP:O    | 1:A:350:LYS:N    | 2.39                     | 0.50              |
| 1:A:449:GLU:N    | 1:A:449:GLU:OE1  | 2.44                     | 0.50              |
| 1:A:606:HIS:NE2  | 2:D:206:MET:HB3  | 2.25                     | 0.50              |
| 1:A:767:LEU:N    | 1:A:768:PRO:HD3  | 2.26                     | 0.50              |
| 1:B:115:ASN:OD1  | 1:B:118:HIS:NE2  | 2.45                     | 0.50              |
| 1:B:203:LEU:O    | 1:B:207:ILE:HG22 | 2.11                     | 0.50              |
| 1:B:469:CYS:HB3  | 1:B:539:TYR:CZ   | 2.46                     | 0.50              |
| 1:E:128:HIS:HD1  | 1:E:166:TYR:H    | 1.59                     | 0.50              |
| 1:E:475:GLN:CD   | 1:E:478:ARG:HH22 | 2.18                     | 0.50              |
| 1:E:780:VAL:HG21 | 1:E:819:ARG:HH12 | 1.76                     | 0.50              |
| 1:E:866:MET:HE2  | 1:E:866:MET:N    | 2.27                     | 0.50              |
| 1:F:396:MET:SD   | 1:F:397:ALA:N    | 2.85                     | 0.50              |
| 1:F:906:THR:HG22 | 2:G:234:VAL:H    | 1.76                     | 0.50              |
| 2:H:175:TYR:HB2  | 2:H:193:ILE:HB   | 1.93                     | 0.50              |
| 2:H:219:LYS:HD2  | 2:H:220:PHE:N    | 2.26                     | 0.50              |
| 1:A:118:HIS:HE1  | 1:A:137:LEU:C    | 2.20                     | 0.50              |
| 1:A:332:HIS:CE1  | 1:A:540:LYS:HD2  | 2.46                     | 0.50              |
| 1:A:593:ARG:O    | 1:A:597:GLU:HG3  | 2.11                     | 0.50              |
| 1:B:720:LEU:HD13 | 1:B:740:LEU:HD12 | 1.92                     | 0.50              |
| 1:F:712:PHE:O    | 1:F:713:ILE:C    | 2.50                     | 0.50              |
| 1:F:720:LEU:HD22 | 1:F:736:ILE:HD13 | 1.93                     | 0.50              |
| 1:F:905:GLN:H    | 2:G:234:VAL:HG12 | 1.76                     | 0.50              |
| 1:B:475:GLN:HG3  | 1:B:478:ARG:NH1  | 2.27                     | 0.50              |
| 1:B:491:GLN:NE2  | 2:C:206:MET:HG2  | 2.26                     | 0.50              |
| 1:E:162:THR:O    | 1:F:533:PHE:HE2  | 1.95                     | 0.50              |
| 1:E:339:HIS:N    | 1:E:347:VAL:O    | 2.34                     | 0.50              |
| 1:E:946:PRO:HG2  | 1:E:975:HIS:NE2  | 2.27                     | 0.50              |
| 2:G:13:PHE:HD1   | 2:G:173:VAL:HG22 | 1.76                     | 0.50              |
| 1:A:750:ASP:CG   | 1:A:751:ILE:H    | 2.19                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:326:ARG:HG2  | 1:E:329:ASP:OD2  | 2.11                     | 0.50              |
| 1:E:479:TYR:CZ   | 1:E:524:ILE:HG21 | 2.47                     | 0.50              |
| 1:F:30:ILE:HD11  | 1:F:292:LEU:HD11 | 1.92                     | 0.50              |
| 1:A:840:LYS:HA   | 1:A:871:ILE:HG21 | 1.93                     | 0.50              |
| 1:B:277:SER:HB2  | 1:B:281:ASP:OD2  | 2.11                     | 0.50              |
| 1:E:205:LYS:NZ   | 1:F:199:LEU:HD23 | 2.26                     | 0.50              |
| 1:E:635:GLY:HA2  | 1:E:638:PHE:CE2  | 2.46                     | 0.50              |
| 1:F:71:TYR:HE1   | 1:F:86:ARG:HH21  | 1.58                     | 0.50              |
| 1:F:101:ASP:HA   | 1:F:104:LEU:HG   | 1.93                     | 0.50              |
| 1:A:692:ALA:O    | 1:A:695:ILE:HG12 | 2.12                     | 0.50              |
| 1:B:23:ASP:O     | 1:B:27:VAL:HG12  | 2.12                     | 0.50              |
| 1:B:135:ASP:HA   | 1:B:174:PHE:CE2  | 2.47                     | 0.50              |
| 1:F:109:GLN:OE1  | 1:F:109:GLN:N    | 2.36                     | 0.50              |
| 1:F:692:ALA:O    | 1:F:696:THR:HG23 | 2.11                     | 0.50              |
| 2:H:64:LYS:HA    | 2:H:217:GLU:HA   | 1.92                     | 0.50              |
| 1:E:633:GLU:C    | 1:E:635:GLY:H    | 2.18                     | 0.50              |
| 1:E:634:LEU:HG   | 1:F:905:GLN:OE1  | 2.12                     | 0.50              |
| 1:F:472:TYR:HB2  | 1:F:535:PHE:CE2  | 2.46                     | 0.50              |
| 1:F:724:LYS:HG2  | 1:F:760:ARG:HG3  | 1.94                     | 0.50              |
| 1:F:861:ASN:CG   | 1:F:863:ASN:H    | 2.20                     | 0.50              |
| 2:G:188:TYR:O    | 2:G:238:SER:HA   | 2.11                     | 0.50              |
| 1:A:566:ARG:HA   | 1:A:569:MET:HG3  | 1.93                     | 0.50              |
| 1:A:885:ILE:HG12 | 1:A:916:PHE:HE1  | 1.77                     | 0.50              |
| 1:B:59:TRP:HE3   | 1:B:62:LEU:HD12  | 1.77                     | 0.50              |
| 1:E:59:TRP:CD1   | 1:E:62:LEU:HD23  | 2.46                     | 0.50              |
| 1:E:148:TYR:CE2  | 1:E:163:SER:HB3  | 2.47                     | 0.50              |
| 1:E:154:ALA:N    | 1:E:157:ASP:OD2  | 2.24                     | 0.50              |
| 1:E:227:MET:O    | 1:E:227:MET:HE3  | 2.11                     | 0.50              |
| 1:E:576:PHE:HB2  | 2:G:30:ALA:HB3   | 1.94                     | 0.50              |
| 1:F:905:GLN:H    | 2:G:234:VAL:CG1  | 2.24                     | 0.50              |
| 1:A:86:ARG:HH22  | 1:A:90:ILE:HD11  | 1.77                     | 0.50              |
| 1:A:215:PHE:CE1  | 1:A:243:PRO:HB2  | 2.47                     | 0.50              |
| 1:A:487:GLN:O    | 1:A:491:GLN:NE2  | 2.44                     | 0.50              |
| 1:A:501:GLY:HA3  | 1:A:747:ARG:NH2  | 2.27                     | 0.50              |
| 1:A:717:LYS:HZ2  | 1:A:749:LEU:HB3  | 1.76                     | 0.50              |
| 1:B:607:GLU:HG3  | 1:B:608:PHE:HD1  | 1.77                     | 0.50              |
| 1:F:649:TYR:HE1  | 1:F:687:TYR:HB2  | 1.77                     | 0.50              |
| 1:F:930:MET:HE3  | 1:F:930:MET:H    | 1.77                     | 0.50              |
| 1:B:44:PHE:CE2   | 1:B:126:PRO:HB3  | 2.47                     | 0.49              |
| 1:B:472:TYR:O    | 1:B:476:ILE:HG12 | 2.12                     | 0.49              |
| 1:B:557:LYS:HG3  | 1:B:587:ARG:HH12 | 1.77                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:729:SER:HB3  | 1:B:731:GLU:OE1   | 2.12                     | 0.49              |
| 1:E:482:TYR:C    | 1:E:482:TYR:CD1   | 2.90                     | 0.49              |
| 1:E:635:GLY:O    | 1:E:638:PHE:N     | 2.45                     | 0.49              |
| 1:A:332:HIS:NE2  | 1:A:540:LYS:HB3   | 2.27                     | 0.49              |
| 1:B:286:TYR:HA   | 1:B:289:VAL:HG12  | 1.93                     | 0.49              |
| 1:B:661:ILE:HG13 | 1:B:663:ASP:N     | 2.23                     | 0.49              |
| 1:E:417:LYS:HD3  | 1:E:420:VAL:HG22  | 1.95                     | 0.49              |
| 1:F:128:HIS:CE1  | 1:F:165:ARG:HA    | 2.48                     | 0.49              |
| 1:F:967:LEU:HA   | 1:F:970:ILE:HB    | 1.94                     | 0.49              |
| 1:A:566:ARG:O    | 1:A:569:MET:HG3   | 2.12                     | 0.49              |
| 1:B:94:VAL:HG21  | 1:F:256:GLU:HB2   | 1.93                     | 0.49              |
| 1:E:569:MET:HE2  | 1:E:569:MET:HA    | 1.95                     | 0.49              |
| 1:E:850:LYS:O    | 1:E:854:LEU:HG    | 2.11                     | 0.49              |
| 1:F:130:ILE:HD12 | 1:F:168:LEU:O     | 2.12                     | 0.49              |
| 1:F:409:ILE:HG13 | 1:F:650:TYR:CZ    | 2.46                     | 0.49              |
| 1:F:738:LYS:O    | 1:F:742:PHE:HB2   | 2.12                     | 0.49              |
| 1:F:801:SER:O    | 1:F:840:LYS:CE    | 2.55                     | 0.49              |
| 1:F:831:LYS:HB3  | 1:F:833:LYS:HG2   | 1.93                     | 0.49              |
| 2:G:198:VAL:HG22 | 2:G:222:ALA:HA    | 1.93                     | 0.49              |
| 1:A:713:ILE:CG2  | 1:A:717:LYS:H     | 2.26                     | 0.49              |
| 1:B:688:LEU:HD23 | 1:B:732:GLY:CA    | 2.42                     | 0.49              |
| 1:E:744:PHE:HD1  | 1:E:745:PRO:HD2   | 1.77                     | 0.49              |
| 1:E:815:PHE:HE2  | 1:E:844:LEU:HA    | 1.77                     | 0.49              |
| 1:E:936:MET:SD   | 1:E:936:MET:N     | 2.77                     | 0.49              |
| 1:E:1004:PHE:HB2 | 1:E:1005:ILE:HD12 | 1.93                     | 0.49              |
| 1:F:696:THR:O    | 1:F:700:SER:HB3   | 2.11                     | 0.49              |
| 1:F:768:PRO:O    | 1:F:772:ILE:HG12  | 2.12                     | 0.49              |
| 1:F:987:ARG:HA   | 1:F:987:ARG:NE    | 2.27                     | 0.49              |
| 2:G:28:GLN:HB3   | 2:G:64:LYS:CD     | 2.38                     | 0.49              |
| 1:B:134:TYR:CE2  | 1:B:171:ALA:HB1   | 2.48                     | 0.49              |
| 1:E:488:ALA:HA   | 1:E:491:GLN:NE2   | 2.27                     | 0.49              |
| 1:E:786:HIS:CD2  | 1:E:791:TYR:HB3   | 2.47                     | 0.49              |
| 1:F:56:TYR:CD1   | 1:F:57:PRO:HD2    | 2.47                     | 0.49              |
| 1:F:331:LYS:HD2  | 1:F:336:TYR:HA    | 1.93                     | 0.49              |
| 1:F:533:PHE:O    | 1:F:537:LYS:HE2   | 2.13                     | 0.49              |
| 2:H:14:LYS:NZ    | 2:H:21:LEU:HA     | 2.27                     | 0.49              |
| 1:B:558:LEU:HD11 | 1:B:614:ASN:HB2   | 1.95                     | 0.49              |
| 1:F:376:LYS:NZ   | 1:F:379:GLU:OE2   | 2.41                     | 0.49              |
| 1:F:418:TYR:O    | 1:F:421:MET:HG3   | 2.12                     | 0.49              |
| 2:H:229:ASP:O    | 2:H:230:GLU:HB2   | 2.11                     | 0.49              |
| 1:A:472:TYR:O    | 1:A:476:ILE:HG22  | 2.11                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:990:ASN:HB3  | 1:B:992:ASN:ND2  | 2.28                     | 0.49              |
| 2:C:10:ASP:HB2   | 2:C:176:ARG:HB3  | 1.94                     | 0.49              |
| 2:C:70:LEU:HD13  | 2:C:74:ALA:HB2   | 1.95                     | 0.49              |
| 1:E:547:ASP:OD1  | 1:E:547:ASP:N    | 2.41                     | 0.49              |
| 1:F:246:ILE:HG22 | 1:F:247:ARG:H    | 1.77                     | 0.49              |
| 1:F:404:ASN:HA   | 2:H:4:VAL:O      | 2.13                     | 0.49              |
| 1:F:769:LYS:HD2  | 1:F:769:LYS:O    | 2.12                     | 0.49              |
| 2:H:192:TYR:HD2  | 2:H:235:ILE:HB   | 1.78                     | 0.49              |
| 1:A:313:TYR:HA   | 1:A:380:ARG:HH21 | 1.77                     | 0.49              |
| 1:A:614:ASN:O    | 1:A:618:LEU:HB2  | 2.12                     | 0.49              |
| 1:A:839:PHE:HA   | 1:A:853:LEU:HD21 | 1.94                     | 0.49              |
| 1:B:639:PHE:C    | 1:B:641:LYS:H    | 2.21                     | 0.49              |
| 1:B:649:TYR:CD1  | 1:B:684:ILE:HG12 | 2.48                     | 0.49              |
| 2:C:69:ASP:HB2   | 2:C:72:TRP:CD1   | 2.48                     | 0.49              |
| 2:D:41:LEU:HD12  | 2:D:42:ARG:HG3   | 1.95                     | 0.49              |
| 1:E:406:SER:HB2  | 2:G:2:LYS:HB2    | 1.95                     | 0.49              |
| 1:F:388:PHE:CD1  | 1:F:393:VAL:HG13 | 2.47                     | 0.49              |
| 2:H:228:THR:HG22 | 2:H:229:ASP:CG   | 2.38                     | 0.49              |
| 1:A:516:GLU:O    | 1:A:519:MET:HE3  | 2.13                     | 0.49              |
| 1:B:453:ASP:O    | 1:B:456:SER:OG   | 2.19                     | 0.49              |
| 1:E:89:GLN:HE22  | 1:E:188:ASP:H    | 1.60                     | 0.49              |
| 1:E:706:VAL:CA   | 1:E:709:TYR:HB3  | 2.42                     | 0.49              |
| 1:E:832:GLN:HA   | 1:E:835:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:408:GLU:HA   | 1:A:650:TYR:OH   | 2.13                     | 0.49              |
| 1:A:607:GLU:OE1  | 1:A:610:GLN:HG2  | 2.12                     | 0.49              |
| 1:B:299:ASN:OD1  | 1:B:299:ASN:N    | 2.42                     | 0.49              |
| 1:B:631:ILE:HG21 | 1:B:636:PHE:HB3  | 1.95                     | 0.49              |
| 2:D:208:LEU:HD11 | 2:D:212:ASN:HB3  | 1.95                     | 0.49              |
| 1:E:286:TYR:O    | 1:E:290:MET:HG2  | 2.13                     | 0.49              |
| 1:E:349:HIS:HE1  | 2:G:213:ALA:HA   | 1.77                     | 0.49              |
| 1:E:396:MET:SD   | 1:E:398:LYS:N    | 2.85                     | 0.49              |
| 1:E:803:ASP:HA   | 1:E:806:ALA:HB3  | 1.94                     | 0.49              |
| 1:F:639:PHE:O    | 1:F:641:LYS:N    | 2.42                     | 0.49              |
| 1:F:955:ILE:HG21 | 1:F:958:TRP:CE2  | 2.47                     | 0.49              |
| 2:H:69:ASP:O     | 2:H:70:LEU:HB2   | 2.12                     | 0.49              |
| 1:A:180:GLY:HA2  | 1:A:183:VAL:HG12 | 1.95                     | 0.48              |
| 1:A:218:TYR:OH   | 1:A:224:ASN:N    | 2.34                     | 0.48              |
| 1:A:357:MET:H    | 1:A:357:MET:CE   | 2.21                     | 0.48              |
| 1:A:655:ILE:HD12 | 1:A:659:PHE:CZ   | 2.47                     | 0.48              |
| 1:A:751:ILE:O    | 1:A:752:GLY:C    | 2.53                     | 0.48              |
| 1:A:899:GLU:O    | 1:A:903:GLY:N    | 2.46                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:551:LEU:HD11 | 1:E:608:PHE:HD1  | 1.78                     | 0.48              |
| 1:E:705:ASN:O    | 1:E:708:PHE:N    | 2.45                     | 0.48              |
| 1:F:821:SER:O    | 1:F:824:THR:OG1  | 2.27                     | 0.48              |
| 1:A:433:GLU:O    | 1:A:437:LYS:HG2  | 2.13                     | 0.48              |
| 1:B:231:TRP:HA   | 1:B:234:LYS:HD3  | 1.95                     | 0.48              |
| 2:C:171:TYR:O    | 2:C:198:VAL:O    | 2.30                     | 0.48              |
| 1:E:190:TYR:HA   | 1:E:193:TYR:HB2  | 1.94                     | 0.48              |
| 1:E:629:ARG:CG   | 1:E:630:ASP:O    | 2.61                     | 0.48              |
| 1:E:750:ASP:O    | 1:E:753:LYS:HG2  | 2.13                     | 0.48              |
| 1:E:906:THR:HG22 | 2:H:233:VAL:HG13 | 1.94                     | 0.48              |
| 2:G:14:LYS:CA    | 2:G:20:LYS:HE3   | 2.43                     | 0.48              |
| 2:G:190:ASP:H    | 2:G:237:ALA:HB3  | 1.78                     | 0.48              |
| 1:A:43:VAL:HG13  | 1:A:213:ILE:HD13 | 1.95                     | 0.48              |
| 1:A:310:ASP:HA   | 1:A:313:TYR:HB3  | 1.94                     | 0.48              |
| 1:A:615:SER:HA   | 1:A:618:LEU:HB2  | 1.96                     | 0.48              |
| 1:B:44:PHE:CD2   | 1:B:126:PRO:HB3  | 2.49                     | 0.48              |
| 1:B:553:ASP:OD1  | 1:B:553:ASP:N    | 2.47                     | 0.48              |
| 1:F:724:LYS:HD2  | 1:F:725:TYR:CD1  | 2.48                     | 0.48              |
| 2:G:192:TYR:HD2  | 2:G:235:ILE:HG21 | 1.78                     | 0.48              |
| 2:H:16:LYS:HE2   | 2:H:170:ARG:HH21 | 1.78                     | 0.48              |
| 1:A:277:SER:HB3  | 1:A:285:ARG:NH2  | 2.28                     | 0.48              |
| 1:A:419:ASP:N    | 1:A:419:ASP:OD1  | 2.45                     | 0.48              |
| 1:B:242:LYS:HB2  | 1:B:267:ARG:NH2  | 2.28                     | 0.48              |
| 1:E:1000:LEU:HA  | 1:E:1004:PHE:HE2 | 1.79                     | 0.48              |
| 1:F:449:GLU:HG3  | 1:F:450:GLU:OE1  | 2.13                     | 0.48              |
| 1:F:579:SER:HB3  | 1:F:582:ILE:HG12 | 1.94                     | 0.48              |
| 1:A:163:SER:HA   | 1:B:533:PHE:CE1  | 2.48                     | 0.48              |
| 1:A:204:MET:HE1  | 1:A:228:LEU:HD13 | 1.94                     | 0.48              |
| 1:A:205:LYS:CB   | 1:B:202:ASN:HD21 | 2.27                     | 0.48              |
| 1:A:444:CYS:HA   | 1:A:601:TRP:HZ3  | 1.77                     | 0.48              |
| 1:A:456:SER:HA   | 1:A:459:ILE:HG22 | 1.96                     | 0.48              |
| 1:A:693:GLU:O    | 1:A:696:THR:OG1  | 2.24                     | 0.48              |
| 1:B:111:ASP:OD1  | 1:B:111:ASP:N    | 2.46                     | 0.48              |
| 1:B:129:VAL:HB   | 1:B:167:LEU:HD13 | 1.95                     | 0.48              |
| 1:B:632:ASP:OD1  | 1:B:632:ASP:N    | 2.40                     | 0.48              |
| 1:E:481:ILE:O    | 1:E:484:SER:OG   | 2.21                     | 0.48              |
| 1:E:630:ASP:HB3  | 1:F:956:PRO:HG3  | 1.95                     | 0.48              |
| 1:A:733:LEU:O    | 1:A:736:ILE:HG22 | 2.13                     | 0.48              |
| 1:A:787:ILE:HG22 | 1:A:788:ASP:H    | 1.78                     | 0.48              |
| 1:E:163:SER:HA   | 1:F:533:PHE:CE2  | 2.49                     | 0.48              |
| 1:E:767:LEU:HD12 | 1:E:811:PHE:HD2  | 1.78                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:79:TYR:HB3   | 1:F:84:TYR:CG    | 2.48                     | 0.48              |
| 1:F:188:ASP:O    | 1:F:192:ASN:N    | 2.47                     | 0.48              |
| 1:F:744:PHE:HB3  | 1:F:749:LEU:HD23 | 1.95                     | 0.48              |
| 2:G:14:LYS:HG2   | 2:G:172:GLU:O    | 2.13                     | 0.48              |
| 1:A:131:THR:HG22 | 1:A:133:ASN:H    | 1.79                     | 0.48              |
| 1:A:512:LEU:HD13 | 1:A:515:ILE:HD11 | 1.95                     | 0.48              |
| 1:A:688:LEU:O    | 1:A:691:ILE:HG13 | 2.14                     | 0.48              |
| 1:E:186:LYS:HE3  | 1:E:186:LYS:HB3  | 1.67                     | 0.48              |
| 1:E:254:GLU:H    | 1:E:254:GLU:CD   | 2.21                     | 0.48              |
| 1:E:458:ILE:O    | 1:E:462:SER:OG   | 2.24                     | 0.48              |
| 1:E:544:PHE:CE2  | 1:E:550:PHE:HB2  | 2.48                     | 0.48              |
| 1:E:729:SER:O    | 1:E:733:LEU:N    | 2.36                     | 0.48              |
| 1:F:657:ARG:HG2  | 1:F:715:GLU:CD   | 2.39                     | 0.48              |
| 1:F:913:MET:H    | 1:F:913:MET:CE   | 2.24                     | 0.48              |
| 1:F:982:GLU:O    | 1:F:985:LYS:HB2  | 2.13                     | 0.48              |
| 1:A:86:ARG:NH2   | 1:E:260:TYR:CZ   | 2.82                     | 0.48              |
| 1:A:131:THR:HB   | 1:A:169:LYS:HA   | 1.96                     | 0.48              |
| 1:A:481:ILE:O    | 1:A:484:SER:OG   | 2.25                     | 0.48              |
| 1:A:548:ASN:HD22 | 2:D:209:GLU:CB   | 2.26                     | 0.48              |
| 1:B:130:ILE:HD11 | 1:B:170:VAL:HG22 | 1.95                     | 0.48              |
| 2:D:206:MET:N    | 2:D:206:MET:SD   | 2.86                     | 0.48              |
| 1:E:334:PHE:O    | 1:E:335:GLU:HG3  | 2.14                     | 0.48              |
| 1:E:428:GLN:NE2  | 1:E:429:SER:O    | 2.46                     | 0.48              |
| 1:E:493:ASN:HA   | 1:E:503:HIS:CE1  | 2.44                     | 0.48              |
| 1:E:839:PHE:HA   | 1:E:842:LEU:HB2  | 1.95                     | 0.48              |
| 1:F:331:LYS:O    | 1:F:331:LYS:HD3  | 2.14                     | 0.48              |
| 1:F:511:PHE:O    | 1:F:515:ILE:HG12 | 2.14                     | 0.48              |
| 2:H:20:LYS:HE2   | 2:H:71:GLU:OE2   | 2.13                     | 0.48              |
| 2:H:172:GLU:HB3  | 2:H:196:PRO:O    | 2.14                     | 0.48              |
| 1:B:688:LEU:HD23 | 1:B:732:GLY:HA2  | 1.96                     | 0.48              |
| 1:F:848:ASN:O    | 1:F:852:HIS:ND1  | 2.45                     | 0.48              |
| 1:F:957:SER:O    | 1:F:959:LEU:N    | 2.47                     | 0.48              |
| 1:B:28:GLU:O     | 1:B:32:GLU:HG2   | 2.13                     | 0.48              |
| 1:B:66:TYR:HE1   | 1:B:103:ILE:HG21 | 1.77                     | 0.48              |
| 1:B:249:ASP:OD2  | 1:B:251:SER:OG   | 2.24                     | 0.48              |
| 1:B:417:LYS:C    | 1:B:421:MET:HE3  | 2.38                     | 0.48              |
| 1:B:588:LEU:HD12 | 1:B:588:LEU:HA   | 1.58                     | 0.48              |
| 1:B:616:MET:HB2  | 1:B:659:PHE:HZ   | 1.79                     | 0.48              |
| 1:E:326:ARG:HD2  | 1:E:328:ILE:HD11 | 1.96                     | 0.48              |
| 1:E:330:LEU:HB3  | 1:E:340:PHE:HE2  | 1.79                     | 0.48              |
| 1:E:791:TYR:O    | 1:E:833:LYS:NZ   | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:966:LEU:HD12 | 2:G:51:TYR:HB3   | 1.96                     | 0.48              |
| 1:A:46:VAL:HG12  | 1:A:130:ILE:O    | 2.14                     | 0.47              |
| 1:A:904:ILE:HG12 | 2:D:235:ILE:HG23 | 1.96                     | 0.47              |
| 1:B:222:ASP:OD1  | 1:B:225:ILE:HG23 | 2.14                     | 0.47              |
| 1:B:245:PHE:O    | 1:B:269:ILE:HD12 | 2.13                     | 0.47              |
| 1:B:522:PHE:CD1  | 1:B:522:PHE:C    | 2.92                     | 0.47              |
| 1:B:675:LYS:HD3  | 1:B:675:LYS:HA   | 1.36                     | 0.47              |
| 1:B:741:LEU:HD22 | 1:B:778:PHE:CG   | 2.49                     | 0.47              |
| 1:B:982:GLU:O    | 1:B:985:LYS:HG3  | 2.13                     | 0.47              |
| 1:E:711:GLN:O    | 1:E:712:PHE:HD1  | 1.96                     | 0.47              |
| 1:E:1002:ASN:O   | 1:E:1003:TYR:C   | 2.57                     | 0.47              |
| 1:F:336:TYR:O    | 1:F:350:LYS:HE2  | 2.14                     | 0.47              |
| 1:F:820:LEU:HA   | 1:F:823:ILE:HG12 | 1.96                     | 0.47              |
| 2:G:38:GLU:CA    | 2:G:54:LYS:HZ1   | 2.27                     | 0.47              |
| 2:H:23:PHE:HE1   | 2:H:66:ALA:CB    | 2.23                     | 0.47              |
| 2:H:52:ILE:HG13  | 2:H:53:LEU:H     | 1.79                     | 0.47              |
| 1:A:370:ARG:HD3  | 1:A:381:PHE:CZ   | 2.49                     | 0.47              |
| 1:B:83:GLU:HA    | 1:B:86:ARG:HG2   | 1.96                     | 0.47              |
| 1:B:114:THR:HB   | 1:B:118:HIS:HD2  | 1.79                     | 0.47              |
| 1:B:377:GLN:O    | 1:B:380:ARG:HG2  | 2.14                     | 0.47              |
| 1:B:626:GLU:HA   | 1:B:629:ARG:NE   | 2.27                     | 0.47              |
| 1:E:59:TRP:CZ2   | 1:E:185:LEU:HG   | 2.49                     | 0.47              |
| 1:F:134:TYR:CZ   | 1:F:183:VAL:HB   | 2.49                     | 0.47              |
| 1:F:284:GLU:O    | 1:F:287:SER:OG   | 2.29                     | 0.47              |
| 1:F:290:MET:O    | 1:F:294:ILE:HG13 | 2.13                     | 0.47              |
| 1:F:906:THR:HB   | 2:G:233:VAL:CA   | 2.44                     | 0.47              |
| 2:H:10:ASP:OD2   | 2:H:12:TYR:OH    | 2.30                     | 0.47              |
| 1:A:206:THR:HG22 | 1:B:203:LEU:HD22 | 1.96                     | 0.47              |
| 1:A:270:ASP:HB3  | 1:A:273:SER:HB3  | 1.95                     | 0.47              |
| 1:A:736:ILE:HG21 | 1:A:761:LEU:CD2  | 2.44                     | 0.47              |
| 1:A:862:ILE:HD12 | 1:A:866:MET:HE3  | 1.96                     | 0.47              |
| 1:B:257:THR:O    | 1:B:261:TYR:HD1  | 1.97                     | 0.47              |
| 1:E:655:ILE:HG23 | 1:E:659:PHE:CE2  | 2.49                     | 0.47              |
| 1:E:861:ASN:C    | 1:E:861:ASN:OD1  | 2.56                     | 0.47              |
| 1:E:861:ASN:ND2  | 1:E:864:ASP:OD2  | 2.46                     | 0.47              |
| 1:F:527:LEU:HD12 | 1:F:531:MET:HE3  | 1.94                     | 0.47              |
| 1:B:578:MET:CA   | 1:B:582:ILE:HG13 | 2.44                     | 0.47              |
| 1:B:675:LYS:C    | 1:B:676:ILE:HG12 | 2.39                     | 0.47              |
| 1:E:215:PHE:HE2  | 1:E:243:PRO:HB2  | 1.80                     | 0.47              |
| 1:E:927:ASN:ND2  | 1:E:929:LYS:HD3  | 2.30                     | 0.47              |
| 2:G:36:ILE:HG23  | 2:G:54:LYS:HE2   | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:36:ILE:HA    | 2:H:56:GLU:O     | 2.14                     | 0.47              |
| 1:A:186:LYS:O    | 1:A:189:ASP:HB2  | 2.14                     | 0.47              |
| 1:A:487:GLN:OE1  | 2:D:207:SER:N    | 2.47                     | 0.47              |
| 1:A:606:HIS:CD2  | 2:D:206:MET:HB3  | 2.49                     | 0.47              |
| 1:B:205:LYS:HZ2  | 1:B:232:VAL:HG22 | 1.79                     | 0.47              |
| 1:B:205:LYS:O    | 1:B:208:ILE:HG22 | 2.15                     | 0.47              |
| 1:B:260:TYR:HA   | 1:B:263:ASN:HD21 | 1.79                     | 0.47              |
| 1:B:322:LEU:HD21 | 1:B:542:LEU:HD22 | 1.95                     | 0.47              |
| 1:B:367:CYS:SG   | 1:B:370:ARG:NH2  | 2.88                     | 0.47              |
| 1:B:455:TYR:O    | 1:B:458:ILE:HG22 | 2.13                     | 0.47              |
| 1:B:569:MET:HE3  | 1:B:570:SER:N    | 2.23                     | 0.47              |
| 1:B:802:ARG:HD3  | 1:B:840:LYS:HD2  | 1.96                     | 0.47              |
| 1:E:242:LYS:NZ   | 1:E:243:PRO:HD2  | 2.29                     | 0.47              |
| 1:F:481:ILE:HD12 | 1:F:484:SER:OG   | 2.14                     | 0.47              |
| 2:G:15:ARG:H     | 2:G:20:LYS:CB    | 2.27                     | 0.47              |
| 2:H:64:LYS:CG    | 2:H:217:GLU:HB3  | 2.39                     | 0.47              |
| 1:A:30:ILE:O     | 1:A:34:THR:HG23  | 2.15                     | 0.47              |
| 1:A:206:THR:HG21 | 1:B:206:THR:OG1  | 2.15                     | 0.47              |
| 1:A:345:THR:HB   | 1:A:397:ALA:N    | 2.29                     | 0.47              |
| 1:A:488:ALA:HA   | 1:A:491:GLN:NE2  | 2.29                     | 0.47              |
| 1:B:249:ASP:CG   | 1:B:251:SER:HG   | 2.20                     | 0.47              |
| 1:B:483:GLN:OE1  | 1:B:483:GLN:HA   | 2.15                     | 0.47              |
| 1:E:207:ILE:HG22 | 1:E:213:ILE:HD11 | 1.96                     | 0.47              |
| 2:H:63:VAL:HG22  | 2:H:220:PHE:CZ   | 2.49                     | 0.47              |
| 1:A:85:LEU:O     | 1:A:187:GLU:HG2  | 2.15                     | 0.47              |
| 1:A:247:ARG:HH12 | 1:A:249:ASP:N    | 2.13                     | 0.47              |
| 1:A:337:ASP:HA   | 1:A:350:LYS:HB2  | 1.97                     | 0.47              |
| 1:A:549:GLN:HA   | 1:A:552:TYR:CG   | 2.49                     | 0.47              |
| 1:B:59:TRP:CE3   | 1:B:62:LEU:HD12  | 2.50                     | 0.47              |
| 1:B:491:GLN:HE22 | 2:C:205:GLU:N    | 2.12                     | 0.47              |
| 1:E:233:ARG:HH21 | 1:E:264:LYS:C    | 2.23                     | 0.47              |
| 1:E:635:GLY:HA2  | 1:E:638:PHE:CD2  | 2.50                     | 0.47              |
| 1:E:891:THR:O    | 1:E:894:VAL:HG22 | 2.15                     | 0.47              |
| 1:F:174:PHE:HD2  | 1:F:178:PHE:HA   | 1.79                     | 0.47              |
| 1:F:244:PHE:CD1  | 1:F:267:ARG:HB2  | 2.49                     | 0.47              |
| 1:F:744:PHE:HE1  | 1:F:748:ASP:HB3  | 1.79                     | 0.47              |
| 1:F:770:SER:O    | 1:F:774:ILE:HG13 | 2.14                     | 0.47              |
| 1:F:825:LEU:HB3  | 1:F:852:HIS:NE2  | 2.29                     | 0.47              |
| 2:G:15:ARG:H     | 2:G:20:LYS:HB3   | 1.80                     | 0.47              |
| 1:A:38:ARG:NE    | 1:A:537:LYS:HD3  | 2.30                     | 0.47              |
| 1:A:220:LEU:HB3  | 1:A:223:TYR:OH   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:225:ILE:O    | 1:A:229:LEU:CB   | 2.63                     | 0.47              |
| 1:B:31:LYS:O     | 1:B:35:GLU:HG3   | 2.14                     | 0.47              |
| 1:B:114:THR:HB   | 1:B:118:HIS:CD2  | 2.50                     | 0.47              |
| 1:E:49:GLY:O     | 1:E:52:THR:OG1   | 2.24                     | 0.47              |
| 1:E:233:ARG:NE   | 1:E:264:LYS:O    | 2.37                     | 0.47              |
| 1:E:526:ASP:OD2  | 1:E:529:ASN:N    | 2.48                     | 0.47              |
| 1:E:535:PHE:CE2  | 1:E:539:TYR:HD2  | 2.32                     | 0.47              |
| 1:E:629:ARG:CG   | 1:E:631:ILE:HB   | 2.38                     | 0.47              |
| 1:E:721:TYR:HD1  | 1:E:757:TRP:CE2  | 2.32                     | 0.47              |
| 1:F:118:HIS:NE2  | 1:F:138:ILE:HD13 | 2.30                     | 0.47              |
| 1:F:565:VAL:O    | 1:F:568:GLU:HG3  | 2.15                     | 0.47              |
| 1:F:904:ILE:HG22 | 2:G:235:ILE:N    | 2.30                     | 0.47              |
| 1:A:45:PHE:CE2   | 1:A:130:ILE:HG13 | 2.50                     | 0.47              |
| 1:A:473:LEU:HA   | 1:A:476:ILE:HG22 | 1.97                     | 0.47              |
| 1:A:606:HIS:CE1  | 2:D:206:MET:HB3  | 2.50                     | 0.47              |
| 1:A:649:TYR:O    | 1:A:653:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:694:GLU:CD   | 1:A:694:GLU:H    | 2.23                     | 0.47              |
| 1:A:717:LYS:NZ   | 1:A:749:LEU:HD23 | 2.30                     | 0.47              |
| 1:A:801:SER:HB3  | 1:A:837:PHE:HE1  | 1.79                     | 0.47              |
| 1:E:111:ASP:N    | 1:E:111:ASP:OD1  | 2.42                     | 0.47              |
| 1:E:370:ARG:HH12 | 1:E:373:LEU:HD22 | 1.80                     | 0.47              |
| 1:F:312:ILE:HG13 | 1:F:313:TYR:N    | 2.30                     | 0.47              |
| 2:H:38:GLU:HA    | 2:H:54:LYS:HZ1   | 1.79                     | 0.47              |
| 1:A:235:LEU:HD13 | 1:B:195:GLN:O    | 2.14                     | 0.47              |
| 1:A:422:LYS:HA   | 1:A:422:LYS:HD2  | 1.49                     | 0.47              |
| 1:B:491:GLN:HE22 | 2:C:206:MET:H    | 1.63                     | 0.47              |
| 1:B:964:ASP:HB2  | 1:B:965:LYS:HZ3  | 1.79                     | 0.47              |
| 2:D:31:SER:O     | 2:D:61:LEU:HD12  | 2.15                     | 0.47              |
| 1:E:375:LYS:HD3  | 1:E:375:LYS:C    | 2.40                     | 0.47              |
| 1:E:681:GLN:NE2  | 1:E:682:GLU:HA   | 2.30                     | 0.47              |
| 1:E:866:MET:HA   | 1:E:869:ILE:HG12 | 1.97                     | 0.47              |
| 1:F:358:GLU:OE1  | 1:F:362:GLU:HG2  | 2.15                     | 0.47              |
| 1:F:801:SER:H    | 1:F:840:LYS:HZ1  | 1.62                     | 0.47              |
| 1:F:861:ASN:HB3  | 1:F:863:ASN:O    | 2.15                     | 0.47              |
| 1:F:906:THR:HB   | 2:G:233:VAL:HA   | 1.96                     | 0.47              |
| 2:G:170:ARG:NH1  | 2:G:199:SER:HB2  | 2.30                     | 0.47              |
| 1:A:90:ILE:O     | 1:A:94:VAL:HG12  | 2.14                     | 0.46              |
| 1:B:89:GLN:OE1   | 1:B:187:GLU:HG3  | 2.15                     | 0.46              |
| 1:B:518:GLU:HG3  | 1:B:519:MET:HE2  | 1.97                     | 0.46              |
| 2:C:11:VAL:HG11  | 2:C:63:VAL:HG11  | 1.98                     | 0.46              |
| 1:F:218:TYR:OH   | 1:F:224:ASN:ND2  | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:751:ILE:HD13 | 1:F:754:ARG:NE   | 2.30                     | 0.46              |
| 2:G:13:PHE:HD2   | 2:G:22:VAL:HG12  | 1.81                     | 0.46              |
| 1:A:964:ASP:N    | 1:A:964:ASP:OD1  | 2.47                     | 0.46              |
| 1:B:439:ALA:HB1  | 1:B:455:TYR:CE1  | 2.51                     | 0.46              |
| 1:E:448:TRP:CH2  | 1:E:707:VAL:HB   | 2.51                     | 0.46              |
| 1:F:323:GLN:HE21 | 1:F:597:GLU:HG3  | 1.81                     | 0.46              |
| 1:F:965:LYS:HE3  | 1:F:966:LEU:HG   | 1.98                     | 0.46              |
| 1:A:241:HIS:HE2  | 1:B:159:ALA:HB1  | 1.80                     | 0.46              |
| 1:B:313:TYR:HA   | 1:B:316:ILE:HG22 | 1.98                     | 0.46              |
| 1:B:374:SER:OG   | 1:B:375:LYS:N    | 2.48                     | 0.46              |
| 1:E:195:GLN:HA   | 1:E:198:PRO:HG3  | 1.97                     | 0.46              |
| 1:E:699:PHE:CD2  | 1:E:743:TYR:HB3  | 2.50                     | 0.46              |
| 1:F:328:ILE:HG13 | 1:F:329:ASP:N    | 2.31                     | 0.46              |
| 1:F:439:ALA:HB2  | 1:F:454:LEU:CD2  | 2.45                     | 0.46              |
| 1:F:752:GLY:N    | 1:F:799:LEU:HD21 | 2.31                     | 0.46              |
| 1:A:174:PHE:CD1  | 1:A:178:PHE:HA   | 2.51                     | 0.46              |
| 1:A:608:PHE:CZ   | 1:A:612:ILE:HD11 | 2.51                     | 0.46              |
| 1:B:62:LEU:HD13  | 1:B:66:TYR:CE2   | 2.51                     | 0.46              |
| 1:B:664:ILE:HD13 | 1:B:722:PHE:HE2  | 1.81                     | 0.46              |
| 1:F:952:LYS:HE2  | 1:F:952:LYS:HA   | 1.97                     | 0.46              |
| 1:F:960:LYS:HD2  | 1:F:962:TYR:HE2  | 1.80                     | 0.46              |
| 1:B:290:MET:HA   | 1:B:293:LEU:HG   | 1.97                     | 0.46              |
| 1:E:407:ILE:HD11 | 1:E:593:ARG:HB2  | 1.97                     | 0.46              |
| 1:E:749:LEU:O    | 1:E:754:ARG:NH1  | 2.49                     | 0.46              |
| 1:E:907:PHE:HD2  | 2:H:232:ALA:HB3  | 1.79                     | 0.46              |
| 1:F:118:HIS:HE1  | 1:F:137:LEU:C    | 2.23                     | 0.46              |
| 1:F:207:ILE:HA   | 1:F:210:THR:HG22 | 1.98                     | 0.46              |
| 2:H:22:VAL:HG13  | 2:H:22:VAL:O     | 2.16                     | 0.46              |
| 1:A:332:HIS:O    | 1:A:333:VAL:C    | 2.57                     | 0.46              |
| 1:A:548:ASN:OD1  | 1:A:548:ASN:N    | 2.48                     | 0.46              |
| 1:A:740:LEU:O    | 1:A:741:LEU:C    | 2.56                     | 0.46              |
| 1:B:569:MET:SD   | 1:B:570:SER:OG   | 2.65                     | 0.46              |
| 1:B:664:ILE:HB   | 1:B:722:PHE:CZ   | 2.51                     | 0.46              |
| 1:B:685:GLU:OE2  | 1:B:688:LEU:HD23 | 2.15                     | 0.46              |
| 1:B:817:SER:OG   | 1:B:844:LEU:O    | 2.30                     | 0.46              |
| 1:E:455:TYR:CE2  | 1:E:481:ILE:HG21 | 2.51                     | 0.46              |
| 1:E:550:PHE:H    | 1:E:550:PHE:HD1  | 1.64                     | 0.46              |
| 1:F:652:PHE:CE1  | 1:F:722:PHE:HD2  | 2.34                     | 0.46              |
| 1:F:911:ASP:HA   | 1:F:913:MET:HE1  | 1.98                     | 0.46              |
| 2:H:70:LEU:HD23  | 2:H:70:LEU:HA    | 1.75                     | 0.46              |
| 1:A:491:GLN:HB2  | 1:A:495:LEU:HB3  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:712:PHE:CG   | 1:A:713:ILE:N    | 2.83                     | 0.46              |
| 1:B:204:MET:HE2  | 1:B:204:MET:HA   | 1.97                     | 0.46              |
| 1:B:326:ARG:HB2  | 1:B:329:ASP:HB2  | 1.97                     | 0.46              |
| 1:B:482:TYR:HE2  | 1:B:519:MET:HB2  | 1.80                     | 0.46              |
| 1:B:643:SER:HB3  | 2:D:5:ILE:HG12   | 1.96                     | 0.46              |
| 1:B:659:PHE:CD2  | 1:B:662:ASP:HA   | 2.50                     | 0.46              |
| 2:C:70:LEU:O     | 2:C:71:GLU:C     | 2.58                     | 0.46              |
| 1:E:367:CYS:O    | 1:E:370:ARG:HB2  | 2.16                     | 0.46              |
| 1:E:449:GLU:HG3  | 1:E:511:PHE:CE2  | 2.51                     | 0.46              |
| 1:E:737:VAL:HG21 | 1:E:771:ILE:HG23 | 1.96                     | 0.46              |
| 1:F:187:GLU:HA   | 1:F:190:TYR:CD2  | 2.50                     | 0.46              |
| 2:G:15:ARG:HG2   | 2:G:20:LYS:CG    | 2.43                     | 0.46              |
| 2:G:225:ASP:OD2  | 2:G:227:ASP:HB3  | 2.16                     | 0.46              |
| 2:H:192:TYR:HB2  | 2:H:235:ILE:HB   | 1.98                     | 0.46              |
| 1:A:491:GLN:HB2  | 1:A:495:LEU:CB   | 2.46                     | 0.46              |
| 1:A:549:GLN:HB2  | 1:A:552:TYR:CB   | 2.45                     | 0.46              |
| 1:A:655:ILE:HG23 | 1:A:659:PHE:CE2  | 2.51                     | 0.46              |
| 1:B:222:ASP:CG   | 1:B:225:ILE:HG23 | 2.40                     | 0.46              |
| 1:B:290:MET:O    | 1:B:294:ILE:HG12 | 2.15                     | 0.46              |
| 1:E:202:ASN:ND2  | 1:F:205:LYS:HE2  | 2.30                     | 0.46              |
| 1:E:434:ASP:O    | 1:E:438:LYS:HG2  | 2.16                     | 0.46              |
| 1:E:456:SER:HA   | 1:E:459:ILE:HD12 | 1.97                     | 0.46              |
| 1:F:229:LEU:O    | 1:F:233:ARG:HG2  | 2.15                     | 0.46              |
| 1:F:332:HIS:CE1  | 1:F:543:GLU:HG2  | 2.50                     | 0.46              |
| 1:A:187:GLU:HA   | 1:A:190:TYR:CD2  | 2.51                     | 0.46              |
| 1:B:31:LYS:HD2   | 1:B:31:LYS:C     | 2.41                     | 0.46              |
| 1:B:62:LEU:HD23  | 1:B:107:PHE:CG   | 2.51                     | 0.46              |
| 2:D:54:LYS:HB3   | 2:D:54:LYS:HE3   | 1.67                     | 0.46              |
| 1:E:574:TYR:OH   | 1:E:629:ARG:NH1  | 2.47                     | 0.46              |
| 1:F:612:ILE:HG21 | 1:F:658:HIS:ND1  | 2.30                     | 0.46              |
| 1:F:728:LEU:HD12 | 1:F:728:LEU:HA   | 1.78                     | 0.46              |
| 1:F:786:HIS:HA   | 1:F:791:TYR:HD2  | 1.80                     | 0.46              |
| 1:A:188:ASP:O    | 1:A:192:ASN:ND2  | 2.49                     | 0.46              |
| 1:A:581:ASP:HA   | 1:A:584:VAL:HG23 | 1.97                     | 0.46              |
| 1:A:750:ASP:CG   | 1:A:796:SER:CB   | 2.89                     | 0.46              |
| 1:B:588:LEU:HD11 | 1:B:615:SER:CB   | 2.46                     | 0.46              |
| 2:C:37:SER:N     | 2:C:56:GLU:OE2   | 2.49                     | 0.46              |
| 1:E:781:LEU:O    | 1:E:784:GLU:HG3  | 2.16                     | 0.46              |
| 1:F:506:PRO:HG2  | 1:F:507:PHE:CE2  | 2.51                     | 0.46              |
| 1:F:776:ASP:HA   | 1:F:779:LEU:HG   | 1.97                     | 0.46              |
| 1:A:336:TYR:O    | 1:A:349:HIS:ND1  | 2.49                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:197:TYR:O    | 1:B:197:TYR:HD1  | 1.98                     | 0.45              |
| 1:B:279:GLU:O    | 1:B:285:ARG:NH2  | 2.49                     | 0.45              |
| 1:B:533:PHE:CD1  | 1:B:533:PHE:N    | 2.83                     | 0.45              |
| 1:B:891:THR:HA   | 1:B:894:VAL:HG22 | 1.98                     | 0.45              |
| 2:D:177:THR:OG1  | 2:D:191:ILE:HB   | 2.16                     | 0.45              |
| 1:E:45:PHE:HE1   | 1:E:213:ILE:HD12 | 1.81                     | 0.45              |
| 1:E:436:TYR:OH   | 1:E:598:ASN:O    | 2.30                     | 0.45              |
| 1:E:883:GLU:O    | 1:E:886:ILE:HG22 | 2.16                     | 0.45              |
| 1:F:842:LEU:O    | 1:F:845:LEU:HB2  | 2.16                     | 0.45              |
| 1:F:892:ARG:HA   | 1:F:895:ASN:ND2  | 2.29                     | 0.45              |
| 1:F:963:ASN:ND2  | 2:G:52:ILE:HG22  | 2.30                     | 0.45              |
| 1:F:965:LYS:O    | 1:F:966:LEU:C    | 2.57                     | 0.45              |
| 2:G:197:ASN:HB3  | 2:G:223:LEU:O    | 2.15                     | 0.45              |
| 1:A:116:PRO:HG2  | 1:A:120:LYS:HZ2  | 1.81                     | 0.45              |
| 1:A:487:GLN:CD   | 2:D:207:SER:H    | 2.24                     | 0.45              |
| 1:A:649:TYR:CE1  | 1:A:683:LYS:HB3  | 2.51                     | 0.45              |
| 1:A:655:ILE:HG23 | 1:A:659:PHE:CZ   | 2.51                     | 0.45              |
| 1:B:573:SER:OG   | 2:D:31:SER:HB2   | 2.16                     | 0.45              |
| 2:D:198:VAL:HG13 | 2:D:220:PHE:HB3  | 1.97                     | 0.45              |
| 1:E:606:HIS:CE1  | 2:H:206:MET:HA   | 2.51                     | 0.45              |
| 1:E:721:TYR:O    | 1:E:760:ARG:NH2  | 2.43                     | 0.45              |
| 1:E:923:GLU:O    | 1:E:923:GLU:HG2  | 2.16                     | 0.45              |
| 1:F:130:ILE:HD13 | 1:F:168:LEU:HD23 | 1.98                     | 0.45              |
| 1:F:326:ARG:HD3  | 1:F:594:PHE:CD2  | 2.51                     | 0.45              |
| 1:F:827:LEU:HG   | 1:F:834:GLN:NE2  | 2.31                     | 0.45              |
| 1:F:932:GLU:H    | 1:F:932:GLU:HG2  | 1.34                     | 0.45              |
| 1:A:145:ARG:CZ   | 1:A:147:LYS:HG2  | 2.46                     | 0.45              |
| 1:A:674:ASP:OD1  | 1:A:724:LYS:HB3  | 2.17                     | 0.45              |
| 1:B:960:LYS:O    | 1:B:961:ASN:C    | 2.58                     | 0.45              |
| 1:E:205:LYS:HB2  | 1:E:231:TRP:HZ2  | 1.81                     | 0.45              |
| 1:E:448:TRP:HB3  | 1:E:481:ILE:HD11 | 1.98                     | 0.45              |
| 1:E:862:ILE:HD12 | 1:E:866:MET:HE3  | 1.97                     | 0.45              |
| 2:G:215:ALA:O    | 2:G:217:GLU:N    | 2.49                     | 0.45              |
| 1:A:792:SER:HA   | 1:A:833:LYS:HD3  | 1.98                     | 0.45              |
| 1:B:730:GLU:HG2  | 1:B:733:LEU:HD12 | 1.98                     | 0.45              |
| 1:E:79:TYR:HA    | 1:E:83:GLU:OE1   | 2.15                     | 0.45              |
| 1:E:328:ILE:C    | 1:E:328:ILE:HD12 | 2.41                     | 0.45              |
| 1:E:632:ASP:CG   | 1:F:955:ILE:HD11 | 2.41                     | 0.45              |
| 1:F:53:LEU:O     | 1:F:115:ASN:ND2  | 2.49                     | 0.45              |
| 1:F:59:TRP:CH2   | 1:F:185:LEU:HG   | 2.51                     | 0.45              |
| 1:F:151:VAL:HG22 | 1:F:167:LEU:HB3  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:472:TYR:HB2  | 1:F:535:PHE:HE2  | 1.81                     | 0.45              |
| 1:F:727:LYS:HA   | 1:F:727:LYS:HD2  | 1.34                     | 0.45              |
| 1:F:880:GLU:CD   | 1:F:880:GLU:H    | 2.24                     | 0.45              |
| 1:A:331:LYS:O    | 1:A:332:HIS:C    | 2.59                     | 0.45              |
| 1:A:475:GLN:HA   | 1:A:478:ARG:HH12 | 1.80                     | 0.45              |
| 1:A:657:ARG:HA   | 1:A:715:GLU:OE2  | 2.15                     | 0.45              |
| 1:A:768:PRO:HA   | 1:A:772:ILE:HB   | 1.99                     | 0.45              |
| 1:B:289:VAL:O    | 1:B:293:LEU:HG   | 2.16                     | 0.45              |
| 1:B:316:ILE:CD1  | 1:B:319:LEU:HD11 | 2.46                     | 0.45              |
| 1:B:741:LEU:HD12 | 1:B:774:ILE:HG22 | 1.97                     | 0.45              |
| 1:E:417:LYS:HD2  | 1:E:417:LYS:O    | 2.17                     | 0.45              |
| 1:E:651:ASP:HA   | 1:E:654:ASN:HD21 | 1.81                     | 0.45              |
| 1:E:664:ILE:O    | 1:E:667:LEU:HG   | 2.16                     | 0.45              |
| 1:F:210:THR:HG23 | 1:F:211:HIS:ND1  | 2.31                     | 0.45              |
| 1:F:566:ARG:O    | 1:F:569:MET:HB3  | 2.16                     | 0.45              |
| 1:F:873:LEU:O    | 1:F:874:ILE:C    | 2.60                     | 0.45              |
| 1:F:956:PRO:O    | 1:F:960:LYS:HG2  | 2.15                     | 0.45              |
| 1:A:246:ILE:HA   | 1:A:269:ILE:HG23 | 1.99                     | 0.45              |
| 1:B:89:GLN:HA    | 1:B:186:LYS:HZ3  | 1.82                     | 0.45              |
| 1:B:660:LYS:HD3  | 1:B:660:LYS:HA   | 1.76                     | 0.45              |
| 1:B:751:ILE:HD13 | 1:B:754:ARG:HH21 | 1.81                     | 0.45              |
| 1:E:749:LEU:HB3  | 1:E:754:ARG:CZ   | 2.47                     | 0.45              |
| 1:F:227:MET:SD   | 1:F:228:LEU:N    | 2.90                     | 0.45              |
| 1:F:425:ILE:HD11 | 1:F:442:LEU:HD23 | 1.98                     | 0.45              |
| 1:F:958:TRP:N    | 1:F:958:TRP:CD1  | 2.84                     | 0.45              |
| 1:F:979:HIS:O    | 1:F:983:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:409:ILE:HD13 | 1:A:414:TYR:CE1  | 2.52                     | 0.45              |
| 1:A:866:MET:N    | 1:A:866:MET:HE2  | 2.31                     | 0.45              |
| 1:B:170:VAL:HG12 | 1:B:200:ILE:HG22 | 1.99                     | 0.45              |
| 1:B:331:LYS:HE3  | 1:B:336:TYR:HE1  | 1.82                     | 0.45              |
| 1:B:640:GLY:C    | 1:B:641:LYS:HG3  | 2.40                     | 0.45              |
| 1:E:208:ILE:HA   | 1:E:213:ILE:CG1  | 2.46                     | 0.45              |
| 1:E:297:GLN:O    | 1:E:299:ASN:N    | 2.50                     | 0.45              |
| 1:E:767:LEU:HB2  | 1:E:811:PHE:CE2  | 2.52                     | 0.45              |
| 1:E:847:THR:HA   | 1:E:850:LYS:HE3  | 1.99                     | 0.45              |
| 1:F:59:TRP:O     | 1:F:63:VAL:HG23  | 2.16                     | 0.45              |
| 1:F:79:TYR:HB3   | 1:F:84:TYR:HA    | 1.99                     | 0.45              |
| 1:F:976:MET:HB3  | 1:F:979:HIS:NE2  | 2.32                     | 0.45              |
| 1:A:388:PHE:HA   | 1:A:391:ASN:HD21 | 1.80                     | 0.45              |
| 1:A:997:LEU:HG   | 1:A:1001:MET:HE3 | 1.98                     | 0.45              |
| 1:B:240:PHE:CZ   | 1:B:243:PRO:HD3  | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:342:VAL:HG12 | 1:B:586:LEU:HB3  | 1.98                     | 0.45              |
| 1:B:442:LEU:HB3  | 1:B:447:ARG:HH22 | 1.82                     | 0.45              |
| 1:B:489:VAL:O    | 1:B:493:ASN:N    | 2.48                     | 0.45              |
| 1:B:609:HIS:HD1  | 1:B:609:HIS:C    | 2.24                     | 0.45              |
| 1:B:965:LYS:H    | 1:B:965:LYS:HG3  | 1.55                     | 0.45              |
| 1:E:195:GLN:HE22 | 1:F:237:LYS:HE3  | 1.82                     | 0.45              |
| 1:E:877:PHE:HE2  | 1:E:924:GLU:HB3  | 1.81                     | 0.45              |
| 1:F:326:ARG:HB2  | 1:F:329:ASP:HB2  | 1.99                     | 0.45              |
| 1:F:338:TYR:HE1  | 1:F:351:ASN:HB2  | 1.81                     | 0.45              |
| 1:F:502:ARG:O    | 1:F:502:ARG:HD3  | 2.17                     | 0.45              |
| 1:F:749:LEU:HD11 | 1:F:754:ARG:HG3  | 1.99                     | 0.45              |
| 1:F:904:ILE:HG22 | 2:G:235:ILE:HA   | 1.99                     | 0.45              |
| 1:F:906:THR:O    | 1:F:907:PHE:C    | 2.59                     | 0.45              |
| 1:F:955:ILE:HD13 | 1:F:958:TRP:NE1  | 2.31                     | 0.45              |
| 1:A:23:ASP:O     | 1:A:27:VAL:HG23  | 2.17                     | 0.45              |
| 1:E:43:VAL:HG22  | 1:E:128:HIS:H    | 1.81                     | 0.45              |
| 1:E:186:LYS:NZ   | 1:E:188:ASP:HB2  | 2.31                     | 0.45              |
| 1:E:500:PHE:HD1  | 1:E:747:ARG:HH22 | 1.64                     | 0.45              |
| 1:E:726:VAL:HG22 | 1:E:727:LYS:H    | 1.82                     | 0.45              |
| 1:F:342:VAL:HG22 | 1:F:586:LEU:HD13 | 1.98                     | 0.45              |
| 1:F:681:GLN:O    | 1:F:685:GLU:HG3  | 2.17                     | 0.45              |
| 1:F:932:GLU:O    | 1:F:934:ILE:HG12 | 2.17                     | 0.45              |
| 1:F:979:HIS:ND1  | 1:F:980:VAL:HG23 | 2.31                     | 0.45              |
| 1:A:547:ASP:O    | 1:A:550:PHE:CD1  | 2.69                     | 0.45              |
| 1:A:772:ILE:HA   | 1:A:775:ILE:HD12 | 1.99                     | 0.45              |
| 1:E:124:MET:N    | 1:E:124:MET:SD   | 2.90                     | 0.45              |
| 1:E:163:SER:OG   | 1:E:165:ARG:O    | 2.35                     | 0.45              |
| 1:E:815:PHE:CE2  | 1:E:844:LEU:HA   | 2.52                     | 0.45              |
| 1:E:818:LYS:HA   | 1:E:821:SER:HB2  | 1.99                     | 0.45              |
| 1:E:865:LEU:HD23 | 1:E:865:LEU:HA   | 1.83                     | 0.45              |
| 1:F:279:GLU:HA   | 1:F:285:ARG:HH22 | 1.82                     | 0.45              |
| 1:F:909:SER:HB3  | 2:G:231:MET:HG2  | 1.98                     | 0.45              |
| 1:A:87:ILE:HA    | 1:A:90:ILE:HG12  | 1.98                     | 0.44              |
| 1:A:231:TRP:HA   | 1:A:234:LYS:HE2  | 1.99                     | 0.44              |
| 1:A:257:THR:HA   | 1:E:86:ARG:HH22  | 1.83                     | 0.44              |
| 1:B:152:ILE:HB   | 1:B:168:LEU:HD12 | 1.99                     | 0.44              |
| 1:B:222:ASP:O    | 1:B:225:ILE:HG12 | 2.17                     | 0.44              |
| 1:B:223:TYR:HA   | 1:B:226:ASN:HD21 | 1.82                     | 0.44              |
| 1:E:61:ARG:NH1   | 1:E:64:ASP:HB2   | 2.32                     | 0.44              |
| 1:E:105:LYS:CE   | 1:E:178:PHE:HB2  | 2.47                     | 0.44              |
| 1:E:422:LYS:NZ   | 1:E:447:ARG:HH22 | 2.15                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:495:LEU:O    | 1:E:498:LEU:HG   | 2.17                     | 0.44              |
| 1:E:973:ASN:O    | 1:E:977:LYS:HB2  | 2.17                     | 0.44              |
| 1:F:294:ILE:HG22 | 1:F:295:GLU:N    | 2.32                     | 0.44              |
| 2:G:20:LYS:HA    | 2:G:72:TRP:CH2   | 2.52                     | 0.44              |
| 1:A:229:LEU:O    | 1:A:233:ARG:HB2  | 2.17                     | 0.44              |
| 1:B:67:HIS:O     | 1:B:70:LEU:HB2   | 2.17                     | 0.44              |
| 1:B:661:ILE:O    | 1:B:665:LYS:CB   | 2.64                     | 0.44              |
| 1:F:963:ASN:O    | 1:F:967:LEU:HD23 | 2.11                     | 0.44              |
| 1:F:965:LYS:O    | 1:F:968:GLY:N    | 2.50                     | 0.44              |
| 2:H:72:TRP:HA    | 2:H:72:TRP:HE3   | 1.74                     | 0.44              |
| 1:A:44:PHE:CE2   | 1:A:121:ILE:HD12 | 2.53                     | 0.44              |
| 1:A:86:ARG:NH2   | 1:A:90:ILE:HD11  | 2.31                     | 0.44              |
| 1:A:193:TYR:O    | 1:A:193:TYR:HD1  | 2.00                     | 0.44              |
| 1:A:469:CYS:O    | 1:A:473:LEU:HD23 | 2.17                     | 0.44              |
| 1:A:537:LYS:HA   | 1:A:537:LYS:HD2  | 1.76                     | 0.44              |
| 1:A:620:ILE:HG21 | 1:A:667:LEU:HD21 | 1.99                     | 0.44              |
| 1:A:794:VAL:HG12 | 1:A:796:SER:H    | 1.83                     | 0.44              |
| 1:A:836:ASP:O    | 1:A:839:PHE:HB3  | 2.18                     | 0.44              |
| 1:B:92:TYR:CD1   | 1:B:92:TYR:C     | 2.95                     | 0.44              |
| 1:B:317:SER:HA   | 1:B:320:PHE:CZ   | 2.53                     | 0.44              |
| 1:E:143:TRP:CE2  | 1:F:463:ILE:HG22 | 2.52                     | 0.44              |
| 1:E:1001:MET:HG3 | 1:F:985:LYS:HE3  | 1.99                     | 0.44              |
| 1:F:322:LEU:HD12 | 1:F:323:GLN:H    | 1.82                     | 0.44              |
| 1:F:535:PHE:HA   | 1:F:538:LYS:HZ2  | 1.82                     | 0.44              |
| 1:F:650:TYR:O    | 1:F:654:ASN:ND2  | 2.51                     | 0.44              |
| 1:F:666:ASN:OD1  | 1:F:666:ASN:C    | 2.60                     | 0.44              |
| 2:H:42:ARG:NH1   | 2:H:52:ILE:HD13  | 2.32                     | 0.44              |
| 1:B:169:LYS:HE2  | 1:B:172:GLY:O    | 2.17                     | 0.44              |
| 1:B:368:ASP:N    | 1:B:368:ASP:OD1  | 2.49                     | 0.44              |
| 1:B:892:ARG:HA   | 1:B:895:ASN:HD21 | 1.82                     | 0.44              |
| 1:F:32:GLU:O     | 1:F:35:GLU:HG3   | 2.18                     | 0.44              |
| 1:F:119:ASP:OD1  | 1:F:119:ASP:N    | 2.50                     | 0.44              |
| 2:H:205:GLU:HG3  | 2:H:207:SER:OG   | 2.18                     | 0.44              |
| 1:A:827:LEU:HD13 | 1:A:835:ILE:HG22 | 1.99                     | 0.44              |
| 1:A:914:SER:O    | 1:A:918:ILE:HG13 | 2.17                     | 0.44              |
| 1:A:955:ILE:HD12 | 1:A:958:TRP:HZ2  | 1.81                     | 0.44              |
| 1:B:245:PHE:O    | 1:B:268:ILE:HD12 | 2.17                     | 0.44              |
| 1:B:685:GLU:CD   | 1:B:731:GLU:HB2  | 2.42                     | 0.44              |
| 2:C:11:VAL:HB    | 2:C:24:THR:HB    | 1.99                     | 0.44              |
| 2:C:15:ARG:HE    | 2:C:20:LYS:HE2   | 1.83                     | 0.44              |
| 1:E:283:LEU:O    | 1:E:283:LEU:HD12 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:312:ILE:HD13 | 1:E:312:ILE:HA   | 1.78                     | 0.44              |
| 1:E:333:VAL:HA   | 1:E:540:LYS:HD3  | 1.99                     | 0.44              |
| 1:E:523:ASN:C    | 1:E:525:ASP:H    | 2.25                     | 0.44              |
| 1:E:549:GLN:HA   | 1:E:552:TYR:CD2  | 2.51                     | 0.44              |
| 1:F:725:TYR:CD1  | 1:F:725:TYR:N    | 2.84                     | 0.44              |
| 1:F:789:GLN:HG3  | 1:F:831:LYS:NZ   | 2.33                     | 0.44              |
| 1:F:863:ASN:CG   | 1:F:864:ASP:H    | 2.26                     | 0.44              |
| 1:F:975:HIS:HD1  | 1:F:976:MET:CG   | 2.30                     | 0.44              |
| 1:A:685:GLU:OE1  | 1:A:685:GLU:N    | 2.51                     | 0.44              |
| 1:B:169:LYS:HG2  | 1:B:172:GLY:H    | 1.83                     | 0.44              |
| 1:B:412:LEU:HA   | 1:B:415:HIS:CD2  | 2.52                     | 0.44              |
| 1:B:475:GLN:HA   | 1:B:478:ARG:CZ   | 2.47                     | 0.44              |
| 1:B:664:ILE:HG23 | 1:B:668:GLU:HG2  | 1.99                     | 0.44              |
| 1:E:45:PHE:HA    | 1:E:130:ILE:O    | 2.18                     | 0.44              |
| 1:E:629:ARG:HH11 | 1:E:631:ILE:HD12 | 1.83                     | 0.44              |
| 1:E:725:TYR:O    | 1:E:726:VAL:HG12 | 2.17                     | 0.44              |
| 1:E:963:ASN:ND2  | 1:E:965:LYS:HB3  | 2.32                     | 0.44              |
| 1:E:974:LYS:O    | 1:E:974:LYS:HD3  | 2.17                     | 0.44              |
| 1:F:75:LYS:HZ1   | 1:F:83:GLU:HB3   | 1.81                     | 0.44              |
| 1:F:104:LEU:HD13 | 1:F:174:PHE:HE2  | 1.82                     | 0.44              |
| 1:F:205:LYS:O    | 1:F:208:ILE:HG22 | 2.18                     | 0.44              |
| 2:G:56:GLU:CD    | 2:G:57:LYS:N     | 2.75                     | 0.44              |
| 1:A:147:LYS:NZ   | 1:B:526:ASP:O    | 2.51                     | 0.44              |
| 1:A:605:PHE:O    | 1:A:609:HIS:NE2  | 2.51                     | 0.44              |
| 1:B:197:TYR:O    | 1:B:197:TYR:CD1  | 2.71                     | 0.44              |
| 1:B:279:GLU:C    | 1:B:285:ARG:HH22 | 2.26                     | 0.44              |
| 1:B:363:LEU:HD23 | 1:B:369:GLU:HB3  | 1.99                     | 0.44              |
| 1:B:593:ARG:HA   | 1:B:596:TYR:CB   | 2.46                     | 0.44              |
| 1:B:864:ASP:OD1  | 1:B:865:LEU:N    | 2.50                     | 0.44              |
| 1:E:61:ARG:HH12  | 1:E:64:ASP:HB2   | 1.83                     | 0.44              |
| 1:E:156:GLU:OE1  | 1:F:239:SER:HB3  | 2.18                     | 0.44              |
| 1:E:995:ARG:O    | 1:E:999:ILE:HB   | 2.17                     | 0.44              |
| 1:F:224:ASN:O    | 1:F:228:LEU:HB3  | 2.16                     | 0.44              |
| 1:F:316:ILE:HD12 | 1:F:316:ILE:HA   | 1.85                     | 0.44              |
| 1:F:778:PHE:CD1  | 1:F:778:PHE:C    | 2.95                     | 0.44              |
| 1:F:827:LEU:HD13 | 1:F:827:LEU:HA   | 1.81                     | 0.44              |
| 1:F:909:SER:HB3  | 2:G:231:MET:HE3  | 1.99                     | 0.44              |
| 1:F:940:TYR:HA   | 1:F:943:PHE:CD2  | 2.53                     | 0.44              |
| 2:G:65:ASN:OD1   | 2:G:65:ASN:C     | 2.61                     | 0.44              |
| 1:A:174:PHE:CE1  | 1:A:178:PHE:HA   | 2.53                     | 0.44              |
| 1:A:225:ILE:O    | 1:A:229:LEU:HB2  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:439:ALA:HB2  | 1:A:454:LEU:HD23 | 2.00                     | 0.44              |
| 1:A:580:SER:O    | 1:A:583:VAL:N    | 2.46                     | 0.44              |
| 1:A:919:TRP:HE1  | 2:D:51:TYR:HB2   | 1.81                     | 0.44              |
| 1:B:135:ASP:OD1  | 1:B:135:ASP:N    | 2.42                     | 0.44              |
| 1:B:348:ARG:HG3  | 1:B:351:ASN:HB3  | 1.99                     | 0.44              |
| 2:D:20:LYS:HA    | 2:D:72:TRP:CE2   | 2.52                     | 0.44              |
| 1:E:115:ASN:HB2  | 1:E:116:PRO:HD2  | 1.99                     | 0.44              |
| 1:E:994:LYS:NZ   | 1:F:989:LYS:O    | 2.45                     | 0.44              |
| 1:F:58:GLN:HG3   | 1:F:61:ARG:NH1   | 2.33                     | 0.44              |
| 1:F:735:LYS:HD2  | 1:F:735:LYS:HA   | 1.82                     | 0.44              |
| 1:A:290:MET:SD   | 1:A:293:LEU:HD21 | 2.58                     | 0.44              |
| 1:A:674:ASP:OD1  | 1:A:724:LYS:NZ   | 2.49                     | 0.44              |
| 2:C:201:SER:O    | 2:C:201:SER:OG   | 2.33                     | 0.44              |
| 1:E:359:ARG:NH1  | 1:E:359:ARG:HA   | 2.33                     | 0.44              |
| 1:F:326:ARG:NH1  | 1:F:591:ASN:HA   | 2.33                     | 0.44              |
| 1:F:407:ILE:H    | 2:H:2:LYS:CB     | 2.30                     | 0.44              |
| 1:F:918:ILE:O    | 1:F:922:LEU:HB2  | 2.18                     | 0.44              |
| 1:F:927:ASN:OD1  | 1:F:928:SER:N    | 2.51                     | 0.44              |
| 1:F:939:GLN:HG3  | 1:F:958:TRP:HB3  | 1.99                     | 0.44              |
| 1:F:956:PRO:HB2  | 1:F:996:TYR:OH   | 2.18                     | 0.44              |
| 1:F:981:ILE:HG23 | 1:F:982:GLU:OE1  | 2.18                     | 0.44              |
| 1:A:44:PHE:CD2   | 1:A:121:ILE:HG23 | 2.53                     | 0.43              |
| 1:A:85:LEU:O     | 1:A:88:PRO:HG2   | 2.18                     | 0.43              |
| 1:A:152:ILE:HG21 | 1:A:158:VAL:HG23 | 2.00                     | 0.43              |
| 1:A:315:LYS:O    | 1:A:318:PRO:HD2  | 2.18                     | 0.43              |
| 1:A:404:ASN:OD1  | 2:C:5:ILE:HA     | 2.17                     | 0.43              |
| 1:A:772:ILE:HA   | 1:A:772:ILE:HD12 | 1.83                     | 0.43              |
| 1:B:333:VAL:HG23 | 1:B:541:ILE:HD12 | 2.00                     | 0.43              |
| 1:B:583:VAL:O    | 1:B:587:ARG:HG2  | 2.18                     | 0.43              |
| 1:E:51:SER:OG    | 1:E:133:ASN:OD1  | 2.21                     | 0.43              |
| 1:E:83:GLU:O     | 1:E:87:ILE:HG12  | 2.18                     | 0.43              |
| 1:E:404:ASN:HB3  | 2:G:1:MET:HA     | 2.00                     | 0.43              |
| 1:E:480:ARG:HG3  | 1:E:605:PHE:CZ   | 2.53                     | 0.43              |
| 1:E:673:ILE:HG23 | 1:E:725:TYR:CE2  | 2.52                     | 0.43              |
| 1:E:840:LYS:C    | 1:E:841:LEU:HD12 | 2.43                     | 0.43              |
| 1:F:89:GLN:HA    | 1:F:186:LYS:CE   | 2.47                     | 0.43              |
| 2:H:36:ILE:HD13  | 2:H:57:LYS:HZ1   | 1.83                     | 0.43              |
| 1:A:662:ASP:OD1  | 1:A:663:ASP:N    | 2.51                     | 0.43              |
| 1:A:764:CYS:O    | 1:A:765:ASN:ND2  | 2.51                     | 0.43              |
| 1:B:134:TYR:CZ   | 1:B:171:ALA:HB1  | 2.53                     | 0.43              |
| 1:B:312:ILE:HD13 | 1:B:312:ILE:HA   | 1.85                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:345:THR:HA   | 1:B:395:CYS:O    | 2.18                     | 0.43              |
| 1:E:76:LYS:HE2   | 1:E:76:LYS:HA    | 1.99                     | 0.43              |
| 1:E:507:PHE:N    | 1:E:507:PHE:CD1  | 2.83                     | 0.43              |
| 1:E:544:PHE:CE1  | 1:E:550:PHE:HB2  | 2.53                     | 0.43              |
| 1:E:706:VAL:O    | 1:E:710:THR:HG23 | 2.18                     | 0.43              |
| 1:F:27:VAL:HA    | 1:F:30:ILE:HD12  | 2.00                     | 0.43              |
| 1:F:60:TRP:CZ3   | 1:F:61:ARG:HG2   | 2.53                     | 0.43              |
| 1:F:994:LYS:HD3  | 1:F:994:LYS:HA   | 1.72                     | 0.43              |
| 2:H:29:THR:HG23  | 2:H:64:LYS:HZ2   | 1.83                     | 0.43              |
| 1:A:140:THR:C    | 1:A:144:LYS:HZ2  | 2.26                     | 0.43              |
| 1:A:706:VAL:HA   | 1:A:709:TYR:HD2  | 1.84                     | 0.43              |
| 1:A:722:PHE:CZ   | 1:A:725:TYR:HD2  | 2.36                     | 0.43              |
| 1:B:916:PHE:HA   | 1:B:919:TRP:HD1  | 1.83                     | 0.43              |
| 1:B:956:PRO:O    | 1:B:996:TYR:OH   | 2.31                     | 0.43              |
| 2:C:70:LEU:HD23  | 2:C:73:LEU:HD23  | 2.00                     | 0.43              |
| 2:D:10:ASP:CG    | 2:D:176:ARG:HE   | 2.26                     | 0.43              |
| 2:D:24:THR:N     | 2:D:68:PHE:HA    | 2.33                     | 0.43              |
| 1:E:390:LYS:HD2  | 1:E:390:LYS:C    | 2.43                     | 0.43              |
| 1:E:755:TYR:CE1  | 1:E:807:LEU:HB3  | 2.52                     | 0.43              |
| 1:E:965:LYS:HA   | 1:E:965:LYS:HD2  | 1.90                     | 0.43              |
| 1:F:322:LEU:HD11 | 1:F:598:ASN:HB3  | 1.99                     | 0.43              |
| 1:F:724:LYS:HD3  | 1:F:760:ARG:CZ   | 2.48                     | 0.43              |
| 2:G:65:ASN:O     | 2:G:216:PRO:HD2  | 2.18                     | 0.43              |
| 1:A:548:ASN:CB   | 2:D:210:ASN:ND2  | 2.79                     | 0.43              |
| 1:A:688:LEU:HD11 | 1:A:736:ILE:HD13 | 2.00                     | 0.43              |
| 1:B:45:PHE:HB2   | 1:B:214:VAL:O    | 2.19                     | 0.43              |
| 1:B:69:GLU:HB2   | 1:B:91:PHE:HE1   | 1.84                     | 0.43              |
| 1:B:286:TYR:HB3  | 1:B:290:MET:HE2  | 2.01                     | 0.43              |
| 1:B:326:ARG:NH1  | 1:B:329:ASP:OD2  | 2.51                     | 0.43              |
| 1:B:913:MET:HE3  | 1:B:940:TYR:CG   | 2.53                     | 0.43              |
| 1:B:978:HIS:NE2  | 1:B:982:GLU:OE2  | 2.51                     | 0.43              |
| 1:E:137:LEU:O    | 1:E:140:THR:OG1  | 2.31                     | 0.43              |
| 1:E:240:PHE:CD1  | 1:E:240:PHE:C    | 2.96                     | 0.43              |
| 1:E:635:GLY:C    | 1:E:637:SER:N    | 2.76                     | 0.43              |
| 1:E:893:LYS:HZ3  | 1:E:933:PHE:HA   | 1.84                     | 0.43              |
| 1:F:357:MET:HG2  | 1:F:361:PHE:CZ   | 2.53                     | 0.43              |
| 1:F:569:MET:CE   | 1:F:621:GLU:HB3  | 2.48                     | 0.43              |
| 1:A:97:GLU:HA    | 1:A:100:PHE:HB2  | 2.00                     | 0.43              |
| 1:A:261:TYR:HD1  | 1:A:261:TYR:HA   | 1.68                     | 0.43              |
| 1:A:955:ILE:HB   | 1:A:958:TRP:CE2  | 2.54                     | 0.43              |
| 1:B:231:TRP:CE2  | 1:B:235:LEU:HD11 | 2.54                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:256:GLU:O     | 1:B:259:ILE:HG22 | 2.18                     | 0.43              |
| 1:B:369:GLU:HA    | 1:B:372:LYS:HD3  | 2.01                     | 0.43              |
| 1:B:577:GLY:N     | 2:D:7:ASP:OD1    | 2.47                     | 0.43              |
| 1:B:646:PHE:HB3   | 1:B:677:ARG:CZ   | 2.49                     | 0.43              |
| 1:B:964:ASP:C     | 1:B:966:LEU:N    | 2.72                     | 0.43              |
| 1:E:282:TYR:O     | 1:E:283:LEU:HB3  | 2.18                     | 0.43              |
| 1:E:315:LYS:HD2   | 1:E:315:LYS:HA   | 1.77                     | 0.43              |
| 1:E:528:PHE:O     | 1:E:531:MET:HB2  | 2.18                     | 0.43              |
| 1:E:987:ARG:O     | 1:E:991:SER:HB3  | 2.18                     | 0.43              |
| 1:F:94:VAL:HG13   | 1:F:95:LYS:HG2   | 2.00                     | 0.43              |
| 1:F:412:LEU:O     | 1:F:416:GLY:N    | 2.51                     | 0.43              |
| 1:A:206:THR:O     | 1:A:210:THR:HG23 | 2.19                     | 0.43              |
| 1:A:326:ARG:NH1   | 1:A:328:ILE:HB   | 2.33                     | 0.43              |
| 1:A:395:CYS:SG    | 1:A:396:MET:N    | 2.91                     | 0.43              |
| 1:A:421:MET:HA    | 1:A:424:PHE:HB3  | 2.01                     | 0.43              |
| 1:B:304:LYS:HE3   | 1:B:306:ASP:HB2  | 1.99                     | 0.43              |
| 1:E:247:ARG:O     | 1:E:271:ALA:N    | 2.52                     | 0.43              |
| 1:E:373:LEU:HD12  | 1:E:373:LEU:HA   | 1.72                     | 0.43              |
| 1:E:479:TYR:CG    | 1:E:524:ILE:HG12 | 2.54                     | 0.43              |
| 1:E:729:SER:C     | 1:E:732:GLY:H    | 2.26                     | 0.43              |
| 1:E:850:LYS:C     | 1:E:854:LEU:HG   | 2.43                     | 0.43              |
| 1:E:1000:LEU:HD12 | 1:E:1004:PHE:HD2 | 1.84                     | 0.43              |
| 1:F:25:ASN:OD1    | 1:F:25:ASN:C     | 2.61                     | 0.43              |
| 1:F:152:ILE:HA    | 1:F:157:ASP:CG   | 2.43                     | 0.43              |
| 1:F:376:LYS:O     | 1:F:379:GLU:HG3  | 2.17                     | 0.43              |
| 1:F:620:ILE:O     | 1:F:620:ILE:HG13 | 2.18                     | 0.43              |
| 1:F:751:ILE:HA    | 1:F:754:ARG:HE   | 1.83                     | 0.43              |
| 1:F:815:PHE:HD2   | 1:F:844:LEU:HD23 | 1.84                     | 0.43              |
| 1:F:906:THR:HB    | 2:G:232:ALA:C    | 2.43                     | 0.43              |
| 1:A:304:LYS:HE2   | 1:A:306:ASP:HB2  | 2.00                     | 0.43              |
| 1:A:717:LYS:HG3   | 1:A:757:TRP:HH2  | 1.84                     | 0.43              |
| 1:A:751:ILE:HA    | 1:A:754:ARG:CB   | 2.48                     | 0.43              |
| 1:A:766:GLU:HB2   | 1:A:768:PRO:HD3  | 2.00                     | 0.43              |
| 1:A:774:ILE:HD12  | 1:A:774:ILE:N    | 2.34                     | 0.43              |
| 1:B:42:LEU:HB3    | 1:B:44:PHE:CE1   | 2.53                     | 0.43              |
| 1:B:118:HIS:HA    | 1:B:121:ILE:CG2  | 2.46                     | 0.43              |
| 1:B:661:ILE:HA    | 1:B:665:LYS:CE   | 2.48                     | 0.43              |
| 1:B:696:THR:O     | 1:B:700:SER:CB   | 2.67                     | 0.43              |
| 2:D:32:PHE:CD1    | 2:D:61:LEU:HD13  | 2.53                     | 0.43              |
| 1:E:657:ARG:HB3   | 1:E:658:HIS:CE1  | 2.54                     | 0.43              |
| 1:E:892:ARG:HD2   | 1:E:892:ARG:HA   | 1.70                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:119:ASP:HB2  | 1:F:120:LYS:HZ2  | 1.82                     | 0.43              |
| 1:F:136:ASN:O    | 1:F:140:THR:HG23 | 2.19                     | 0.43              |
| 1:F:827:LEU:HG   | 1:F:834:GLN:HE21 | 1.84                     | 0.43              |
| 1:A:473:LEU:HD12 | 1:A:600:LEU:CD2  | 2.47                     | 0.43              |
| 1:A:515:ILE:O    | 1:A:518:GLU:HG3  | 2.19                     | 0.43              |
| 1:A:998:GLU:O    | 1:A:1002:ASN:HB2 | 2.19                     | 0.43              |
| 1:B:136:ASN:C    | 1:B:136:ASN:OD1  | 2.61                     | 0.43              |
| 1:B:493:ASN:C    | 1:B:494:GLY:O    | 2.60                     | 0.43              |
| 1:B:608:PHE:O    | 1:B:612:ILE:HG13 | 2.19                     | 0.43              |
| 1:E:886:ILE:HD12 | 1:E:886:ILE:HA   | 1.85                     | 0.43              |
| 1:F:29:CYS:SG    | 1:F:244:PHE:HE1  | 2.42                     | 0.43              |
| 1:F:89:GLN:HB3   | 1:F:186:LYS:HZ3  | 1.82                     | 0.43              |
| 1:A:237:LYS:HB2  | 1:A:238:ASP:OD1  | 2.18                     | 0.43              |
| 1:A:531:MET:HE3  | 1:A:532:PRO:CD   | 2.48                     | 0.43              |
| 1:B:425:ILE:HG12 | 1:B:442:LEU:HD23 | 2.01                     | 0.43              |
| 1:B:589:TYR:HA   | 1:B:592:LEU:HB3  | 1.99                     | 0.43              |
| 1:B:607:GLU:HG3  | 1:B:608:PHE:N    | 2.32                     | 0.43              |
| 2:C:5:ILE:O      | 2:C:6:GLN:HB3    | 2.18                     | 0.43              |
| 1:E:100:PHE:O    | 1:E:104:LEU:HG   | 2.19                     | 0.43              |
| 1:E:317:SER:OG   | 1:E:318:PRO:HD3  | 2.18                     | 0.43              |
| 1:E:627:ARG:CZ   | 1:E:675:LYS:HB3  | 2.48                     | 0.43              |
| 1:E:767:LEU:HB2  | 1:E:811:PHE:HE2  | 1.82                     | 0.43              |
| 1:F:224:ASN:OD1  | 1:F:225:ILE:N    | 2.52                     | 0.43              |
| 1:F:549:GLN:O    | 1:F:552:TYR:N    | 2.51                     | 0.43              |
| 1:F:627:ARG:HE   | 1:F:675:LYS:HZ2  | 1.67                     | 0.43              |
| 1:F:631:ILE:HG21 | 1:F:635:GLY:HA3  | 2.00                     | 0.43              |
| 1:F:672:SER:OG   | 1:F:672:SER:O    | 2.36                     | 0.43              |
| 1:A:396:MET:O    | 1:A:400:ALA:N    | 2.52                     | 0.43              |
| 1:A:661:ILE:HD11 | 2:D:219:LYS:NZ   | 2.33                     | 0.43              |
| 1:B:79:TYR:HB3   | 1:B:83:GLU:HB2   | 2.00                     | 0.43              |
| 1:B:661:ILE:HA   | 1:B:665:LYS:HE3  | 2.00                     | 0.43              |
| 1:E:148:TYR:CD2  | 1:F:532:PRO:HG3  | 2.54                     | 0.43              |
| 1:E:435:ASP:HA   | 1:E:438:LYS:HE2  | 2.01                     | 0.43              |
| 1:E:807:LEU:HD12 | 1:E:808:ILE:HG22 | 2.01                     | 0.43              |
| 1:F:41:LYS:NZ    | 1:F:211:HIS:HA   | 2.31                     | 0.43              |
| 1:F:950:ASP:OD1  | 1:F:950:ASP:O    | 2.37                     | 0.43              |
| 1:A:225:ILE:HG13 | 1:A:226:ASN:N    | 2.33                     | 0.42              |
| 1:A:551:LEU:HA   | 1:A:554:ASP:OD2  | 2.18                     | 0.42              |
| 1:A:626:GLU:OE2  | 1:A:629:ARG:HD2  | 2.18                     | 0.42              |
| 1:A:802:ARG:CZ   | 1:A:867:ASN:HA   | 2.49                     | 0.42              |
| 1:A:866:MET:HA   | 1:A:869:ILE:HG22 | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:85:LEU:O     | 1:B:187:GLU:HB3  | 2.19                     | 0.42              |
| 1:B:254:GLU:OE1  | 1:B:254:GLU:N    | 2.52                     | 0.42              |
| 1:B:438:LYS:HA   | 1:B:441:PHE:HD1  | 1.83                     | 0.42              |
| 1:B:902:LYS:HB3  | 1:B:904:ILE:HD11 | 2.00                     | 0.42              |
| 2:C:170:ARG:O    | 2:C:171:TYR:C    | 2.42                     | 0.42              |
| 1:E:487:GLN:HG2  | 1:E:491:GLN:NE2  | 2.34                     | 0.42              |
| 1:E:880:GLU:HA   | 1:E:883:GLU:OE1  | 2.19                     | 0.42              |
| 1:F:851:SER:OG   | 1:F:852:HIS:N    | 2.50                     | 0.42              |
| 2:G:72:TRP:N     | 2:G:72:TRP:CD1   | 2.87                     | 0.42              |
| 1:A:170:VAL:HA   | 1:A:200:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:660:LYS:O    | 1:A:664:ILE:HD13 | 2.18                     | 0.42              |
| 1:B:105:LYS:HE3  | 1:B:105:LYS:HB3  | 1.68                     | 0.42              |
| 1:E:213:ILE:HB   | 1:E:243:PRO:HB3  | 2.01                     | 0.42              |
| 1:E:220:LEU:HD21 | 1:E:247:ARG:HH22 | 1.84                     | 0.42              |
| 1:E:322:LEU:HD13 | 1:E:322:LEU:HA   | 1.86                     | 0.42              |
| 1:E:605:PHE:HA   | 2:H:207:SER:CB   | 2.42                     | 0.42              |
| 1:E:695:ILE:HB   | 1:E:699:PHE:CE2  | 2.54                     | 0.42              |
| 1:E:724:LYS:NZ   | 1:E:764:CYS:HB2  | 2.33                     | 0.42              |
| 1:E:869:ILE:HD12 | 2:H:50:LEU:HG    | 2.01                     | 0.42              |
| 1:F:346:VAL:H    | 1:F:396:MET:HA   | 1.83                     | 0.42              |
| 1:F:802:ARG:HE   | 1:F:840:LYS:HA   | 1.85                     | 0.42              |
| 1:F:921:PHE:CE2  | 1:F:970:ILE:HD13 | 2.54                     | 0.42              |
| 2:G:212:ASN:C    | 2:G:214:LEU:N    | 2.72                     | 0.42              |
| 2:H:22:VAL:HA    | 2:H:69:ASP:H     | 1.84                     | 0.42              |
| 1:A:87:ILE:N     | 1:A:88:PRO:HD2   | 2.34                     | 0.42              |
| 1:A:491:GLN:C    | 1:A:494:GLY:H    | 2.27                     | 0.42              |
| 1:B:533:PHE:N    | 1:B:533:PHE:HD1  | 2.17                     | 0.42              |
| 1:E:24:ASN:OD1   | 1:E:25:ASN:N     | 2.52                     | 0.42              |
| 1:E:53:LEU:HD11  | 1:E:286:TYR:HE2  | 1.81                     | 0.42              |
| 1:F:216:ILE:HG22 | 1:F:246:ILE:HG13 | 2.01                     | 0.42              |
| 1:F:965:LYS:HZ2  | 2:G:49:PRO:HA    | 1.83                     | 0.42              |
| 2:H:21:LEU:O     | 2:H:71:GLU:HB3   | 2.19                     | 0.42              |
| 2:H:63:VAL:HG22  | 2:H:220:PHE:HZ   | 1.83                     | 0.42              |
| 1:A:214:VAL:HG12 | 1:A:244:PHE:HD2  | 1.85                     | 0.42              |
| 1:A:215:PHE:HB2  | 1:A:245:PHE:HD1  | 1.82                     | 0.42              |
| 1:A:286:TYR:N    | 1:A:286:TYR:CD1  | 2.87                     | 0.42              |
| 1:A:581:ASP:O    | 1:A:582:ILE:C    | 2.54                     | 0.42              |
| 1:A:581:ASP:O    | 1:A:585:LEU:N    | 2.39                     | 0.42              |
| 1:B:27:VAL:HA    | 1:B:30:ILE:HG22  | 2.01                     | 0.42              |
| 1:B:606:HIS:ND1  | 1:B:609:HIS:HB3  | 2.35                     | 0.42              |
| 1:B:696:THR:O    | 1:B:700:SER:OG   | 2.36                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:130:ILE:HA   | 1:E:168:LEU:O    | 2.19                     | 0.42              |
| 1:F:626:GLU:HG2  | 1:F:629:ARG:NH2  | 2.35                     | 0.42              |
| 2:H:192:TYR:O    | 2:H:234:VAL:HA   | 2.20                     | 0.42              |
| 1:A:248:THR:HB   | 1:A:286:TYR:CZ   | 2.54                     | 0.42              |
| 1:A:657:ARG:HA   | 1:A:715:GLU:CD   | 2.44                     | 0.42              |
| 1:A:659:PHE:HD2  | 1:A:718:ALA:HB1  | 1.85                     | 0.42              |
| 1:A:744:PHE:HD1  | 1:A:745:PRO:HD2  | 1.84                     | 0.42              |
| 1:B:75:LYS:HB3   | 1:B:79:TYR:CZ    | 2.54                     | 0.42              |
| 1:E:304:LYS:CD   | 1:E:307:GLU:H    | 2.32                     | 0.42              |
| 1:E:326:ARG:HD2  | 1:E:328:ILE:CD1  | 2.49                     | 0.42              |
| 1:E:556:VAL:HG11 | 1:F:552:TYR:CE2  | 2.53                     | 0.42              |
| 1:E:687:TYR:O    | 1:E:691:ILE:HG12 | 2.19                     | 0.42              |
| 1:E:801:SER:OG   | 1:E:841:LEU:HD11 | 2.20                     | 0.42              |
| 1:F:117:ILE:HD12 | 1:F:290:MET:SD   | 2.60                     | 0.42              |
| 1:F:697:LYS:HE2  | 1:F:697:LYS:HB2  | 1.87                     | 0.42              |
| 1:A:128:HIS:CE1  | 1:A:165:ARG:HA   | 2.54                     | 0.42              |
| 1:A:473:LEU:HA   | 1:A:476:ILE:CG2  | 2.49                     | 0.42              |
| 1:B:438:LYS:O    | 1:B:442:LEU:HG   | 2.19                     | 0.42              |
| 1:B:547:ASP:N    | 1:B:547:ASP:OD1  | 2.49                     | 0.42              |
| 2:D:27:ALA:HB1   | 2:D:64:LYS:H     | 1.85                     | 0.42              |
| 1:E:131:THR:HG22 | 1:E:169:LYS:HB2  | 2.01                     | 0.42              |
| 1:E:477:ASN:O    | 1:E:481:ILE:HG22 | 2.18                     | 0.42              |
| 1:E:955:ILE:HB   | 1:E:958:TRP:CE2  | 2.55                     | 0.42              |
| 1:F:66:TYR:CB    | 1:F:87:ILE:HG12  | 2.50                     | 0.42              |
| 1:F:255:ASN:O    | 1:F:258:LEU:HG   | 2.19                     | 0.42              |
| 1:F:289:VAL:HG23 | 1:F:290:MET:CE   | 2.50                     | 0.42              |
| 1:F:450:GLU:H    | 1:F:450:GLU:CD   | 2.28                     | 0.42              |
| 1:F:724:LYS:HD3  | 1:F:760:ARG:NH2  | 2.35                     | 0.42              |
| 2:H:227:ASP:O    | 2:H:228:THR:OG1  | 2.25                     | 0.42              |
| 1:A:585:LEU:HA   | 1:A:588:LEU:HB2  | 2.02                     | 0.42              |
| 1:A:750:ASP:O    | 1:A:753:LYS:HB2  | 2.20                     | 0.42              |
| 1:A:949:PHE:CE2  | 1:A:951:TYR:HA   | 2.54                     | 0.42              |
| 1:B:69:GLU:N     | 1:B:69:GLU:OE1   | 2.52                     | 0.42              |
| 1:B:247:ARG:HD3  | 1:B:249:ASP:HB2  | 2.02                     | 0.42              |
| 1:E:454:LEU:O    | 1:E:458:ILE:HG23 | 2.19                     | 0.42              |
| 1:E:606:HIS:CE1  | 2:H:205:GLU:O    | 2.73                     | 0.42              |
| 1:E:613:ARG:O    | 1:E:616:MET:HG3  | 2.20                     | 0.42              |
| 1:E:660:LYS:HD2  | 1:E:661:ILE:HG22 | 2.00                     | 0.42              |
| 1:E:869:ILE:HG22 | 1:E:874:ILE:HB   | 2.02                     | 0.42              |
| 1:E:916:PHE:HA   | 1:E:919:TRP:CE3  | 2.55                     | 0.42              |
| 1:F:656:SER:C    | 1:F:715:GLU:HG3  | 2.45                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:865:LEU:O    | 1:F:866:MET:C    | 2.62                     | 0.42              |
| 1:F:984:LEU:HD22 | 1:F:1000:LEU:HB2 | 2.02                     | 0.42              |
| 2:G:170:ARG:HB3  | 2:G:172:GLU:OE2  | 2.19                     | 0.42              |
| 2:H:15:ARG:HB2   | 2:H:171:TYR:CE1  | 2.55                     | 0.42              |
| 1:A:208:ILE:HD13 | 1:A:213:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:345:THR:HG22 | 1:A:395:CYS:O    | 2.20                     | 0.42              |
| 1:A:757:TRP:HA   | 1:A:760:ARG:HB2  | 2.00                     | 0.42              |
| 1:A:937:ASP:HB3  | 1:A:940:TYR:HB2  | 2.01                     | 0.42              |
| 1:B:231:TRP:NE1  | 1:B:235:LEU:HD11 | 2.34                     | 0.42              |
| 1:B:664:ILE:HG13 | 1:B:668:GLU:OE1  | 2.20                     | 0.42              |
| 1:B:830:ASP:OD1  | 1:B:830:ASP:N    | 2.52                     | 0.42              |
| 1:B:870:ARG:HA   | 2:C:51:TYR:CZ    | 2.55                     | 0.42              |
| 2:D:189:SER:HA   | 2:D:238:SER:HB3  | 2.01                     | 0.42              |
| 1:E:304:LYS:HD2  | 1:E:306:ASP:N    | 2.35                     | 0.42              |
| 1:E:574:TYR:HD2  | 2:G:32:PHE:HB2   | 1.85                     | 0.42              |
| 1:E:618:LEU:O    | 1:E:621:GLU:HB2  | 2.20                     | 0.42              |
| 1:F:44:PHE:HD1   | 1:F:214:VAL:HB   | 1.84                     | 0.42              |
| 1:F:305:ASP:O    | 1:F:309:ILE:HG12 | 2.19                     | 0.42              |
| 1:A:676:ILE:CG2  | 1:A:677:ARG:N    | 2.78                     | 0.42              |
| 1:A:747:ARG:HD3  | 1:A:747:ARG:HA   | 1.66                     | 0.42              |
| 1:B:528:PHE:C    | 1:B:528:PHE:CD1  | 2.98                     | 0.42              |
| 1:B:708:PHE:HA   | 1:B:711:GLN:HG2  | 2.02                     | 0.42              |
| 2:C:70:LEU:HD22  | 2:C:74:ALA:N     | 2.35                     | 0.42              |
| 1:E:130:ILE:HD12 | 1:E:168:LEU:HB3  | 2.02                     | 0.42              |
| 1:E:279:GLU:OE1  | 1:E:279:GLU:N    | 2.45                     | 0.42              |
| 1:E:606:HIS:CD2  | 2:H:206:MET:O    | 2.73                     | 0.42              |
| 1:F:186:LYS:HZ2  | 1:F:188:ASP:H    | 1.66                     | 0.42              |
| 1:F:245:PHE:N    | 1:F:267:ARG:O    | 2.51                     | 0.42              |
| 1:F:409:ILE:HG13 | 1:F:650:TYR:CE2  | 2.55                     | 0.42              |
| 1:F:657:ARG:NH1  | 1:F:715:GLU:OE1  | 2.53                     | 0.42              |
| 1:F:782:GLN:OE1  | 1:F:785:LYS:HD2  | 2.20                     | 0.42              |
| 2:G:212:ASN:CG   | 2:G:214:LEU:H    | 2.28                     | 0.42              |
| 1:A:91:PHE:CE2   | 1:A:103:ILE:HD12 | 2.54                     | 0.42              |
| 1:A:481:ILE:O    | 1:A:485:ILE:HG13 | 2.20                     | 0.42              |
| 1:A:606:HIS:HA   | 2:D:206:MET:O    | 2.19                     | 0.42              |
| 1:A:772:ILE:HD12 | 1:A:775:ILE:HD13 | 2.02                     | 0.42              |
| 1:B:391:ASN:ND2  | 1:B:393:VAL:HG23 | 2.34                     | 0.42              |
| 1:B:418:TYR:O    | 1:B:422:LYS:HG3  | 2.20                     | 0.42              |
| 1:B:473:LEU:HD21 | 1:B:542:LEU:HD21 | 2.00                     | 0.42              |
| 1:B:560:GLU:OE1  | 1:B:564:LYS:HD2  | 2.20                     | 0.42              |
| 1:B:655:ILE:O    | 1:B:659:PHE:HB2  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:892:ARG:HH21 | 1:B:908:SER:HB2  | 1.83                     | 0.42              |
| 2:C:36:ILE:HA    | 2:C:56:GLU:O     | 2.20                     | 0.42              |
| 1:E:432:ILE:H    | 1:E:432:ILE:HG12 | 1.64                     | 0.42              |
| 1:E:660:LYS:N    | 1:E:663:ASP:OD2  | 2.45                     | 0.42              |
| 1:E:801:SER:CB   | 1:E:841:LEU:HD11 | 2.50                     | 0.42              |
| 1:F:71:TYR:O     | 1:F:73:SER:N     | 2.53                     | 0.42              |
| 1:F:185:LEU:HD12 | 1:F:185:LEU:HA   | 1.88                     | 0.42              |
| 1:F:871:ILE:HG13 | 1:F:872:GLY:N    | 2.35                     | 0.42              |
| 1:F:899:GLU:CD   | 1:F:904:ILE:HG13 | 2.45                     | 0.42              |
| 2:H:23:PHE:CE1   | 2:H:66:ALA:HB2   | 2.37                     | 0.42              |
| 2:H:192:TYR:CD2  | 2:H:235:ILE:HB   | 2.55                     | 0.42              |
| 1:A:117:ILE:O    | 1:A:121:ILE:HG12 | 2.19                     | 0.41              |
| 1:A:258:LEU:O    | 1:A:262:GLU:HG3  | 2.20                     | 0.41              |
| 1:A:607:GLU:OE1  | 1:A:607:GLU:HA   | 2.19                     | 0.41              |
| 1:A:699:PHE:CB   | 1:A:704:MET:HG3  | 2.48                     | 0.41              |
| 1:A:709:TYR:O    | 1:A:712:PHE:HB2  | 2.20                     | 0.41              |
| 1:A:861:ASN:O    | 1:A:865:LEU:N    | 2.48                     | 0.41              |
| 1:A:997:LEU:O    | 1:A:1000:LEU:HG  | 2.19                     | 0.41              |
| 1:B:147:LYS:N    | 1:B:147:LYS:HD3  | 2.33                     | 0.41              |
| 1:E:115:ASN:OD1  | 1:E:118:HIS:ND1  | 2.53                     | 0.41              |
| 1:E:627:ARG:NH1  | 1:E:675:LYS:HB3  | 2.35                     | 0.41              |
| 1:E:755:TYR:CE1  | 1:E:807:LEU:HD23 | 2.54                     | 0.41              |
| 1:E:834:GLN:HA   | 1:E:837:PHE:HB3  | 2.01                     | 0.41              |
| 1:E:919:TRP:O    | 1:E:924:GLU:HB2  | 2.20                     | 0.41              |
| 1:F:68:GLU:OE1   | 1:F:74:PRO:HD3   | 2.20                     | 0.41              |
| 1:F:385:PHE:CE1  | 1:F:389:GLU:HG3  | 2.55                     | 0.41              |
| 1:F:647:MET:SD   | 1:F:678:PHE:HD1  | 2.43                     | 0.41              |
| 1:F:795:SER:OG   | 1:F:799:LEU:HG   | 2.20                     | 0.41              |
| 2:H:170:ARG:O    | 2:H:171:TYR:HB2  | 2.19                     | 0.41              |
| 1:A:195:GLN:HG2  | 1:A:196:ASN:N    | 2.34                     | 0.41              |
| 1:A:198:PRO:HG3  | 1:B:235:LEU:HD22 | 2.02                     | 0.41              |
| 1:A:367:CYS:HA   | 1:A:370:ARG:NE   | 2.35                     | 0.41              |
| 1:B:286:TYR:O    | 1:B:290:MET:HE2  | 2.20                     | 0.41              |
| 1:B:332:HIS:HB2  | 1:B:541:ILE:HG13 | 2.02                     | 0.41              |
| 1:B:407:ILE:HD12 | 1:B:589:TYR:CB   | 2.50                     | 0.41              |
| 1:B:509:ASP:N    | 1:B:509:ASP:OD1  | 2.53                     | 0.41              |
| 2:D:178:ILE:HG12 | 2:D:190:ASP:OD1  | 2.20                     | 0.41              |
| 1:E:92:TYR:HA    | 1:E:96:GLY:O     | 2.19                     | 0.41              |
| 1:E:472:TYR:CD2  | 1:E:542:LEU:HG   | 2.55                     | 0.41              |
| 1:E:491:GLN:O    | 1:E:495:LEU:HD23 | 2.20                     | 0.41              |
| 1:E:801:SER:HB3  | 1:E:841:LEU:HD11 | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:946:PRO:HG2  | 1:E:975:HIS:CE1  | 2.55                     | 0.41              |
| 1:F:43:VAL:HG12  | 1:F:212:THR:O    | 2.19                     | 0.41              |
| 1:F:256:GLU:HA   | 1:F:259:ILE:HG12 | 2.02                     | 0.41              |
| 1:F:569:MET:SD   | 1:F:625:TYR:HD2  | 2.44                     | 0.41              |
| 1:F:711:GLN:C    | 1:F:712:PHE:CD1  | 2.98                     | 0.41              |
| 1:F:959:LEU:O    | 1:F:960:LYS:C    | 2.61                     | 0.41              |
| 2:H:66:ALA:HB3   | 2:H:218:ILE:HD11 | 2.03                     | 0.41              |
| 1:A:338:TYR:HE1  | 1:A:351:ASN:HB2  | 1.84                     | 0.41              |
| 1:A:411:SER:HB2  | 1:A:415:HIS:CE1  | 2.54                     | 0.41              |
| 1:A:531:MET:HE3  | 1:A:531:MET:HA   | 2.03                     | 0.41              |
| 1:A:582:ILE:O    | 1:A:585:LEU:N    | 2.52                     | 0.41              |
| 1:A:750:ASP:CG   | 1:A:796:SER:HB3  | 2.44                     | 0.41              |
| 1:B:657:ARG:HA   | 1:B:715:GLU:HG3  | 2.01                     | 0.41              |
| 1:B:857:LYS:HA   | 1:B:857:LYS:HD3  | 1.83                     | 0.41              |
| 1:B:960:LYS:HD3  | 1:B:996:TYR:CE1  | 2.55                     | 0.41              |
| 1:E:298:GLU:C    | 1:E:300:LYS:N    | 2.78                     | 0.41              |
| 1:E:674:ASP:HA   | 1:E:725:TYR:CZ   | 2.54                     | 0.41              |
| 1:E:816:ILE:HG22 | 1:E:818:LYS:HG2  | 2.02                     | 0.41              |
| 1:E:887:GLU:O    | 1:E:890:GLU:HG3  | 2.20                     | 0.41              |
| 1:E:889:LEU:HB3  | 1:E:933:PHE:CE2  | 2.55                     | 0.41              |
| 1:F:422:LYS:HD2  | 1:F:422:LYS:C    | 2.45                     | 0.41              |
| 1:F:615:SER:O    | 1:F:619:LEU:HG   | 2.21                     | 0.41              |
| 1:F:653:VAL:HG22 | 1:F:687:TYR:CE1  | 2.56                     | 0.41              |
| 1:F:677:ARG:HG2  | 1:F:678:PHE:H    | 1.85                     | 0.41              |
| 1:F:821:SER:O    | 1:F:825:LEU:HG   | 2.19                     | 0.41              |
| 1:A:208:ILE:HA   | 1:A:213:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:675:LYS:O    | 1:A:678:PHE:HB3  | 2.20                     | 0.41              |
| 1:A:890:GLU:O    | 1:A:893:LYS:HG2  | 2.20                     | 0.41              |
| 1:B:48:ALA:HA    | 1:B:133:ASN:HB3  | 2.02                     | 0.41              |
| 1:B:283:LEU:HD12 | 1:B:284:GLU:HG3  | 2.01                     | 0.41              |
| 1:B:286:TYR:O    | 1:B:289:VAL:HG12 | 2.20                     | 0.41              |
| 1:B:420:VAL:HB   | 1:B:424:PHE:CZ   | 2.55                     | 0.41              |
| 1:E:124:MET:CE   | 1:E:124:MET:H    | 2.33                     | 0.41              |
| 1:E:375:LYS:NZ   | 1:E:379:GLU:OE1  | 2.46                     | 0.41              |
| 1:E:705:ASN:O    | 1:E:705:ASN:OD1  | 2.38                     | 0.41              |
| 1:E:708:PHE:CD1  | 1:E:711:GLN:HB3  | 2.55                     | 0.41              |
| 1:E:1002:ASN:N   | 1:E:1005:ILE:OXT | 2.50                     | 0.41              |
| 1:E:1003:TYR:O   | 1:E:1004:PHE:C   | 2.62                     | 0.41              |
| 1:F:41:LYS:NZ    | 1:F:210:THR:O    | 2.53                     | 0.41              |
| 1:F:383:ALA:O    | 1:F:386:ASN:HB2  | 2.20                     | 0.41              |
| 1:F:435:ASP:O    | 1:F:438:LYS:HB2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:660:LYS:HE2  | 2:G:203:GLU:OE2  | 2.20                     | 0.41              |
| 1:F:804:TYR:O    | 1:F:808:ILE:HD12 | 2.21                     | 0.41              |
| 1:F:845:LEU:HD13 | 1:F:849:ALA:HB1  | 2.03                     | 0.41              |
| 2:G:14:LYS:NZ    | 2:G:174:GLU:HB2  | 2.35                     | 0.41              |
| 1:A:82:ASP:OD1   | 1:A:82:ASP:C     | 2.64                     | 0.41              |
| 1:A:652:PHE:CD1  | 1:A:684:ILE:HG23 | 2.55                     | 0.41              |
| 1:B:33:ILE:HG12  | 1:B:33:ILE:H     | 1.72                     | 0.41              |
| 1:B:813:LYS:HE2  | 1:B:813:LYS:HB2  | 1.93                     | 0.41              |
| 2:C:240:ASP:N    | 2:C:240:ASP:OD1  | 2.50                     | 0.41              |
| 1:E:741:LEU:HD12 | 1:E:778:PHE:CG   | 2.56                     | 0.41              |
| 1:E:769:LYS:HA   | 1:E:772:ILE:HD13 | 2.02                     | 0.41              |
| 1:E:777:ASP:OD1  | 1:E:819:ARG:NH2  | 2.53                     | 0.41              |
| 1:F:362:GLU:O    | 1:F:365:GLU:HG2  | 2.20                     | 0.41              |
| 2:G:15:ARG:N     | 2:G:20:LYS:HE3   | 2.35                     | 0.41              |
| 1:A:85:LEU:HB2   | 1:A:187:GLU:OE2  | 2.20                     | 0.41              |
| 1:A:235:LEU:O    | 1:A:237:LYS:HG2  | 2.20                     | 0.41              |
| 1:A:326:ARG:HA   | 1:A:593:ARG:HH21 | 1.86                     | 0.41              |
| 1:A:404:ASN:OD1  | 2:C:5:ILE:HG23   | 2.21                     | 0.41              |
| 1:A:607:GLU:HB3  | 1:A:610:GLN:HB2  | 2.02                     | 0.41              |
| 1:A:713:ILE:HG23 | 1:A:717:LYS:H    | 1.86                     | 0.41              |
| 1:A:800:TYR:C    | 1:A:802:ARG:N    | 2.78                     | 0.41              |
| 1:A:885:ILE:HG12 | 1:A:916:PHE:CE1  | 2.55                     | 0.41              |
| 1:B:337:ASP:OD1  | 1:B:338:TYR:N    | 2.54                     | 0.41              |
| 1:B:437:LYS:O    | 1:B:441:PHE:CD1  | 2.74                     | 0.41              |
| 1:B:801:SER:HA   | 1:B:804:TYR:CD2  | 2.55                     | 0.41              |
| 1:E:635:GLY:O    | 1:E:636:PHE:C    | 2.61                     | 0.41              |
| 1:E:892:ARG:HG3  | 1:E:913:MET:HE1  | 2.03                     | 0.41              |
| 1:F:449:GLU:CB   | 1:F:511:PHE:HE2  | 2.34                     | 0.41              |
| 1:F:799:LEU:HA   | 1:F:799:LEU:HD23 | 1.58                     | 0.41              |
| 1:F:869:ILE:HD12 | 1:F:874:ILE:O    | 2.17                     | 0.41              |
| 1:A:86:ARG:NH1   | 1:A:89:GLN:HB3   | 2.33                     | 0.41              |
| 1:A:198:PRO:HG2  | 1:B:235:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:277:SER:HB3  | 1:A:285:ARG:HH21 | 1.86                     | 0.41              |
| 1:A:284:GLU:OE1  | 1:A:285:ARG:NH2  | 2.53                     | 0.41              |
| 1:A:578:MET:O    | 1:A:578:MET:HG3  | 2.19                     | 0.41              |
| 1:B:479:TYR:CE2  | 1:B:524:ILE:HG21 | 2.56                     | 0.41              |
| 1:B:491:GLN:CD   | 2:C:206:MET:HG2  | 2.46                     | 0.41              |
| 1:B:961:ASN:OD1  | 1:B:961:ASN:N    | 2.52                     | 0.41              |
| 1:E:23:ASP:O     | 1:E:27:VAL:HG23  | 2.20                     | 0.41              |
| 1:E:552:TYR:CE1  | 1:F:556:VAL:HG11 | 2.56                     | 0.41              |
| 1:E:880:GLU:HA   | 1:E:883:GLU:CD   | 2.45                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:952:LYS:HB2  | 1:E:952:LYS:HE3  | 1.77                     | 0.41              |
| 1:F:131:THR:O    | 1:F:169:LYS:HA   | 2.20                     | 0.41              |
| 1:F:173:ASP:N    | 1:F:173:ASP:OD1  | 2.53                     | 0.41              |
| 1:F:376:LYS:HA   | 1:F:376:LYS:HD2  | 1.93                     | 0.41              |
| 1:F:610:GLN:CD   | 1:F:613:ARG:HH22 | 2.28                     | 0.41              |
| 1:F:625:TYR:C    | 1:F:625:TYR:CD1  | 2.99                     | 0.41              |
| 1:F:802:ARG:HB2  | 1:F:840:LYS:CA   | 2.50                     | 0.41              |
| 2:G:214:LEU:HA   | 2:G:214:LEU:HD13 | 1.59                     | 0.41              |
| 1:A:323:GLN:HB2  | 1:A:597:GLU:OE1  | 2.21                     | 0.41              |
| 1:A:331:LYS:C    | 1:A:332:HIS:CG   | 2.99                     | 0.41              |
| 1:B:54:SER:O     | 1:B:54:SER:OG    | 2.30                     | 0.41              |
| 1:B:95:LYS:HA    | 1:B:95:LYS:HD2   | 1.65                     | 0.41              |
| 1:B:148:TYR:HE2  | 1:B:163:SER:HB2  | 1.85                     | 0.41              |
| 1:B:173:ASP:C    | 1:B:183:VAL:HG23 | 2.46                     | 0.41              |
| 1:B:729:SER:O    | 1:B:731:GLU:N    | 2.54                     | 0.41              |
| 2:C:70:LEU:HD23  | 2:C:73:LEU:HB3   | 2.03                     | 0.41              |
| 1:E:116:PRO:HA   | 1:E:119:ASP:OD2  | 2.20                     | 0.41              |
| 1:E:163:SER:HA   | 1:F:533:PHE:CZ   | 2.55                     | 0.41              |
| 1:E:254:GLU:CD   | 1:E:254:GLU:N    | 2.79                     | 0.41              |
| 1:E:661:ILE:HA   | 1:E:664:ILE:HD12 | 2.03                     | 0.41              |
| 1:E:692:ALA:O    | 1:E:695:ILE:HG12 | 2.21                     | 0.41              |
| 1:E:954:PHE:HB2  | 1:E:958:TRP:HZ3  | 1.86                     | 0.41              |
| 1:F:80:SER:O     | 1:F:83:GLU:N     | 2.54                     | 0.41              |
| 1:F:455:TYR:OH   | 1:F:477:ASN:OD1  | 2.23                     | 0.41              |
| 1:F:723:ALA:O    | 1:F:726:VAL:HG22 | 2.21                     | 0.41              |
| 1:A:127:ALA:O    | 1:A:128:HIS:ND1  | 2.53                     | 0.41              |
| 1:A:316:ILE:O    | 1:A:319:LEU:HB2  | 2.20                     | 0.41              |
| 1:A:549:GLN:O    | 1:A:552:TYR:HB2  | 2.20                     | 0.41              |
| 1:A:583:VAL:HA   | 1:A:586:LEU:CD1  | 2.51                     | 0.41              |
| 1:A:655:ILE:HG21 | 1:A:722:PHE:CE1  | 2.56                     | 0.41              |
| 1:B:245:PHE:N    | 1:B:267:ARG:O    | 2.54                     | 0.41              |
| 1:B:536:GLN:HG2  | 1:B:537:LYS:N    | 2.36                     | 0.41              |
| 2:C:170:ARG:NE   | 2:C:197:ASN:OD1  | 2.54                     | 0.41              |
| 1:E:235:LEU:CG   | 1:E:236:GLN:H    | 2.34                     | 0.41              |
| 1:E:304:LYS:NZ   | 1:E:307:GLU:HB2  | 2.31                     | 0.41              |
| 1:E:324:TYR:HA   | 1:E:390:LYS:NZ   | 2.35                     | 0.41              |
| 1:E:383:ALA:HA   | 1:E:386:ASN:HD21 | 1.86                     | 0.41              |
| 1:E:440:PHE:CD1  | 1:E:440:PHE:C    | 2.94                     | 0.41              |
| 1:E:540:LYS:HE2  | 1:E:540:LYS:HB2  | 1.92                     | 0.41              |
| 1:E:606:HIS:HB3  | 1:E:610:GLN:HE21 | 1.85                     | 0.41              |
| 1:E:963:ASN:O    | 1:E:967:LEU:N    | 2.46                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:37:SER:HB3  | 1:F:42:LEU:HD22  | 2.03                     | 0.41              |
| 1:F:197:TYR:HD1 | 1:F:197:TYR:HA   | 1.81                     | 0.41              |
| 1:F:478:ARG:HA  | 1:F:481:ILE:HG22 | 2.03                     | 0.41              |
| 1:F:578:MET:HG2 | 1:F:582:ILE:HD11 | 2.03                     | 0.41              |
| 1:F:614:ASN:O   | 1:F:618:LEU:HD12 | 2.21                     | 0.41              |
| 1:F:696:THR:O   | 1:F:700:SER:OG   | 2.30                     | 0.41              |
| 1:F:706:VAL:O   | 1:F:709:TYR:N    | 2.54                     | 0.41              |
| 1:F:956:PRO:HB3 | 1:F:987:ARG:HG3  | 2.03                     | 0.41              |
| 2:G:15:ARG:HG2  | 2:G:20:LYS:HB2   | 2.03                     | 0.41              |
| 2:H:32:PHE:CE1  | 2:H:59:ILE:HG23  | 2.49                     | 0.41              |
| 2:H:206:MET:O   | 2:H:207:SER:C    | 2.64                     | 0.41              |
| 1:A:31:LYS:O    | 1:A:34:THR:OG1   | 2.36                     | 0.41              |
| 1:A:656:SER:C   | 1:A:715:GLU:HB2  | 2.46                     | 0.41              |
| 1:A:735:LYS:HD3 | 1:A:735:LYS:HA   | 1.80                     | 0.41              |
| 1:B:192:ASN:HB3 | 1:B:196:ASN:OD1  | 2.20                     | 0.41              |
| 1:B:414:TYR:OH  | 1:B:654:ASN:ND2  | 2.54                     | 0.41              |
| 2:D:64:LYS:HB2  | 2:D:217:GLU:HA   | 2.02                     | 0.41              |
| 1:E:105:LYS:HD3 | 1:E:178:PHE:HB2  | 2.03                     | 0.41              |
| 1:E:754:ARG:HB2 | 1:E:804:TYR:OH   | 2.21                     | 0.41              |
| 1:E:954:PHE:HB2 | 1:E:958:TRP:CZ3  | 2.55                     | 0.41              |
| 1:F:95:LYS:HD3  | 1:F:95:LYS:HA    | 1.94                     | 0.41              |
| 2:G:56:GLU:OE2  | 2:G:58:GLU:N     | 2.52                     | 0.41              |
| 2:G:56:GLU:OE2  | 2:G:57:LYS:N     | 2.54                     | 0.41              |
| 2:G:75:MET:O    | 2:G:75:MET:HE3   | 2.20                     | 0.41              |
| 1:A:85:LEU:HD13 | 1:A:190:TYR:CZ   | 2.56                     | 0.40              |
| 1:A:188:ASP:HA  | 1:A:191:LEU:HB3  | 2.03                     | 0.40              |
| 1:A:596:TYR:N   | 1:A:596:TYR:CD1  | 2.89                     | 0.40              |
| 1:A:740:LEU:C   | 1:A:742:PHE:N    | 2.77                     | 0.40              |
| 1:A:795:SER:OG  | 1:A:799:LEU:C    | 2.64                     | 0.40              |
| 1:A:802:ARG:CB  | 1:A:840:LYS:CB   | 2.99                     | 0.40              |
| 1:B:79:TYR:HB2  | 1:B:84:TYR:CZ    | 2.56                     | 0.40              |
| 1:B:280:TYR:HA  | 1:B:282:TYR:CZ   | 2.56                     | 0.40              |
| 1:B:412:LEU:HA  | 1:B:415:HIS:HD2  | 1.85                     | 0.40              |
| 1:B:491:GLN:NE2 | 2:C:206:MET:H    | 2.19                     | 0.40              |
| 1:B:598:ASN:OD1 | 1:B:600:LEU:N    | 2.54                     | 0.40              |
| 2:C:29:THR:OG1  | 2:C:64:LYS:HE3   | 2.21                     | 0.40              |
| 1:E:448:TRP:HZ3 | 1:E:707:VAL:HG21 | 1.86                     | 0.40              |
| 1:E:544:PHE:O   | 1:E:550:PHE:HB3  | 2.20                     | 0.40              |
| 1:F:359:ARG:HA  | 1:F:362:GLU:HB2  | 2.02                     | 0.40              |
| 1:F:407:ILE:O   | 1:F:650:TYR:HE2  | 2.05                     | 0.40              |
| 1:F:448:TRP:HB3 | 1:F:481:ILE:HD11 | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:614:ASN:OD1  | 1:F:614:ASN:C    | 2.64                     | 0.40              |
| 1:F:750:ASP:OD1  | 1:F:753:LYS:HB3  | 2.21                     | 0.40              |
| 1:F:755:TYR:HE1  | 1:F:807:LEU:HD23 | 1.86                     | 0.40              |
| 1:F:776:ASP:HB3  | 1:F:820:LEU:HD22 | 2.04                     | 0.40              |
| 1:F:960:LYS:NZ   | 1:F:999:ILE:HG13 | 2.33                     | 0.40              |
| 2:G:240:ASP:N    | 2:G:240:ASP:OD1  | 2.51                     | 0.40              |
| 2:H:11:VAL:HG13  | 2:H:175:TYR:CE1  | 2.49                     | 0.40              |
| 2:H:175:TYR:HD1  | 2:H:175:TYR:HA   | 1.75                     | 0.40              |
| 2:H:177:THR:OG1  | 2:H:191:ILE:HB   | 2.22                     | 0.40              |
| 1:A:487:GLN:HG3  | 2:D:207:SER:H    | 1.86                     | 0.40              |
| 1:A:605:PHE:HD1  | 1:A:605:PHE:HA   | 1.78                     | 0.40              |
| 1:A:711:GLN:CD   | 1:A:711:GLN:N    | 2.79                     | 0.40              |
| 1:A:717:LYS:HZ3  | 1:A:749:LEU:HD23 | 1.86                     | 0.40              |
| 1:A:780:VAL:HG13 | 1:A:820:LEU:HB3  | 2.02                     | 0.40              |
| 1:B:98:MET:HA    | 1:B:101:ASP:OD2  | 2.21                     | 0.40              |
| 1:B:442:LEU:HB3  | 1:B:447:ARG:NH1  | 2.34                     | 0.40              |
| 1:B:685:GLU:O    | 1:B:689:VAL:HG13 | 2.20                     | 0.40              |
| 2:C:61:LEU:HD23  | 2:C:175:TYR:CZ   | 2.56                     | 0.40              |
| 2:D:23:PHE:CZ    | 2:D:220:PHE:HZ   | 2.39                     | 0.40              |
| 1:E:32:GLU:CD    | 1:E:267:ARG:HH22 | 2.24                     | 0.40              |
| 1:E:235:LEU:HD23 | 1:F:198:PRO:HG2  | 2.02                     | 0.40              |
| 1:E:375:LYS:HD3  | 1:E:376:LYS:N    | 2.36                     | 0.40              |
| 1:E:415:HIS:HA   | 1:E:649:TYR:OH   | 2.20                     | 0.40              |
| 1:E:475:GLN:HB2  | 1:E:527:LEU:HD21 | 2.03                     | 0.40              |
| 1:F:64:ASP:OD1   | 1:F:64:ASP:C     | 2.64                     | 0.40              |
| 1:F:452:TYR:OH   | 1:F:514:ARG:NE   | 2.55                     | 0.40              |
| 1:F:459:ILE:HA   | 1:F:459:ILE:HD12 | 1.77                     | 0.40              |
| 1:F:869:ILE:HG12 | 1:F:919:TRP:CZ2  | 2.49                     | 0.40              |
| 1:F:888:TYR:CZ   | 1:F:912:TYR:HB2  | 2.56                     | 0.40              |
| 1:F:900:LYS:HE2  | 1:F:900:LYS:HB2  | 1.90                     | 0.40              |
| 2:G:68:PHE:O     | 2:G:68:PHE:CG    | 2.75                     | 0.40              |
| 2:G:201:SER:O    | 2:G:219:LYS:HB2  | 2.21                     | 0.40              |
| 2:H:177:THR:OG1  | 2:H:191:ILE:O    | 2.32                     | 0.40              |
| 2:H:219:LYS:HD2  | 2:H:219:LYS:C    | 2.46                     | 0.40              |
| 1:A:733:LEU:HD23 | 1:A:761:LEU:HD23 | 2.03                     | 0.40              |
| 1:A:804:TYR:O    | 1:A:808:ILE:HG12 | 2.21                     | 0.40              |
| 1:B:483:GLN:NE2  | 2:C:209:GLU:O    | 2.54                     | 0.40              |
| 1:B:622:LYS:HG3  | 1:B:623:ALA:N    | 2.36                     | 0.40              |
| 1:B:681:GLN:HE21 | 1:B:684:ILE:N    | 2.20                     | 0.40              |
| 2:C:4:VAL:O      | 2:C:4:VAL:HG12   | 2.21                     | 0.40              |
| 1:E:225:ILE:O    | 1:E:229:LEU:HD13 | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:228:LEU:O    | 1:E:229:LEU:C    | 2.64                     | 0.40              |
| 1:E:332:HIS:ND1  | 1:E:336:TYR:HE1  | 2.18                     | 0.40              |
| 1:E:452:TYR:CE1  | 1:E:478:ARG:HG3  | 2.56                     | 0.40              |
| 1:F:364:LYS:HD2  | 1:F:364:LYS:HA   | 1.61                     | 0.40              |
| 1:F:589:TYR:OH   | 1:F:651:ASP:OD1  | 2.38                     | 0.40              |
| 1:F:625:TYR:C    | 1:F:625:TYR:HD1  | 2.29                     | 0.40              |
| 1:F:767:LEU:HD13 | 1:F:811:PHE:CD1  | 2.57                     | 0.40              |
| 1:F:862:ILE:H    | 1:F:862:ILE:CD1  | 2.28                     | 0.40              |
| 2:H:169:GLU:C    | 2:H:170:ARG:O    | 2.56                     | 0.40              |
| 2:H:218:ILE:HG13 | 2:H:220:PHE:CE1  | 2.56                     | 0.40              |
| 1:A:223:TYR:HB2  | 1:A:226:ASN:HB3  | 2.03                     | 0.40              |
| 1:A:257:THR:HG23 | 1:E:86:ARG:HH22  | 1.86                     | 0.40              |
| 1:A:783:ALA:HB2  | 1:A:841:LEU:HD12 | 2.02                     | 0.40              |
| 1:B:675:LYS:NZ   | 1:B:678:PHE:HZ   | 2.19                     | 0.40              |
| 1:B:754:ARG:O    | 1:B:758:LEU:HG   | 2.21                     | 0.40              |
| 1:E:186:LYS:HD2  | 1:E:188:ASP:N    | 2.35                     | 0.40              |
| 1:E:338:TYR:CD2  | 1:E:348:ARG:HA   | 2.56                     | 0.40              |
| 1:E:538:LYS:HB3  | 1:E:538:LYS:HE2  | 1.80                     | 0.40              |
| 1:E:660:LYS:O    | 1:E:663:ASP:N    | 2.53                     | 0.40              |
| 1:E:802:ARG:H    | 1:E:840:LYS:HE2  | 1.87                     | 0.40              |
| 1:E:890:GLU:O    | 1:E:894:VAL:HG13 | 2.21                     | 0.40              |
| 1:F:70:LEU:HA    | 1:F:70:LEU:HD23  | 1.71                     | 0.40              |
| 2:G:14:LYS:HB3   | 2:G:20:LYS:O     | 2.21                     | 0.40              |
| 2:H:23:PHE:CG    | 2:H:24:THR:N     | 2.89                     | 0.40              |
| 1:A:109:GLN:O    | 1:A:109:GLN:HG2  | 2.21                     | 0.40              |
| 1:A:118:HIS:HE1  | 1:A:138:ILE:N    | 2.19                     | 0.40              |
| 1:A:491:GLN:O    | 1:A:495:LEU:N    | 2.55                     | 0.40              |
| 1:A:595:LEU:HD12 | 1:A:602:SER:HB2  | 2.03                     | 0.40              |
| 1:A:969:LYS:HA   | 1:A:969:LYS:HD3  | 1.83                     | 0.40              |
| 1:B:610:GLN:HG3  | 1:B:613:ARG:HH21 | 1.87                     | 0.40              |
| 1:B:661:ILE:HA   | 1:B:665:LYS:HD2  | 2.03                     | 0.40              |
| 2:D:45:ILE:C     | 2:D:47:ASN:H     | 2.30                     | 0.40              |
| 1:E:392:GLY:O    | 1:E:394:ILE:HG12 | 2.22                     | 0.40              |
| 1:E:634:LEU:O    | 1:E:637:SER:OG   | 2.33                     | 0.40              |
| 1:E:649:TYR:O    | 1:E:653:VAL:HG12 | 2.21                     | 0.40              |
| 1:E:811:PHE:HD1  | 1:E:811:PHE:HA   | 1.75                     | 0.40              |
| 1:E:998:GLU:OE2  | 1:E:999:ILE:HG13 | 2.21                     | 0.40              |
| 1:F:47:GLY:HA3   | 1:F:217:GLY:C    | 2.47                     | 0.40              |
| 1:F:279:GLU:OE1  | 1:F:279:GLU:C    | 2.64                     | 0.40              |
| 1:F:605:PHE:CD2  | 2:G:209:GLU:HB2  | 2.49                     | 0.40              |
| 1:F:616:MET:HA   | 1:F:619:LEU:HD12 | 2.03                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:720:LEU:HB2 | 1:F:757:TRP:CZ3  | 2.56                     | 0.40              |
| 1:F:793:GLU:OE2 | 1:F:799:LEU:HD13 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 981/1005 (98%)  | 883 (90%)  | 95 (10%)  | 3 (0%)   | 36          | 71  |
| 1   | B     | 981/1005 (98%)  | 908 (93%)  | 71 (7%)   | 2 (0%)   | 43          | 77  |
| 1   | E     | 981/1005 (98%)  | 867 (88%)  | 108 (11%) | 6 (1%)   | 21          | 58  |
| 1   | F     | 981/1005 (98%)  | 848 (86%)  | 129 (13%) | 4 (0%)   | 30          | 66  |
| 2   | C     | 147/264 (56%)   | 122 (83%)  | 25 (17%)  | 0        | 100         | 100 |
| 2   | D     | 147/264 (56%)   | 111 (76%)  | 35 (24%)  | 1 (1%)   | 18          | 55  |
| 2   | G     | 147/264 (56%)   | 116 (79%)  | 30 (20%)  | 1 (1%)   | 18          | 55  |
| 2   | H     | 147/264 (56%)   | 109 (74%)  | 38 (26%)  | 0        | 100         | 100 |
| All | All   | 4512/5076 (89%) | 3964 (88%) | 531 (12%) | 17 (0%)  | 31          | 66  |

All (17) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 768 | PRO  |
| 1   | E     | 298 | GLU  |
| 1   | E     | 726 | VAL  |
| 1   | F     | 864 | ASP  |
| 1   | A     | 676 | ILE  |
| 1   | B     | 72  | GLY  |
| 1   | B     | 580 | SER  |
| 1   | E     | 978 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 1002 | ASN  |
| 1   | F     | 934  | ILE  |
| 1   | F     | 958  | TRP  |
| 1   | E     | 299  | ASN  |
| 1   | F     | 874  | ILE  |
| 1   | A     | 332  | HIS  |
| 2   | G     | 216  | PRO  |
| 2   | D     | 214  | LEU  |
| 1   | E     | 237  | LYS  |

### 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     | 901/922 (98%)   | 885 (98%)  | 16 (2%)  | 51          | 67 |
| 1   | B     | 901/922 (98%)   | 880 (98%)  | 21 (2%)  | 44          | 63 |
| 1   | E     | 901/922 (98%)   | 886 (98%)  | 15 (2%)  | 53          | 67 |
| 1   | F     | 901/922 (98%)   | 874 (97%)  | 27 (3%)  | 36          | 57 |
| 2   | C     | 130/225 (58%)   | 124 (95%)  | 6 (5%)   | 24          | 46 |
| 2   | D     | 130/225 (58%)   | 129 (99%)  | 1 (1%)   | 73          | 77 |
| 2   | G     | 130/225 (58%)   | 123 (95%)  | 7 (5%)   | 20          | 42 |
| 2   | H     | 130/225 (58%)   | 125 (96%)  | 5 (4%)   | 29          | 50 |
| All | All   | 4124/4588 (90%) | 4026 (98%) | 98 (2%)  | 43          | 63 |

All (98) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 238 | ASP  |
| 1   | A     | 547 | ASP  |
| 1   | A     | 550 | PHE  |
| 1   | A     | 579 | SER  |
| 1   | A     | 580 | SER  |
| 1   | A     | 581 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 592 | LEU  |
| 1   | A     | 674 | ASP  |
| 1   | A     | 676 | ILE  |
| 1   | A     | 727 | LYS  |
| 1   | A     | 728 | LEU  |
| 1   | A     | 738 | LYS  |
| 1   | A     | 740 | LEU  |
| 1   | A     | 749 | LEU  |
| 1   | A     | 750 | ASP  |
| 1   | A     | 802 | ARG  |
| 1   | B     | 28  | GLU  |
| 1   | B     | 67  | HIS  |
| 1   | B     | 71  | TYR  |
| 1   | B     | 184 | VAL  |
| 1   | B     | 194 | ASP  |
| 1   | B     | 208 | ILE  |
| 1   | B     | 224 | ASN  |
| 1   | B     | 420 | VAL  |
| 1   | B     | 495 | LEU  |
| 1   | B     | 664 | ILE  |
| 1   | B     | 674 | ASP  |
| 1   | B     | 675 | LYS  |
| 1   | B     | 676 | ILE  |
| 1   | B     | 730 | GLU  |
| 1   | B     | 740 | LEU  |
| 1   | B     | 904 | ILE  |
| 1   | B     | 905 | GLN  |
| 1   | B     | 906 | THR  |
| 1   | B     | 960 | LYS  |
| 1   | B     | 961 | ASN  |
| 1   | B     | 965 | LYS  |
| 2   | C     | 5   | ILE  |
| 2   | C     | 68  | PHE  |
| 2   | C     | 69  | ASP  |
| 2   | C     | 70  | LEU  |
| 2   | C     | 71  | GLU  |
| 2   | C     | 169 | GLU  |
| 2   | D     | 231 | MET  |
| 1   | E     | 231 | TRP  |
| 1   | E     | 303 | THR  |
| 1   | E     | 304 | LYS  |
| 1   | E     | 312 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 351  | ASN  |
| 1   | E     | 357  | MET  |
| 1   | E     | 419  | ASP  |
| 1   | E     | 432  | ILE  |
| 1   | E     | 467  | ASN  |
| 1   | E     | 618  | LEU  |
| 1   | E     | 631  | ILE  |
| 1   | E     | 633  | GLU  |
| 1   | E     | 634  | LEU  |
| 1   | E     | 733  | LEU  |
| 1   | E     | 1004 | PHE  |
| 1   | F     | 119  | ASP  |
| 1   | F     | 208  | ILE  |
| 1   | F     | 512  | LEU  |
| 1   | F     | 596  | TYR  |
| 1   | F     | 636  | PHE  |
| 1   | F     | 647  | MET  |
| 1   | F     | 683  | LYS  |
| 1   | F     | 711  | GLN  |
| 1   | F     | 713  | ILE  |
| 1   | F     | 724  | LYS  |
| 1   | F     | 725  | TYR  |
| 1   | F     | 726  | VAL  |
| 1   | F     | 727  | LYS  |
| 1   | F     | 827  | LEU  |
| 1   | F     | 829  | GLN  |
| 1   | F     | 862  | ILE  |
| 1   | F     | 863  | ASN  |
| 1   | F     | 864  | ASP  |
| 1   | F     | 869  | ILE  |
| 1   | F     | 874  | ILE  |
| 1   | F     | 904  | ILE  |
| 1   | F     | 905  | GLN  |
| 1   | F     | 906  | THR  |
| 1   | F     | 922  | LEU  |
| 1   | F     | 931  | GLU  |
| 1   | F     | 932  | GLU  |
| 1   | F     | 965  | LYS  |
| 2   | G     | 28   | GLN  |
| 2   | G     | 168  | SER  |
| 2   | G     | 214  | LEU  |
| 2   | G     | 233  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 234 | VAL  |
| 2   | G     | 235 | ILE  |
| 2   | G     | 239 | ARG  |
| 2   | H     | 70  | LEU  |
| 2   | H     | 72  | TRP  |
| 2   | H     | 169 | GLU  |
| 2   | H     | 207 | SER  |
| 2   | H     | 210 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 118 | HIS  |
| 1   | A     | 133 | ASN  |
| 1   | A     | 136 | ASN  |
| 1   | A     | 263 | ASN  |
| 1   | A     | 299 | ASN  |
| 1   | A     | 493 | ASN  |
| 1   | A     | 548 | ASN  |
| 1   | A     | 609 | HIS  |
| 1   | A     | 711 | GLN  |
| 1   | A     | 765 | ASN  |
| 1   | B     | 236 | GLN  |
| 1   | B     | 263 | ASN  |
| 1   | B     | 491 | GLN  |
| 1   | B     | 521 | ASN  |
| 1   | B     | 698 | GLN  |
| 1   | B     | 939 | GLN  |
| 1   | B     | 963 | ASN  |
| 1   | B     | 992 | ASN  |
| 2   | C     | 6   | GLN  |
| 2   | D     | 194 | GLN  |
| 1   | E     | 67  | HIS  |
| 1   | E     | 89  | GLN  |
| 1   | E     | 349 | HIS  |
| 1   | E     | 404 | ASN  |
| 1   | E     | 487 | GLN  |
| 1   | E     | 491 | GLN  |
| 1   | E     | 591 | ASN  |
| 1   | E     | 610 | GLN  |
| 1   | E     | 681 | GLN  |
| 1   | E     | 790 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 115 | ASN  |
| 1   | F     | 160 | ASN  |
| 1   | F     | 202 | ASN  |
| 1   | F     | 211 | HIS  |
| 1   | F     | 339 | HIS  |
| 1   | F     | 654 | ASN  |
| 1   | F     | 658 | HIS  |
| 1   | F     | 848 | ASN  |
| 1   | F     | 863 | ASN  |
| 1   | F     | 881 | HIS  |
| 1   | F     | 895 | ASN  |
| 1   | F     | 910 | ASN  |
| 1   | F     | 973 | ASN  |
| 1   | F     | 990 | 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.

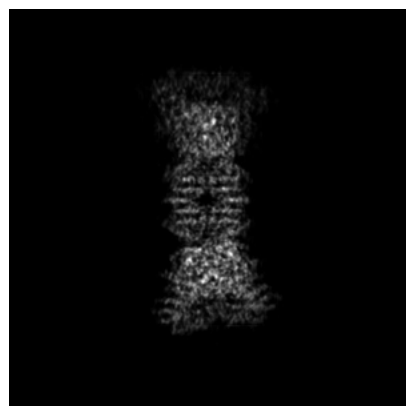
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39259. 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](#)

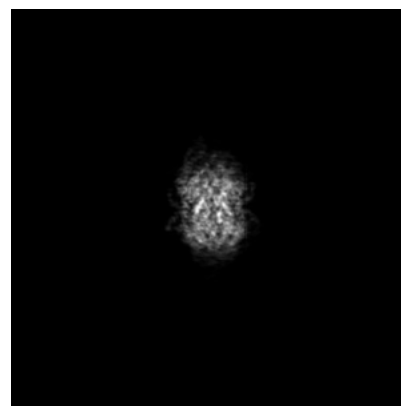
#### 6.1.1 Primary map



X

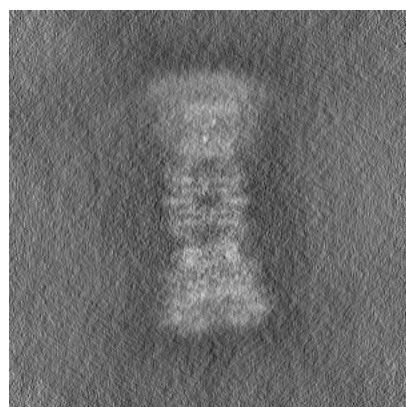


Y

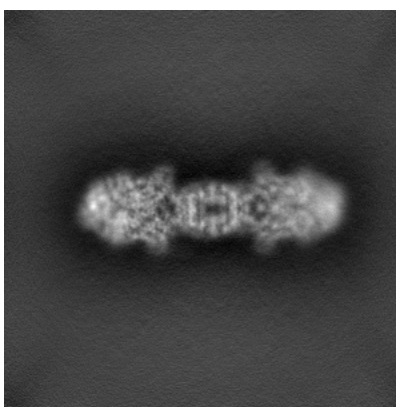


Z

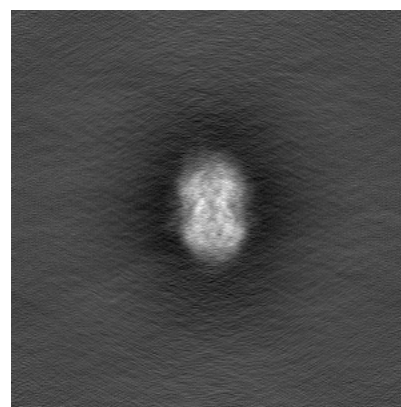
#### 6.1.2 Raw map



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: 230

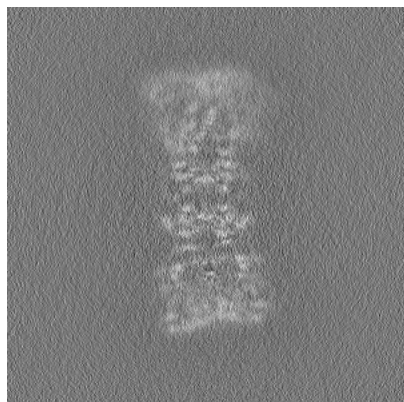


Y Index: 230

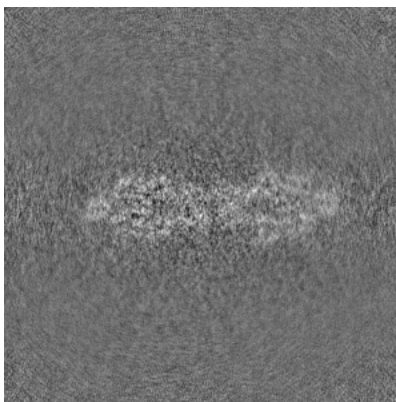


Z Index: 230

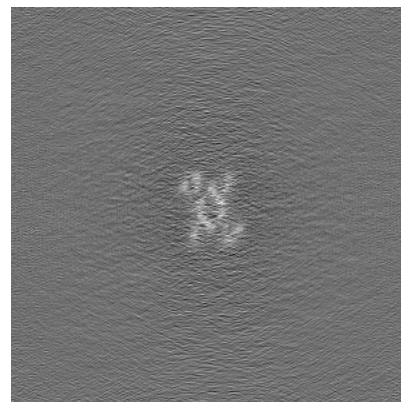
### 6.2.2 Raw map



X Index: 230



Y Index: 230



Z Index: 230

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: 245

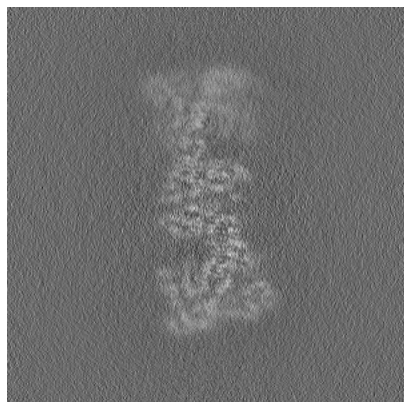


Y Index: 225

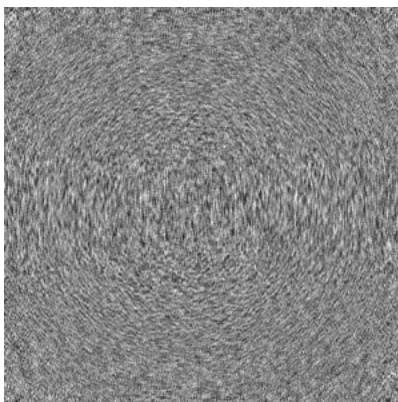


Z Index: 144

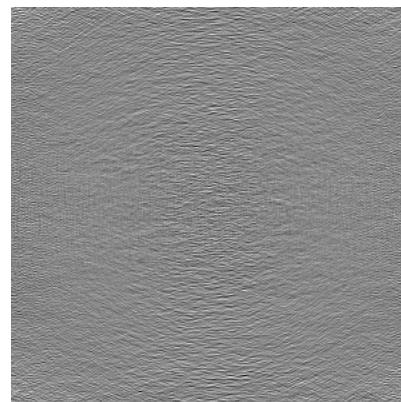
### 6.3.2 Raw map



X Index: 223



Y Index: 0

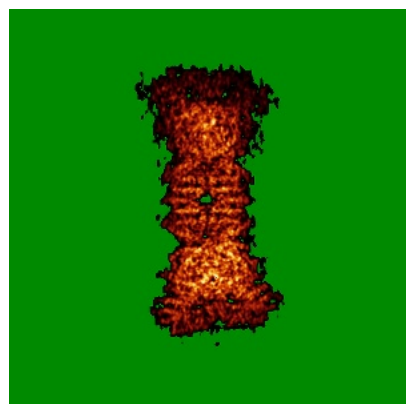


Z Index: 0

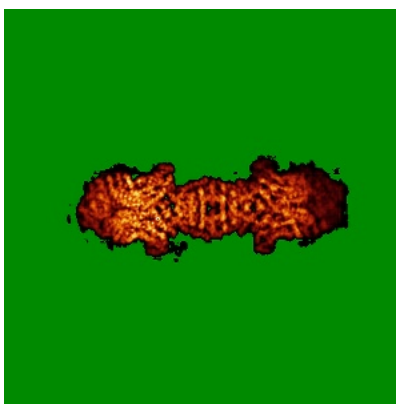
The images above show the largest variance slices of the map in three orthogonal directions.

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

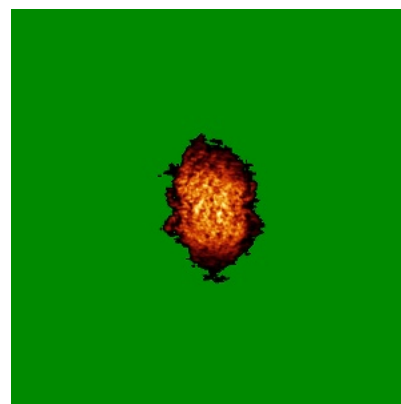
### 6.4.1 Primary map



X

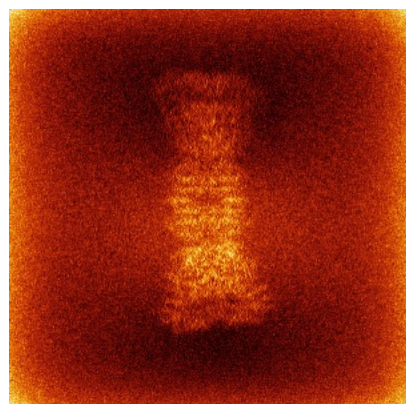


Y

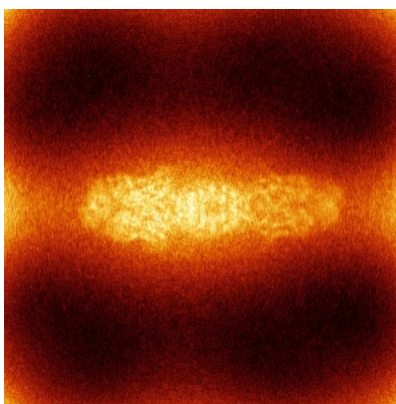


Z

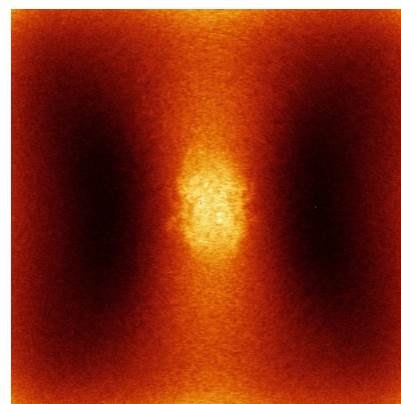
### 6.4.2 Raw map



X



Y

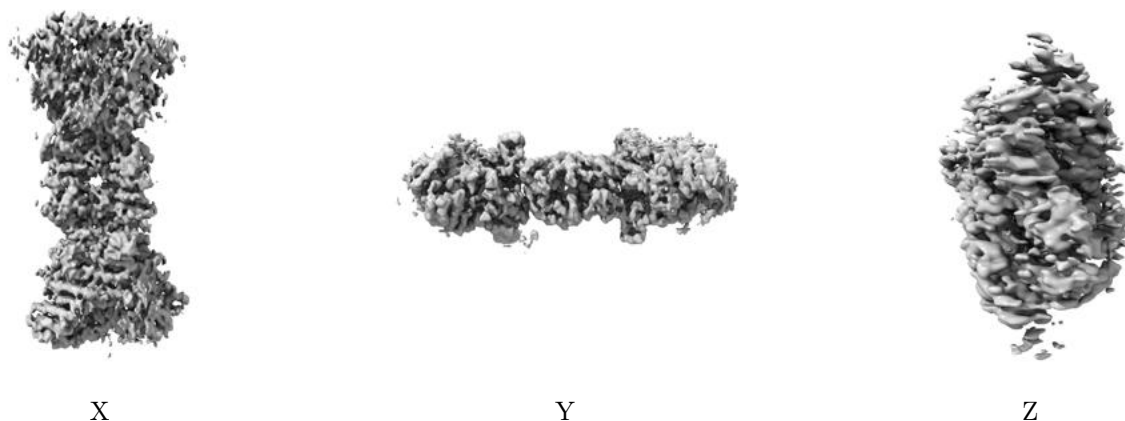


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

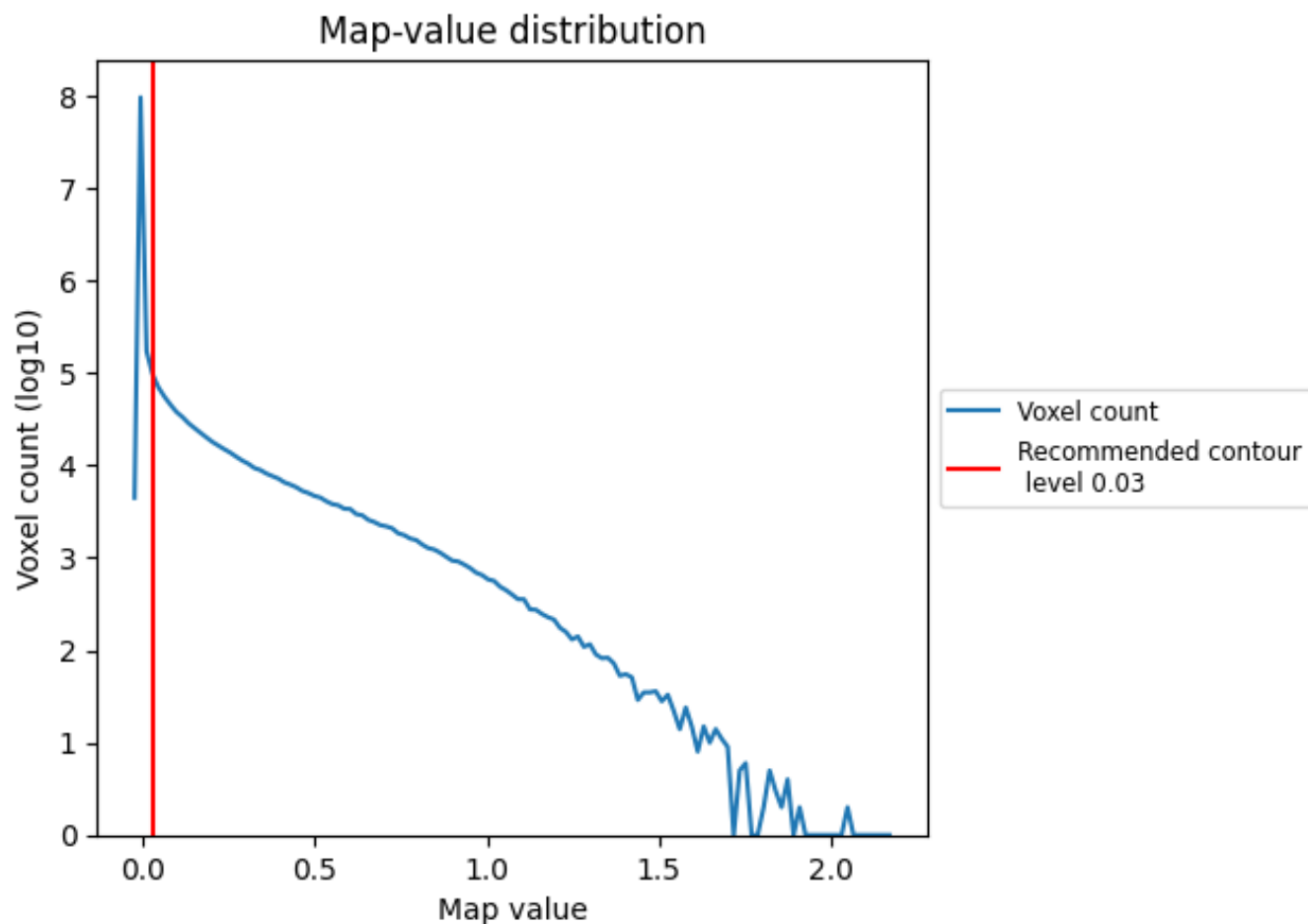
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

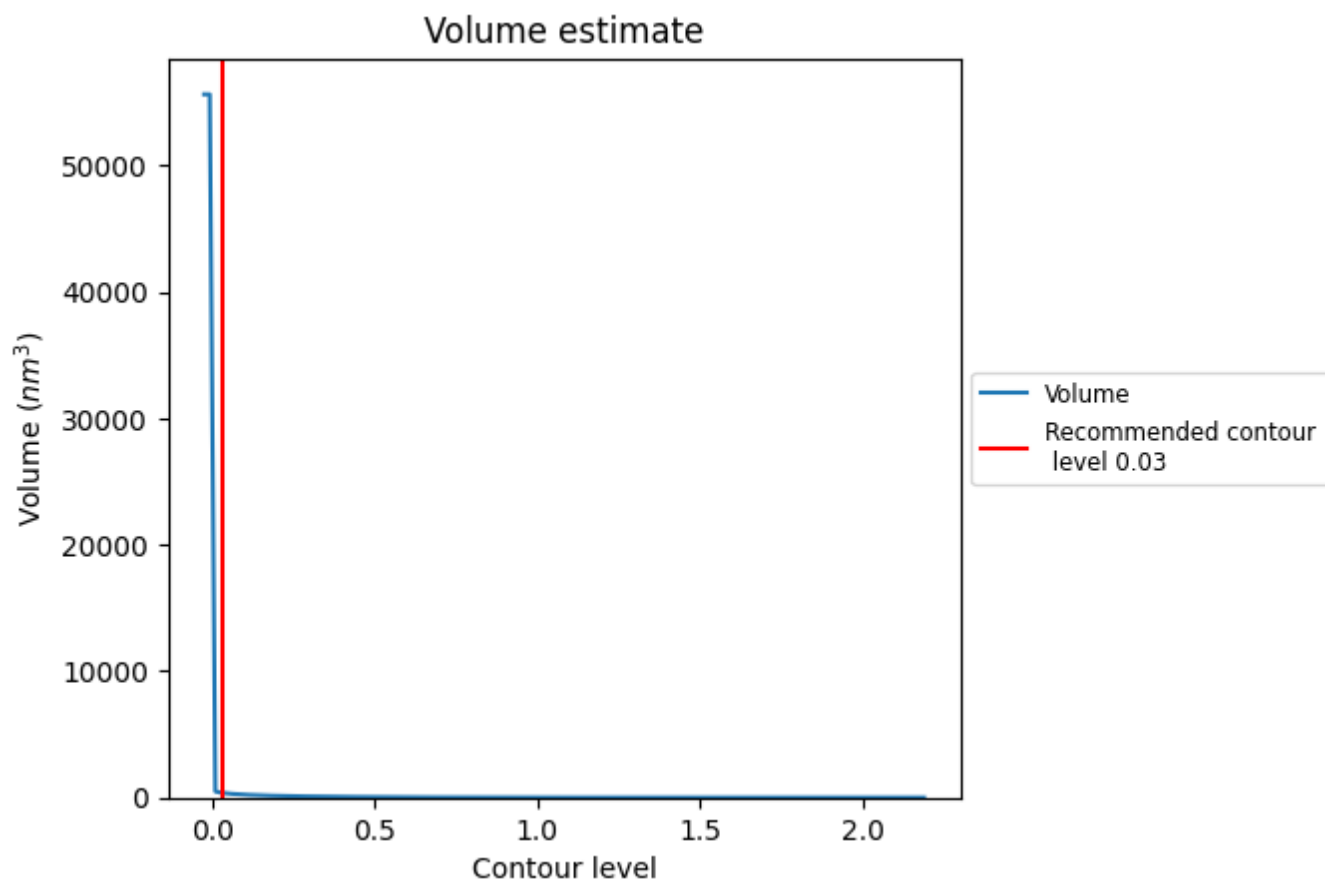
This section contains the results of statistical analysis of the map.

### 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.

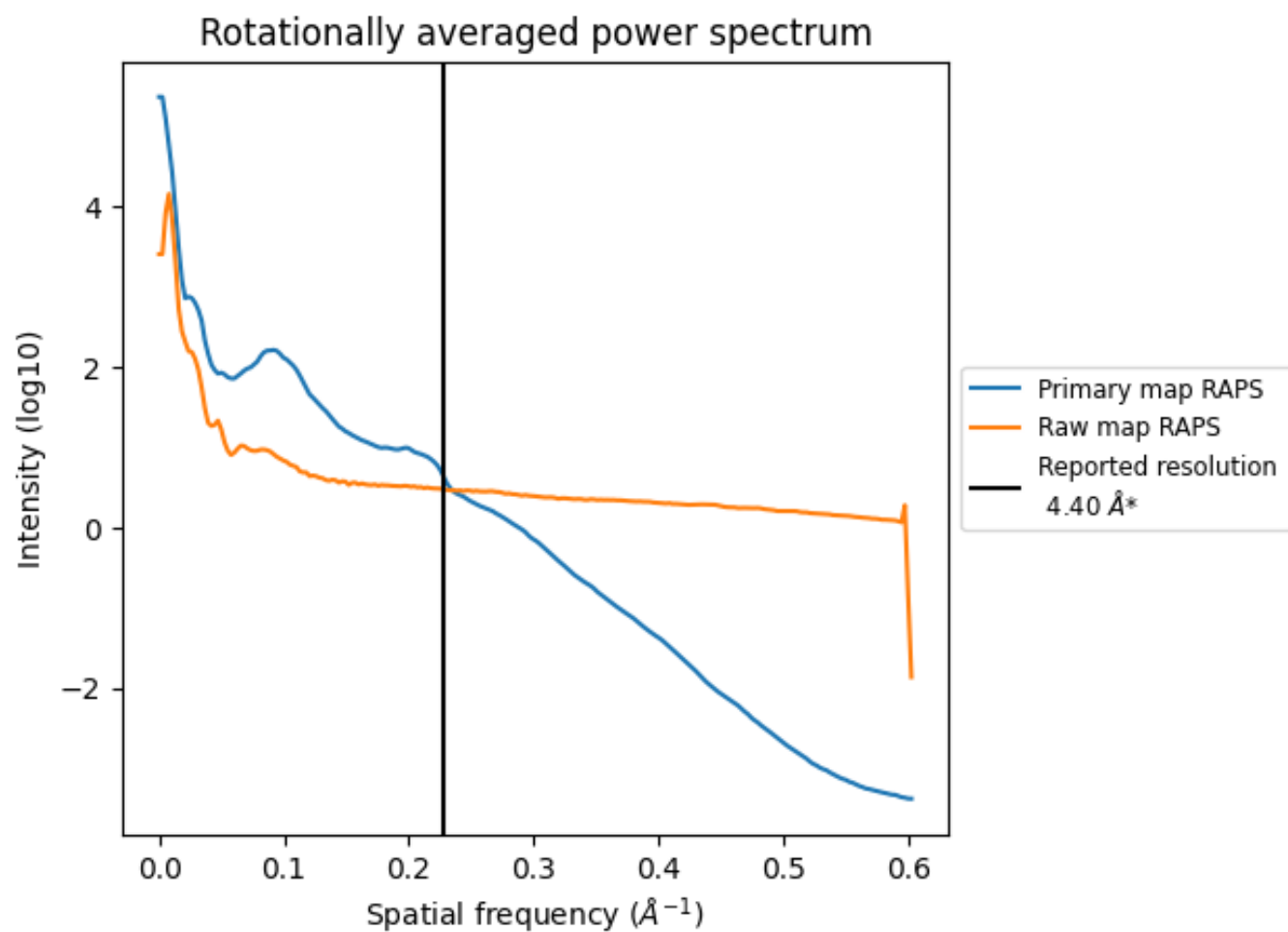
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376  $\text{nm}^3$ ; this corresponds to an approximate mass of 340 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 ⓘ

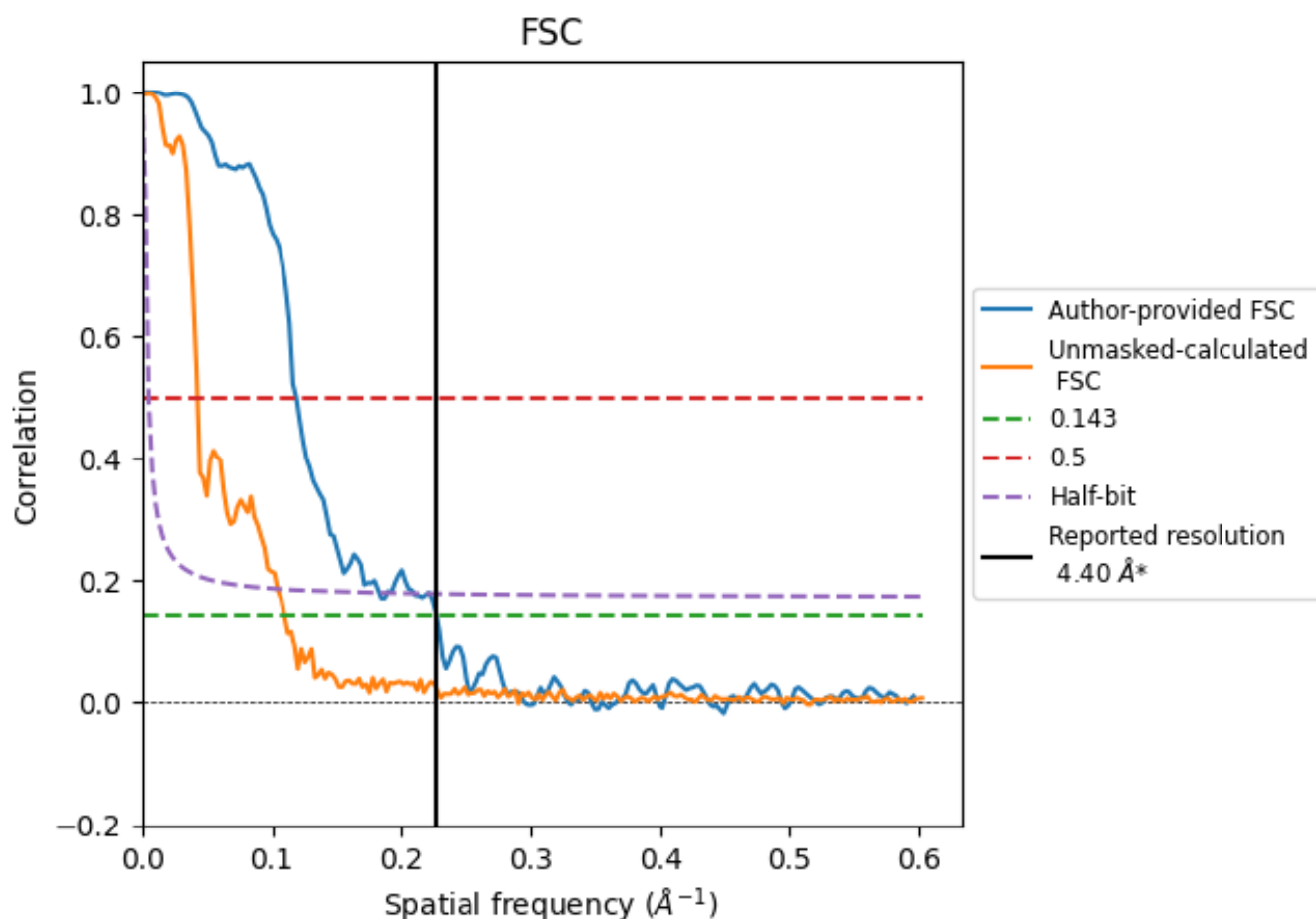


\*Reported resolution corresponds to spatial frequency of 0.227  $\text{\AA}^{-1}$

## 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  $0.227 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

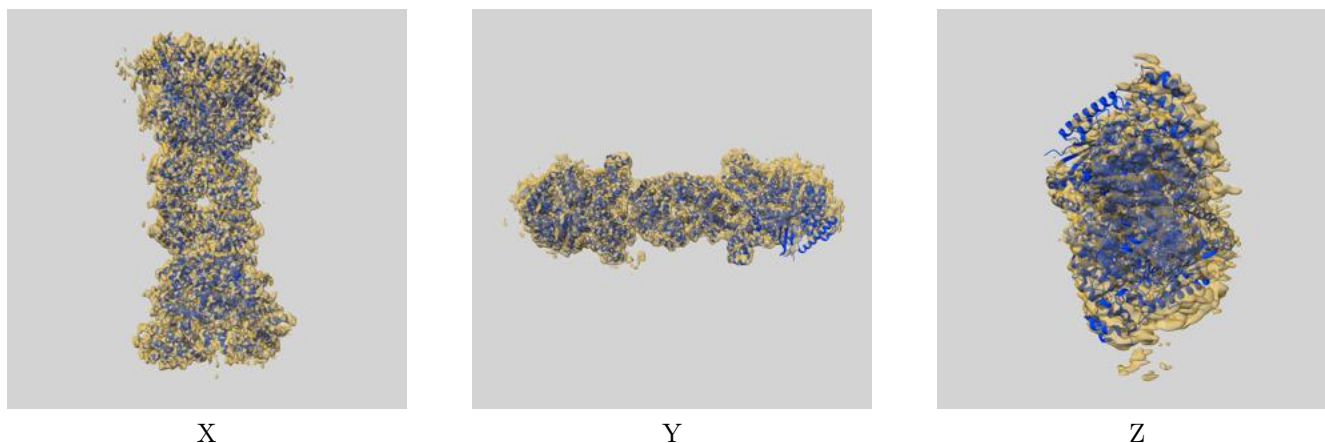
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 4.40                               | -     | -        |
| Author-provided FSC curve | 4.40                               | 8.39  | 5.46     |
| Unmasked-calculated*      | 9.11                               | 23.47 | 9.57     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.11 differs from the reported value 4.4 by more than 10 %

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

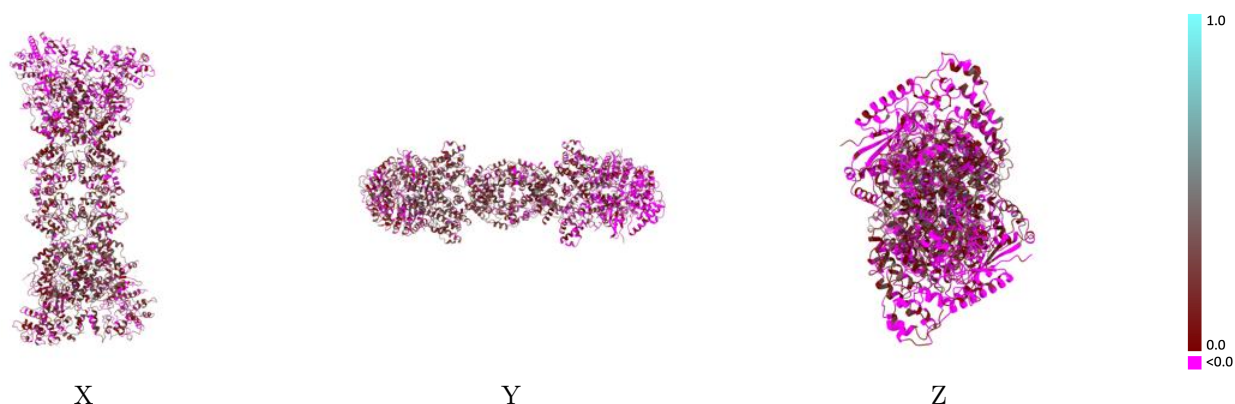
This section contains information regarding the fit between EMDB map EMD-39259 and PDB model 8YGP. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



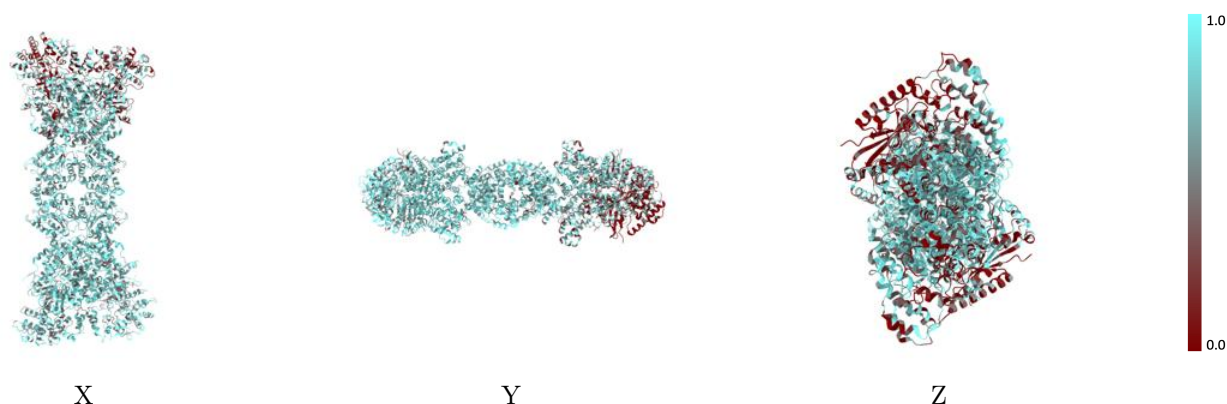
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



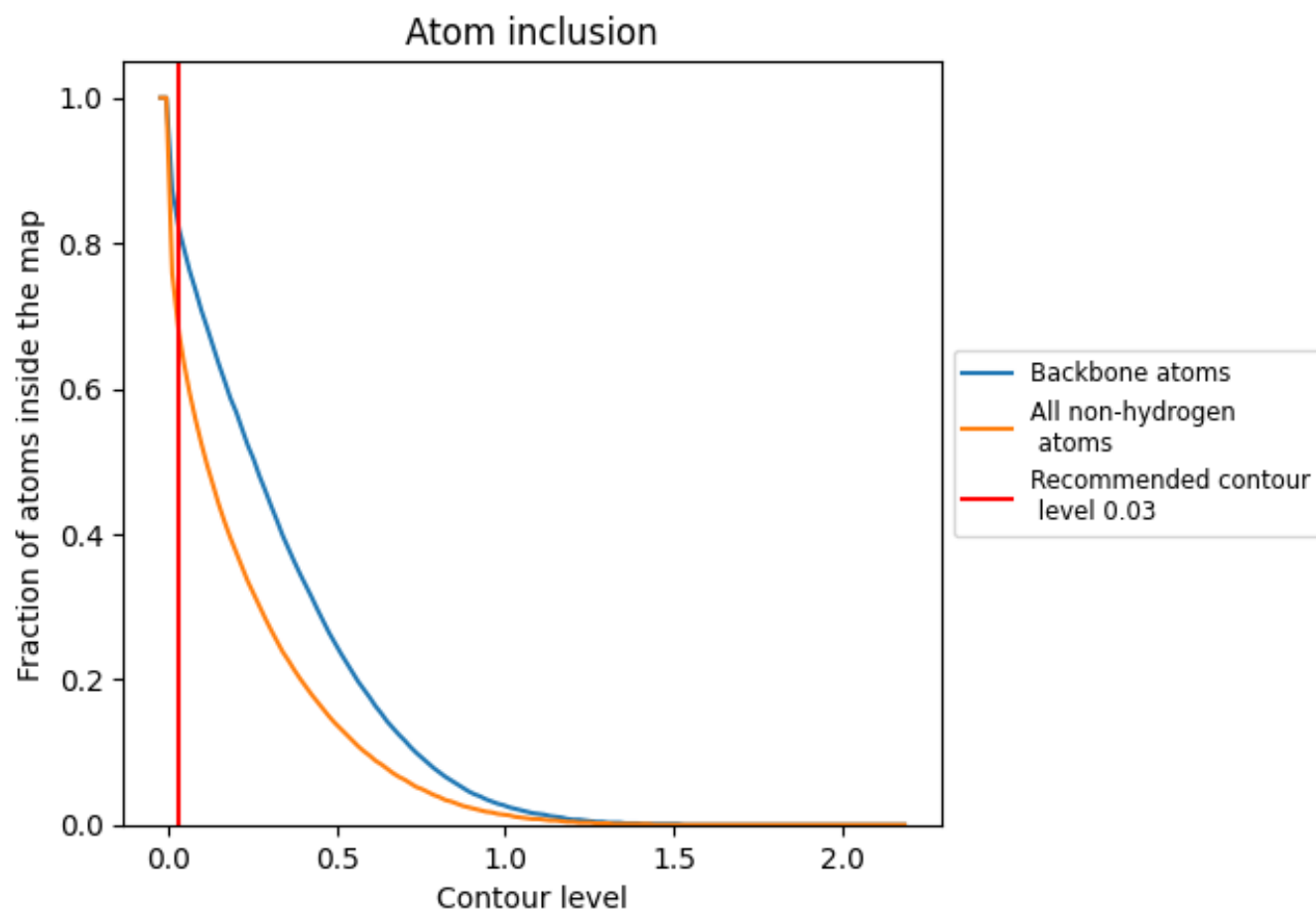
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 68% 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 (0.03) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score             |
|-------|--------------------|---------------------|
| All   | <div></div> 0.6760 | <div></div> 0.1320  |
| A     | <div></div> 0.6410 | <div></div> 0.0940  |
| B     | <div></div> 0.6190 | <div></div> 0.0910  |
| C     | <div></div> 0.2820 | <div></div> -0.0230 |
| D     | <div></div> 0.3460 | <div></div> -0.0400 |
| E     | <div></div> 0.7880 | <div></div> 0.2000  |
| F     | <div></div> 0.7840 | <div></div> 0.1980  |
| G     | <div></div> 0.6330 | <div></div> 0.1260  |
| H     | <div></div> 0.5710 | <div></div> 0.0810  |

