



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:39 PM UTC

PDB ID : 5FM1 / pdb\_00005fm1  
EMDB ID : EMD-1731  
Title : Structure of gamma-tubulin small complex based on a cryo-EM map, chemical cross-links, and a remotely related structure  
Authors : Greenberg, C.H.; Kollman, J.; Zelter, A.; Johnson, R.; MacCoss, M.J.; Davis, T.N.; Agard, D.A.; Sali, A.  
Deposited on : 2015-10-30  
Resolution : 8.00 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 : **NOT EXECUTED**  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

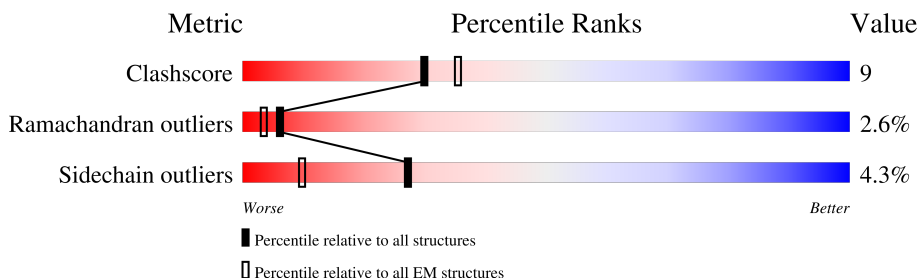
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.00 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) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 229148                      | 23984                       |
| Ramachandran outliers | 224038                      | 23583                       |
| Sidechain outliers    | 223484                      | 23102                       |

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   | 1-A   | 823    | <div> <div>70%</div> <div> <div>55%</div> <div>13%</div> <div>•</div> <div>30%</div> </div> </div> |
| 1   | 10-A  | 823    | <div> <div>54%</div> <div>15%</div> <div>•</div> <div>30%</div> </div>                             |
| 1   | 2-A   | 823    | <div> <div>56%</div> <div>12%</div> <div>•</div> <div>30%</div> </div>                             |
| 1   | 3-A   | 823    | <div> <div>57%</div> <div>11%</div> <div>•</div> <div>30%</div> </div>                             |
| 1   | 4-A   | 823    | <div> <div>57%</div> <div>11%</div> <div>•</div> <div>30%</div> </div>                             |
| 1   | 5-A   | 823    | <div> <div>53%</div> <div>14%</div> <div>•</div> <div>30%</div> </div>                             |
| 1   | 6-A   | 823    | <div> <div>57%</div> <div>12%</div> <div>•</div> <div>30%</div> </div>                             |
| 1   | 7-A   | 823    | <div> <div>56%</div> <div>14%</div> <div>•</div> <div>30%</div> </div>                             |

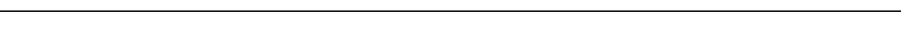
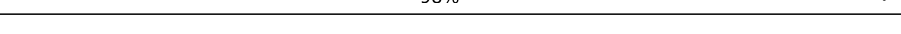
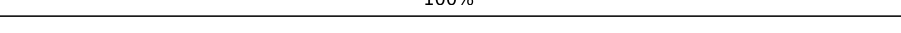
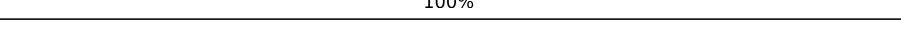
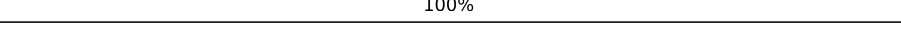
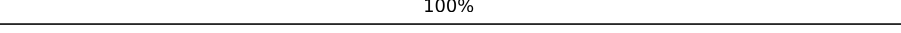
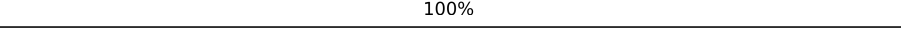
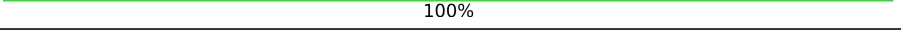
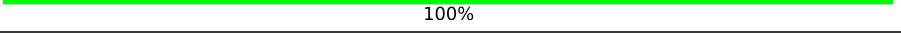
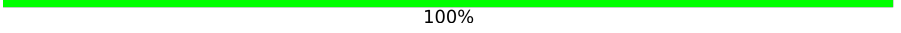
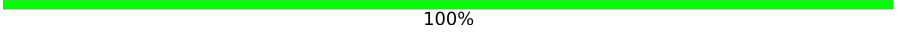
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | 8-A   | 823    |    |
| 1   | 9-A   | 823    |    |
| 2   | 1-B   | 846    |    |
| 2   | 10-B  | 846    |    |
| 2   | 2-B   | 846    |    |
| 2   | 3-B   | 846    |    |
| 2   | 4-B   | 846    |    |
| 2   | 5-B   | 846    |    |
| 2   | 6-B   | 846    |    |
| 2   | 7-B   | 846    |    |
| 2   | 8-B   | 846    |    |
| 2   | 9-B   | 846    |   |
| 3   | 1-C   | 473    |  |
| 3   | 1-D   | 473    |  |
| 3   | 10-C  | 473    |  |
| 3   | 10-D  | 473    |  |
| 3   | 2-C   | 473    |  |
| 3   | 2-D   | 473    |  |
| 3   | 3-C   | 473    |  |
| 3   | 3-D   | 473    |  |
| 3   | 4-C   | 473    |  |
| 3   | 4-D   | 473    |  |
| 3   | 5-C   | 473    |  |
| 3   | 5-D   | 473    |  |
| 3   | 6-C   | 473    |  |

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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 3   | 6-D   | 473    |  79%15% • 6%   |
| 3   | 7-C   | 473    |  79%15% • 6%   |
| 3   | 7-D   | 473    |  79%14% • 6%   |
| 3   | 8-C   | 473    |  78%15% • 6%   |
| 3   | 8-D   | 473    |  79%15% • 6%   |
| 3   | 9-C   | 473    |  81%12% • 6%   |
| 3   | 9-D   | 473    |  80%13% • 6%   |
| 4   | 1-E   | 44     |  100%<br>100%  |
| 4   | 1-F   | 44     |  100%<br>98% • |
| 4   | 10-E  | 44     |  95%5%         |
| 4   | 10-F  | 44     |  100%          |
| 4   | 2-E   | 44     |  100%          |
| 4   | 2-F   | 44     |  100%        |
| 4   | 3-E   | 44     |  100%        |
| 4   | 3-F   | 44     |  98% •       |
| 4   | 4-E   | 44     |  100%        |
| 4   | 4-F   | 44     |  100%        |
| 4   | 5-E   | 44     |  100%        |
| 4   | 5-F   | 44     |  100%        |
| 4   | 6-E   | 44     |  100%        |
| 4   | 6-F   | 44     |  100%        |
| 4   | 7-E   | 44     |  100%        |
| 4   | 7-F   | 44     |  100%        |
| 4   | 8-E   | 44     |  100%        |
| 4   | 8-F   | 44     |  100%        |

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| Mol | Chain | Length | Quality of chain                                                                        |
|-----|-------|--------|-----------------------------------------------------------------------------------------|
| 4   | 9-E   | 44     |  100% |
| 4   | 9-F   | 44     |  100% |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 169380 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 SPINDLE POLE BODY COMPONENT SPC97.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 1-A   | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3110 | 806 | 889 | 26 |         |       |
| 1   | 2-A   | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3110 | 806 | 889 | 26 |         |       |
| 1   | 3-A   | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3110 | 806 | 889 | 26 |         |       |
| 1   | 4-A   | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3110 | 806 | 889 | 26 |         |       |
| 1   | 5-A   | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3110 | 806 | 889 | 26 |         |       |
| 1   | 6-A   | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3110 | 806 | 889 | 26 |         |       |
| 1   | 7-A   | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3110 | 806 | 889 | 26 |         |       |
| 1   | 8-A   | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3110 | 806 | 889 | 26 |         |       |
| 1   | 9-A   | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3110 | 806 | 889 | 26 |         |       |
| 1   | 10-A  | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4831  | 3110 | 806 | 889 | 26 |         |       |

- Molecule 2 is a protein called SPINDLE POLE BODY COMPONENT SPC98.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | 1-B   | 565      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4701  | 3058 | 775 | 853 | 15 |         |       |
| 2   | 2-B   | 565      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4701  | 3058 | 775 | 853 | 15 |         |       |
| 2   | 3-B   | 565      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4701  | 3058 | 775 | 853 | 15 |         |       |
| 2   | 4-B   | 565      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4701  | 3058 | 775 | 853 | 15 |         |       |
| 2   | 5-B   | 565      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4701  | 3058 | 775 | 853 | 15 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | 6-B   | 565      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4701  | 3058 | 775 | 853 | 15 |         |       |
| 2   | 7-B   | 565      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4701  | 3058 | 775 | 853 | 15 |         |       |
| 2   | 8-B   | 565      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4701  | 3058 | 775 | 853 | 15 |         |       |
| 2   | 9-B   | 565      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4701  | 3058 | 775 | 853 | 15 |         |       |
| 2   | 10-B  | 565      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4701  | 3058 | 775 | 853 | 15 |         |       |

- Molecule 3 is a protein called TUBULIN GAMMA CHAIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | 1-C   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 2-C   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 3-C   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 4-C   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 5-C   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 6-C   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 7-C   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 8-C   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 9-C   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 10-C  | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 1-D   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 2-D   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 3-D   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 4-D   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | 5-D   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 6-D   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 7-D   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 8-D   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 9-D   | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |
| 3   | 10-D  | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3483  | 2179 | 591 | 696 | 17 |         |       |

- Molecule 4 is a protein called SPINDLE POLE BODY COMPONENT 110.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4   | 1-E   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 2-E   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 3-E   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 4-E   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 5-E   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 6-E   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 7-E   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 8-E   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 9-E   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 10-E  | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 1-F   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 2-F   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |
| 4   | 3-F   | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 220   | 132 | 44 | 44 |         |       |

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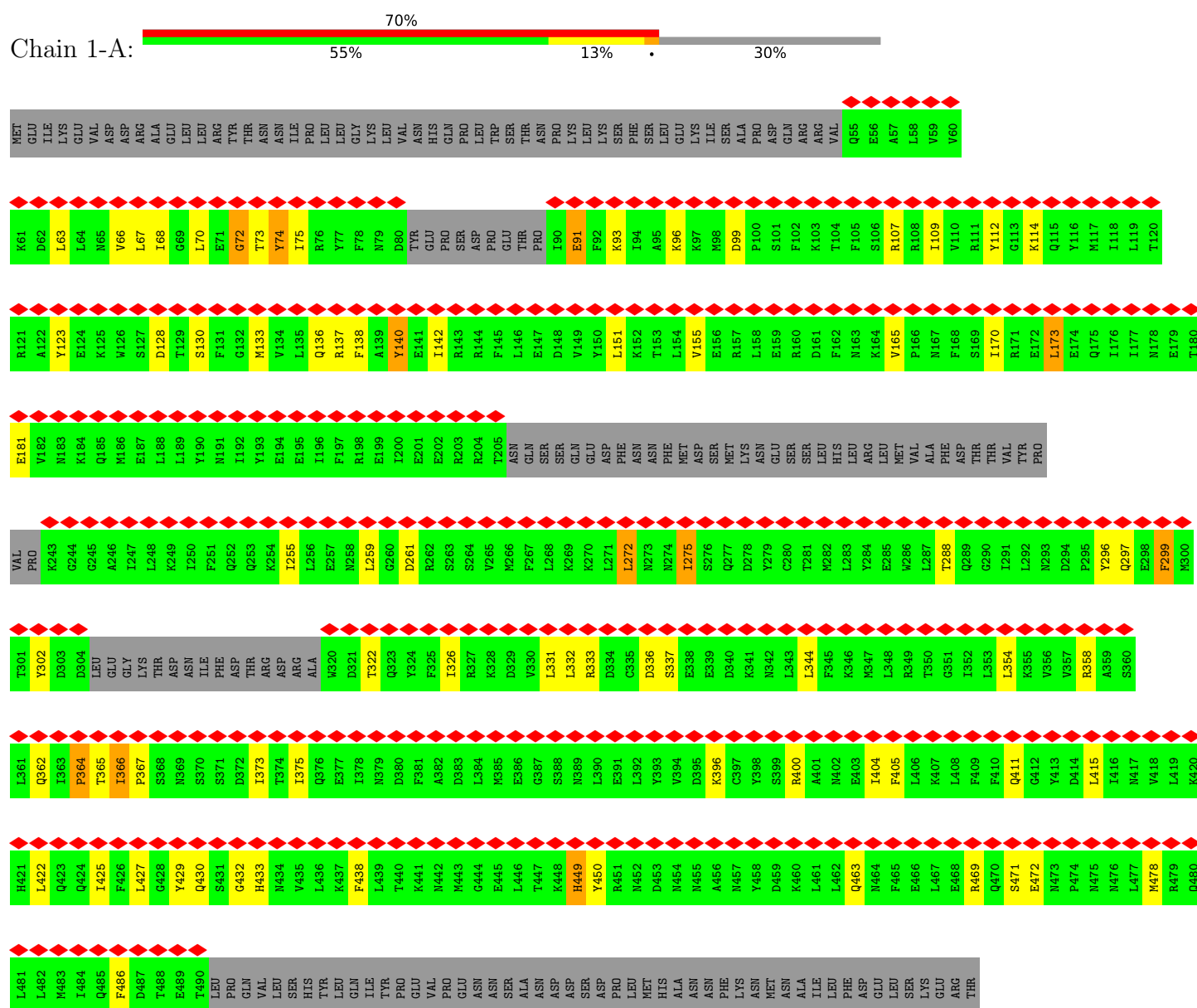
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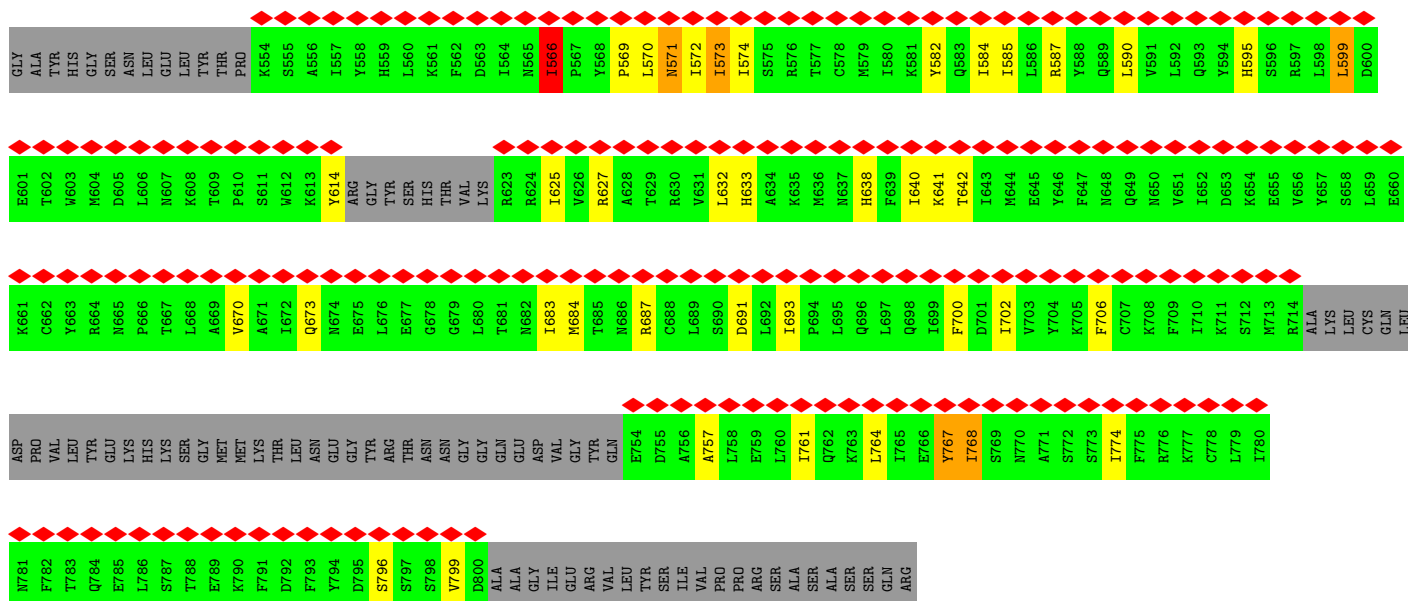
| Mol | Chain | Residues | Atoms        |          |         |         | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 4   | 4-F   | 44       | Total<br>220 | C<br>132 | N<br>44 | O<br>44 | 0       | 0     |
| 4   | 5-F   | 44       | Total<br>220 | C<br>132 | N<br>44 | O<br>44 | 0       | 0     |
| 4   | 6-F   | 44       | Total<br>220 | C<br>132 | N<br>44 | O<br>44 | 0       | 0     |
| 4   | 7-F   | 44       | Total<br>220 | C<br>132 | N<br>44 | O<br>44 | 0       | 0     |
| 4   | 8-F   | 44       | Total<br>220 | C<br>132 | N<br>44 | O<br>44 | 0       | 0     |
| 4   | 9-F   | 44       | Total<br>220 | C<br>132 | N<br>44 | O<br>44 | 0       | 0     |
| 4   | 10-F  | 44       | Total<br>220 | C<br>132 | N<br>44 | O<br>44 | 0       | 0     |

### 3 Residue-property plots

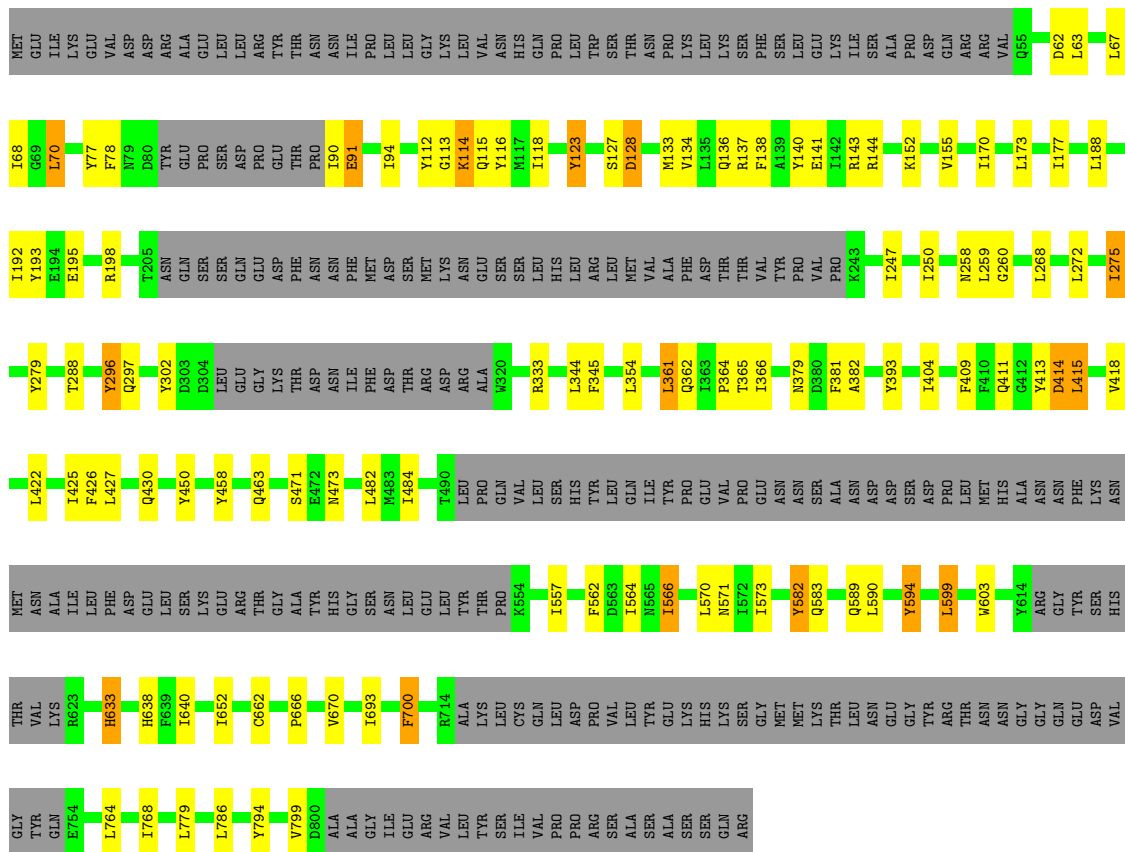
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: SPINDLE POLE BODY COMPONENT SPC97



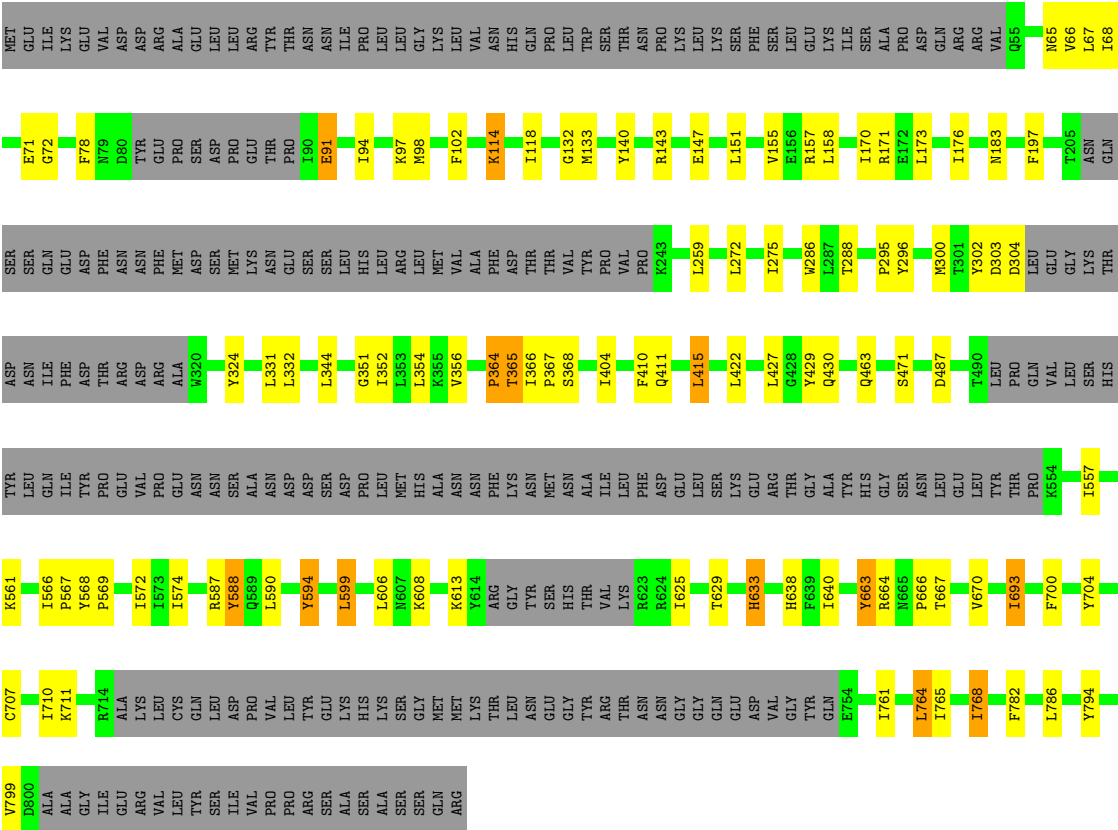


● Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

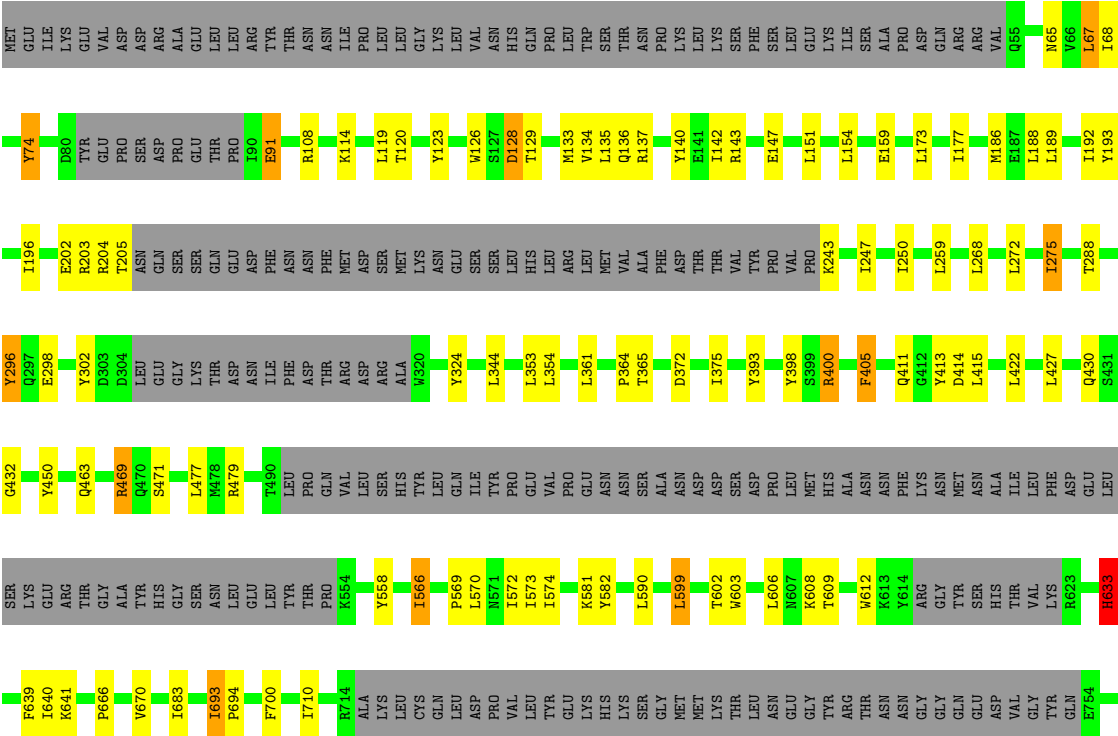


- Molecule 1: SPINDLE POLE BODY COMPONENT SPC97



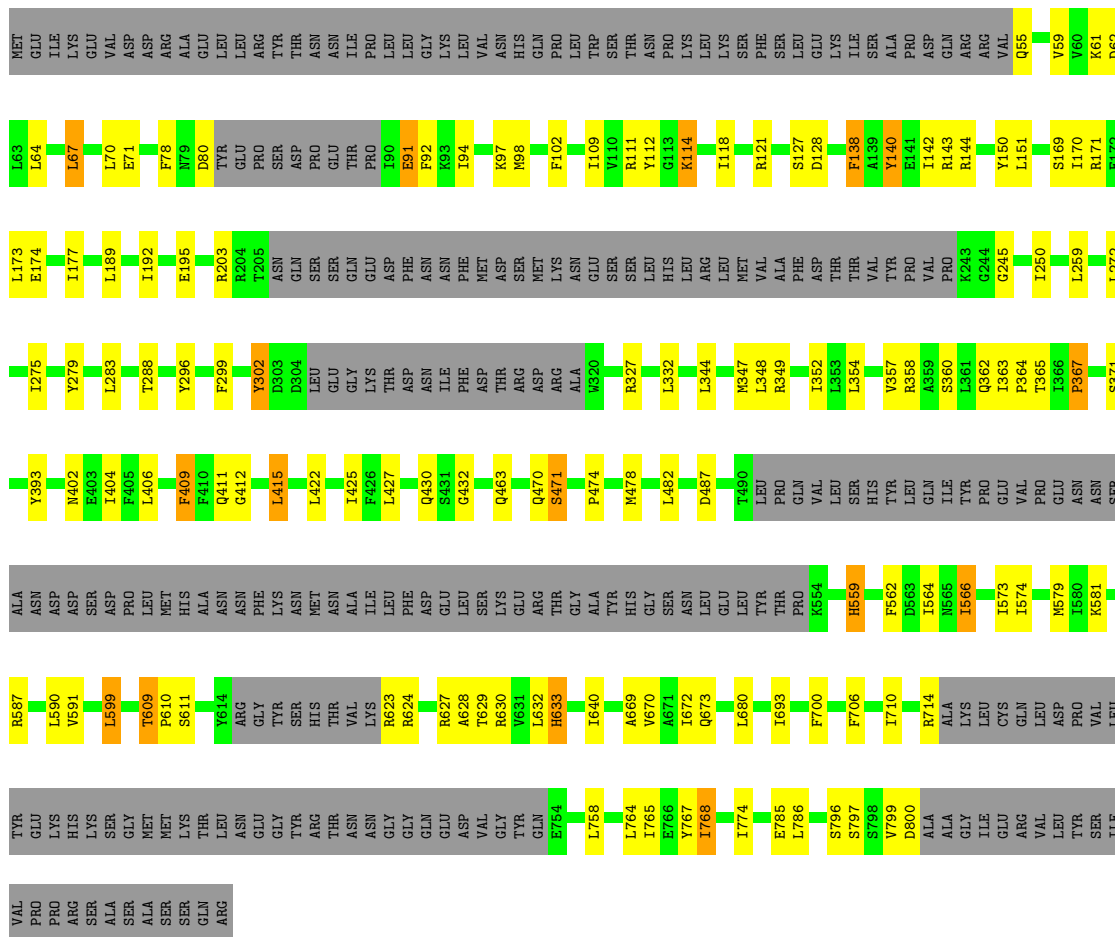


● Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

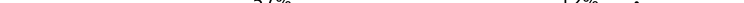


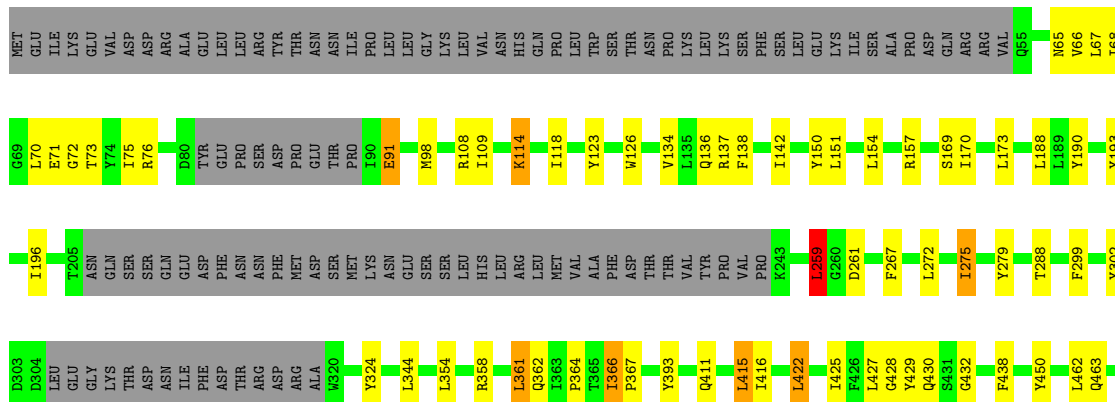
- Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

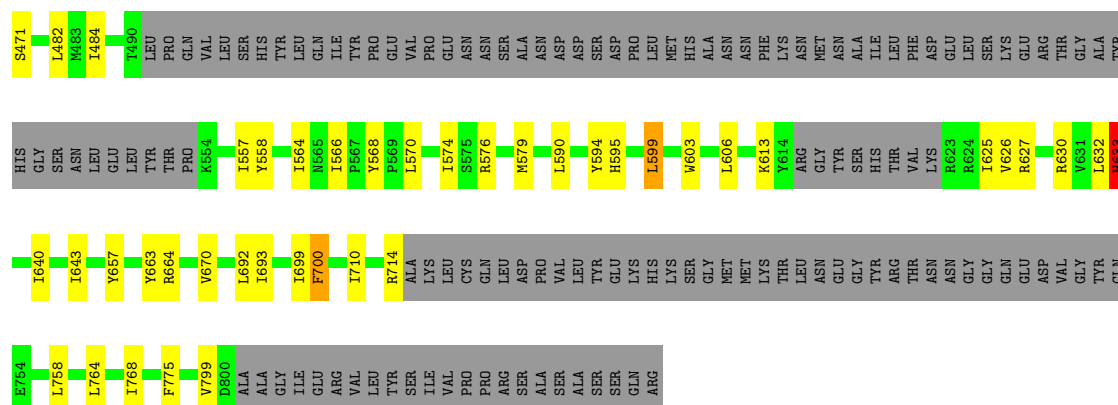
Chain 5-A:  53% 14% . 30%



- Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

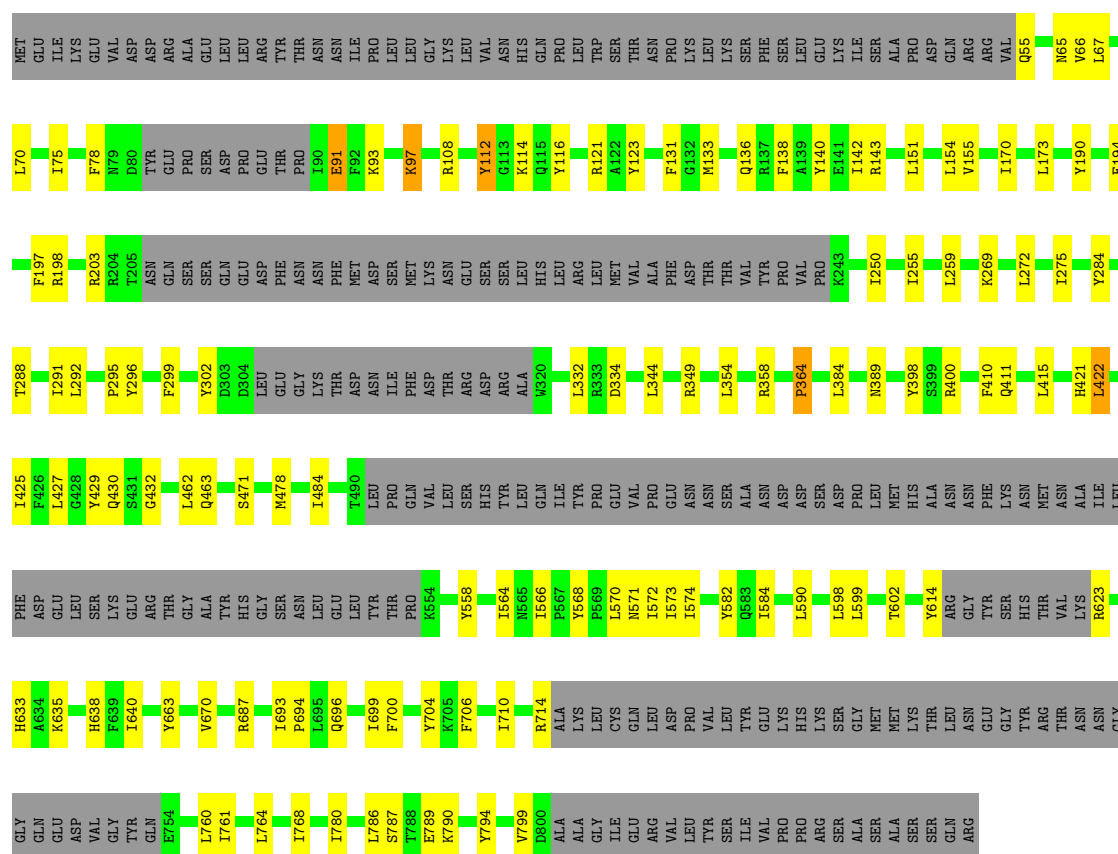
Chain 6-A:  57% 12% 30%





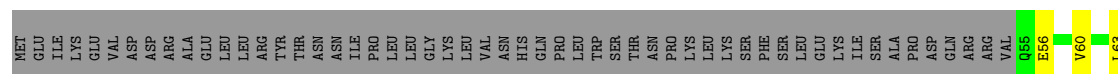
• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

Chain 7-A: 56% 14% 30%



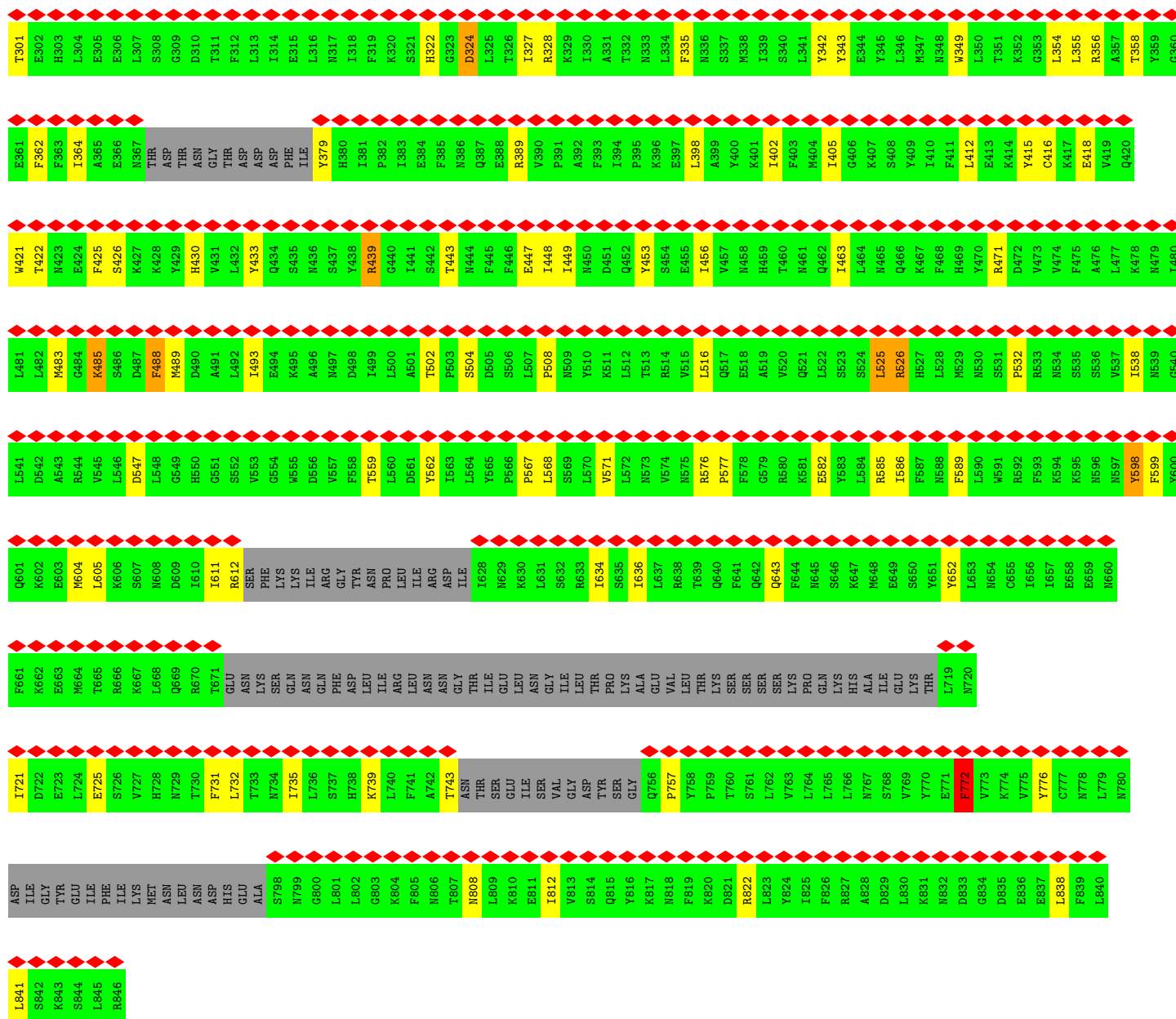
• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

Chain 8-A: 56% 13% 30%



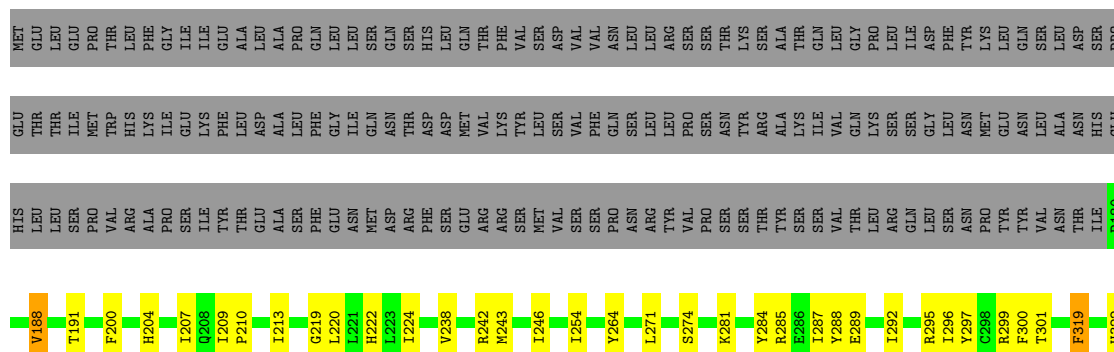




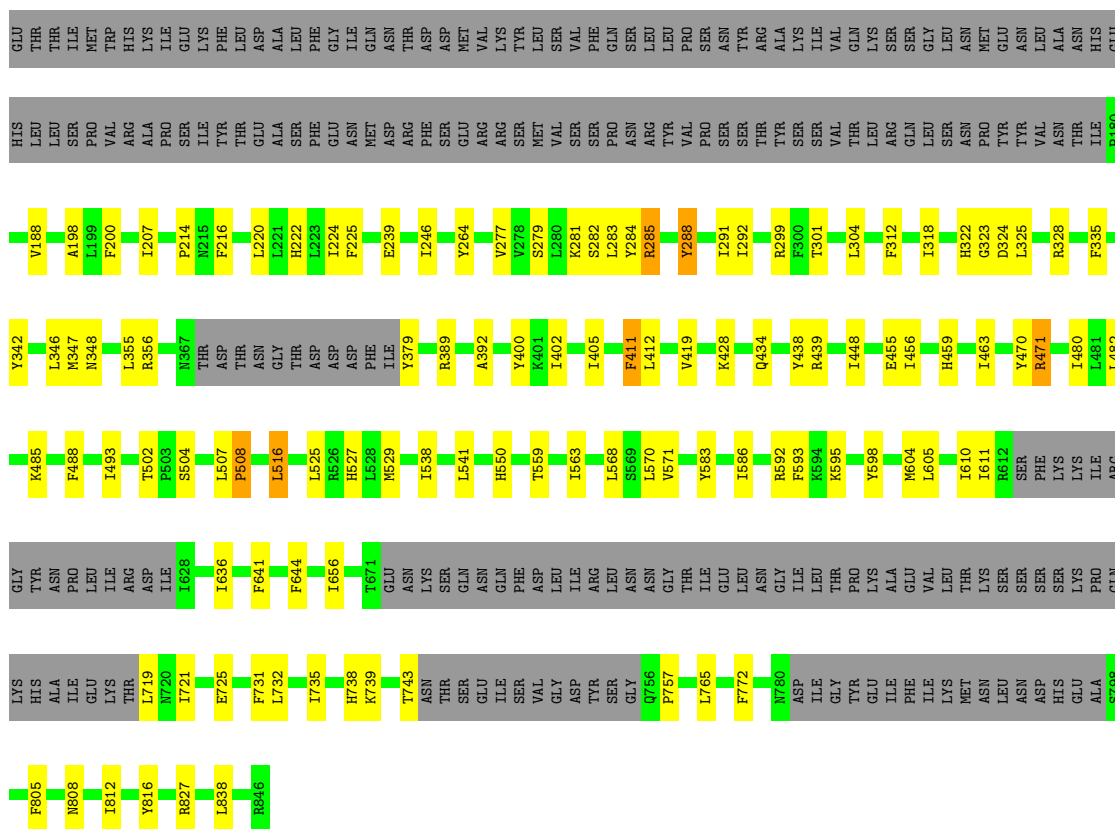


● Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Chain 2-B: 54% 12% 33%

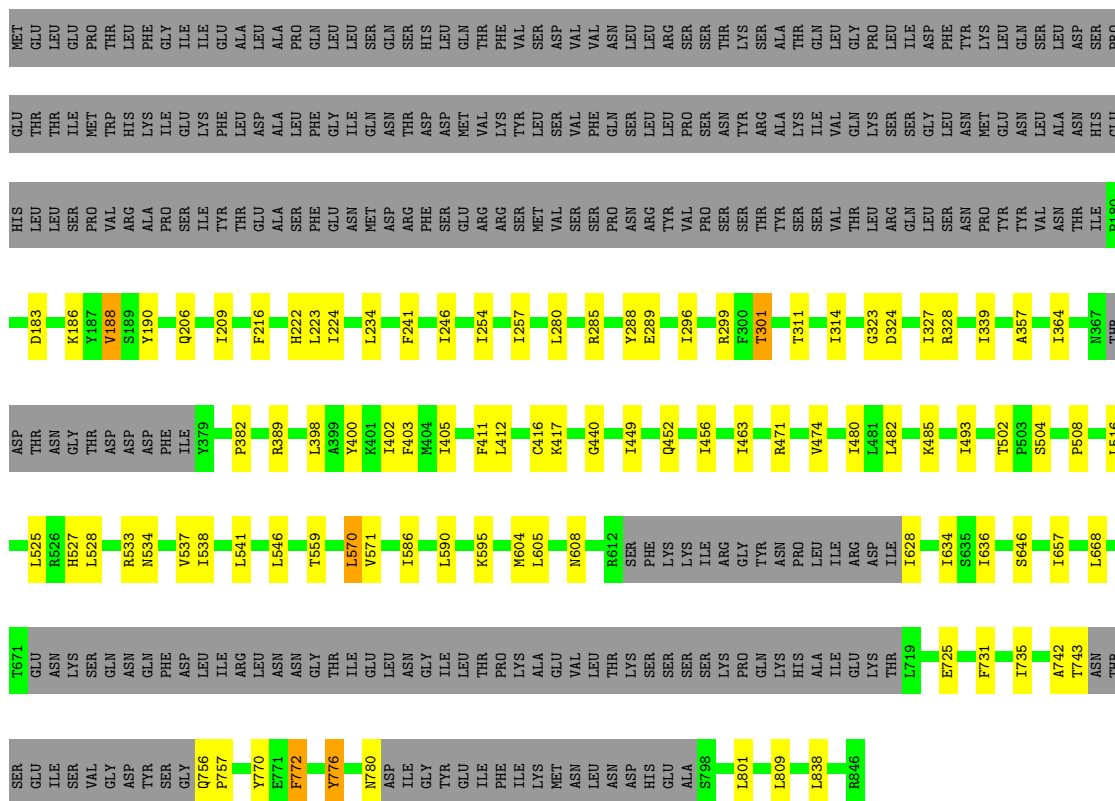






- Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Chain 5-B:  56% 11% • 33%

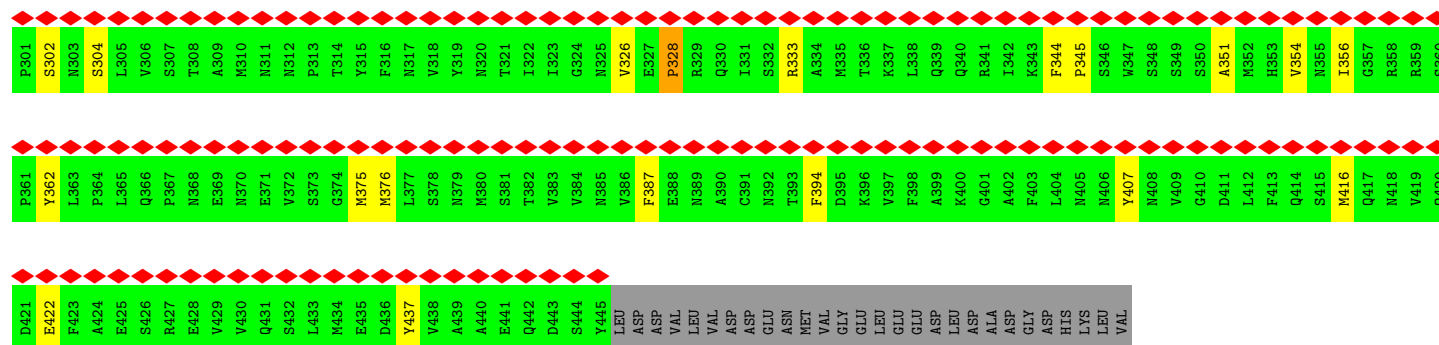






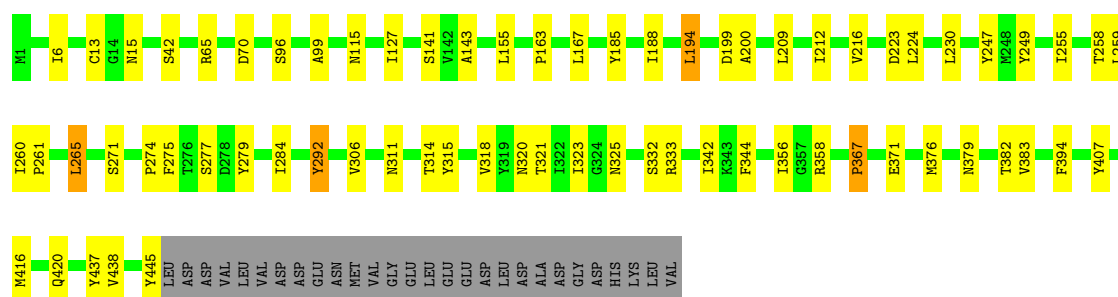






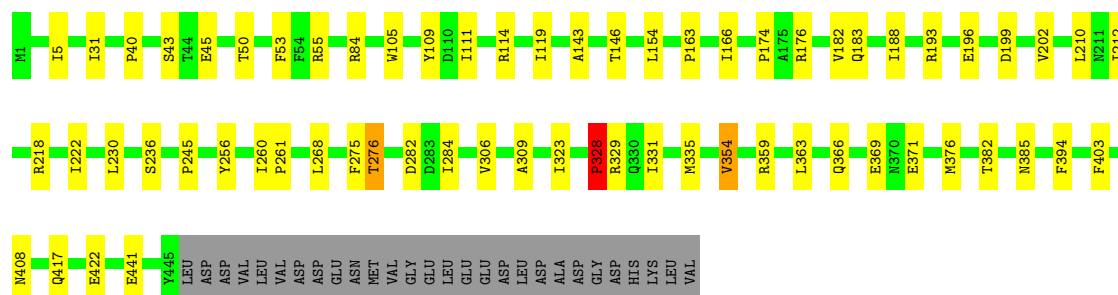
### • Molecule 3: TUBULIN GAMMA CHAIN

Chain 2-C: 79% 14% 6%



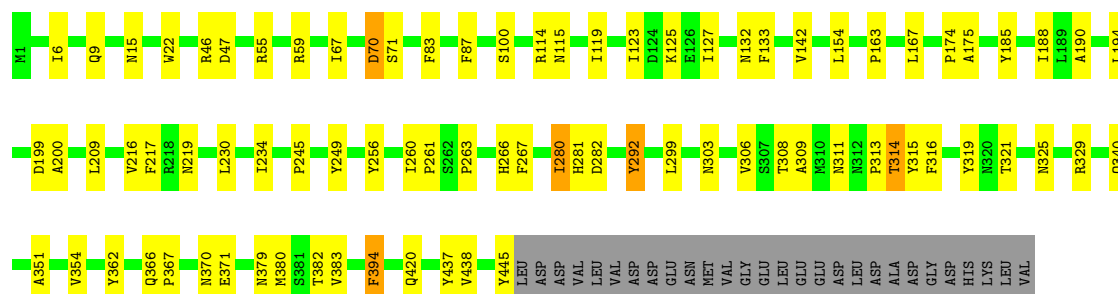
### • Molecule 3: TUBULIN GAMMA CHAIN

Chain 2-D: 80% 13% 6%

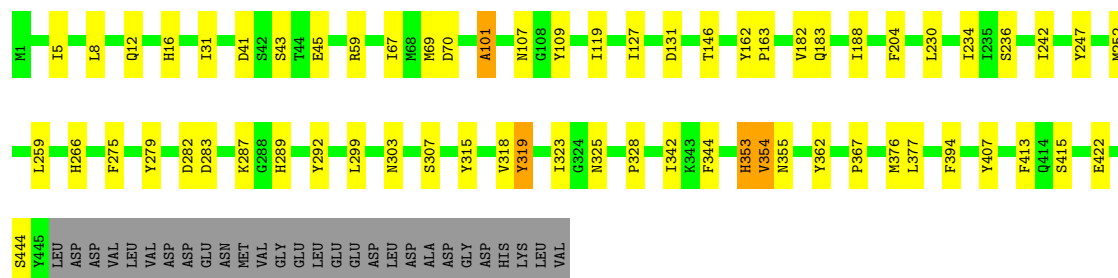


### • Molecule 3: TUBULIN GAMMA CHAIN

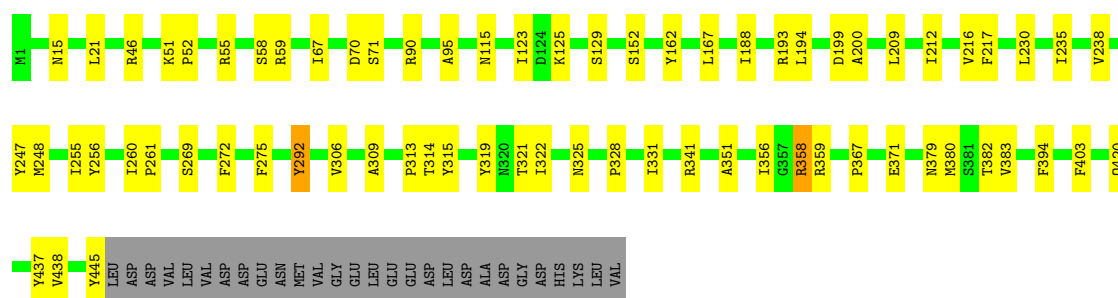
Chain 3-C: 77% 16% 6%



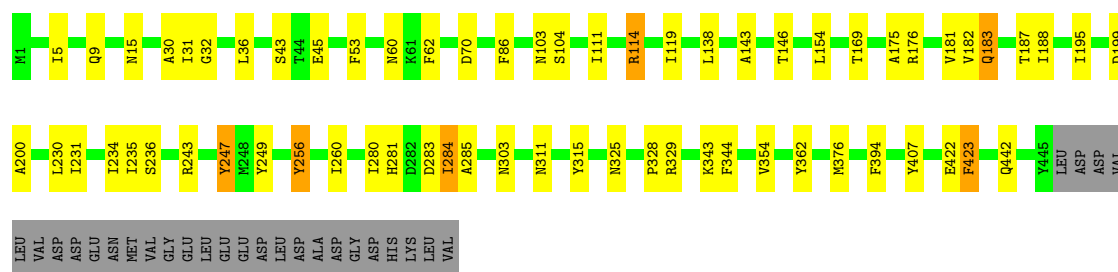
## • Molecule 3: TUBULIN GAMMA CHAIN

Chain 3-D:  81% 13% 6%

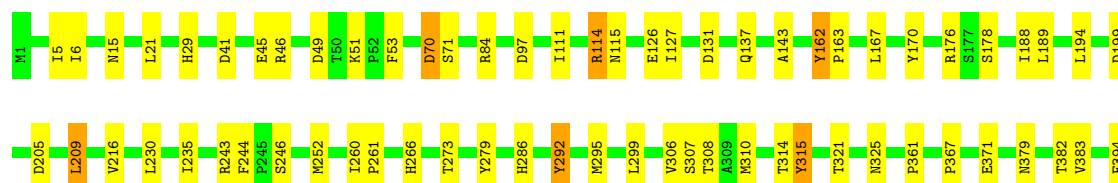
## • Molecule 3: TUBULIN GAMMA CHAIN

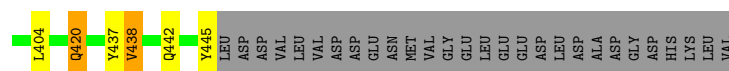
Chain 4-C:  79% 14% 6%

## • Molecule 3: TUBULIN GAMMA CHAIN

Chain 4-D:  80% 12% 6%

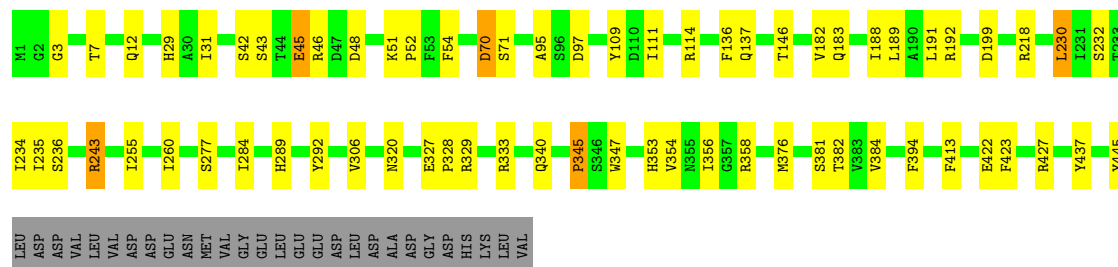
## • Molecule 3: TUBULIN GAMMA CHAIN

Chain 5-C:  79% 14% 6%



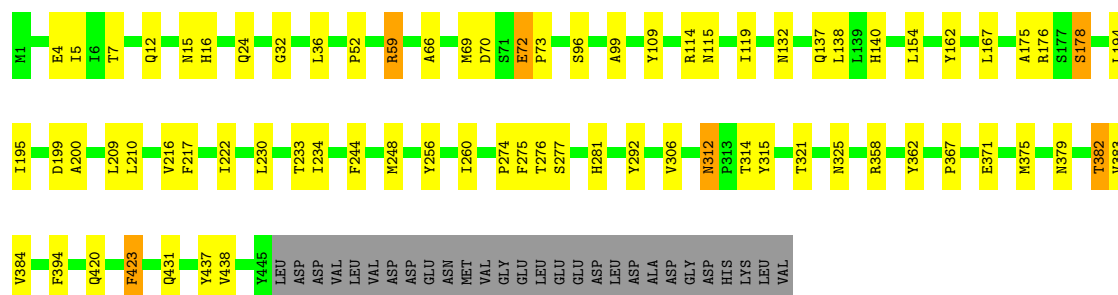
### • Molecule 3: TUBULIN GAMMA CHAIN

Chain 5-D: 80% 13% • 6%



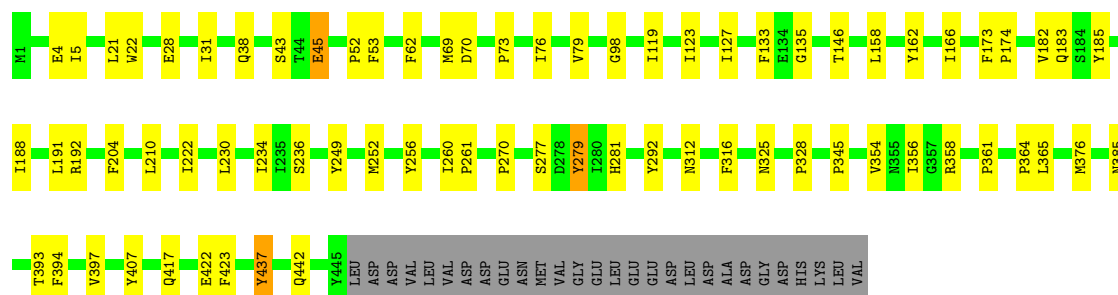
### • Molecule 3: TUBULIN GAMMA CHAIN

Chain 6-C: 78% 15% • 6%



### • Molecule 3: TUBULIN GAMMA CHAIN

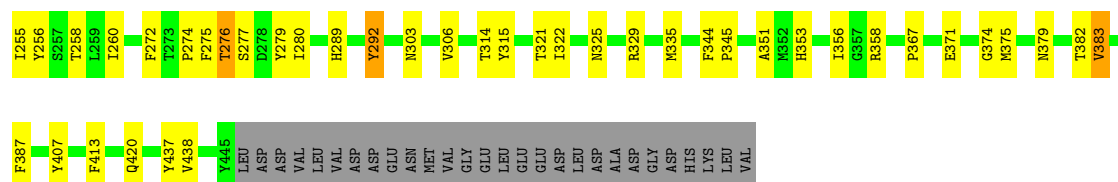
Chain 6-D: 79% 15% • 6%



### • Molecule 3: TUBULIN GAMMA CHAIN

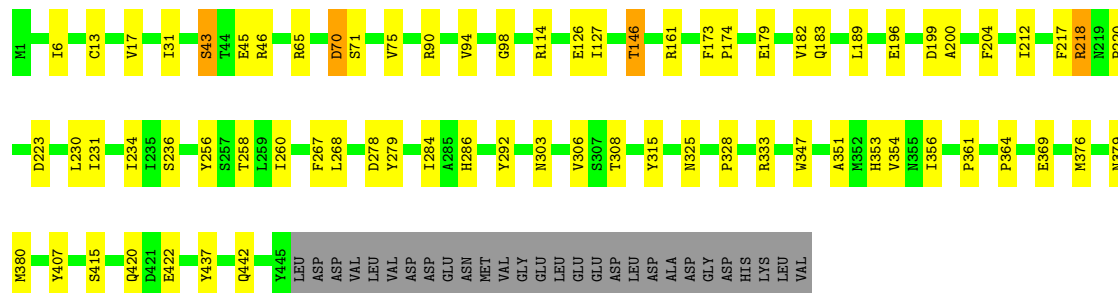
Chain 7-C: 79% 15% • 6%





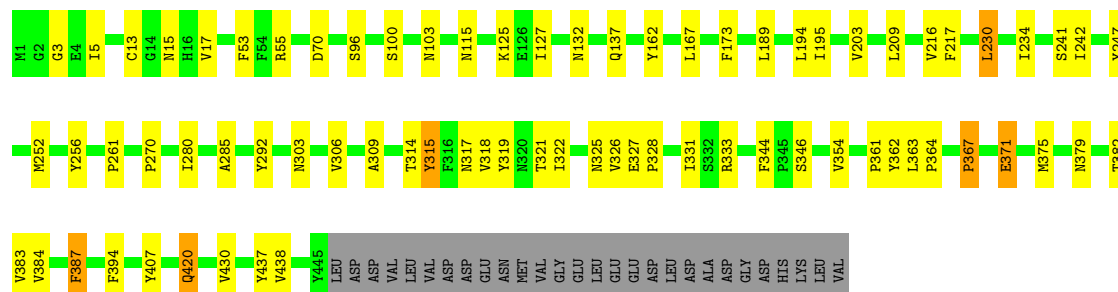
### • Molecule 3: TUBULIN GAMMA CHAIN

Chain 7-D: 79% 14% • 6%



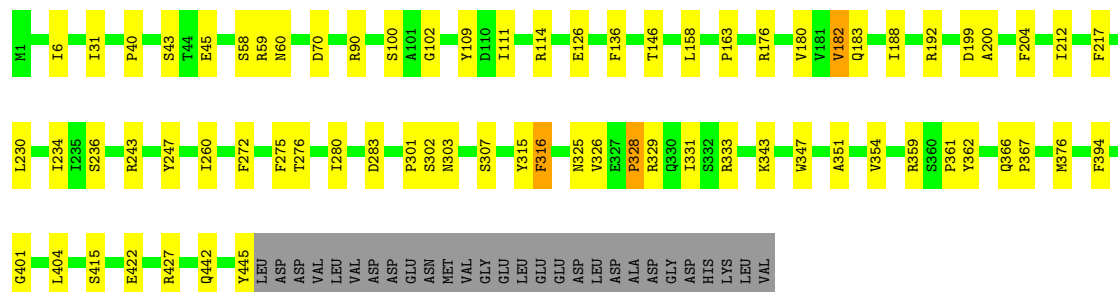
### • Molecule 3: TUBULIN GAMMA CHAIN

Chain 8-C: 78% 15% • 6%



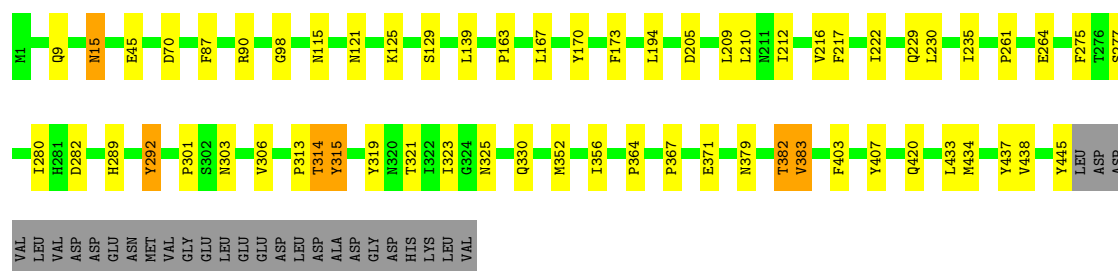
### • Molecule 3: TUBULIN GAMMA CHAIN

Chain 8-D: 79% 15% • 6%

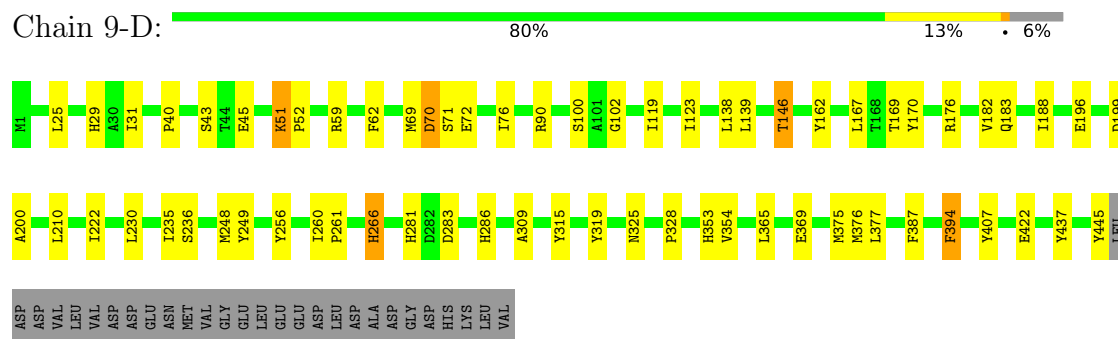


### • Molecule 3: TUBULIN GAMMA CHAIN

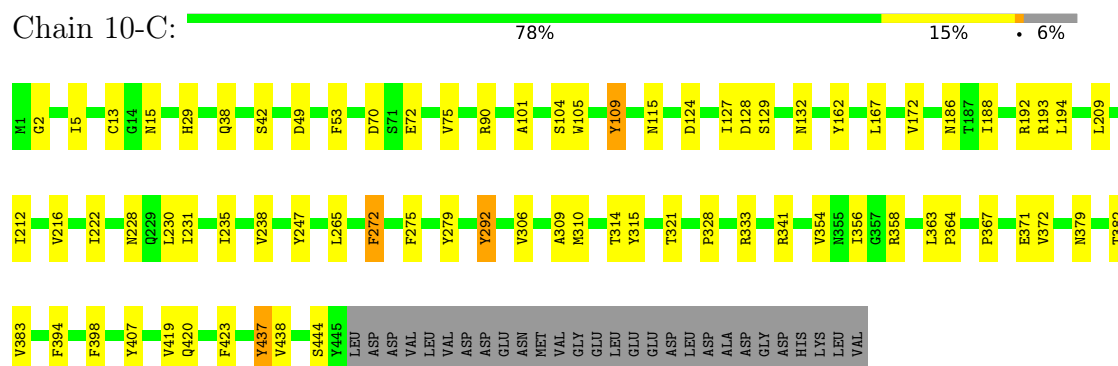
Chain 9-C: 81% 12% • 6%



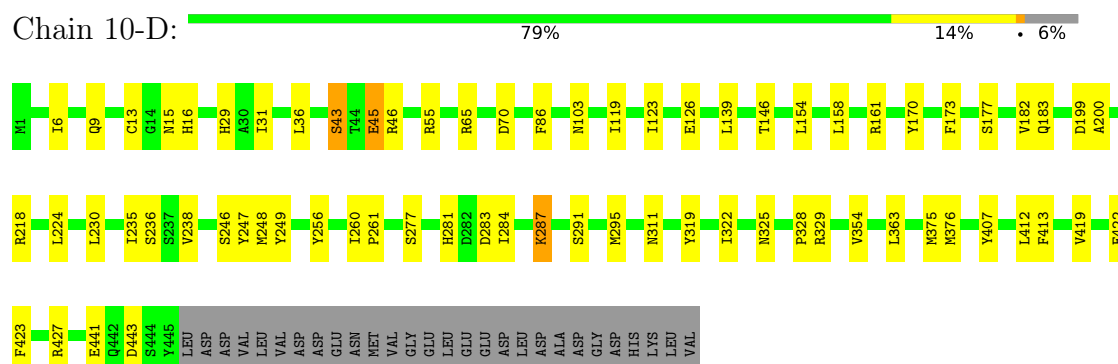
• Molecule 3: TUBULIN GAMMA CHAIN



• Molecule 3: TUBULIN GAMMA CHAIN



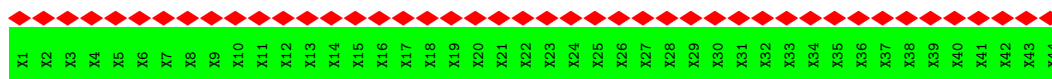
• Molecule 3: TUBULIN GAMMA CHAIN



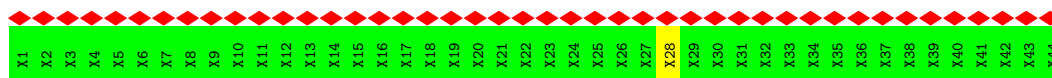
• Molecule 4: SPINDLE POLE BODY COMPONENT 110

100%





• Molecule 4: SPINDLE POLE BODY COMPONENT 110



• Molecule 4: SPINDLE POLE BODY COMPONENT 110



There are no outlier residues recorded for this chain.

• Molecule 4: SPINDLE POLE BODY COMPONENT 110



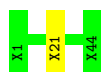
There are no outlier residues recorded for this chain.

• Molecule 4: SPINDLE POLE BODY COMPONENT 110



There are no outlier residues recorded for this chain.

• Molecule 4: SPINDLE POLE BODY COMPONENT 110



• Molecule 4: SPINDLE POLE BODY COMPONENT 110



There are no outlier residues recorded for this chain.

• Molecule 4: SPINDLE POLE BODY COMPONENT 110



There are no outlier residues recorded for this chain.

• Molecule 4: SPINDLE POLE BODY COMPONENT 110



There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 5-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 6-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 6-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 7-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 7-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 8-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 8-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 9-E:  100%

There are no outlier residues recorded for this chain.

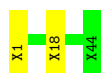
- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 9-F:  100%

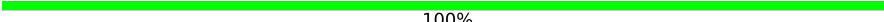
There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 10-E:  95% 5%



- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 10-F:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

| Property                             | Value                                                                     | Source    |
|--------------------------------------|---------------------------------------------------------------------------|-----------|
| EM reconstruction method             | HELICAL                                                                   | Depositor |
| Imposed symmetry                     | HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided | Depositor |
| Number of segments used              | Not provided                                                              |           |
| Resolution determination method      | Not provided                                                              |           |
| CTF correction method                | WHOLE MICROGRAPH                                                          | Depositor |
| Microscope                           | FEI TECNAI F20                                                            | Depositor |
| Voltage (kV)                         | 200                                                                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20                                                                        | Depositor |
| Minimum defocus (nm)                 | 800                                                                       | Depositor |
| Maximum defocus (nm)                 | 3000                                                                      | Depositor |
| Magnification                        | 60000                                                                     | Depositor |
| Image detector                       | TVIPS TEMCAM-F816 (8k x 8k)                                               | Depositor |
| Maximum map value                    | 6.278                                                                     | Depositor |
| Minimum map value                    | -3.005                                                                    | Depositor |
| Average map value                    | 1.000                                                                     | Depositor |
| Map value standard deviation         | 1.000                                                                     | Depositor |
| Recommended contour level            | 2.5                                                                       | Depositor |
| Map size (Å)                         | 380.8, 380.8, 380.8                                                       | wwPDB     |
| Map dimensions                       | 320, 320, 320                                                             | wwPDB     |
| Map angles (°)                       | 90, 90, 90                                                                | wwPDB     |
| Pixel spacing (Å)                    | 1.19, 1.19, 1.19                                                          | 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   | 1-A   | 0.40         | 0/4917      | 0.48        | 0/6616      |
| 1   | 2-A   | 0.40         | 0/4917      | 0.48        | 0/6616      |
| 1   | 3-A   | 0.40         | 0/4917      | 0.48        | 0/6616      |
| 1   | 4-A   | 0.40         | 0/4917      | 0.48        | 0/6616      |
| 1   | 5-A   | 0.40         | 0/4917      | 0.48        | 0/6616      |
| 1   | 6-A   | 0.40         | 0/4917      | 0.48        | 0/6616      |
| 1   | 7-A   | 0.40         | 0/4917      | 0.48        | 0/6616      |
| 1   | 8-A   | 0.40         | 0/4917      | 0.48        | 0/6616      |
| 1   | 9-A   | 0.40         | 0/4917      | 0.48        | 0/6616      |
| 1   | 10-A  | 0.40         | 0/4917      | 0.48        | 0/6616      |
| 2   | 1-B   | 0.41         | 0/4803      | 0.47        | 0/6481      |
| 2   | 2-B   | 0.41         | 0/4803      | 0.47        | 0/6481      |
| 2   | 3-B   | 0.41         | 0/4803      | 0.47        | 0/6481      |
| 2   | 4-B   | 0.41         | 0/4803      | 0.47        | 0/6481      |
| 2   | 5-B   | 0.41         | 0/4803      | 0.47        | 0/6481      |
| 2   | 6-B   | 0.41         | 0/4803      | 0.47        | 0/6481      |
| 2   | 7-B   | 0.41         | 0/4803      | 0.47        | 0/6481      |
| 2   | 8-B   | 0.41         | 0/4803      | 0.47        | 0/6481      |
| 2   | 9-B   | 0.41         | 0/4803      | 0.47        | 0/6481      |
| 2   | 10-B  | 0.41         | 0/4803      | 0.47        | 0/6481      |
| 3   | 1-C   | 0.42         | 0/3558      | 0.47        | 0/4831      |
| 3   | 1-D   | 0.41         | 0/3558      | 0.45        | 0/4831      |
| 3   | 2-C   | 0.42         | 0/3558      | 0.47        | 0/4831      |
| 3   | 2-D   | 0.41         | 0/3558      | 0.45        | 0/4831      |
| 3   | 3-C   | 0.42         | 0/3558      | 0.47        | 0/4831      |
| 3   | 3-D   | 0.41         | 0/3558      | 0.45        | 0/4831      |
| 3   | 4-C   | 0.42         | 0/3558      | 0.47        | 0/4831      |
| 3   | 4-D   | 0.41         | 0/3558      | 0.45        | 0/4831      |
| 3   | 5-C   | 0.42         | 0/3558      | 0.47        | 0/4831      |
| 3   | 5-D   | 0.41         | 0/3558      | 0.45        | 0/4831      |
| 3   | 6-C   | 0.42         | 0/3558      | 0.47        | 0/4831      |
| 3   | 6-D   | 0.41         | 0/3558      | 0.45        | 0/4831      |
| 3   | 7-C   | 0.42         | 0/3558      | 0.47        | 0/4831      |
| 3   | 7-D   | 0.41         | 0/3558      | 0.45        | 0/4831      |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 3   | 8-C   | 0.42         | 0/3558   | 0.47        | 0/4831   |
| 3   | 8-D   | 0.41         | 0/3558   | 0.45        | 0/4831   |
| 3   | 9-C   | 0.42         | 0/3558   | 0.47        | 0/4831   |
| 3   | 9-D   | 0.41         | 0/3558   | 0.45        | 0/4831   |
| 3   | 10-C  | 0.42         | 0/3558   | 0.47        | 0/4831   |
| 3   | 10-D  | 0.41         | 0/3558   | 0.45        | 0/4831   |
| All | All   | 0.41         | 0/168360 | 0.47        | 0/227590 |

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   | 1-A   | 0                   | 19                  |
| 1   | 2-A   | 0                   | 16                  |
| 1   | 3-A   | 0                   | 15                  |
| 1   | 4-A   | 0                   | 16                  |
| 1   | 5-A   | 0                   | 18                  |
| 1   | 6-A   | 0                   | 24                  |
| 1   | 7-A   | 0                   | 19                  |
| 1   | 8-A   | 0                   | 21                  |
| 1   | 9-A   | 0                   | 19                  |
| 1   | 10-A  | 0                   | 20                  |
| 2   | 1-B   | 0                   | 25                  |
| 2   | 2-B   | 0                   | 18                  |
| 2   | 3-B   | 0                   | 17                  |
| 2   | 4-B   | 0                   | 21                  |
| 2   | 5-B   | 0                   | 7                   |
| 2   | 6-B   | 0                   | 19                  |
| 2   | 7-B   | 0                   | 23                  |
| 2   | 8-B   | 0                   | 28                  |
| 2   | 9-B   | 0                   | 15                  |
| 2   | 10-B  | 0                   | 25                  |
| 3   | 1-C   | 0                   | 15                  |
| 3   | 1-D   | 0                   | 9                   |
| 3   | 2-C   | 0                   | 9                   |
| 3   | 2-D   | 0                   | 6                   |
| 3   | 3-C   | 0                   | 16                  |
| 3   | 3-D   | 0                   | 12                  |
| 3   | 4-C   | 0                   | 13                  |
| 3   | 4-D   | 0                   | 13                  |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | 5-C   | 0                   | 8                   |
| 3   | 5-D   | 0                   | 10                  |
| 3   | 6-C   | 0                   | 12                  |
| 3   | 6-D   | 1                   | 8                   |
| 3   | 7-C   | 0                   | 9                   |
| 3   | 7-D   | 0                   | 11                  |
| 3   | 8-C   | 0                   | 9                   |
| 3   | 8-D   | 0                   | 14                  |
| 3   | 9-C   | 0                   | 8                   |
| 3   | 9-D   | 0                   | 14                  |
| 3   | 10-C  | 0                   | 11                  |
| 3   | 10-D  | 0                   | 17                  |
| All | All   | 1                   | 609                 |

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | 6-D   | 73  | PRO  | CA   |

All (609) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 1-A   | 112 | TYR  | Sidechain |
| 1   | 1-A   | 123 | TYR  | Sidechain |
| 1   | 1-A   | 140 | TYR  | Sidechain |
| 1   | 1-A   | 181 | GLU  | Peptide   |
| 1   | 1-A   | 299 | PHE  | Sidechain |
| 1   | 1-A   | 333 | ARG  | Sidechain |
| 1   | 1-A   | 400 | ARG  | Sidechain |
| 1   | 1-A   | 405 | PHE  | Sidechain |
| 1   | 1-A   | 429 | TYR  | Sidechain |
| 1   | 1-A   | 438 | PHE  | Sidechain |
| 1   | 1-A   | 469 | ARG  | Sidechain |
| 1   | 1-A   | 486 | PHE  | Sidechain |
| 1   | 1-A   | 582 | TYR  | Sidechain |
| 1   | 1-A   | 587 | ARG  | Sidechain |
| 1   | 1-A   | 614 | TYR  | Sidechain |
| 1   | 1-A   | 627 | ARG  | Sidechain |
| 1   | 1-A   | 706 | PHE  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 1-A   | 74  | TYR  | Sidechain |
| 1   | 1-A   | 767 | TYR  | Sidechain |
| 2   | 1-B   | 187 | TYR  | Sidechain |
| 2   | 1-B   | 190 | TYR  | Sidechain |
| 2   | 1-B   | 222 | HIS  | Sidechain |
| 2   | 1-B   | 264 | TYR  | Sidechain |
| 2   | 1-B   | 293 | ARG  | Sidechain |
| 2   | 1-B   | 297 | TYR  | Sidechain |
| 2   | 1-B   | 299 | ARG  | Sidechain |
| 2   | 1-B   | 342 | TYR  | Sidechain |
| 2   | 1-B   | 343 | TYR  | Sidechain |
| 2   | 1-B   | 356 | ARG  | Sidechain |
| 2   | 1-B   | 379 | TYR  | Sidechain |
| 2   | 1-B   | 415 | TYR  | Sidechain |
| 2   | 1-B   | 425 | PHE  | Sidechain |
| 2   | 1-B   | 433 | TYR  | Sidechain |
| 2   | 1-B   | 439 | ARG  | Sidechain |
| 2   | 1-B   | 488 | PHE  | Sidechain |
| 2   | 1-B   | 526 | ARG  | Sidechain |
| 2   | 1-B   | 562 | TYR  | Sidechain |
| 2   | 1-B   | 576 | ARG  | Sidechain |
| 2   | 1-B   | 598 | TYR  | Sidechain |
| 2   | 1-B   | 599 | PHE  | Sidechain |
| 2   | 1-B   | 612 | ARG  | Sidechain |
| 2   | 1-B   | 652 | TYR  | Sidechain |
| 2   | 1-B   | 772 | PHE  | Sidechain |
| 2   | 1-B   | 776 | TYR  | Sidechain |
| 3   | 1-C   | 109 | TYR  | Sidechain |
| 3   | 1-C   | 185 | TYR  | Sidechain |
| 3   | 1-C   | 20  | PHE  | Sidechain |
| 3   | 1-C   | 249 | TYR  | Sidechain |
| 3   | 1-C   | 256 | TYR  | Sidechain |
| 3   | 1-C   | 279 | TYR  | Sidechain |
| 3   | 1-C   | 281 | HIS  | Sidechain |
| 3   | 1-C   | 292 | TYR  | Sidechain |
| 3   | 1-C   | 319 | TYR  | Sidechain |
| 3   | 1-C   | 362 | TYR  | Sidechain |
| 3   | 1-C   | 394 | PHE  | Sidechain |
| 3   | 1-C   | 407 | TYR  | Sidechain |
| 3   | 1-C   | 437 | TYR  | Sidechain |
| 3   | 1-C   | 445 | TYR  | Sidechain |
| 3   | 1-C   | 86  | PHE  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | 1-D   | 109 | TYR  | Sidechain |
| 3   | 1-D   | 136 | PHE  | Sidechain |
| 3   | 1-D   | 170 | TYR  | Sidechain |
| 3   | 1-D   | 249 | TYR  | Sidechain |
| 3   | 1-D   | 279 | TYR  | Sidechain |
| 3   | 1-D   | 333 | ARG  | Sidechain |
| 3   | 1-D   | 362 | TYR  | Sidechain |
| 3   | 1-D   | 387 | PHE  | Sidechain |
| 3   | 1-D   | 437 | TYR  | Sidechain |
| 1   | 10-A  | 143 | ARG  | Sidechain |
| 1   | 10-A  | 150 | TYR  | Sidechain |
| 1   | 10-A  | 171 | ARG  | Sidechain |
| 1   | 10-A  | 190 | TYR  | Sidechain |
| 1   | 10-A  | 198 | ARG  | Sidechain |
| 1   | 10-A  | 333 | ARG  | Sidechain |
| 1   | 10-A  | 381 | PHE  | Sidechain |
| 1   | 10-A  | 413 | TYR  | Sidechain |
| 1   | 10-A  | 449 | HIS  | Sidechain |
| 1   | 10-A  | 450 | TYR  | Sidechain |
| 1   | 10-A  | 479 | ARG  | Sidechain |
| 1   | 10-A  | 558 | TYR  | Sidechain |
| 1   | 10-A  | 594 | TYR  | Sidechain |
| 1   | 10-A  | 623 | ARG  | Sidechain |
| 1   | 10-A  | 630 | ARG  | Sidechain |
| 1   | 10-A  | 663 | TYR  | Sidechain |
| 1   | 10-A  | 664 | ARG  | Sidechain |
| 1   | 10-A  | 706 | PHE  | Sidechain |
| 1   | 10-A  | 76  | ARG  | Sidechain |
| 1   | 10-A  | 791 | PHE  | Sidechain |
| 2   | 10-B  | 190 | TYR  | Sidechain |
| 2   | 10-B  | 231 | TYR  | Sidechain |
| 2   | 10-B  | 242 | ARG  | Sidechain |
| 2   | 10-B  | 288 | TYR  | Sidechain |
| 2   | 10-B  | 297 | TYR  | Sidechain |
| 2   | 10-B  | 342 | TYR  | Sidechain |
| 2   | 10-B  | 343 | TYR  | Sidechain |
| 2   | 10-B  | 356 | ARG  | Sidechain |
| 2   | 10-B  | 411 | PHE  | Sidechain |
| 2   | 10-B  | 429 | TYR  | Sidechain |
| 2   | 10-B  | 438 | TYR  | Sidechain |
| 2   | 10-B  | 446 | PHE  | Sidechain |
| 2   | 10-B  | 453 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | 10-B  | 470 | TYR  | Sidechain |
| 2   | 10-B  | 471 | ARG  | Sidechain |
| 2   | 10-B  | 562 | TYR  | Sidechain |
| 2   | 10-B  | 592 | ARG  | Sidechain |
| 2   | 10-B  | 598 | TYR  | Sidechain |
| 2   | 10-B  | 652 | TYR  | Sidechain |
| 2   | 10-B  | 670 | ARG  | Sidechain |
| 2   | 10-B  | 731 | PHE  | Sidechain |
| 2   | 10-B  | 741 | PHE  | Sidechain |
| 2   | 10-B  | 772 | PHE  | Sidechain |
| 2   | 10-B  | 805 | PHE  | Sidechain |
| 2   | 10-B  | 824 | TYR  | Sidechain |
| 3   | 10-C  | 109 | TYR  | Sidechain |
| 3   | 10-C  | 192 | ARG  | Sidechain |
| 3   | 10-C  | 247 | TYR  | Sidechain |
| 3   | 10-C  | 272 | PHE  | Sidechain |
| 3   | 10-C  | 333 | ARG  | Sidechain |
| 3   | 10-C  | 341 | ARG  | Sidechain |
| 3   | 10-C  | 358 | ARG  | Sidechain |
| 3   | 10-C  | 398 | PHE  | Sidechain |
| 3   | 10-C  | 407 | TYR  | Sidechain |
| 3   | 10-C  | 437 | TYR  | Sidechain |
| 3   | 10-C  | 90  | ARG  | Sidechain |
| 3   | 10-D  | 16  | HIS  | Sidechain |
| 3   | 10-D  | 161 | ARG  | Sidechain |
| 3   | 10-D  | 170 | TYR  | Sidechain |
| 3   | 10-D  | 173 | PHE  | Sidechain |
| 3   | 10-D  | 218 | ARG  | Sidechain |
| 3   | 10-D  | 247 | TYR  | Sidechain |
| 3   | 10-D  | 249 | TYR  | Sidechain |
| 3   | 10-D  | 256 | TYR  | Sidechain |
| 3   | 10-D  | 319 | TYR  | Sidechain |
| 3   | 10-D  | 407 | TYR  | Sidechain |
| 3   | 10-D  | 413 | PHE  | Sidechain |
| 3   | 10-D  | 423 | PHE  | Sidechain |
| 3   | 10-D  | 427 | ARG  | Sidechain |
| 3   | 10-D  | 46  | ARG  | Sidechain |
| 3   | 10-D  | 55  | ARG  | Sidechain |
| 3   | 10-D  | 65  | ARG  | Sidechain |
| 3   | 10-D  | 86  | PHE  | Sidechain |
| 1   | 2-A   | 123 | TYR  | Sidechain |
| 1   | 2-A   | 140 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 2-A   | 193 | TYR  | Sidechain |
| 1   | 2-A   | 198 | ARG  | Sidechain |
| 1   | 2-A   | 279 | TYR  | Sidechain |
| 1   | 2-A   | 296 | TYR  | Sidechain |
| 1   | 2-A   | 345 | PHE  | Sidechain |
| 1   | 2-A   | 381 | PHE  | Sidechain |
| 1   | 2-A   | 393 | TYR  | Sidechain |
| 1   | 2-A   | 413 | TYR  | Sidechain |
| 1   | 2-A   | 450 | TYR  | Sidechain |
| 1   | 2-A   | 582 | TYR  | Sidechain |
| 1   | 2-A   | 594 | TYR  | Sidechain |
| 1   | 2-A   | 638 | HIS  | Sidechain |
| 1   | 2-A   | 77  | TYR  | Sidechain |
| 1   | 2-A   | 794 | TYR  | Sidechain |
| 2   | 2-B   | 200 | PHE  | Sidechain |
| 2   | 2-B   | 264 | TYR  | Sidechain |
| 2   | 2-B   | 284 | TYR  | Sidechain |
| 2   | 2-B   | 319 | PHE  | Sidechain |
| 2   | 2-B   | 328 | ARG  | Sidechain |
| 2   | 2-B   | 345 | TYR  | Sidechain |
| 2   | 2-B   | 400 | TYR  | Sidechain |
| 2   | 2-B   | 411 | PHE  | Sidechain |
| 2   | 2-B   | 415 | TYR  | Sidechain |
| 2   | 2-B   | 429 | TYR  | Sidechain |
| 2   | 2-B   | 439 | ARG  | Sidechain |
| 2   | 2-B   | 470 | TYR  | Sidechain |
| 2   | 2-B   | 558 | PHE  | Sidechain |
| 2   | 2-B   | 578 | PHE  | Sidechain |
| 2   | 2-B   | 612 | ARG  | Sidechain |
| 2   | 2-B   | 641 | PHE  | Sidechain |
| 2   | 2-B   | 742 | ALA  | Peptide   |
| 2   | 2-B   | 822 | ARG  | Sidechain |
| 3   | 2-C   | 185 | TYR  | Sidechain |
| 3   | 2-C   | 247 | TYR  | Sidechain |
| 3   | 2-C   | 249 | TYR  | Sidechain |
| 3   | 2-C   | 279 | TYR  | Sidechain |
| 3   | 2-C   | 292 | TYR  | Sidechain |
| 3   | 2-C   | 333 | ARG  | Sidechain |
| 3   | 2-C   | 407 | TYR  | Sidechain |
| 3   | 2-C   | 445 | TYR  | Sidechain |
| 3   | 2-C   | 65  | ARG  | Sidechain |
| 3   | 2-D   | 176 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | 2-D   | 218 | ARG  | Sidechain |
| 3   | 2-D   | 329 | ARG  | Sidechain |
| 3   | 2-D   | 359 | ARG  | Sidechain |
| 3   | 2-D   | 55  | ARG  | Sidechain |
| 3   | 2-D   | 84  | ARG  | Sidechain |
| 1   | 3-A   | 171 | ARG  | Sidechain |
| 1   | 3-A   | 183 | ASN  | Mainchain |
| 1   | 3-A   | 197 | PHE  | Sidechain |
| 1   | 3-A   | 324 | TYR  | Sidechain |
| 1   | 3-A   | 410 | PHE  | Sidechain |
| 1   | 3-A   | 429 | TYR  | Sidechain |
| 1   | 3-A   | 568 | TYR  | Sidechain |
| 1   | 3-A   | 588 | TYR  | Sidechain |
| 1   | 3-A   | 594 | TYR  | Sidechain |
| 1   | 3-A   | 633 | HIS  | Sidechain |
| 1   | 3-A   | 663 | TYR  | Sidechain |
| 1   | 3-A   | 664 | ARG  | Sidechain |
| 1   | 3-A   | 704 | TYR  | Sidechain |
| 1   | 3-A   | 782 | PHE  | Sidechain |
| 1   | 3-A   | 794 | TYR  | Sidechain |
| 2   | 3-B   | 264 | TYR  | Sidechain |
| 2   | 3-B   | 288 | TYR  | Sidechain |
| 2   | 3-B   | 297 | TYR  | Sidechain |
| 2   | 3-B   | 345 | TYR  | Sidechain |
| 2   | 3-B   | 356 | ARG  | Sidechain |
| 2   | 3-B   | 359 | TYR  | Sidechain |
| 2   | 3-B   | 389 | ARG  | Sidechain |
| 2   | 3-B   | 445 | PHE  | Sidechain |
| 2   | 3-B   | 471 | ARG  | Sidechain |
| 2   | 3-B   | 488 | PHE  | Sidechain |
| 2   | 3-B   | 598 | TYR  | Sidechain |
| 2   | 3-B   | 641 | PHE  | Sidechain |
| 2   | 3-B   | 651 | TYR  | Sidechain |
| 2   | 3-B   | 652 | TYR  | Sidechain |
| 2   | 3-B   | 770 | TYR  | Sidechain |
| 2   | 3-B   | 816 | TYR  | Sidechain |
| 2   | 3-B   | 827 | ARG  | Sidechain |
| 3   | 3-C   | 114 | ARG  | Sidechain |
| 3   | 3-C   | 133 | PHE  | Sidechain |
| 3   | 3-C   | 185 | TYR  | Sidechain |
| 3   | 3-C   | 249 | TYR  | Sidechain |
| 3   | 3-C   | 267 | PHE  | Sidechain |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 3   | 3-C   | 292 | TYR  | Sidechain         |
| 3   | 3-C   | 319 | TYR  | Sidechain         |
| 3   | 3-C   | 329 | ARG  | Sidechain         |
| 3   | 3-C   | 362 | TYR  | Sidechain         |
| 3   | 3-C   | 394 | PHE  | Sidechain         |
| 3   | 3-C   | 445 | TYR  | Sidechain         |
| 3   | 3-C   | 46  | ARG  | Sidechain         |
| 3   | 3-C   | 55  | ARG  | Sidechain         |
| 3   | 3-C   | 59  | ARG  | Sidechain         |
| 3   | 3-C   | 83  | PHE  | Sidechain         |
| 3   | 3-C   | 87  | PHE  | Sidechain         |
| 3   | 3-D   | 109 | TYR  | Sidechain         |
| 3   | 3-D   | 204 | PHE  | Sidechain         |
| 3   | 3-D   | 247 | TYR  | Sidechain         |
| 3   | 3-D   | 275 | PHE  | Sidechain         |
| 3   | 3-D   | 279 | TYR  | Sidechain         |
| 3   | 3-D   | 292 | TYR  | Sidechain         |
| 3   | 3-D   | 315 | TYR  | Sidechain         |
| 3   | 3-D   | 319 | TYR  | Sidechain         |
| 3   | 3-D   | 362 | TYR  | Sidechain         |
| 3   | 3-D   | 407 | TYR  | Sidechain         |
| 3   | 3-D   | 413 | PHE  | Sidechain         |
| 3   | 3-D   | 59  | ARG  | Sidechain         |
| 1   | 4-A   | 193 | TYR  | Sidechain         |
| 1   | 4-A   | 204 | ARG  | Sidechain         |
| 1   | 4-A   | 296 | TYR  | Sidechain         |
| 1   | 4-A   | 324 | TYR  | Sidechain         |
| 1   | 4-A   | 393 | TYR  | Sidechain         |
| 1   | 4-A   | 398 | TYR  | Sidechain         |
| 1   | 4-A   | 400 | ARG  | Sidechain         |
| 1   | 4-A   | 405 | PHE  | Sidechain         |
| 1   | 4-A   | 450 | TYR  | Sidechain         |
| 1   | 4-A   | 469 | ARG  | Sidechain         |
| 1   | 4-A   | 479 | ARG  | Peptide,Sidechain |
| 1   | 4-A   | 633 | HIS  | Sidechain         |
| 1   | 4-A   | 639 | PHE  | Sidechain         |
| 1   | 4-A   | 74  | TYR  | Sidechain         |
| 1   | 4-A   | 767 | TYR  | Sidechain         |
| 2   | 4-B   | 222 | HIS  | Sidechain         |
| 2   | 4-B   | 264 | TYR  | Sidechain         |
| 2   | 4-B   | 285 | ARG  | Sidechain         |
| 2   | 4-B   | 288 | TYR  | Sidechain         |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | 4-B   | 328 | ARG  | Sidechain |
| 2   | 4-B   | 342 | TYR  | Sidechain |
| 2   | 4-B   | 379 | TYR  | Sidechain |
| 2   | 4-B   | 400 | TYR  | Sidechain |
| 2   | 4-B   | 411 | PHE  | Sidechain |
| 2   | 4-B   | 438 | TYR  | Sidechain |
| 2   | 4-B   | 470 | TYR  | Sidechain |
| 2   | 4-B   | 471 | ARG  | Sidechain |
| 2   | 4-B   | 488 | PHE  | Sidechain |
| 2   | 4-B   | 583 | TYR  | Sidechain |
| 2   | 4-B   | 592 | ARG  | Sidechain |
| 2   | 4-B   | 593 | PHE  | Sidechain |
| 2   | 4-B   | 598 | TYR  | Sidechain |
| 2   | 4-B   | 644 | PHE  | Sidechain |
| 2   | 4-B   | 805 | PHE  | Sidechain |
| 2   | 4-B   | 816 | TYR  | Sidechain |
| 2   | 4-B   | 827 | ARG  | Sidechain |
| 3   | 4-C   | 162 | TYR  | Sidechain |
| 3   | 4-C   | 217 | PHE  | Sidechain |
| 3   | 4-C   | 247 | TYR  | Sidechain |
| 3   | 4-C   | 256 | TYR  | Sidechain |
| 3   | 4-C   | 272 | PHE  | Sidechain |
| 3   | 4-C   | 292 | TYR  | Sidechain |
| 3   | 4-C   | 319 | TYR  | Sidechain |
| 3   | 4-C   | 341 | ARG  | Sidechain |
| 3   | 4-C   | 358 | ARG  | Sidechain |
| 3   | 4-C   | 359 | ARG  | Sidechain |
| 3   | 4-C   | 445 | TYR  | Sidechain |
| 3   | 4-C   | 46  | ARG  | Sidechain |
| 3   | 4-C   | 90  | ARG  | Sidechain |
| 3   | 4-D   | 114 | ARG  | Sidechain |
| 3   | 4-D   | 176 | ARG  | Sidechain |
| 3   | 4-D   | 243 | ARG  | Sidechain |
| 3   | 4-D   | 247 | TYR  | Sidechain |
| 3   | 4-D   | 256 | TYR  | Sidechain |
| 3   | 4-D   | 315 | TYR  | Sidechain |
| 3   | 4-D   | 329 | ARG  | Sidechain |
| 3   | 4-D   | 344 | PHE  | Sidechain |
| 3   | 4-D   | 362 | TYR  | Sidechain |
| 3   | 4-D   | 407 | TYR  | Sidechain |
| 3   | 4-D   | 423 | PHE  | Sidechain |
| 3   | 4-D   | 62  | PHE  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | 4-D   | 86  | PHE  | Sidechain |
| 1   | 5-A   | 111 | ARG  | Sidechain |
| 1   | 5-A   | 121 | ARG  | Sidechain |
| 1   | 5-A   | 138 | PHE  | Sidechain |
| 1   | 5-A   | 140 | TYR  | Sidechain |
| 1   | 5-A   | 144 | ARG  | Sidechain |
| 1   | 5-A   | 203 | ARG  | Sidechain |
| 1   | 5-A   | 279 | TYR  | Sidechain |
| 1   | 5-A   | 296 | TYR  | Sidechain |
| 1   | 5-A   | 302 | TYR  | Sidechain |
| 1   | 5-A   | 327 | ARG  | Sidechain |
| 1   | 5-A   | 349 | ARG  | Sidechain |
| 1   | 5-A   | 393 | TYR  | Sidechain |
| 1   | 5-A   | 409 | PHE  | Sidechain |
| 1   | 5-A   | 559 | HIS  | Sidechain |
| 1   | 5-A   | 623 | ARG  | Sidechain |
| 1   | 5-A   | 627 | ARG  | Sidechain |
| 1   | 5-A   | 767 | TYR  | Sidechain |
| 1   | 5-A   | 92  | PHE  | Sidechain |
| 2   | 5-B   | 190 | TYR  | Sidechain |
| 2   | 5-B   | 328 | ARG  | Sidechain |
| 2   | 5-B   | 400 | TYR  | Sidechain |
| 2   | 5-B   | 570 | LEU  | Mainchain |
| 2   | 5-B   | 742 | ALA  | Peptide   |
| 2   | 5-B   | 770 | TYR  | Sidechain |
| 2   | 5-B   | 776 | TYR  | Sidechain |
| 3   | 5-C   | 114 | ARG  | Sidechain |
| 3   | 5-C   | 162 | TYR  | Sidechain |
| 3   | 5-C   | 170 | TYR  | Sidechain |
| 3   | 5-C   | 176 | ARG  | Sidechain |
| 3   | 5-C   | 243 | ARG  | Sidechain |
| 3   | 5-C   | 292 | TYR  | Sidechain |
| 3   | 5-C   | 445 | TYR  | Sidechain |
| 3   | 5-C   | 84  | ARG  | Sidechain |
| 3   | 5-D   | 109 | TYR  | Sidechain |
| 3   | 5-D   | 114 | ARG  | Sidechain |
| 3   | 5-D   | 136 | PHE  | Sidechain |
| 3   | 5-D   | 243 | ARG  | Sidechain |
| 3   | 5-D   | 292 | TYR  | Sidechain |
| 3   | 5-D   | 329 | ARG  | Sidechain |
| 3   | 5-D   | 413 | PHE  | Sidechain |
| 3   | 5-D   | 423 | PHE  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | 5-D   | 445 | TYR  | Sidechain |
| 3   | 5-D   | 54  | PHE  | Sidechain |
| 1   | 6-A   | 108 | ARG  | Sidechain |
| 1   | 6-A   | 123 | TYR  | Sidechain |
| 1   | 6-A   | 138 | PHE  | Sidechain |
| 1   | 6-A   | 150 | TYR  | Sidechain |
| 1   | 6-A   | 157 | ARG  | Sidechain |
| 1   | 6-A   | 190 | TYR  | Sidechain |
| 1   | 6-A   | 193 | TYR  | Sidechain |
| 1   | 6-A   | 267 | PHE  | Sidechain |
| 1   | 6-A   | 279 | TYR  | Sidechain |
| 1   | 6-A   | 299 | PHE  | Sidechain |
| 1   | 6-A   | 324 | TYR  | Sidechain |
| 1   | 6-A   | 358 | ARG  | Sidechain |
| 1   | 6-A   | 393 | TYR  | Sidechain |
| 1   | 6-A   | 450 | TYR  | Sidechain |
| 1   | 6-A   | 558 | TYR  | Sidechain |
| 1   | 6-A   | 568 | TYR  | Sidechain |
| 1   | 6-A   | 576 | ARG  | Sidechain |
| 1   | 6-A   | 594 | TYR  | Sidechain |
| 1   | 6-A   | 627 | ARG  | Sidechain |
| 1   | 6-A   | 633 | HIS  | Sidechain |
| 1   | 6-A   | 657 | TYR  | Sidechain |
| 1   | 6-A   | 663 | TYR  | Sidechain |
| 1   | 6-A   | 76  | ARG  | Sidechain |
| 1   | 6-A   | 775 | PHE  | Sidechain |
| 2   | 6-B   | 216 | PHE  | Sidechain |
| 2   | 6-B   | 236 | TYR  | Sidechain |
| 2   | 6-B   | 241 | PHE  | Sidechain |
| 2   | 6-B   | 284 | TYR  | Sidechain |
| 2   | 6-B   | 293 | ARG  | Sidechain |
| 2   | 6-B   | 295 | ARG  | Sidechain |
| 2   | 6-B   | 297 | TYR  | Sidechain |
| 2   | 6-B   | 299 | ARG  | Sidechain |
| 2   | 6-B   | 322 | HIS  | Peptide   |
| 2   | 6-B   | 328 | ARG  | Sidechain |
| 2   | 6-B   | 345 | TYR  | Sidechain |
| 2   | 6-B   | 409 | TYR  | Sidechain |
| 2   | 6-B   | 430 | HIS  | Sidechain |
| 2   | 6-B   | 438 | TYR  | Sidechain |
| 2   | 6-B   | 469 | HIS  | Sidechain |
| 2   | 6-B   | 470 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | 6-B   | 590 | LEU  | Mainchain |
| 2   | 6-B   | 824 | TYR  | Sidechain |
| 2   | 6-B   | 827 | ARG  | Sidechain |
| 3   | 6-C   | 109 | TYR  | Sidechain |
| 3   | 6-C   | 114 | ARG  | Sidechain |
| 3   | 6-C   | 162 | TYR  | Sidechain |
| 3   | 6-C   | 176 | ARG  | Sidechain |
| 3   | 6-C   | 244 | PHE  | Sidechain |
| 3   | 6-C   | 256 | TYR  | Sidechain |
| 3   | 6-C   | 275 | PHE  | Sidechain |
| 3   | 6-C   | 358 | ARG  | Sidechain |
| 3   | 6-C   | 362 | TYR  | Sidechain |
| 3   | 6-C   | 394 | PHE  | Sidechain |
| 3   | 6-C   | 423 | PHE  | Sidechain |
| 3   | 6-C   | 59  | ARG  | Sidechain |
| 3   | 6-D   | 185 | TYR  | Sidechain |
| 3   | 6-D   | 192 | ARG  | Sidechain |
| 3   | 6-D   | 249 | TYR  | Sidechain |
| 3   | 6-D   | 279 | TYR  | Sidechain |
| 3   | 6-D   | 292 | TYR  | Sidechain |
| 3   | 6-D   | 407 | TYR  | Sidechain |
| 3   | 6-D   | 437 | TYR  | Sidechain |
| 3   | 6-D   | 62  | PHE  | Sidechain |
| 1   | 7-A   | 112 | TYR  | Sidechain |
| 1   | 7-A   | 116 | TYR  | Sidechain |
| 1   | 7-A   | 121 | ARG  | Sidechain |
| 1   | 7-A   | 143 | ARG  | Sidechain |
| 1   | 7-A   | 190 | TYR  | Sidechain |
| 1   | 7-A   | 197 | PHE  | Sidechain |
| 1   | 7-A   | 198 | ARG  | Sidechain |
| 1   | 7-A   | 203 | ARG  | Sidechain |
| 1   | 7-A   | 284 | TYR  | Sidechain |
| 1   | 7-A   | 349 | ARG  | Sidechain |
| 1   | 7-A   | 398 | TYR  | Sidechain |
| 1   | 7-A   | 400 | ARG  | Sidechain |
| 1   | 7-A   | 410 | PHE  | Sidechain |
| 1   | 7-A   | 429 | TYR  | Sidechain |
| 1   | 7-A   | 558 | TYR  | Sidechain |
| 1   | 7-A   | 568 | TYR  | Sidechain |
| 1   | 7-A   | 582 | TYR  | Sidechain |
| 1   | 7-A   | 663 | TYR  | Sidechain |
| 1   | 7-A   | 704 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | 7-B   | 190 | TYR  | Sidechain |
| 2   | 7-B   | 285 | ARG  | Sidechain |
| 2   | 7-B   | 297 | TYR  | Sidechain |
| 2   | 7-B   | 312 | PHE  | Sidechain |
| 2   | 7-B   | 356 | ARG  | Sidechain |
| 2   | 7-B   | 359 | TYR  | Sidechain |
| 2   | 7-B   | 389 | ARG  | Sidechain |
| 2   | 7-B   | 400 | TYR  | Sidechain |
| 2   | 7-B   | 403 | PHE  | Sidechain |
| 2   | 7-B   | 429 | TYR  | Sidechain |
| 2   | 7-B   | 562 | TYR  | Sidechain |
| 2   | 7-B   | 565 | TYR  | Sidechain |
| 2   | 7-B   | 583 | TYR  | Sidechain |
| 2   | 7-B   | 585 | ARG  | Sidechain |
| 2   | 7-B   | 592 | ARG  | Sidechain |
| 2   | 7-B   | 598 | TYR  | Sidechain |
| 2   | 7-B   | 600 | TYR  | Sidechain |
| 2   | 7-B   | 641 | PHE  | Sidechain |
| 2   | 7-B   | 670 | ARG  | Sidechain |
| 2   | 7-B   | 758 | TYR  | Sidechain |
| 2   | 7-B   | 770 | TYR  | Sidechain |
| 2   | 7-B   | 776 | TYR  | Sidechain |
| 2   | 7-B   | 827 | ARG  | Sidechain |
| 3   | 7-C   | 193 | ARG  | Sidechain |
| 3   | 7-C   | 20  | PHE  | Sidechain |
| 3   | 7-C   | 247 | TYR  | Sidechain |
| 3   | 7-C   | 249 | TYR  | Sidechain |
| 3   | 7-C   | 329 | ARG  | Sidechain |
| 3   | 7-C   | 407 | TYR  | Sidechain |
| 3   | 7-C   | 413 | PHE  | Sidechain |
| 3   | 7-C   | 46  | ARG  | Sidechain |
| 3   | 7-C   | 65  | ARG  | Sidechain |
| 3   | 7-D   | 114 | ARG  | Sidechain |
| 3   | 7-D   | 217 | PHE  | Sidechain |
| 3   | 7-D   | 218 | ARG  | Sidechain |
| 3   | 7-D   | 267 | PHE  | Sidechain |
| 3   | 7-D   | 292 | TYR  | Sidechain |
| 3   | 7-D   | 315 | TYR  | Sidechain |
| 3   | 7-D   | 407 | TYR  | Sidechain |
| 3   | 7-D   | 437 | TYR  | Sidechain |
| 3   | 7-D   | 46  | ARG  | Sidechain |
| 3   | 7-D   | 65  | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | 7-D   | 90  | ARG  | Sidechain |
| 1   | 8-A   | 105 | PHE  | Sidechain |
| 1   | 8-A   | 116 | TYR  | Sidechain |
| 1   | 8-A   | 123 | TYR  | Sidechain |
| 1   | 8-A   | 140 | TYR  | Sidechain |
| 1   | 8-A   | 145 | PHE  | Sidechain |
| 1   | 8-A   | 190 | TYR  | Sidechain |
| 1   | 8-A   | 198 | ARG  | Sidechain |
| 1   | 8-A   | 203 | ARG  | Sidechain |
| 1   | 8-A   | 302 | TYR  | Sidechain |
| 1   | 8-A   | 349 | ARG  | Sidechain |
| 1   | 8-A   | 393 | TYR  | Sidechain |
| 1   | 8-A   | 458 | TYR  | Sidechain |
| 1   | 8-A   | 465 | PHE  | Sidechain |
| 1   | 8-A   | 469 | ARG  | Sidechain |
| 1   | 8-A   | 486 | PHE  | Sidechain |
| 1   | 8-A   | 568 | TYR  | Sidechain |
| 1   | 8-A   | 588 | TYR  | Sidechain |
| 1   | 8-A   | 627 | ARG  | Sidechain |
| 1   | 8-A   | 647 | PHE  | Sidechain |
| 1   | 8-A   | 767 | TYR  | Sidechain |
| 1   | 8-A   | 77  | TYR  | Sidechain |
| 2   | 8-B   | 231 | TYR  | Sidechain |
| 2   | 8-B   | 242 | ARG  | Sidechain |
| 2   | 8-B   | 264 | TYR  | Sidechain |
| 2   | 8-B   | 288 | TYR  | Sidechain |
| 2   | 8-B   | 293 | ARG  | Sidechain |
| 2   | 8-B   | 297 | TYR  | Sidechain |
| 2   | 8-B   | 299 | ARG  | Sidechain |
| 2   | 8-B   | 342 | TYR  | Sidechain |
| 2   | 8-B   | 359 | TYR  | Sidechain |
| 2   | 8-B   | 429 | TYR  | Sidechain |
| 2   | 8-B   | 430 | HIS  | Sidechain |
| 2   | 8-B   | 433 | TYR  | Sidechain |
| 2   | 8-B   | 438 | TYR  | Sidechain |
| 2   | 8-B   | 453 | TYR  | Sidechain |
| 2   | 8-B   | 470 | TYR  | Sidechain |
| 2   | 8-B   | 475 | PHE  | Sidechain |
| 2   | 8-B   | 510 | TYR  | Sidechain |
| 2   | 8-B   | 514 | ARG  | Sidechain |
| 2   | 8-B   | 544 | ARG  | Sidechain |
| 2   | 8-B   | 558 | PHE  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | 8-B   | 583 | TYR  | Sidechain |
| 2   | 8-B   | 585 | ARG  | Sidechain |
| 2   | 8-B   | 592 | ARG  | Sidechain |
| 2   | 8-B   | 644 | PHE  | Sidechain |
| 2   | 8-B   | 670 | ARG  | Sidechain |
| 2   | 8-B   | 758 | TYR  | Sidechain |
| 2   | 8-B   | 805 | PHE  | Sidechain |
| 2   | 8-B   | 816 | TYR  | Sidechain |
| 3   | 8-C   | 217 | PHE  | Sidechain |
| 3   | 8-C   | 247 | TYR  | Sidechain |
| 3   | 8-C   | 256 | TYR  | Sidechain |
| 3   | 8-C   | 319 | TYR  | Sidechain |
| 3   | 8-C   | 344 | PHE  | Sidechain |
| 3   | 8-C   | 387 | PHE  | Sidechain |
| 3   | 8-C   | 394 | PHE  | Sidechain |
| 3   | 8-C   | 407 | TYR  | Sidechain |
| 3   | 8-C   | 55  | ARG  | Sidechain |
| 3   | 8-D   | 109 | TYR  | Sidechain |
| 3   | 8-D   | 176 | ARG  | Sidechain |
| 3   | 8-D   | 243 | ARG  | Sidechain |
| 3   | 8-D   | 247 | TYR  | Sidechain |
| 3   | 8-D   | 272 | PHE  | Sidechain |
| 3   | 8-D   | 315 | TYR  | Sidechain |
| 3   | 8-D   | 316 | PHE  | Sidechain |
| 3   | 8-D   | 329 | ARG  | Sidechain |
| 3   | 8-D   | 333 | ARG  | Sidechain |
| 3   | 8-D   | 359 | ARG  | Sidechain |
| 3   | 8-D   | 362 | TYR  | Sidechain |
| 3   | 8-D   | 427 | ARG  | Sidechain |
| 3   | 8-D   | 445 | TYR  | Sidechain |
| 3   | 8-D   | 90  | ARG  | Sidechain |
| 1   | 9-A   | 123 | TYR  | Sidechain |
| 1   | 9-A   | 129 | THR  | Peptide   |
| 1   | 9-A   | 190 | TYR  | Sidechain |
| 1   | 9-A   | 203 | ARG  | Sidechain |
| 1   | 9-A   | 279 | TYR  | Sidechain |
| 1   | 9-A   | 302 | TYR  | Sidechain |
| 1   | 9-A   | 405 | PHE  | Sidechain |
| 1   | 9-A   | 451 | ARG  | Sidechain |
| 1   | 9-A   | 458 | TYR  | Sidechain |
| 1   | 9-A   | 568 | TYR  | Sidechain |
| 1   | 9-A   | 588 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 9-A   | 594 | TYR  | Sidechain |
| 1   | 9-A   | 597 | ARG  | Sidechain |
| 1   | 9-A   | 624 | ARG  | Sidechain |
| 1   | 9-A   | 646 | TYR  | Sidechain |
| 1   | 9-A   | 657 | TYR  | Sidechain |
| 1   | 9-A   | 664 | ARG  | Sidechain |
| 1   | 9-A   | 77  | TYR  | Sidechain |
| 1   | 9-A   | 791 | PHE  | Sidechain |
| 2   | 9-B   | 187 | TYR  | Sidechain |
| 2   | 9-B   | 264 | TYR  | Sidechain |
| 2   | 9-B   | 328 | ARG  | Sidechain |
| 2   | 9-B   | 342 | TYR  | Sidechain |
| 2   | 9-B   | 345 | TYR  | Sidechain |
| 2   | 9-B   | 359 | TYR  | Sidechain |
| 2   | 9-B   | 385 | PHE  | Sidechain |
| 2   | 9-B   | 438 | TYR  | Sidechain |
| 2   | 9-B   | 544 | ARG  | Sidechain |
| 2   | 9-B   | 562 | TYR  | Sidechain |
| 2   | 9-B   | 600 | TYR  | Sidechain |
| 2   | 9-B   | 651 | TYR  | Sidechain |
| 2   | 9-B   | 776 | TYR  | Sidechain |
| 2   | 9-B   | 816 | TYR  | Sidechain |
| 2   | 9-B   | 826 | PHE  | Sidechain |
| 3   | 9-C   | 173 | PHE  | Sidechain |
| 3   | 9-C   | 217 | PHE  | Sidechain |
| 3   | 9-C   | 315 | TYR  | Sidechain |
| 3   | 9-C   | 319 | TYR  | Sidechain |
| 3   | 9-C   | 407 | TYR  | Sidechain |
| 3   | 9-C   | 445 | TYR  | Sidechain |
| 3   | 9-C   | 87  | PHE  | Sidechain |
| 3   | 9-C   | 90  | ARG  | Sidechain |
| 3   | 9-D   | 162 | TYR  | Sidechain |
| 3   | 9-D   | 170 | TYR  | Sidechain |
| 3   | 9-D   | 176 | ARG  | Sidechain |
| 3   | 9-D   | 249 | TYR  | Sidechain |
| 3   | 9-D   | 315 | TYR  | Sidechain |
| 3   | 9-D   | 319 | TYR  | Sidechain |
| 3   | 9-D   | 353 | HIS  | Sidechain |
| 3   | 9-D   | 387 | PHE  | Sidechain |
| 3   | 9-D   | 394 | PHE  | Sidechain |
| 3   | 9-D   | 407 | TYR  | Sidechain |
| 3   | 9-D   | 445 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | 9-D   | 59  | ARG  | Sidechain |
| 3   | 9-D   | 62  | PHE  | Sidechain |
| 3   | 9-D   | 90  | ARG  | Sidechain |

## 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   | 1-A   | 4831  | 0        | 4863     | 192     | 0            |
| 1   | 2-A   | 4831  | 0        | 4863     | 140     | 0            |
| 1   | 3-A   | 4831  | 0        | 4863     | 117     | 0            |
| 1   | 4-A   | 4831  | 0        | 4862     | 121     | 0            |
| 1   | 5-A   | 4831  | 0        | 4863     | 128     | 0            |
| 1   | 6-A   | 4831  | 0        | 4862     | 115     | 0            |
| 1   | 7-A   | 4831  | 0        | 4863     | 113     | 0            |
| 1   | 8-A   | 4831  | 0        | 4862     | 146     | 0            |
| 1   | 9-A   | 4831  | 0        | 4863     | 148     | 0            |
| 1   | 10-A  | 4831  | 0        | 4863     | 153     | 0            |
| 2   | 1-B   | 4701  | 0        | 4728     | 183     | 0            |
| 2   | 2-B   | 4701  | 0        | 4731     | 143     | 0            |
| 2   | 3-B   | 4701  | 0        | 4731     | 122     | 0            |
| 2   | 4-B   | 4701  | 0        | 4729     | 136     | 0            |
| 2   | 5-B   | 4701  | 0        | 4729     | 144     | 0            |
| 2   | 6-B   | 4701  | 0        | 4729     | 180     | 0            |
| 2   | 7-B   | 4701  | 0        | 4729     | 127     | 0            |
| 2   | 8-B   | 4701  | 0        | 4731     | 183     | 0            |
| 2   | 9-B   | 4701  | 0        | 4727     | 124     | 0            |
| 2   | 10-B  | 4701  | 0        | 4729     | 135     | 0            |
| 3   | 1-C   | 3483  | 0        | 3340     | 47      | 0            |
| 3   | 1-D   | 3483  | 0        | 3340     | 38      | 0            |
| 3   | 2-C   | 3483  | 0        | 3340     | 43      | 0            |
| 3   | 2-D   | 3483  | 0        | 3340     | 49      | 0            |
| 3   | 3-C   | 3483  | 0        | 3340     | 51      | 0            |
| 3   | 3-D   | 3483  | 0        | 3340     | 38      | 0            |
| 3   | 4-C   | 3483  | 0        | 3340     | 54      | 0            |
| 3   | 4-D   | 3483  | 0        | 3340     | 43      | 0            |
| 3   | 5-C   | 3483  | 0        | 3340     | 34      | 0            |
| 3   | 5-D   | 3483  | 0        | 3340     | 51      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 3   | 6-C   | 3483   | 0        | 3340     | 28      | 0            |
| 3   | 6-D   | 3483   | 0        | 3340     | 62      | 0            |
| 3   | 7-C   | 3483   | 0        | 3340     | 34      | 0            |
| 3   | 7-D   | 3483   | 0        | 3340     | 48      | 0            |
| 3   | 8-C   | 3483   | 0        | 3340     | 24      | 0            |
| 3   | 8-D   | 3483   | 0        | 3340     | 45      | 0            |
| 3   | 9-C   | 3483   | 0        | 3340     | 29      | 0            |
| 3   | 9-D   | 3483   | 0        | 3340     | 42      | 0            |
| 3   | 10-C  | 3483   | 0        | 3340     | 44      | 0            |
| 3   | 10-D  | 3483   | 0        | 3340     | 28      | 0            |
| 4   | 1-E   | 220    | 0        | 46       | 0       | 0            |
| 4   | 1-F   | 220    | 0        | 46       | 1       | 0            |
| 4   | 2-E   | 220    | 0        | 46       | 0       | 0            |
| 4   | 2-F   | 220    | 0        | 46       | 0       | 0            |
| 4   | 3-E   | 220    | 0        | 46       | 0       | 0            |
| 4   | 3-F   | 220    | 0        | 46       | 1       | 0            |
| 4   | 4-E   | 220    | 0        | 46       | 0       | 0            |
| 4   | 4-F   | 220    | 0        | 46       | 0       | 0            |
| 4   | 5-E   | 220    | 0        | 46       | 0       | 0            |
| 4   | 5-F   | 220    | 0        | 46       | 0       | 0            |
| 4   | 6-E   | 220    | 0        | 46       | 0       | 0            |
| 4   | 6-F   | 220    | 0        | 46       | 0       | 0            |
| 4   | 7-E   | 220    | 0        | 46       | 0       | 0            |
| 4   | 7-F   | 220    | 0        | 46       | 0       | 0            |
| 4   | 8-E   | 220    | 0        | 46       | 0       | 0            |
| 4   | 8-F   | 220    | 0        | 46       | 0       | 0            |
| 4   | 9-E   | 220    | 0        | 46       | 0       | 0            |
| 4   | 9-F   | 220    | 0        | 46       | 0       | 0            |
| 4   | 10-E  | 220    | 0        | 46       | 2       | 0            |
| 4   | 10-F  | 220    | 0        | 46       | 0       | 0            |
| All | All   | 169380 | 0        | 163640   | 3046    | 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 9.

All (3046) 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:A:68:ILE:HD13 | 2:B:216:PHE:CG   | 1.27                     | 1.67              |
| 2:B:405:ILE:CG2 | 2:B:456:ILE:HD12 | 1.28                     | 1.57              |
| 1:A:68:ILE:CD1  | 2:B:216:PHE:HB3  | 1.21                     | 1.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:131:PHE:CE2  | 2:B:322:HIS:NE2  | 1.71                     | 1.54              |
| 1:A:68:ILE:HD13  | 2:B:216:PHE:CB   | 1.30                     | 1.53              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:HE   | 1.25                     | 1.50              |
| 1:A:68:ILE:CD1   | 2:B:216:PHE:CB   | 1.76                     | 1.49              |
| 1:A:296:TYR:OH   | 2:B:322:HIS:CD2  | 1.70                     | 1.45              |
| 2:B:257:ILE:HD12 | 2:B:297:TYR:CD1  | 1.51                     | 1.45              |
| 1:A:151:LEU:CG   | 2:B:285:ARG:HD3  | 1.49                     | 1.41              |
| 1:A:151:LEU:HD23 | 2:B:285:ARG:NH2  | 1.25                     | 1.40              |
| 1:A:65:ASN:HD21  | 2:B:215:ASN:CB   | 1.35                     | 1.40              |
| 1:A:151:LEU:HD22 | 2:B:285:ARG:NE   | 1.33                     | 1.39              |
| 1:A:131:PHE:HE2  | 2:B:322:HIS:NE2  | 0.92                     | 1.39              |
| 2:B:257:ILE:HD12 | 2:B:297:TYR:CE1  | 1.59                     | 1.38              |
| 2:B:288:TYR:CE2  | 2:B:292:ILE:HD11 | 1.57                     | 1.37              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:HG12 | 1.52                     | 1.37              |
| 2:B:405:ILE:HA   | 2:B:456:ILE:CD1  | 1.54                     | 1.36              |
| 1:A:152:LYS:HD3  | 2:B:285:ARG:NH1  | 1.08                     | 1.36              |
| 1:A:158:LEU:HD23 | 2:B:281:LYS:NZ   | 1.37                     | 1.36              |
| 1:A:566:ILE:CD1  | 1:A:574:ILE:HD12 | 1.55                     | 1.36              |
| 1:A:151:LEU:HG   | 2:B:285:ARG:CD   | 1.53                     | 1.36              |
| 1:A:588:TYR:CD1  | 1:A:693:ILE:HD11 | 1.61                     | 1.35              |
| 1:A:425:ILE:HD11 | 1:A:482:LEU:CD2  | 1.51                     | 1.35              |
| 1:A:68:ILE:CD1   | 2:B:281:LYS:HD2  | 1.54                     | 1.35              |
| 1:A:65:ASN:ND2   | 2:B:215:ASN:CB   | 1.90                     | 1.34              |
| 1:A:365:THR:HG23 | 1:A:404:ILE:CD1  | 1.55                     | 1.33              |
| 1:A:152:LYS:CD   | 2:B:285:ARG:NH1  | 1.91                     | 1.33              |
| 1:A:426:PHE:CZ   | 1:A:564:ILE:HD11 | 1.62                     | 1.33              |
| 2:B:628:ILE:HD12 | 2:B:780:ASN:ND2  | 1.38                     | 1.33              |
| 2:B:264:TYR:CZ   | 2:B:287:ILE:HD11 | 1.61                     | 1.32              |
| 1:A:68:ILE:CD1   | 2:B:216:PHE:CG   | 2.02                     | 1.32              |
| 2:B:634:ILE:HD11 | 2:B:772:PHE:CE1  | 1.61                     | 1.31              |
| 1:A:137:ARG:HH21 | 2:B:328:ARG:CZ   | 1.43                     | 1.31              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:CD1  | 2.08                     | 1.31              |
| 3:C:199:ASP:O    | 3:C:260:ILE:HD13 | 1.23                     | 1.31              |
| 1:A:140:TYR:OH   | 2:B:296:ILE:HD11 | 1.31                     | 1.31              |
| 2:B:335:PHE:CZ   | 2:B:339:ILE:HD11 | 1.65                     | 1.31              |
| 1:A:140:TYR:OH   | 2:B:292:ILE:HG22 | 1.27                     | 1.30              |
| 2:B:610:ILE:CD1  | 3:D:196:GLU:O    | 1.78                     | 1.30              |
| 2:B:586:ILE:HD12 | 2:B:732:LEU:CD2  | 1.59                     | 1.30              |
| 1:A:152:LYS:HG2  | 2:B:285:ARG:NH1  | 1.41                     | 1.30              |
| 2:B:412:LEU:CD2  | 2:B:463:ILE:HD12 | 1.58                     | 1.30              |
| 2:B:349:TRP:HE1  | 2:B:364:ILE:CD1  | 1.43                     | 1.30              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:335:PHE:CE1  | 2:B:339:ILE:HD11 | 1.67                     | 1.30              |
| 1:A:65:ASN:ND2   | 2:B:215:ASN:HB3  | 1.43                     | 1.29              |
| 3:D:256:TYR:CZ   | 3:D:260:ILE:HD11 | 1.65                     | 1.29              |
| 2:B:405:ILE:CG2  | 2:B:456:ILE:CD1  | 2.09                     | 1.28              |
| 1:A:133:MET:HE3  | 2:B:328:ARG:NH2  | 1.47                     | 1.28              |
| 1:A:70:LEU:O     | 2:B:216:PHE:CE2  | 1.86                     | 1.28              |
| 3:D:256:TYR:CE1  | 3:D:260:ILE:HD12 | 1.68                     | 1.28              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CG   | 1.65                     | 1.28              |
| 1:A:140:TYR:OH   | 2:B:292:ILE:CG2  | 1.81                     | 1.27              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:CD1  | 1.63                     | 1.27              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CB   | 1.63                     | 1.27              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:HG3  | 1.64                     | 1.26              |
| 2:B:349:TRP:CD1  | 2:B:364:ILE:HD11 | 1.70                     | 1.26              |
| 1:A:62:ASP:OD1   | 1:A:94:ILE:HD11  | 1.27                     | 1.26              |
| 3:D:119:ILE:CD1  | 3:D:154:LEU:HD22 | 1.66                     | 1.25              |
| 1:A:151:LEU:HB3  | 2:B:285:ARG:NE   | 1.48                     | 1.25              |
| 2:B:209:ILE:HD12 | 2:B:222:HIS:NE2  | 1.50                     | 1.25              |
| 2:B:184:ILE:HD12 | 2:B:217:GLU:OE1  | 1.37                     | 1.25              |
| 1:A:136:GLN:NE2  | 2:B:327:ILE:CD1  | 1.99                     | 1.25              |
| 1:A:147:GLU:OE1  | 2:B:292:ILE:CD1  | 1.86                     | 1.24              |
| 1:A:74:TYR:CD2   | 2:B:216:PHE:HZ   | 1.55                     | 1.24              |
| 1:A:570:LEU:CD2  | 1:A:573:ILE:HD12 | 1.67                     | 1.24              |
| 2:B:586:ILE:HG22 | 2:B:735:ILE:CD1  | 1.68                     | 1.24              |
| 2:B:349:TRP:CE2  | 2:B:364:ILE:HD13 | 1.72                     | 1.24              |
| 2:B:412:LEU:HD22 | 2:B:463:ILE:CD1  | 1.68                     | 1.24              |
| 1:A:70:LEU:HG    | 2:B:216:PHE:CE1  | 1.72                     | 1.24              |
| 2:B:405:ILE:CD1  | 2:B:453:TYR:HA   | 1.67                     | 1.23              |
| 2:B:610:ILE:HD12 | 3:D:196:GLU:O    | 1.35                     | 1.23              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CB   | 2.16                     | 1.23              |
| 1:A:68:ILE:C     | 2:B:281:LYS:HZ2  | 1.47                     | 1.23              |
| 1:A:133:MET:CE   | 2:B:328:ARG:NH2  | 2.00                     | 1.22              |
| 2:B:339:ILE:CD1  | 2:B:440:GLY:HA3  | 1.69                     | 1.22              |
| 1:A:65:ASN:OD1   | 2:B:216:PHE:CE1  | 1.91                     | 1.22              |
| 1:A:356:VAL:HG21 | 1:A:572:ILE:CD1  | 1.70                     | 1.22              |
| 1:A:458:TYR:CD1  | 1:A:484:ILE:CD1  | 2.22                     | 1.22              |
| 2:B:586:ILE:HG23 | 2:B:735:ILE:CD1  | 1.70                     | 1.22              |
| 1:A:70:LEU:O     | 2:B:216:PHE:CD2  | 1.92                     | 1.22              |
| 2:B:586:ILE:HG23 | 2:B:735:ILE:CD1  | 1.70                     | 1.21              |
| 2:B:493:ILE:CD1  | 2:B:598:TYR:HB3  | 1.69                     | 1.21              |
| 2:B:349:TRP:NE1  | 2:B:364:ILE:HD12 | 1.55                     | 1.21              |
| 1:A:138:PHE:CZ   | 1:A:275:ILE:CD1  | 2.24                     | 1.21              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:297:TYR:CZ   | 2:B:330:ILE:HD12 | 1.76                     | 1.21              |
| 1:A:138:PHE:CZ   | 1:A:275:ILE:HD11 | 1.75                     | 1.21              |
| 2:B:825:ILE:HD11 | 2:B:841:LEU:CD1  | 1.70                     | 1.20              |
| 1:A:566:ILE:HD11 | 1:A:574:ILE:CD1  | 1.68                     | 1.20              |
| 1:A:137:ARG:HE   | 2:B:325:LEU:CD1  | 1.54                     | 1.20              |
| 1:A:151:LEU:HD23 | 2:B:285:ARG:CZ   | 1.72                     | 1.20              |
| 1:A:140:TYR:CZ   | 2:B:292:ILE:HG21 | 1.75                     | 1.20              |
| 2:B:241:PHE:CB   | 2:B:254:ILE:HD13 | 1.70                     | 1.20              |
| 1:A:151:LEU:CB   | 2:B:285:ARG:NE   | 2.02                     | 1.20              |
| 1:A:152:LYS:CG   | 2:B:285:ARG:HH11 | 1.55                     | 1.20              |
| 3:C:125:LYS:HG2  | 3:D:283:ASP:OD1  | 1.37                     | 1.20              |
| 1:A:625:ILE:CD1  | 1:A:764:LEU:HB3  | 1.71                     | 1.20              |
| 3:C:125:LYS:HG3  | 3:D:283:ASP:OD2  | 1.37                     | 1.20              |
| 1:A:356:VAL:HG21 | 1:A:572:ILE:HD11 | 1.24                     | 1.19              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:CD1  | 2.21                     | 1.19              |
| 2:B:349:TRP:CD1  | 2:B:364:ILE:CD1  | 2.26                     | 1.19              |
| 2:B:529:MET:CE   | 2:B:538:ILE:HD11 | 1.72                     | 1.19              |
| 2:B:349:TRP:CD1  | 2:B:364:ILE:HD11 | 1.78                     | 1.19              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:NE   | 1.92                     | 1.18              |
| 1:A:68:ILE:CD1   | 1:A:158:LEU:HD21 | 1.73                     | 1.18              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:HD11 | 1.21                     | 1.18              |
| 3:D:256:TYR:CZ   | 3:D:260:ILE:CD1  | 2.27                     | 1.18              |
| 1:A:573:ILE:CD1  | 1:A:673:GLN:HB3  | 1.72                     | 1.18              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CG   | 2.26                     | 1.18              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:HD2  | 1.73                     | 1.18              |
| 1:A:426:PHE:CE2  | 1:A:564:ILE:HD13 | 1.78                     | 1.18              |
| 1:A:566:ILE:HD13 | 1:A:574:ILE:CD1  | 1.72                     | 1.17              |
| 1:A:595:HIS:ND1  | 1:A:640:ILE:HD13 | 1.59                     | 1.17              |
| 2:B:586:ILE:HD12 | 2:B:732:LEU:HD22 | 1.20                     | 1.17              |
| 1:A:114:LYS:CE   | 1:A:118:ILE:HD11 | 1.73                     | 1.17              |
| 2:B:412:LEU:CD2  | 2:B:463:ILE:CD1  | 2.22                     | 1.17              |
| 1:A:151:LEU:HD21 | 2:B:285:ARG:CG   | 1.75                     | 1.17              |
| 1:A:154:LEU:HD21 | 1:A:177:ILE:HD12 | 1.17                     | 1.17              |
| 2:B:586:ILE:HG23 | 2:B:735:ILE:HD11 | 1.27                     | 1.17              |
| 1:A:151:LEU:CB   | 2:B:285:ARG:CD   | 2.22                     | 1.16              |
| 3:C:212:ILE:HD13 | 3:C:275:PHE:CZ   | 1.81                     | 1.16              |
| 2:B:264:TYR:CZ   | 2:B:287:ILE:CD1  | 2.28                     | 1.16              |
| 1:A:629:THR:HG21 | 1:A:710:ILE:HD11 | 1.21                     | 1.16              |
| 1:A:138:PHE:CE2  | 1:A:275:ILE:CD1  | 2.29                     | 1.16              |
| 1:A:147:GLU:OE1  | 2:B:292:ILE:HD11 | 1.01                     | 1.16              |
| 2:B:398:LEU:CD2  | 2:B:449:ILE:HD12 | 1.75                     | 1.16              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:137:ARG:NH2  | 2:B:325:LEU:HD21 | 1.59                     | 1.15              |
| 1:A:558:TYR:HB2  | 1:A:693:ILE:HD11 | 1.15                     | 1.15              |
| 2:B:586:ILE:HD12 | 2:B:735:ILE:HD11 | 1.26                     | 1.15              |
| 1:A:136:GLN:NE2  | 2:B:323:GLY:HA2  | 1.58                     | 1.15              |
| 1:A:73:THR:HG22  | 2:B:215:ASN:HA   | 1.29                     | 1.15              |
| 2:B:188:VAL:HG13 | 2:B:224:ILE:HD13 | 1.27                     | 1.15              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:CG   | 1.80                     | 1.15              |
| 1:A:573:ILE:HD12 | 1:A:673:GLN:CB   | 1.77                     | 1.14              |
| 1:A:70:LEU:CD1   | 2:B:281:LYS:NZ   | 2.11                     | 1.14              |
| 1:A:70:LEU:HG    | 2:B:281:LYS:HZ1  | 1.05                     | 1.14              |
| 1:A:255:ILE:HD11 | 1:A:272:LEU:HD22 | 1.16                     | 1.14              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:HB3  | 1.77                     | 1.14              |
| 2:B:570:LEU:CD2  | 2:B:721:ILE:CD1  | 2.25                     | 1.14              |
| 1:A:70:LEU:HD12  | 2:B:281:LYS:CE   | 1.77                     | 1.14              |
| 3:D:199:ASP:O    | 3:D:260:ILE:HD13 | 1.46                     | 1.14              |
| 1:A:70:LEU:HD11  | 2:B:220:LEU:HD11 | 1.21                     | 1.14              |
| 1:A:151:LEU:CB   | 2:B:285:ARG:HD3  | 1.76                     | 1.14              |
| 2:B:200:PHE:CZ   | 2:B:207:ILE:HD11 | 1.81                     | 1.14              |
| 2:B:493:ILE:HD13 | 2:B:598:TYR:HB3  | 1.20                     | 1.14              |
| 1:A:137:ARG:NE   | 2:B:325:LEU:HD11 | 1.63                     | 1.13              |
| 1:A:151:LEU:HD12 | 2:B:285:ARG:HG3  | 1.27                     | 1.13              |
| 1:A:138:PHE:CD2  | 1:A:275:ILE:HD11 | 1.82                     | 1.13              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:HD11 | 1.22                     | 1.13              |
| 1:A:142:ILE:HD12 | 1:A:189:LEU:HG   | 1.17                     | 1.13              |
| 1:A:66:VAL:HB    | 1:A:94:ILE:HD12  | 1.30                     | 1.13              |
| 1:A:70:LEU:CG    | 2:B:216:PHE:CE1  | 2.31                     | 1.13              |
| 2:B:412:LEU:CD1  | 2:B:463:ILE:HD12 | 1.77                     | 1.13              |
| 1:A:438:PHE:CZ   | 1:A:484:ILE:HD12 | 1.83                     | 1.13              |
| 3:D:210:LEU:HD22 | 3:D:222:ILE:CD1  | 1.77                     | 1.13              |
| 1:A:131:PHE:CE2  | 2:B:322:HIS:CD2  | 2.35                     | 1.13              |
| 1:A:426:PHE:CZ   | 1:A:564:ILE:CD1  | 2.30                     | 1.13              |
| 2:B:571:VAL:CG2  | 2:B:721:ILE:HD11 | 1.77                     | 1.13              |
| 1:A:137:ARG:HE   | 2:B:325:LEU:HD11 | 1.08                     | 1.12              |
| 3:D:210:LEU:CD2  | 3:D:222:ILE:HD11 | 1.77                     | 1.12              |
| 3:D:5:ILE:HD11   | 3:D:252:MET:HE2  | 1.14                     | 1.12              |
| 2:B:209:ILE:HD11 | 2:B:218:SER:HB3  | 1.15                     | 1.12              |
| 1:A:195:GLU:HG3  | 1:A:250:ILE:HD13 | 1.25                     | 1.12              |
| 1:A:137:ARG:HH21 | 2:B:328:ARG:NH2  | 1.47                     | 1.12              |
| 2:B:339:ILE:HD13 | 2:B:440:GLY:HA3  | 1.22                     | 1.12              |
| 2:B:405:ILE:CD1  | 2:B:456:ILE:HD12 | 1.79                     | 1.12              |
| 1:A:367:PRO:HB3  | 1:A:404:ILE:HD13 | 1.19                     | 1.12              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:418:GLU:OE2  | 2:B:463:ILE:HD11 | 1.50                     | 1.12              |
| 1:A:570:LEU:HD22 | 1:A:573:ILE:HD12 | 1.25                     | 1.12              |
| 3:D:210:LEU:HD11 | 3:D:222:ILE:HD11 | 1.31                     | 1.11              |
| 2:B:570:LEU:CD2  | 2:B:721:ILE:HD12 | 1.78                     | 1.11              |
| 2:B:241:PHE:HB3  | 2:B:254:ILE:CD1  | 1.80                     | 1.11              |
| 2:B:480:ILE:HD11 | 2:B:537:VAL:CG2  | 1.80                     | 1.11              |
| 1:A:70:LEU:HG    | 2:B:281:LYS:NZ   | 1.64                     | 1.11              |
| 2:B:570:LEU:HD23 | 2:B:721:ILE:HD12 | 1.21                     | 1.11              |
| 1:A:438:PHE:CE2  | 1:A:484:ILE:HD12 | 1.84                     | 1.11              |
| 2:B:412:LEU:HD22 | 2:B:463:ILE:HD13 | 1.32                     | 1.11              |
| 2:B:586:ILE:HD12 | 2:B:735:ILE:CD1  | 1.80                     | 1.11              |
| 1:A:151:LEU:HD22 | 2:B:285:ARG:CD   | 1.80                     | 1.11              |
| 1:A:640:ILE:HD13 | 1:A:696:GLN:NE2  | 1.65                     | 1.11              |
| 3:D:256:TYR:CE1  | 3:D:260:ILE:HD12 | 1.85                     | 1.11              |
| 1:A:133:MET:HE1  | 2:B:328:ARG:HH22 | 1.10                     | 1.11              |
| 2:B:482:LEU:HD22 | 2:B:735:ILE:CD1  | 1.79                     | 1.11              |
| 1:A:128:ASP:HA   | 2:B:322:HIS:CE1  | 1.85                     | 1.11              |
| 1:A:63:LEU:HB3   | 1:A:170:ILE:CD1  | 1.81                     | 1.10              |
| 2:B:383:ILE:HD12 | 2:B:410:ILE:CD1  | 1.79                     | 1.10              |
| 1:A:70:LEU:HD13  | 2:B:220:LEU:HD22 | 1.27                     | 1.10              |
| 2:B:257:ILE:CD1  | 2:B:297:TYR:CD1  | 2.32                     | 1.10              |
| 1:A:66:VAL:HG22  | 2:B:216:PHE:HE1  | 1.15                     | 1.10              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:HD22 | 1.80                     | 1.10              |
| 2:B:342:TYR:HE2  | 2:B:394:ILE:HD11 | 1.06                     | 1.10              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CD1  | 1.86                     | 1.10              |
| 3:D:356:ILE:HD13 | 3:D:358:ARG:HH12 | 1.12                     | 1.10              |
| 1:A:70:LEU:HD12  | 2:B:281:LYS:HE2  | 1.32                     | 1.10              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:CD1  | 1.80                     | 1.10              |
| 1:A:585:ILE:HD11 | 1:A:683:ILE:HG12 | 1.14                     | 1.10              |
| 3:C:121:ASN:ND2  | 3:D:218:ARG:HH12 | 1.49                     | 1.10              |
| 2:B:241:PHE:HB3  | 2:B:254:ILE:HD13 | 1.24                     | 1.09              |
| 1:A:130:SER:OG   | 2:B:322:HIS:ND1  | 1.85                     | 1.09              |
| 1:A:570:LEU:HD23 | 1:A:573:ILE:HD12 | 1.30                     | 1.09              |
| 2:B:296:ILE:HD12 | 2:B:327:ILE:HG12 | 1.14                     | 1.09              |
| 1:A:70:LEU:HG    | 2:B:216:PHE:CZ   | 1.88                     | 1.09              |
| 2:B:257:ILE:CD1  | 2:B:297:TYR:CE2  | 2.33                     | 1.09              |
| 2:B:209:ILE:CD1  | 2:B:218:SER:HB3  | 1.82                     | 1.09              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CG   | 1.86                     | 1.09              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:HD13 | 1.80                     | 1.09              |
| 3:C:195:ILE:HD13 | 3:C:423:PHE:HE1  | 1.08                     | 1.09              |
| 1:A:255:ILE:HD11 | 1:A:272:LEU:CD2  | 1.83                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:573:ILE:HD12 | 1:A:673:GLN:HB3  | 1.14                     | 1.09              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:HD13 | 1.80                     | 1.09              |
| 1:A:65:ASN:HD21  | 2:B:215:ASN:CG   | 1.59                     | 1.09              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:HD11 | 1.11                     | 1.08              |
| 2:B:209:ILE:HD11 | 2:B:218:SER:HB3  | 1.29                     | 1.08              |
| 1:A:65:ASN:HB3   | 2:B:216:PHE:CE1  | 1.87                     | 1.08              |
| 3:D:204:PHE:HE2  | 3:D:234:ILE:HD12 | 1.15                     | 1.08              |
| 3:D:210:LEU:HD22 | 3:D:222:ILE:HD11 | 1.24                     | 1.08              |
| 1:A:599:LEU:HD22 | 1:A:640:ILE:HD12 | 1.33                     | 1.08              |
| 3:D:200:ALA:HB2  | 3:D:260:ILE:HD11 | 1.32                     | 1.08              |
| 2:B:209:ILE:HD13 | 2:B:222:HIS:CD2  | 1.88                     | 1.08              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:NH2  | 2.16                     | 1.08              |
| 1:A:566:ILE:HD12 | 1:A:574:ILE:HG23 | 1.36                     | 1.08              |
| 1:A:438:PHE:CZ   | 1:A:484:ILE:HD13 | 1.86                     | 1.08              |
| 3:D:119:ILE:CD1  | 3:D:154:LEU:CD2  | 2.31                     | 1.08              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:CZ   | 2.31                     | 1.08              |
| 1:A:151:LEU:HD12 | 2:B:285:ARG:CG   | 1.68                     | 1.08              |
| 1:A:640:ILE:HD13 | 1:A:696:GLN:HE22 | 0.97                     | 1.08              |
| 2:B:209:ILE:HD11 | 2:B:218:SER:CB   | 1.84                     | 1.08              |
| 1:A:426:PHE:CE2  | 1:A:564:ILE:CD1  | 2.37                     | 1.08              |
| 1:A:566:ILE:HD13 | 1:A:571:ASN:HB3  | 1.30                     | 1.08              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:HD12 | 1.17                     | 1.08              |
| 2:B:610:ILE:HD11 | 3:D:196:GLU:O    | 1.52                     | 1.08              |
| 2:B:257:ILE:HD11 | 2:B:297:TYR:CE2  | 1.86                     | 1.08              |
| 1:A:138:PHE:CZ   | 1:A:275:ILE:HD12 | 1.89                     | 1.08              |
| 2:B:335:PHE:CE2  | 2:B:339:ILE:HD11 | 1.87                     | 1.08              |
| 1:A:625:ILE:HD11 | 1:A:764:LEU:HB3  | 1.16                     | 1.08              |
| 1:A:584:ILE:HD12 | 1:A:687:ARG:HD2  | 1.29                     | 1.07              |
| 1:A:152:LYS:CD   | 2:B:285:ARG:HH12 | 1.58                     | 1.07              |
| 1:A:195:GLU:CD   | 1:A:250:ILE:CD1  | 2.27                     | 1.07              |
| 1:A:74:TYR:HD2   | 2:B:216:PHE:CZ   | 1.70                     | 1.07              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:HD11 | 1.34                     | 1.07              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:HB2  | 1.14                     | 1.07              |
| 1:A:70:LEU:HD12  | 2:B:220:LEU:CD1  | 1.83                     | 1.07              |
| 1:A:68:ILE:HD11  | 2:B:216:PHE:CD1  | 1.90                     | 1.07              |
| 3:C:212:ILE:HD13 | 3:C:275:PHE:CZ   | 1.89                     | 1.07              |
| 1:A:363:ILE:HD13 | 1:A:413:TYR:HB2  | 1.36                     | 1.07              |
| 3:D:97:ASP:O     | 3:D:111:ILE:HD12 | 1.52                     | 1.07              |
| 1:A:137:ARG:NH2  | 2:B:328:ARG:CZ   | 2.18                     | 1.07              |
| 1:A:584:ILE:HD12 | 1:A:687:ARG:HG3  | 1.34                     | 1.07              |
| 2:B:405:ILE:HD12 | 2:B:453:TYR:HA   | 1.13                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:458:TYR:CD1  | 1:A:484:ILE:HD11 | 1.90                     | 1.06              |
| 2:B:527:HIS:CE1  | 2:B:538:ILE:CD1  | 2.38                     | 1.06              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:CD2  | 2.32                     | 1.06              |
| 3:D:258:THR:HG23 | 3:D:356:ILE:CD1  | 1.84                     | 1.06              |
| 1:A:70:LEU:HD11  | 2:B:220:LEU:CD1  | 1.84                     | 1.06              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CG   | 2.36                     | 1.06              |
| 2:B:480:ILE:HD11 | 2:B:537:VAL:HG21 | 1.36                     | 1.06              |
| 2:B:493:ILE:HD12 | 2:B:598:TYR:CD2  | 1.89                     | 1.06              |
| 1:A:438:PHE:CE2  | 1:A:484:ILE:CD1  | 2.37                     | 1.06              |
| 2:B:405:ILE:HD13 | 2:B:452:GLN:HB3  | 1.38                     | 1.06              |
| 2:B:628:ILE:CD1  | 2:B:780:ASN:ND2  | 2.17                     | 1.06              |
| 2:B:636:ILE:HD11 | 3:D:437:TYR:CZ   | 1.89                     | 1.06              |
| 1:A:136:GLN:HE22 | 2:B:327:ILE:HD13 | 1.14                     | 1.06              |
| 1:A:151:LEU:HD21 | 2:B:285:ARG:HG3  | 1.10                     | 1.06              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:HB2  | 1.37                     | 1.06              |
| 1:A:138:PHE:CZ   | 1:A:275:ILE:CD1  | 2.39                     | 1.05              |
| 2:B:656:ILE:HD13 | 2:B:738:HIS:NE2  | 1.71                     | 1.05              |
| 1:A:199:GLU:CD   | 1:A:250:ILE:HD12 | 1.80                     | 1.05              |
| 1:A:367:PRO:CB   | 1:A:404:ILE:HD13 | 1.85                     | 1.05              |
| 2:B:739:LYS:O    | 2:B:743:THR:O    | 1.75                     | 1.05              |
| 1:A:136:GLN:NE2  | 2:B:327:ILE:HD13 | 1.66                     | 1.05              |
| 2:B:355:LEU:CD2  | 2:B:364:ILE:HD12 | 1.85                     | 1.05              |
| 1:A:138:PHE:CE1  | 1:A:275:ILE:HD12 | 1.91                     | 1.05              |
| 2:B:355:LEU:O    | 2:B:364:ILE:HD12 | 1.57                     | 1.05              |
| 1:A:68:ILE:HD12  | 2:B:281:LYS:HD2  | 1.34                     | 1.05              |
| 3:D:200:ALA:HB2  | 3:D:260:ILE:HD11 | 1.31                     | 1.05              |
| 3:D:204:PHE:CE2  | 3:D:234:ILE:HD12 | 1.91                     | 1.05              |
| 2:B:349:TRP:HE1  | 2:B:364:ILE:HD12 | 0.89                     | 1.05              |
| 3:D:200:ALA:HB2  | 3:D:260:ILE:HD11 | 1.36                     | 1.05              |
| 2:B:394:ILE:HD13 | 2:B:445:PHE:CE2  | 1.92                     | 1.04              |
| 2:B:402:ILE:CD1  | 2:B:449:ILE:HD11 | 1.85                     | 1.04              |
| 2:B:349:TRP:NE1  | 2:B:364:ILE:CD1  | 2.21                     | 1.04              |
| 2:B:586:ILE:HG23 | 2:B:735:ILE:HD13 | 1.06                     | 1.04              |
| 3:D:256:TYR:CE1  | 3:D:260:ILE:HD11 | 1.91                     | 1.04              |
| 1:A:151:LEU:HB2  | 2:B:285:ARG:CD   | 1.86                     | 1.04              |
| 2:B:405:ILE:HG22 | 2:B:456:ILE:CD1  | 1.84                     | 1.04              |
| 3:C:195:ILE:HD13 | 3:C:423:PHE:CE1  | 1.91                     | 1.04              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:HD11 | 1.86                     | 1.04              |
| 1:A:144:ARG:CZ   | 2:B:289:GLU:OE2  | 2.06                     | 1.04              |
| 3:D:210:LEU:CD2  | 3:D:222:ILE:HD11 | 1.87                     | 1.04              |
| 1:A:128:ASP:HA   | 2:B:322:HIS:NE2  | 1.72                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:566:ILE:HD11 | 1:A:574:ILE:HD12 | 1.04                     | 1.03              |
| 2:B:412:LEU:HD23 | 2:B:463:ILE:HD12 | 1.36                     | 1.03              |
| 1:A:151:LEU:HB3  | 2:B:285:ARG:HE   | 0.88                     | 1.03              |
| 1:A:363:ILE:CD1  | 1:A:413:TYR:HB2  | 1.88                     | 1.03              |
| 3:C:256:TYR:CE2  | 3:C:260:ILE:HD12 | 1.93                     | 1.03              |
| 2:B:264:TYR:CE1  | 2:B:287:ILE:HD11 | 1.93                     | 1.03              |
| 1:A:114:LYS:HE3  | 1:A:118:ILE:CD1  | 1.88                     | 1.03              |
| 2:B:482:LEU:HD22 | 2:B:735:ILE:HD11 | 1.36                     | 1.03              |
| 2:B:570:LEU:HD23 | 2:B:721:ILE:CD1  | 1.84                     | 1.03              |
| 1:A:68:ILE:CD1   | 2:B:216:PHE:CD1  | 2.40                     | 1.03              |
| 1:A:130:SER:OG   | 2:B:322:HIS:CE1  | 2.12                     | 1.03              |
| 2:B:586:ILE:CD1  | 2:B:732:LEU:CD2  | 2.36                     | 1.03              |
| 1:A:625:ILE:CD1  | 1:A:764:LEU:CB   | 2.36                     | 1.03              |
| 1:A:558:TYR:CB   | 1:A:693:ILE:HD11 | 1.89                     | 1.03              |
| 2:B:402:ILE:HG13 | 2:B:449:ILE:HD13 | 1.35                     | 1.03              |
| 2:B:412:LEU:HD21 | 2:B:463:ILE:HD12 | 1.40                     | 1.03              |
| 1:A:641:LYS:HD2  | 3:C:356:ILE:CD1  | 1.89                     | 1.02              |
| 1:A:68:ILE:HD11  | 2:B:281:LYS:HD2  | 1.37                     | 1.02              |
| 2:B:586:ILE:CD1  | 2:B:735:ILE:HD11 | 1.87                     | 1.02              |
| 2:B:493:ILE:CD1  | 2:B:598:TYR:CB   | 2.36                     | 1.02              |
| 1:A:567:PRO:HD2  | 1:A:574:ILE:HD13 | 1.39                     | 1.02              |
| 2:B:480:ILE:HD13 | 2:B:541:LEU:HD11 | 1.39                     | 1.02              |
| 2:B:405:ILE:HA   | 2:B:456:ILE:HD12 | 1.42                     | 1.02              |
| 2:B:335:PHE:HE1  | 2:B:339:ILE:HD11 | 1.03                     | 1.02              |
| 1:A:61:LYS:HE3   | 2:B:216:PHE:HE1  | 1.17                     | 1.02              |
| 1:A:595:HIS:ND1  | 1:A:640:ILE:CD1  | 2.23                     | 1.02              |
| 2:B:191:THR:CG2  | 2:B:207:ILE:HD13 | 1.89                     | 1.02              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CG   | 2.43                     | 1.02              |
| 1:A:147:GLU:CD   | 2:B:292:ILE:HD11 | 1.85                     | 1.02              |
| 1:A:158:LEU:CD2  | 2:B:281:LYS:NZ   | 2.21                     | 1.02              |
| 2:B:335:PHE:CE2  | 2:B:339:ILE:HD11 | 1.95                     | 1.02              |
| 3:D:5:ILE:CD1    | 3:D:252:MET:HE2  | 1.88                     | 1.02              |
| 2:B:527:HIS:CE1  | 2:B:538:ILE:HD12 | 1.93                     | 1.02              |
| 2:B:656:ILE:CD1  | 2:B:738:HIS:CE1  | 2.43                     | 1.02              |
| 1:A:70:LEU:CD1   | 2:B:281:LYS:HZ3  | 1.72                     | 1.02              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:CG   | 1.94                     | 1.01              |
| 1:A:155:VAL:HG11 | 2:B:285:ARG:HH11 | 1.25                     | 1.01              |
| 2:B:405:ILE:HD11 | 2:B:456:ILE:CD1  | 1.89                     | 1.01              |
| 2:B:234:LEU:HD22 | 2:B:257:ILE:HD11 | 1.43                     | 1.01              |
| 2:B:412:LEU:CD1  | 2:B:463:ILE:CD1  | 2.37                     | 1.01              |
| 3:C:121:ASN:HD21 | 3:D:218:ARG:NH1  | 1.57                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:349:TRP:CD2  | 2:B:364:ILE:HD13 | 1.96                     | 1.01              |
| 1:A:68:ILE:O     | 2:B:281:LYS:NZ   | 1.94                     | 1.01              |
| 2:B:586:ILE:HD12 | 2:B:732:LEU:HD23 | 1.41                     | 1.01              |
| 1:A:142:ILE:HD12 | 1:A:189:LEU:CG   | 1.89                     | 1.01              |
| 2:B:529:MET:HE1  | 2:B:538:ILE:HD11 | 1.39                     | 1.01              |
| 2:B:570:LEU:HD22 | 2:B:721:ILE:CD1  | 1.91                     | 1.01              |
| 2:B:739:LYS:O    | 2:B:743:THR:O    | 1.79                     | 1.01              |
| 1:A:595:HIS:CE1  | 1:A:640:ILE:HD13 | 1.95                     | 1.01              |
| 3:C:121:ASN:ND2  | 3:D:218:ARG:NH1  | 2.09                     | 1.01              |
| 2:B:257:ILE:CD1  | 2:B:297:TYR:CE1  | 2.44                     | 1.01              |
| 1:A:154:LEU:HD23 | 2:B:281:LYS:NZ   | 1.75                     | 1.00              |
| 3:D:256:TYR:CE1  | 3:D:260:ILE:HD12 | 1.96                     | 1.00              |
| 1:A:65:ASN:HD21  | 2:B:215:ASN:HB3  | 0.97                     | 1.00              |
| 1:A:356:VAL:CG2  | 1:A:572:ILE:HD11 | 1.90                     | 1.00              |
| 1:A:133:MET:HE3  | 2:B:328:ARG:HH21 | 1.19                     | 1.00              |
| 3:C:258:THR:CG2  | 3:C:356:ILE:CD1  | 2.39                     | 1.00              |
| 3:D:95:ALA:HB1   | 3:D:111:ILE:HD11 | 1.42                     | 1.00              |
| 2:B:527:HIS:HE1  | 2:B:538:ILE:HD11 | 1.25                     | 1.00              |
| 2:B:264:TYR:CE2  | 2:B:287:ILE:HD11 | 1.96                     | 1.00              |
| 2:B:191:THR:HG23 | 2:B:207:ILE:HD13 | 1.43                     | 1.00              |
| 1:A:74:TYR:CD2   | 2:B:216:PHE:CZ   | 2.46                     | 1.00              |
| 2:B:656:ILE:HD13 | 2:B:738:HIS:CE1  | 1.96                     | 1.00              |
| 1:A:570:LEU:CD2  | 1:A:573:ILE:HD12 | 1.90                     | 1.00              |
| 1:A:66:VAL:HG21  | 1:A:94:ILE:HD13  | 1.39                     | 1.00              |
| 2:B:349:TRP:CD2  | 2:B:364:ILE:HD13 | 1.97                     | 1.00              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:HD11 | 1.43                     | 0.99              |
| 1:A:625:ILE:HD11 | 1:A:764:LEU:CB   | 1.92                     | 0.99              |
| 1:A:123:TYR:HE1  | 2:B:295:ARG:NH2  | 1.58                     | 0.99              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CD2  | 2.44                     | 0.99              |
| 1:A:138:PHE:CD2  | 1:A:192:ILE:CD1  | 2.45                     | 0.99              |
| 2:B:184:ILE:CD1  | 2:B:217:GLU:OE1  | 2.10                     | 0.99              |
| 3:D:200:ALA:HA   | 3:D:260:ILE:HD11 | 1.38                     | 0.99              |
| 1:A:426:PHE:CE1  | 1:A:564:ILE:HD11 | 1.96                     | 0.99              |
| 2:B:383:ILE:HD12 | 2:B:410:ILE:HD13 | 1.42                     | 0.99              |
| 3:C:5:ILE:HD11   | 3:C:252:MET:HG3  | 1.44                     | 0.99              |
| 2:B:355:LEU:HD21 | 2:B:364:ILE:CD1  | 1.92                     | 0.99              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:CD1  | 1.92                     | 0.99              |
| 3:C:256:TYR:CE1  | 3:C:260:ILE:HD12 | 1.97                     | 0.99              |
| 2:B:586:ILE:HG21 | 2:B:735:ILE:CD1  | 1.87                     | 0.99              |
| 1:A:356:VAL:CG2  | 1:A:572:ILE:HD11 | 1.92                     | 0.99              |
| 1:A:640:ILE:HD11 | 1:A:699:ILE:CD1  | 1.93                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:349:TRP:CE2  | 2:B:364:ILE:HD13 | 1.98                     | 0.99              |
| 1:A:623:ARG:CZ   | 1:A:761:ILE:HD11 | 1.93                     | 0.99              |
| 1:A:138:PHE:CE2  | 1:A:275:ILE:HD13 | 1.98                     | 0.99              |
| 3:C:342:ILE:HD13 | 3:C:344:PHE:CZ   | 1.98                     | 0.99              |
| 1:A:144:ARG:NH2  | 2:B:288:TYR:CD2  | 2.31                     | 0.99              |
| 1:A:109:ILE:HD11 | 1:A:174:GLU:OE1  | 1.61                     | 0.99              |
| 1:A:138:PHE:CE1  | 1:A:275:ILE:HD11 | 1.97                     | 0.99              |
| 3:C:256:TYR:CE1  | 3:C:260:ILE:CD1  | 2.46                     | 0.98              |
| 1:A:66:VAL:CG2   | 2:B:216:PHE:HE1  | 1.76                     | 0.98              |
| 2:B:586:ILE:HG23 | 2:B:735:ILE:CD1  | 1.93                     | 0.98              |
| 3:D:200:ALA:HB2  | 3:D:260:ILE:HD11 | 1.43                     | 0.98              |
| 1:A:70:LEU:CD1   | 2:B:216:PHE:CZ   | 2.46                     | 0.98              |
| 3:C:255:ILE:HD13 | 3:C:358:ARG:HD3  | 1.43                     | 0.98              |
| 2:B:586:ILE:HG23 | 2:B:735:ILE:HD13 | 1.01                     | 0.98              |
| 1:A:70:LEU:HB3   | 2:B:219:GLY:HA3  | 1.43                     | 0.98              |
| 2:B:288:TYR:CE2  | 2:B:292:ILE:CD1  | 2.46                     | 0.98              |
| 2:B:398:LEU:HD23 | 2:B:449:ILE:HD12 | 1.45                     | 0.98              |
| 1:A:65:ASN:CB    | 2:B:216:PHE:CE1  | 2.46                     | 0.98              |
| 2:B:349:TRP:NE1  | 2:B:364:ILE:HD11 | 1.78                     | 0.98              |
| 3:C:256:TYR:CD2  | 3:C:260:ILE:HD12 | 1.99                     | 0.98              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:CG1  | 2.41                     | 0.98              |
| 2:B:405:ILE:CA   | 2:B:456:ILE:CD1  | 2.41                     | 0.98              |
| 3:D:256:TYR:CE1  | 3:D:260:ILE:CD1  | 2.46                     | 0.98              |
| 1:A:641:LYS:CD   | 3:C:356:ILE:CD1  | 2.41                     | 0.98              |
| 3:C:258:THR:HG21 | 3:C:356:ILE:HD13 | 1.44                     | 0.98              |
| 3:C:188:ILE:HD11 | 3:C:394:PHE:CB   | 1.92                     | 0.98              |
| 3:D:210:LEU:HD11 | 3:D:222:ILE:CD1  | 1.94                     | 0.98              |
| 1:A:70:LEU:CG    | 2:B:281:LYS:HZ1  | 1.77                     | 0.98              |
| 1:A:425:ILE:HD13 | 1:A:478:MET:HA   | 1.45                     | 0.98              |
| 2:B:209:ILE:CD1  | 2:B:222:HIS:NE2  | 2.26                     | 0.97              |
| 2:B:571:VAL:HG23 | 2:B:721:ILE:HD11 | 1.46                     | 0.97              |
| 3:C:121:ASN:HD21 | 3:D:218:ARG:HH12 | 1.09                     | 0.97              |
| 1:A:629:THR:OG1  | 1:A:710:ILE:HD12 | 1.64                     | 0.97              |
| 1:A:70:LEU:HB2   | 2:B:216:PHE:HE1  | 1.26                     | 0.97              |
| 2:B:342:TYR:CE2  | 2:B:394:ILE:HD11 | 1.97                     | 0.97              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:CD1  | 1.94                     | 0.97              |
| 1:A:133:MET:CE   | 2:B:328:ARG:HH22 | 1.63                     | 0.97              |
| 2:B:586:ILE:HD13 | 2:B:732:LEU:HD23 | 1.45                     | 0.97              |
| 1:A:73:THR:H     | 2:B:215:ASN:HB3  | 1.27                     | 0.97              |
| 1:A:68:ILE:O     | 2:B:216:PHE:CE2  | 2.18                     | 0.97              |
| 1:A:70:LEU:CG    | 2:B:281:LYS:NZ   | 2.27                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:212:ILE:HD13 | 3:C:275:PHE:CE1  | 1.98                     | 0.97              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:CD1  | 2.41                     | 0.97              |
| 1:A:70:LEU:HD11  | 2:B:281:LYS:HZ3  | 1.27                     | 0.97              |
| 1:A:66:VAL:HG22  | 2:B:216:PHE:CE1  | 2.00                     | 0.97              |
| 2:B:568:LEU:HA   | 2:B:721:ILE:HD12 | 1.47                     | 0.97              |
| 2:B:288:TYR:HE2  | 2:B:292:ILE:HD11 | 1.26                     | 0.97              |
| 1:A:137:ARG:NE   | 2:B:325:LEU:CD1  | 2.25                     | 0.97              |
| 2:B:296:ILE:HD11 | 2:B:327:ILE:HG12 | 1.45                     | 0.97              |
| 1:A:151:LEU:HG   | 2:B:285:ARG:CG   | 1.94                     | 0.97              |
| 1:A:199:GLU:OE1  | 1:A:250:ILE:HD12 | 1.64                     | 0.97              |
| 2:B:634:ILE:HD11 | 2:B:772:PHE:CZ   | 1.99                     | 0.97              |
| 2:B:412:LEU:HD12 | 2:B:463:ILE:HD12 | 1.42                     | 0.97              |
| 2:B:772:PHE:CE1  | 2:B:812:ILE:HD12 | 2.00                     | 0.97              |
| 2:B:296:ILE:HD11 | 2:B:327:ILE:HG23 | 1.44                     | 0.96              |
| 3:C:125:LYS:CG   | 3:D:283:ASP:OD2  | 2.12                     | 0.96              |
| 2:B:412:LEU:CD2  | 2:B:463:ILE:CD1  | 2.42                     | 0.96              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:HB2  | 1.95                     | 0.96              |
| 1:A:68:ILE:HD12  | 2:B:216:PHE:CB   | 1.61                     | 0.96              |
| 1:A:135:LEU:CD2  | 1:A:247:ILE:CD1  | 2.43                     | 0.96              |
| 1:A:65:ASN:OD1   | 2:B:216:PHE:CD1  | 2.18                     | 0.96              |
| 1:A:640:ILE:CD1  | 1:A:696:GLN:HE22 | 1.78                     | 0.96              |
| 3:C:275:PHE:H    | 3:C:284:ILE:CD1  | 1.78                     | 0.96              |
| 2:B:586:ILE:HG22 | 2:B:735:ILE:HD12 | 1.45                     | 0.96              |
| 1:A:73:THR:CG2   | 2:B:215:ASN:HD22 | 1.78                     | 0.96              |
| 1:A:365:THR:HG23 | 1:A:404:ILE:HD13 | 1.44                     | 0.96              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:CD1  | 2.42                     | 0.96              |
| 1:A:140:TYR:CZ   | 2:B:292:ILE:CG2  | 2.44                     | 0.96              |
| 1:A:566:ILE:CD1  | 1:A:574:ILE:HD12 | 1.96                     | 0.96              |
| 1:A:599:LEU:CD1  | 1:A:640:ILE:HD11 | 1.95                     | 0.96              |
| 3:D:210:LEU:HD12 | 3:D:222:ILE:HD11 | 1.47                     | 0.96              |
| 2:B:241:PHE:HB3  | 2:B:254:ILE:CD1  | 1.96                     | 0.96              |
| 2:B:257:ILE:HD13 | 2:B:297:TYR:CZ   | 2.01                     | 0.96              |
| 1:A:570:LEU:HD23 | 1:A:573:ILE:HD12 | 1.47                     | 0.96              |
| 1:A:570:LEU:HD23 | 1:A:573:ILE:HD12 | 1.46                     | 0.96              |
| 2:B:209:ILE:HD11 | 2:B:222:HIS:NE2  | 1.79                     | 0.96              |
| 2:B:656:ILE:CD1  | 2:B:738:HIS:NE2  | 2.27                     | 0.96              |
| 1:A:566:ILE:CD1  | 1:A:574:ILE:HG23 | 1.95                     | 0.95              |
| 2:B:394:ILE:CD1  | 2:B:445:PHE:CE2  | 2.49                     | 0.95              |
| 1:A:195:GLU:HG3  | 1:A:250:ILE:CD1  | 1.94                     | 0.95              |
| 2:B:402:ILE:CG1  | 2:B:449:ILE:HD13 | 1.96                     | 0.95              |
| 2:B:527:HIS:HE1  | 2:B:538:ILE:CD1  | 1.73                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:825:ILE:HD11 | 2:B:841:LEU:HD12 | 1.44                     | 0.95              |
| 1:A:438:PHE:HZ   | 1:A:484:ILE:HD13 | 1.21                     | 0.95              |
| 2:B:241:PHE:CB   | 2:B:254:ILE:CD1  | 2.42                     | 0.95              |
| 1:A:138:PHE:CD2  | 1:A:275:ILE:CD1  | 2.46                     | 0.95              |
| 2:B:405:ILE:HG22 | 2:B:456:ILE:HD12 | 1.44                     | 0.95              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:HH21 | 1.74                     | 0.95              |
| 1:A:62:ASP:OD1   | 1:A:94:ILE:CD1   | 2.13                     | 0.95              |
| 2:B:634:ILE:HD12 | 2:B:809:LEU:CD2  | 1.97                     | 0.95              |
| 3:D:199:ASP:O    | 3:D:260:ILE:HD13 | 1.67                     | 0.95              |
| 2:B:188:VAL:HG13 | 2:B:224:ILE:HD13 | 1.45                     | 0.95              |
| 2:B:412:LEU:CD2  | 2:B:463:ILE:HD13 | 1.90                     | 0.95              |
| 3:D:212:ILE:HD11 | 3:D:302:SER:O    | 1.67                     | 0.95              |
| 1:A:66:VAL:CG2   | 2:B:216:PHE:CE1  | 2.50                     | 0.94              |
| 2:B:586:ILE:CD1  | 2:B:732:LEU:HD23 | 1.96                     | 0.94              |
| 1:A:70:LEU:CB    | 2:B:216:PHE:CE1  | 2.50                     | 0.94              |
| 3:D:119:ILE:HD12 | 3:D:154:LEU:HD22 | 1.49                     | 0.94              |
| 2:B:209:ILE:HD12 | 2:B:222:HIS:CE1  | 2.02                     | 0.94              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:HB2  | 1.48                     | 0.94              |
| 1:A:70:LEU:CD1   | 2:B:281:LYS:CE   | 2.44                     | 0.94              |
| 1:A:564:ILE:HD12 | 1:A:582:TYR:CD2  | 2.01                     | 0.94              |
| 2:B:586:ILE:CD1  | 2:B:732:LEU:HD23 | 1.95                     | 0.94              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CG   | 2.50                     | 0.94              |
| 3:D:127:ILE:HD13 | 3:D:162:TYR:CZ   | 2.02                     | 0.94              |
| 3:C:255:ILE:CD1  | 3:C:358:ARG:CZ   | 2.44                     | 0.94              |
| 3:D:127:ILE:CD1  | 3:D:161:ARG:HH12 | 1.81                     | 0.94              |
| 1:A:366:ILE:N    | 1:A:404:ILE:HD11 | 1.80                     | 0.94              |
| 1:A:774:ILE:HD12 | 1:A:796:SER:CB   | 1.97                     | 0.94              |
| 1:A:458:TYR:CD1  | 1:A:484:ILE:HD13 | 2.02                     | 0.94              |
| 1:A:137:ARG:CZ   | 2:B:325:LEU:HD11 | 1.98                     | 0.94              |
| 1:A:70:LEU:HD12  | 2:B:220:LEU:HD11 | 1.49                     | 0.94              |
| 1:A:696:GLN:NE2  | 1:A:699:ILE:HD12 | 1.82                     | 0.94              |
| 1:A:696:GLN:HE21 | 1:A:699:ILE:HD12 | 1.33                     | 0.94              |
| 1:A:137:ARG:NH2  | 2:B:325:LEU:HD11 | 1.83                     | 0.94              |
| 1:A:131:PHE:CD2  | 2:B:322:HIS:NE2  | 2.36                     | 0.94              |
| 2:B:296:ILE:HD12 | 2:B:327:ILE:CD1  | 1.97                     | 0.94              |
| 1:A:365:THR:HG23 | 1:A:404:ILE:HD12 | 1.47                     | 0.94              |
| 1:A:588:TYR:CD1  | 1:A:693:ILE:CD1  | 2.51                     | 0.94              |
| 1:A:643:ILE:HD13 | 1:A:692:LEU:HD23 | 1.50                     | 0.94              |
| 3:C:125:LYS:HG2  | 3:D:283:ASP:CG   | 1.93                     | 0.93              |
| 1:A:135:LEU:HD21 | 1:A:247:ILE:HD11 | 1.48                     | 0.93              |
| 1:A:65:ASN:ND2   | 2:B:215:ASN:CG   | 2.23                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:188:ILE:HD13 | 3:D:394:PHE:CD2  | 2.02                     | 0.93              |
| 2:B:241:PHE:HB3  | 2:B:254:ILE:HD11 | 1.49                     | 0.93              |
| 2:B:349:TRP:CD1  | 2:B:364:ILE:CD1  | 2.50                     | 0.93              |
| 1:A:581:LYS:HB3  | 1:A:683:ILE:HD12 | 1.50                     | 0.93              |
| 3:D:210:LEU:HD22 | 3:D:222:ILE:HD11 | 1.49                     | 0.93              |
| 2:B:570:LEU:HD22 | 2:B:721:ILE:HD13 | 1.50                     | 0.93              |
| 1:A:362:GLN:NE2  | 2:B:447:GLU:CG   | 2.31                     | 0.93              |
| 3:D:5:ILE:HD11   | 3:D:252:MET:HE2  | 1.50                     | 0.93              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:HD13 | 1.96                     | 0.93              |
| 3:C:125:LYS:CG   | 3:D:283:ASP:CG   | 2.41                     | 0.93              |
| 1:A:585:ILE:HD11 | 1:A:683:ILE:CG1  | 1.99                     | 0.93              |
| 1:A:65:ASN:HB3   | 2:B:216:PHE:CZ   | 2.03                     | 0.93              |
| 1:A:425:ILE:HD13 | 1:A:482:LEU:HD11 | 1.51                     | 0.93              |
| 1:A:367:PRO:HG3  | 1:A:404:ILE:HD12 | 1.50                     | 0.93              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:CD2  | 2.46                     | 0.93              |
| 2:B:349:TRP:CE2  | 2:B:364:ILE:CD1  | 2.52                     | 0.93              |
| 1:A:151:LEU:HG   | 2:B:285:ARG:HD3  | 0.94                     | 0.93              |
| 2:B:586:ILE:HG21 | 2:B:735:ILE:CD1  | 1.97                     | 0.93              |
| 3:D:210:LEU:CD1  | 3:D:222:ILE:HD11 | 1.99                     | 0.92              |
| 1:A:70:LEU:HD13  | 2:B:220:LEU:CD2  | 1.97                     | 0.92              |
| 2:B:349:TRP:CG   | 2:B:364:ILE:CD1  | 2.51                     | 0.92              |
| 2:B:586:ILE:HG21 | 2:B:735:ILE:HD12 | 1.52                     | 0.92              |
| 2:B:405:ILE:HD11 | 2:B:456:ILE:HD12 | 0.96                     | 0.92              |
| 1:A:356:VAL:HG21 | 1:A:572:ILE:HD11 | 0.96                     | 0.92              |
| 1:A:73:THR:HG22  | 2:B:215:ASN:CA   | 1.95                     | 0.92              |
| 1:A:123:TYR:CE1  | 2:B:295:ARG:NH2  | 2.36                     | 0.92              |
| 1:A:158:LEU:HD23 | 2:B:281:LYS:HZ1  | 0.94                     | 0.92              |
| 1:A:367:PRO:CB   | 1:A:404:ILE:CD1  | 2.47                     | 0.92              |
| 1:A:65:ASN:OD1   | 2:B:216:PHE:HE1  | 1.40                     | 0.92              |
| 2:B:480:ILE:CD1  | 2:B:537:VAL:HG22 | 1.99                     | 0.92              |
| 1:A:68:ILE:HG13  | 2:B:281:LYS:NZ   | 1.85                     | 0.92              |
| 2:B:482:LEU:CD2  | 2:B:735:ILE:CD1  | 2.47                     | 0.92              |
| 1:A:202:GLU:O    | 1:A:205:THR:O    | 1.88                     | 0.92              |
| 2:B:636:ILE:HD13 | 3:D:442:GLN:OE1  | 1.69                     | 0.92              |
| 2:B:257:ILE:HD11 | 2:B:297:TYR:CZ   | 2.04                     | 0.92              |
| 1:A:458:TYR:CE1  | 1:A:484:ILE:CD1  | 2.52                     | 0.92              |
| 1:A:438:PHE:CZ   | 1:A:484:ILE:CD1  | 2.52                     | 0.92              |
| 1:A:70:LEU:CD1   | 2:B:281:LYS:HE2  | 2.00                     | 0.92              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:HD12 | 1.49                     | 0.92              |
| 2:B:586:ILE:HG12 | 2:B:735:ILE:HD12 | 1.47                     | 0.92              |
| 1:A:195:GLU:CG   | 1:A:250:ILE:HD13 | 1.99                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:586:ILE:CG2  | 2:B:735:ILE:HD12 | 1.99                     | 0.92              |
| 1:A:73:THR:HG23  | 2:B:215:ASN:HD22 | 1.34                     | 0.92              |
| 2:B:570:LEU:HD22 | 2:B:721:ILE:CD1  | 1.99                     | 0.92              |
| 1:A:367:PRO:HB3  | 1:A:404:ILE:CD1  | 1.99                     | 0.92              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CG   | 2.52                     | 0.92              |
| 1:A:70:LEU:CD1   | 2:B:216:PHE:HZ   | 1.83                     | 0.92              |
| 1:A:71:GLU:O     | 2:B:208:GLN:CD   | 2.12                     | 0.92              |
| 1:A:566:ILE:CD1  | 1:A:574:ILE:CD1  | 2.47                     | 0.92              |
| 1:A:366:ILE:C    | 1:A:404:ILE:HD12 | 1.95                     | 0.92              |
| 1:A:699:ILE:HD11 | 1:A:782:PHE:HE2  | 1.35                     | 0.91              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:HD12 | 0.92                     | 0.91              |
| 3:C:212:ILE:CD1  | 3:C:275:PHE:CZ   | 2.54                     | 0.91              |
| 3:C:6:ILE:HD12   | 3:C:127:ILE:HG12 | 1.52                     | 0.91              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:HG12 | 1.98                     | 0.91              |
| 1:A:131:PHE:CE2  | 2:B:322:HIS:CE1  | 2.57                     | 0.91              |
| 2:B:241:PHE:HB3  | 2:B:254:ILE:CD1  | 1.99                     | 0.91              |
| 1:A:135:LEU:HD21 | 1:A:247:ILE:CD1  | 2.00                     | 0.91              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:HB3  | 1.97                     | 0.91              |
| 3:D:200:ALA:CA   | 3:D:260:ILE:HD11 | 1.99                     | 0.91              |
| 3:D:210:LEU:CD1  | 3:D:222:ILE:HD11 | 2.00                     | 0.91              |
| 1:A:425:ILE:HD11 | 1:A:482:LEU:HD22 | 0.92                     | 0.91              |
| 1:A:131:PHE:CD2  | 2:B:322:HIS:CE1  | 2.58                     | 0.91              |
| 1:A:425:ILE:HD13 | 1:A:482:LEU:CD1  | 1.98                     | 0.91              |
| 1:A:66:VAL:CB    | 1:A:94:ILE:HD12  | 2.01                     | 0.91              |
| 2:B:427:LYS:HE2  | 2:B:456:ILE:HD11 | 1.49                     | 0.91              |
| 2:B:241:PHE:CB   | 2:B:254:ILE:HD13 | 1.99                     | 0.91              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:HD13 | 2.00                     | 0.91              |
| 2:B:241:PHE:HB2  | 2:B:254:ILE:HD13 | 1.51                     | 0.91              |
| 2:B:634:ILE:HD13 | 2:B:776:TYR:HE1  | 1.35                     | 0.91              |
| 3:D:256:TYR:CD1  | 3:D:260:ILE:HD12 | 2.06                     | 0.91              |
| 2:B:533:ARG:O    | 2:B:538:ILE:HD12 | 1.71                     | 0.91              |
| 1:A:158:LEU:CD2  | 2:B:281:LYS:HZ1  | 1.81                     | 0.91              |
| 1:A:70:LEU:HD12  | 2:B:220:LEU:HD13 | 1.51                     | 0.91              |
| 1:A:65:ASN:CG    | 2:B:216:PHE:CE1  | 2.49                     | 0.90              |
| 1:A:643:ILE:CD1  | 1:A:692:LEU:HD23 | 2.01                     | 0.90              |
| 2:B:355:LEU:HD21 | 2:B:364:ILE:HD13 | 1.51                     | 0.90              |
| 3:C:188:ILE:HD13 | 3:C:394:PHE:CD1  | 2.05                     | 0.90              |
| 1:A:61:LYS:HE3   | 2:B:216:PHE:CE1  | 2.06                     | 0.90              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:CD1  | 2.48                     | 0.90              |
| 2:B:586:ILE:CD1  | 2:B:732:LEU:HD22 | 1.99                     | 0.90              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CB   | 2.49                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:406:LEU:HD21 | 1:A:672:ILE:HD11 | 1.52                     | 0.90              |
| 2:B:405:ILE:HA   | 2:B:456:ILE:HD13 | 1.52                     | 0.90              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:CD1  | 2.50                     | 0.90              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:HD22 | 2.01                     | 0.90              |
| 3:D:119:ILE:HD11 | 3:D:154:LEU:HD22 | 1.52                     | 0.90              |
| 1:A:114:LYS:HE3  | 1:A:118:ILE:HD11 | 0.94                     | 0.90              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CB   | 2.45                     | 0.90              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:CG   | 2.42                     | 0.90              |
| 3:C:212:ILE:HD13 | 3:C:275:PHE:CE2  | 2.05                     | 0.90              |
| 1:A:70:LEU:CG    | 2:B:216:PHE:CZ   | 2.51                     | 0.90              |
| 1:A:70:LEU:CB    | 2:B:216:PHE:HE1  | 1.85                     | 0.90              |
| 1:A:641:LYS:HD3  | 3:C:356:ILE:HD11 | 1.52                     | 0.90              |
| 1:A:303:ASP:O    | 1:A:304:ASP:O    | 1.88                     | 0.90              |
| 1:A:425:ILE:HD11 | 1:A:478:MET:HG3  | 1.54                     | 0.90              |
| 1:A:65:ASN:HD21  | 2:B:215:ASN:ND2  | 1.70                     | 0.90              |
| 1:A:130:SER:OG   | 2:B:322:HIS:CG   | 2.24                     | 0.90              |
| 1:A:63:LEU:HB3   | 1:A:170:ILE:HD13 | 1.54                     | 0.90              |
| 1:A:70:LEU:HD11  | 2:B:220:LEU:CD1  | 2.01                     | 0.90              |
| 1:A:599:LEU:HD12 | 1:A:640:ILE:HD11 | 1.54                     | 0.90              |
| 1:A:68:ILE:HD11  | 1:A:158:LEU:HD21 | 1.53                     | 0.90              |
| 2:B:398:LEU:HD11 | 2:B:449:ILE:HD12 | 1.54                     | 0.90              |
| 1:A:706:PHE:HE2  | 1:A:768:ILE:CD1  | 1.85                     | 0.90              |
| 3:D:217:PHE:CD1  | 3:D:280:ILE:HD13 | 2.07                     | 0.90              |
| 1:A:126:TRP:CH2  | 1:A:196:ILE:HD12 | 2.07                     | 0.89              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:CB   | 1.99                     | 0.89              |
| 1:A:641:LYS:HG3  | 3:C:356:ILE:CD1  | 2.02                     | 0.89              |
| 2:B:293:ARG:HB3  | 2:B:330:ILE:HD11 | 1.54                     | 0.89              |
| 2:B:355:LEU:CD2  | 2:B:364:ILE:CD1  | 2.46                     | 0.89              |
| 1:A:425:ILE:HD11 | 1:A:482:LEU:HB2  | 1.52                     | 0.89              |
| 3:D:258:THR:HG23 | 3:D:356:ILE:HD13 | 1.54                     | 0.89              |
| 3:C:188:ILE:HD11 | 3:C:394:PHE:HB3  | 1.54                     | 0.89              |
| 1:A:71:GLU:HA    | 2:B:216:PHE:CE2  | 2.06                     | 0.89              |
| 2:B:412:LEU:HD11 | 2:B:463:ILE:CD1  | 2.01                     | 0.89              |
| 1:A:70:LEU:HB3   | 2:B:216:PHE:HB3  | 1.52                     | 0.89              |
| 1:A:138:PHE:CZ   | 1:A:275:ILE:HD13 | 2.05                     | 0.89              |
| 3:C:188:ILE:HD13 | 3:C:394:PHE:CD2  | 2.08                     | 0.89              |
| 1:A:584:ILE:CD1  | 1:A:687:ARG:HD2  | 2.02                     | 0.89              |
| 2:B:634:ILE:HD11 | 2:B:772:PHE:HE1  | 1.13                     | 0.89              |
| 2:B:342:TYR:HE2  | 2:B:394:ILE:CD1  | 1.85                     | 0.89              |
| 1:A:65:ASN:OD1   | 2:B:215:ASN:CG   | 2.14                     | 0.89              |
| 1:A:774:ILE:HD12 | 1:A:796:SER:HB2  | 1.54                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:412:LEU:CD2  | 2:B:463:ILE:HD11 | 2.02                     | 0.89              |
| 2:B:402:ILE:CG1  | 2:B:449:ILE:HD13 | 2.03                     | 0.89              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:HB2  | 1.93                     | 0.89              |
| 2:B:772:PHE:HE1  | 2:B:812:ILE:HD12 | 1.33                     | 0.88              |
| 1:A:367:PRO:HA   | 1:A:404:ILE:HD11 | 1.53                     | 0.88              |
| 2:B:241:PHE:HB3  | 2:B:254:ILE:HD13 | 1.41                     | 0.88              |
| 2:B:296:ILE:HD12 | 2:B:327:ILE:HD12 | 1.55                     | 0.88              |
| 2:B:335:PHE:CE2  | 2:B:339:ILE:CD1  | 2.55                     | 0.88              |
| 2:B:412:LEU:CD2  | 2:B:463:ILE:HD12 | 1.95                     | 0.88              |
| 1:A:71:GLU:O     | 2:B:208:GLN:NE2  | 2.06                     | 0.88              |
| 1:A:140:TYR:HH   | 2:B:296:ILE:HD11 | 1.36                     | 0.88              |
| 1:A:357:VAL:HB   | 1:A:363:ILE:HD12 | 1.55                     | 0.88              |
| 1:A:425:ILE:HD12 | 1:A:482:LEU:HD13 | 1.54                     | 0.88              |
| 1:A:151:LEU:HD22 | 2:B:285:ARG:HB2  | 1.55                     | 0.88              |
| 1:A:365:THR:CG2  | 1:A:404:ILE:CD1  | 2.49                     | 0.88              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:HD11 | 1.54                     | 0.88              |
| 1:A:195:GLU:CD   | 1:A:250:ILE:HD12 | 1.98                     | 0.88              |
| 2:B:628:ILE:HD12 | 2:B:780:ASN:HD21 | 1.31                     | 0.88              |
| 2:B:825:ILE:CD1  | 2:B:841:LEU:CD1  | 2.51                     | 0.88              |
| 1:A:625:ILE:HD13 | 1:A:764:LEU:CB   | 2.03                     | 0.88              |
| 1:A:114:LYS:HE3  | 1:A:118:ILE:CD1  | 2.03                     | 0.88              |
| 1:A:70:LEU:O     | 2:B:216:PHE:HE2  | 1.51                     | 0.88              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CD2  | 2.57                     | 0.88              |
| 1:A:641:LYS:HB3  | 3:C:356:ILE:CD1  | 2.04                     | 0.88              |
| 1:A:68:ILE:C     | 2:B:281:LYS:NZ   | 2.32                     | 0.88              |
| 1:A:136:GLN:HE22 | 2:B:296:ILE:HD11 | 1.39                     | 0.88              |
| 1:A:195:GLU:CG   | 1:A:250:ILE:CD1  | 2.50                     | 0.88              |
| 3:C:238:VAL:HG23 | 3:C:322:ILE:HD12 | 1.56                     | 0.88              |
| 3:C:255:ILE:HD13 | 3:C:358:ARG:CZ   | 2.03                     | 0.88              |
| 1:A:151:LEU:CG   | 2:B:285:ARG:CD   | 2.25                     | 0.88              |
| 1:A:699:ILE:HD11 | 1:A:782:PHE:CE2  | 2.08                     | 0.88              |
| 1:A:68:ILE:CD1   | 2:B:281:LYS:CD   | 2.48                     | 0.87              |
| 1:A:425:ILE:HD11 | 1:A:482:LEU:CB   | 2.04                     | 0.87              |
| 1:A:425:ILE:HD12 | 1:A:478:MET:HB3  | 1.54                     | 0.87              |
| 2:B:656:ILE:HD12 | 2:B:738:HIS:CD2  | 2.10                     | 0.87              |
| 1:A:356:VAL:HG21 | 1:A:572:ILE:HD13 | 1.54                     | 0.87              |
| 3:D:258:THR:HG23 | 3:D:356:ILE:HD12 | 1.55                     | 0.87              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:HD11 | 1.56                     | 0.87              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:HD12 | 2.04                     | 0.87              |
| 1:A:458:TYR:CE1  | 1:A:484:ILE:HD13 | 2.09                     | 0.87              |
| 1:A:73:THR:N     | 2:B:215:ASN:HB3  | 1.88                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:136:GLN:HE22 | 2:B:322:HIS:HB3  | 1.38                     | 0.87              |
| 2:B:297:TYR:CE2  | 2:B:330:ILE:HD12 | 2.10                     | 0.87              |
| 1:A:557:ILE:HD12 | 1:A:594:TYR:CE2  | 2.10                     | 0.87              |
| 2:B:192:LEU:HD21 | 2:B:287:ILE:HD12 | 1.56                     | 0.87              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CB   | 2.03                     | 0.87              |
| 3:D:199:ASP:O    | 3:D:260:ILE:HD13 | 1.74                     | 0.87              |
| 1:A:70:LEU:HD12  | 2:B:216:PHE:CZ   | 2.08                     | 0.87              |
| 1:A:199:GLU:CD   | 1:A:250:ILE:CD1  | 2.48                     | 0.87              |
| 3:D:127:ILE:HD11 | 3:D:161:ARG:HH12 | 1.37                     | 0.87              |
| 3:C:6:ILE:CD1    | 3:C:127:ILE:HG12 | 2.03                     | 0.87              |
| 3:C:238:VAL:CG2  | 3:C:322:ILE:CD1  | 2.52                     | 0.87              |
| 3:C:200:ALA:CB   | 3:C:260:ILE:HD11 | 2.03                     | 0.87              |
| 1:A:629:THR:HG21 | 1:A:710:ILE:CD1  | 2.04                     | 0.87              |
| 2:B:586:ILE:HG23 | 2:B:735:ILE:HD13 | 1.55                     | 0.87              |
| 1:A:566:ILE:HD12 | 1:A:574:ILE:HG21 | 1.57                     | 0.86              |
| 3:C:255:ILE:HD13 | 3:C:358:ARG:NH2  | 1.90                     | 0.86              |
| 2:B:586:ILE:HG12 | 2:B:735:ILE:CD1  | 2.04                     | 0.86              |
| 2:B:405:ILE:HD12 | 2:B:453:TYR:CA   | 2.04                     | 0.86              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:CD1  | 1.87                     | 0.86              |
| 2:B:224:ILE:HD13 | 2:B:280:LEU:HD11 | 1.55                     | 0.86              |
| 3:C:195:ILE:HD12 | 3:C:430:VAL:HG11 | 1.57                     | 0.86              |
| 1:A:70:LEU:HD11  | 2:B:220:LEU:HD11 | 1.58                     | 0.86              |
| 1:A:142:ILE:CD1  | 1:A:189:LEU:HG   | 2.02                     | 0.86              |
| 2:B:493:ILE:CD1  | 2:B:598:TYR:CG   | 2.59                     | 0.86              |
| 1:A:68:ILE:HD12  | 2:B:281:LYS:CD   | 2.05                     | 0.86              |
| 2:B:405:ILE:HD13 | 2:B:452:GLN:CB   | 2.04                     | 0.86              |
| 1:A:154:LEU:HD23 | 2:B:281:LYS:CE   | 2.05                     | 0.86              |
| 2:B:402:ILE:HG13 | 2:B:449:ILE:HD13 | 1.58                     | 0.86              |
| 2:B:532:PRO:HB2  | 2:B:538:ILE:HD13 | 1.58                     | 0.86              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CD2  | 2.57                     | 0.86              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:HD11 | 1.56                     | 0.86              |
| 1:A:567:PRO:HD2  | 1:A:574:ILE:CD1  | 2.05                     | 0.86              |
| 2:B:296:ILE:HD11 | 2:B:327:ILE:HG23 | 1.57                     | 0.86              |
| 2:B:349:TRP:CD2  | 2:B:364:ILE:HD13 | 2.10                     | 0.86              |
| 1:A:362:GLN:HE21 | 2:B:447:GLU:CG   | 1.89                     | 0.86              |
| 1:A:366:ILE:N    | 1:A:404:ILE:CD1  | 2.38                     | 0.86              |
| 1:A:137:ARG:HH21 | 2:B:325:LEU:HD11 | 1.40                     | 0.86              |
| 1:A:151:LEU:CB   | 2:B:285:ARG:HE   | 1.72                     | 0.86              |
| 2:B:339:ILE:HD13 | 2:B:440:GLY:CA   | 2.05                     | 0.86              |
| 3:D:199:ASP:O    | 3:D:260:ILE:HD13 | 1.76                     | 0.86              |
| 2:B:527:HIS:HA   | 2:B:538:ILE:CD1  | 2.06                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:362:GLN:HE21 | 2:B:447:GLU:HG2  | 1.41                     | 0.85              |
| 3:C:258:THR:OG1  | 3:C:356:ILE:HD11 | 1.76                     | 0.85              |
| 3:D:5:ILE:HD12   | 3:D:53:PHE:CZ    | 2.11                     | 0.85              |
| 1:A:72:GLY:HA3   | 2:B:222:HIS:CE1  | 2.10                     | 0.85              |
| 1:A:151:LEU:HD23 | 2:B:285:ARG:HH21 | 0.85                     | 0.85              |
| 1:A:70:LEU:HB2   | 2:B:216:PHE:CE1  | 2.09                     | 0.85              |
| 1:A:641:LYS:CD   | 3:C:356:ILE:HD11 | 2.04                     | 0.85              |
| 2:B:383:ILE:HD11 | 2:B:410:ILE:HD13 | 1.55                     | 0.85              |
| 1:A:136:GLN:NE2  | 2:B:296:ILE:HD11 | 1.92                     | 0.85              |
| 2:B:191:THR:CG2  | 2:B:207:ILE:CD1  | 2.54                     | 0.85              |
| 1:A:68:ILE:HD13  | 2:B:216:PHE:HB2  | 1.57                     | 0.85              |
| 3:C:188:ILE:HD11 | 3:C:394:PHE:CD2  | 2.12                     | 0.85              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:CD1  | 2.06                     | 0.85              |
| 3:D:95:ALA:HB1   | 3:D:111:ILE:CD1  | 2.05                     | 0.85              |
| 1:A:362:GLN:HB3  | 2:B:446:PHE:CE2  | 2.12                     | 0.85              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:CB   | 2.06                     | 0.85              |
| 3:D:356:ILE:CD1  | 3:D:358:ARG:HH12 | 1.88                     | 0.85              |
| 1:A:70:LEU:HD11  | 2:B:220:LEU:HD13 | 1.58                     | 0.85              |
| 1:A:588:TYR:CE1  | 1:A:693:ILE:HD11 | 2.11                     | 0.85              |
| 1:A:152:LYS:HD3  | 2:B:285:ARG:HH11 | 1.03                     | 0.85              |
| 3:C:188:ILE:HD13 | 3:C:394:PHE:HD1  | 1.39                     | 0.85              |
| 2:B:184:ILE:CD1  | 2:B:217:GLU:OE1  | 2.24                     | 0.85              |
| 2:B:192:LEU:CD2  | 2:B:287:ILE:HD12 | 2.05                     | 0.85              |
| 2:B:349:TRP:CE2  | 2:B:364:ILE:CD1  | 2.58                     | 0.85              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:HD11 | 2.07                     | 0.85              |
| 2:B:643:GLN:CD   | 3:D:356:ILE:HD11 | 2.02                     | 0.85              |
| 1:A:564:ILE:HD12 | 1:A:582:TYR:HD2  | 1.37                     | 0.85              |
| 2:B:570:LEU:HD12 | 2:B:721:ILE:HD13 | 1.55                     | 0.85              |
| 2:B:257:ILE:HD13 | 2:B:297:TYR:CE2  | 2.10                     | 0.85              |
| 2:B:412:LEU:HD11 | 2:B:463:ILE:HD11 | 1.57                     | 0.85              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CG   | 2.60                     | 0.84              |
| 3:D:256:TYR:CE1  | 3:D:260:ILE:HD12 | 2.11                     | 0.84              |
| 2:B:349:TRP:CD2  | 2:B:364:ILE:CD1  | 2.59                     | 0.84              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:HB3  | 1.60                     | 0.84              |
| 2:B:412:LEU:HD21 | 2:B:463:ILE:HD12 | 1.59                     | 0.84              |
| 1:A:566:ILE:CD1  | 1:A:574:ILE:HB   | 2.07                     | 0.84              |
| 1:A:584:ILE:CD1  | 1:A:687:ARG:HG3  | 2.07                     | 0.84              |
| 2:B:412:LEU:HD23 | 2:B:463:ILE:CD1  | 2.07                     | 0.84              |
| 2:B:402:ILE:CG1  | 2:B:449:ILE:HD13 | 2.07                     | 0.84              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:HB3  | 1.55                     | 0.84              |
| 1:A:62:ASP:CG    | 1:A:94:ILE:HD11  | 2.03                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:140:TYR:OH   | 2:B:296:ILE:CD1  | 2.22                     | 0.84              |
| 2:B:383:ILE:CD1  | 2:B:410:ILE:CD1  | 2.55                     | 0.84              |
| 3:D:127:ILE:CD1  | 3:D:161:ARG:NH1  | 2.39                     | 0.84              |
| 3:D:199:ASP:O    | 3:D:260:ILE:CD1  | 2.26                     | 0.84              |
| 2:B:398:LEU:CD1  | 2:B:449:ILE:HD12 | 2.08                     | 0.84              |
| 2:B:412:LEU:HD23 | 2:B:463:ILE:HD11 | 1.58                     | 0.84              |
| 1:A:780:ILE:CD1  | 1:A:789:GLU:CD   | 2.51                     | 0.84              |
| 2:B:349:TRP:CG   | 2:B:364:ILE:CD1  | 2.61                     | 0.84              |
| 1:A:151:LEU:HD22 | 2:B:285:ARG:HD2  | 0.87                     | 0.84              |
| 3:D:200:ALA:CB   | 3:D:260:ILE:HD11 | 2.08                     | 0.84              |
| 3:C:212:ILE:HD13 | 3:C:275:PHE:CZ   | 2.13                     | 0.84              |
| 2:B:349:TRP:CE2  | 2:B:364:ILE:HD13 | 2.13                     | 0.83              |
| 1:A:137:ARG:NH2  | 2:B:325:LEU:CD2  | 2.41                     | 0.83              |
| 1:A:425:ILE:HD11 | 1:A:482:LEU:HD21 | 1.60                     | 0.83              |
| 1:A:599:LEU:HD22 | 1:A:640:ILE:HD11 | 1.60                     | 0.83              |
| 1:A:74:TYR:HB3   | 2:B:215:ASN:OD1  | 1.77                     | 0.83              |
| 2:B:349:TRP:NE1  | 2:B:364:ILE:HD11 | 1.93                     | 0.83              |
| 2:B:634:ILE:CD1  | 2:B:772:PHE:CE1  | 2.55                     | 0.83              |
| 1:A:584:ILE:HD12 | 1:A:687:ARG:CG   | 2.08                     | 0.83              |
| 1:A:70:LEU:O     | 2:B:216:PHE:HD2  | 1.54                     | 0.83              |
| 1:A:136:GLN:CD   | 2:B:323:GLY:HA2  | 2.03                     | 0.83              |
| 1:A:291:ILE:HD11 | 1:A:358:ARG:HH11 | 1.41                     | 0.83              |
| 1:A:135:LEU:HD22 | 1:A:247:ILE:HD12 | 1.60                     | 0.83              |
| 1:A:365:THR:C    | 1:A:404:ILE:HD11 | 2.02                     | 0.83              |
| 2:B:480:ILE:CD1  | 2:B:537:VAL:CG2  | 2.55                     | 0.83              |
| 2:B:493:ILE:CD1  | 2:B:598:TYR:CD2  | 2.60                     | 0.83              |
| 2:B:209:ILE:HD12 | 2:B:222:HIS:HE1  | 1.40                     | 0.83              |
| 1:A:136:GLN:NE2  | 2:B:327:ILE:HD11 | 1.93                     | 0.83              |
| 1:A:74:TYR:HB3   | 2:B:215:ASN:CG   | 2.02                     | 0.83              |
| 3:D:200:ALA:CB   | 3:D:260:ILE:HD11 | 2.07                     | 0.83              |
| 1:A:154:LEU:CD2  | 2:B:281:LYS:HE2  | 2.09                     | 0.83              |
| 1:A:136:GLN:HE21 | 2:B:327:ILE:HD11 | 1.43                     | 0.83              |
| 2:B:808:ASN:ND2  | 2:B:812:ILE:HD12 | 1.92                     | 0.83              |
| 2:B:349:TRP:NE1  | 2:B:364:ILE:CD1  | 2.26                     | 0.83              |
| 1:A:155:VAL:HG11 | 2:B:285:ARG:NH1  | 1.92                     | 0.83              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:CD1  | 2.07                     | 0.83              |
| 1:A:625:ILE:HD12 | 1:A:758:LEU:HD21 | 1.61                     | 0.83              |
| 1:A:641:LYS:HB3  | 3:C:356:ILE:HD12 | 1.59                     | 0.83              |
| 1:A:151:LEU:HD22 | 2:B:285:ARG:HE   | 0.67                     | 0.83              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:CD1  | 2.57                     | 0.82              |
| 3:C:258:THR:HG23 | 3:C:356:ILE:CD1  | 2.08                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:102:PHE:HB3  | 1:A:170:ILE:HD12 | 1.61                     | 0.82              |
| 1:A:629:THR:OG1  | 1:A:710:ILE:HD11 | 1.79                     | 0.82              |
| 1:A:141:GLU:OE2  | 2:B:324:ASP:OD2  | 1.97                     | 0.82              |
| 3:D:127:ILE:HD13 | 3:D:162:TYR:OH   | 1.77                     | 0.82              |
| 3:D:210:LEU:HD12 | 3:D:222:ILE:CD1  | 2.09                     | 0.82              |
| 1:A:143:ARG:NH1  | 2:B:292:ILE:HD13 | 1.92                     | 0.82              |
| 1:A:154:LEU:HD23 | 2:B:281:LYS:HZ3  | 1.44                     | 0.82              |
| 1:A:114:LYS:HE3  | 1:A:118:ILE:HD11 | 1.60                     | 0.82              |
| 2:B:634:ILE:HD11 | 2:B:772:PHE:HE1  | 1.45                     | 0.82              |
| 3:D:255:ILE:HD12 | 3:D:358:ARG:CZ   | 2.09                     | 0.82              |
| 1:A:588:TYR:CD1  | 1:A:693:ILE:CD1  | 2.62                     | 0.82              |
| 2:B:636:ILE:CD1  | 3:D:442:GLN:OE1  | 2.27                     | 0.82              |
| 1:A:73:THR:HG22  | 2:B:215:ASN:HA   | 1.60                     | 0.82              |
| 2:B:634:ILE:CD1  | 2:B:772:PHE:HE1  | 1.91                     | 0.82              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:HD11 | 2.08                     | 0.82              |
| 3:C:212:ILE:CD1  | 3:C:275:PHE:CZ   | 2.62                     | 0.82              |
| 1:A:584:ILE:CD1  | 1:A:687:ARG:CD   | 2.57                     | 0.82              |
| 2:B:264:TYR:CE1  | 2:B:287:ILE:CD1  | 2.57                     | 0.82              |
| 1:A:142:ILE:HD11 | 1:A:186:MET:HG2  | 1.62                     | 0.82              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:HD13 | 1.61                     | 0.82              |
| 1:A:365:THR:HG23 | 1:A:404:ILE:HD13 | 1.62                     | 0.82              |
| 1:A:143:ARG:HD2  | 2:B:292:ILE:HD11 | 1.62                     | 0.82              |
| 1:A:138:PHE:CD2  | 1:A:192:ILE:HD12 | 2.14                     | 0.82              |
| 1:A:291:ILE:HD11 | 1:A:358:ARG:NH1  | 1.95                     | 0.82              |
| 2:B:656:ILE:HD12 | 2:B:738:HIS:CG   | 2.15                     | 0.82              |
| 1:A:363:ILE:HD11 | 1:A:413:TYR:CD1  | 2.14                     | 0.82              |
| 1:A:702:ILE:HD11 | 1:A:767:TYR:CE2  | 2.14                     | 0.82              |
| 2:B:493:ILE:HD12 | 2:B:598:TYR:CG   | 2.14                     | 0.82              |
| 1:A:640:ILE:HD11 | 1:A:699:ILE:HD13 | 1.62                     | 0.81              |
| 1:A:599:LEU:CD1  | 1:A:640:ILE:HD12 | 2.10                     | 0.81              |
| 2:B:241:PHE:HB3  | 2:B:254:ILE:HD11 | 1.58                     | 0.81              |
| 1:A:367:PRO:CA   | 1:A:404:ILE:HD11 | 2.09                     | 0.81              |
| 2:B:570:LEU:CD2  | 2:B:721:ILE:HD13 | 2.09                     | 0.81              |
| 1:A:641:LYS:HG3  | 3:C:356:ILE:HD13 | 1.62                     | 0.81              |
| 2:B:480:ILE:HD12 | 2:B:541:LEU:HD21 | 1.59                     | 0.81              |
| 3:C:238:VAL:HG22 | 3:C:322:ILE:CD1  | 2.10                     | 0.81              |
| 3:D:212:ILE:HD12 | 3:D:303:ASN:OD1  | 1.80                     | 0.81              |
| 1:A:128:ASP:CA   | 2:B:322:HIS:CE1  | 2.64                     | 0.81              |
| 1:A:425:ILE:HD13 | 1:A:482:LEU:HD22 | 1.62                     | 0.81              |
| 2:B:349:TRP:NE1  | 2:B:364:ILE:HD12 | 1.95                     | 0.81              |
| 1:A:68:ILE:O     | 2:B:281:LYS:HD2  | 1.80                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:70:LEU:HA    | 1:A:75:ILE:HD13  | 1.61                     | 0.81              |
| 3:D:119:ILE:HD11 | 3:D:154:LEU:CD2  | 2.07                     | 0.81              |
| 1:A:629:THR:OG1  | 1:A:768:ILE:HD11 | 1.81                     | 0.81              |
| 1:A:774:ILE:CD1  | 1:A:796:SER:HB3  | 2.10                     | 0.81              |
| 2:B:296:ILE:HD13 | 2:B:327:ILE:HD13 | 1.62                     | 0.81              |
| 1:A:588:TYR:CD1  | 1:A:693:ILE:HD12 | 2.16                     | 0.81              |
| 2:B:493:ILE:HD12 | 2:B:598:TYR:HB2  | 1.60                     | 0.81              |
| 1:A:133:MET:HG3  | 2:B:328:ARG:HH21 | 1.43                     | 0.81              |
| 1:A:137:ARG:HH21 | 2:B:325:LEU:HD21 | 1.46                     | 0.81              |
| 2:B:586:ILE:HG22 | 2:B:735:ILE:HD11 | 1.48                     | 0.81              |
| 1:A:152:LYS:HD3  | 2:B:285:ARG:HH12 | 1.07                     | 0.81              |
| 1:A:136:GLN:HE21 | 2:B:327:ILE:CD1  | 1.90                     | 0.81              |
| 1:A:629:THR:CG2  | 1:A:710:ILE:HD11 | 2.09                     | 0.81              |
| 1:A:137:ARG:HE   | 2:B:325:LEU:HD12 | 1.45                     | 0.81              |
| 2:B:257:ILE:HD13 | 2:B:297:TYR:CE2  | 2.15                     | 0.81              |
| 2:B:349:TRP:CD2  | 2:B:364:ILE:HD11 | 2.16                     | 0.81              |
| 2:B:402:ILE:HG12 | 2:B:449:ILE:HD13 | 1.63                     | 0.81              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:HD13 | 2.10                     | 0.81              |
| 2:B:297:TYR:CE2  | 2:B:330:ILE:CD1  | 2.63                     | 0.81              |
| 3:C:6:ILE:CD1    | 3:C:127:ILE:HG22 | 2.10                     | 0.81              |
| 3:C:129:SER:OG   | 3:D:284:ILE:HG13 | 1.81                     | 0.81              |
| 2:B:335:PHE:CE1  | 2:B:339:ILE:CD1  | 2.59                     | 0.81              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:CB   | 2.09                     | 0.81              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CE2  | 2.64                     | 0.81              |
| 3:C:200:ALA:CB   | 3:C:260:ILE:HD11 | 2.11                     | 0.81              |
| 1:A:567:PRO:CD   | 1:A:574:ILE:HD13 | 2.11                     | 0.81              |
| 3:C:195:ILE:CD1  | 3:C:430:VAL:HG11 | 2.11                     | 0.81              |
| 2:B:480:ILE:CD1  | 2:B:541:LEU:HD11 | 2.11                     | 0.80              |
| 1:A:135:LEU:CD2  | 1:A:247:ILE:HD12 | 2.10                     | 0.80              |
| 1:A:573:ILE:HD12 | 1:A:673:GLN:CG   | 2.11                     | 0.80              |
| 2:B:568:LEU:CA   | 2:B:721:ILE:HD12 | 2.11                     | 0.80              |
| 2:B:636:ILE:HD13 | 3:D:351:ALA:HB2  | 1.63                     | 0.80              |
| 3:D:188:ILE:HD13 | 3:D:394:PHE:CG   | 2.15                     | 0.80              |
| 3:C:200:ALA:CB   | 3:C:260:ILE:HD11 | 2.08                     | 0.80              |
| 2:B:586:ILE:HG21 | 2:B:735:ILE:HD13 | 1.56                     | 0.80              |
| 3:C:188:ILE:HD13 | 3:C:394:PHE:CG   | 2.17                     | 0.80              |
| 2:B:188:VAL:CG1  | 2:B:224:ILE:HD13 | 2.10                     | 0.80              |
| 3:D:255:ILE:CD1  | 3:D:358:ARG:CZ   | 2.59                     | 0.80              |
| 1:A:136:GLN:NE2  | 2:B:296:ILE:CD1  | 2.44                     | 0.80              |
| 2:B:257:ILE:CD1  | 2:B:297:TYR:CZ   | 2.64                     | 0.80              |
| 3:C:258:THR:CG2  | 3:C:356:ILE:HD13 | 2.08                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:582:TYR:HD1  | 1:A:683:ILE:HD11 | 1.45                     | 0.80              |
| 1:A:71:GLU:OE1   | 2:B:222:HIS:NE2  | 2.14                     | 0.80              |
| 2:B:335:PHE:HE1  | 2:B:339:ILE:CD1  | 1.92                     | 0.80              |
| 2:B:349:TRP:CE2  | 2:B:364:ILE:HD11 | 2.17                     | 0.80              |
| 2:B:739:LYS:O    | 2:B:743:THR:O    | 2.00                     | 0.80              |
| 1:A:570:LEU:CD2  | 1:A:573:ILE:CD1  | 2.57                     | 0.80              |
| 1:A:584:ILE:HD12 | 1:A:687:ARG:CD   | 2.09                     | 0.80              |
| 2:B:533:ARG:HA   | 2:B:538:ILE:HD12 | 1.64                     | 0.80              |
| 1:A:588:TYR:CE1  | 1:A:693:ILE:CD1  | 2.64                     | 0.80              |
| 1:A:570:LEU:HD22 | 1:A:573:ILE:CD1  | 2.07                     | 0.80              |
| 1:A:606:LEU:HD13 | 1:A:710:ILE:HD11 | 1.64                     | 0.80              |
| 2:B:480:ILE:HD12 | 2:B:562:TYR:OH   | 1.82                     | 0.80              |
| 2:B:808:ASN:HD21 | 2:B:812:ILE:CD1  | 1.95                     | 0.79              |
| 1:A:699:ILE:HD11 | 1:A:775:PHE:CZ   | 2.16                     | 0.79              |
| 1:A:62:ASP:CG    | 1:A:94:ILE:CD1   | 2.55                     | 0.79              |
| 2:B:296:ILE:HD11 | 2:B:327:ILE:CG1  | 2.10                     | 0.79              |
| 2:B:241:PHE:HB3  | 2:B:254:ILE:HD12 | 1.63                     | 0.79              |
| 1:A:133:MET:CG   | 2:B:328:ARG:NH2  | 2.45                     | 0.79              |
| 1:A:566:ILE:HD13 | 1:A:574:ILE:HD12 | 0.83                     | 0.79              |
| 3:D:199:ASP:O    | 3:D:260:ILE:HD13 | 1.82                     | 0.79              |
| 2:B:242:ARG:HA   | 2:B:254:ILE:HD11 | 1.64                     | 0.79              |
| 2:B:493:ILE:HD11 | 2:B:598:TYR:HB3  | 1.64                     | 0.79              |
| 1:A:65:ASN:ND2   | 2:B:215:ASN:ND2  | 2.27                     | 0.79              |
| 3:D:5:ILE:HD11   | 3:D:252:MET:CE   | 2.05                     | 0.79              |
| 1:A:136:GLN:OE1  | 2:B:323:GLY:HA2  | 1.83                     | 0.79              |
| 1:A:66:VAL:HG21  | 1:A:170:ILE:HD12 | 1.65                     | 0.79              |
| 3:D:127:ILE:HD11 | 3:D:161:ARG:NH1  | 1.96                     | 0.79              |
| 1:A:140:TYR:HE2  | 2:B:327:ILE:HD11 | 1.47                     | 0.79              |
| 1:A:365:THR:CG2  | 1:A:404:ILE:HD13 | 2.12                     | 0.79              |
| 3:C:255:ILE:HD13 | 3:C:358:ARG:CD   | 2.13                     | 0.79              |
| 1:A:158:LEU:HD23 | 2:B:281:LYS:HZ3  | 1.48                     | 0.79              |
| 1:A:356:VAL:HG21 | 1:A:572:ILE:CD1  | 2.09                     | 0.79              |
| 1:A:128:ASP:OD1  | 2:B:296:ILE:HD11 | 1.83                     | 0.79              |
| 1:A:137:ARG:NH2  | 2:B:324:ASP:OD1  | 2.16                     | 0.79              |
| 1:A:126:TRP:HH2  | 1:A:196:ILE:HD12 | 1.44                     | 0.79              |
| 3:D:127:ILE:HD12 | 3:D:161:ARG:HH22 | 1.48                     | 0.79              |
| 2:B:402:ILE:CG1  | 2:B:449:ILE:CD1  | 2.60                     | 0.79              |
| 1:A:155:VAL:CG1  | 2:B:285:ARG:NH1  | 2.46                     | 0.79              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CD1  | 2.18                     | 0.79              |
| 2:B:586:ILE:HG21 | 2:B:735:ILE:CD1  | 2.13                     | 0.79              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:CD1  | 2.13                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:493:ILE:HD11 | 2:B:598:TYR:CB   | 2.12                     | 0.79              |
| 1:A:68:ILE:HD13  | 1:A:158:LEU:HD21 | 1.64                     | 0.79              |
| 2:B:405:ILE:HA   | 2:B:456:ILE:HD11 | 1.64                     | 0.79              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:CG   | 2.18                     | 0.79              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:HG23 | 2.13                     | 0.78              |
| 1:A:557:ILE:HD12 | 1:A:594:TYR:HE2  | 1.45                     | 0.78              |
| 2:B:405:ILE:CG2  | 2:B:456:ILE:HD12 | 2.09                     | 0.78              |
| 3:C:258:THR:HG23 | 3:C:356:ILE:HD12 | 1.65                     | 0.78              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:CG1  | 2.61                     | 0.78              |
| 2:B:412:LEU:HD13 | 2:B:463:ILE:HD12 | 1.66                     | 0.78              |
| 3:D:188:ILE:HD13 | 3:D:394:PHE:CD2  | 2.17                     | 0.78              |
| 2:B:825:ILE:HD11 | 2:B:841:LEU:HD11 | 1.64                     | 0.78              |
| 1:A:606:LEU:HD22 | 1:A:710:ILE:CD1  | 2.13                     | 0.78              |
| 2:B:570:LEU:CD1  | 2:B:721:ILE:HD13 | 2.13                     | 0.78              |
| 2:B:529:MET:SD   | 2:B:538:ILE:CD1  | 2.72                     | 0.78              |
| 2:B:405:ILE:CD1  | 2:B:453:TYR:CA   | 2.59                     | 0.78              |
| 2:B:570:LEU:HD22 | 2:B:721:ILE:HD11 | 1.65                     | 0.78              |
| 1:A:614:TYR:O    | 1:A:623:ARG:HB2  | 1.83                     | 0.78              |
| 1:A:137:ARG:NH2  | 2:B:328:ARG:NH2  | 2.28                     | 0.78              |
| 3:D:200:ALA:HA   | 3:D:260:ILE:CD1  | 2.12                     | 0.78              |
| 3:C:256:TYR:CE2  | 3:C:260:ILE:CD1  | 2.67                     | 0.78              |
| 1:A:144:ARG:NE   | 2:B:289:GLU:OE2  | 2.17                     | 0.78              |
| 3:C:125:LYS:CG   | 3:D:283:ASP:OD1  | 2.24                     | 0.78              |
| 1:A:154:LEU:HD23 | 2:B:281:LYS:HE2  | 1.66                     | 0.78              |
| 2:B:339:ILE:HD12 | 2:B:439:ARG:HD2  | 1.66                     | 0.78              |
| 1:A:606:LEU:HD21 | 1:A:710:ILE:HD12 | 1.64                     | 0.78              |
| 1:A:641:LYS:HD2  | 3:C:356:ILE:HD12 | 1.64                     | 0.78              |
| 1:A:138:PHE:CG   | 1:A:192:ILE:HD12 | 2.19                     | 0.78              |
| 1:A:570:LEU:HD22 | 1:A:573:ILE:HD12 | 1.64                     | 0.77              |
| 1:A:158:LEU:HD23 | 2:B:281:LYS:CE   | 2.12                     | 0.77              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:CE1  | 2.19                     | 0.77              |
| 1:A:702:ILE:CD1  | 1:A:767:TYR:CD2  | 2.68                     | 0.77              |
| 1:A:68:ILE:HG13  | 2:B:281:LYS:CE   | 2.14                     | 0.77              |
| 1:A:158:LEU:CD2  | 2:B:281:LYS:HZ3  | 1.98                     | 0.77              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CB   | 2.13                     | 0.77              |
| 1:A:135:LEU:HD22 | 1:A:247:ILE:CD1  | 2.12                     | 0.77              |
| 1:A:66:VAL:HB    | 1:A:94:ILE:CD1   | 2.13                     | 0.77              |
| 2:B:571:VAL:HG21 | 2:B:721:ILE:HD11 | 1.67                     | 0.77              |
| 1:A:425:ILE:HD13 | 1:A:482:LEU:HD13 | 1.66                     | 0.77              |
| 1:A:151:LEU:CD1  | 2:B:285:ARG:HG3  | 2.15                     | 0.77              |
| 1:A:367:PRO:CB   | 1:A:404:ILE:HD11 | 2.14                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:623:ARG:NE   | 1:A:761:ILE:HD11 | 1.98                     | 0.77              |
| 1:A:63:LEU:CB    | 1:A:170:ILE:CD1  | 2.60                     | 0.77              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CB   | 2.60                     | 0.77              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:HB2  | 2.14                     | 0.77              |
| 3:D:256:TYR:CD1  | 3:D:260:ILE:HD12 | 2.20                     | 0.77              |
| 2:B:355:LEU:HD22 | 2:B:364:ILE:HD12 | 1.67                     | 0.77              |
| 1:A:138:PHE:CG   | 1:A:275:ILE:HD11 | 2.19                     | 0.77              |
| 1:A:405:PHE:CZ   | 1:A:573:ILE:HD11 | 2.20                     | 0.77              |
| 3:D:119:ILE:HD13 | 3:D:154:LEU:CD2  | 2.15                     | 0.77              |
| 1:A:599:LEU:HD21 | 1:A:640:ILE:HD12 | 1.65                     | 0.77              |
| 1:A:109:ILE:CD1  | 1:A:170:ILE:HD11 | 2.15                     | 0.77              |
| 1:A:641:LYS:HD2  | 3:C:356:ILE:CD1  | 2.14                     | 0.77              |
| 3:C:212:ILE:CD1  | 3:C:275:PHE:CZ   | 2.68                     | 0.77              |
| 3:C:123:ILE:HD13 | 3:C:161:ARG:HH22 | 1.50                     | 0.77              |
| 1:A:141:GLU:CD   | 2:B:324:ASP:OD2  | 2.28                     | 0.77              |
| 1:A:74:TYR:HD2   | 2:B:216:PHE:HZ   | 0.87                     | 0.77              |
| 2:B:825:ILE:CD1  | 2:B:841:LEU:HD12 | 2.13                     | 0.76              |
| 1:A:155:VAL:HG11 | 2:B:285:ARG:HH22 | 1.50                     | 0.76              |
| 1:A:425:ILE:HD12 | 1:A:478:MET:CB   | 2.15                     | 0.76              |
| 1:A:144:ARG:NH1  | 2:B:289:GLU:OE2  | 2.18                     | 0.76              |
| 1:A:589:GLN:NE2  | 1:A:652:ILE:HD13 | 2.01                     | 0.76              |
| 2:B:571:VAL:HG23 | 2:B:721:ILE:CD1  | 2.14                     | 0.76              |
| 2:B:634:ILE:CD1  | 2:B:809:LEU:HG   | 2.15                     | 0.76              |
| 1:A:255:ILE:HD13 | 1:A:269:LYS:HG2  | 1.65                     | 0.76              |
| 1:A:66:VAL:CG2   | 1:A:94:ILE:HD13  | 2.16                     | 0.76              |
| 3:C:67:ILE:HD12  | 3:C:123:ILE:CG2  | 2.15                     | 0.76              |
| 1:A:599:LEU:CD2  | 1:A:640:ILE:HD12 | 2.12                     | 0.76              |
| 1:A:641:LYS:HD3  | 3:C:356:ILE:CD1  | 2.16                     | 0.76              |
| 2:B:349:TRP:HE1  | 2:B:364:ILE:HD13 | 1.48                     | 0.76              |
| 1:A:65:ASN:CG    | 2:B:215:ASN:CG   | 2.53                     | 0.76              |
| 1:A:157:ARG:HD3  | 1:A:176:ILE:HD13 | 1.67                     | 0.76              |
| 2:B:209:ILE:HD11 | 2:B:218:SER:CB   | 2.12                     | 0.76              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CB   | 2.62                     | 0.76              |
| 2:B:586:ILE:HG21 | 2:B:735:ILE:HD11 | 1.56                     | 0.76              |
| 2:B:570:LEU:HD12 | 2:B:721:ILE:CD1  | 2.13                     | 0.76              |
| 2:B:808:ASN:ND2  | 2:B:812:ILE:CD1  | 2.48                     | 0.76              |
| 1:A:114:LYS:CE   | 1:A:118:ILE:CD1  | 2.58                     | 0.76              |
| 2:B:207:ILE:CD1  | 2:B:221:LEU:HD23 | 2.16                     | 0.76              |
| 2:B:349:TRP:NE1  | 2:B:364:ILE:CD1  | 2.48                     | 0.76              |
| 1:A:63:LEU:HB3   | 1:A:170:ILE:HD11 | 1.66                     | 0.76              |
| 1:A:296:TYR:HH   | 2:B:322:HIS:CD2  | 1.72                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:151:LEU:HB2  | 2:B:285:ARG:HD3  | 1.52                     | 0.76              |
| 1:A:68:ILE:HD11  | 2:B:216:PHE:HD1  | 1.51                     | 0.76              |
| 1:A:68:ILE:HG21  | 2:B:216:PHE:HB2  | 1.66                     | 0.76              |
| 2:B:405:ILE:HD11 | 2:B:453:TYR:HA   | 1.64                     | 0.76              |
| 1:A:133:MET:HG3  | 2:B:328:ARG:NH2  | 2.01                     | 0.76              |
| 2:B:529:MET:SD   | 2:B:538:ILE:HD11 | 2.25                     | 0.76              |
| 1:A:425:ILE:HD12 | 1:A:564:ILE:HD12 | 1.68                     | 0.76              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:CD2  | 2.21                     | 0.76              |
| 3:D:255:ILE:CD1  | 3:D:358:ARG:NE   | 2.48                     | 0.76              |
| 2:B:293:ARG:HB3  | 2:B:330:ILE:CD1  | 2.16                     | 0.76              |
| 2:B:200:PHE:HZ   | 2:B:207:ILE:HD11 | 1.49                     | 0.76              |
| 2:B:188:VAL:HG11 | 2:B:224:ILE:CD1  | 2.16                     | 0.76              |
| 1:A:66:VAL:HG23  | 2:B:216:PHE:CE1  | 2.20                     | 0.75              |
| 3:D:356:ILE:HD13 | 3:D:358:ARG:NH1  | 1.96                     | 0.75              |
| 1:A:66:VAL:CB    | 1:A:94:ILE:CD1   | 2.63                     | 0.75              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CG   | 2.22                     | 0.75              |
| 1:A:131:PHE:CD2  | 2:B:322:HIS:CD2  | 2.74                     | 0.75              |
| 1:A:65:ASN:OD1   | 2:B:216:PHE:HE1  | 1.69                     | 0.75              |
| 1:A:202:GLU:O    | 1:A:205:THR:O    | 2.04                     | 0.75              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:HB2  | 2.16                     | 0.75              |
| 1:A:141:GLU:OE1  | 2:B:324:ASP:OD2  | 2.04                     | 0.75              |
| 1:A:706:PHE:CE2  | 1:A:768:ILE:CD1  | 2.69                     | 0.75              |
| 2:B:628:ILE:HD12 | 2:B:780:ASN:HD22 | 1.50                     | 0.75              |
| 1:A:68:ILE:HG21  | 2:B:215:ASN:HD22 | 1.50                     | 0.75              |
| 3:C:238:VAL:HG23 | 3:C:322:ILE:CD1  | 2.15                     | 0.75              |
| 1:A:138:PHE:CD2  | 1:A:192:ILE:HD13 | 2.19                     | 0.75              |
| 2:B:743:THR:O    | 2:B:756:GLN:NE2  | 2.18                     | 0.75              |
| 1:A:131:PHE:HD2  | 2:B:322:HIS:CE1  | 2.04                     | 0.75              |
| 1:A:625:ILE:HD13 | 1:A:764:LEU:HB2  | 1.67                     | 0.75              |
| 2:B:570:LEU:CD2  | 2:B:721:ILE:CD1  | 2.65                     | 0.75              |
| 1:A:774:ILE:HD12 | 1:A:796:SER:HB3  | 1.66                     | 0.75              |
| 2:B:398:LEU:HD21 | 2:B:449:ILE:HD12 | 1.69                     | 0.75              |
| 3:D:210:LEU:HD23 | 3:D:222:ILE:HD11 | 1.65                     | 0.75              |
| 1:A:361:LEU:HD11 | 2:B:443:THR:HG22 | 1.69                     | 0.75              |
| 1:A:625:ILE:HD12 | 1:A:758:LEU:CD2  | 2.15                     | 0.75              |
| 3:D:210:LEU:HD22 | 3:D:222:ILE:HD13 | 1.66                     | 0.75              |
| 2:B:184:ILE:HD12 | 2:B:217:GLU:OE1  | 1.85                     | 0.75              |
| 1:A:126:TRP:CZ2  | 1:A:196:ILE:CD1  | 2.70                     | 0.75              |
| 1:A:66:VAL:HA    | 2:B:216:PHE:CD1  | 2.22                     | 0.75              |
| 2:B:349:TRP:CG   | 2:B:364:ILE:CD1  | 2.70                     | 0.75              |
| 2:B:634:ILE:HD13 | 2:B:805:PHE:CZ   | 2.22                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:128:ASP:OD2  | 3:D:281:HIS:CG   | 2.40                     | 0.75              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CG   | 2.70                     | 0.75              |
| 2:B:241:PHE:HB3  | 2:B:254:ILE:HD13 | 1.69                     | 0.74              |
| 2:B:636:ILE:HD11 | 3:D:437:TYR:CE1  | 2.22                     | 0.74              |
| 2:B:568:LEU:HA   | 2:B:721:ILE:CD1  | 2.16                     | 0.74              |
| 2:B:412:LEU:HD22 | 2:B:463:ILE:HD12 | 1.68                     | 0.74              |
| 1:A:133:MET:SD   | 2:B:328:ARG:NH2  | 2.60                     | 0.74              |
| 3:D:139:LEU:CD2  | 3:D:235:ILE:HD13 | 2.16                     | 0.74              |
| 2:B:643:GLN:CG   | 3:D:356:ILE:HD11 | 2.18                     | 0.74              |
| 1:A:71:GLU:CB    | 2:B:215:ASN:CG   | 2.38                     | 0.74              |
| 1:A:625:ILE:HD11 | 1:A:764:LEU:C    | 2.11                     | 0.74              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:CD1  | 2.17                     | 0.74              |
| 1:A:70:LEU:HD12  | 2:B:216:PHE:HZ   | 1.46                     | 0.74              |
| 1:A:109:ILE:HD13 | 1:A:173:LEU:HD13 | 1.68                     | 0.74              |
| 2:B:402:ILE:HG13 | 2:B:449:ILE:HD13 | 1.69                     | 0.74              |
| 3:D:188:ILE:HD13 | 3:D:394:PHE:CG   | 2.23                     | 0.74              |
| 3:D:256:TYR:CE2  | 3:D:260:ILE:HD12 | 2.22                     | 0.74              |
| 2:B:296:ILE:HD13 | 2:B:327:ILE:CD1  | 2.16                     | 0.74              |
| 3:C:6:ILE:HD12   | 3:C:127:ILE:HG22 | 1.70                     | 0.74              |
| 2:B:335:PHE:CE1  | 2:B:339:ILE:HD11 | 2.22                     | 0.74              |
| 1:A:582:TYR:CD1  | 1:A:683:ILE:HD11 | 2.22                     | 0.74              |
| 2:B:480:ILE:HD11 | 2:B:537:VAL:HG22 | 1.69                     | 0.74              |
| 2:B:480:ILE:HD12 | 2:B:537:VAL:HG22 | 1.68                     | 0.74              |
| 3:C:199:ASP:C    | 3:C:260:ILE:HD13 | 2.11                     | 0.74              |
| 1:A:143:ARG:HD2  | 2:B:292:ILE:CD1  | 2.18                     | 0.74              |
| 2:B:586:ILE:CG1  | 2:B:735:ILE:HD12 | 2.18                     | 0.74              |
| 1:A:140:TYR:CE1  | 2:B:292:ILE:HD13 | 2.23                     | 0.73              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CG   | 2.72                     | 0.73              |
| 1:A:780:ILE:HD11 | 1:A:789:GLU:OE1  | 1.88                     | 0.73              |
| 3:C:212:ILE:HD13 | 3:C:275:PHE:CE1  | 2.23                     | 0.73              |
| 2:B:643:GLN:HG2  | 3:D:356:ILE:CD1  | 2.18                     | 0.73              |
| 2:B:586:ILE:CD1  | 2:B:732:LEU:CD2  | 2.65                     | 0.73              |
| 3:C:123:ILE:CD1  | 3:C:161:ARG:HH22 | 2.01                     | 0.73              |
| 1:A:155:VAL:CG1  | 2:B:285:ARG:HH11 | 2.01                     | 0.73              |
| 2:B:349:TRP:NE1  | 2:B:364:ILE:HD13 | 1.88                     | 0.73              |
| 2:B:209:ILE:CD1  | 2:B:218:SER:HB3  | 2.16                     | 0.73              |
| 1:A:581:LYS:HB3  | 1:A:683:ILE:HD12 | 1.70                     | 0.73              |
| 1:A:566:ILE:CD1  | 1:A:574:ILE:CG2  | 2.66                     | 0.73              |
| 1:A:566:ILE:CD1  | 1:A:574:ILE:HD13 | 2.17                     | 0.73              |
| 3:C:275:PHE:H    | 3:C:284:ILE:HD12 | 1.53                     | 0.73              |
| 2:B:427:LYS:HE2  | 2:B:456:ILE:CD1  | 2.18                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:212:ILE:CD1  | 3:D:303:ASN:OD1  | 2.36                     | 0.73              |
| 1:A:566:ILE:HD11 | 1:A:574:ILE:HB   | 1.69                     | 0.73              |
| 3:D:139:LEU:HD21 | 3:D:235:ILE:HD13 | 1.69                     | 0.73              |
| 1:A:155:VAL:HG12 | 2:B:281:LYS:HD3  | 1.71                     | 0.73              |
| 2:B:527:HIS:HA   | 2:B:538:ILE:HD11 | 1.71                     | 0.73              |
| 2:B:532:PRO:O    | 2:B:538:ILE:HD12 | 1.88                     | 0.73              |
| 1:A:138:PHE:HZ   | 1:A:275:ILE:CD1  | 1.98                     | 0.73              |
| 3:C:129:SER:OG   | 3:D:284:ILE:CG1  | 2.36                     | 0.73              |
| 1:A:706:PHE:CE2  | 1:A:768:ILE:HD12 | 2.22                     | 0.73              |
| 2:B:493:ILE:CD1  | 2:B:598:TYR:HB2  | 2.19                     | 0.73              |
| 1:A:140:TYR:HH   | 2:B:292:ILE:CG2  | 1.99                     | 0.73              |
| 2:B:407:LYS:NZ   | 2:B:721:ILE:HD12 | 2.03                     | 0.73              |
| 1:A:566:ILE:CD1  | 1:A:574:ILE:HD13 | 2.18                     | 0.73              |
| 3:D:258:THR:CG2  | 3:D:356:ILE:HD12 | 2.18                     | 0.73              |
| 2:B:242:ARG:HG3  | 2:B:254:ILE:CD1  | 2.19                     | 0.73              |
| 1:A:375:ILE:HD11 | 1:A:400:ARG:NH2  | 2.04                     | 0.73              |
| 3:C:255:ILE:CD1  | 3:C:358:ARG:NH1  | 2.51                     | 0.73              |
| 2:B:628:ILE:CD1  | 2:B:780:ASN:HD22 | 2.01                     | 0.73              |
| 1:A:566:ILE:CD1  | 1:A:571:ASN:HA   | 2.19                     | 0.73              |
| 3:C:275:PHE:N    | 3:C:284:ILE:CD1  | 2.52                     | 0.73              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:HB2  | 1.71                     | 0.73              |
| 1:A:425:ILE:HD12 | 1:A:478:MET:CB   | 2.18                     | 0.73              |
| 1:A:458:TYR:CG   | 1:A:484:ILE:HD11 | 2.24                     | 0.73              |
| 2:B:656:ILE:CD1  | 2:B:738:HIS:CD2  | 2.72                     | 0.73              |
| 2:B:349:TRP:CD1  | 2:B:364:ILE:HD11 | 2.24                     | 0.72              |
| 3:C:275:PHE:N    | 3:C:284:ILE:HD12 | 2.04                     | 0.72              |
| 3:C:255:ILE:HD11 | 3:C:358:ARG:NH1  | 2.04                     | 0.72              |
| 3:C:256:TYR:CE1  | 3:C:260:ILE:HD11 | 2.22                     | 0.72              |
| 1:A:367:PRO:CB   | 1:A:404:ILE:CD1  | 2.67                     | 0.72              |
| 2:B:405:ILE:CA   | 2:B:456:ILE:HD13 | 2.15                     | 0.72              |
| 3:C:199:ASP:O    | 3:C:260:ILE:CD1  | 2.19                     | 0.72              |
| 1:A:128:ASP:HA   | 2:B:322:HIS:HE2  | 1.51                     | 0.72              |
| 1:A:566:ILE:HD13 | 1:A:571:ASN:CB   | 2.15                     | 0.72              |
| 2:B:224:ILE:HD11 | 2:B:283:LEU:HD23 | 1.71                     | 0.72              |
| 1:A:114:LYS:HE2  | 1:A:118:ILE:HD11 | 1.70                     | 0.72              |
| 1:A:152:LYS:HD2  | 2:B:285:ARG:HH12 | 1.53                     | 0.72              |
| 1:A:144:ARG:NH2  | 2:B:288:TYR:HD2  | 1.86                     | 0.72              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CD1  | 2.73                     | 0.72              |
| 3:D:127:ILE:HD12 | 3:D:161:ARG:NH2  | 2.04                     | 0.72              |
| 1:A:72:GLY:HA3   | 2:B:215:ASN:O    | 1.89                     | 0.72              |
| 2:B:296:ILE:HD11 | 2:B:327:ILE:CG2  | 2.18                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:780:ILE:HD12 | 1:A:789:GLU:HB2  | 1.70                     | 0.72              |
| 2:B:405:ILE:HG21 | 2:B:456:ILE:HD12 | 1.61                     | 0.72              |
| 1:A:65:ASN:CG    | 2:B:216:PHE:CD1  | 2.66                     | 0.72              |
| 2:B:493:ILE:HD13 | 2:B:598:TYR:CB   | 2.08                     | 0.72              |
| 2:B:634:ILE:HD13 | 2:B:805:PHE:HZ   | 1.55                     | 0.72              |
| 2:B:355:LEU:O    | 2:B:364:ILE:CD1  | 2.37                     | 0.72              |
| 1:A:566:ILE:HD12 | 1:A:574:ILE:CG2  | 2.16                     | 0.72              |
| 1:A:109:ILE:HD12 | 1:A:170:ILE:HD11 | 1.70                     | 0.72              |
| 2:B:412:LEU:CG   | 2:B:463:ILE:CD1  | 2.67                     | 0.72              |
| 1:A:71:GLU:HB2   | 2:B:208:GLN:OE1  | 1.90                     | 0.72              |
| 3:C:255:ILE:CD1  | 3:C:358:ARG:HD3  | 2.17                     | 0.72              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CG   | 2.72                     | 0.72              |
| 1:A:102:PHE:CE1  | 1:A:170:ILE:HD11 | 2.25                     | 0.72              |
| 1:A:151:LEU:HB2  | 2:B:285:ARG:NE   | 1.92                     | 0.72              |
| 2:B:342:TYR:CE2  | 2:B:394:ILE:CD1  | 2.66                     | 0.72              |
| 1:A:780:ILE:HD11 | 1:A:789:GLU:CD   | 2.14                     | 0.71              |
| 2:B:394:ILE:HD11 | 2:B:445:PHE:CZ   | 2.25                     | 0.71              |
| 2:B:480:ILE:HD12 | 2:B:537:VAL:HG21 | 1.69                     | 0.71              |
| 1:A:73:THR:HG22  | 2:B:215:ASN:CA   | 2.16                     | 0.71              |
| 1:A:151:LEU:CG   | 2:B:285:ARG:HG3  | 2.20                     | 0.71              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CZ   | 2.72                     | 0.71              |
| 1:A:130:SER:CB   | 2:B:322:HIS:CE1  | 2.73                     | 0.71              |
| 3:D:212:ILE:HD11 | 3:D:302:SER:O    | 1.89                     | 0.71              |
| 1:A:152:LYS:HG2  | 2:B:285:ARG:HH11 | 0.64                     | 0.71              |
| 2:B:209:ILE:CD1  | 2:B:222:HIS:NE2  | 2.44                     | 0.71              |
| 3:C:125:LYS:HG3  | 3:D:283:ASP:CG   | 2.07                     | 0.71              |
| 3:D:255:ILE:HD12 | 3:D:358:ARG:NE   | 2.05                     | 0.71              |
| 1:A:291:ILE:CD1  | 1:A:358:ARG:NH1  | 2.54                     | 0.71              |
| 3:D:210:LEU:CD2  | 3:D:222:ILE:CD1  | 2.67                     | 0.71              |
| 2:B:339:ILE:CD1  | 2:B:440:GLY:N    | 2.53                     | 0.71              |
| 2:B:349:TRP:CD2  | 2:B:364:ILE:CD1  | 2.73                     | 0.71              |
| 1:A:138:PHE:CE1  | 1:A:142:ILE:HD11 | 2.25                     | 0.71              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:HD11 | 1.69                     | 0.71              |
| 1:A:367:PRO:CG   | 1:A:404:ILE:HD12 | 2.18                     | 0.71              |
| 1:A:564:ILE:CD1  | 1:A:582:TYR:CD2  | 2.74                     | 0.71              |
| 1:A:367:PRO:HB3  | 1:A:404:ILE:CD1  | 2.20                     | 0.71              |
| 3:D:256:TYR:CE1  | 3:D:260:ILE:CD1  | 2.71                     | 0.71              |
| 1:A:151:LEU:HD11 | 2:B:285:ARG:HG3  | 1.73                     | 0.71              |
| 1:A:126:TRP:CH2  | 1:A:196:ILE:CD1  | 2.74                     | 0.71              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CD2  | 2.74                     | 0.71              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:HD1  | 2.03                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:402:ILE:HD11 | 2:B:449:ILE:HD11 | 1.72                     | 0.71              |
| 1:A:130:SER:CB   | 2:B:322:HIS:ND1  | 2.53                     | 0.71              |
| 2:B:184:ILE:HD13 | 2:B:217:GLU:CD   | 2.14                     | 0.71              |
| 3:C:275:PHE:HB2  | 3:C:284:ILE:HD11 | 1.73                     | 0.71              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:HB2  | 2.20                     | 0.71              |
| 3:D:234:ILE:HD13 | 3:D:270:PRO:HB2  | 1.72                     | 0.71              |
| 1:A:352:ILE:HG22 | 1:A:572:ILE:HD13 | 1.72                     | 0.71              |
| 1:A:136:GLN:CD   | 2:B:323:GLY:HA2  | 2.16                     | 0.71              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CD2  | 2.74                     | 0.71              |
| 1:A:363:ILE:HD11 | 1:A:413:TYR:CG   | 2.25                     | 0.71              |
| 2:B:188:VAL:HG13 | 2:B:224:ILE:CD1  | 2.15                     | 0.70              |
| 1:A:566:ILE:HD13 | 1:A:571:ASN:HA   | 1.73                     | 0.70              |
| 1:A:425:ILE:HD13 | 1:A:482:LEU:HD13 | 1.73                     | 0.70              |
| 2:B:342:TYR:OH   | 2:B:394:ILE:HD12 | 1.90                     | 0.70              |
| 2:B:586:ILE:HD12 | 2:B:735:ILE:HD12 | 1.70                     | 0.70              |
| 1:A:154:LEU:HD23 | 2:B:281:LYS:HE3  | 1.71                     | 0.70              |
| 1:A:70:LEU:HD22  | 2:B:216:PHE:O    | 1.92                     | 0.70              |
| 1:A:585:ILE:HD11 | 1:A:683:ILE:HD11 | 1.71                     | 0.70              |
| 1:A:365:THR:HG23 | 1:A:404:ILE:HD11 | 1.69                     | 0.70              |
| 3:C:67:ILE:CD1   | 3:C:123:ILE:HG23 | 2.21                     | 0.70              |
| 2:B:257:ILE:CD1  | 2:B:297:TYR:OH   | 2.39                     | 0.70              |
| 1:A:68:ILE:HD13  | 2:B:216:PHE:CD2  | 2.18                     | 0.70              |
| 1:A:155:VAL:HG23 | 2:B:281:LYS:HD3  | 1.73                     | 0.70              |
| 1:A:159:GLU:OE1  | 2:B:277:VAL:HG11 | 1.92                     | 0.70              |
| 2:B:634:ILE:HD13 | 2:B:776:TYR:CE1  | 2.23                     | 0.70              |
| 1:A:142:ILE:HD11 | 1:A:188:LEU:HD12 | 1.73                     | 0.70              |
| 2:B:570:LEU:CD1  | 2:B:721:ILE:CD1  | 2.70                     | 0.70              |
| 1:A:155:VAL:HG11 | 2:B:281:LYS:HG2  | 1.73                     | 0.70              |
| 1:A:625:ILE:CD1  | 1:A:764:LEU:HB2  | 2.22                     | 0.70              |
| 1:A:255:ILE:CD1  | 1:A:272:LEU:HD22 | 2.10                     | 0.70              |
| 2:B:823:LEU:HD13 | 2:B:823:LEU:C    | 2.16                     | 0.70              |
| 3:C:67:ILE:CD1   | 3:C:123:ILE:HG23 | 2.20                     | 0.70              |
| 1:A:114:LYS:CE   | 1:A:118:ILE:HD11 | 2.21                     | 0.70              |
| 1:A:425:ILE:CD1  | 1:A:478:MET:HG3  | 2.21                     | 0.70              |
| 2:B:636:ILE:CD1  | 3:D:437:TYR:CZ   | 2.72                     | 0.70              |
| 2:B:380:HIS:CE1  | 2:B:573:ASN:HA   | 2.27                     | 0.70              |
| 1:A:71:GLU:H     | 2:B:216:PHE:HB3  | 1.56                     | 0.70              |
| 3:D:256:TYR:CD1  | 3:D:260:ILE:HD12 | 2.27                     | 0.70              |
| 1:A:780:ILE:HD13 | 1:A:789:GLU:CD   | 2.16                     | 0.70              |
| 3:D:139:LEU:HD22 | 3:D:235:ILE:CD1  | 2.21                     | 0.70              |
| 1:A:362:GLN:NE2  | 2:B:447:GLU:OE2  | 2.25                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:595:HIS:ND1  | 1:A:640:ILE:CD1  | 2.55                     | 0.70              |
| 1:A:425:ILE:HD11 | 1:A:482:LEU:HD22 | 1.73                     | 0.70              |
| 2:B:412:LEU:CD2  | 2:B:463:ILE:CD1  | 2.69                     | 0.70              |
| 1:A:570:LEU:CD2  | 1:A:573:ILE:HD12 | 2.17                     | 0.70              |
| 3:C:125:LYS:HD3  | 3:D:283:ASP:CG   | 2.17                     | 0.70              |
| 2:B:610:ILE:HD13 | 3:D:196:GLU:O    | 1.86                     | 0.70              |
| 1:A:74:TYR:HB2   | 2:B:215:ASN:ND2  | 2.07                     | 0.69              |
| 2:B:209:ILE:HD11 | 2:B:222:HIS:HE2  | 1.57                     | 0.69              |
| 1:A:296:TYR:OH   | 2:B:322:HIS:NE2  | 1.92                     | 0.69              |
| 2:B:434:GLN:HE21 | 2:B:448:ILE:HD12 | 1.56                     | 0.69              |
| 3:D:188:ILE:HD13 | 3:D:394:PHE:CD2  | 2.27                     | 0.69              |
| 1:A:140:TYR:HD2  | 2:B:324:ASP:OD1  | 1.58                     | 0.69              |
| 1:A:142:ILE:HD12 | 1:A:193:TYR:OH   | 1.92                     | 0.69              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:CD1  | 2.69                     | 0.69              |
| 3:C:292:TYR:OH   | 3:C:323:ILE:HD13 | 1.92                     | 0.69              |
| 1:A:72:GLY:HA2   | 2:B:215:ASN:O    | 1.92                     | 0.69              |
| 1:A:296:TYR:OH   | 2:B:322:HIS:CG   | 2.43                     | 0.69              |
| 1:A:150:TYR:CD1  | 1:A:177:ILE:CD1  | 2.75                     | 0.69              |
| 2:B:188:VAL:HG11 | 2:B:224:ILE:HD13 | 1.74                     | 0.69              |
| 1:A:70:LEU:CD1   | 2:B:216:PHE:CE1  | 2.73                     | 0.69              |
| 2:B:349:TRP:CH2  | 2:B:383:ILE:CD1  | 2.75                     | 0.69              |
| 1:A:365:THR:CG2  | 1:A:404:ILE:HD12 | 2.18                     | 0.69              |
| 2:B:430:HIS:HB3  | 2:B:448:ILE:HD12 | 1.72                     | 0.69              |
| 2:B:493:ILE:HD11 | 2:B:598:TYR:HB2  | 1.75                     | 0.69              |
| 2:B:636:ILE:CD1  | 3:D:351:ALA:HB2  | 2.23                     | 0.69              |
| 2:B:586:ILE:HD13 | 2:B:732:LEU:CD2  | 2.22                     | 0.69              |
| 1:A:68:ILE:O     | 2:B:216:PHE:CD2  | 2.46                     | 0.69              |
| 1:A:629:THR:HG21 | 1:A:710:ILE:CD1  | 2.22                     | 0.69              |
| 2:B:656:ILE:HD13 | 2:B:738:HIS:HB2  | 1.74                     | 0.69              |
| 1:A:367:PRO:HB3  | 1:A:404:ILE:HD11 | 1.73                     | 0.69              |
| 1:A:66:VAL:HG21  | 1:A:94:ILE:CD1   | 2.19                     | 0.69              |
| 3:D:200:ALA:CB   | 3:D:260:ILE:HD11 | 2.19                     | 0.69              |
| 2:B:402:ILE:CD1  | 2:B:449:ILE:CD1  | 2.60                     | 0.69              |
| 3:D:289:HIS:HE1  | 3:D:323:ILE:HD13 | 1.58                     | 0.69              |
| 3:C:21:LEU:HD22  | 3:C:235:ILE:HD11 | 1.75                     | 0.69              |
| 1:A:357:VAL:CG2  | 1:A:363:ILE:HD12 | 2.23                     | 0.69              |
| 2:B:634:ILE:HD12 | 2:B:809:LEU:CG   | 2.23                     | 0.69              |
| 2:B:412:LEU:HG   | 2:B:463:ILE:CD1  | 2.23                     | 0.69              |
| 2:B:533:ARG:O    | 2:B:538:ILE:CD1  | 2.41                     | 0.69              |
| 3:D:234:ILE:HD13 | 3:D:270:PRO:CB   | 2.23                     | 0.69              |
| 2:B:293:ARG:HD3  | 2:B:330:ILE:HD12 | 1.74                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:195:ILE:CD1  | 3:C:430:VAL:CG1  | 2.70                     | 0.69              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:HB3  | 1.68                     | 0.69              |
| 1:A:73:THR:HG23  | 2:B:215:ASN:ND2  | 2.05                     | 0.69              |
| 1:A:595:HIS:ND1  | 1:A:640:ILE:HD11 | 2.08                     | 0.69              |
| 2:B:402:ILE:CD1  | 2:B:449:ILE:CD1  | 2.71                     | 0.69              |
| 1:A:584:ILE:CD1  | 1:A:687:ARG:NE   | 2.55                     | 0.69              |
| 1:A:602:THR:HG23 | 1:A:710:ILE:HD12 | 1.74                     | 0.69              |
| 2:B:264:TYR:CZ   | 2:B:287:ILE:HD13 | 2.27                     | 0.69              |
| 1:A:599:LEU:HD11 | 1:A:640:ILE:HD12 | 1.75                     | 0.69              |
| 2:B:364:ILE:HD13 | 2:B:403:PHE:HD1  | 1.57                     | 0.69              |
| 2:B:398:LEU:HD11 | 2:B:449:ILE:HD12 | 1.74                     | 0.69              |
| 3:C:256:TYR:CE1  | 3:C:260:ILE:HD12 | 2.28                     | 0.68              |
| 3:D:127:ILE:CD1  | 3:D:162:TYR:OH   | 2.41                     | 0.68              |
| 1:A:109:ILE:HG22 | 1:A:177:ILE:HD11 | 1.75                     | 0.68              |
| 2:B:296:ILE:HD12 | 2:B:327:ILE:HG12 | 1.72                     | 0.68              |
| 2:B:188:VAL:CG1  | 2:B:224:ILE:HD13 | 2.22                     | 0.68              |
| 2:B:296:ILE:HG21 | 2:B:327:ILE:HD13 | 1.74                     | 0.68              |
| 2:B:296:ILE:HD13 | 2:B:327:ILE:HD11 | 1.74                     | 0.68              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:CG   | 2.29                     | 0.68              |
| 3:D:5:ILE:HD12   | 3:D:53:PHE:CE1   | 2.28                     | 0.68              |
| 1:A:154:LEU:CD2  | 2:B:281:LYS:HE3  | 2.24                     | 0.68              |
| 1:A:194:GLU:HB3  | 1:A:250:ILE:CD1  | 2.23                     | 0.68              |
| 1:A:640:ILE:CD1  | 1:A:696:GLN:NE2  | 2.47                     | 0.68              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CD2  | 2.75                     | 0.68              |
| 2:B:480:ILE:CD1  | 2:B:541:LEU:HD21 | 2.23                     | 0.68              |
| 2:B:646:SER:OG   | 3:D:356:ILE:HD12 | 1.93                     | 0.68              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CG   | 2.29                     | 0.68              |
| 2:B:284:TYR:CE1  | 2:B:291:ILE:HD13 | 2.28                     | 0.68              |
| 2:B:567:PRO:HG2  | 2:B:721:ILE:HD13 | 1.76                     | 0.68              |
| 3:C:210:LEU:HG   | 3:C:222:ILE:HD11 | 1.74                     | 0.68              |
| 3:D:256:TYR:CZ   | 3:D:260:ILE:HD12 | 2.22                     | 0.68              |
| 2:B:402:ILE:CG1  | 2:B:449:ILE:HD13 | 2.24                     | 0.68              |
| 2:B:257:ILE:HD13 | 2:B:297:TYR:CD2  | 2.29                     | 0.68              |
| 2:B:586:ILE:CG1  | 2:B:735:ILE:CD1  | 2.72                     | 0.68              |
| 1:A:136:GLN:CD   | 2:B:323:GLY:CA   | 2.66                     | 0.68              |
| 1:A:699:ILE:HD12 | 1:A:782:PHE:HZ   | 1.58                     | 0.68              |
| 2:B:412:LEU:CD1  | 2:B:463:ILE:HD12 | 2.24                     | 0.68              |
| 2:B:209:ILE:CD1  | 2:B:222:HIS:CD2  | 2.65                     | 0.68              |
| 1:A:566:ILE:CG1  | 1:A:574:ILE:HD12 | 2.21                     | 0.68              |
| 1:A:68:ILE:CD1   | 1:A:158:LEU:CD2  | 2.63                     | 0.68              |
| 1:A:148:ASP:CG   | 2:B:285:ARG:HH21 | 2.02                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:349:TRP:CH2  | 2:B:383:ILE:HD11 | 2.29                     | 0.68              |
| 2:B:296:ILE:HD13 | 2:B:327:ILE:HA   | 1.74                     | 0.68              |
| 2:B:634:ILE:HD12 | 2:B:809:LEU:HG   | 1.76                     | 0.68              |
| 3:C:193:ARG:HH12 | 3:C:419:VAL:HG13 | 1.58                     | 0.68              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:CD1  | 2.14                     | 0.67              |
| 1:A:599:LEU:HD11 | 1:A:640:ILE:HD11 | 1.75                     | 0.67              |
| 1:A:585:ILE:HD13 | 1:A:683:ILE:HG12 | 1.76                     | 0.67              |
| 3:C:129:SER:OG   | 3:D:283:ASP:CG   | 2.37                     | 0.67              |
| 1:A:641:LYS:HD2  | 3:C:356:ILE:HD12 | 1.75                     | 0.67              |
| 1:A:136:GLN:HB3  | 2:B:324:ASP:OD2  | 1.95                     | 0.67              |
| 3:C:6:ILE:CD1    | 3:C:127:ILE:CG1  | 2.72                     | 0.67              |
| 2:B:412:LEU:CG   | 2:B:463:ILE:HD12 | 2.24                     | 0.67              |
| 3:C:195:ILE:HD12 | 3:C:430:VAL:CG1  | 2.25                     | 0.67              |
| 2:B:405:ILE:HG12 | 2:B:456:ILE:HD12 | 1.77                     | 0.67              |
| 1:A:62:ASP:CG    | 1:A:94:ILE:HD13  | 2.19                     | 0.67              |
| 1:A:570:LEU:HD12 | 1:A:573:ILE:HD11 | 1.74                     | 0.67              |
| 1:A:68:ILE:HD12  | 2:B:216:PHE:HB3  | 0.67                     | 0.67              |
| 2:B:339:ILE:CD1  | 2:B:440:GLY:CA   | 2.63                     | 0.67              |
| 2:B:209:ILE:HD13 | 2:B:222:HIS:NE2  | 1.99                     | 0.67              |
| 3:D:127:ILE:CD1  | 3:D:162:TYR:CZ   | 2.77                     | 0.67              |
| 1:A:140:TYR:HH   | 2:B:292:ILE:HG22 | 1.52                     | 0.67              |
| 1:A:109:ILE:CG2  | 1:A:177:ILE:HD11 | 2.25                     | 0.67              |
| 3:C:67:ILE:CD1   | 3:C:123:ILE:CG2  | 2.73                     | 0.67              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:HD13 | 2.25                     | 0.67              |
| 3:D:127:ILE:HD12 | 3:D:161:ARG:HH12 | 1.59                     | 0.67              |
| 2:B:296:ILE:HD12 | 2:B:327:ILE:HD11 | 1.75                     | 0.67              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:CD2  | 2.24                     | 0.67              |
| 3:D:210:LEU:HD21 | 3:D:222:ILE:HD11 | 1.73                     | 0.67              |
| 3:C:199:ASP:O    | 3:C:260:ILE:HD13 | 1.94                     | 0.67              |
| 2:B:412:LEU:HG   | 2:B:463:ILE:HD13 | 1.77                     | 0.67              |
| 1:A:640:ILE:CD1  | 1:A:699:ILE:CD1  | 2.73                     | 0.67              |
| 2:B:380:HIS:HE1  | 2:B:573:ASN:HA   | 1.60                     | 0.67              |
| 2:B:394:ILE:HD11 | 2:B:445:PHE:CE2  | 2.28                     | 0.67              |
| 2:B:777:CYS:O    | 2:B:780:ASN:O    | 2.13                     | 0.67              |
| 1:A:73:THR:HG22  | 2:B:215:ASN:HD22 | 1.58                     | 0.67              |
| 1:A:133:MET:HE1  | 2:B:328:ARG:NH2  | 1.82                     | 0.67              |
| 1:A:143:ARG:NH1  | 2:B:292:ILE:CD1  | 2.57                     | 0.67              |
| 2:B:586:ILE:HD11 | 2:B:732:LEU:HD23 | 1.77                     | 0.67              |
| 1:A:75:ILE:HD12  | 2:B:216:PHE:CE1  | 2.29                     | 0.67              |
| 3:C:212:ILE:HD11 | 3:C:301:PRO:HA   | 1.75                     | 0.67              |
| 1:A:70:LEU:N     | 2:B:216:PHE:CD1  | 2.62                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:363:ILE:CD1  | 1:A:413:TYR:CB   | 2.69                     | 0.67              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:CD1  | 2.24                     | 0.67              |
| 1:A:143:ARG:CZ   | 2:B:292:ILE:HD13 | 2.25                     | 0.67              |
| 2:B:364:ILE:HD13 | 2:B:403:PHE:HA   | 1.76                     | 0.67              |
| 2:B:407:LYS:HZ3  | 2:B:721:ILE:HD12 | 1.60                     | 0.67              |
| 2:B:335:PHE:CZ   | 2:B:339:ILE:CD1  | 2.59                     | 0.67              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:HD11 | 1.75                     | 0.67              |
| 2:B:241:PHE:CB   | 2:B:254:ILE:HD11 | 2.24                     | 0.66              |
| 2:B:480:ILE:HD11 | 2:B:520:VAL:HG13 | 1.77                     | 0.66              |
| 1:A:65:ASN:ND2   | 2:B:215:ASN:HB2  | 2.04                     | 0.66              |
| 1:A:566:ILE:HD11 | 1:A:571:ASN:HB3  | 1.77                     | 0.66              |
| 2:B:610:ILE:HD11 | 3:D:196:GLU:O    | 1.95                     | 0.66              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CD2  | 2.78                     | 0.66              |
| 2:B:634:ILE:HD11 | 2:B:772:PHE:CE1  | 2.28                     | 0.66              |
| 2:B:402:ILE:CG1  | 2:B:449:ILE:HD13 | 2.26                     | 0.66              |
| 2:B:296:ILE:HD13 | 2:B:327:ILE:CD1  | 2.24                     | 0.66              |
| 1:A:362:GLN:NE2  | 2:B:447:GLU:CD   | 2.52                     | 0.66              |
| 3:D:127:ILE:HD12 | 3:D:162:TYR:OH   | 1.94                     | 0.66              |
| 3:D:36:LEU:HD22  | 3:D:36:LEU:H     | 1.61                     | 0.66              |
| 1:A:641:LYS:HD3  | 3:C:356:ILE:HD12 | 1.75                     | 0.66              |
| 1:A:607:ASN:HA   | 1:A:630:ARG:HH22 | 1.60                     | 0.66              |
| 1:A:641:LYS:HB3  | 3:C:356:ILE:HD11 | 1.76                     | 0.66              |
| 3:D:5:ILE:HD12   | 3:D:53:PHE:CE1   | 2.30                     | 0.66              |
| 2:B:364:ILE:CD1  | 2:B:403:PHE:HA   | 2.25                     | 0.66              |
| 1:A:142:ILE:HD12 | 1:A:193:TYR:CZ   | 2.30                     | 0.66              |
| 2:B:207:ILE:HD13 | 2:B:221:LEU:HD23 | 1.78                     | 0.66              |
| 2:B:264:TYR:CE1  | 2:B:287:ILE:HD11 | 2.30                     | 0.66              |
| 3:D:210:LEU:HD21 | 3:D:222:ILE:CD1  | 2.26                     | 0.66              |
| 2:B:209:ILE:HD12 | 2:B:222:HIS:CE1  | 2.28                     | 0.66              |
| 2:B:349:TRP:CD1  | 2:B:364:ILE:HD12 | 2.29                     | 0.66              |
| 1:A:154:LEU:HD21 | 1:A:177:ILE:CD1  | 2.10                     | 0.66              |
| 1:A:70:LEU:HD12  | 2:B:216:PHE:CE1  | 2.30                     | 0.66              |
| 1:A:135:LEU:CD1  | 1:A:247:ILE:HD11 | 2.26                     | 0.66              |
| 2:B:412:LEU:HD22 | 2:B:463:ILE:HD11 | 1.76                     | 0.66              |
| 2:B:412:LEU:CD2  | 2:B:463:ILE:HD12 | 2.25                     | 0.66              |
| 2:B:349:TRP:CD2  | 2:B:364:ILE:CD1  | 2.78                     | 0.66              |
| 2:B:739:LYS:HD2  | 2:B:743:THR:O    | 1.95                     | 0.66              |
| 3:C:188:ILE:HD11 | 3:C:394:PHE:HA   | 1.76                     | 0.66              |
| 1:A:566:ILE:CD1  | 1:A:574:ILE:CD1  | 2.50                     | 0.66              |
| 3:C:5:ILE:CD1    | 3:C:252:MET:HG3  | 2.25                     | 0.66              |
| 2:B:512:LEU:HD23 | 2:B:558:PHE:CD2  | 2.31                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:127:ILE:HD13 | 3:C:162:TYR:OH   | 1.96                     | 0.66              |
| 2:B:636:ILE:CD1  | 3:D:437:TYR:CE1  | 2.79                     | 0.66              |
| 2:B:296:ILE:HD11 | 2:B:327:ILE:HG12 | 1.76                     | 0.66              |
| 2:B:586:ILE:HD13 | 2:B:736:LEU:HD13 | 1.75                     | 0.66              |
| 3:D:284:ILE:HD11 | 3:D:287:LYS:HA   | 1.78                     | 0.66              |
| 3:C:229:GLN:OE1  | 3:C:280:ILE:HD11 | 1.96                     | 0.66              |
| 3:D:139:LEU:HD21 | 3:D:235:ILE:HD13 | 1.77                     | 0.66              |
| 2:B:482:LEU:CD2  | 2:B:735:ILE:HD12 | 2.24                     | 0.65              |
| 2:B:586:ILE:HD11 | 2:B:732:LEU:CD2  | 2.26                     | 0.65              |
| 1:A:148:ASP:OD1  | 2:B:285:ARG:NH2  | 2.29                     | 0.65              |
| 1:A:702:ILE:HD11 | 1:A:767:TYR:CD2  | 2.31                     | 0.65              |
| 3:D:258:THR:CG2  | 3:D:356:ILE:CD1  | 2.70                     | 0.65              |
| 1:A:68:ILE:HG13  | 2:B:281:LYS:HZ3  | 1.62                     | 0.65              |
| 1:A:599:LEU:HD11 | 1:A:640:ILE:HD12 | 1.78                     | 0.65              |
| 1:A:641:LYS:CG   | 3:C:356:ILE:HD13 | 2.26                     | 0.65              |
| 1:A:706:PHE:HE2  | 1:A:768:ILE:HD11 | 1.61                     | 0.65              |
| 3:D:200:ALA:CB   | 3:D:260:ILE:CD1  | 2.75                     | 0.65              |
| 1:A:72:GLY:HA3   | 2:B:222:HIS:HE1  | 1.58                     | 0.65              |
| 3:C:131:ASP:OD1  | 3:D:284:ILE:HD12 | 1.96                     | 0.65              |
| 1:A:625:ILE:HD11 | 1:A:765:ILE:HD11 | 1.79                     | 0.65              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:CD2  | 2.31                     | 0.65              |
| 2:B:206:GLN:HE21 | 2:B:209:ILE:CD1  | 2.09                     | 0.65              |
| 2:B:402:ILE:CG1  | 2:B:449:ILE:CD1  | 2.72                     | 0.65              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:CD1  | 2.31                     | 0.65              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:CD1  | 2.31                     | 0.65              |
| 2:B:825:ILE:CD1  | 2:B:841:LEU:HD11 | 2.22                     | 0.65              |
| 2:B:405:ILE:CG2  | 2:B:456:ILE:CD1  | 2.59                     | 0.65              |
| 2:B:527:HIS:HA   | 2:B:538:ILE:HD13 | 1.77                     | 0.65              |
| 1:A:129:THR:N    | 2:B:322:HIS:CE1  | 2.65                     | 0.65              |
| 1:A:136:GLN:HE21 | 2:B:296:ILE:CD1  | 2.10                     | 0.65              |
| 3:D:5:ILE:HD12   | 3:D:53:PHE:CZ    | 2.32                     | 0.65              |
| 3:D:256:TYR:CE1  | 3:D:260:ILE:CD1  | 2.79                     | 0.65              |
| 1:A:71:GLU:CA    | 2:B:216:PHE:CE2  | 2.79                     | 0.65              |
| 1:A:129:THR:N    | 2:B:322:HIS:HE1  | 1.94                     | 0.65              |
| 1:A:151:LEU:HD21 | 2:B:285:ARG:HG2  | 1.77                     | 0.65              |
| 1:A:68:ILE:CG1   | 2:B:281:LYS:HD2  | 2.27                     | 0.65              |
| 1:A:137:ARG:HH21 | 2:B:325:LEU:CD1  | 2.08                     | 0.65              |
| 3:C:328:PRO:HD2  | 3:C:331:ILE:HD12 | 1.78                     | 0.65              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:HD13 | 2.27                     | 0.65              |
| 3:D:123:ILE:HG22 | 3:D:127:ILE:HD12 | 1.78                     | 0.65              |
| 1:A:255:ILE:CD1  | 1:A:272:LEU:CD2  | 2.67                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:585:ILE:CD1  | 1:A:683:ILE:HG12 | 2.09                     | 0.65              |
| 2:B:339:ILE:HD13 | 2:B:439:ARG:HG3  | 1.79                     | 0.65              |
| 1:A:137:ARG:NH2  | 2:B:325:LEU:CD1  | 2.58                     | 0.65              |
| 1:A:68:ILE:HD12  | 2:B:216:PHE:CG   | 2.31                     | 0.65              |
| 3:C:67:ILE:HD12  | 3:C:123:ILE:HG23 | 1.79                     | 0.65              |
| 1:A:65:ASN:OD1   | 2:B:215:ASN:ND2  | 2.30                     | 0.65              |
| 1:A:155:VAL:HG11 | 2:B:285:ARG:NH2  | 2.12                     | 0.65              |
| 1:A:584:ILE:CD1  | 1:A:687:ARG:CG   | 2.72                     | 0.65              |
| 2:B:412:LEU:HD13 | 2:B:463:ILE:CD1  | 2.26                     | 0.65              |
| 3:C:188:ILE:HD11 | 3:C:394:PHE:HB3  | 1.79                     | 0.65              |
| 1:A:154:LEU:CD2  | 2:B:281:LYS:NZ   | 2.55                     | 0.65              |
| 1:A:641:LYS:HG2  | 3:C:356:ILE:HD11 | 1.79                     | 0.65              |
| 1:A:102:PHE:HB3  | 1:A:170:ILE:CD1  | 2.26                     | 0.64              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:CB   | 2.19                     | 0.64              |
| 2:B:405:ILE:HG12 | 2:B:456:ILE:CD1  | 2.27                     | 0.64              |
| 1:A:68:ILE:O     | 2:B:281:LYS:CE   | 2.44                     | 0.64              |
| 1:A:606:LEU:HG   | 1:A:710:ILE:CD1  | 2.27                     | 0.64              |
| 1:A:127:SER:HB3  | 2:B:299:ARG:HH12 | 1.62                     | 0.64              |
| 2:B:656:ILE:HD11 | 2:B:738:HIS:CE1  | 2.30                     | 0.64              |
| 3:D:210:LEU:CD1  | 3:D:222:ILE:CD1  | 2.75                     | 0.64              |
| 2:B:586:ILE:HD13 | 2:B:735:ILE:HD12 | 1.79                     | 0.64              |
| 1:A:699:ILE:HD12 | 1:A:782:PHE:CZ   | 2.32                     | 0.64              |
| 1:A:632:LEU:CD2  | 1:A:768:ILE:HD12 | 2.27                     | 0.64              |
| 3:D:256:TYR:CD1  | 3:D:260:ILE:CD1  | 2.80                     | 0.64              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CG   | 2.32                     | 0.64              |
| 3:C:127:ILE:HD13 | 3:C:162:TYR:HE2  | 1.62                     | 0.64              |
| 1:A:64:LEU:HG    | 2:B:216:PHE:HE2  | 1.63                     | 0.64              |
| 3:D:200:ALA:HB2  | 3:D:260:ILE:CD1  | 2.27                     | 0.64              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:CB   | 2.74                     | 0.64              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CD1  | 2.32                     | 0.64              |
| 2:B:634:ILE:HD12 | 2:B:809:LEU:HD23 | 1.77                     | 0.64              |
| 2:B:398:LEU:CD1  | 2:B:449:ILE:HD12 | 2.27                     | 0.64              |
| 1:A:573:ILE:CD1  | 1:A:673:GLN:CB   | 2.51                     | 0.64              |
| 2:B:402:ILE:HG12 | 2:B:449:ILE:CD1  | 2.25                     | 0.64              |
| 1:A:151:LEU:HD13 | 2:B:285:ARG:HG3  | 1.80                     | 0.64              |
| 2:B:188:VAL:HB   | 2:B:224:ILE:HD12 | 1.79                     | 0.64              |
| 1:A:152:LYS:HD2  | 2:B:285:ARG:NH1  | 2.06                     | 0.64              |
| 1:A:623:ARG:NH2  | 1:A:761:ILE:HD11 | 2.11                     | 0.64              |
| 2:B:398:LEU:HD11 | 2:B:449:ILE:HD12 | 1.77                     | 0.64              |
| 1:A:195:GLU:CD   | 1:A:250:ILE:HD11 | 2.21                     | 0.64              |
| 3:D:306:VAL:HG23 | 3:D:382:THR:HG21 | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:209:ILE:HD13 | 2:B:222:HIS:CE1  | 2.33                     | 0.64              |
| 2:B:405:ILE:CB   | 2:B:456:ILE:HD13 | 2.28                     | 0.64              |
| 2:B:257:ILE:HD13 | 2:B:297:TYR:OH   | 1.97                     | 0.64              |
| 1:A:152:LYS:CG   | 2:B:285:ARG:NH1  | 2.32                     | 0.64              |
| 1:A:558:TYR:CD1  | 1:A:693:ILE:CD1  | 2.80                     | 0.64              |
| 3:C:21:LEU:HD11  | 3:C:235:ILE:HD13 | 1.80                     | 0.64              |
| 1:A:66:VAL:HG11  | 1:A:94:ILE:CD1   | 2.28                     | 0.64              |
| 1:A:66:VAL:HG23  | 1:A:94:ILE:HD13  | 1.80                     | 0.63              |
| 1:A:606:LEU:HD22 | 1:A:710:ILE:HD11 | 1.79                     | 0.63              |
| 2:B:418:GLU:OE2  | 2:B:463:ILE:CD1  | 2.39                     | 0.63              |
| 2:B:349:TRP:CD1  | 2:B:364:ILE:CD1  | 2.80                     | 0.63              |
| 2:B:184:ILE:HD13 | 2:B:217:GLU:OE1  | 1.98                     | 0.63              |
| 2:B:412:LEU:HD22 | 2:B:463:ILE:HD12 | 1.72                     | 0.63              |
| 1:A:570:LEU:HD23 | 1:A:573:ILE:CD1  | 2.26                     | 0.63              |
| 1:A:425:ILE:HD12 | 1:A:482:LEU:HB2  | 1.79                     | 0.63              |
| 1:A:63:LEU:CD2   | 1:A:170:ILE:HD12 | 2.29                     | 0.63              |
| 1:A:151:LEU:HD11 | 2:B:285:ARG:NE   | 2.13                     | 0.63              |
| 1:A:63:LEU:CD2   | 1:A:170:ILE:HD12 | 2.29                     | 0.63              |
| 1:A:152:LYS:CG   | 2:B:285:ARG:HD2  | 2.28                     | 0.63              |
| 1:A:706:PHE:HE2  | 1:A:768:ILE:HD12 | 1.57                     | 0.63              |
| 1:A:366:ILE:C    | 1:A:404:ILE:CD1  | 2.72                     | 0.63              |
| 2:B:209:ILE:HD13 | 2:B:213:ILE:CD1  | 2.29                     | 0.63              |
| 2:B:257:ILE:HD12 | 2:B:301:THR:OG1  | 1.98                     | 0.63              |
| 3:D:256:TYR:CE2  | 3:D:260:ILE:CD1  | 2.81                     | 0.63              |
| 1:A:599:LEU:HD22 | 1:A:640:ILE:CD1  | 2.18                     | 0.63              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CE1  | 2.81                     | 0.63              |
| 3:C:128:ASP:OD2  | 3:D:281:HIS:ND1  | 2.31                     | 0.63              |
| 2:B:412:LEU:HD22 | 2:B:463:ILE:CD1  | 2.28                     | 0.63              |
| 3:C:137:GLN:NE2  | 3:C:235:ILE:HD11 | 2.13                     | 0.63              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CB   | 2.76                     | 0.63              |
| 1:A:74:TYR:CB    | 2:B:215:ASN:CG   | 2.71                     | 0.63              |
| 1:A:155:VAL:HG12 | 2:B:281:LYS:CD   | 2.28                     | 0.63              |
| 1:A:136:GLN:HB3  | 2:B:323:GLY:HA2  | 1.79                     | 0.63              |
| 1:A:606:LEU:HD21 | 1:A:710:ILE:CD1  | 2.28                     | 0.63              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:CD1  | 2.29                     | 0.63              |
| 1:A:362:GLN:NE2  | 2:B:447:GLU:HG3  | 2.12                     | 0.63              |
| 3:C:67:ILE:HD12  | 3:C:123:ILE:HG22 | 1.80                     | 0.63              |
| 1:A:150:TYR:HD1  | 1:A:177:ILE:CD1  | 2.12                     | 0.63              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:HD22 | 2.27                     | 0.63              |
| 2:B:349:TRP:CG   | 2:B:364:ILE:HD13 | 2.33                     | 0.63              |
| 2:B:634:ILE:CD1  | 2:B:809:LEU:CD2  | 2.76                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:581:LYS:O    | 1:A:683:ILE:HD13 | 1.99                     | 0.63              |
| 1:A:366:ILE:H    | 1:A:404:ILE:CD1  | 2.11                     | 0.62              |
| 2:B:418:GLU:HB3  | 2:B:463:ILE:HD13 | 1.81                     | 0.62              |
| 1:A:140:TYR:CB   | 2:B:324:ASP:OD1  | 2.47                     | 0.62              |
| 1:A:135:LEU:CD1  | 1:A:247:ILE:HD13 | 2.29                     | 0.62              |
| 2:B:296:ILE:HD11 | 2:B:327:ILE:CB   | 2.29                     | 0.62              |
| 1:A:74:TYR:CB    | 2:B:215:ASN:ND2  | 2.62                     | 0.62              |
| 3:C:200:ALA:CB   | 3:C:260:ILE:HD11 | 2.29                     | 0.62              |
| 3:C:238:VAL:CG2  | 3:C:322:ILE:HD12 | 2.23                     | 0.62              |
| 3:C:255:ILE:HD11 | 3:C:358:ARG:CZ   | 2.29                     | 0.62              |
| 3:D:255:ILE:HD12 | 3:D:358:ARG:CD   | 2.29                     | 0.62              |
| 1:A:426:PHE:CD2  | 1:A:564:ILE:CD1  | 2.82                     | 0.62              |
| 1:A:151:LEU:HD22 | 2:B:285:ARG:CB   | 2.28                     | 0.62              |
| 1:A:133:MET:SD   | 2:B:328:ARG:NH2  | 2.72                     | 0.62              |
| 2:B:394:ILE:HD13 | 2:B:445:PHE:CD2  | 2.34                     | 0.62              |
| 1:A:137:ARG:HA   | 2:B:324:ASP:OD1  | 1.99                     | 0.62              |
| 1:A:126:TRP:CZ2  | 1:A:196:ILE:HD11 | 2.35                     | 0.62              |
| 3:D:139:LEU:HD22 | 3:D:235:ILE:HD11 | 1.80                     | 0.62              |
| 2:B:412:LEU:HD22 | 2:B:463:ILE:CD1  | 2.29                     | 0.62              |
| 1:A:74:TYR:CE2   | 2:B:216:PHE:HZ   | 2.14                     | 0.62              |
| 1:A:137:ARG:NH2  | 2:B:328:ARG:NE   | 2.47                     | 0.62              |
| 1:A:585:ILE:CD1  | 1:A:683:ILE:HD11 | 2.29                     | 0.62              |
| 2:B:335:PHE:CE2  | 2:B:339:ILE:CD1  | 2.74                     | 0.62              |
| 1:A:157:ARG:CD   | 1:A:176:ILE:HD13 | 2.29                     | 0.62              |
| 2:B:568:LEU:HD22 | 2:B:568:LEU:H    | 1.63                     | 0.62              |
| 1:A:363:ILE:HD11 | 1:A:404:ILE:CG2  | 2.29                     | 0.62              |
| 1:A:416:ILE:HD11 | 1:A:664:ARG:HG2  | 1.82                     | 0.62              |
| 1:A:66:VAL:HA    | 1:A:75:ILE:HD11  | 1.82                     | 0.62              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:HB2  | 1.78                     | 0.62              |
| 3:D:127:ILE:HD12 | 3:D:161:ARG:NH1  | 2.12                     | 0.62              |
| 1:A:66:VAL:CG2   | 1:A:94:ILE:CD1   | 2.77                     | 0.62              |
| 1:A:68:ILE:O     | 2:B:281:LYS:CD   | 2.47                     | 0.62              |
| 1:A:126:TRP:HZ2  | 1:A:196:ILE:HD11 | 1.64                     | 0.62              |
| 1:A:628:ALA:HB1  | 1:A:765:ILE:HD13 | 1.82                     | 0.62              |
| 2:B:184:ILE:HD13 | 2:B:213:ILE:CD1  | 2.30                     | 0.62              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:CD1  | 2.30                     | 0.62              |
| 2:B:191:THR:HG22 | 2:B:207:ILE:CD1  | 2.30                     | 0.62              |
| 1:A:137:ARG:HH22 | 2:B:325:LEU:HD21 | 1.61                     | 0.62              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:CZ   | 2.35                     | 0.62              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CE2  | 2.35                     | 0.62              |
| 2:B:192:LEU:HD21 | 2:B:287:ILE:CD1  | 2.29                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:772:PHE:HD1  | 2:B:812:ILE:HD12 | 1.65                     | 0.61              |
| 2:B:739:LYS:O    | 2:B:743:THR:O    | 2.19                     | 0.61              |
| 3:D:255:ILE:HD12 | 3:D:358:ARG:HD3  | 1.83                     | 0.61              |
| 3:C:175:ALA:HB3  | 3:C:178:SER:HB3  | 1.82                     | 0.61              |
| 1:A:699:ILE:CD1  | 1:A:782:PHE:CE2  | 2.81                     | 0.61              |
| 1:A:699:ILE:CD1  | 1:A:782:PHE:CZ   | 2.83                     | 0.61              |
| 2:B:210:PRO:HG2  | 2:B:213:ILE:HD13 | 1.81                     | 0.61              |
| 1:A:78:PHE:CE1   | 4:F:21:UNK:CB    | 2.83                     | 0.61              |
| 3:D:188:ILE:HD13 | 3:D:394:PHE:CG   | 2.35                     | 0.61              |
| 3:D:111:ILE:HG12 | 3:D:114:ARG:HH21 | 1.65                     | 0.61              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CD1  | 2.35                     | 0.61              |
| 1:A:65:ASN:O     | 2:B:216:PHE:CE2  | 2.53                     | 0.61              |
| 2:B:355:LEU:HD23 | 2:B:355:LEU:H    | 1.65                     | 0.61              |
| 1:A:425:ILE:HD12 | 1:A:478:MET:HB3  | 1.81                     | 0.61              |
| 1:A:296:TYR:OH   | 2:B:322:HIS:CE1  | 2.53                     | 0.61              |
| 2:B:412:LEU:HD13 | 2:B:463:ILE:HD13 | 1.82                     | 0.61              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:CD1  | 2.70                     | 0.61              |
| 1:A:365:THR:HA   | 1:A:404:ILE:HD11 | 1.81                     | 0.61              |
| 1:A:68:ILE:HD11  | 2:B:216:PHE:HD1  | 1.64                     | 0.61              |
| 1:A:624:ARG:H    | 1:A:624:ARG:HE   | 1.48                     | 0.61              |
| 3:C:6:ILE:CD1    | 3:C:126:GLU:HG3  | 2.30                     | 0.61              |
| 2:B:383:ILE:CD1  | 2:B:410:ILE:HG21 | 2.31                     | 0.61              |
| 2:B:284:TYR:CE1  | 2:B:291:ILE:HD13 | 2.36                     | 0.61              |
| 1:A:599:LEU:HD11 | 1:A:640:ILE:CD1  | 2.31                     | 0.61              |
| 1:A:588:TYR:HD1  | 1:A:693:ILE:CD1  | 2.14                     | 0.61              |
| 1:A:558:TYR:CD1  | 1:A:693:ILE:HD13 | 2.35                     | 0.61              |
| 1:A:128:ASP:OD2  | 2:B:295:ARG:HG2  | 2.00                     | 0.61              |
| 3:D:200:ALA:HB2  | 3:D:260:ILE:CD1  | 2.23                     | 0.61              |
| 2:B:772:PHE:HB2  | 2:B:812:ILE:HD13 | 1.82                     | 0.61              |
| 3:D:166:ILE:HD12 | 3:D:256:TYR:CD2  | 2.36                     | 0.61              |
| 3:D:127:ILE:CD1  | 3:D:162:TYR:OH   | 2.49                     | 0.61              |
| 2:B:241:PHE:CG   | 2:B:254:ILE:HD13 | 2.33                     | 0.61              |
| 1:A:73:THR:HB    | 2:B:215:ASN:HA   | 1.82                     | 0.61              |
| 1:A:375:ILE:HD13 | 1:A:396:LYS:HD2  | 1.83                     | 0.60              |
| 1:A:138:PHE:CG   | 1:A:192:ILE:CD1  | 2.80                     | 0.60              |
| 1:A:362:GLN:HB3  | 2:B:446:PHE:HE2  | 1.66                     | 0.60              |
| 1:A:570:LEU:CD2  | 1:A:573:ILE:CD1  | 2.73                     | 0.60              |
| 1:A:137:ARG:NH2  | 2:B:325:LEU:HD22 | 2.16                     | 0.60              |
| 1:A:148:ASP:OD1  | 2:B:285:ARG:NE   | 2.34                     | 0.60              |
| 2:B:742:ALA:HB1  | 2:B:743:THR:HG23 | 1.82                     | 0.60              |
| 1:A:353:LEU:HD13 | 1:A:572:ILE:HD13 | 1.81                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:195:ILE:HD12 | 3:D:423:PHE:HE1  | 1.66                     | 0.60              |
| 2:B:296:ILE:HD11 | 2:B:327:ILE:CD1  | 2.31                     | 0.60              |
| 2:B:634:ILE:HD13 | 2:B:772:PHE:CZ   | 2.36                     | 0.60              |
| 1:A:151:LEU:HG   | 2:B:285:ARG:HG2  | 1.82                     | 0.60              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:HD11 | 1.83                     | 0.60              |
| 1:A:567:PRO:CD   | 1:A:574:ILE:CD1  | 2.77                     | 0.60              |
| 2:B:346:LEU:HD13 | 2:B:402:ILE:HD13 | 1.82                     | 0.60              |
| 2:B:366:GLU:OE1  | 2:B:381:ILE:HD13 | 2.00                     | 0.60              |
| 1:A:641:LYS:HD2  | 3:C:356:ILE:HD13 | 1.82                     | 0.60              |
| 3:D:139:LEU:CD2  | 3:D:235:ILE:HD13 | 2.31                     | 0.60              |
| 2:B:209:ILE:CD1  | 2:B:222:HIS:CE1  | 2.84                     | 0.60              |
| 2:B:383:ILE:CD1  | 2:B:410:ILE:HD11 | 2.31                     | 0.60              |
| 1:A:641:LYS:CG   | 3:C:356:ILE:CD1  | 2.78                     | 0.60              |
| 1:A:65:ASN:CG    | 2:B:215:ASN:ND2  | 2.60                     | 0.60              |
| 2:B:482:LEU:HD22 | 2:B:657:ILE:HG21 | 1.83                     | 0.60              |
| 1:A:142:ILE:CD1  | 1:A:189:LEU:HD21 | 2.31                     | 0.60              |
| 3:C:131:ASP:CG   | 3:D:284:ILE:HD12 | 2.27                     | 0.60              |
| 1:A:426:PHE:CD2  | 1:A:564:ILE:HD13 | 2.35                     | 0.60              |
| 1:A:66:VAL:HG11  | 1:A:94:ILE:HD11  | 1.83                     | 0.60              |
| 1:A:147:GLU:HB2  | 2:B:285:ARG:HD3  | 1.83                     | 0.60              |
| 3:C:6:ILE:CD1    | 3:C:127:ILE:CG2  | 2.80                     | 0.60              |
| 3:C:70:ASP:CG    | 3:C:71:SER:H     | 2.09                     | 0.60              |
| 2:B:242:ARG:N    | 2:B:254:ILE:CD1  | 2.64                     | 0.60              |
| 2:B:480:ILE:CD1  | 2:B:537:VAL:HG21 | 2.31                     | 0.60              |
| 1:A:366:ILE:HG12 | 1:A:368:SER:H    | 1.67                     | 0.60              |
| 1:A:68:ILE:HG12  | 2:B:281:LYS:HD2  | 1.84                     | 0.60              |
| 2:B:634:ILE:HG21 | 2:B:809:LEU:HD21 | 1.84                     | 0.60              |
| 2:B:224:ILE:HD13 | 2:B:280:LEU:CD1  | 2.30                     | 0.60              |
| 2:B:728:HIS:CE1  | 2:B:732:LEU:HD11 | 2.35                     | 0.60              |
| 1:A:137:ARG:HH21 | 2:B:328:ARG:NE   | 1.95                     | 0.60              |
| 2:B:772:PHE:HD1  | 2:B:812:ILE:CD1  | 2.15                     | 0.60              |
| 1:A:138:PHE:CE2  | 1:A:275:ILE:HD13 | 2.36                     | 0.60              |
| 2:B:668:LEU:O    | 2:B:671:THR:O    | 2.19                     | 0.60              |
| 3:D:255:ILE:HD13 | 3:D:358:ARG:CZ   | 2.32                     | 0.60              |
| 3:C:255:ILE:HD11 | 3:C:358:ARG:CZ   | 2.31                     | 0.60              |
| 1:A:606:LEU:HD22 | 1:A:710:ILE:HD12 | 1.82                     | 0.60              |
| 1:A:65:ASN:CG    | 2:B:215:ASN:CB   | 2.70                     | 0.60              |
| 2:B:296:ILE:HD13 | 2:B:327:ILE:HD12 | 1.84                     | 0.60              |
| 2:B:289:GLU:CD   | 2:B:289:GLU:H    | 2.10                     | 0.60              |
| 1:A:74:TYR:HB2   | 2:B:215:ASN:HD21 | 1.66                     | 0.59              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:HB2  | 2.31                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:590:LEU:HD22 | 2:B:657:ILE:HD13 | 1.83                     | 0.59              |
| 2:B:349:TRP:CG   | 2:B:364:ILE:HD12 | 2.37                     | 0.59              |
| 1:A:129:THR:H    | 2:B:322:HIS:HE1  | 1.48                     | 0.59              |
| 1:A:152:LYS:HA   | 2:B:285:ARG:CZ   | 2.31                     | 0.59              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CD2  | 2.85                     | 0.59              |
| 1:A:599:LEU:HD11 | 1:A:640:ILE:CD1  | 2.32                     | 0.59              |
| 1:A:558:TYR:CB   | 1:A:693:ILE:CD1  | 2.75                     | 0.59              |
| 1:A:774:ILE:HD13 | 1:A:796:SER:HB3  | 1.81                     | 0.59              |
| 3:D:139:LEU:HD22 | 3:D:235:ILE:HD11 | 1.82                     | 0.59              |
| 1:A:137:ARG:HH22 | 2:B:328:ARG:CZ   | 2.15                     | 0.59              |
| 2:B:296:ILE:HD13 | 2:B:327:ILE:HD13 | 1.84                     | 0.59              |
| 2:B:418:GLU:HG3  | 2:B:463:ILE:HD12 | 1.83                     | 0.59              |
| 1:A:357:VAL:CB   | 1:A:363:ILE:HD12 | 2.29                     | 0.59              |
| 1:A:140:TYR:CE1  | 2:B:292:ILE:HG21 | 2.35                     | 0.59              |
| 1:A:599:LEU:CD2  | 1:A:640:ILE:HD12 | 2.32                     | 0.59              |
| 1:A:65:ASN:HB2   | 1:A:94:ILE:HD11  | 1.84                     | 0.59              |
| 3:C:188:ILE:HD13 | 3:C:394:PHE:CB   | 2.32                     | 0.59              |
| 2:B:349:TRP:CH2  | 2:B:383:ILE:HD13 | 2.37                     | 0.59              |
| 2:B:398:LEU:CD1  | 2:B:449:ILE:HD12 | 2.27                     | 0.59              |
| 1:A:138:PHE:CE1  | 1:A:275:ILE:CD1  | 2.73                     | 0.59              |
| 2:B:386:ASN:HD21 | 2:B:389:ARG:H    | 1.51                     | 0.59              |
| 1:A:71:GLU:HA    | 2:B:216:PHE:CZ   | 2.37                     | 0.59              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:HB2  | 1.83                     | 0.59              |
| 3:D:200:ALA:HB2  | 3:D:260:ILE:HD12 | 1.84                     | 0.59              |
| 1:A:641:LYS:CB   | 3:C:356:ILE:HD12 | 2.31                     | 0.59              |
| 1:A:109:ILE:HD11 | 1:A:170:ILE:HD11 | 1.83                     | 0.59              |
| 1:A:151:LEU:HD11 | 2:B:285:ARG:CD   | 2.32                     | 0.59              |
| 1:A:143:ARG:NH2  | 2:B:288:TYR:OH   | 2.36                     | 0.59              |
| 2:B:493:ILE:CD1  | 2:B:598:TYR:CB   | 2.81                     | 0.59              |
| 1:A:566:ILE:HD12 | 1:A:574:ILE:HB   | 1.83                     | 0.59              |
| 3:D:210:LEU:HD11 | 3:D:222:ILE:HD11 | 1.83                     | 0.59              |
| 2:B:808:ASN:HD21 | 2:B:812:ILE:HD11 | 1.65                     | 0.59              |
| 2:B:398:LEU:HD23 | 2:B:449:ILE:CD1  | 2.29                     | 0.59              |
| 1:A:152:LYS:HG2  | 2:B:285:ARG:CZ   | 2.29                     | 0.59              |
| 3:C:274:PRO:HB2  | 3:C:284:ILE:HD12 | 1.84                     | 0.59              |
| 2:B:480:ILE:HD13 | 2:B:541:LEU:CD1  | 2.26                     | 0.59              |
| 3:C:289:HIS:CD2  | 3:C:335:MET:HE2  | 2.37                     | 0.59              |
| 2:B:257:ILE:HD12 | 2:B:297:TYR:CG   | 2.29                     | 0.59              |
| 2:B:743:THR:O    | 2:B:756:GLN:N    | 2.36                     | 0.59              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:HD12 | 1.85                     | 0.59              |
| 2:B:739:LYS:O    | 2:B:743:THR:O    | 2.20                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:631:LEU:O    | 2:B:634:ILE:HG12 | 2.03                     | 0.59              |
| 2:B:405:ILE:CG1  | 2:B:456:ILE:HD12 | 2.32                     | 0.58              |
| 1:A:134:VAL:HG12 | 1:A:275:ILE:HG23 | 1.85                     | 0.58              |
| 1:A:65:ASN:ND2   | 2:B:215:ASN:HD22 | 2.01                     | 0.58              |
| 2:B:643:GLN:CG   | 3:D:356:ILE:CD1  | 2.80                     | 0.58              |
| 2:B:643:GLN:HG2  | 3:D:356:ILE:HD13 | 1.84                     | 0.58              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CD1  | 2.83                     | 0.58              |
| 2:B:634:ILE:HD11 | 2:B:809:LEU:HG   | 1.84                     | 0.58              |
| 1:A:154:LEU:CD2  | 2:B:281:LYS:CE   | 2.74                     | 0.58              |
| 2:B:242:ARG:CA   | 2:B:254:ILE:HD11 | 2.32                     | 0.58              |
| 1:A:144:ARG:CD   | 2:B:289:GLU:OE2  | 2.51                     | 0.58              |
| 1:A:588:TYR:CE1  | 1:A:693:ILE:HD12 | 2.37                     | 0.58              |
| 2:B:207:ILE:HD11 | 2:B:221:LEU:HD23 | 1.84                     | 0.58              |
| 2:B:184:ILE:HD13 | 2:B:217:GLU:OE2  | 2.02                     | 0.58              |
| 1:A:63:LEU:CB    | 1:A:170:ILE:HD11 | 2.29                     | 0.58              |
| 3:C:258:THR:HG21 | 3:C:356:ILE:CD1  | 2.09                     | 0.58              |
| 3:D:200:ALA:CA   | 3:D:260:ILE:CD1  | 2.74                     | 0.58              |
| 1:A:151:LEU:CD1  | 2:B:285:ARG:HE   | 2.16                     | 0.58              |
| 1:A:71:GLU:CD    | 2:B:222:HIS:NE2  | 2.62                     | 0.58              |
| 2:B:383:ILE:HD11 | 2:B:410:ILE:CD1  | 2.31                     | 0.58              |
| 3:C:255:ILE:CD1  | 3:C:358:ARG:NH2  | 2.63                     | 0.58              |
| 2:B:284:TYR:HE1  | 2:B:291:ILE:HD13 | 1.68                     | 0.58              |
| 2:B:288:TYR:HE2  | 2:B:292:ILE:CD1  | 1.97                     | 0.58              |
| 2:B:405:ILE:HG22 | 2:B:456:ILE:HD13 | 1.83                     | 0.58              |
| 1:A:425:ILE:HD11 | 1:A:478:MET:CG   | 2.30                     | 0.58              |
| 2:B:634:ILE:CD1  | 2:B:772:PHE:CZ   | 2.81                     | 0.58              |
| 2:B:656:ILE:CD1  | 2:B:738:HIS:CG   | 2.86                     | 0.58              |
| 3:D:139:LEU:HD22 | 3:D:235:ILE:CD1  | 2.32                     | 0.58              |
| 1:A:375:ILE:CD1  | 1:A:396:LYS:HD2  | 2.33                     | 0.58              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CG   | 2.86                     | 0.58              |
| 3:D:166:ILE:HD12 | 3:D:256:TYR:CE2  | 2.39                     | 0.58              |
| 3:C:195:ILE:CD1  | 3:C:423:PHE:CE1  | 2.79                     | 0.58              |
| 2:B:739:LYS:O    | 2:B:743:THR:O    | 2.20                     | 0.58              |
| 2:B:405:ILE:CD1  | 2:B:452:GLN:CB   | 2.80                     | 0.58              |
| 1:A:606:LEU:CD1  | 1:A:710:ILE:HD11 | 2.34                     | 0.58              |
| 3:D:188:ILE:HD13 | 3:D:394:PHE:CD1  | 2.38                     | 0.58              |
| 1:A:255:ILE:CD1  | 1:A:269:LYS:HG2  | 2.34                     | 0.58              |
| 1:A:625:ILE:HD13 | 1:A:765:ILE:HG13 | 1.85                     | 0.58              |
| 3:D:284:ILE:HD11 | 3:D:371:GLU:HG2  | 1.86                     | 0.58              |
| 1:A:68:ILE:HD11  | 2:B:216:PHE:CD1  | 2.39                     | 0.58              |
| 3:C:255:ILE:HD13 | 3:C:358:ARG:NH2  | 2.17                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:493:ILE:HD12 | 2:B:598:TYR:CB   | 2.34                     | 0.58              |
| 1:A:136:GLN:HE21 | 2:B:296:ILE:HD12 | 1.69                     | 0.57              |
| 2:B:768:SER:HB3  | 2:B:812:ILE:HD13 | 1.86                     | 0.57              |
| 3:C:200:ALA:CB   | 3:C:260:ILE:CD1  | 2.71                     | 0.57              |
| 1:A:62:ASP:CG    | 1:A:94:ILE:HD13  | 2.27                     | 0.57              |
| 1:A:140:TYR:HB3  | 2:B:324:ASP:OD1  | 2.04                     | 0.57              |
| 2:B:634:ILE:HD12 | 2:B:809:LEU:HD21 | 1.85                     | 0.57              |
| 2:B:207:ILE:HD13 | 2:B:221:LEU:CD2  | 2.34                     | 0.57              |
| 1:A:136:GLN:C    | 2:B:324:ASP:OD1  | 2.48                     | 0.57              |
| 1:A:142:ILE:HD12 | 1:A:189:LEU:CD2  | 2.35                     | 0.57              |
| 3:D:200:ALA:HB2  | 3:D:260:ILE:CD1  | 2.27                     | 0.57              |
| 1:A:570:LEU:HD22 | 1:A:573:ILE:CD1  | 2.34                     | 0.57              |
| 1:A:599:LEU:CD1  | 1:A:640:ILE:CD1  | 2.82                     | 0.57              |
| 2:B:571:VAL:HG23 | 2:B:721:ILE:HD11 | 1.86                     | 0.57              |
| 2:B:567:PRO:O    | 2:B:570:LEU:HD12 | 2.04                     | 0.57              |
| 3:C:242:ILE:HD11 | 3:C:252:MET:SD   | 2.45                     | 0.57              |
| 1:A:258:ASN:HD22 | 1:A:260:GLY:H    | 1.53                     | 0.57              |
| 3:C:258:THR:OG1  | 3:C:356:ILE:CD1  | 2.51                     | 0.57              |
| 1:A:352:ILE:CG2  | 1:A:572:ILE:HD13 | 2.35                     | 0.57              |
| 2:B:634:ILE:HD11 | 2:B:776:TYR:CD2  | 2.38                     | 0.57              |
| 1:A:134:VAL:HG13 | 1:A:275:ILE:HB   | 1.86                     | 0.57              |
| 1:A:487:ASP:H    | 1:A:559:HIS:HB3  | 1.68                     | 0.57              |
| 1:A:70:LEU:C     | 2:B:216:PHE:CE2  | 2.79                     | 0.57              |
| 1:A:643:ILE:HD12 | 1:A:692:LEU:HD23 | 1.85                     | 0.57              |
| 3:C:72:GLU:H     | 3:C:73:PRO:CD    | 2.17                     | 0.57              |
| 1:A:65:ASN:HD21  | 2:B:215:ASN:HD22 | 1.49                     | 0.57              |
| 3:D:238:VAL:HG22 | 3:D:375:MET:SD   | 2.45                     | 0.57              |
| 2:B:194:ALA:HA   | 2:B:232:GLN:HG2  | 1.85                     | 0.57              |
| 1:A:150:TYR:CD1  | 1:A:177:ILE:HD11 | 2.38                     | 0.57              |
| 2:B:383:ILE:HD12 | 2:B:410:ILE:HG21 | 1.87                     | 0.57              |
| 1:A:348:LEU:HD21 | 1:A:352:ILE:HD11 | 1.86                     | 0.57              |
| 3:D:5:ILE:HD12   | 3:D:53:PHE:CZ    | 2.39                     | 0.57              |
| 1:A:365:THR:HG23 | 1:A:404:ILE:CD1  | 2.34                     | 0.57              |
| 1:A:458:TYR:CE1  | 1:A:484:ILE:HD12 | 2.36                     | 0.57              |
| 1:A:70:LEU:CG    | 2:B:281:LYS:HZ3  | 2.05                     | 0.57              |
| 1:A:135:LEU:CD1  | 1:A:247:ILE:CD1  | 2.82                     | 0.57              |
| 2:B:241:PHE:CG   | 2:B:254:ILE:CD1  | 2.87                     | 0.57              |
| 2:B:260:GLU:OE2  | 2:B:330:ILE:CD1  | 2.53                     | 0.57              |
| 2:B:772:PHE:CE1  | 2:B:812:ILE:CD1  | 2.84                     | 0.57              |
| 3:D:199:ASP:O    | 3:D:260:ILE:CD1  | 2.49                     | 0.57              |
| 1:A:75:ILE:HD12  | 2:B:216:PHE:HE1  | 1.67                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CD1  | 2.32                     | 0.57              |
| 1:A:137:ARG:NH2  | 2:B:328:ARG:CZ   | 2.68                     | 0.56              |
| 3:D:210:LEU:HD11 | 3:D:222:ILE:HD13 | 1.87                     | 0.56              |
| 1:A:66:VAL:CG2   | 1:A:94:ILE:HD13  | 2.35                     | 0.56              |
| 3:D:234:ILE:HD13 | 3:D:303:ASN:ND2  | 2.19                     | 0.56              |
| 1:A:136:GLN:HG3  | 2:B:323:GLY:O    | 2.04                     | 0.56              |
| 2:B:222:HIS:HA   | 2:B:225:PHE:CE2  | 2.40                     | 0.56              |
| 1:A:80:ASP:O     | 1:A:90:ILE:N     | 2.37                     | 0.56              |
| 2:B:335:PHE:CD1  | 2:B:339:ILE:HD11 | 2.35                     | 0.56              |
| 3:D:234:ILE:HD11 | 3:D:303:ASN:ND2  | 2.20                     | 0.56              |
| 1:A:375:ILE:HD11 | 1:A:396:LYS:CB   | 2.34                     | 0.56              |
| 1:A:72:GLY:CA    | 2:B:215:ASN:O    | 2.53                     | 0.56              |
| 1:A:137:ARG:CZ   | 2:B:325:LEU:CD1  | 2.74                     | 0.56              |
| 3:C:127:ILE:CD1  | 3:C:162:TYR:CE2  | 2.88                     | 0.56              |
| 3:D:200:ALA:CB   | 3:D:260:ILE:HD11 | 2.22                     | 0.56              |
| 1:A:66:VAL:CG1   | 1:A:94:ILE:CD1   | 2.83                     | 0.56              |
| 1:A:147:GLU:CG   | 2:B:285:ARG:CD   | 2.66                     | 0.56              |
| 3:C:125:LYS:HE3  | 3:D:282:ASP:O    | 2.05                     | 0.56              |
| 2:B:241:PHE:CB   | 2:B:254:ILE:HD13 | 2.34                     | 0.56              |
| 1:A:73:THR:CG2   | 2:B:215:ASN:HA   | 2.33                     | 0.56              |
| 2:B:241:PHE:C    | 2:B:254:ILE:CD1  | 2.78                     | 0.56              |
| 2:B:571:VAL:CG2  | 2:B:721:ILE:CD1  | 2.66                     | 0.56              |
| 1:A:194:GLU:HB3  | 1:A:250:ILE:HD11 | 1.86                     | 0.56              |
| 3:C:383:VAL:HG12 | 3:C:387:PHE:CZ   | 2.41                     | 0.56              |
| 3:D:127:ILE:HD12 | 3:D:161:ARG:CZ   | 2.36                     | 0.56              |
| 1:A:410:PHE:HA   | 1:A:415:LEU:H    | 1.70                     | 0.56              |
| 3:D:175:ALA:HB2  | 3:D:206:ASN:HB3  | 1.88                     | 0.56              |
| 2:B:563:ILE:HG12 | 2:B:564:LEU:HD23 | 1.86                     | 0.56              |
| 1:A:625:ILE:CD1  | 1:A:758:LEU:CD2  | 2.84                     | 0.56              |
| 3:D:234:ILE:HD11 | 3:D:303:ASN:CG   | 2.31                     | 0.56              |
| 1:A:628:ALA:CB   | 1:A:765:ILE:HD13 | 2.36                     | 0.56              |
| 1:A:641:LYS:CD   | 3:C:356:ILE:CD1  | 2.83                     | 0.56              |
| 2:B:209:ILE:CD1  | 2:B:213:ILE:CD1  | 2.83                     | 0.56              |
| 1:A:135:LEU:HD11 | 1:A:247:ILE:CD1  | 2.35                     | 0.56              |
| 3:C:212:ILE:CD1  | 3:C:275:PHE:CE2  | 2.86                     | 0.56              |
| 1:A:363:ILE:HD13 | 1:A:413:TYR:CB   | 2.25                     | 0.56              |
| 1:A:128:ASP:HB3  | 2:B:299:ARG:HD3  | 1.87                     | 0.56              |
| 1:A:296:TYR:CE2  | 2:B:322:HIS:HD2  | 2.23                     | 0.56              |
| 2:B:570:LEU:CD2  | 2:B:721:ILE:HD13 | 2.30                     | 0.56              |
| 1:A:68:ILE:HG13  | 2:B:281:LYS:HE3  | 1.87                     | 0.56              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:CB   | 2.84                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:188:ILE:HD11 | 3:C:394:PHE:CB   | 2.36                     | 0.56              |
| 2:B:209:ILE:CD1  | 2:B:222:HIS:CE1  | 2.89                     | 0.56              |
| 3:D:12:GLN:CD    | 3:D:12:GLN:H     | 2.13                     | 0.56              |
| 1:A:641:LYS:HG2  | 3:C:356:ILE:CD1  | 2.35                     | 0.56              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CD1  | 2.89                     | 0.56              |
| 3:D:210:LEU:HD11 | 3:D:222:ILE:CD1  | 2.35                     | 0.56              |
| 1:A:140:TYR:CG   | 2:B:324:ASP:OD1  | 2.58                     | 0.56              |
| 1:A:72:GLY:H     | 1:A:75:ILE:HB    | 1.71                     | 0.56              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:HB2  | 2.35                     | 0.56              |
| 2:B:412:LEU:CG   | 2:B:463:ILE:HD12 | 2.36                     | 0.56              |
| 1:A:352:ILE:HG22 | 1:A:572:ILE:CD1  | 2.36                     | 0.56              |
| 1:A:68:ILE:HD12  | 2:B:216:PHE:CB   | 2.36                     | 0.56              |
| 3:C:256:TYR:CD1  | 3:C:260:ILE:CD1  | 2.88                     | 0.56              |
| 1:A:155:VAL:CG1  | 2:B:285:ARG:HH22 | 2.17                     | 0.56              |
| 1:A:296:TYR:OH   | 2:B:322:HIS:HB2  | 2.05                     | 0.56              |
| 1:A:151:LEU:HD11 | 2:B:285:ARG:CG   | 2.36                     | 0.55              |
| 2:B:532:PRO:O    | 2:B:538:ILE:HD11 | 2.06                     | 0.55              |
| 2:B:608:ASN:HB3  | 3:D:260:ILE:HD13 | 1.87                     | 0.55              |
| 2:B:349:TRP:CG   | 2:B:364:ILE:HD12 | 2.41                     | 0.55              |
| 1:A:406:LEU:HD21 | 1:A:672:ILE:CD1  | 2.30                     | 0.55              |
| 2:B:634:ILE:CD1  | 2:B:809:LEU:CG   | 2.82                     | 0.55              |
| 1:A:365:THR:CA   | 1:A:404:ILE:HD11 | 2.36                     | 0.55              |
| 2:B:297:TYR:OH   | 2:B:330:ILE:HD12 | 2.04                     | 0.55              |
| 2:B:482:LEU:HD22 | 2:B:657:ILE:CG2  | 2.37                     | 0.55              |
| 2:B:339:ILE:HD12 | 2:B:440:GLY:H    | 1.71                     | 0.55              |
| 3:D:356:ILE:HD11 | 3:D:358:ARG:HH22 | 1.71                     | 0.55              |
| 3:C:75:VAL:HG21  | 3:C:94:VAL:HG22  | 1.88                     | 0.55              |
| 3:C:72:GLU:HA    | 3:C:75:VAL:HG12  | 1.87                     | 0.55              |
| 2:B:200:PHE:CZ   | 2:B:207:ILE:CD1  | 2.74                     | 0.55              |
| 1:A:595:HIS:ND1  | 1:A:640:ILE:HD12 | 2.15                     | 0.55              |
| 1:A:68:ILE:CD1   | 2:B:216:PHE:HB2  | 2.14                     | 0.55              |
| 1:A:61:LYS:CE    | 2:B:216:PHE:CE1  | 2.86                     | 0.55              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:HD13 | 2.26                     | 0.55              |
| 1:A:367:PRO:CG   | 1:A:404:ILE:HD13 | 2.35                     | 0.55              |
| 1:A:780:ILE:HD13 | 1:A:789:GLU:OE2  | 2.06                     | 0.55              |
| 1:A:630:ARG:HA   | 1:A:633:HIS:CD2  | 2.42                     | 0.55              |
| 1:A:632:LEU:HD22 | 1:A:768:ILE:HD12 | 1.88                     | 0.55              |
| 1:A:641:LYS:CD   | 3:C:356:ILE:HD12 | 2.30                     | 0.55              |
| 3:C:342:ILE:CD1  | 3:C:344:PHE:CZ   | 2.83                     | 0.55              |
| 1:A:606:LEU:HG   | 1:A:710:ILE:HD11 | 1.87                     | 0.55              |
| 1:A:68:ILE:O     | 2:B:220:LEU:HD11 | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:137:ARG:HH21 | 2:B:325:LEU:CD2  | 2.15                     | 0.55              |
| 3:C:69:MET:HE1   | 3:C:154:LEU:HD11 | 1.89                     | 0.55              |
| 1:A:133:MET:HG3  | 2:B:322:HIS:HA   | 1.87                     | 0.55              |
| 3:C:256:TYR:CD1  | 3:C:260:ILE:HD12 | 2.40                     | 0.55              |
| 2:B:779:LEU:HD21 | 2:B:805:PHE:HB3  | 1.88                     | 0.55              |
| 1:A:138:PHE:CD1  | 1:A:275:ILE:HD12 | 2.39                     | 0.55              |
| 1:A:203:ARG:HH22 | 1:A:243:LYS:HD3  | 1.71                     | 0.55              |
| 2:B:296:ILE:HD13 | 2:B:327:ILE:CG2  | 2.37                     | 0.55              |
| 1:A:136:GLN:CD   | 2:B:323:GLY:N    | 2.65                     | 0.55              |
| 1:A:140:TYR:HE2  | 2:B:327:ILE:HD11 | 1.72                     | 0.55              |
| 1:A:375:ILE:CD1  | 1:A:396:LYS:CB   | 2.84                     | 0.55              |
| 2:B:209:ILE:HD11 | 2:B:222:HIS:CE1  | 2.41                     | 0.55              |
| 2:B:271:LEU:CD1  | 2:B:287:ILE:HD11 | 2.37                     | 0.55              |
| 1:A:126:TRP:HZ2  | 1:A:196:ILE:CD1  | 2.17                     | 0.55              |
| 1:A:714:ARG:O    | 1:A:760:LEU:HD22 | 2.07                     | 0.55              |
| 2:B:636:ILE:HD13 | 3:D:437:TYR:CD1  | 2.42                     | 0.55              |
| 3:D:309:ALA:H    | 3:D:385:ASN:HD21 | 1.55                     | 0.55              |
| 3:C:5:ILE:HD11   | 3:C:137:GLN:HB2  | 1.88                     | 0.55              |
| 1:A:702:ILE:HG23 | 1:A:768:ILE:CD1  | 2.37                     | 0.55              |
| 1:A:102:PHE:CB   | 1:A:170:ILE:HD12 | 2.34                     | 0.54              |
| 1:A:133:MET:HG3  | 2:B:322:HIS:HA   | 1.89                     | 0.54              |
| 1:A:150:TYR:HD1  | 1:A:177:ILE:HD12 | 1.72                     | 0.54              |
| 2:B:206:GLN:NE2  | 2:B:209:ILE:CD1  | 2.71                     | 0.54              |
| 2:B:656:ILE:CD1  | 2:B:738:HIS:HE1  | 2.18                     | 0.54              |
| 2:B:610:ILE:HD11 | 3:D:196:GLU:O    | 1.96                     | 0.54              |
| 1:A:366:ILE:O    | 1:A:404:ILE:HD12 | 2.07                     | 0.54              |
| 2:B:271:LEU:HD11 | 2:B:287:ILE:HD11 | 1.87                     | 0.54              |
| 3:C:255:ILE:CD1  | 3:C:358:ARG:CZ   | 2.85                     | 0.54              |
| 3:C:277:SER:HB3  | 3:C:279:TYR:H    | 1.71                     | 0.54              |
| 1:A:137:ARG:HH12 | 2:B:325:LEU:HD13 | 1.73                     | 0.54              |
| 1:A:595:HIS:ND1  | 1:A:640:ILE:CD1  | 2.70                     | 0.54              |
| 3:C:127:ILE:HD13 | 3:C:162:TYR:CE2  | 2.42                     | 0.54              |
| 1:A:137:ARG:NE   | 2:B:325:LEU:HB2  | 2.21                     | 0.54              |
| 3:D:139:LEU:CD2  | 3:D:235:ILE:CD1  | 2.80                     | 0.54              |
| 1:A:425:ILE:HD13 | 1:A:482:LEU:CD2  | 2.34                     | 0.54              |
| 3:C:189:LEU:HD21 | 3:C:420:GLN:HG2  | 1.89                     | 0.54              |
| 1:A:109:ILE:HD11 | 1:A:170:ILE:HD11 | 1.89                     | 0.54              |
| 2:B:405:ILE:CG2  | 2:B:456:ILE:HD12 | 2.28                     | 0.54              |
| 2:B:402:ILE:HG13 | 2:B:449:ILE:HD13 | 1.87                     | 0.54              |
| 1:A:62:ASP:OD1   | 1:A:94:ILE:CD1   | 2.56                     | 0.54              |
| 3:C:212:ILE:HD13 | 3:C:275:PHE:CE1  | 2.42                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:150:TYR:CD1  | 1:A:177:ILE:HD12 | 2.42                     | 0.54              |
| 3:D:139:LEU:CD2  | 3:D:235:ILE:CD1  | 2.86                     | 0.54              |
| 1:A:138:PHE:CG   | 1:A:275:ILE:CD1  | 2.85                     | 0.54              |
| 1:A:422:LEU:HD13 | 1:A:564:ILE:CD1  | 2.38                     | 0.54              |
| 2:B:453:TYR:O    | 2:B:457:VAL:HG22 | 2.07                     | 0.54              |
| 3:C:238:VAL:HG11 | 3:C:375:MET:HE2  | 1.88                     | 0.54              |
| 1:A:367:PRO:CB   | 1:A:404:ILE:HD12 | 2.37                     | 0.54              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:CD1  | 2.28                     | 0.54              |
| 1:A:638:HIS:CE1  | 3:C:340:GLN:HE22 | 2.25                     | 0.54              |
| 3:D:393:THR:O    | 3:D:397:VAL:HG23 | 2.06                     | 0.54              |
| 1:A:109:ILE:HG22 | 1:A:177:ILE:CD1  | 2.37                     | 0.54              |
| 3:D:217:PHE:CG   | 3:D:280:ILE:HD13 | 2.42                     | 0.54              |
| 3:C:128:ASP:OD2  | 3:D:281:HIS:CE1  | 2.61                     | 0.54              |
| 3:D:188:ILE:HD12 | 3:D:394:PHE:CE1  | 2.40                     | 0.54              |
| 1:A:365:THR:HA   | 1:A:404:ILE:HD11 | 1.89                     | 0.54              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:HD13 | 1.90                     | 0.54              |
| 2:B:455:GLU:O    | 2:B:459:HIS:CD2  | 2.61                     | 0.54              |
| 1:A:433:HIS:CD2  | 3:C:2:GLY:HA3    | 2.41                     | 0.54              |
| 3:D:255:ILE:CD1  | 3:D:320:ASN:HD21 | 2.20                     | 0.54              |
| 1:A:63:LEU:HD23  | 1:A:109:ILE:HD11 | 1.90                     | 0.54              |
| 3:C:67:ILE:CD1   | 3:C:123:ILE:CG2  | 2.86                     | 0.54              |
| 1:A:613:LYS:HG3  | 1:A:714:ARG:O    | 2.07                     | 0.54              |
| 2:B:335:PHE:CZ   | 2:B:339:ILE:HD12 | 2.43                     | 0.54              |
| 1:A:71:GLU:OE1   | 2:B:216:PHE:CD1  | 2.61                     | 0.54              |
| 1:A:140:TYR:CD2  | 2:B:324:ASP:HB3  | 2.43                     | 0.54              |
| 1:A:142:ILE:HD12 | 1:A:193:TYR:OH   | 2.08                     | 0.54              |
| 3:C:139:LEU:CD2  | 3:C:235:ILE:HD13 | 2.38                     | 0.54              |
| 3:C:315:TYR:HA   | 3:C:346:SER:HB2  | 1.89                     | 0.54              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:HD21 | 2.34                     | 0.53              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:HD13 | 2.38                     | 0.53              |
| 3:C:271:SER:HB3  | 3:C:376:MET:HE2  | 1.89                     | 0.53              |
| 1:A:142:ILE:HD11 | 1:A:186:MET:CG   | 2.37                     | 0.53              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:HA   | 2.38                     | 0.53              |
| 1:A:641:LYS:HD2  | 3:C:356:ILE:HD13 | 1.86                     | 0.53              |
| 3:C:200:ALA:HB2  | 3:C:260:ILE:HD13 | 1.85                     | 0.53              |
| 2:B:284:TYR:CE1  | 2:B:291:ILE:HD13 | 2.43                     | 0.53              |
| 2:B:493:ILE:HD12 | 2:B:598:TYR:HB2  | 1.90                     | 0.53              |
| 3:D:268:LEU:HD23 | 3:D:379:ASN:HD22 | 1.74                     | 0.53              |
| 1:A:135:LEU:HD13 | 1:A:247:ILE:HD13 | 1.90                     | 0.53              |
| 1:A:367:PRO:HG3  | 1:A:404:ILE:CD1  | 2.30                     | 0.53              |
| 2:B:284:TYR:CE1  | 2:B:291:ILE:CD1  | 2.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:349:TRP:HE1  | 2:B:364:ILE:CD1  | 2.19                     | 0.53              |
| 1:A:151:LEU:CD1  | 2:B:285:ARG:NE   | 2.71                     | 0.53              |
| 3:C:238:VAL:HG22 | 3:C:322:ILE:HD13 | 1.91                     | 0.53              |
| 1:A:66:VAL:CG2   | 1:A:170:ILE:HD12 | 2.36                     | 0.53              |
| 1:A:147:GLU:CG   | 2:B:285:ARG:HD3  | 2.38                     | 0.53              |
| 1:A:405:PHE:HZ   | 1:A:573:ILE:HD11 | 1.69                     | 0.53              |
| 3:C:6:ILE:HD13   | 3:C:126:GLU:HG3  | 1.91                     | 0.53              |
| 1:A:62:ASP:OD1   | 1:A:94:ILE:HD11  | 2.08                     | 0.53              |
| 1:A:143:ARG:HH11 | 2:B:292:ILE:CD1  | 2.20                     | 0.53              |
| 2:B:568:LEU:N    | 2:B:721:ILE:HD12 | 2.23                     | 0.53              |
| 1:A:567:PRO:CG   | 1:A:574:ILE:HD13 | 2.38                     | 0.53              |
| 3:C:238:VAL:HG22 | 3:C:322:ILE:HD11 | 1.90                     | 0.53              |
| 1:A:62:ASP:OD2   | 1:A:94:ILE:HD13  | 2.09                     | 0.53              |
| 2:B:656:ILE:HD12 | 2:B:738:HIS:NE2  | 2.19                     | 0.53              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:CD1  | 2.77                     | 0.53              |
| 1:A:358:ARG:NH2  | 2:B:443:THR:CG2  | 2.71                     | 0.53              |
| 2:B:586:ILE:HD11 | 2:B:732:LEU:HB3  | 1.90                     | 0.53              |
| 2:B:192:LEU:CD2  | 2:B:287:ILE:CD1  | 2.81                     | 0.53              |
| 2:B:583:TYR:CE1  | 2:B:732:LEU:HD13 | 2.43                     | 0.53              |
| 2:B:529:MET:SD   | 2:B:538:ILE:HD13 | 2.49                     | 0.53              |
| 1:A:142:ILE:CD1  | 1:A:189:LEU:CD2  | 2.87                     | 0.53              |
| 3:C:32:GLY:H     | 3:C:36:LEU:H     | 1.57                     | 0.53              |
| 3:D:234:ILE:HD11 | 3:D:303:ASN:CG   | 2.34                     | 0.53              |
| 2:B:586:ILE:CB   | 2:B:735:ILE:HD13 | 2.38                     | 0.53              |
| 1:A:151:LEU:HD13 | 2:B:285:ARG:HE   | 1.74                     | 0.53              |
| 1:A:326:ILE:HD12 | 1:A:332:LEU:HD22 | 1.91                     | 0.53              |
| 1:A:625:ILE:HA   | 1:A:761:ILE:HD11 | 1.90                     | 0.53              |
| 1:A:154:LEU:HD23 | 2:B:281:LYS:HZ1  | 1.71                     | 0.53              |
| 1:A:566:ILE:HD13 | 1:A:574:ILE:O    | 2.09                     | 0.53              |
| 3:D:29:HIS:HA    | 3:D:46:ARG:HH12  | 1.74                     | 0.53              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:CG   | 2.85                     | 0.53              |
| 3:D:13:CYS:O     | 3:D:17:VAL:HG23  | 2.09                     | 0.53              |
| 3:C:188:ILE:HD11 | 3:C:394:PHE:CG   | 2.43                     | 0.53              |
| 3:D:13:CYS:SG    | 3:D:224:LEU:HD11 | 2.49                     | 0.53              |
| 2:B:568:LEU:HG   | 2:B:721:ILE:HD12 | 1.91                     | 0.53              |
| 2:B:339:ILE:HD13 | 2:B:439:ARG:CG   | 2.38                     | 0.53              |
| 2:B:586:ILE:CD1  | 2:B:735:ILE:CD1  | 2.64                     | 0.53              |
| 2:B:646:SER:CB   | 3:D:356:ILE:HD12 | 2.38                     | 0.53              |
| 1:A:570:LEU:HD23 | 1:A:573:ILE:CD1  | 2.29                     | 0.53              |
| 1:A:143:ARG:NH1  | 2:B:292:ILE:HD13 | 2.23                     | 0.53              |
| 1:A:348:LEU:HD23 | 1:A:348:LEU:O    | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:13:CYS:HA    | 3:C:228:ASN:HD21 | 1.74                     | 0.53              |
| 1:A:55:GLN:HE22  | 1:A:97:LYS:HD2   | 1.74                     | 0.53              |
| 1:A:714:ARG:NH2  | 1:A:761:ILE:HD12 | 2.23                     | 0.53              |
| 1:A:684:MET:HA   | 1:A:687:ARG:HE   | 1.74                     | 0.53              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:HB2  | 2.33                     | 0.52              |
| 2:B:209:ILE:HD13 | 2:B:213:ILE:HD11 | 1.91                     | 0.52              |
| 2:B:567:PRO:C    | 2:B:721:ILE:CD1  | 2.82                     | 0.52              |
| 1:A:112:TYR:OH   | 1:A:177:ILE:HD11 | 2.08                     | 0.52              |
| 1:A:137:ARG:NH2  | 2:B:325:LEU:CG   | 2.72                     | 0.52              |
| 2:B:480:ILE:CD1  | 2:B:541:LEU:HD11 | 2.39                     | 0.52              |
| 1:A:137:ARG:HH22 | 2:B:325:LEU:HD23 | 1.73                     | 0.52              |
| 1:A:136:GLN:CD   | 2:B:323:GLY:H    | 2.16                     | 0.52              |
| 2:B:820:LYS:HA   | 2:B:823:LEU:HD12 | 1.91                     | 0.52              |
| 1:A:155:VAL:HG11 | 2:B:282:SER:OG   | 2.08                     | 0.52              |
| 1:A:587:ARG:O    | 1:A:591:VAL:HG23 | 2.10                     | 0.52              |
| 1:A:64:LEU:CD2   | 1:A:68:ILE:HD12  | 2.39                     | 0.52              |
| 3:C:188:ILE:HD11 | 3:C:394:PHE:CB   | 2.39                     | 0.52              |
| 3:D:276:THR:HG21 | 3:D:284:ILE:HD12 | 1.91                     | 0.52              |
| 1:A:367:PRO:CB   | 1:A:404:ILE:HD11 | 2.35                     | 0.52              |
| 2:B:206:GLN:HE21 | 2:B:209:ILE:HD11 | 1.75                     | 0.52              |
| 2:B:405:ILE:CA   | 2:B:456:ILE:HD11 | 2.30                     | 0.52              |
| 3:C:4:GLU:HA     | 3:C:52:PRO:HA    | 1.92                     | 0.52              |
| 3:D:256:TYR:OH   | 3:D:260:ILE:CD1  | 2.56                     | 0.52              |
| 3:D:75:VAL:HG21  | 3:D:94:VAL:CG1   | 2.39                     | 0.52              |
| 3:C:383:VAL:HG21 | 3:C:434:MET:HE2  | 1.91                     | 0.52              |
| 1:A:365:THR:HG22 | 1:A:404:ILE:HD13 | 1.90                     | 0.52              |
| 1:A:696:GLN:HE21 | 1:A:699:ILE:CD1  | 2.14                     | 0.52              |
| 1:A:581:LYS:CB   | 1:A:683:ILE:HD12 | 2.33                     | 0.52              |
| 1:A:138:PHE:CZ   | 1:A:275:ILE:HD13 | 2.26                     | 0.52              |
| 1:A:108:ARG:HG3  | 1:A:177:ILE:HD11 | 1.90                     | 0.52              |
| 1:A:357:VAL:CG2  | 1:A:363:ILE:CD1  | 2.88                     | 0.52              |
| 3:C:55:ARG:HH11  | 3:D:284:ILE:HD13 | 1.74                     | 0.52              |
| 2:B:296:ILE:HD13 | 2:B:327:ILE:CD1  | 2.32                     | 0.52              |
| 1:A:640:ILE:HD11 | 1:A:699:ILE:HD11 | 1.86                     | 0.52              |
| 1:A:632:LEU:HD23 | 1:A:768:ILE:HD12 | 1.91                     | 0.52              |
| 2:B:264:TYR:CZ   | 2:B:287:ILE:HD11 | 2.44                     | 0.52              |
| 1:A:581:LYS:CB   | 1:A:683:ILE:HD12 | 2.39                     | 0.52              |
| 1:A:71:GLU:CD    | 2:B:222:HIS:CD2  | 2.87                     | 0.52              |
| 1:A:195:GLU:CD   | 1:A:250:ILE:CD1  | 2.82                     | 0.52              |
| 2:B:206:GLN:NE2  | 2:B:209:ILE:HD12 | 2.24                     | 0.52              |
| 1:A:65:ASN:OD1   | 2:B:216:PHE:CE1  | 2.58                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:296:ILE:HD12 | 2:B:327:ILE:HD13 | 1.90                     | 0.52              |
| 1:A:70:LEU:HD11  | 2:B:281:LYS:NZ   | 1.96                     | 0.52              |
| 1:A:585:ILE:CD1  | 1:A:683:ILE:CD1  | 2.87                     | 0.52              |
| 3:C:170:TYR:CE2  | 3:C:235:ILE:HD12 | 2.45                     | 0.52              |
| 2:B:207:ILE:CD1  | 2:B:221:LEU:CD2  | 2.86                     | 0.52              |
| 1:A:66:VAL:HA    | 2:B:216:PHE:CE1  | 2.45                     | 0.52              |
| 3:C:6:ILE:HD12   | 3:C:127:ILE:CG2  | 2.40                     | 0.52              |
| 1:A:72:GLY:HA3   | 2:B:222:HIS:ND1  | 2.23                     | 0.52              |
| 1:A:72:GLY:O     | 2:B:222:HIS:HE1  | 1.92                     | 0.52              |
| 1:A:143:ARG:HH22 | 2:B:296:ILE:HD11 | 1.74                     | 0.52              |
| 3:D:256:TYR:CD1  | 3:D:260:ILE:HD12 | 2.45                     | 0.52              |
| 1:A:630:ARG:HA   | 1:A:633:HIS:CD2  | 2.44                     | 0.52              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CD1  | 2.93                     | 0.52              |
| 3:D:212:ILE:HD13 | 3:D:275:PHE:CZ   | 2.45                     | 0.52              |
| 2:B:191:THR:CG2  | 2:B:207:ILE:HD13 | 2.39                     | 0.52              |
| 1:A:64:LEU:HD21  | 1:A:68:ILE:HD12  | 1.91                     | 0.52              |
| 2:B:355:LEU:C    | 2:B:364:ILE:HD12 | 2.33                     | 0.52              |
| 3:D:119:ILE:HD13 | 3:D:154:LEU:HD21 | 1.90                     | 0.52              |
| 1:A:367:PRO:CG   | 1:A:404:ILE:CD1  | 2.88                     | 0.52              |
| 2:B:634:ILE:CD1  | 2:B:809:LEU:HD21 | 2.40                     | 0.52              |
| 2:B:398:LEU:HD13 | 2:B:449:ILE:HD12 | 1.88                     | 0.52              |
| 1:A:696:GLN:NE2  | 1:A:699:ILE:CD1  | 2.67                     | 0.52              |
| 2:B:468:PHE:HA   | 2:B:529:MET:HE3  | 1.91                     | 0.52              |
| 1:A:128:ASP:OD1  | 2:B:295:ARG:HD3  | 2.10                     | 0.52              |
| 3:C:6:ILE:HD13   | 3:C:126:GLU:CG   | 2.40                     | 0.52              |
| 1:A:567:PRO:CG   | 1:A:574:ILE:CD1  | 2.87                     | 0.52              |
| 2:B:386:ASN:ND2  | 2:B:389:ARG:H    | 2.07                     | 0.52              |
| 2:B:527:HIS:CE1  | 2:B:538:ILE:HD11 | 2.14                     | 0.52              |
| 1:A:361:LEU:HD21 | 2:B:443:THR:HG23 | 1.90                     | 0.52              |
| 2:B:218:SER:O    | 2:B:222:HIS:CD2  | 2.63                     | 0.52              |
| 3:D:289:HIS:CE1  | 3:D:323:ILE:HD13 | 2.44                     | 0.52              |
| 2:B:296:ILE:HD11 | 2:B:327:ILE:CG1  | 2.38                     | 0.52              |
| 1:A:595:HIS:O    | 1:A:599:LEU:HD13 | 2.09                     | 0.52              |
| 3:D:5:ILE:HD12   | 3:D:53:PHE:HZ    | 1.72                     | 0.51              |
| 2:B:349:TRP:CD2  | 2:B:364:ILE:HD11 | 2.45                     | 0.51              |
| 1:A:62:ASP:CG    | 1:A:94:ILE:CD1   | 2.82                     | 0.51              |
| 1:A:68:ILE:HD13  | 2:B:216:PHE:N    | 2.24                     | 0.51              |
| 1:A:706:PHE:CE2  | 1:A:768:ILE:HD11 | 2.40                     | 0.51              |
| 1:A:405:PHE:CZ   | 1:A:573:ILE:HD11 | 2.45                     | 0.51              |
| 3:D:217:PHE:CD1  | 3:D:280:ILE:CD1  | 2.90                     | 0.51              |
| 2:B:412:LEU:HD22 | 2:B:463:ILE:CD1  | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:114:LYS:HE3  | 1:A:118:ILE:HD12 | 1.87                     | 0.51              |
| 2:B:405:ILE:HG23 | 2:B:456:ILE:HD13 | 1.91                     | 0.51              |
| 3:D:204:PHE:HE1  | 3:D:234:ILE:HD12 | 1.74                     | 0.51              |
| 1:A:614:TYR:O    | 1:A:714:ARG:NH2  | 2.44                     | 0.51              |
| 2:B:662:LYS:HD3  | 3:D:329:ARG:HH12 | 1.75                     | 0.51              |
| 1:A:93:LYS:HD3   | 4:F:28:UNK:CB    | 2.40                     | 0.51              |
| 1:A:595:HIS:ND1  | 1:A:640:ILE:HD13 | 2.24                     | 0.51              |
| 3:D:123:ILE:CD1  | 3:D:154:LEU:HD11 | 2.40                     | 0.51              |
| 1:A:707:CYS:O    | 1:A:711:LYS:HG3  | 2.10                     | 0.51              |
| 3:C:316:PHE:CE1  | 3:C:380:MET:HE2  | 2.45                     | 0.51              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:HD11 | 2.33                     | 0.51              |
| 1:A:126:TRP:CH2  | 1:A:196:ILE:HD11 | 2.46                     | 0.51              |
| 2:B:430:HIS:CB   | 2:B:448:ILE:HD12 | 2.40                     | 0.51              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:HB3  | 1.92                     | 0.51              |
| 2:B:586:ILE:CB   | 2:B:735:ILE:CD1  | 2.87                     | 0.51              |
| 3:C:173:PHE:CD1  | 3:C:203:VAL:HG13 | 2.46                     | 0.51              |
| 1:A:584:ILE:CD1  | 1:A:687:ARG:HB2  | 2.41                     | 0.51              |
| 3:D:299:LEU:H    | 3:D:299:LEU:HD22 | 1.75                     | 0.51              |
| 1:A:599:LEU:HD22 | 1:A:640:ILE:HD13 | 1.91                     | 0.51              |
| 1:A:409:PHE:HB3  | 1:A:415:LEU:HB2  | 1.93                     | 0.51              |
| 3:D:256:TYR:HE1  | 3:D:260:ILE:CD1  | 2.16                     | 0.51              |
| 1:A:68:ILE:CG1   | 2:B:281:LYS:HE3  | 2.40                     | 0.51              |
| 1:A:70:LEU:CG    | 2:B:216:PHE:HE1  | 2.01                     | 0.51              |
| 3:C:281:HIS:CD2  | 3:C:282:ASP:H    | 2.29                     | 0.51              |
| 1:A:283:LEU:HD11 | 1:A:347:MET:HE2  | 1.93                     | 0.51              |
| 1:A:367:PRO:HB2  | 1:A:404:ILE:HD11 | 1.93                     | 0.51              |
| 2:B:405:ILE:HD13 | 2:B:453:TYR:HA   | 1.93                     | 0.51              |
| 3:D:328:PRO:HG2  | 3:D:331:ILE:HG22 | 1.93                     | 0.51              |
| 1:A:155:VAL:CG1  | 2:B:281:LYS:HG2  | 2.40                     | 0.51              |
| 3:D:342:ILE:HD13 | 3:D:344:PHE:CZ   | 2.46                     | 0.51              |
| 1:A:296:TYR:OH   | 2:B:322:HIS:NE2  | 2.43                     | 0.51              |
| 2:B:242:ARG:HG3  | 2:B:254:ILE:HD13 | 1.93                     | 0.51              |
| 2:B:297:TYR:CZ   | 2:B:330:ILE:CD1  | 2.67                     | 0.51              |
| 1:A:135:LEU:HD13 | 1:A:247:ILE:HD11 | 1.92                     | 0.51              |
| 2:B:346:LEU:HD13 | 2:B:402:ILE:HD13 | 1.91                     | 0.51              |
| 1:A:138:PHE:CE1  | 1:A:192:ILE:HD13 | 2.45                     | 0.51              |
| 1:A:102:PHE:CE1  | 1:A:170:ILE:CD1  | 2.94                     | 0.51              |
| 2:B:590:LEU:CD2  | 2:B:657:ILE:HD13 | 2.40                     | 0.51              |
| 1:A:625:ILE:HD12 | 1:A:761:ILE:HG23 | 1.92                     | 0.51              |
| 1:A:641:LYS:HD3  | 3:C:356:ILE:CD1  | 2.19                     | 0.51              |
| 1:A:195:GLU:OE1  | 1:A:250:ILE:HD12 | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:308:THR:HG22 | 3:C:310:MET:H    | 1.76                     | 0.51              |
| 1:A:135:LEU:CD2  | 1:A:247:ILE:HD11 | 2.19                     | 0.51              |
| 1:A:282:MET:HB3  | 1:A:292:LEU:HD11 | 1.93                     | 0.51              |
| 1:A:357:VAL:HG23 | 1:A:363:ILE:HD12 | 1.93                     | 0.50              |
| 3:D:188:ILE:HD13 | 3:D:394:PHE:CG   | 2.45                     | 0.50              |
| 3:D:232:SER:HA   | 3:D:235:ILE:HG22 | 1.93                     | 0.50              |
| 1:A:422:LEU:CD1  | 1:A:564:ILE:HD12 | 2.41                     | 0.50              |
| 1:A:462:LEU:HD13 | 1:A:484:ILE:HG13 | 1.93                     | 0.50              |
| 2:B:264:TYR:OH   | 2:B:287:ILE:HD13 | 2.11                     | 0.50              |
| 3:D:284:ILE:HD12 | 3:D:369:GLU:OE1  | 2.11                     | 0.50              |
| 1:A:135:LEU:HD11 | 1:A:247:ILE:HD11 | 1.94                     | 0.50              |
| 2:B:765:LEU:O    | 2:B:769:VAL:HG23 | 2.11                     | 0.50              |
| 3:D:192:ARG:HE   | 3:D:192:ARG:C    | 2.19                     | 0.50              |
| 2:B:408:SER:HA   | 2:B:411:PHE:CE2  | 2.46                     | 0.50              |
| 3:D:242:ILE:HD13 | 3:D:252:MET:SD   | 2.50                     | 0.50              |
| 1:A:135:LEU:HD13 | 1:A:247:ILE:CD1  | 2.41                     | 0.50              |
| 1:A:142:ILE:HD11 | 1:A:188:LEU:CD1  | 2.40                     | 0.50              |
| 3:C:330:GLN:CD   | 3:C:330:GLN:H    | 2.18                     | 0.50              |
| 1:A:757:ALA:O    | 1:A:761:ILE:HG13 | 2.12                     | 0.50              |
| 3:D:210:LEU:HD11 | 3:D:222:ILE:HD13 | 1.88                     | 0.50              |
| 1:A:137:ARG:NE   | 2:B:324:ASP:HA   | 2.26                     | 0.50              |
| 1:A:589:GLN:CD   | 1:A:652:ILE:HD13 | 2.36                     | 0.50              |
| 1:A:62:ASP:CB    | 1:A:94:ILE:HD13  | 2.41                     | 0.50              |
| 1:A:296:TYR:OH   | 2:B:322:HIS:CE1  | 2.63                     | 0.50              |
| 2:B:184:ILE:O    | 2:B:188:VAL:HG23 | 2.12                     | 0.50              |
| 3:D:189:LEU:HD23 | 3:D:192:ARG:HH22 | 1.77                     | 0.50              |
| 2:B:586:ILE:HG21 | 2:B:735:ILE:HD11 | 1.92                     | 0.50              |
| 1:A:332:LEU:HB3  | 1:A:334:ASP:H    | 1.76                     | 0.50              |
| 2:B:339:ILE:HD11 | 2:B:440:GLY:HA3  | 1.83                     | 0.50              |
| 2:B:479:ASN:HB3  | 2:B:485:LYS:HE3  | 1.92                     | 0.50              |
| 1:A:606:LEU:HB2  | 1:A:710:ILE:HD13 | 1.93                     | 0.50              |
| 1:A:635:LYS:HA   | 1:A:638:HIS:CD2  | 2.47                     | 0.50              |
| 1:A:247:ILE:HD13 | 1:A:275:ILE:HG21 | 1.94                     | 0.50              |
| 3:C:205:ASP:H    | 3:C:303:ASN:HB3  | 1.75                     | 0.50              |
| 2:B:775:VAL:HG12 | 2:B:780:ASN:HD21 | 1.77                     | 0.50              |
| 3:C:51:LYS:HB3   | 3:C:52:PRO:HD3   | 1.94                     | 0.50              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:HG23 | 2.42                     | 0.50              |
| 2:B:312:PHE:CZ   | 2:B:316:LEU:HD11 | 2.46                     | 0.50              |
| 1:A:189:LEU:O    | 1:A:192:ILE:HG12 | 2.12                     | 0.50              |
| 3:D:123:ILE:HD11 | 3:D:154:LEU:HD11 | 1.93                     | 0.50              |
| 1:A:134:VAL:HG11 | 1:A:247:ILE:HD12 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:152:LYS:HG2  | 2:B:285:ARG:HD2  | 1.94                     | 0.50              |
| 1:A:72:GLY:HA2   | 2:B:215:ASN:C    | 2.37                     | 0.50              |
| 1:A:422:LEU:CD1  | 1:A:564:ILE:CD1  | 2.90                     | 0.50              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:HD21 | 2.27                     | 0.50              |
| 1:A:606:LEU:HD13 | 1:A:710:ILE:HG21 | 1.93                     | 0.50              |
| 2:B:656:ILE:CD1  | 2:B:738:HIS:HB2  | 2.40                     | 0.50              |
| 1:A:599:LEU:CD2  | 1:A:640:ILE:CD1  | 2.83                     | 0.50              |
| 1:A:566:ILE:HD13 | 1:A:574:ILE:CG1  | 2.39                     | 0.50              |
| 1:A:609:THR:H    | 1:A:610:PRO:CD   | 2.25                     | 0.50              |
| 1:A:72:GLY:N     | 2:B:216:PHE:CE1  | 2.80                     | 0.50              |
| 1:A:361:LEU:HD11 | 2:B:443:THR:HG23 | 1.93                     | 0.50              |
| 2:B:185:LEU:HD11 | 2:B:272:VAL:HA   | 1.92                     | 0.50              |
| 1:A:638:HIS:CD2  | 3:C:354:VAL:HG21 | 2.47                     | 0.50              |
| 1:A:130:SER:OG   | 2:B:322:HIS:CD2  | 2.64                     | 0.50              |
| 2:B:643:GLN:HG2  | 3:D:356:ILE:HD11 | 1.83                     | 0.50              |
| 1:A:141:GLU:OE2  | 2:B:324:ASP:CG   | 2.54                     | 0.50              |
| 1:A:98:MET:HE1   | 1:A:170:ILE:HD11 | 1.93                     | 0.50              |
| 3:D:143:ALA:HA   | 3:D:183:GLN:HE22 | 1.76                     | 0.50              |
| 1:A:142:ILE:HD13 | 1:A:189:LEU:HD21 | 1.92                     | 0.50              |
| 2:B:480:ILE:HD12 | 2:B:541:LEU:HD11 | 1.94                     | 0.50              |
| 3:D:69:MET:HE2   | 3:D:119:ILE:HD11 | 1.94                     | 0.50              |
| 2:B:319:PHE:HA   | 2:B:322:HIS:CD2  | 2.46                     | 0.50              |
| 1:A:73:THR:H     | 2:B:215:ASN:HA   | 1.75                     | 0.49              |
| 3:C:323:ILE:HD12 | 3:C:332:SER:HB3  | 1.94                     | 0.49              |
| 3:C:67:ILE:HD12  | 3:C:123:ILE:CG2  | 2.42                     | 0.49              |
| 1:A:70:LEU:HD11  | 2:B:223:LEU:HD11 | 1.94                     | 0.49              |
| 1:A:142:ILE:HD13 | 1:A:189:LEU:CD2  | 2.42                     | 0.49              |
| 3:D:28:GLU:O     | 3:D:365:LEU:HD12 | 2.12                     | 0.49              |
| 3:C:272:PHE:HB2  | 3:C:303:ASN:HD21 | 1.77                     | 0.49              |
| 3:D:75:VAL:HG21  | 3:D:94:VAL:HG13  | 1.93                     | 0.49              |
| 1:A:137:ARG:NH1  | 2:B:325:LEU:HD13 | 2.27                     | 0.49              |
| 1:A:367:PRO:CG   | 1:A:404:ILE:CD1  | 2.86                     | 0.49              |
| 1:A:612:TRP:HA   | 1:A:630:ARG:HH22 | 1.76                     | 0.49              |
| 3:D:205:ASP:H    | 3:D:304:SER:HA   | 1.76                     | 0.49              |
| 1:A:140:TYR:HB2  | 2:B:324:ASP:OD1  | 2.11                     | 0.49              |
| 1:A:629:THR:HG21 | 1:A:710:ILE:HD12 | 1.93                     | 0.49              |
| 3:C:276:THR:HG22 | 3:C:277:SER:H    | 1.77                     | 0.49              |
| 3:C:312:ASN:HD22 | 3:C:382:THR:HG21 | 1.78                     | 0.49              |
| 3:D:70:ASP:CG    | 3:D:71:SER:H     | 2.20                     | 0.49              |
| 1:A:66:VAL:CG1   | 1:A:94:ILE:HD12  | 2.42                     | 0.49              |
| 1:A:63:LEU:HD11  | 1:A:109:ILE:HD12 | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:584:ILE:HD11 | 1:A:687:ARG:HB2  | 1.94                     | 0.49              |
| 1:A:561:LYS:HG3  | 1:A:587:ARG:HH11 | 1.77                     | 0.49              |
| 3:D:101:ALA:HB1  | 3:D:107:ASN:HB2  | 1.94                     | 0.49              |
| 3:C:32:GLY:H     | 3:C:36:LEU:N     | 2.11                     | 0.49              |
| 3:C:326:VAL:HG23 | 3:C:362:TYR:CD2  | 2.47                     | 0.49              |
| 3:C:327:GLU:HB3  | 3:C:331:ILE:HD12 | 1.93                     | 0.49              |
| 1:A:585:ILE:HD12 | 1:A:683:ILE:CG1  | 2.41                     | 0.49              |
| 1:A:366:ILE:O    | 1:A:404:ILE:HD12 | 2.13                     | 0.49              |
| 2:B:418:GLU:HB3  | 2:B:463:ILE:CD1  | 2.43                     | 0.49              |
| 2:B:742:ALA:CB   | 2:B:743:THR:HG23 | 2.42                     | 0.49              |
| 3:C:70:ASP:CG    | 3:C:71:SER:H     | 2.20                     | 0.49              |
| 1:A:67:LEU:HD13  | 1:A:109:ILE:HD13 | 1.94                     | 0.49              |
| 2:B:264:TYR:CE2  | 2:B:287:ILE:CD1  | 2.81                     | 0.49              |
| 3:C:258:THR:OG1  | 3:C:356:ILE:CD1  | 2.61                     | 0.49              |
| 1:A:425:ILE:HD11 | 1:A:482:LEU:HA   | 1.93                     | 0.49              |
| 1:A:142:ILE:HD12 | 1:A:193:TYR:CE1  | 2.46                     | 0.49              |
| 1:A:425:ILE:HD11 | 1:A:482:LEU:HB3  | 1.92                     | 0.49              |
| 3:D:9:GLN:HE21   | 3:D:15:ASN:HA    | 1.77                     | 0.49              |
| 3:C:6:ILE:HD11   | 3:C:126:GLU:HG3  | 1.94                     | 0.49              |
| 1:A:462:LEU:HD13 | 1:A:484:ILE:HD12 | 1.93                     | 0.49              |
| 1:A:714:ARG:O    | 1:A:760:LEU:CD2  | 2.60                     | 0.49              |
| 2:B:586:ILE:HG12 | 2:B:735:ILE:HD13 | 1.89                     | 0.49              |
| 1:A:584:ILE:HD12 | 1:A:687:ARG:CB   | 2.43                     | 0.49              |
| 2:B:335:PHE:CZ   | 2:B:339:ILE:HD11 | 2.43                     | 0.49              |
| 2:B:493:ILE:HD13 | 2:B:595:LYS:HA   | 1.95                     | 0.49              |
| 2:B:296:ILE:HD12 | 2:B:327:ILE:CG1  | 2.09                     | 0.49              |
| 3:C:111:ILE:HG23 | 3:C:114:ARG:HH21 | 1.77                     | 0.49              |
| 1:A:438:PHE:CE1  | 1:A:484:ILE:CD1  | 2.95                     | 0.49              |
| 2:B:363:PHE:CG   | 2:B:390:VAL:HG12 | 2.47                     | 0.49              |
| 2:B:402:ILE:CG1  | 2:B:449:ILE:CD1  | 2.86                     | 0.49              |
| 2:B:402:ILE:HG12 | 2:B:449:ILE:HD13 | 1.90                     | 0.49              |
| 1:A:72:GLY:CA    | 2:B:222:HIS:HE1  | 2.23                     | 0.49              |
| 3:C:234:ILE:HD13 | 3:C:303:ASN:CG   | 2.37                     | 0.49              |
| 2:B:284:TYR:CE1  | 2:B:291:ILE:CD1  | 2.94                     | 0.49              |
| 2:B:634:ILE:HD12 | 2:B:809:LEU:HD21 | 1.86                     | 0.49              |
| 3:C:12:GLN:O     | 3:C:16:HIS:CD2   | 2.66                     | 0.49              |
| 3:C:5:ILE:HD12   | 3:C:53:PHE:CZ    | 2.48                     | 0.49              |
| 2:B:402:ILE:HG12 | 2:B:449:ILE:HD13 | 1.94                     | 0.49              |
| 1:A:137:ARG:N    | 2:B:324:ASP:OD1  | 2.46                     | 0.49              |
| 1:A:367:PRO:N    | 1:A:404:ILE:HD12 | 2.26                     | 0.49              |
| 3:D:48:ASP:H     | 3:D:243:ARG:HA   | 1.78                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:78:PHE:HB2   | 1:A:93:LYS:HD2   | 1.95                     | 0.49              |
| 1:A:780:ILE:CD1  | 1:A:789:GLU:HB2  | 2.40                     | 0.49              |
| 1:A:641:LYS:CG   | 3:C:356:ILE:CD1  | 2.90                     | 0.49              |
| 1:A:140:TYR:CD2  | 2:B:324:ASP:OD2  | 2.66                     | 0.49              |
| 2:B:463:ILE:HG12 | 2:B:467:LYS:HD2  | 1.94                     | 0.49              |
| 2:B:586:ILE:CB   | 2:B:735:ILE:HD13 | 2.43                     | 0.49              |
| 1:A:127:SER:HB3  | 1:A:143:ARG:HH22 | 1.78                     | 0.49              |
| 2:B:434:GLN:HG3  | 2:B:448:ILE:HD11 | 1.95                     | 0.49              |
| 2:B:402:ILE:CD1  | 2:B:449:ILE:HD11 | 2.21                     | 0.49              |
| 2:B:184:ILE:CD1  | 2:B:213:ILE:HG13 | 2.43                     | 0.49              |
| 1:A:606:LEU:CD2  | 1:A:710:ILE:HD11 | 2.43                     | 0.49              |
| 2:B:407:LYS:HZ3  | 2:B:721:ILE:CD1  | 2.25                     | 0.49              |
| 2:B:568:LEU:N    | 2:B:721:ILE:CD1  | 2.76                     | 0.49              |
| 3:C:1:MET:HG3    | 3:C:3:GLY:H      | 1.77                     | 0.49              |
| 3:D:127:ILE:HD12 | 3:D:161:ARG:NH1  | 2.27                     | 0.49              |
| 3:D:70:ASP:CG    | 3:D:71:SER:H     | 2.21                     | 0.49              |
| 1:A:625:ILE:CD1  | 1:A:758:LEU:HD22 | 2.43                     | 0.49              |
| 3:C:69:MET:SD    | 3:C:119:ILE:HD13 | 2.52                     | 0.49              |
| 1:A:422:LEU:CD1  | 1:A:574:ILE:HD13 | 2.43                     | 0.49              |
| 1:A:640:ILE:CD1  | 1:A:699:ILE:HD13 | 2.36                     | 0.49              |
| 1:A:367:PRO:CA   | 1:A:404:ILE:CD1  | 2.87                     | 0.49              |
| 2:B:230:LEU:HD22 | 2:B:295:ARG:HA   | 1.95                     | 0.49              |
| 1:A:641:LYS:CD   | 3:C:356:ILE:HD12 | 2.42                     | 0.49              |
| 1:A:566:ILE:CD1  | 1:A:574:ILE:HG21 | 2.38                     | 0.48              |
| 2:B:731:PHE:CE2  | 2:B:735:ILE:HD11 | 2.48                     | 0.48              |
| 1:A:74:TYR:CE2   | 2:B:216:PHE:CZ   | 2.96                     | 0.48              |
| 2:B:224:ILE:HG22 | 2:B:284:TYR:CD1  | 2.48                     | 0.48              |
| 2:B:480:ILE:HD11 | 2:B:520:VAL:CG1  | 2.43                     | 0.48              |
| 3:D:268:LEU:CD2  | 3:D:379:ASN:HD22 | 2.25                     | 0.48              |
| 1:A:267:PHE:CE2  | 1:A:271:LEU:HD11 | 2.48                     | 0.48              |
| 1:A:195:GLU:HG3  | 1:A:250:ILE:HD13 | 1.94                     | 0.48              |
| 2:B:455:GLU:O    | 2:B:459:HIS:CG   | 2.66                     | 0.48              |
| 3:C:124:ASP:OD2  | 3:D:281:HIS:NE2  | 2.46                     | 0.48              |
| 1:A:566:ILE:HD12 | 1:A:574:ILE:HD13 | 1.91                     | 0.48              |
| 1:A:602:THR:HG22 | 1:A:710:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:143:ARG:CD   | 2:B:292:ILE:HD11 | 2.40                     | 0.48              |
| 1:A:588:TYR:CD1  | 1:A:693:ILE:HD11 | 2.47                     | 0.48              |
| 3:C:139:LEU:HD23 | 3:C:170:TYR:HB2  | 1.95                     | 0.48              |
| 1:A:68:ILE:HD13  | 1:A:158:LEU:CD2  | 2.37                     | 0.48              |
| 2:B:503:PRO:HG2  | 2:B:550:HIS:CE1  | 2.48                     | 0.48              |
| 1:A:112:TYR:HE2  | 1:A:177:ILE:HD13 | 1.77                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:296:ILE:HD12 | 2:B:327:ILE:HG23 | 1.96                     | 0.48              |
| 3:C:384:VAL:HG11 | 3:C:431:GLN:HG2  | 1.95                     | 0.48              |
| 1:A:438:PHE:CE2  | 1:A:484:ILE:HD11 | 2.43                     | 0.48              |
| 2:B:362:PHE:CE2  | 2:B:364:ILE:HD11 | 2.49                     | 0.48              |
| 2:B:427:LYS:NZ   | 2:B:456:ILE:HD13 | 2.29                     | 0.48              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:HB2  | 1.93                     | 0.48              |
| 1:A:599:LEU:HD22 | 1:A:640:ILE:CD1  | 2.43                     | 0.48              |
| 2:B:257:ILE:CD1  | 2:B:301:THR:OG1  | 2.61                     | 0.48              |
| 2:B:313:LEU:HD13 | 2:B:391:PRO:HA   | 1.96                     | 0.48              |
| 2:B:402:ILE:CG1  | 2:B:449:ILE:CD1  | 2.92                     | 0.48              |
| 1:A:375:ILE:CD1  | 1:A:396:LYS:HB2  | 2.43                     | 0.48              |
| 1:A:603:TRP:CZ2  | 1:A:633:HIS:HB2  | 2.48                     | 0.48              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:CD2  | 2.46                     | 0.48              |
| 3:C:55:ARG:HB3   | 3:C:65:ARG:CZ    | 2.43                     | 0.48              |
| 1:A:366:ILE:HG23 | 1:A:367:PRO:HD2  | 1.96                     | 0.48              |
| 1:A:587:ARG:O    | 1:A:591:VAL:HG23 | 2.13                     | 0.48              |
| 3:D:76:ILE:HA    | 3:D:79:VAL:HG22  | 1.95                     | 0.48              |
| 2:B:349:TRP:HH2  | 2:B:383:ILE:HD13 | 1.78                     | 0.48              |
| 2:B:430:HIS:CD2  | 2:B:448:ILE:HG22 | 2.48                     | 0.48              |
| 3:D:123:ILE:HD13 | 3:D:158:LEU:HD21 | 1.95                     | 0.48              |
| 1:A:152:LYS:HG3  | 2:B:285:ARG:HD2  | 1.94                     | 0.48              |
| 2:B:288:TYR:CZ   | 2:B:292:ILE:HD11 | 2.34                     | 0.48              |
| 3:C:199:ASP:O    | 3:C:260:ILE:HD13 | 2.14                     | 0.48              |
| 1:A:75:ILE:HD12  | 2:B:216:PHE:CZ   | 2.48                     | 0.48              |
| 2:B:241:PHE:CB   | 2:B:254:ILE:HD13 | 2.44                     | 0.48              |
| 1:A:625:ILE:CD1  | 1:A:761:ILE:HG23 | 2.44                     | 0.48              |
| 1:A:641:LYS:HD3  | 3:C:356:ILE:HD13 | 1.95                     | 0.48              |
| 2:B:349:TRP:CZ3  | 2:B:383:ILE:CD1  | 2.96                     | 0.48              |
| 2:B:207:ILE:HD13 | 2:B:221:LEU:HG   | 1.95                     | 0.48              |
| 1:A:134:VAL:CG1  | 1:A:247:ILE:HD12 | 2.43                     | 0.48              |
| 3:D:166:ILE:HD12 | 3:D:256:TYR:CG   | 2.48                     | 0.48              |
| 1:A:588:TYR:CG   | 1:A:693:ILE:HD11 | 2.37                     | 0.48              |
| 3:C:127:ILE:HD11 | 3:C:162:TYR:HE2  | 1.77                     | 0.48              |
| 3:C:234:ILE:HA   | 3:C:375:MET:HE1  | 1.94                     | 0.48              |
| 3:D:204:PHE:CE2  | 3:D:234:ILE:CD1  | 2.81                     | 0.48              |
| 1:A:706:PHE:CE2  | 1:A:710:ILE:HD11 | 2.48                     | 0.48              |
| 2:B:493:ILE:CD1  | 2:B:598:TYR:HD2  | 2.23                     | 0.48              |
| 2:B:533:ARG:HA   | 2:B:538:ILE:CD1  | 2.40                     | 0.48              |
| 3:C:5:ILE:HD12   | 3:C:53:PHE:CE1   | 2.49                     | 0.48              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:HB2  | 1.81                     | 0.48              |
| 1:A:128:ASP:CG   | 2:B:295:ARG:HD3  | 2.39                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:12:GLN:O     | 3:C:16:HIS:CD2   | 2.66                     | 0.48              |
| 3:C:188:ILE:CD1  | 3:C:394:PHE:CB   | 2.90                     | 0.48              |
| 1:A:63:LEU:HD22  | 1:A:170:ILE:HD12 | 1.96                     | 0.48              |
| 3:C:199:ASP:O    | 3:C:260:ILE:HD13 | 2.14                     | 0.48              |
| 1:A:557:ILE:CD1  | 1:A:594:TYR:CD2  | 2.96                     | 0.48              |
| 2:B:284:TYR:CZ   | 2:B:291:ILE:HD13 | 2.48                     | 0.48              |
| 3:C:152:SER:HB3  | 3:C:193:ARG:HG3  | 1.96                     | 0.48              |
| 1:A:131:PHE:CD2  | 2:B:322:HIS:CG   | 3.02                     | 0.48              |
| 1:A:128:ASP:CA   | 2:B:322:HIS:HE1  | 2.22                     | 0.48              |
| 2:B:322:HIS:HD2  | 2:B:327:ILE:HD13 | 1.77                     | 0.48              |
| 3:D:326:VAL:HG12 | 3:D:361:PRO:HB3  | 1.96                     | 0.48              |
| 2:B:779:LEU:HD13 | 2:B:780:ASN:O    | 2.14                     | 0.48              |
| 1:A:136:GLN:NE2  | 2:B:327:ILE:HD12 | 2.13                     | 0.48              |
| 1:A:140:TYR:CE1  | 2:B:292:ILE:CD1  | 2.95                     | 0.48              |
| 3:C:344:PHE:HB3  | 3:C:345:PRO:HD3  | 1.95                     | 0.48              |
| 1:A:425:ILE:HD13 | 1:A:482:LEU:CD1  | 2.43                     | 0.48              |
| 1:A:702:ILE:CD1  | 1:A:767:TYR:CE2  | 2.88                     | 0.48              |
| 2:B:412:LEU:HD22 | 2:B:463:ILE:HD13 | 1.95                     | 0.48              |
| 2:B:610:ILE:CD1  | 3:D:196:GLU:O    | 2.60                     | 0.48              |
| 1:A:625:ILE:HD13 | 1:A:764:LEU:HB3  | 1.64                     | 0.48              |
| 1:A:133:MET:HA   | 2:B:323:GLY:H    | 1.79                     | 0.48              |
| 3:C:67:ILE:CD1   | 3:C:123:ILE:HG22 | 2.42                     | 0.48              |
| 3:C:205:ASP:O    | 3:C:209:LEU:HD13 | 2.14                     | 0.48              |
| 3:C:138:LEU:HG   | 3:C:140:HIS:CD2  | 2.49                     | 0.48              |
| 3:D:180:VAL:HB   | 3:D:182:VAL:HG22 | 1.96                     | 0.48              |
| 1:A:128:ASP:OD2  | 2:B:295:ARG:HD3  | 2.14                     | 0.47              |
| 3:D:143:ALA:HB2  | 3:D:174:PRO:HB3  | 1.96                     | 0.47              |
| 3:C:234:ILE:CD1  | 3:C:303:ASN:CG   | 2.87                     | 0.47              |
| 1:A:425:ILE:HD11 | 1:A:482:LEU:CA   | 2.44                     | 0.47              |
| 1:A:585:ILE:HD12 | 1:A:683:ILE:HG12 | 1.97                     | 0.47              |
| 3:D:12:GLN:O     | 3:D:16:HIS:CD2   | 2.68                     | 0.47              |
| 3:D:280:ILE:HG23 | 3:D:281:HIS:CD2  | 2.48                     | 0.47              |
| 1:A:109:ILE:HD11 | 1:A:174:GLU:CD   | 2.35                     | 0.47              |
| 3:C:322:ILE:HD11 | 3:C:358:ARG:NH2  | 2.29                     | 0.47              |
| 3:D:188:ILE:HD13 | 3:D:394:PHE:CD2  | 2.49                     | 0.47              |
| 1:A:66:VAL:HG13  | 1:A:75:ILE:HD12  | 1.96                     | 0.47              |
| 3:C:8:LEU:HD13   | 3:C:154:LEU:HD21 | 1.97                     | 0.47              |
| 2:B:529:MET:HE2  | 2:B:538:ILE:HD11 | 1.83                     | 0.47              |
| 2:B:398:LEU:CD2  | 2:B:449:ILE:CD1  | 2.69                     | 0.47              |
| 3:D:316:PHE:HB2  | 3:D:347:TRP:CZ3  | 2.49                     | 0.47              |
| 3:C:212:ILE:HD13 | 3:C:275:PHE:CE2  | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:155:LEU:HD11 | 3:C:194:LEU:HD12 | 1.96                     | 0.47              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CD2  | 2.94                     | 0.47              |
| 2:B:293:ARG:CD   | 2:B:330:ILE:HD12 | 2.44                     | 0.47              |
| 2:B:323:GLY:O    | 2:B:327:ILE:HD12 | 2.15                     | 0.47              |
| 3:C:9:GLN:HE21   | 3:C:15:ASN:HA    | 1.79                     | 0.47              |
| 2:B:563:ILE:HG12 | 2:B:564:LEU:H    | 1.79                     | 0.47              |
| 2:B:188:VAL:CG1  | 2:B:224:ILE:CD1  | 2.86                     | 0.47              |
| 2:B:304:LEU:HD22 | 2:B:312:PHE:CE1  | 2.49                     | 0.47              |
| 2:B:405:ILE:HG12 | 2:B:456:ILE:HD13 | 1.94                     | 0.47              |
| 3:C:199:ASP:O    | 3:C:260:ILE:HD13 | 2.15                     | 0.47              |
| 3:C:13:CYS:O     | 3:C:17:VAL:HG23  | 2.15                     | 0.47              |
| 1:A:573:ILE:HD12 | 1:A:673:GLN:HG2  | 1.92                     | 0.47              |
| 3:D:363:LEU:HD22 | 3:D:363:LEU:H    | 1.78                     | 0.47              |
| 1:A:151:LEU:CD1  | 2:B:285:ARG:HG3  | 2.43                     | 0.47              |
| 2:B:402:ILE:CD1  | 2:B:449:ILE:HD13 | 2.39                     | 0.47              |
| 3:C:17:VAL:HG21  | 3:C:231:ILE:HD12 | 1.96                     | 0.47              |
| 1:A:566:ILE:HD11 | 1:A:571:ASN:HA   | 1.95                     | 0.47              |
| 1:A:108:ARG:HB3  | 1:A:177:ILE:HD13 | 1.97                     | 0.47              |
| 2:B:634:ILE:HD11 | 2:B:772:PHE:CD1  | 2.50                     | 0.47              |
| 2:B:335:PHE:CD2  | 2:B:339:ILE:HD12 | 2.50                     | 0.47              |
| 3:C:67:ILE:HD11  | 3:C:123:ILE:HG23 | 1.96                     | 0.47              |
| 2:B:405:ILE:HG21 | 2:B:456:ILE:CD1  | 2.28                     | 0.47              |
| 2:B:570:LEU:HD23 | 2:B:721:ILE:HD13 | 1.85                     | 0.47              |
| 3:C:129:SER:CB   | 3:D:284:ILE:HD12 | 2.45                     | 0.47              |
| 2:B:405:ILE:HG12 | 2:B:456:ILE:HD11 | 1.96                     | 0.47              |
| 3:C:127:ILE:HD11 | 3:C:162:TYR:CE2  | 2.50                     | 0.47              |
| 2:B:407:LYS:HZ1  | 2:B:721:ILE:HD12 | 1.76                     | 0.47              |
| 3:C:317:ASN:O    | 3:C:318:VAL:HG13 | 2.15                     | 0.47              |
| 1:A:140:TYR:HE1  | 2:B:292:ILE:CD1  | 2.28                     | 0.47              |
| 1:A:155:VAL:CG1  | 2:B:285:ARG:NH2  | 2.77                     | 0.47              |
| 2:B:464:LEU:HD22 | 2:B:470:TYR:CE2  | 2.49                     | 0.47              |
| 2:B:586:ILE:CB   | 2:B:735:ILE:CD1  | 2.93                     | 0.47              |
| 2:B:589:PHE:CD2  | 2:B:739:LYS:HG3  | 2.50                     | 0.47              |
| 3:C:6:ILE:HD11   | 3:C:127:ILE:HG22 | 1.94                     | 0.47              |
| 3:D:353:HIS:CE1  | 3:D:355:ASN:H    | 2.33                     | 0.47              |
| 1:A:348:LEU:CD2  | 1:A:352:ILE:HD11 | 2.45                     | 0.47              |
| 3:D:255:ILE:HD11 | 3:D:320:ASN:HD21 | 1.79                     | 0.47              |
| 2:B:480:ILE:HD11 | 2:B:537:VAL:HG22 | 1.97                     | 0.47              |
| 3:C:104:SER:HA   | 3:C:186:ASN:HD21 | 1.80                     | 0.47              |
| 1:A:70:LEU:CD1   | 2:B:220:LEU:CG   | 2.93                     | 0.47              |
| 1:A:140:TYR:OH   | 2:B:326:THR:HG23 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:557:ILE:HD12 | 1:A:594:TYR:CD2  | 2.48                     | 0.47              |
| 3:C:125:LYS:CE   | 3:D:282:ASP:O    | 2.63                     | 0.47              |
| 3:C:127:ILE:HD13 | 3:C:162:TYR:CZ   | 2.50                     | 0.47              |
| 3:D:188:ILE:HD11 | 3:D:427:ARG:NH2  | 2.30                     | 0.47              |
| 1:A:422:LEU:HD13 | 1:A:564:ILE:HD11 | 1.97                     | 0.47              |
| 2:B:493:ILE:HD11 | 2:B:598:TYR:CB   | 2.43                     | 0.47              |
| 1:A:706:PHE:CZ   | 1:A:710:ILE:HD11 | 2.50                     | 0.47              |
| 1:A:352:ILE:CD1  | 1:A:572:ILE:HG21 | 2.44                     | 0.47              |
| 1:A:73:THR:CG2   | 2:B:215:ASN:ND2  | 2.62                     | 0.47              |
| 1:A:572:ILE:O    | 1:A:572:ILE:HG12 | 2.15                     | 0.47              |
| 1:A:638:HIS:HE1  | 3:C:340:GLN:HE22 | 1.62                     | 0.47              |
| 2:B:207:ILE:HD13 | 2:B:225:PHE:HA   | 1.97                     | 0.47              |
| 3:C:127:ILE:CD1  | 3:C:162:TYR:HE2  | 2.28                     | 0.47              |
| 1:A:68:ILE:CD1   | 2:B:216:PHE:CB   | 2.93                     | 0.47              |
| 1:A:458:TYR:CG   | 1:A:484:ILE:CD1  | 2.85                     | 0.46              |
| 2:B:383:ILE:HD11 | 2:B:410:ILE:HD11 | 1.96                     | 0.46              |
| 3:C:119:ILE:HD12 | 3:C:154:LEU:HD13 | 1.97                     | 0.46              |
| 1:A:609:THR:HA   | 1:A:612:TRP:CE2  | 2.50                     | 0.46              |
| 1:A:78:PHE:HD2   | 1:A:80:ASP:O     | 1.98                     | 0.46              |
| 1:A:142:ILE:HD11 | 1:A:189:LEU:HD21 | 1.97                     | 0.46              |
| 2:B:405:ILE:CB   | 2:B:456:ILE:CD1  | 2.92                     | 0.46              |
| 3:C:188:ILE:HD13 | 3:C:394:PHE:CD2  | 2.48                     | 0.46              |
| 1:A:65:ASN:CB    | 2:B:216:PHE:CD1  | 2.98                     | 0.46              |
| 2:B:339:ILE:CD1  | 2:B:440:GLY:CA   | 2.93                     | 0.46              |
| 1:A:71:GLU:CB    | 2:B:208:GLN:OE1  | 2.61                     | 0.46              |
| 1:A:138:PHE:CE2  | 1:A:192:ILE:HD13 | 2.50                     | 0.46              |
| 1:A:154:LEU:HD21 | 2:B:281:LYS:HE3  | 1.98                     | 0.46              |
| 3:D:258:THR:HG21 | 3:D:356:ILE:HD13 | 1.97                     | 0.46              |
| 3:D:306:VAL:HG22 | 3:D:380:MET:HE1  | 1.96                     | 0.46              |
| 3:C:125:LYS:HG3  | 3:D:283:ASP:CG   | 2.41                     | 0.46              |
| 2:B:191:THR:HG23 | 2:B:207:ILE:HD13 | 1.97                     | 0.46              |
| 1:A:148:ASP:OD1  | 2:B:285:ARG:CZ   | 2.64                     | 0.46              |
| 1:A:702:ILE:HG23 | 1:A:768:ILE:HD13 | 1.97                     | 0.46              |
| 1:A:195:GLU:OE2  | 1:A:250:ILE:HD11 | 2.14                     | 0.46              |
| 1:A:662:CYS:O    | 1:A:666:PRO:HD2  | 2.15                     | 0.46              |
| 3:D:195:ILE:HD12 | 3:D:423:PHE:CE1  | 2.48                     | 0.46              |
| 1:A:574:ILE:HD11 | 1:A:579:MET:HG2  | 1.98                     | 0.46              |
| 1:A:564:ILE:HD13 | 1:A:574:ILE:HG21 | 1.96                     | 0.46              |
| 1:A:71:GLU:H     | 2:B:216:PHE:CB   | 2.27                     | 0.46              |
| 1:A:140:TYR:CD2  | 2:B:324:ASP:CB   | 2.98                     | 0.46              |
| 3:C:125:LYS:NZ   | 3:D:281:HIS:O    | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:302:GLU:HB2  | 4:E:1:UNK:H2     | 1.79                     | 0.46              |
| 1:A:63:LEU:HD21  | 1:A:170:ILE:CD1  | 2.46                     | 0.46              |
| 3:C:123:ILE:HG21 | 3:C:161:ARG:HH12 | 1.81                     | 0.46              |
| 2:B:362:PHE:CD2  | 2:B:364:ILE:CD1  | 2.98                     | 0.46              |
| 2:B:284:TYR:CE1  | 2:B:291:ILE:CD1  | 2.98                     | 0.46              |
| 1:A:67:LEU:HD22  | 1:A:154:LEU:HD11 | 1.98                     | 0.46              |
| 2:B:239:GLU:OE1  | 2:B:239:GLU:HA   | 2.14                     | 0.46              |
| 1:A:643:ILE:HD12 | 1:A:692:LEU:CD2  | 2.45                     | 0.46              |
| 2:B:775:VAL:HG11 | 2:B:805:PHE:HA   | 1.97                     | 0.46              |
| 1:A:136:GLN:NE2  | 2:B:323:GLY:CA   | 2.51                     | 0.46              |
| 1:A:91:GLU:HG3   | 1:A:92:PHE:H     | 1.80                     | 0.46              |
| 1:A:799:VAL:HG12 | 1:A:800:ASP:O    | 2.15                     | 0.46              |
| 1:A:638:HIS:CE1  | 1:A:642:THR:HG21 | 2.51                     | 0.46              |
| 3:D:138:LEU:HB3  | 3:D:169:THR:HG22 | 1.97                     | 0.46              |
| 1:A:195:GLU:OE2  | 1:A:250:ILE:CD1  | 2.62                     | 0.46              |
| 2:B:482:LEU:HD21 | 2:B:735:ILE:HD12 | 1.96                     | 0.46              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:CB   | 2.91                     | 0.46              |
| 2:B:264:TYR:CE2  | 2:B:287:ILE:HD11 | 2.51                     | 0.46              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:CG2  | 2.93                     | 0.46              |
| 1:A:66:VAL:HG21  | 1:A:170:ILE:CD1  | 2.41                     | 0.46              |
| 3:C:97:ASP:HB3   | 3:C:114:ARG:HH11 | 1.81                     | 0.46              |
| 2:B:260:GLU:OE2  | 2:B:330:ILE:HD13 | 2.14                     | 0.46              |
| 2:B:349:TRP:CZ2  | 2:B:364:ILE:HG21 | 2.51                     | 0.46              |
| 1:A:612:TRP:CG   | 1:A:630:ARG:HH12 | 2.34                     | 0.46              |
| 2:B:731:PHE:CE1  | 2:B:735:ILE:HD11 | 2.51                     | 0.46              |
| 3:C:46:ARG:HA    | 3:C:244:PHE:CE2  | 2.51                     | 0.46              |
| 3:C:292:TYR:CZ   | 3:C:374:GLY:HA3  | 2.50                     | 0.46              |
| 2:B:339:ILE:CD1  | 2:B:439:ARG:NH1  | 2.79                     | 0.46              |
| 2:B:493:ILE:HD13 | 2:B:595:LYS:HA   | 1.97                     | 0.46              |
| 2:B:545:VAL:HB   | 2:B:550:HIS:CD2  | 2.50                     | 0.46              |
| 1:A:366:ILE:HG22 | 1:A:368:SER:H    | 1.80                     | 0.46              |
| 1:A:638:HIS:CE1  | 3:C:340:GLN:NE2  | 2.84                     | 0.46              |
| 1:A:140:TYR:CG   | 2:B:324:ASP:CG   | 2.94                     | 0.46              |
| 1:A:55:GLN:O     | 1:A:59:VAL:HG23  | 2.16                     | 0.46              |
| 2:B:339:ILE:CD1  | 2:B:440:GLY:H    | 2.21                     | 0.46              |
| 2:B:405:ILE:CG1  | 2:B:456:ILE:CD1  | 2.93                     | 0.46              |
| 1:A:780:ILE:HD12 | 1:A:789:GLU:CB   | 2.43                     | 0.46              |
| 2:B:339:ILE:HD11 | 2:B:440:GLY:CA   | 2.46                     | 0.46              |
| 1:A:641:LYS:CD   | 3:C:356:ILE:HD12 | 2.45                     | 0.46              |
| 1:A:628:ALA:HB3  | 1:A:765:ILE:HD13 | 1.97                     | 0.46              |
| 1:A:375:ILE:CD1  | 1:A:396:LYS:CD   | 2.94                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:349:TRP:CE2  | 2:B:364:ILE:CD1  | 2.92                     | 0.46              |
| 1:A:135:LEU:HD11 | 1:A:247:ILE:HD11 | 1.97                     | 0.46              |
| 3:C:269:SER:HB3  | 3:C:380:MET:HE2  | 1.98                     | 0.46              |
| 3:D:7:THR:HG23   | 3:D:137:GLN:HE21 | 1.80                     | 0.46              |
| 1:A:120:THR:HA   | 1:A:123:TYR:CD2  | 2.51                     | 0.46              |
| 1:A:367:PRO:HA   | 1:A:404:ILE:CD1  | 2.36                     | 0.46              |
| 3:D:138:LEU:HB2  | 3:D:169:THR:HG22 | 1.98                     | 0.46              |
| 2:B:548:LEU:HD12 | 2:B:548:LEU:H    | 1.81                     | 0.46              |
| 1:A:142:ILE:CD1  | 1:A:186:MET:HG2  | 2.41                     | 0.46              |
| 1:A:66:VAL:CG1   | 1:A:109:ILE:HD12 | 2.46                     | 0.46              |
| 1:A:140:TYR:CD1  | 2:B:324:ASP:OD2  | 2.69                     | 0.46              |
| 2:B:364:ILE:HD11 | 2:B:403:PHE:CA   | 2.45                     | 0.46              |
| 1:A:63:LEU:HD21  | 1:A:170:ILE:HD12 | 1.97                     | 0.46              |
| 1:A:362:GLN:NE2  | 2:B:447:GLU:HG2  | 2.08                     | 0.46              |
| 1:A:603:TRP:CG   | 1:A:633:HIS:HD1  | 2.33                     | 0.46              |
| 2:B:335:PHE:CD2  | 2:B:339:ILE:CD1  | 2.98                     | 0.46              |
| 2:B:381:ILE:O    | 2:B:381:ILE:HG22 | 2.16                     | 0.46              |
| 2:B:192:LEU:HD22 | 2:B:227:ALA:HB3  | 1.98                     | 0.46              |
| 2:B:349:TRP:CZ3  | 2:B:383:ILE:HD11 | 2.50                     | 0.46              |
| 3:D:49:ASP:HA    | 3:D:52:PRO:HD2   | 1.99                     | 0.45              |
| 1:A:147:GLU:CD   | 2:B:292:ILE:CD1  | 2.69                     | 0.45              |
| 1:A:128:ASP:CG   | 2:B:299:ARG:HD2  | 2.32                     | 0.45              |
| 2:B:279:SER:H    | 2:B:282:SER:HB2  | 1.81                     | 0.45              |
| 2:B:241:PHE:C    | 2:B:254:ILE:HD13 | 2.41                     | 0.45              |
| 3:C:217:PHE:CD1  | 3:C:281:HIS:CD2  | 3.04                     | 0.45              |
| 2:B:772:PHE:HB2  | 2:B:812:ILE:HD13 | 1.98                     | 0.45              |
| 3:D:25:LEU:O     | 3:D:29:HIS:CD2   | 2.69                     | 0.45              |
| 1:A:585:ILE:CD1  | 1:A:683:ILE:CD1  | 2.94                     | 0.45              |
| 3:C:217:PHE:CD2  | 3:C:280:ILE:HD13 | 2.50                     | 0.45              |
| 1:A:138:PHE:CE2  | 1:A:192:ILE:CD1  | 2.98                     | 0.45              |
| 1:A:470:GLN:HE22 | 1:A:474:PRO:HA   | 1.81                     | 0.45              |
| 2:B:405:ILE:CD1  | 2:B:452:GLN:HB2  | 2.45                     | 0.45              |
| 3:D:191:LEU:HD13 | 3:D:427:ARG:CD   | 2.46                     | 0.45              |
| 1:A:595:HIS:ND1  | 1:A:640:ILE:HD13 | 2.31                     | 0.45              |
| 3:D:401:GLY:HA2  | 3:D:404:LEU:HD13 | 1.99                     | 0.45              |
| 3:C:129:SER:HA   | 3:D:283:ASP:HB3  | 1.98                     | 0.45              |
| 2:B:640:GLN:HG2  | 3:D:354:VAL:HG11 | 1.98                     | 0.45              |
| 2:B:224:ILE:CD1  | 2:B:283:LEU:HD23 | 2.43                     | 0.45              |
| 2:B:335:PHE:HB3  | 2:B:439:ARG:HH21 | 1.81                     | 0.45              |
| 3:C:248:MET:HE2  | 3:C:248:MET:H    | 1.81                     | 0.45              |
| 1:A:352:ILE:HD13 | 1:A:572:ILE:HG21 | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:184:ILE:O    | 2:B:188:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:138:PHE:CD1  | 1:A:275:ILE:CD1  | 2.97                     | 0.45              |
| 1:A:625:ILE:HA   | 1:A:761:ILE:CD1  | 2.46                     | 0.45              |
| 1:A:414:ASP:O    | 1:A:418:VAL:HG23 | 2.16                     | 0.45              |
| 2:B:541:LEU:HD12 | 2:B:541:LEU:H    | 1.81                     | 0.45              |
| 1:A:151:LEU:HD11 | 2:B:282:SER:HA   | 1.98                     | 0.45              |
| 1:A:142:ILE:CD1  | 1:A:188:LEU:HD12 | 2.45                     | 0.45              |
| 1:A:108:ARG:HH12 | 1:A:112:TYR:HB2  | 1.80                     | 0.45              |
| 2:B:600:TYR:CE2  | 2:B:604:MET:HE1  | 2.51                     | 0.45              |
| 1:A:585:ILE:HD13 | 1:A:683:ILE:CG1  | 2.45                     | 0.45              |
| 1:A:577:THR:HG23 | 1:A:680:LEU:HD22 | 1.97                     | 0.45              |
| 3:C:193:ARG:NH1  | 3:C:419:VAL:HG13 | 2.29                     | 0.45              |
| 1:A:68:ILE:HG13  | 2:B:281:LYS:HZ2  | 1.78                     | 0.45              |
| 3:D:212:ILE:HD13 | 3:D:275:PHE:CZ   | 2.51                     | 0.45              |
| 3:C:219:ASN:HD21 | 3:C:280:ILE:HD11 | 1.81                     | 0.45              |
| 1:A:154:LEU:HD12 | 1:A:154:LEU:HA   | 1.73                     | 0.45              |
| 1:A:641:LYS:HG3  | 3:C:356:ILE:HD11 | 1.96                     | 0.45              |
| 2:B:411:PHE:HB2  | 2:B:570:LEU:HD22 | 1.98                     | 0.45              |
| 3:D:9:GLN:HE21   | 3:D:15:ASN:HA    | 1.81                     | 0.45              |
| 1:A:70:LEU:CD1   | 2:B:223:LEU:HD11 | 2.46                     | 0.45              |
| 1:A:402:ASN:HB3  | 1:A:669:ALA:H    | 1.80                     | 0.45              |
| 1:A:65:ASN:O     | 2:B:216:PHE:CZ   | 2.70                     | 0.45              |
| 1:A:595:HIS:CE1  | 1:A:640:ILE:HG21 | 2.51                     | 0.45              |
| 1:A:128:ASP:C    | 2:B:322:HIS:CE1  | 2.94                     | 0.45              |
| 1:A:109:ILE:HD13 | 1:A:173:LEU:CD1  | 2.44                     | 0.45              |
| 3:D:284:ILE:HD13 | 3:D:284:ILE:HG21 | 1.77                     | 0.45              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:CD1  | 2.90                     | 0.45              |
| 3:D:323:ILE:HD13 | 3:D:335:MET:HE1  | 1.99                     | 0.45              |
| 1:A:567:PRO:HG2  | 1:A:574:ILE:CD1  | 2.47                     | 0.45              |
| 1:A:65:ASN:HB3   | 2:B:216:PHE:CE2  | 2.52                     | 0.45              |
| 3:D:138:LEU:HB3  | 3:D:169:THR:HG22 | 1.99                     | 0.45              |
| 1:A:72:GLY:CA    | 2:B:215:ASN:HB3  | 2.46                     | 0.45              |
| 2:B:639:THR:HA   | 2:B:642:GLN:HE21 | 1.82                     | 0.45              |
| 3:D:127:ILE:CD1  | 3:D:161:ARG:CZ   | 2.91                     | 0.45              |
| 1:A:96:LYS:HE3   | 1:A:107:ARG:HH12 | 1.82                     | 0.45              |
| 1:A:774:ILE:CD1  | 1:A:796:SER:HB2  | 2.47                     | 0.45              |
| 3:C:6:ILE:HD11   | 3:C:127:ILE:HA   | 1.98                     | 0.45              |
| 1:A:694:PRO:HB2  | 1:A:794:TYR:CE2  | 2.52                     | 0.45              |
| 2:B:245:ASN:HD21 | 2:B:254:ILE:HD12 | 1.81                     | 0.45              |
| 2:B:334:LEU:O    | 2:B:338:MET:HE2  | 2.17                     | 0.45              |
| 1:A:147:GLU:OE2  | 2:B:288:TYR:CD2  | 2.70                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:611:SER:HB3  | 1:A:630:ARG:HH11 | 1.82                     | 0.45              |
| 3:D:51:LYS:HB3   | 3:D:52:PRO:HD3   | 1.99                     | 0.45              |
| 3:D:4:GLU:HA     | 3:D:52:PRO:HB3   | 1.97                     | 0.45              |
| 3:D:21:LEU:HD23  | 3:D:22:TRP:CZ3   | 2.52                     | 0.45              |
| 2:B:426:SER:O    | 2:B:430:HIS:CD2  | 2.70                     | 0.45              |
| 2:B:480:ILE:HD11 | 2:B:537:VAL:HG13 | 1.99                     | 0.45              |
| 3:D:318:VAL:HG22 | 3:D:319:TYR:N    | 2.31                     | 0.45              |
| 1:A:797:SER:O    | 1:A:800:ASP:O    | 2.35                     | 0.45              |
| 2:B:780:ASN:O    | 2:B:801:LEU:HD23 | 2.17                     | 0.45              |
| 2:B:412:LEU:HD23 | 2:B:419:VAL:H    | 1.82                     | 0.45              |
| 3:C:384:VAL:HA   | 3:C:387:PHE:CD2  | 2.52                     | 0.45              |
| 1:A:629:THR:OG1  | 1:A:710:ILE:CD1  | 2.50                     | 0.45              |
| 2:B:251:LYS:O    | 2:B:255:ILE:HG13 | 2.16                     | 0.45              |
| 1:A:379:ASN:O    | 1:A:382:ALA:HB3  | 2.17                     | 0.45              |
| 1:A:188:LEU:HD13 | 1:A:268:LEU:HD11 | 1.98                     | 0.45              |
| 1:A:195:GLU:CD   | 1:A:250:ILE:HD11 | 2.42                     | 0.45              |
| 2:B:646:SER:OG   | 3:D:356:ILE:HD12 | 2.17                     | 0.45              |
| 2:B:227:ALA:HB2  | 2:B:291:ILE:CD1  | 2.46                     | 0.45              |
| 1:A:137:ARG:HH12 | 2:B:325:LEU:CD1  | 2.30                     | 0.45              |
| 2:B:402:ILE:HD11 | 2:B:449:ILE:CD1  | 2.45                     | 0.45              |
| 2:B:582:GLU:HG2  | 2:B:585:ARG:HH21 | 1.81                     | 0.44              |
| 2:B:362:PHE:CD2  | 2:B:364:ILE:HD12 | 2.53                     | 0.44              |
| 3:D:366:GLN:HB3  | 3:D:369:GLU:HG3  | 1.98                     | 0.44              |
| 1:A:625:ILE:HD12 | 1:A:765:ILE:CG2  | 2.48                     | 0.44              |
| 3:C:188:ILE:HD11 | 3:C:394:PHE:CD2  | 2.39                     | 0.44              |
| 1:A:573:ILE:HG22 | 1:A:673:GLN:HE22 | 1.82                     | 0.44              |
| 3:D:312:ASN:HB3  | 3:D:385:ASN:HD21 | 1.82                     | 0.44              |
| 1:A:194:GLU:HB3  | 1:A:250:ILE:HD12 | 1.98                     | 0.44              |
| 2:B:184:ILE:HD12 | 2:B:280:LEU:HG   | 1.99                     | 0.44              |
| 2:B:325:LEU:HD22 | 2:B:325:LEU:H    | 1.81                     | 0.44              |
| 2:B:339:ILE:CD1  | 2:B:439:ARG:HD2  | 2.41                     | 0.44              |
| 2:B:405:ILE:CG2  | 2:B:456:ILE:HD12 | 2.46                     | 0.44              |
| 3:D:189:LEU:HG   | 3:D:420:GLN:HE21 | 1.81                     | 0.44              |
| 2:B:528:LEU:HG   | 2:B:529:MET:H    | 1.81                     | 0.44              |
| 1:A:64:LEU:HD13  | 1:A:168:PHE:HB3  | 1.99                     | 0.44              |
| 2:B:257:ILE:CD1  | 2:B:297:TYR:HE2  | 2.17                     | 0.44              |
| 2:B:583:TYR:CD1  | 2:B:732:LEU:HD13 | 2.52                     | 0.44              |
| 1:A:296:TYR:OH   | 2:B:318:ILE:HD11 | 2.17                     | 0.44              |
| 2:B:455:GLU:HG2  | 2:B:459:HIS:CE1  | 2.52                     | 0.44              |
| 1:A:581:LYS:HD3  | 1:A:680:LEU:HD22 | 2.00                     | 0.44              |
| 3:C:188:ILE:HD13 | 3:C:394:PHE:CE2  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:70:LEU:C     | 2:B:216:PHE:HE2  | 2.22                     | 0.44              |
| 2:B:739:LYS:C    | 2:B:743:THR:O    | 2.57                     | 0.44              |
| 1:A:425:ILE:CD1  | 1:A:478:MET:HB3  | 2.38                     | 0.44              |
| 1:A:363:ILE:CD1  | 1:A:413:TYR:CG   | 2.94                     | 0.44              |
| 3:C:188:ILE:HG23 | 3:C:423:PHE:CD2  | 2.52                     | 0.44              |
| 1:A:137:ARG:CA   | 2:B:324:ASP:OD1  | 2.66                     | 0.44              |
| 1:A:585:ILE:HD11 | 1:A:683:ILE:CD1  | 2.47                     | 0.44              |
| 2:B:634:ILE:HD11 | 2:B:772:PHE:HD1  | 1.83                     | 0.44              |
| 2:B:808:ASN:ND2  | 2:B:812:ILE:HD11 | 2.25                     | 0.44              |
| 3:D:188:ILE:HD13 | 3:D:394:PHE:CG   | 2.51                     | 0.44              |
| 1:A:192:ILE:HG22 | 1:A:250:ILE:HG21 | 1.99                     | 0.44              |
| 3:C:71:SER:HA    | 3:C:95:ALA:H     | 1.82                     | 0.44              |
| 1:A:348:LEU:CD2  | 1:A:352:ILE:CD1  | 2.95                     | 0.44              |
| 2:B:646:SER:HB2  | 3:D:356:ILE:CD1  | 2.48                     | 0.44              |
| 2:B:191:THR:CG2  | 2:B:207:ILE:CD1  | 2.95                     | 0.44              |
| 3:C:235:ILE:O    | 3:C:238:VAL:HG22 | 2.17                     | 0.44              |
| 3:D:29:HIS:CE1   | 3:D:363:LEU:HG   | 2.53                     | 0.44              |
| 1:A:373:ILE:HD13 | 1:A:373:ILE:HG21 | 1.84                     | 0.44              |
| 3:C:259:LEU:HA   | 3:C:318:VAL:HG11 | 1.98                     | 0.44              |
| 3:D:183:GLN:HE21 | 3:D:187:THR:HG23 | 1.82                     | 0.44              |
| 1:A:64:LEU:HG    | 2:B:216:PHE:CE2  | 2.49                     | 0.44              |
| 2:B:474:VAL:HG21 | 2:B:668:LEU:HD13 | 1.98                     | 0.44              |
| 2:B:293:ARG:HE   | 2:B:326:THR:HB   | 1.81                     | 0.44              |
| 2:B:245:ASN:ND2  | 2:B:254:ILE:HD12 | 2.33                     | 0.44              |
| 2:B:293:ARG:HD3  | 2:B:330:ILE:CD1  | 2.45                     | 0.44              |
| 3:C:241:SER:HB3  | 3:C:322:ILE:HD12 | 2.00                     | 0.44              |
| 3:C:313:PRO:HG2  | 3:C:382:THR:HA   | 1.99                     | 0.44              |
| 2:B:421:TRP:HB3  | 2:B:422:THR:H    | 1.62                     | 0.44              |
| 3:C:265:LEU:HD12 | 3:C:265:LEU:HA   | 1.91                     | 0.44              |
| 3:D:111:ILE:HG12 | 3:D:114:ARG:HH21 | 1.83                     | 0.44              |
| 1:A:365:THR:CG2  | 1:A:404:ILE:HD13 | 2.32                     | 0.44              |
| 2:B:656:ILE:HD13 | 2:B:738:HIS:CG   | 2.52                     | 0.44              |
| 1:A:171:ARG:H    | 1:A:171:ARG:HD2  | 1.83                     | 0.44              |
| 3:D:166:ILE:HD13 | 3:D:256:TYR:CD2  | 2.52                     | 0.44              |
| 1:A:151:LEU:O    | 1:A:155:VAL:HG12 | 2.18                     | 0.44              |
| 1:A:356:VAL:CG2  | 1:A:572:ILE:CD1  | 2.65                     | 0.44              |
| 2:B:206:GLN:HE22 | 4:E:18:UNK:CB    | 2.31                     | 0.44              |
| 3:C:29:HIS:CE1   | 3:C:49:ASP:HB3   | 2.52                     | 0.44              |
| 3:C:363:LEU:HD22 | 3:C:363:LEU:H    | 1.82                     | 0.44              |
| 3:D:105:TRP:CH2  | 3:D:109:TYR:CD1  | 3.05                     | 0.44              |
| 3:D:119:ILE:HD11 | 3:D:154:LEU:HD23 | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:567:PRO:HG2  | 1:A:574:ILE:HD13 | 2.00                     | 0.44              |
| 3:C:9:GLN:HE22   | 3:C:22:TRP:HE1   | 1.66                     | 0.44              |
| 2:B:183:ASP:HA   | 2:B:186:LYS:HE2  | 1.99                     | 0.44              |
| 2:B:636:ILE:HD11 | 3:D:437:TYR:CD1  | 2.52                     | 0.44              |
| 1:A:384:LEU:HB2  | 1:A:389:ASN:HD22 | 1.82                     | 0.44              |
| 3:D:6:ILE:HG21   | 3:D:126:GLU:HB3  | 2.00                     | 0.44              |
| 3:D:199:ASP:O    | 3:D:260:ILE:HD13 | 2.18                     | 0.44              |
| 1:A:140:TYR:CB   | 2:B:324:ASP:HB2  | 2.48                     | 0.44              |
| 3:D:217:PHE:CE1  | 3:D:280:ILE:HD13 | 2.49                     | 0.44              |
| 1:A:151:LEU:CD1  | 2:B:285:ARG:CG   | 2.91                     | 0.44              |
| 3:D:344:PHE:HB2  | 3:D:345:PRO:HD3  | 2.00                     | 0.44              |
| 2:B:505:ASP:HA   | 2:B:550:HIS:HE1  | 1.83                     | 0.44              |
| 3:D:195:ILE:CD1  | 3:D:423:PHE:HE1  | 2.30                     | 0.44              |
| 2:B:296:ILE:CD1  | 2:B:327:ILE:CA   | 2.95                     | 0.44              |
| 2:B:604:MET:SD   | 2:B:769:VAL:HG21 | 2.58                     | 0.44              |
| 3:C:5:ILE:HD13   | 3:C:137:GLN:NE2  | 2.32                     | 0.44              |
| 2:B:570:LEU:HD11 | 2:B:721:ILE:HD13 | 1.98                     | 0.44              |
| 1:A:562:PHE:O    | 1:A:583:GLN:HB3  | 2.18                     | 0.44              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CD1  | 2.76                     | 0.44              |
| 1:A:286:TRP:CE2  | 1:A:351:GLY:HA3  | 2.53                     | 0.44              |
| 2:B:544:ARG:HA   | 2:B:544:ARG:CZ   | 2.47                     | 0.44              |
| 1:A:62:ASP:OD2   | 1:A:98:MET:HE3   | 2.18                     | 0.44              |
| 2:B:227:ALA:HB2  | 2:B:291:ILE:HD13 | 2.00                     | 0.44              |
| 1:A:303:ASP:OD1  | 1:A:304:ASP:O    | 2.36                     | 0.44              |
| 1:A:155:VAL:CG1  | 2:B:281:LYS:HE3  | 2.48                     | 0.43              |
| 1:A:195:GLU:CG   | 1:A:250:ILE:HD11 | 2.41                     | 0.43              |
| 2:B:418:GLU:CB   | 2:B:463:ILE:CD1  | 2.96                     | 0.43              |
| 3:C:188:ILE:HD13 | 3:C:394:PHE:CE2  | 2.50                     | 0.43              |
| 2:B:411:PHE:HB2  | 2:B:721:ILE:HD11 | 1.99                     | 0.43              |
| 2:B:636:ILE:HD12 | 3:D:442:GLN:HA   | 1.99                     | 0.43              |
| 1:A:78:PHE:CD2   | 1:A:80:ASP:O     | 2.71                     | 0.43              |
| 3:C:6:ILE:HD13   | 3:C:126:GLU:HG3  | 2.00                     | 0.43              |
| 1:A:584:ILE:HD11 | 1:A:687:ARG:NE   | 2.29                     | 0.43              |
| 2:B:188:VAL:CG1  | 2:B:224:ILE:HD13 | 2.45                     | 0.43              |
| 1:A:327:ARG:HE   | 1:A:328:LYS:H    | 1.65                     | 0.43              |
| 2:B:483:MET:HG2  | 2:B:489:MET:SD   | 2.58                     | 0.43              |
| 3:C:72:GLU:H     | 3:C:72:GLU:CD    | 2.26                     | 0.43              |
| 3:D:234:ILE:HD13 | 3:D:303:ASN:OD1  | 2.18                     | 0.43              |
| 3:C:70:ASP:CG    | 3:C:71:SER:N     | 2.76                     | 0.43              |
| 3:D:340:GLN:HB3  | 3:D:353:HIS:ND1  | 2.33                     | 0.43              |
| 1:A:599:LEU:HD22 | 1:A:640:ILE:CD1  | 2.41                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:398:LEU:HG   | 2:B:449:ILE:HD12 | 2.00                     | 0.43              |
| 2:B:489:MET:O    | 2:B:493:ILE:HG13 | 2.18                     | 0.43              |
| 3:C:289:HIS:H    | 3:C:289:HIS:CD2  | 2.36                     | 0.43              |
| 3:D:167:LEU:N    | 3:D:167:LEU:HD22 | 2.33                     | 0.43              |
| 2:B:586:ILE:HA   | 2:B:735:ILE:HD13 | 1.99                     | 0.43              |
| 3:C:200:ALA:HB1  | 3:C:260:ILE:HD11 | 1.96                     | 0.43              |
| 3:C:258:THR:HG1  | 3:C:356:ILE:HD11 | 1.80                     | 0.43              |
| 2:B:482:LEU:CD2  | 2:B:657:ILE:HG22 | 2.48                     | 0.43              |
| 1:A:438:PHE:CZ   | 1:A:484:ILE:HD11 | 2.48                     | 0.43              |
| 1:A:557:ILE:HD13 | 1:A:700:PHE:CD2  | 2.53                     | 0.43              |
| 1:A:603:TRP:CZ2  | 1:A:633:HIS:HB2  | 2.54                     | 0.43              |
| 3:D:173:PHE:CE2  | 3:D:191:LEU:HD21 | 2.53                     | 0.43              |
| 3:D:347:TRP:CD1  | 3:D:353:HIS:H    | 2.36                     | 0.43              |
| 1:A:595:HIS:CD2  | 1:A:696:GLN:HE21 | 2.36                     | 0.43              |
| 2:B:364:ILE:HD11 | 2:B:403:PHE:HA   | 1.98                     | 0.43              |
| 2:B:465:ASN:HB3  | 2:B:471:ARG:HE   | 1.83                     | 0.43              |
| 3:C:189:LEU:HD21 | 3:C:420:GLN:HG2  | 2.00                     | 0.43              |
| 1:A:599:LEU:HD21 | 1:A:640:ILE:HD12 | 1.99                     | 0.43              |
| 1:A:112:TYR:OH   | 1:A:177:ILE:CD1  | 2.67                     | 0.43              |
| 2:B:383:ILE:HD12 | 2:B:410:ILE:HD12 | 1.88                     | 0.43              |
| 1:A:151:LEU:HD22 | 2:B:285:ARG:CD   | 2.35                     | 0.43              |
| 2:B:405:ILE:CG2  | 2:B:456:ILE:HD13 | 2.47                     | 0.43              |
| 2:B:323:GLY:CA   | 2:B:327:ILE:HD12 | 2.48                     | 0.43              |
| 1:A:140:TYR:CE1  | 2:B:292:ILE:HD13 | 2.52                     | 0.43              |
| 1:A:439:LEU:HD22 | 1:A:594:TYR:HA   | 2.00                     | 0.43              |
| 3:C:264:GLU:HB2  | 3:C:433:LEU:HG   | 2.00                     | 0.43              |
| 3:D:70:ASP:CG    | 3:D:71:SER:H     | 2.27                     | 0.43              |
| 1:A:199:GLU:CD   | 1:A:250:ILE:HD11 | 2.39                     | 0.43              |
| 2:B:398:LEU:CD1  | 2:B:449:ILE:HD12 | 2.48                     | 0.43              |
| 2:B:586:ILE:HD11 | 2:B:732:LEU:CB   | 2.49                     | 0.43              |
| 3:D:328:PRO:HG2  | 3:D:331:ILE:CD1  | 2.49                     | 0.43              |
| 3:D:111:ILE:HG12 | 3:D:114:ARG:NH2  | 2.33                     | 0.43              |
| 1:A:150:TYR:CE1  | 1:A:177:ILE:CD1  | 3.01                     | 0.43              |
| 2:B:480:ILE:CD1  | 2:B:520:VAL:HG13 | 2.47                     | 0.43              |
| 1:A:147:GLU:CB   | 2:B:285:ARG:HD3  | 2.47                     | 0.43              |
| 1:A:138:PHE:O    | 1:A:142:ILE:HG13 | 2.18                     | 0.43              |
| 2:B:209:ILE:CD1  | 2:B:213:ILE:HD13 | 2.48                     | 0.43              |
| 2:B:525:LEU:O    | 2:B:525:LEU:HD13 | 2.19                     | 0.43              |
| 1:A:78:PHE:HB3   | 1:A:90:ILE:HD12  | 2.01                     | 0.43              |
| 1:A:557:ILE:CD1  | 1:A:700:PHE:CE2  | 3.01                     | 0.43              |
| 1:A:606:LEU:CG   | 1:A:710:ILE:HD11 | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:362:PHE:HE2  | 2:B:364:ILE:HD12 | 1.84                     | 0.43              |
| 2:B:631:LEU:HD12 | 2:B:780:ASN:HD22 | 1.83                     | 0.43              |
| 1:A:363:ILE:HD11 | 1:A:404:ILE:HG21 | 1.99                     | 0.43              |
| 2:B:608:ASN:HD21 | 3:D:260:ILE:HB   | 1.83                     | 0.43              |
| 2:B:362:PHE:CE2  | 2:B:364:ILE:HD12 | 2.54                     | 0.43              |
| 2:B:427:LYS:HE3  | 2:B:431:VAL:HG13 | 2.01                     | 0.43              |
| 1:A:425:ILE:HD12 | 1:A:478:MET:CG   | 2.49                     | 0.43              |
| 1:A:152:LYS:HA   | 2:B:285:ARG:NH2  | 2.33                     | 0.43              |
| 3:C:275:PHE:CB   | 3:C:284:ILE:HD11 | 2.45                     | 0.43              |
| 2:B:339:ILE:HG21 | 2:B:439:ARG:HG2  | 2.01                     | 0.43              |
| 1:A:120:THR:HA   | 1:A:123:TYR:CE2  | 2.53                     | 0.43              |
| 1:A:296:TYR:CZ   | 2:B:318:ILE:HD11 | 2.54                     | 0.43              |
| 1:A:151:LEU:HD12 | 2:B:285:ARG:HH21 | 1.84                     | 0.43              |
| 2:B:204:HIS:O    | 2:B:204:HIS:CG   | 2.72                     | 0.43              |
| 1:A:66:VAL:O     | 1:A:75:ILE:HD11  | 2.18                     | 0.43              |
| 1:A:367:PRO:HB3  | 1:A:404:ILE:HD12 | 1.97                     | 0.43              |
| 2:B:560:LEU:HB2  | 2:B:587:PHE:CE2  | 2.54                     | 0.43              |
| 1:A:595:HIS:CE1  | 1:A:640:ILE:HD11 | 2.54                     | 0.43              |
| 1:A:425:ILE:HD11 | 1:A:482:LEU:CD2  | 2.46                     | 0.43              |
| 1:A:158:LEU:HD22 | 2:B:281:LYS:HZ3  | 1.82                     | 0.43              |
| 1:A:366:ILE:HB   | 1:A:367:PRO:HD3  | 2.00                     | 0.43              |
| 1:A:135:LEU:HD11 | 1:A:247:ILE:HD13 | 1.99                     | 0.43              |
| 2:B:743:THR:HG22 | 2:B:759:PRO:HD3  | 2.01                     | 0.43              |
| 3:C:230:LEU:O    | 3:C:234:ILE:HG13 | 2.18                     | 0.43              |
| 3:D:51:LYS:H     | 3:D:52:PRO:CD    | 2.32                     | 0.43              |
| 3:C:5:ILE:HD12   | 3:C:53:PHE:CZ    | 2.53                     | 0.43              |
| 2:B:822:ARG:HH22 | 2:B:841:LEU:HD22 | 1.84                     | 0.43              |
| 3:C:212:ILE:HD13 | 3:C:275:PHE:CE1  | 2.53                     | 0.43              |
| 3:D:270:PRO:CB   | 3:D:375:MET:HE1  | 2.49                     | 0.43              |
| 3:C:67:ILE:HD12  | 3:C:123:ILE:HG23 | 1.96                     | 0.43              |
| 3:D:127:ILE:CD1  | 3:D:162:TYR:CE2  | 3.01                     | 0.43              |
| 3:D:188:ILE:HD11 | 3:D:394:PHE:CG   | 2.37                     | 0.43              |
| 1:A:421:HIS:O    | 1:A:425:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:140:TYR:CG   | 2:B:324:ASP:CB   | 3.01                     | 0.43              |
| 1:A:129:THR:C    | 2:B:322:HIS:CE1  | 2.96                     | 0.43              |
| 1:A:425:ILE:CD1  | 1:A:482:LEU:HD13 | 2.46                     | 0.43              |
| 2:B:430:HIS:HB3  | 2:B:448:ILE:HG21 | 2.01                     | 0.43              |
| 3:C:393:THR:O    | 3:C:397:VAL:HG23 | 2.18                     | 0.43              |
| 1:A:557:ILE:HD11 | 1:A:594:TYR:HD2  | 1.83                     | 0.43              |
| 2:B:602:LYS:HE3  | 2:B:602:LYS:HB3  | 1.95                     | 0.43              |
| 3:D:259:LEU:HD21 | 3:D:377:LEU:HB3  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:808:ASN:ND2  | 2:B:812:ILE:HD11 | 2.34                     | 0.43              |
| 1:A:632:LEU:HD11 | 1:A:765:ILE:HA   | 2.01                     | 0.43              |
| 3:D:333:ARG:HD3  | 3:D:333:ARG:C    | 2.43                     | 0.43              |
| 1:A:780:ILE:CD1  | 1:A:789:GLU:CB   | 2.96                     | 0.43              |
| 3:C:9:GLN:HE22   | 3:C:22:TRP:HE1   | 1.67                     | 0.43              |
| 1:A:641:LYS:CG   | 3:C:356:ILE:HD12 | 2.49                     | 0.43              |
| 3:D:322:ILE:HD12 | 3:D:375:MET:HE2  | 2.01                     | 0.43              |
| 3:D:70:ASP:HA    | 3:D:146:THR:HG21 | 2.00                     | 0.42              |
| 3:C:292:TYR:CD2  | 3:C:372:VAL:HG12 | 2.54                     | 0.42              |
| 3:D:412:LEU:HG   | 3:D:419:VAL:HG11 | 2.00                     | 0.42              |
| 1:A:62:ASP:HB3   | 1:A:94:ILE:HD13  | 2.01                     | 0.42              |
| 1:A:425:ILE:HG23 | 1:A:426:PHE:CD1  | 2.54                     | 0.42              |
| 2:B:199:LEU:HD23 | 2:B:200:PHE:CE2  | 2.53                     | 0.42              |
| 2:B:636:ILE:HD13 | 2:B:636:ILE:HG21 | 1.87                     | 0.42              |
| 3:D:255:ILE:CD1  | 3:D:358:ARG:CD   | 2.95                     | 0.42              |
| 2:B:184:ILE:HD11 | 2:B:213:ILE:HG13 | 2.01                     | 0.42              |
| 2:B:350:LEU:HD22 | 2:B:405:ILE:HG13 | 2.00                     | 0.42              |
| 2:B:398:LEU:CD1  | 2:B:449:ILE:CD1  | 2.90                     | 0.42              |
| 3:C:7:THR:O      | 3:C:66:ALA:HA    | 2.19                     | 0.42              |
| 3:D:133:PHE:CZ   | 3:D:135:GLY:O    | 2.72                     | 0.42              |
| 1:A:123:TYR:OH   | 2:B:288:TYR:CZ   | 2.51                     | 0.42              |
| 1:A:128:ASP:C    | 2:B:322:HIS:HE1  | 2.28                     | 0.42              |
| 2:B:214:PRO:HB2  | 2:B:217:GLU:CB   | 2.49                     | 0.42              |
| 2:B:261:LEU:HD12 | 2:B:293:ARG:HH22 | 1.84                     | 0.42              |
| 3:C:210:LEU:HD22 | 3:C:222:ILE:CD1  | 2.49                     | 0.42              |
| 2:B:216:PHE:O    | 2:B:216:PHE:CG   | 2.72                     | 0.42              |
| 3:D:209:LEU:HD21 | 3:D:231:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:779:LEU:HD22 | 1:A:779:LEU:HA   | 1.84                     | 0.42              |
| 3:D:127:ILE:CD1  | 3:D:162:TYR:CZ   | 3.02                     | 0.42              |
| 1:A:348:LEU:HD23 | 1:A:352:ILE:CD1  | 2.49                     | 0.42              |
| 3:C:299:LEU:HD22 | 3:C:299:LEU:H    | 1.84                     | 0.42              |
| 3:C:24:GLN:HE22  | 3:C:233:THR:HA   | 1.85                     | 0.42              |
| 3:D:316:PHE:CD1  | 3:D:345:PRO:HB3  | 2.55                     | 0.42              |
| 3:D:204:PHE:CD2  | 3:D:231:ILE:HG23 | 2.54                     | 0.42              |
| 1:A:68:ILE:HG22  | 1:A:158:LEU:HD13 | 2.00                     | 0.42              |
| 1:A:372:ASP:OD1  | 1:A:375:ILE:HD12 | 2.18                     | 0.42              |
| 2:B:188:VAL:HG21 | 2:B:280:LEU:HD22 | 2.00                     | 0.42              |
| 2:B:209:ILE:CD1  | 2:B:218:SER:CB   | 2.66                     | 0.42              |
| 1:A:123:TYR:HA   | 1:A:126:TRP:CE3  | 2.54                     | 0.42              |
| 2:B:405:ILE:CG2  | 2:B:456:ILE:CD1  | 2.74                     | 0.42              |
| 1:A:630:ARG:HA   | 1:A:633:HIS:CD2  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:527:HIS:CG   | 2:B:527:HIS:O    | 2.70                     | 0.42              |
| 3:C:266:HIS:CD2  | 3:C:266:HIS:H    | 2.38                     | 0.42              |
| 3:D:202:VAL:HG22 | 3:D:268:LEU:HD23 | 2.00                     | 0.42              |
| 2:B:348:ASN:OD1  | 2:B:355:LEU:HD23 | 2.20                     | 0.42              |
| 2:B:634:ILE:CD1  | 2:B:776:TYR:HE1  | 2.16                     | 0.42              |
| 2:B:500:LEU:HD21 | 2:B:558:PHE:HB2  | 2.00                     | 0.42              |
| 2:B:660:ASN:HD22 | 2:B:735:ILE:HG23 | 1.85                     | 0.42              |
| 2:B:402:ILE:CD1  | 2:B:449:ILE:CD1  | 2.96                     | 0.42              |
| 2:B:463:ILE:HD13 | 2:B:463:ILE:HG21 | 1.79                     | 0.42              |
| 3:C:188:ILE:HD11 | 3:C:394:PHE:CG   | 2.21                     | 0.42              |
| 1:A:154:LEU:CD2  | 2:B:281:LYS:HZ1  | 2.29                     | 0.42              |
| 1:A:693:ILE:HG23 | 1:A:694:PRO:HD3  | 2.00                     | 0.42              |
| 3:D:231:ILE:O    | 3:D:235:ILE:HG13 | 2.18                     | 0.42              |
| 1:A:357:VAL:HG23 | 1:A:363:ILE:CD1  | 2.49                     | 0.42              |
| 2:B:427:LYS:HD3  | 2:B:452:GLN:HE22 | 1.83                     | 0.42              |
| 3:C:238:VAL:CG1  | 3:C:375:MET:HE2  | 2.50                     | 0.42              |
| 1:A:70:LEU:HG    | 2:B:281:LYS:HZ3  | 1.67                     | 0.42              |
| 1:A:151:LEU:HD12 | 2:B:282:SER:HA   | 2.02                     | 0.42              |
| 1:A:625:ILE:HD13 | 1:A:765:ILE:CG1  | 2.49                     | 0.42              |
| 2:B:526:ARG:O    | 2:B:538:ILE:HD11 | 2.19                     | 0.42              |
| 1:A:137:ARG:CZ   | 2:B:325:LEU:HD22 | 2.49                     | 0.42              |
| 3:D:6:ILE:HD11   | 3:D:126:GLU:HB3  | 2.02                     | 0.42              |
| 3:C:188:ILE:HD11 | 3:C:394:PHE:CG   | 2.52                     | 0.42              |
| 1:A:63:LEU:HD23  | 1:A:170:ILE:HD12 | 2.02                     | 0.42              |
| 1:A:114:LYS:HE3  | 1:A:118:ILE:HD12 | 2.00                     | 0.42              |
| 3:D:188:ILE:CD1  | 3:D:394:PHE:CG   | 3.02                     | 0.42              |
| 1:A:603:TRP:CD2  | 1:A:633:HIS:HB2  | 2.55                     | 0.42              |
| 2:B:482:LEU:HD13 | 2:B:731:PHE:CZ   | 2.55                     | 0.42              |
| 2:B:641:PHE:CD1  | 2:B:765:LEU:HD21 | 2.55                     | 0.42              |
| 3:C:238:VAL:CG2  | 3:C:322:ILE:HD13 | 2.43                     | 0.42              |
| 2:B:188:VAL:HB   | 2:B:224:ILE:CD1  | 2.48                     | 0.42              |
| 3:C:29:HIS:CE1   | 3:C:49:ASP:HA    | 2.54                     | 0.42              |
| 3:D:356:ILE:CD1  | 3:D:358:ARG:NH1  | 2.69                     | 0.42              |
| 3:C:275:PHE:O    | 3:C:276:THR:HG23 | 2.20                     | 0.42              |
| 1:A:375:ILE:HD11 | 1:A:396:LYS:CG   | 2.50                     | 0.42              |
| 1:A:375:ILE:HD11 | 1:A:396:LYS:HB3  | 2.00                     | 0.42              |
| 3:D:72:GLU:O     | 3:D:76:ILE:HG13  | 2.19                     | 0.42              |
| 2:B:349:TRP:CE2  | 2:B:364:ILE:CD1  | 3.03                     | 0.42              |
| 2:B:449:ILE:HD13 | 2:B:449:ILE:HG21 | 1.87                     | 0.42              |
| 3:D:142:VAL:O    | 3:D:142:VAL:HG12 | 2.20                     | 0.42              |
| 3:D:69:MET:SD    | 3:D:119:ILE:HD11 | 2.59                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:405:ILE:CG1  | 2:B:456:ILE:HD13 | 2.49                     | 0.42              |
| 1:A:598:LEU:HD13 | 1:A:598:LEU:HA   | 1.89                     | 0.42              |
| 3:D:75:VAL:HG11  | 3:D:94:VAL:HG22  | 2.02                     | 0.42              |
| 2:B:253:LEU:HD22 | 2:B:334:LEU:HD23 | 2.00                     | 0.42              |
| 2:B:322:HIS:HD2  | 2:B:327:ILE:CD1  | 2.33                     | 0.42              |
| 2:B:586:ILE:CG2  | 2:B:735:ILE:HD12 | 2.14                     | 0.42              |
| 3:C:270:PRO:HB2  | 3:C:375:MET:HE1  | 2.02                     | 0.42              |
| 3:D:119:ILE:O    | 3:D:123:ILE:HG13 | 2.20                     | 0.42              |
| 1:A:425:ILE:HD12 | 1:A:478:MET:O    | 2.20                     | 0.42              |
| 2:B:349:TRP:CD1  | 2:B:364:ILE:HD12 | 2.52                     | 0.42              |
| 3:C:272:PHE:O    | 3:C:275:PHE:CE1  | 2.73                     | 0.42              |
| 3:D:9:GLN:HE21   | 3:D:15:ASN:HA    | 1.84                     | 0.42              |
| 1:A:73:THR:H     | 2:B:215:ASN:CA   | 2.33                     | 0.42              |
| 1:A:570:LEU:HB3  | 1:A:573:ILE:HD12 | 2.00                     | 0.42              |
| 3:C:258:THR:CB   | 3:C:356:ILE:CD1  | 2.97                     | 0.42              |
| 1:A:415:LEU:HD22 | 1:A:663:TYR:CE1  | 2.55                     | 0.42              |
| 2:B:311:THR:O    | 2:B:314:ILE:HG12 | 2.20                     | 0.42              |
| 2:B:480:ILE:CD1  | 2:B:541:LEU:CD1  | 2.98                     | 0.42              |
| 3:D:289:HIS:CD2  | 3:D:289:HIS:H    | 2.37                     | 0.42              |
| 1:A:632:LEU:C    | 1:A:632:LEU:HD13 | 2.45                     | 0.42              |
| 2:B:264:TYR:CD2  | 2:B:287:ILE:HD11 | 2.47                     | 0.42              |
| 2:B:287:ILE:HG23 | 2:B:291:ILE:HD11 | 2.01                     | 0.42              |
| 2:B:651:TYR:CE1  | 3:D:333:ARG:HG2  | 2.55                     | 0.42              |
| 3:C:256:TYR:CZ   | 3:C:260:ILE:HD12 | 2.52                     | 0.42              |
| 3:D:173:PHE:CD1  | 3:D:174:PRO:HD2  | 2.54                     | 0.42              |
| 1:A:405:PHE:HZ   | 1:A:573:ILE:HD11 | 1.83                     | 0.42              |
| 3:C:105:TRP:CH2  | 3:C:109:TYR:CE2  | 3.08                     | 0.42              |
| 3:C:320:ASN:HD21 | 3:C:358:ARG:HG3  | 1.84                     | 0.42              |
| 2:B:574:VAL:O    | 2:B:574:VAL:HG13 | 2.19                     | 0.42              |
| 3:C:299:LEU:H    | 3:C:299:LEU:CD2  | 2.33                     | 0.42              |
| 1:A:136:GLN:HG2  | 2:B:324:ASP:H    | 1.85                     | 0.42              |
| 1:A:566:ILE:HG22 | 1:A:579:MET:HE2  | 2.02                     | 0.42              |
| 1:A:259:LEU:HD22 | 1:A:259:LEU:HA   | 1.96                     | 0.42              |
| 1:A:450:TYR:CE1  | 1:A:559:HIS:CE1  | 3.08                     | 0.42              |
| 1:A:650:ASN:HD21 | 3:C:333:ARG:HD3  | 1.84                     | 0.42              |
| 2:B:499:ILE:HD13 | 2:B:511:LYS:CB   | 2.49                     | 0.42              |
| 1:A:80:ASP:O     | 1:A:90:ILE:N     | 2.53                     | 0.42              |
| 1:A:585:ILE:CD1  | 1:A:683:ILE:HD11 | 2.49                     | 0.42              |
| 3:C:5:ILE:HD12   | 3:C:53:PHE:CE2   | 2.55                     | 0.42              |
| 1:A:375:ILE:HD13 | 1:A:396:LYS:CD   | 2.48                     | 0.42              |
| 1:A:449:HIS:CG   | 1:A:450:TYR:H    | 2.37                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:584:ILE:CD1  | 1:A:687:ARG:CB   | 2.98                     | 0.42              |
| 2:B:238:VAL:O    | 2:B:254:ILE:HD12 | 2.20                     | 0.42              |
| 1:A:245:GLY:HA3  | 1:A:332:LEU:HA   | 2.02                     | 0.42              |
| 2:B:411:PHE:CE1  | 2:B:570:LEU:HD23 | 2.55                     | 0.42              |
| 2:B:485:LYS:HG2  | 2:B:488:PHE:H    | 1.85                     | 0.41              |
| 2:B:567:PRO:C    | 2:B:721:ILE:HD11 | 2.44                     | 0.41              |
| 2:B:772:PHE:HB2  | 2:B:812:ILE:CD1  | 2.46                     | 0.41              |
| 2:B:210:PRO:HG2  | 2:B:213:ILE:CD1  | 2.47                     | 0.41              |
| 1:A:66:VAL:HG23  | 1:A:94:ILE:CD1   | 2.47                     | 0.41              |
| 3:D:234:ILE:HD13 | 3:D:303:ASN:CG   | 2.45                     | 0.41              |
| 1:A:595:HIS:HE2  | 1:A:699:ILE:HG22 | 1.85                     | 0.41              |
| 1:A:602:THR:CG2  | 1:A:710:ILE:HD12 | 2.48                     | 0.41              |
| 1:A:105:PHE:CZ   | 1:A:177:ILE:HD12 | 2.55                     | 0.41              |
| 1:A:137:ARG:HE   | 2:B:328:ARG:NH2  | 2.18                     | 0.41              |
| 2:B:192:LEU:CD2  | 2:B:227:ALA:HB3  | 2.50                     | 0.41              |
| 2:B:533:ARG:O    | 2:B:538:ILE:HD12 | 2.19                     | 0.41              |
| 3:D:69:MET:O     | 3:D:70:ASP:HB2   | 2.20                     | 0.41              |
| 1:A:585:ILE:HD12 | 1:A:683:ILE:HD11 | 2.01                     | 0.41              |
| 3:C:193:ARG:HH12 | 3:C:419:VAL:CG1  | 2.32                     | 0.41              |
| 3:D:119:ILE:HD12 | 3:D:154:LEU:HD23 | 2.01                     | 0.41              |
| 1:A:449:HIS:CD2  | 1:A:450:TYR:H    | 2.38                     | 0.41              |
| 1:A:115:GLN:O    | 1:A:118:ILE:HG22 | 2.20                     | 0.41              |
| 1:A:119:LEU:HD21 | 1:A:143:ARG:HA   | 2.00                     | 0.41              |
| 1:A:714:ARG:HH12 | 1:A:758:LEU:HD13 | 1.84                     | 0.41              |
| 1:A:65:ASN:OD1   | 2:B:216:PHE:HD1  | 1.93                     | 0.41              |
| 2:B:543:ALA:HB2  | 2:B:558:PHE:CE2  | 2.55                     | 0.41              |
| 2:B:192:LEU:HD22 | 2:B:268:VAL:HG21 | 2.02                     | 0.41              |
| 3:C:256:TYR:CD1  | 3:C:260:ILE:HD11 | 2.52                     | 0.41              |
| 3:D:333:ARG:HH11 | 3:D:333:ARG:HD3  | 1.68                     | 0.41              |
| 1:A:56:GLU:O     | 1:A:60:VAL:HG23  | 2.20                     | 0.41              |
| 1:A:140:TYR:CE1  | 2:B:292:ILE:CD1  | 3.03                     | 0.41              |
| 1:A:425:ILE:CD1  | 1:A:478:MET:HA   | 2.33                     | 0.41              |
| 1:A:363:ILE:HD11 | 1:A:413:TYR:CB   | 2.45                     | 0.41              |
| 1:A:151:LEU:O    | 1:A:155:VAL:HG23 | 2.20                     | 0.41              |
| 2:B:349:TRP:CD1  | 2:B:362:PHE:CE2  | 3.08                     | 0.41              |
| 1:A:557:ILE:HD11 | 1:A:594:TYR:CD2  | 2.55                     | 0.41              |
| 1:A:71:GLU:OE1   | 2:B:222:HIS:CE1  | 2.71                     | 0.41              |
| 2:B:323:GLY:O    | 2:B:327:ILE:HD12 | 2.20                     | 0.41              |
| 1:A:416:ILE:CD1  | 1:A:664:ARG:HG2  | 2.48                     | 0.41              |
| 1:A:70:LEU:HD22  | 2:B:219:GLY:HA2  | 2.01                     | 0.41              |
| 1:A:787:SER:HB2  | 1:A:790:LYS:HG2  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:121:ASN:HD22 | 3:D:218:ARG:HH12 | 1.50                     | 0.41              |
| 1:A:489:GLU:HG3  | 1:A:559:HIS:CE1  | 2.55                     | 0.41              |
| 1:A:606:LEU:CG   | 1:A:710:ILE:HD11 | 2.50                     | 0.41              |
| 1:A:795:ASP:O    | 1:A:799:VAL:HG23 | 2.20                     | 0.41              |
| 3:D:70:ASP:HA    | 3:D:146:THR:HG21 | 2.02                     | 0.41              |
| 1:A:63:LEU:HD13  | 1:A:98:MET:HE2   | 2.02                     | 0.41              |
| 2:B:269:ASN:HA   | 2:B:272:VAL:HG22 | 2.01                     | 0.41              |
| 2:B:342:TYR:CZ   | 2:B:394:ILE:HD12 | 2.56                     | 0.41              |
| 1:A:409:PHE:HB3  | 1:A:415:LEU:HD22 | 2.02                     | 0.41              |
| 3:D:199:ASP:HB3  | 3:D:260:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:151:LEU:HD23 | 2:B:285:ARG:NE   | 1.82                     | 0.41              |
| 1:A:372:ASP:CG   | 1:A:375:ILE:HD12 | 2.44                     | 0.41              |
| 2:B:719:LEU:HD23 | 2:B:719:LEU:HA   | 1.82                     | 0.41              |
| 2:B:527:HIS:HB2  | 2:B:533:ARG:HD2  | 2.02                     | 0.41              |
| 3:C:72:GLU:H     | 3:C:73:PRO:HD2   | 1.85                     | 0.41              |
| 1:A:138:PHE:CZ   | 1:A:142:ILE:HD11 | 2.56                     | 0.41              |
| 2:B:214:PRO:HB2  | 2:B:217:GLU:HB3  | 2.02                     | 0.41              |
| 1:A:173:LEU:C    | 1:A:173:LEU:HD23 | 2.45                     | 0.41              |
| 3:C:292:TYR:CD2  | 3:C:372:VAL:HB   | 2.56                     | 0.41              |
| 1:A:70:LEU:HD13  | 2:B:220:LEU:CG   | 2.50                     | 0.41              |
| 3:C:273:THR:HG23 | 3:C:295:MET:HE2  | 2.02                     | 0.41              |
| 3:D:381:SER:O    | 3:D:384:VAL:HG22 | 2.20                     | 0.41              |
| 2:B:242:ARG:N    | 2:B:254:ILE:HD11 | 2.33                     | 0.41              |
| 2:B:405:ILE:HG12 | 2:B:456:ILE:HD12 | 2.03                     | 0.41              |
| 2:B:823:LEU:HD13 | 2:B:824:TYR:N    | 2.35                     | 0.41              |
| 1:A:695:LEU:HD22 | 1:A:793:PHE:CE2  | 2.55                     | 0.41              |
| 2:B:644:PHE:HB3  | 2:B:648:MET:HE3  | 2.03                     | 0.41              |
| 1:A:128:ASP:OD2  | 2:B:295:ARG:CD   | 2.67                     | 0.41              |
| 2:B:564:LEU:HD12 | 2:B:568:LEU:HD23 | 2.03                     | 0.41              |
| 3:D:408:ASN:ND2  | 3:D:417:GLN:HE21 | 2.19                     | 0.41              |
| 1:A:296:TYR:HH   | 2:B:322:HIS:CE1  | 2.24                     | 0.41              |
| 3:D:188:ILE:HG23 | 3:D:423:PHE:CD2  | 2.56                     | 0.41              |
| 1:A:151:LEU:CD2  | 2:B:285:ARG:HD3  | 2.39                     | 0.41              |
| 2:B:335:PHE:CD1  | 2:B:339:ILE:CD1  | 2.99                     | 0.41              |
| 3:C:234:ILE:HD11 | 3:C:303:ASN:ND2  | 2.35                     | 0.41              |
| 1:A:73:THR:CB    | 2:B:215:ASN:HA   | 2.50                     | 0.41              |
| 1:A:143:ARG:HD2  | 2:B:292:ILE:HD13 | 1.99                     | 0.41              |
| 1:A:425:ILE:HD13 | 1:A:482:LEU:CG   | 2.51                     | 0.41              |
| 2:B:572:LEU:HD23 | 2:B:572:LEU:HA   | 1.89                     | 0.41              |
| 1:A:684:MET:HE1  | 1:A:687:ARG:NH2  | 2.36                     | 0.41              |
| 2:B:430:HIS:HB3  | 2:B:448:ILE:HD13 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:305:LEU:O    | 3:C:306:VAL:HG13 | 2.20                     | 0.41              |
| 1:A:606:LEU:CD2  | 1:A:710:ILE:HD11 | 2.51                     | 0.41              |
| 3:C:67:ILE:HD11  | 3:C:123:ILE:HA   | 2.03                     | 0.41              |
| 2:B:296:ILE:HD13 | 2:B:327:ILE:CA   | 2.44                     | 0.41              |
| 2:B:636:ILE:HD11 | 3:D:437:TYR:CE2  | 2.47                     | 0.41              |
| 3:C:260:ILE:HD13 | 3:C:266:HIS:HB2  | 2.03                     | 0.41              |
| 3:D:95:ALA:HB1   | 3:D:111:ILE:HD13 | 1.97                     | 0.41              |
| 3:D:345:PRO:O    | 3:D:347:TRP:CE2  | 2.74                     | 0.41              |
| 3:D:222:ILE:HD13 | 3:D:222:ILE:HG21 | 1.78                     | 0.41              |
| 1:A:128:ASP:CA   | 2:B:322:HIS:HE2  | 2.29                     | 0.41              |
| 1:A:68:ILE:HD12  | 1:A:158:LEU:HD21 | 1.87                     | 0.41              |
| 1:A:113:GLY:HA2  | 1:A:116:TYR:CE2  | 2.55                     | 0.41              |
| 1:A:247:ILE:CG2  | 1:A:275:ILE:HD13 | 2.51                     | 0.41              |
| 2:B:591:TRP:CD1  | 2:B:595:LYS:HZ2  | 2.39                     | 0.41              |
| 3:C:342:ILE:HD12 | 3:C:344:PHE:CE1  | 2.56                     | 0.41              |
| 3:C:142:VAL:HG13 | 3:C:190:ALA:CB   | 2.50                     | 0.41              |
| 1:A:469:ARG:HH21 | 1:A:477:LEU:HG   | 1.84                     | 0.41              |
| 3:C:5:ILE:HD12   | 3:C:53:PHE:CZ    | 2.55                     | 0.41              |
| 1:A:626:VAL:O    | 1:A:630:ARG:HG2  | 2.21                     | 0.41              |
| 3:D:111:ILE:HA   | 3:D:114:ARG:HE   | 1.85                     | 0.41              |
| 3:D:136:PHE:CZ   | 3:D:158:LEU:HD12 | 2.55                     | 0.41              |
| 3:D:347:TRP:CE3  | 3:D:347:TRP:HA   | 2.56                     | 0.41              |
| 3:D:366:GLN:CD   | 3:D:367:PRO:HD2  | 2.46                     | 0.41              |
| 2:B:257:ILE:HD13 | 2:B:257:ILE:HG21 | 1.93                     | 0.41              |
| 1:A:68:ILE:CD1   | 2:B:215:ASN:HB3  | 2.50                     | 0.41              |
| 1:A:98:MET:CE    | 1:A:170:ILE:HD11 | 2.51                     | 0.41              |
| 2:B:346:LEU:CD1  | 2:B:402:ILE:HD13 | 2.49                     | 0.41              |
| 2:B:507:LEU:HB3  | 2:B:508:PRO:HD3  | 2.03                     | 0.41              |
| 1:A:348:LEU:HD23 | 1:A:352:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:358:ARG:HA   | 1:A:363:ILE:HB   | 2.03                     | 0.41              |
| 3:C:188:ILE:HD12 | 3:C:394:PHE:HD2  | 1.82                     | 0.41              |
| 3:D:230:LEU:O    | 3:D:234:ILE:HG13 | 2.20                     | 0.41              |
| 1:A:362:GLN:HB3  | 2:B:446:PHE:CZ   | 2.53                     | 0.41              |
| 2:B:600:TYR:CE1  | 2:B:765:LEU:HB3  | 2.55                     | 0.41              |
| 2:B:634:ILE:HD13 | 2:B:634:ILE:HG21 | 1.92                     | 0.41              |
| 1:A:159:GLU:OE1  | 2:B:277:VAL:HG12 | 2.21                     | 0.41              |
| 1:A:365:THR:C    | 1:A:404:ILE:CD1  | 2.94                     | 0.41              |
| 1:A:564:ILE:HD13 | 1:A:564:ILE:HG21 | 1.91                     | 0.41              |
| 3:D:6:ILE:HD13   | 3:D:126:GLU:HB2  | 2.03                     | 0.41              |
| 3:D:212:ILE:HD13 | 3:D:275:PHE:CE2  | 2.55                     | 0.41              |
| 1:A:247:ILE:CD1  | 1:A:275:ILE:HD13 | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:248:LEU:HD11 | 1:A:279:TYR:CG   | 2.56                     | 0.41              |
| 2:B:546:LEU:HB3  | 2:B:547:ASP:H    | 1.68                     | 0.41              |
| 1:A:195:GLU:CG   | 1:A:250:ILE:HD13 | 2.51                     | 0.41              |
| 1:A:778:CYS:HA   | 1:A:781:ASN:HD22 | 1.86                     | 0.41              |
| 2:B:405:ILE:CG2  | 2:B:456:ILE:CD1  | 2.96                     | 0.41              |
| 2:B:563:ILE:HG12 | 2:B:564:LEU:N    | 2.36                     | 0.41              |
| 3:D:95:ALA:HB1   | 3:D:111:ILE:CD1  | 2.51                     | 0.41              |
| 1:A:247:ILE:HG21 | 1:A:275:ILE:HD13 | 2.03                     | 0.41              |
| 2:B:656:ILE:HG21 | 2:B:738:HIS:CE1  | 2.56                     | 0.41              |
| 1:A:68:ILE:CD1   | 2:B:216:PHE:HB3  | 2.51                     | 0.41              |
| 1:A:303:ASP:C    | 1:A:304:ASP:O    | 2.59                     | 0.41              |
| 1:A:558:TYR:CA   | 1:A:693:ILE:HD11 | 2.48                     | 0.41              |
| 2:B:516:LEU:HD21 | 2:B:541:LEU:HB3  | 2.02                     | 0.41              |
| 1:A:415:LEU:HD13 | 1:A:570:LEU:HG   | 2.03                     | 0.41              |
| 1:A:630:ARG:HA   | 1:A:633:HIS:ND1  | 2.36                     | 0.41              |
| 2:B:470:TYR:HE2  | 2:B:724:LEU:HD22 | 1.86                     | 0.41              |
| 2:B:665:THR:O    | 2:B:669:GLN:HG2  | 2.21                     | 0.41              |
| 3:D:238:VAL:HG13 | 3:D:322:ILE:HD12 | 2.02                     | 0.41              |
| 2:B:349:TRP:CE3  | 2:B:364:ILE:HD11 | 2.56                     | 0.40              |
| 2:B:822:ARG:NH2  | 2:B:841:LEU:HD22 | 2.35                     | 0.40              |
| 3:C:188:ILE:HD13 | 3:C:394:PHE:CD2  | 2.52                     | 0.40              |
| 1:A:188:LEU:HD22 | 1:A:268:LEU:HD11 | 2.03                     | 0.40              |
| 3:C:125:LYS:HD3  | 3:D:283:ASP:OD2  | 2.20                     | 0.40              |
| 3:C:129:SER:HB3  | 3:D:284:ILE:HB   | 2.03                     | 0.40              |
| 3:C:315:TYR:CE2  | 3:C:438:VAL:O    | 2.74                     | 0.40              |
| 2:B:765:LEU:O    | 2:B:769:VAL:HG23 | 2.20                     | 0.40              |
| 1:A:291:ILE:HD12 | 1:A:358:ARG:NH1  | 2.33                     | 0.40              |
| 1:A:292:LEU:HD21 | 1:A:299:PHE:CD2  | 2.56                     | 0.40              |
| 2:B:535:SER:H    | 2:B:538:ILE:HD11 | 1.86                     | 0.40              |
| 3:D:256:TYR:HE1  | 3:D:260:ILE:CD1  | 2.23                     | 0.40              |
| 3:D:375:MET:HE3  | 3:D:377:LEU:HD22 | 2.01                     | 0.40              |
| 3:C:128:ASP:OD2  | 3:D:281:HIS:CD2  | 2.74                     | 0.40              |
| 3:D:291:SER:O    | 3:D:295:MET:HG3  | 2.22                     | 0.40              |
| 1:A:774:ILE:HD13 | 1:A:796:SER:HB2  | 2.01                     | 0.40              |
| 3:C:107:ASN:HD21 | 3:C:409:VAL:HG23 | 1.86                     | 0.40              |
| 3:D:106:ALA:CB   | 3:D:407:TYR:HA   | 2.51                     | 0.40              |
| 2:B:300:PHE:CE2  | 2:B:319:PHE:CE1  | 3.09                     | 0.40              |
| 3:C:13:CYS:HB2   | 3:C:141:SER:HB3  | 2.02                     | 0.40              |
| 1:A:143:ARG:CZ   | 2:B:292:ILE:HG23 | 2.51                     | 0.40              |
| 2:B:346:LEU:CD1  | 2:B:402:ILE:HD13 | 2.51                     | 0.40              |
| 2:B:347:MET:SD   | 2:B:428:LYS:HA   | 2.61                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:247:TYR:C    | 3:D:249:TYR:H    | 2.30                     | 0.40              |
| 2:B:493:ILE:HD13 | 2:B:595:LYS:HA   | 2.03                     | 0.40              |
| 3:C:120:LEU:HD22 | 3:C:161:ARG:NH1  | 2.36                     | 0.40              |
| 2:B:499:ILE:HD13 | 2:B:511:LYS:HB2  | 2.03                     | 0.40              |
| 3:C:328:PRO:HD2  | 3:C:331:ILE:CD1  | 2.51                     | 0.40              |
| 1:A:434:ASN:CB   | 1:A:469:ARG:HE   | 2.34                     | 0.40              |
| 2:B:591:TRP:CZ2  | 2:B:595:LYS:HD3  | 2.56                     | 0.40              |
| 1:A:761:ILE:O    | 1:A:765:ILE:HG23 | 2.21                     | 0.40              |
| 2:B:735:ILE:HD13 | 2:B:735:ILE:HG21 | 1.90                     | 0.40              |
| 2:B:742:ALA:C    | 2:B:743:THR:O    | 2.62                     | 0.40              |
| 3:D:8:LEU:HD23   | 3:D:67:ILE:CG2   | 2.52                     | 0.40              |
| 3:C:129:SER:OG   | 3:D:284:ILE:CB   | 2.70                     | 0.40              |
| 3:D:255:ILE:CD1  | 3:D:358:ARG:HD3  | 2.49                     | 0.40              |
| 3:D:306:VAL:HG13 | 3:D:382:THR:HG21 | 2.03                     | 0.40              |
| 2:B:339:ILE:CD1  | 2:B:440:GLY:N    | 2.85                     | 0.40              |
| 3:C:127:ILE:HD13 | 3:C:162:TYR:CE2  | 2.48                     | 0.40              |
| 1:A:73:THR:HG21  | 2:B:213:ILE:O    | 2.21                     | 0.40              |
| 1:A:335:CYS:HA   | 1:A:340:ASP:HB3  | 2.04                     | 0.40              |
| 3:C:121:ASN:O    | 3:C:125:LYS:HG3  | 2.21                     | 0.40              |
| 1:A:70:LEU:HB3   | 1:A:92:PHE:CE1   | 2.55                     | 0.40              |
| 1:A:589:GLN:NE2  | 1:A:652:ILE:HD13 | 2.36                     | 0.40              |
| 1:A:592:LEU:HA   | 1:A:696:GLN:OE1  | 2.21                     | 0.40              |
| 3:C:2:GLY:HA3    | 3:C:132:ASN:HD22 | 1.86                     | 0.40              |
| 3:C:182:VAL:HG12 | 3:C:403:PHE:HB3  | 2.02                     | 0.40              |
| 3:C:223:ASP:CG   | 3:C:224:LEU:H    | 2.29                     | 0.40              |
| 2:B:564:LEU:HD23 | 2:B:564:LEU:H    | 1.86                     | 0.40              |
| 2:B:455:GLU:HG2  | 2:B:459:HIS:NE2  | 2.36                     | 0.40              |
| 2:B:241:PHE:HB3  | 2:B:254:ILE:HD13 | 2.03                     | 0.40              |
| 2:B:253:LEU:HD12 | 2:B:334:LEU:HG   | 2.02                     | 0.40              |
| 3:D:123:ILE:HD13 | 3:D:158:LEU:HD21 | 2.03                     | 0.40              |
| 2:B:364:ILE:CD1  | 2:B:403:PHE:CA   | 2.98                     | 0.40              |
| 2:B:739:LYS:O    | 2:B:743:THR:O    | 2.40                     | 0.40              |
| 3:D:261:PRO:HD2  | 3:D:266:HIS:HA   | 2.04                     | 0.40              |
| 1:A:69:GLY:HA2   | 2:B:216:PHE:CG   | 2.56                     | 0.40              |
| 1:A:639:PHE:CE2  | 1:A:775:PHE:HB3  | 2.57                     | 0.40              |
| 2:B:200:PHE:HB2  | 2:B:207:ILE:CD1  | 2.51                     | 0.40              |
| 3:C:172:VAL:HG22 | 3:C:231:ILE:HD13 | 2.04                     | 0.40              |
| 2:B:287:ILE:HD13 | 2:B:287:ILE:HG21 | 1.91                     | 0.40              |
| 2:B:335:PHE:CD2  | 2:B:439:ARG:HG2  | 2.57                     | 0.40              |
| 3:D:105:TRP:CZ2  | 3:D:193:ARG:NH2  | 2.90                     | 0.40              |
| 3:C:129:SER:OG   | 3:D:284:ILE:HB   | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:119:ILE:HG21 | 3:D:154:LEU:HD11 | 2.03                     | 0.40              |
| 1:A:482:LEU:HD11 | 1:A:562:PHE:HB3  | 2.03                     | 0.40              |
| 3:C:404:LEU:HD12 | 3:C:404:LEU:HA   | 1.97                     | 0.40              |
| 1:A:136:GLN:OE1  | 2:B:323:GLY:N    | 2.53                     | 0.40              |
| 1:A:201:GLU:HA   | 1:A:204:ARG:HH21 | 1.87                     | 0.40              |
| 1:A:566:ILE:H    | 1:A:566:ILE:HG12 | 1.64                     | 0.40              |
| 2:B:199:LEU:HD13 | 2:B:199:LEU:O    | 2.21                     | 0.40              |
| 1:A:140:TYR:CE2  | 2:B:292:ILE:HG21 | 2.57                     | 0.40              |
| 1:A:776:ARG:HH11 | 1:A:776:ARG:HD2  | 1.74                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | 1-A   | 561/823 (68%) | 518 (92%) | 20 (4%) | 23 (4%)  | 2           | 18 |
| 1   | 2-A   | 561/823 (68%) | 534 (95%) | 17 (3%) | 10 (2%)  | 6           | 34 |
| 1   | 3-A   | 561/823 (68%) | 522 (93%) | 23 (4%) | 16 (3%)  | 3           | 23 |
| 1   | 4-A   | 561/823 (68%) | 529 (94%) | 20 (4%) | 12 (2%)  | 5           | 30 |
| 1   | 5-A   | 561/823 (68%) | 525 (94%) | 20 (4%) | 16 (3%)  | 3           | 23 |
| 1   | 6-A   | 561/823 (68%) | 538 (96%) | 13 (2%) | 10 (2%)  | 6           | 34 |
| 1   | 7-A   | 561/823 (68%) | 529 (94%) | 23 (4%) | 9 (2%)   | 7           | 38 |
| 1   | 8-A   | 561/823 (68%) | 523 (93%) | 23 (4%) | 15 (3%)  | 4           | 25 |
| 1   | 9-A   | 561/823 (68%) | 530 (94%) | 23 (4%) | 8 (1%)   | 9           | 40 |
| 1   | 10-A  | 561/823 (68%) | 521 (93%) | 29 (5%) | 11 (2%)  | 6           | 31 |
| 2   | 1-B   | 553/846 (65%) | 519 (94%) | 23 (4%) | 11 (2%)  | 6           | 31 |
| 2   | 2-B   | 553/846 (65%) | 520 (94%) | 21 (4%) | 12 (2%)  | 5           | 29 |
| 2   | 3-B   | 553/846 (65%) | 521 (94%) | 20 (4%) | 12 (2%)  | 5           | 29 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|-----------|----------|-------------|----|
| 2   | 4-B   | 553/846 (65%)     | 515 (93%)   | 28 (5%)   | 10 (2%)  | 6           | 34 |
| 2   | 5-B   | 553/846 (65%)     | 516 (93%)   | 30 (5%)   | 7 (1%)   | 9           | 42 |
| 2   | 6-B   | 553/846 (65%)     | 513 (93%)   | 27 (5%)   | 13 (2%)  | 4           | 27 |
| 2   | 7-B   | 553/846 (65%)     | 514 (93%)   | 23 (4%)   | 16 (3%)  | 3           | 23 |
| 2   | 8-B   | 553/846 (65%)     | 525 (95%)   | 19 (3%)   | 9 (2%)   | 7           | 38 |
| 2   | 9-B   | 553/846 (65%)     | 521 (94%)   | 24 (4%)   | 8 (1%)   | 9           | 40 |
| 2   | 10-B  | 553/846 (65%)     | 517 (94%)   | 22 (4%)   | 14 (2%)  | 4           | 26 |
| 3   | 1-C   | 443/473 (94%)     | 392 (88%)   | 32 (7%)   | 19 (4%)  | 2           | 17 |
| 3   | 1-D   | 443/473 (94%)     | 404 (91%)   | 28 (6%)   | 11 (2%)  | 4           | 26 |
| 3   | 2-C   | 443/473 (94%)     | 400 (90%)   | 30 (7%)   | 13 (3%)  | 3           | 23 |
| 3   | 2-D   | 443/473 (94%)     | 411 (93%)   | 22 (5%)   | 10 (2%)  | 5           | 28 |
| 3   | 3-C   | 443/473 (94%)     | 384 (87%)   | 37 (8%)   | 22 (5%)  | 1           | 16 |
| 3   | 3-D   | 443/473 (94%)     | 402 (91%)   | 27 (6%)   | 14 (3%)  | 3           | 21 |
| 3   | 4-C   | 443/473 (94%)     | 399 (90%)   | 35 (8%)   | 9 (2%)   | 6           | 31 |
| 3   | 4-D   | 443/473 (94%)     | 392 (88%)   | 38 (9%)   | 13 (3%)  | 3           | 23 |
| 3   | 5-C   | 443/473 (94%)     | 408 (92%)   | 19 (4%)   | 16 (4%)  | 2           | 20 |
| 3   | 5-D   | 443/473 (94%)     | 399 (90%)   | 36 (8%)   | 8 (2%)   | 6           | 34 |
| 3   | 6-C   | 443/473 (94%)     | 396 (89%)   | 36 (8%)   | 11 (2%)  | 4           | 26 |
| 3   | 6-D   | 443/473 (94%)     | 400 (90%)   | 29 (6%)   | 14 (3%)  | 3           | 21 |
| 3   | 7-C   | 443/473 (94%)     | 406 (92%)   | 26 (6%)   | 11 (2%)  | 4           | 26 |
| 3   | 7-D   | 443/473 (94%)     | 393 (89%)   | 34 (8%)   | 16 (4%)  | 2           | 20 |
| 3   | 8-C   | 443/473 (94%)     | 399 (90%)   | 27 (6%)   | 17 (4%)  | 2           | 19 |
| 3   | 8-D   | 443/473 (94%)     | 395 (89%)   | 32 (7%)   | 16 (4%)  | 2           | 20 |
| 3   | 9-C   | 443/473 (94%)     | 396 (89%)   | 35 (8%)   | 12 (3%)  | 4           | 25 |
| 3   | 9-D   | 443/473 (94%)     | 399 (90%)   | 32 (7%)   | 12 (3%)  | 4           | 25 |
| 3   | 10-C  | 443/473 (94%)     | 404 (91%)   | 27 (6%)   | 12 (3%)  | 4           | 25 |
| 3   | 10-D  | 443/473 (94%)     | 390 (88%)   | 38 (9%)   | 15 (3%)  | 3           | 21 |
| All | All   | 20000/26150 (76%) | 18419 (92%) | 1068 (5%) | 513 (3%) | 6           | 25 |

All (513) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 91  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 99  | ASP  |
| 1   | 1-A   | 261 | ASP  |
| 1   | 1-A   | 322 | THR  |
| 1   | 1-A   | 364 | PRO  |
| 1   | 1-A   | 571 | ASN  |
| 2   | 1-B   | 212 | LYS  |
| 3   | 1-C   | 51  | LYS  |
| 3   | 1-C   | 275 | PHE  |
| 3   | 1-C   | 280 | ILE  |
| 3   | 1-C   | 315 | TYR  |
| 3   | 1-C   | 416 | MET  |
| 3   | 1-D   | 51  | LYS  |
| 1   | 2-A   | 91  | GLU  |
| 1   | 2-A   | 297 | GLN  |
| 1   | 2-A   | 473 | ASN  |
| 2   | 2-B   | 357 | ALA  |
| 2   | 2-B   | 416 | CYS  |
| 2   | 2-B   | 574 | VAL  |
| 3   | 2-C   | 99  | ALA  |
| 3   | 2-D   | 261 | PRO  |
| 1   | 3-A   | 91  | GLU  |
| 1   | 3-A   | 97  | LYS  |
| 1   | 3-A   | 365 | THR  |
| 2   | 3-B   | 194 | ALA  |
| 3   | 3-C   | 325 | ASN  |
| 3   | 3-C   | 366 | GLN  |
| 3   | 3-C   | 370 | ASN  |
| 3   | 3-D   | 354 | VAL  |
| 3   | 3-D   | 415 | SER  |
| 1   | 4-A   | 91  | GLU  |
| 2   | 4-B   | 611 | ILE  |
| 3   | 4-C   | 59  | ARG  |
| 3   | 4-D   | 60  | ASN  |
| 1   | 5-A   | 91  | GLU  |
| 1   | 5-A   | 609 | THR  |
| 2   | 5-B   | 357 | ALA  |
| 3   | 5-C   | 97  | ASP  |
| 3   | 5-C   | 178 | SER  |
| 3   | 5-C   | 286 | HIS  |
| 3   | 5-C   | 325 | ASN  |
| 1   | 6-A   | 91  | GLU  |
| 1   | 6-A   | 98  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 6-B   | 210 | PRO  |
| 2   | 6-B   | 417 | LYS  |
| 3   | 6-C   | 59  | ARG  |
| 3   | 6-C   | 132 | ASN  |
| 3   | 6-C   | 248 | MET  |
| 3   | 6-C   | 274 | PRO  |
| 3   | 6-C   | 325 | ASN  |
| 3   | 6-D   | 73  | PRO  |
| 3   | 6-D   | 325 | ASN  |
| 1   | 7-A   | 786 | LEU  |
| 2   | 7-B   | 198 | ALA  |
| 2   | 7-B   | 210 | PRO  |
| 2   | 7-B   | 214 | PRO  |
| 2   | 7-B   | 548 | LEU  |
| 3   | 7-C   | 70  | ASP  |
| 3   | 7-C   | 351 | ALA  |
| 3   | 7-D   | 223 | ASP  |
| 3   | 7-D   | 279 | TYR  |
| 3   | 7-D   | 286 | HIS  |
| 3   | 7-D   | 325 | ASN  |
| 3   | 7-D   | 351 | ALA  |
| 1   | 8-A   | 91  | GLU  |
| 1   | 8-A   | 259 | LEU  |
| 1   | 8-A   | 570 | LEU  |
| 3   | 8-C   | 103 | ASN  |
| 3   | 8-C   | 309 | ALA  |
| 3   | 8-C   | 325 | ASN  |
| 3   | 8-C   | 363 | LEU  |
| 3   | 8-D   | 58  | SER  |
| 3   | 8-D   | 325 | ASN  |
| 1   | 9-A   | 91  | GLU  |
| 1   | 9-A   | 130 | SER  |
| 2   | 9-B   | 206 | GLN  |
| 3   | 9-C   | 325 | ASN  |
| 3   | 9-C   | 352 | MET  |
| 3   | 9-C   | 403 | PHE  |
| 3   | 9-D   | 51  | LYS  |
| 3   | 9-D   | 248 | MET  |
| 3   | 9-D   | 325 | ASN  |
| 3   | 9-D   | 365 | LEU  |
| 1   | 10-A  | 91  | GLU  |
| 1   | 10-A  | 362 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 10-B  | 208 | GLN  |
| 2   | 10-B  | 247 | SER  |
| 2   | 10-B  | 547 | ASP  |
| 2   | 10-B  | 610 | ILE  |
| 3   | 10-C  | 310 | MET  |
| 3   | 10-D  | 103 | ASN  |
| 3   | 10-D  | 311 | ASN  |
| 1   | 1-A   | 297 | GLN  |
| 1   | 1-A   | 432 | GLY  |
| 1   | 1-A   | 691 | ASP  |
| 2   | 1-B   | 354 | LEU  |
| 2   | 1-B   | 416 | CYS  |
| 2   | 1-B   | 547 | ASP  |
| 2   | 1-B   | 577 | PRO  |
| 3   | 1-C   | 70  | ASP  |
| 3   | 1-C   | 221 | ASN  |
| 3   | 1-C   | 223 | ASP  |
| 3   | 1-C   | 302 | SER  |
| 3   | 1-C   | 369 | GLU  |
| 3   | 1-D   | 70  | ASP  |
| 3   | 1-D   | 100 | SER  |
| 3   | 1-D   | 278 | ASP  |
| 3   | 1-D   | 326 | VAL  |
| 1   | 2-A   | 128 | ASP  |
| 1   | 2-A   | 333 | ARG  |
| 1   | 2-A   | 361 | LEU  |
| 2   | 2-B   | 204 | HIS  |
| 2   | 2-B   | 382 | PRO  |
| 2   | 2-B   | 537 | VAL  |
| 3   | 2-C   | 265 | LEU  |
| 3   | 2-C   | 277 | SER  |
| 3   | 2-C   | 325 | ASN  |
| 3   | 2-D   | 40  | PRO  |
| 3   | 2-D   | 50  | THR  |
| 3   | 2-D   | 441 | GLU  |
| 1   | 3-A   | 332 | LEU  |
| 1   | 3-A   | 667 | THR  |
| 1   | 3-A   | 786 | LEU  |
| 2   | 3-B   | 279 | SER  |
| 2   | 3-B   | 383 | ILE  |
| 2   | 3-B   | 438 | TYR  |
| 2   | 3-B   | 439 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 3-B   | 533 | ARG  |
| 2   | 3-B   | 576 | ARG  |
| 3   | 3-C   | 70  | ASP  |
| 3   | 3-C   | 100 | SER  |
| 3   | 3-C   | 132 | ASN  |
| 3   | 3-C   | 163 | PRO  |
| 3   | 3-C   | 280 | ILE  |
| 3   | 3-C   | 308 | THR  |
| 3   | 3-C   | 354 | VAL  |
| 3   | 3-D   | 41  | ASP  |
| 3   | 3-D   | 70  | ASP  |
| 3   | 3-D   | 287 | LYS  |
| 3   | 3-D   | 307 | SER  |
| 3   | 3-D   | 325 | ASN  |
| 3   | 3-D   | 444 | SER  |
| 1   | 4-A   | 361 | LEU  |
| 1   | 4-A   | 365 | THR  |
| 1   | 4-A   | 432 | GLY  |
| 1   | 4-A   | 608 | LYS  |
| 2   | 4-B   | 356 | ARG  |
| 2   | 4-B   | 392 | ALA  |
| 3   | 4-C   | 70  | ASP  |
| 3   | 4-C   | 261 | PRO  |
| 3   | 4-C   | 351 | ALA  |
| 3   | 4-D   | 30  | ALA  |
| 3   | 4-D   | 70  | ASP  |
| 3   | 4-D   | 104 | SER  |
| 3   | 4-D   | 175 | ALA  |
| 3   | 4-D   | 284 | ILE  |
| 3   | 4-D   | 285 | ALA  |
| 1   | 5-A   | 169 | SER  |
| 1   | 5-A   | 365 | THR  |
| 1   | 5-A   | 432 | GLY  |
| 1   | 5-A   | 471 | SER  |
| 2   | 5-B   | 417 | LYS  |
| 3   | 5-C   | 41  | ASP  |
| 3   | 5-C   | 163 | PRO  |
| 3   | 5-C   | 246 | SER  |
| 3   | 5-C   | 307 | SER  |
| 3   | 5-D   | 42  | SER  |
| 1   | 6-A   | 429 | TYR  |
| 1   | 6-A   | 432 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 6-B   | 194 | ALA  |
| 2   | 6-B   | 439 | ARG  |
| 2   | 6-B   | 575 | ASN  |
| 3   | 6-C   | 99  | ALA  |
| 3   | 6-D   | 261 | PRO  |
| 3   | 6-D   | 279 | TYR  |
| 3   | 6-D   | 364 | PRO  |
| 1   | 7-A   | 91  | GLU  |
| 1   | 7-A   | 97  | LYS  |
| 1   | 7-A   | 296 | TYR  |
| 1   | 7-A   | 432 | GLY  |
| 1   | 7-A   | 571 | ASN  |
| 1   | 7-A   | 572 | ILE  |
| 2   | 7-B   | 206 | GLN  |
| 2   | 7-B   | 246 | ILE  |
| 2   | 7-B   | 416 | CYS  |
| 2   | 7-B   | 419 | VAL  |
| 3   | 7-C   | 99  | ALA  |
| 3   | 7-D   | 43  | SER  |
| 1   | 8-A   | 388 | SER  |
| 1   | 8-A   | 489 | GLU  |
| 2   | 8-B   | 358 | THR  |
| 2   | 8-B   | 530 | ASN  |
| 3   | 8-C   | 261 | PRO  |
| 3   | 8-C   | 285 | ALA  |
| 3   | 8-D   | 60  | ASN  |
| 3   | 8-D   | 70  | ASP  |
| 3   | 8-D   | 276 | THR  |
| 3   | 8-D   | 301 | PRO  |
| 3   | 8-D   | 351 | ALA  |
| 3   | 8-D   | 442 | GLN  |
| 1   | 9-A   | 555 | SER  |
| 2   | 9-B   | 246 | ILE  |
| 2   | 9-B   | 570 | LEU  |
| 3   | 9-C   | 70  | ASP  |
| 3   | 9-C   | 261 | PRO  |
| 3   | 9-C   | 277 | SER  |
| 3   | 9-D   | 70  | ASP  |
| 3   | 9-D   | 100 | SER  |
| 3   | 9-D   | 309 | ALA  |
| 1   | 10-A  | 432 | GLY  |
| 1   | 10-A  | 666 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 10-B  | 194 | ALA  |
| 2   | 10-B  | 212 | LYS  |
| 2   | 10-B  | 274 | SER  |
| 2   | 10-B  | 524 | SER  |
| 3   | 10-C  | 70  | ASP  |
| 3   | 10-C  | 101 | ALA  |
| 3   | 10-C  | 222 | ILE  |
| 3   | 10-C  | 309 | ALA  |
| 3   | 10-C  | 328 | PRO  |
| 3   | 10-C  | 364 | PRO  |
| 3   | 10-D  | 70  | ASP  |
| 3   | 10-D  | 177 | SER  |
| 3   | 10-D  | 325 | ASN  |
| 1   | 1-A   | 72  | GLY  |
| 1   | 1-A   | 296 | TYR  |
| 1   | 1-A   | 299 | PHE  |
| 1   | 1-A   | 337 | SER  |
| 1   | 1-A   | 570 | LEU  |
| 2   | 1-B   | 204 | HIS  |
| 2   | 1-B   | 243 | MET  |
| 2   | 1-B   | 526 | ARG  |
| 3   | 1-C   | 61  | LYS  |
| 3   | 1-C   | 277 | SER  |
| 3   | 1-D   | 328 | PRO  |
| 1   | 2-A   | 362 | GLN  |
| 1   | 2-A   | 414 | ASP  |
| 2   | 2-B   | 274 | SER  |
| 2   | 2-B   | 532 | PRO  |
| 2   | 2-B   | 533 | ARG  |
| 2   | 2-B   | 577 | PRO  |
| 3   | 2-C   | 70  | ASP  |
| 3   | 2-C   | 416 | MET  |
| 3   | 2-D   | 403 | PHE  |
| 1   | 3-A   | 487 | ASP  |
| 1   | 3-A   | 666 | PRO  |
| 2   | 3-B   | 577 | PRO  |
| 2   | 3-B   | 835 | ASP  |
| 3   | 3-C   | 175 | ALA  |
| 3   | 3-C   | 311 | ASN  |
| 3   | 3-C   | 313 | PRO  |
| 3   | 3-D   | 101 | ALA  |
| 3   | 3-D   | 266 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 4-A   | 128 | ASP  |
| 1   | 4-A   | 129 | THR  |
| 1   | 4-A   | 413 | TYR  |
| 2   | 4-B   | 198 | ALA  |
| 2   | 4-B   | 214 | PRO  |
| 3   | 4-C   | 58  | SER  |
| 3   | 4-C   | 313 | PRO  |
| 3   | 4-C   | 325 | ASN  |
| 1   | 5-A   | 128 | ASP  |
| 2   | 5-B   | 382 | PRO  |
| 3   | 5-C   | 70  | ASP  |
| 3   | 5-C   | 143 | ALA  |
| 3   | 5-C   | 361 | PRO  |
| 3   | 5-D   | 45  | GLU  |
| 3   | 5-D   | 70  | ASP  |
| 3   | 5-D   | 218 | ARG  |
| 3   | 5-D   | 277 | SER  |
| 1   | 6-A   | 261 | ASP  |
| 1   | 6-A   | 366 | ILE  |
| 2   | 6-B   | 198 | ALA  |
| 2   | 6-B   | 204 | HIS  |
| 3   | 6-C   | 70  | ASP  |
| 3   | 6-C   | 72  | GLU  |
| 3   | 6-C   | 96  | SER  |
| 3   | 6-D   | 45  | GLU  |
| 1   | 7-A   | 364 | PRO  |
| 2   | 7-B   | 469 | HIS  |
| 2   | 7-B   | 524 | SER  |
| 2   | 7-B   | 551 | GLY  |
| 3   | 7-C   | 274 | PRO  |
| 3   | 7-C   | 276 | THR  |
| 3   | 7-C   | 325 | ASN  |
| 3   | 7-D   | 70  | ASP  |
| 3   | 7-D   | 179 | GLU  |
| 3   | 7-D   | 278 | ASP  |
| 3   | 7-D   | 308 | THR  |
| 3   | 7-D   | 442 | GLN  |
| 1   | 8-A   | 97  | LYS  |
| 1   | 8-A   | 296 | TYR  |
| 1   | 8-A   | 297 | GLN  |
| 1   | 8-A   | 298 | GLU  |
| 1   | 8-A   | 361 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 8-A   | 412 | GLY  |
| 2   | 8-B   | 439 | ARG  |
| 2   | 8-B   | 529 | MET  |
| 2   | 8-B   | 550 | HIS  |
| 3   | 8-C   | 70  | ASP  |
| 3   | 8-C   | 96  | SER  |
| 3   | 8-C   | 364 | PRO  |
| 3   | 8-D   | 59  | ARG  |
| 3   | 8-D   | 343 | LYS  |
| 1   | 9-A   | 74  | TYR  |
| 1   | 9-A   | 666 | PRO  |
| 2   | 9-B   | 547 | ASP  |
| 2   | 9-B   | 577 | PRO  |
| 3   | 9-C   | 314 | THR  |
| 3   | 9-D   | 102 | GLY  |
| 3   | 9-D   | 266 | HIS  |
| 1   | 10-A  | 259 | LEU  |
| 1   | 10-A  | 295 | PRO  |
| 2   | 10-B  | 204 | HIS  |
| 2   | 10-B  | 358 | THR  |
| 2   | 10-B  | 416 | CYS  |
| 2   | 10-B  | 720 | ASN  |
| 3   | 10-C  | 38  | GLN  |
| 3   | 10-D  | 45  | GLU  |
| 3   | 10-D  | 246 | SER  |
| 3   | 10-D  | 248 | MET  |
| 3   | 10-D  | 443 | ASP  |
| 1   | 1-A   | 331 | LEU  |
| 1   | 1-A   | 366 | ILE  |
| 1   | 1-A   | 449 | HIS  |
| 1   | 1-A   | 472 | GLU  |
| 2   | 1-B   | 324 | ASP  |
| 3   | 1-C   | 178 | SER  |
| 3   | 1-C   | 219 | ASN  |
| 3   | 1-C   | 328 | PRO  |
| 3   | 1-D   | 246 | SER  |
| 1   | 2-A   | 70  | LEU  |
| 3   | 2-C   | 96  | SER  |
| 3   | 2-C   | 143 | ALA  |
| 3   | 2-C   | 163 | PRO  |
| 3   | 2-C   | 311 | ASN  |
| 3   | 2-C   | 367 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2-D   | 276 | THR  |
| 1   | 3-A   | 300 | MET  |
| 1   | 3-A   | 569 | PRO  |
| 1   | 3-A   | 608 | LYS  |
| 2   | 3-B   | 324 | ASP  |
| 2   | 3-B   | 382 | PRO  |
| 3   | 3-C   | 261 | PRO  |
| 3   | 3-C   | 263 | PRO  |
| 3   | 3-C   | 266 | HIS  |
| 3   | 3-C   | 314 | THR  |
| 3   | 3-D   | 131 | ASP  |
| 3   | 3-D   | 163 | PRO  |
| 3   | 3-D   | 353 | HIS  |
| 2   | 4-B   | 527 | HIS  |
| 2   | 4-B   | 563 | ILE  |
| 3   | 4-D   | 103 | ASN  |
| 3   | 4-D   | 311 | ASN  |
| 3   | 4-D   | 325 | ASN  |
| 3   | 4-D   | 343 | LYS  |
| 1   | 5-A   | 97  | LYS  |
| 1   | 5-A   | 360 | SER  |
| 1   | 5-A   | 786 | LEU  |
| 2   | 5-B   | 416 | CYS  |
| 3   | 5-C   | 45  | GLU  |
| 3   | 5-C   | 442 | GLN  |
| 1   | 6-A   | 259 | LEU  |
| 2   | 6-B   | 203 | ASP  |
| 2   | 6-B   | 419 | VAL  |
| 2   | 6-B   | 483 | MET  |
| 3   | 6-C   | 178 | SER  |
| 3   | 6-C   | 312 | ASN  |
| 3   | 6-D   | 38  | GLN  |
| 3   | 6-D   | 70  | ASP  |
| 3   | 6-D   | 98  | GLY  |
| 3   | 6-D   | 361 | PRO  |
| 2   | 7-B   | 247 | SER  |
| 2   | 7-B   | 417 | LYS  |
| 3   | 7-C   | 163 | PRO  |
| 3   | 7-C   | 353 | HIS  |
| 3   | 7-D   | 364 | PRO  |
| 3   | 7-D   | 415 | SER  |
| 1   | 8-A   | 487 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 8-B   | 244 | LEU  |
| 2   | 8-B   | 247 | SER  |
| 2   | 8-B   | 381 | ILE  |
| 2   | 8-B   | 416 | CYS  |
| 3   | 8-C   | 132 | ASN  |
| 3   | 8-C   | 280 | ILE  |
| 3   | 8-C   | 361 | PRO  |
| 3   | 8-D   | 100 | SER  |
| 3   | 8-D   | 102 | GLY  |
| 3   | 8-D   | 307 | SER  |
| 2   | 9-B   | 247 | SER  |
| 2   | 9-B   | 524 | SER  |
| 3   | 9-C   | 163 | PRO  |
| 3   | 9-C   | 364 | PRO  |
| 3   | 9-D   | 286 | HIS  |
| 1   | 10-A  | 296 | TYR  |
| 1   | 10-A  | 610 | PRO  |
| 2   | 10-B  | 324 | ASP  |
| 2   | 10-B  | 381 | ILE  |
| 3   | 10-C  | 42  | SER  |
| 3   | 10-C  | 265 | LEU  |
| 3   | 10-C  | 279 | TYR  |
| 3   | 10-D  | 43  | SER  |
| 1   | 1-A   | 336 | ASP  |
| 1   | 1-A   | 566 | ILE  |
| 2   | 1-B   | 358 | THR  |
| 3   | 1-C   | 248 | MET  |
| 3   | 1-C   | 350 | SER  |
| 3   | 1-C   | 361 | PRO  |
| 3   | 1-D   | 104 | SER  |
| 3   | 1-D   | 416 | MET  |
| 2   | 2-B   | 243 | MET  |
| 3   | 2-D   | 163 | PRO  |
| 1   | 3-A   | 295 | PRO  |
| 1   | 3-A   | 331 | LEU  |
| 1   | 3-A   | 364 | PRO  |
| 1   | 3-A   | 613 | LYS  |
| 2   | 3-B   | 779 | LEU  |
| 3   | 3-C   | 309 | ALA  |
| 3   | 3-C   | 351 | ALA  |
| 1   | 4-A   | 298 | GLU  |
| 2   | 4-B   | 610 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 4-C   | 309 | ALA  |
| 3   | 4-C   | 403 | PHE  |
| 3   | 4-D   | 32  | GLY  |
| 1   | 5-A   | 299 | PHE  |
| 1   | 5-A   | 362 | GLN  |
| 1   | 5-A   | 371 | SER  |
| 1   | 5-A   | 785 | GLU  |
| 2   | 5-B   | 534 | ASN  |
| 3   | 5-C   | 279 | TYR  |
| 1   | 6-A   | 169 | SER  |
| 1   | 6-A   | 361 | LEU  |
| 2   | 6-B   | 246 | ILE  |
| 2   | 6-B   | 552 | SER  |
| 3   | 6-D   | 277 | SER  |
| 3   | 6-D   | 281 | HIS  |
| 3   | 6-D   | 417 | GLN  |
| 3   | 7-C   | 30  | ALA  |
| 3   | 7-D   | 361 | PRO  |
| 3   | 8-C   | 100 | SER  |
| 3   | 8-C   | 371 | GLU  |
| 3   | 8-D   | 415 | SER  |
| 1   | 9-A   | 472 | GLU  |
| 3   | 9-C   | 282 | ASP  |
| 3   | 9-D   | 369 | GLU  |
| 1   | 10-A  | 129 | THR  |
| 1   | 10-A  | 489 | GLU  |
| 1   | 10-A  | 609 | THR  |
| 3   | 10-C  | 444 | SER  |
| 3   | 10-D  | 277 | SER  |
| 3   | 1-D   | 277 | SER  |
| 1   | 2-A   | 786 | LEU  |
| 2   | 2-B   | 526 | ARG  |
| 3   | 2-C   | 42  | SER  |
| 3   | 2-D   | 282 | ASP  |
| 3   | 3-C   | 47  | ASP  |
| 3   | 3-D   | 367 | PRO  |
| 1   | 4-A   | 414 | ASP  |
| 2   | 4-B   | 550 | HIS  |
| 1   | 5-A   | 412 | GLY  |
| 2   | 5-B   | 528 | LEU  |
| 2   | 5-B   | 546 | LEU  |
| 3   | 5-D   | 3   | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 7-B   | 357 | ALA  |
| 2   | 7-B   | 529 | MET  |
| 2   | 7-B   | 546 | LEU  |
| 3   | 7-C   | 44  | THR  |
| 3   | 8-D   | 163 | PRO  |
| 1   | 9-A   | 567 | PRO  |
| 2   | 9-B   | 274 | SER  |
| 3   | 9-C   | 45  | GLU  |
| 3   | 9-C   | 98  | GLY  |
| 3   | 9-D   | 40  | PRO  |
| 3   | 10-D  | 36  | LEU  |
| 3   | 10-D  | 261 | PRO  |
| 3   | 10-D  | 287 | LYS  |
| 3   | 10-D  | 441 | GLU  |
| 1   | 1-A   | 165 | VAL  |
| 2   | 1-B   | 611 | ILE  |
| 3   | 1-C   | 367 | PRO  |
| 3   | 1-D   | 261 | PRO  |
| 3   | 3-C   | 174 | PRO  |
| 1   | 4-A   | 666 | PRO  |
| 2   | 4-B   | 419 | VAL  |
| 1   | 5-A   | 367 | PRO  |
| 3   | 8-C   | 367 | PRO  |
| 3   | 2-C   | 261 | PRO  |
| 3   | 2-D   | 245 | PRO  |
| 3   | 5-D   | 327 | GLU  |
| 1   | 6-A   | 428 | GLY  |
| 3   | 7-D   | 98  | GLY  |
| 3   | 8-C   | 3   | GLY  |
| 3   | 8-D   | 40  | PRO  |
| 3   | 4-D   | 181 | VAL  |
| 3   | 5-D   | 345 | PRO  |
| 2   | 6-B   | 309 | GLY  |
| 3   | 7-C   | 280 | ILE  |
| 3   | 7-D   | 220 | PRO  |
| 1   | 8-A   | 573 | ILE  |
| 1   | 1-A   | 573 | ILE  |
| 3   | 2-D   | 328 | PRO  |
| 1   | 3-A   | 132 | GLY  |
| 3   | 5-C   | 261 | PRO  |
| 1   | 7-A   | 295 | PRO  |
| 1   | 8-A   | 473 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 8-A   | 666 | PRO  |
| 3   | 8-C   | 354 | VAL  |
| 1   | 9-A   | 364 | PRO  |
| 3   | 3-C   | 245 | PRO  |
| 3   | 5-C   | 51  | LYS  |
| 3   | 6-D   | 174 | PRO  |
| 1   | 1-A   | 569 | PRO  |
| 1   | 4-A   | 569 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | 1-A   | 542/766 (71%) | 513 (95%) | 29 (5%)  | 20          | 41 |
| 1   | 2-A   | 542/766 (71%) | 513 (95%) | 29 (5%)  | 20          | 41 |
| 1   | 3-A   | 542/766 (71%) | 513 (95%) | 29 (5%)  | 20          | 41 |
| 1   | 4-A   | 542/766 (71%) | 513 (95%) | 29 (5%)  | 20          | 41 |
| 1   | 5-A   | 542/766 (71%) | 513 (95%) | 29 (5%)  | 20          | 41 |
| 1   | 6-A   | 542/766 (71%) | 513 (95%) | 29 (5%)  | 20          | 41 |
| 1   | 7-A   | 542/766 (71%) | 513 (95%) | 29 (5%)  | 20          | 41 |
| 1   | 8-A   | 542/766 (71%) | 513 (95%) | 29 (5%)  | 20          | 41 |
| 1   | 9-A   | 542/766 (71%) | 513 (95%) | 29 (5%)  | 20          | 41 |
| 1   | 10-A  | 542/766 (71%) | 513 (95%) | 29 (5%)  | 20          | 41 |
| 2   | 1-B   | 528/787 (67%) | 509 (96%) | 19 (4%)  | 31          | 52 |
| 2   | 2-B   | 528/787 (67%) | 509 (96%) | 19 (4%)  | 31          | 52 |
| 2   | 3-B   | 528/787 (67%) | 509 (96%) | 19 (4%)  | 31          | 52 |
| 2   | 4-B   | 528/787 (67%) | 509 (96%) | 19 (4%)  | 31          | 52 |
| 2   | 5-B   | 528/787 (67%) | 509 (96%) | 19 (4%)  | 31          | 52 |
| 2   | 6-B   | 528/787 (67%) | 509 (96%) | 19 (4%)  | 31          | 52 |
| 2   | 7-B   | 528/787 (67%) | 509 (96%) | 19 (4%)  | 31          | 52 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 2   | 8-B   | 528/787 (67%)     | 509 (96%)   | 19 (4%)  | 31          | 52 |
| 2   | 9-B   | 528/787 (67%)     | 509 (96%)   | 19 (4%)  | 31          | 52 |
| 2   | 10-B  | 528/787 (67%)     | 509 (96%)   | 19 (4%)  | 31          | 52 |
| 3   | 1-C   | 395/420 (94%)     | 375 (95%)   | 20 (5%)  | 21          | 42 |
| 3   | 1-D   | 395/420 (94%)     | 383 (97%)   | 12 (3%)  | 36          | 57 |
| 3   | 2-C   | 395/420 (94%)     | 375 (95%)   | 20 (5%)  | 21          | 42 |
| 3   | 2-D   | 395/420 (94%)     | 383 (97%)   | 12 (3%)  | 36          | 57 |
| 3   | 3-C   | 395/420 (94%)     | 375 (95%)   | 20 (5%)  | 21          | 42 |
| 3   | 3-D   | 395/420 (94%)     | 383 (97%)   | 12 (3%)  | 36          | 57 |
| 3   | 4-C   | 395/420 (94%)     | 375 (95%)   | 20 (5%)  | 21          | 42 |
| 3   | 4-D   | 395/420 (94%)     | 383 (97%)   | 12 (3%)  | 36          | 57 |
| 3   | 5-C   | 395/420 (94%)     | 375 (95%)   | 20 (5%)  | 21          | 42 |
| 3   | 5-D   | 395/420 (94%)     | 383 (97%)   | 12 (3%)  | 36          | 57 |
| 3   | 6-C   | 395/420 (94%)     | 375 (95%)   | 20 (5%)  | 21          | 42 |
| 3   | 6-D   | 395/420 (94%)     | 383 (97%)   | 12 (3%)  | 36          | 57 |
| 3   | 7-C   | 395/420 (94%)     | 375 (95%)   | 20 (5%)  | 21          | 42 |
| 3   | 7-D   | 395/420 (94%)     | 383 (97%)   | 12 (3%)  | 36          | 57 |
| 3   | 8-C   | 395/420 (94%)     | 375 (95%)   | 20 (5%)  | 21          | 42 |
| 3   | 8-D   | 395/420 (94%)     | 383 (97%)   | 12 (3%)  | 36          | 57 |
| 3   | 9-C   | 395/420 (94%)     | 375 (95%)   | 20 (5%)  | 21          | 42 |
| 3   | 9-D   | 395/420 (94%)     | 383 (97%)   | 12 (3%)  | 36          | 57 |
| 3   | 10-C  | 395/420 (94%)     | 375 (95%)   | 20 (5%)  | 21          | 42 |
| 3   | 10-D  | 395/420 (94%)     | 383 (97%)   | 12 (3%)  | 36          | 57 |
| All | All   | 18600/23930 (78%) | 17800 (96%) | 800 (4%) | 27          | 47 |

All (800) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 67  | LEU  |
| 1   | 1-A   | 91  | GLU  |
| 1   | 1-A   | 114 | LYS  |
| 1   | 1-A   | 173 | LEU  |
| 1   | 1-A   | 259 | LEU  |
| 1   | 1-A   | 272 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 275 | ILE  |
| 1   | 1-A   | 288 | THR  |
| 1   | 1-A   | 302 | TYR  |
| 1   | 1-A   | 344 | LEU  |
| 1   | 1-A   | 354 | LEU  |
| 1   | 1-A   | 364 | PRO  |
| 1   | 1-A   | 411 | GLN  |
| 1   | 1-A   | 415 | LEU  |
| 1   | 1-A   | 422 | LEU  |
| 1   | 1-A   | 427 | LEU  |
| 1   | 1-A   | 430 | GLN  |
| 1   | 1-A   | 463 | GLN  |
| 1   | 1-A   | 471 | SER  |
| 1   | 1-A   | 566 | ILE  |
| 1   | 1-A   | 590 | LEU  |
| 1   | 1-A   | 599 | LEU  |
| 1   | 1-A   | 633 | HIS  |
| 1   | 1-A   | 670 | VAL  |
| 1   | 1-A   | 693 | ILE  |
| 1   | 1-A   | 700 | PHE  |
| 1   | 1-A   | 764 | LEU  |
| 1   | 1-A   | 768 | ILE  |
| 1   | 1-A   | 799 | VAL  |
| 2   | 1-B   | 188 | VAL  |
| 2   | 1-B   | 246 | ILE  |
| 2   | 1-B   | 301 | THR  |
| 2   | 1-B   | 389 | ARG  |
| 2   | 1-B   | 471 | ARG  |
| 2   | 1-B   | 485 | LYS  |
| 2   | 1-B   | 502 | THR  |
| 2   | 1-B   | 504 | SER  |
| 2   | 1-B   | 508 | PRO  |
| 2   | 1-B   | 516 | LEU  |
| 2   | 1-B   | 525 | LEU  |
| 2   | 1-B   | 559 | THR  |
| 2   | 1-B   | 571 | VAL  |
| 2   | 1-B   | 604 | MET  |
| 2   | 1-B   | 605 | LEU  |
| 2   | 1-B   | 725 | GLU  |
| 2   | 1-B   | 757 | PRO  |
| 2   | 1-B   | 772 | PHE  |
| 2   | 1-B   | 838 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1-C   | 15  | ASN  |
| 3   | 1-C   | 115 | ASN  |
| 3   | 1-C   | 167 | LEU  |
| 3   | 1-C   | 194 | LEU  |
| 3   | 1-C   | 209 | LEU  |
| 3   | 1-C   | 216 | VAL  |
| 3   | 1-C   | 230 | LEU  |
| 3   | 1-C   | 292 | TYR  |
| 3   | 1-C   | 306 | VAL  |
| 3   | 1-C   | 314 | THR  |
| 3   | 1-C   | 315 | TYR  |
| 3   | 1-C   | 321 | THR  |
| 3   | 1-C   | 367 | PRO  |
| 3   | 1-C   | 371 | GLU  |
| 3   | 1-C   | 379 | ASN  |
| 3   | 1-C   | 382 | THR  |
| 3   | 1-C   | 383 | VAL  |
| 3   | 1-C   | 420 | GLN  |
| 3   | 1-C   | 437 | TYR  |
| 3   | 1-C   | 438 | VAL  |
| 3   | 1-D   | 31  | ILE  |
| 3   | 1-D   | 43  | SER  |
| 3   | 1-D   | 45  | GLU  |
| 3   | 1-D   | 146 | THR  |
| 3   | 1-D   | 182 | VAL  |
| 3   | 1-D   | 183 | GLN  |
| 3   | 1-D   | 230 | LEU  |
| 3   | 1-D   | 236 | SER  |
| 3   | 1-D   | 328 | PRO  |
| 3   | 1-D   | 354 | VAL  |
| 3   | 1-D   | 376 | MET  |
| 3   | 1-D   | 422 | GLU  |
| 1   | 2-A   | 67  | LEU  |
| 1   | 2-A   | 91  | GLU  |
| 1   | 2-A   | 114 | LYS  |
| 1   | 2-A   | 173 | LEU  |
| 1   | 2-A   | 259 | LEU  |
| 1   | 2-A   | 272 | LEU  |
| 1   | 2-A   | 275 | ILE  |
| 1   | 2-A   | 288 | THR  |
| 1   | 2-A   | 302 | TYR  |
| 1   | 2-A   | 344 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2-A   | 354 | LEU  |
| 1   | 2-A   | 364 | PRO  |
| 1   | 2-A   | 411 | GLN  |
| 1   | 2-A   | 415 | LEU  |
| 1   | 2-A   | 422 | LEU  |
| 1   | 2-A   | 427 | LEU  |
| 1   | 2-A   | 430 | GLN  |
| 1   | 2-A   | 463 | GLN  |
| 1   | 2-A   | 471 | SER  |
| 1   | 2-A   | 566 | ILE  |
| 1   | 2-A   | 590 | LEU  |
| 1   | 2-A   | 599 | LEU  |
| 1   | 2-A   | 633 | HIS  |
| 1   | 2-A   | 670 | VAL  |
| 1   | 2-A   | 693 | ILE  |
| 1   | 2-A   | 700 | PHE  |
| 1   | 2-A   | 764 | LEU  |
| 1   | 2-A   | 768 | ILE  |
| 1   | 2-A   | 799 | VAL  |
| 2   | 2-B   | 188 | VAL  |
| 2   | 2-B   | 246 | ILE  |
| 2   | 2-B   | 301 | THR  |
| 2   | 2-B   | 389 | ARG  |
| 2   | 2-B   | 471 | ARG  |
| 2   | 2-B   | 485 | LYS  |
| 2   | 2-B   | 502 | THR  |
| 2   | 2-B   | 504 | SER  |
| 2   | 2-B   | 508 | PRO  |
| 2   | 2-B   | 516 | LEU  |
| 2   | 2-B   | 525 | LEU  |
| 2   | 2-B   | 559 | THR  |
| 2   | 2-B   | 571 | VAL  |
| 2   | 2-B   | 604 | MET  |
| 2   | 2-B   | 605 | LEU  |
| 2   | 2-B   | 725 | GLU  |
| 2   | 2-B   | 757 | PRO  |
| 2   | 2-B   | 772 | PHE  |
| 2   | 2-B   | 838 | LEU  |
| 3   | 2-C   | 15  | ASN  |
| 3   | 2-C   | 115 | ASN  |
| 3   | 2-C   | 167 | LEU  |
| 3   | 2-C   | 194 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2-C   | 209 | LEU  |
| 3   | 2-C   | 216 | VAL  |
| 3   | 2-C   | 230 | LEU  |
| 3   | 2-C   | 292 | TYR  |
| 3   | 2-C   | 306 | VAL  |
| 3   | 2-C   | 314 | THR  |
| 3   | 2-C   | 315 | TYR  |
| 3   | 2-C   | 321 | THR  |
| 3   | 2-C   | 367 | PRO  |
| 3   | 2-C   | 371 | GLU  |
| 3   | 2-C   | 379 | ASN  |
| 3   | 2-C   | 382 | THR  |
| 3   | 2-C   | 383 | VAL  |
| 3   | 2-C   | 420 | GLN  |
| 3   | 2-C   | 437 | TYR  |
| 3   | 2-C   | 438 | VAL  |
| 3   | 2-D   | 31  | ILE  |
| 3   | 2-D   | 43  | SER  |
| 3   | 2-D   | 45  | GLU  |
| 3   | 2-D   | 146 | THR  |
| 3   | 2-D   | 182 | VAL  |
| 3   | 2-D   | 183 | GLN  |
| 3   | 2-D   | 230 | LEU  |
| 3   | 2-D   | 236 | SER  |
| 3   | 2-D   | 328 | PRO  |
| 3   | 2-D   | 354 | VAL  |
| 3   | 2-D   | 376 | MET  |
| 3   | 2-D   | 422 | GLU  |
| 1   | 3-A   | 67  | LEU  |
| 1   | 3-A   | 91  | GLU  |
| 1   | 3-A   | 114 | LYS  |
| 1   | 3-A   | 173 | LEU  |
| 1   | 3-A   | 259 | LEU  |
| 1   | 3-A   | 272 | LEU  |
| 1   | 3-A   | 275 | ILE  |
| 1   | 3-A   | 288 | THR  |
| 1   | 3-A   | 302 | TYR  |
| 1   | 3-A   | 344 | LEU  |
| 1   | 3-A   | 354 | LEU  |
| 1   | 3-A   | 364 | PRO  |
| 1   | 3-A   | 411 | GLN  |
| 1   | 3-A   | 415 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3-A   | 422 | LEU  |
| 1   | 3-A   | 427 | LEU  |
| 1   | 3-A   | 430 | GLN  |
| 1   | 3-A   | 463 | GLN  |
| 1   | 3-A   | 471 | SER  |
| 1   | 3-A   | 566 | ILE  |
| 1   | 3-A   | 590 | LEU  |
| 1   | 3-A   | 599 | LEU  |
| 1   | 3-A   | 633 | HIS  |
| 1   | 3-A   | 670 | VAL  |
| 1   | 3-A   | 693 | ILE  |
| 1   | 3-A   | 700 | PHE  |
| 1   | 3-A   | 764 | LEU  |
| 1   | 3-A   | 768 | ILE  |
| 1   | 3-A   | 799 | VAL  |
| 2   | 3-B   | 188 | VAL  |
| 2   | 3-B   | 246 | ILE  |
| 2   | 3-B   | 301 | THR  |
| 2   | 3-B   | 389 | ARG  |
| 2   | 3-B   | 471 | ARG  |
| 2   | 3-B   | 485 | LYS  |
| 2   | 3-B   | 502 | THR  |
| 2   | 3-B   | 504 | SER  |
| 2   | 3-B   | 508 | PRO  |
| 2   | 3-B   | 516 | LEU  |
| 2   | 3-B   | 525 | LEU  |
| 2   | 3-B   | 559 | THR  |
| 2   | 3-B   | 571 | VAL  |
| 2   | 3-B   | 604 | MET  |
| 2   | 3-B   | 605 | LEU  |
| 2   | 3-B   | 725 | GLU  |
| 2   | 3-B   | 757 | PRO  |
| 2   | 3-B   | 772 | PHE  |
| 2   | 3-B   | 838 | LEU  |
| 3   | 3-C   | 15  | ASN  |
| 3   | 3-C   | 115 | ASN  |
| 3   | 3-C   | 167 | LEU  |
| 3   | 3-C   | 194 | LEU  |
| 3   | 3-C   | 209 | LEU  |
| 3   | 3-C   | 216 | VAL  |
| 3   | 3-C   | 230 | LEU  |
| 3   | 3-C   | 292 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3-C   | 306 | VAL  |
| 3   | 3-C   | 314 | THR  |
| 3   | 3-C   | 315 | TYR  |
| 3   | 3-C   | 321 | THR  |
| 3   | 3-C   | 367 | PRO  |
| 3   | 3-C   | 371 | GLU  |
| 3   | 3-C   | 379 | ASN  |
| 3   | 3-C   | 382 | THR  |
| 3   | 3-C   | 383 | VAL  |
| 3   | 3-C   | 420 | GLN  |
| 3   | 3-C   | 437 | TYR  |
| 3   | 3-C   | 438 | VAL  |
| 3   | 3-D   | 31  | ILE  |
| 3   | 3-D   | 43  | SER  |
| 3   | 3-D   | 45  | GLU  |
| 3   | 3-D   | 146 | THR  |
| 3   | 3-D   | 182 | VAL  |
| 3   | 3-D   | 183 | GLN  |
| 3   | 3-D   | 230 | LEU  |
| 3   | 3-D   | 236 | SER  |
| 3   | 3-D   | 328 | PRO  |
| 3   | 3-D   | 354 | VAL  |
| 3   | 3-D   | 376 | MET  |
| 3   | 3-D   | 422 | GLU  |
| 1   | 4-A   | 67  | LEU  |
| 1   | 4-A   | 91  | GLU  |
| 1   | 4-A   | 114 | LYS  |
| 1   | 4-A   | 173 | LEU  |
| 1   | 4-A   | 259 | LEU  |
| 1   | 4-A   | 272 | LEU  |
| 1   | 4-A   | 275 | ILE  |
| 1   | 4-A   | 288 | THR  |
| 1   | 4-A   | 302 | TYR  |
| 1   | 4-A   | 344 | LEU  |
| 1   | 4-A   | 354 | LEU  |
| 1   | 4-A   | 364 | PRO  |
| 1   | 4-A   | 411 | GLN  |
| 1   | 4-A   | 415 | LEU  |
| 1   | 4-A   | 422 | LEU  |
| 1   | 4-A   | 427 | LEU  |
| 1   | 4-A   | 430 | GLN  |
| 1   | 4-A   | 463 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 4-A   | 471 | SER  |
| 1   | 4-A   | 566 | ILE  |
| 1   | 4-A   | 590 | LEU  |
| 1   | 4-A   | 599 | LEU  |
| 1   | 4-A   | 633 | HIS  |
| 1   | 4-A   | 670 | VAL  |
| 1   | 4-A   | 693 | ILE  |
| 1   | 4-A   | 700 | PHE  |
| 1   | 4-A   | 764 | LEU  |
| 1   | 4-A   | 768 | ILE  |
| 1   | 4-A   | 799 | VAL  |
| 2   | 4-B   | 188 | VAL  |
| 2   | 4-B   | 246 | ILE  |
| 2   | 4-B   | 301 | THR  |
| 2   | 4-B   | 389 | ARG  |
| 2   | 4-B   | 471 | ARG  |
| 2   | 4-B   | 485 | LYS  |
| 2   | 4-B   | 502 | THR  |
| 2   | 4-B   | 504 | SER  |
| 2   | 4-B   | 508 | PRO  |
| 2   | 4-B   | 516 | LEU  |
| 2   | 4-B   | 525 | LEU  |
| 2   | 4-B   | 559 | THR  |
| 2   | 4-B   | 571 | VAL  |
| 2   | 4-B   | 604 | MET  |
| 2   | 4-B   | 605 | LEU  |
| 2   | 4-B   | 725 | GLU  |
| 2   | 4-B   | 757 | PRO  |
| 2   | 4-B   | 772 | PHE  |
| 2   | 4-B   | 838 | LEU  |
| 3   | 4-C   | 15  | ASN  |
| 3   | 4-C   | 115 | ASN  |
| 3   | 4-C   | 167 | LEU  |
| 3   | 4-C   | 194 | LEU  |
| 3   | 4-C   | 209 | LEU  |
| 3   | 4-C   | 216 | VAL  |
| 3   | 4-C   | 230 | LEU  |
| 3   | 4-C   | 292 | TYR  |
| 3   | 4-C   | 306 | VAL  |
| 3   | 4-C   | 314 | THR  |
| 3   | 4-C   | 315 | TYR  |
| 3   | 4-C   | 321 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 4-C   | 367 | PRO  |
| 3   | 4-C   | 371 | GLU  |
| 3   | 4-C   | 379 | ASN  |
| 3   | 4-C   | 382 | THR  |
| 3   | 4-C   | 383 | VAL  |
| 3   | 4-C   | 420 | GLN  |
| 3   | 4-C   | 437 | TYR  |
| 3   | 4-C   | 438 | VAL  |
| 3   | 4-D   | 31  | ILE  |
| 3   | 4-D   | 43  | SER  |
| 3   | 4-D   | 45  | GLU  |
| 3   | 4-D   | 146 | THR  |
| 3   | 4-D   | 182 | VAL  |
| 3   | 4-D   | 183 | GLN  |
| 3   | 4-D   | 230 | LEU  |
| 3   | 4-D   | 236 | SER  |
| 3   | 4-D   | 328 | PRO  |
| 3   | 4-D   | 354 | VAL  |
| 3   | 4-D   | 376 | MET  |
| 3   | 4-D   | 422 | GLU  |
| 1   | 5-A   | 67  | LEU  |
| 1   | 5-A   | 91  | GLU  |
| 1   | 5-A   | 114 | LYS  |
| 1   | 5-A   | 173 | LEU  |
| 1   | 5-A   | 259 | LEU  |
| 1   | 5-A   | 272 | LEU  |
| 1   | 5-A   | 275 | ILE  |
| 1   | 5-A   | 288 | THR  |
| 1   | 5-A   | 302 | TYR  |
| 1   | 5-A   | 344 | LEU  |
| 1   | 5-A   | 354 | LEU  |
| 1   | 5-A   | 364 | PRO  |
| 1   | 5-A   | 411 | GLN  |
| 1   | 5-A   | 415 | LEU  |
| 1   | 5-A   | 422 | LEU  |
| 1   | 5-A   | 427 | LEU  |
| 1   | 5-A   | 430 | GLN  |
| 1   | 5-A   | 463 | GLN  |
| 1   | 5-A   | 471 | SER  |
| 1   | 5-A   | 566 | ILE  |
| 1   | 5-A   | 590 | LEU  |
| 1   | 5-A   | 599 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5-A   | 633 | HIS  |
| 1   | 5-A   | 670 | VAL  |
| 1   | 5-A   | 693 | ILE  |
| 1   | 5-A   | 700 | PHE  |
| 1   | 5-A   | 764 | LEU  |
| 1   | 5-A   | 768 | ILE  |
| 1   | 5-A   | 799 | VAL  |
| 2   | 5-B   | 188 | VAL  |
| 2   | 5-B   | 246 | ILE  |
| 2   | 5-B   | 301 | THR  |
| 2   | 5-B   | 389 | ARG  |
| 2   | 5-B   | 471 | ARG  |
| 2   | 5-B   | 485 | LYS  |
| 2   | 5-B   | 502 | THR  |
| 2   | 5-B   | 504 | SER  |
| 2   | 5-B   | 508 | PRO  |
| 2   | 5-B   | 516 | LEU  |
| 2   | 5-B   | 525 | LEU  |
| 2   | 5-B   | 559 | THR  |
| 2   | 5-B   | 571 | VAL  |
| 2   | 5-B   | 604 | MET  |
| 2   | 5-B   | 605 | LEU  |
| 2   | 5-B   | 725 | GLU  |
| 2   | 5-B   | 757 | PRO  |
| 2   | 5-B   | 772 | PHE  |
| 2   | 5-B   | 838 | LEU  |
| 3   | 5-C   | 15  | ASN  |
| 3   | 5-C   | 115 | ASN  |
| 3   | 5-C   | 167 | LEU  |
| 3   | 5-C   | 194 | LEU  |
| 3   | 5-C   | 209 | LEU  |
| 3   | 5-C   | 216 | VAL  |
| 3   | 5-C   | 230 | LEU  |
| 3   | 5-C   | 292 | TYR  |
| 3   | 5-C   | 306 | VAL  |
| 3   | 5-C   | 314 | THR  |
| 3   | 5-C   | 315 | TYR  |
| 3   | 5-C   | 321 | THR  |
| 3   | 5-C   | 367 | PRO  |
| 3   | 5-C   | 371 | GLU  |
| 3   | 5-C   | 379 | ASN  |
| 3   | 5-C   | 382 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 5-C   | 383 | VAL  |
| 3   | 5-C   | 420 | GLN  |
| 3   | 5-C   | 437 | TYR  |
| 3   | 5-C   | 438 | VAL  |
| 3   | 5-D   | 31  | ILE  |
| 3   | 5-D   | 43  | SER  |
| 3   | 5-D   | 45  | GLU  |
| 3   | 5-D   | 146 | THR  |
| 3   | 5-D   | 182 | VAL  |
| 3   | 5-D   | 183 | GLN  |
| 3   | 5-D   | 230 | LEU  |
| 3   | 5-D   | 236 | SER  |
| 3   | 5-D   | 328 | PRO  |
| 3   | 5-D   | 354 | VAL  |
| 3   | 5-D   | 376 | MET  |
| 3   | 5-D   | 422 | GLU  |
| 1   | 6-A   | 67  | LEU  |
| 1   | 6-A   | 91  | GLU  |
| 1   | 6-A   | 114 | LYS  |
| 1   | 6-A   | 173 | LEU  |
| 1   | 6-A   | 259 | LEU  |
| 1   | 6-A   | 272 | LEU  |
| 1   | 6-A   | 275 | ILE  |
| 1   | 6-A   | 288 | THR  |
| 1   | 6-A   | 302 | TYR  |
| 1   | 6-A   | 344 | LEU  |
| 1   | 6-A   | 354 | LEU  |
| 1   | 6-A   | 364 | PRO  |
| 1   | 6-A   | 411 | GLN  |
| 1   | 6-A   | 415 | LEU  |
| 1   | 6-A   | 422 | LEU  |
| 1   | 6-A   | 427 | LEU  |
| 1   | 6-A   | 430 | GLN  |
| 1   | 6-A   | 463 | GLN  |
| 1   | 6-A   | 471 | SER  |
| 1   | 6-A   | 566 | ILE  |
| 1   | 6-A   | 590 | LEU  |
| 1   | 6-A   | 599 | LEU  |
| 1   | 6-A   | 633 | HIS  |
| 1   | 6-A   | 670 | VAL  |
| 1   | 6-A   | 693 | ILE  |
| 1   | 6-A   | 700 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6-A   | 764 | LEU  |
| 1   | 6-A   | 768 | ILE  |
| 1   | 6-A   | 799 | VAL  |
| 2   | 6-B   | 188 | VAL  |
| 2   | 6-B   | 246 | ILE  |
| 2   | 6-B   | 301 | THR  |
| 2   | 6-B   | 389 | ARG  |
| 2   | 6-B   | 471 | ARG  |
| 2   | 6-B   | 485 | LYS  |
| 2   | 6-B   | 502 | THR  |
| 2   | 6-B   | 504 | SER  |
| 2   | 6-B   | 508 | PRO  |
| 2   | 6-B   | 516 | LEU  |
| 2   | 6-B   | 525 | LEU  |
| 2   | 6-B   | 559 | THR  |
| 2   | 6-B   | 571 | VAL  |
| 2   | 6-B   | 604 | MET  |
| 2   | 6-B   | 605 | LEU  |
| 2   | 6-B   | 725 | GLU  |
| 2   | 6-B   | 757 | PRO  |
| 2   | 6-B   | 772 | PHE  |
| 2   | 6-B   | 838 | LEU  |
| 3   | 6-C   | 15  | ASN  |
| 3   | 6-C   | 115 | ASN  |
| 3   | 6-C   | 167 | LEU  |
| 3   | 6-C   | 194 | LEU  |
| 3   | 6-C   | 209 | LEU  |
| 3   | 6-C   | 216 | VAL  |
| 3   | 6-C   | 230 | LEU  |
| 3   | 6-C   | 292 | TYR  |
| 3   | 6-C   | 306 | VAL  |
| 3   | 6-C   | 314 | THR  |
| 3   | 6-C   | 315 | TYR  |
| 3   | 6-C   | 321 | THR  |
| 3   | 6-C   | 367 | PRO  |
| 3   | 6-C   | 371 | GLU  |
| 3   | 6-C   | 379 | ASN  |
| 3   | 6-C   | 382 | THR  |
| 3   | 6-C   | 383 | VAL  |
| 3   | 6-C   | 420 | GLN  |
| 3   | 6-C   | 437 | TYR  |
| 3   | 6-C   | 438 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 6-D   | 31  | ILE  |
| 3   | 6-D   | 43  | SER  |
| 3   | 6-D   | 45  | GLU  |
| 3   | 6-D   | 146 | THR  |
| 3   | 6-D   | 182 | VAL  |
| 3   | 6-D   | 183 | GLN  |
| 3   | 6-D   | 230 | LEU  |
| 3   | 6-D   | 236 | SER  |
| 3   | 6-D   | 328 | PRO  |
| 3   | 6-D   | 354 | VAL  |
| 3   | 6-D   | 376 | MET  |
| 3   | 6-D   | 422 | GLU  |
| 1   | 7-A   | 67  | LEU  |
| 1   | 7-A   | 91  | GLU  |
| 1   | 7-A   | 114 | LYS  |
| 1   | 7-A   | 173 | LEU  |
| 1   | 7-A   | 259 | LEU  |
| 1   | 7-A   | 272 | LEU  |
| 1   | 7-A   | 275 | ILE  |
| 1   | 7-A   | 288 | THR  |
| 1   | 7-A   | 302 | TYR  |
| 1   | 7-A   | 344 | LEU  |
| 1   | 7-A   | 354 | LEU  |
| 1   | 7-A   | 364 | PRO  |
| 1   | 7-A   | 411 | GLN  |
| 1   | 7-A   | 415 | LEU  |
| 1   | 7-A   | 422 | LEU  |
| 1   | 7-A   | 427 | LEU  |
| 1   | 7-A   | 430 | GLN  |
| 1   | 7-A   | 463 | GLN  |
| 1   | 7-A   | 471 | SER  |
| 1   | 7-A   | 566 | ILE  |
| 1   | 7-A   | 590 | LEU  |
| 1   | 7-A   | 599 | LEU  |
| 1   | 7-A   | 633 | HIS  |
| 1   | 7-A   | 670 | VAL  |
| 1   | 7-A   | 693 | ILE  |
| 1   | 7-A   | 700 | PHE  |
| 1   | 7-A   | 764 | LEU  |
| 1   | 7-A   | 768 | ILE  |
| 1   | 7-A   | 799 | VAL  |
| 2   | 7-B   | 188 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 7-B   | 246 | ILE  |
| 2   | 7-B   | 301 | THR  |
| 2   | 7-B   | 389 | ARG  |
| 2   | 7-B   | 471 | ARG  |
| 2   | 7-B   | 485 | LYS  |
| 2   | 7-B   | 502 | THR  |
| 2   | 7-B   | 504 | SER  |
| 2   | 7-B   | 508 | PRO  |
| 2   | 7-B   | 516 | LEU  |
| 2   | 7-B   | 525 | LEU  |
| 2   | 7-B   | 559 | THR  |
| 2   | 7-B   | 571 | VAL  |
| 2   | 7-B   | 604 | MET  |
| 2   | 7-B   | 605 | LEU  |
| 2   | 7-B   | 725 | GLU  |
| 2   | 7-B   | 757 | PRO  |
| 2   | 7-B   | 772 | PHE  |
| 2   | 7-B   | 838 | LEU  |
| 3   | 7-C   | 15  | ASN  |
| 3   | 7-C   | 115 | ASN  |
| 3   | 7-C   | 167 | LEU  |
| 3   | 7-C   | 194 | LEU  |
| 3   | 7-C   | 209 | LEU  |
| 3   | 7-C   | 216 | VAL  |
| 3   | 7-C   | 230 | LEU  |
| 3   | 7-C   | 292 | TYR  |
| 3   | 7-C   | 306 | VAL  |
| 3   | 7-C   | 314 | THR  |
| 3   | 7-C   | 315 | TYR  |
| 3   | 7-C   | 321 | THR  |
| 3   | 7-C   | 367 | PRO  |
| 3   | 7-C   | 371 | GLU  |
| 3   | 7-C   | 379 | ASN  |
| 3   | 7-C   | 382 | THR  |
| 3   | 7-C   | 383 | VAL  |
| 3   | 7-C   | 420 | GLN  |
| 3   | 7-C   | 437 | TYR  |
| 3   | 7-C   | 438 | VAL  |
| 3   | 7-D   | 31  | ILE  |
| 3   | 7-D   | 43  | SER  |
| 3   | 7-D   | 45  | GLU  |
| 3   | 7-D   | 146 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 7-D   | 182 | VAL  |
| 3   | 7-D   | 183 | GLN  |
| 3   | 7-D   | 230 | LEU  |
| 3   | 7-D   | 236 | SER  |
| 3   | 7-D   | 328 | PRO  |
| 3   | 7-D   | 354 | VAL  |
| 3   | 7-D   | 376 | MET  |
| 3   | 7-D   | 422 | GLU  |
| 1   | 8-A   | 67  | LEU  |
| 1   | 8-A   | 91  | GLU  |
| 1   | 8-A   | 114 | LYS  |
| 1   | 8-A   | 173 | LEU  |
| 1   | 8-A   | 259 | LEU  |
| 1   | 8-A   | 272 | LEU  |
| 1   | 8-A   | 275 | ILE  |
| 1   | 8-A   | 288 | THR  |
| 1   | 8-A   | 302 | TYR  |
| 1   | 8-A   | 344 | LEU  |
| 1   | 8-A   | 354 | LEU  |
| 1   | 8-A   | 364 | PRO  |
| 1   | 8-A   | 411 | GLN  |
| 1   | 8-A   | 415 | LEU  |
| 1   | 8-A   | 422 | LEU  |
| 1   | 8-A   | 427 | LEU  |
| 1   | 8-A   | 430 | GLN  |
| 1   | 8-A   | 463 | GLN  |
| 1   | 8-A   | 471 | SER  |
| 1   | 8-A   | 566 | ILE  |
| 1   | 8-A   | 590 | LEU  |
| 1   | 8-A   | 599 | LEU  |
| 1   | 8-A   | 633 | HIS  |
| 1   | 8-A   | 670 | VAL  |
| 1   | 8-A   | 693 | ILE  |
| 1   | 8-A   | 700 | PHE  |
| 1   | 8-A   | 764 | LEU  |
| 1   | 8-A   | 768 | ILE  |
| 1   | 8-A   | 799 | VAL  |
| 2   | 8-B   | 188 | VAL  |
| 2   | 8-B   | 246 | ILE  |
| 2   | 8-B   | 301 | THR  |
| 2   | 8-B   | 389 | ARG  |
| 2   | 8-B   | 471 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 8-B   | 485 | LYS  |
| 2   | 8-B   | 502 | THR  |
| 2   | 8-B   | 504 | SER  |
| 2   | 8-B   | 508 | PRO  |
| 2   | 8-B   | 516 | LEU  |
| 2   | 8-B   | 525 | LEU  |
| 2   | 8-B   | 559 | THR  |
| 2   | 8-B   | 571 | VAL  |
| 2   | 8-B   | 604 | MET  |
| 2   | 8-B   | 605 | LEU  |
| 2   | 8-B   | 725 | GLU  |
| 2   | 8-B   | 757 | PRO  |
| 2   | 8-B   | 772 | PHE  |
| 2   | 8-B   | 838 | LEU  |
| 3   | 8-C   | 15  | ASN  |
| 3   | 8-C   | 115 | ASN  |
| 3   | 8-C   | 167 | LEU  |
| 3   | 8-C   | 194 | LEU  |
| 3   | 8-C   | 209 | LEU  |
| 3   | 8-C   | 216 | VAL  |
| 3   | 8-C   | 230 | LEU  |
| 3   | 8-C   | 292 | TYR  |
| 3   | 8-C   | 306 | VAL  |
| 3   | 8-C   | 314 | THR  |
| 3   | 8-C   | 315 | TYR  |
| 3   | 8-C   | 321 | THR  |
| 3   | 8-C   | 367 | PRO  |
| 3   | 8-C   | 371 | GLU  |
| 3   | 8-C   | 379 | ASN  |
| 3   | 8-C   | 382 | THR  |
| 3   | 8-C   | 383 | VAL  |
| 3   | 8-C   | 420 | GLN  |
| 3   | 8-C   | 437 | TYR  |
| 3   | 8-C   | 438 | VAL  |
| 3   | 8-D   | 31  | ILE  |
| 3   | 8-D   | 43  | SER  |
| 3   | 8-D   | 45  | GLU  |
| 3   | 8-D   | 146 | THR  |
| 3   | 8-D   | 182 | VAL  |
| 3   | 8-D   | 183 | GLN  |
| 3   | 8-D   | 230 | LEU  |
| 3   | 8-D   | 236 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 8-D   | 328 | PRO  |
| 3   | 8-D   | 354 | VAL  |
| 3   | 8-D   | 376 | MET  |
| 3   | 8-D   | 422 | GLU  |
| 1   | 9-A   | 67  | LEU  |
| 1   | 9-A   | 91  | GLU  |
| 1   | 9-A   | 114 | LYS  |
| 1   | 9-A   | 173 | LEU  |
| 1   | 9-A   | 259 | LEU  |
| 1   | 9-A   | 272 | LEU  |
| 1   | 9-A   | 275 | ILE  |
| 1   | 9-A   | 288 | THR  |
| 1   | 9-A   | 302 | TYR  |
| 1   | 9-A   | 344 | LEU  |
| 1   | 9-A   | 354 | LEU  |
| 1   | 9-A   | 364 | PRO  |
| 1   | 9-A   | 411 | GLN  |
| 1   | 9-A   | 415 | LEU  |
| 1   | 9-A   | 422 | LEU  |
| 1   | 9-A   | 427 | LEU  |
| 1   | 9-A   | 430 | GLN  |
| 1   | 9-A   | 463 | GLN  |
| 1   | 9-A   | 471 | SER  |
| 1   | 9-A   | 566 | ILE  |
| 1   | 9-A   | 590 | LEU  |
| 1   | 9-A   | 599 | LEU  |
| 1   | 9-A   | 633 | HIS  |
| 1   | 9-A   | 670 | VAL  |
| 1   | 9-A   | 693 | ILE  |
| 1   | 9-A   | 700 | PHE  |
| 1   | 9-A   | 764 | LEU  |
| 1   | 9-A   | 768 | ILE  |
| 1   | 9-A   | 799 | VAL  |
| 2   | 9-B   | 188 | VAL  |
| 2   | 9-B   | 246 | ILE  |
| 2   | 9-B   | 301 | THR  |
| 2   | 9-B   | 389 | ARG  |
| 2   | 9-B   | 471 | ARG  |
| 2   | 9-B   | 485 | LYS  |
| 2   | 9-B   | 502 | THR  |
| 2   | 9-B   | 504 | SER  |
| 2   | 9-B   | 508 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 9-B   | 516 | LEU  |
| 2   | 9-B   | 525 | LEU  |
| 2   | 9-B   | 559 | THR  |
| 2   | 9-B   | 571 | VAL  |
| 2   | 9-B   | 604 | MET  |
| 2   | 9-B   | 605 | LEU  |
| 2   | 9-B   | 725 | GLU  |
| 2   | 9-B   | 757 | PRO  |
| 2   | 9-B   | 772 | PHE  |
| 2   | 9-B   | 838 | LEU  |
| 3   | 9-C   | 15  | ASN  |
| 3   | 9-C   | 115 | ASN  |
| 3   | 9-C   | 167 | LEU  |
| 3   | 9-C   | 194 | LEU  |
| 3   | 9-C   | 209 | LEU  |
| 3   | 9-C   | 216 | VAL  |
| 3   | 9-C   | 230 | LEU  |
| 3   | 9-C   | 292 | TYR  |
| 3   | 9-C   | 306 | VAL  |
| 3   | 9-C   | 314 | THR  |
| 3   | 9-C   | 315 | TYR  |
| 3   | 9-C   | 321 | THR  |
| 3   | 9-C   | 367 | PRO  |
| 3   | 9-C   | 371 | GLU  |
| 3   | 9-C   | 379 | ASN  |
| 3   | 9-C   | 382 | THR  |
| 3   | 9-C   | 383 | VAL  |
| 3   | 9-C   | 420 | GLN  |
| 3   | 9-C   | 437 | TYR  |
| 3   | 9-C   | 438 | VAL  |
| 3   | 9-D   | 31  | ILE  |
| 3   | 9-D   | 43  | SER  |
| 3   | 9-D   | 45  | GLU  |
| 3   | 9-D   | 146 | THR  |
| 3   | 9-D   | 182 | VAL  |
| 3   | 9-D   | 183 | GLN  |
| 3   | 9-D   | 230 | LEU  |
| 3   | 9-D   | 236 | SER  |
| 3   | 9-D   | 328 | PRO  |
| 3   | 9-D   | 354 | VAL  |
| 3   | 9-D   | 376 | MET  |
| 3   | 9-D   | 422 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 10-A  | 67  | LEU  |
| 1   | 10-A  | 91  | GLU  |
| 1   | 10-A  | 114 | LYS  |
| 1   | 10-A  | 173 | LEU  |
| 1   | 10-A  | 259 | LEU  |
| 1   | 10-A  | 272 | LEU  |
| 1   | 10-A  | 275 | ILE  |
| 1   | 10-A  | 288 | THR  |
| 1   | 10-A  | 302 | TYR  |
| 1   | 10-A  | 344 | LEU  |
| 1   | 10-A  | 354 | LEU  |
| 1   | 10-A  | 364 | PRO  |
| 1   | 10-A  | 411 | GLN  |
| 1   | 10-A  | 415 | LEU  |
| 1   | 10-A  | 422 | LEU  |
| 1   | 10-A  | 427 | LEU  |
| 1   | 10-A  | 430 | GLN  |
| 1   | 10-A  | 463 | GLN  |
| 1   | 10-A  | 471 | SER  |
| 1   | 10-A  | 566 | ILE  |
| 1   | 10-A  | 590 | LEU  |
| 1   | 10-A  | 599 | LEU  |
| 1   | 10-A  | 633 | HIS  |
| 1   | 10-A  | 670 | VAL  |
| 1   | 10-A  | 693 | ILE  |
| 1   | 10-A  | 700 | PHE  |
| 1   | 10-A  | 764 | LEU  |
| 1   | 10-A  | 768 | ILE  |
| 1   | 10-A  | 799 | VAL  |
| 2   | 10-B  | 188 | VAL  |
| 2   | 10-B  | 246 | ILE  |
| 2   | 10-B  | 301 | THR  |
| 2   | 10-B  | 389 | ARG  |
| 2   | 10-B  | 471 | ARG  |
| 2   | 10-B  | 485 | LYS  |
| 2   | 10-B  | 502 | THR  |
| 2   | 10-B  | 504 | SER  |
| 2   | 10-B  | 508 | PRO  |
| 2   | 10-B  | 516 | LEU  |
| 2   | 10-B  | 525 | LEU  |
| 2   | 10-B  | 559 | THR  |
| 2   | 10-B  | 571 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 10-B  | 604 | MET  |
| 2   | 10-B  | 605 | LEU  |
| 2   | 10-B  | 725 | GLU  |
| 2   | 10-B  | 757 | PRO  |
| 2   | 10-B  | 772 | PHE  |
| 2   | 10-B  | 838 | LEU  |
| 3   | 10-C  | 15  | ASN  |
| 3   | 10-C  | 115 | ASN  |
| 3   | 10-C  | 167 | LEU  |
| 3   | 10-C  | 194 | LEU  |
| 3   | 10-C  | 209 | LEU  |
| 3   | 10-C  | 216 | VAL  |
| 3   | 10-C  | 230 | LEU  |
| 3   | 10-C  | 292 | TYR  |
| 3   | 10-C  | 306 | VAL  |
| 3   | 10-C  | 314 | THR  |
| 3   | 10-C  | 315 | TYR  |
| 3   | 10-C  | 321 | THR  |
| 3   | 10-C  | 367 | PRO  |
| 3   | 10-C  | 371 | GLU  |
| 3   | 10-C  | 379 | ASN  |
| 3   | 10-C  | 382 | THR  |
| 3   | 10-C  | 383 | VAL  |
| 3   | 10-C  | 420 | GLN  |
| 3   | 10-C  | 437 | TYR  |
| 3   | 10-C  | 438 | VAL  |
| 3   | 10-D  | 31  | ILE  |
| 3   | 10-D  | 43  | SER  |
| 3   | 10-D  | 45  | GLU  |
| 3   | 10-D  | 146 | THR  |
| 3   | 10-D  | 182 | VAL  |
| 3   | 10-D  | 183 | GLN  |
| 3   | 10-D  | 230 | LEU  |
| 3   | 10-D  | 236 | SER  |
| 3   | 10-D  | 328 | PRO  |
| 3   | 10-D  | 354 | VAL  |
| 3   | 10-D  | 376 | MET  |
| 3   | 10-D  | 422 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (614) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 136 | GLN  |
| 1   | 1-A   | 289 | GLN  |
| 1   | 1-A   | 293 | ASN  |
| 1   | 1-A   | 297 | GLN  |
| 1   | 1-A   | 362 | GLN  |
| 1   | 1-A   | 402 | ASN  |
| 1   | 1-A   | 417 | ASN  |
| 1   | 1-A   | 454 | ASN  |
| 1   | 1-A   | 463 | GLN  |
| 1   | 1-A   | 485 | GLN  |
| 1   | 1-A   | 589 | GLN  |
| 1   | 1-A   | 633 | HIS  |
| 1   | 1-A   | 638 | HIS  |
| 1   | 1-A   | 648 | ASN  |
| 1   | 1-A   | 665 | ASN  |
| 1   | 1-A   | 686 | ASN  |
| 2   | 1-B   | 215 | ASN  |
| 2   | 1-B   | 222 | HIS  |
| 2   | 1-B   | 232 | GLN  |
| 2   | 1-B   | 348 | ASN  |
| 2   | 1-B   | 380 | HIS  |
| 2   | 1-B   | 430 | HIS  |
| 2   | 1-B   | 436 | ASN  |
| 2   | 1-B   | 452 | GLN  |
| 2   | 1-B   | 462 | GLN  |
| 2   | 1-B   | 466 | GLN  |
| 2   | 1-B   | 469 | HIS  |
| 2   | 1-B   | 539 | ASN  |
| 2   | 1-B   | 629 | ASN  |
| 2   | 1-B   | 640 | GLN  |
| 2   | 1-B   | 654 | ASN  |
| 2   | 1-B   | 720 | ASN  |
| 2   | 1-B   | 728 | HIS  |
| 2   | 1-B   | 756 | GLN  |
| 2   | 1-B   | 767 | ASN  |
| 2   | 1-B   | 799 | ASN  |
| 2   | 1-B   | 808 | ASN  |
| 3   | 1-C   | 15  | ASN  |
| 3   | 1-C   | 16  | HIS  |
| 3   | 1-C   | 132 | ASN  |
| 3   | 1-C   | 153 | ASN  |
| 3   | 1-C   | 183 | GLN  |
| 3   | 1-C   | 211 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1-C   | 225 | GLN  |
| 3   | 1-C   | 266 | HIS  |
| 3   | 1-C   | 281 | HIS  |
| 3   | 1-C   | 303 | ASN  |
| 3   | 1-C   | 311 | ASN  |
| 3   | 1-C   | 317 | ASN  |
| 3   | 1-C   | 320 | ASN  |
| 3   | 1-C   | 339 | GLN  |
| 3   | 1-C   | 366 | GLN  |
| 3   | 1-C   | 368 | ASN  |
| 3   | 1-C   | 370 | ASN  |
| 3   | 1-D   | 91  | ASN  |
| 3   | 1-D   | 103 | ASN  |
| 3   | 1-D   | 115 | ASN  |
| 3   | 1-D   | 225 | GLN  |
| 3   | 1-D   | 266 | HIS  |
| 3   | 1-D   | 281 | HIS  |
| 3   | 1-D   | 286 | HIS  |
| 3   | 1-D   | 317 | ASN  |
| 3   | 1-D   | 325 | ASN  |
| 3   | 1-D   | 379 | ASN  |
| 1   | 2-A   | 79  | ASN  |
| 1   | 2-A   | 136 | GLN  |
| 1   | 2-A   | 273 | ASN  |
| 1   | 2-A   | 369 | ASN  |
| 1   | 2-A   | 402 | ASN  |
| 1   | 2-A   | 417 | ASN  |
| 1   | 2-A   | 434 | ASN  |
| 1   | 2-A   | 449 | HIS  |
| 1   | 2-A   | 559 | HIS  |
| 1   | 2-A   | 583 | GLN  |
| 1   | 2-A   | 607 | ASN  |
| 1   | 2-A   | 665 | ASN  |
| 2   | 2-B   | 215 | ASN  |
| 2   | 2-B   | 270 | ASN  |
| 2   | 2-B   | 367 | ASN  |
| 2   | 2-B   | 387 | GLN  |
| 2   | 2-B   | 430 | HIS  |
| 2   | 2-B   | 452 | GLN  |
| 2   | 2-B   | 461 | ASN  |
| 2   | 2-B   | 469 | HIS  |
| 2   | 2-B   | 497 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2-B   | 530 | ASN  |
| 2   | 2-B   | 550 | HIS  |
| 2   | 2-B   | 573 | ASN  |
| 2   | 2-B   | 596 | ASN  |
| 2   | 2-B   | 642 | GLN  |
| 2   | 2-B   | 738 | HIS  |
| 2   | 2-B   | 778 | ASN  |
| 3   | 2-C   | 15  | ASN  |
| 3   | 2-C   | 29  | HIS  |
| 3   | 2-C   | 116 | GLN  |
| 3   | 2-C   | 219 | ASN  |
| 3   | 2-C   | 229 | GLN  |
| 3   | 2-C   | 266 | HIS  |
| 3   | 2-C   | 286 | HIS  |
| 3   | 2-C   | 312 | ASN  |
| 3   | 2-C   | 317 | ASN  |
| 3   | 2-C   | 320 | ASN  |
| 3   | 2-C   | 339 | GLN  |
| 3   | 2-C   | 379 | ASN  |
| 3   | 2-C   | 385 | ASN  |
| 3   | 2-D   | 9   | GLN  |
| 3   | 2-D   | 12  | GLN  |
| 3   | 2-D   | 15  | ASN  |
| 3   | 2-D   | 16  | HIS  |
| 3   | 2-D   | 57  | ASN  |
| 3   | 2-D   | 107 | ASN  |
| 3   | 2-D   | 226 | HIS  |
| 3   | 2-D   | 228 | ASN  |
| 3   | 2-D   | 289 | HIS  |
| 3   | 2-D   | 330 | GLN  |
| 3   | 2-D   | 385 | ASN  |
| 3   | 2-D   | 408 | ASN  |
| 3   | 2-D   | 418 | ASN  |
| 1   | 3-A   | 55  | GLN  |
| 1   | 3-A   | 178 | ASN  |
| 1   | 3-A   | 191 | ASN  |
| 1   | 3-A   | 258 | ASN  |
| 1   | 3-A   | 323 | GLN  |
| 1   | 3-A   | 389 | ASN  |
| 1   | 3-A   | 421 | HIS  |
| 1   | 3-A   | 475 | ASN  |
| 1   | 3-A   | 637 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3-A   | 638 | HIS  |
| 1   | 3-A   | 665 | ASN  |
| 1   | 3-A   | 673 | GLN  |
| 1   | 3-A   | 784 | GLN  |
| 2   | 3-B   | 208 | GLN  |
| 2   | 3-B   | 215 | ASN  |
| 2   | 3-B   | 222 | HIS  |
| 2   | 3-B   | 232 | GLN  |
| 2   | 3-B   | 322 | HIS  |
| 2   | 3-B   | 380 | HIS  |
| 2   | 3-B   | 386 | ASN  |
| 2   | 3-B   | 420 | GLN  |
| 2   | 3-B   | 509 | ASN  |
| 2   | 3-B   | 527 | HIS  |
| 2   | 3-B   | 629 | ASN  |
| 2   | 3-B   | 640 | GLN  |
| 2   | 3-B   | 642 | GLN  |
| 2   | 3-B   | 660 | ASN  |
| 2   | 3-B   | 734 | ASN  |
| 2   | 3-B   | 767 | ASN  |
| 2   | 3-B   | 780 | ASN  |
| 2   | 3-B   | 806 | ASN  |
| 3   | 3-C   | 9   | GLN  |
| 3   | 3-C   | 12  | GLN  |
| 3   | 3-C   | 103 | ASN  |
| 3   | 3-C   | 153 | ASN  |
| 3   | 3-C   | 219 | ASN  |
| 3   | 3-C   | 225 | GLN  |
| 3   | 3-C   | 229 | GLN  |
| 3   | 3-C   | 392 | ASN  |
| 3   | 3-C   | 408 | ASN  |
| 3   | 3-C   | 418 | ASN  |
| 3   | 3-D   | 16  | HIS  |
| 3   | 3-D   | 24  | GLN  |
| 3   | 3-D   | 91  | ASN  |
| 3   | 3-D   | 103 | ASN  |
| 3   | 3-D   | 116 | GLN  |
| 3   | 3-D   | 121 | ASN  |
| 3   | 3-D   | 153 | ASN  |
| 3   | 3-D   | 219 | ASN  |
| 3   | 3-D   | 281 | HIS  |
| 3   | 3-D   | 289 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3-D   | 312 | ASN  |
| 3   | 3-D   | 317 | ASN  |
| 3   | 3-D   | 325 | ASN  |
| 3   | 3-D   | 330 | GLN  |
| 3   | 3-D   | 340 | GLN  |
| 3   | 3-D   | 353 | HIS  |
| 3   | 3-D   | 370 | ASN  |
| 3   | 3-D   | 414 | GLN  |
| 3   | 3-D   | 417 | GLN  |
| 1   | 4-A   | 178 | ASN  |
| 1   | 4-A   | 185 | GLN  |
| 1   | 4-A   | 274 | ASN  |
| 1   | 4-A   | 376 | GLN  |
| 1   | 4-A   | 389 | ASN  |
| 1   | 4-A   | 421 | HIS  |
| 1   | 4-A   | 434 | ASN  |
| 1   | 4-A   | 442 | ASN  |
| 1   | 4-A   | 454 | ASN  |
| 1   | 4-A   | 463 | GLN  |
| 1   | 4-A   | 470 | GLN  |
| 1   | 4-A   | 476 | ASN  |
| 1   | 4-A   | 485 | GLN  |
| 1   | 4-A   | 559 | HIS  |
| 1   | 4-A   | 583 | GLN  |
| 1   | 4-A   | 589 | GLN  |
| 1   | 4-A   | 595 | HIS  |
| 1   | 4-A   | 637 | ASN  |
| 1   | 4-A   | 638 | HIS  |
| 1   | 4-A   | 649 | GLN  |
| 1   | 4-A   | 650 | ASN  |
| 1   | 4-A   | 686 | ASN  |
| 1   | 4-A   | 781 | ASN  |
| 1   | 4-A   | 784 | GLN  |
| 2   | 4-B   | 204 | HIS  |
| 2   | 4-B   | 208 | GLN  |
| 2   | 4-B   | 232 | GLN  |
| 2   | 4-B   | 270 | ASN  |
| 2   | 4-B   | 303 | HIS  |
| 2   | 4-B   | 322 | HIS  |
| 2   | 4-B   | 336 | ASN  |
| 2   | 4-B   | 367 | ASN  |
| 2   | 4-B   | 380 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 4-B   | 386 | ASN  |
| 2   | 4-B   | 387 | GLN  |
| 2   | 4-B   | 423 | ASN  |
| 2   | 4-B   | 430 | HIS  |
| 2   | 4-B   | 434 | GLN  |
| 2   | 4-B   | 459 | HIS  |
| 2   | 4-B   | 462 | GLN  |
| 2   | 4-B   | 466 | GLN  |
| 2   | 4-B   | 469 | HIS  |
| 2   | 4-B   | 497 | ASN  |
| 2   | 4-B   | 509 | ASN  |
| 2   | 4-B   | 601 | GLN  |
| 2   | 4-B   | 608 | ASN  |
| 2   | 4-B   | 640 | GLN  |
| 2   | 4-B   | 642 | GLN  |
| 2   | 4-B   | 669 | GLN  |
| 2   | 4-B   | 738 | HIS  |
| 2   | 4-B   | 780 | ASN  |
| 2   | 4-B   | 815 | GLN  |
| 3   | 4-C   | 29  | HIS  |
| 3   | 4-C   | 115 | ASN  |
| 3   | 4-C   | 116 | GLN  |
| 3   | 4-C   | 121 | ASN  |
| 3   | 4-C   | 140 | HIS  |
| 3   | 4-C   | 221 | ASN  |
| 3   | 4-C   | 225 | GLN  |
| 3   | 4-C   | 228 | ASN  |
| 3   | 4-C   | 229 | GLN  |
| 3   | 4-C   | 266 | HIS  |
| 3   | 4-C   | 325 | ASN  |
| 3   | 4-C   | 368 | ASN  |
| 3   | 4-C   | 392 | ASN  |
| 3   | 4-C   | 405 | ASN  |
| 3   | 4-D   | 9   | GLN  |
| 3   | 4-D   | 16  | HIS  |
| 3   | 4-D   | 29  | HIS  |
| 3   | 4-D   | 60  | ASN  |
| 3   | 4-D   | 183 | GLN  |
| 3   | 4-D   | 281 | HIS  |
| 3   | 4-D   | 286 | HIS  |
| 3   | 4-D   | 303 | ASN  |
| 3   | 4-D   | 317 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 4-D   | 420 | GLN  |
| 1   | 5-A   | 191 | ASN  |
| 1   | 5-A   | 252 | GLN  |
| 1   | 5-A   | 273 | ASN  |
| 1   | 5-A   | 274 | ASN  |
| 1   | 5-A   | 293 | ASN  |
| 1   | 5-A   | 342 | ASN  |
| 1   | 5-A   | 449 | HIS  |
| 1   | 5-A   | 457 | ASN  |
| 1   | 5-A   | 464 | ASN  |
| 1   | 5-A   | 470 | GLN  |
| 1   | 5-A   | 485 | GLN  |
| 1   | 5-A   | 559 | HIS  |
| 1   | 5-A   | 589 | GLN  |
| 1   | 5-A   | 633 | HIS  |
| 1   | 5-A   | 648 | ASN  |
| 1   | 5-A   | 673 | GLN  |
| 1   | 5-A   | 674 | ASN  |
| 1   | 5-A   | 686 | ASN  |
| 1   | 5-A   | 696 | GLN  |
| 1   | 5-A   | 770 | ASN  |
| 2   | 5-B   | 206 | GLN  |
| 2   | 5-B   | 215 | ASN  |
| 2   | 5-B   | 386 | ASN  |
| 2   | 5-B   | 420 | GLN  |
| 2   | 5-B   | 444 | ASN  |
| 2   | 5-B   | 461 | ASN  |
| 2   | 5-B   | 517 | GLN  |
| 2   | 5-B   | 521 | GLN  |
| 2   | 5-B   | 527 | HIS  |
| 2   | 5-B   | 530 | ASN  |
| 2   | 5-B   | 539 | ASN  |
| 2   | 5-B   | 573 | ASN  |
| 2   | 5-B   | 575 | ASN  |
| 2   | 5-B   | 608 | ASN  |
| 2   | 5-B   | 629 | ASN  |
| 2   | 5-B   | 734 | ASN  |
| 2   | 5-B   | 756 | GLN  |
| 2   | 5-B   | 780 | ASN  |
| 2   | 5-B   | 808 | ASN  |
| 2   | 5-B   | 818 | ASN  |
| 2   | 5-B   | 832 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 5-C   | 16  | HIS  |
| 3   | 5-C   | 60  | ASN  |
| 3   | 5-C   | 81  | ASN  |
| 3   | 5-C   | 91  | ASN  |
| 3   | 5-C   | 103 | ASN  |
| 3   | 5-C   | 115 | ASN  |
| 3   | 5-C   | 116 | GLN  |
| 3   | 5-C   | 137 | GLN  |
| 3   | 5-C   | 140 | HIS  |
| 3   | 5-C   | 186 | ASN  |
| 3   | 5-C   | 389 | ASN  |
| 3   | 5-C   | 418 | ASN  |
| 3   | 5-C   | 420 | GLN  |
| 3   | 5-C   | 431 | GLN  |
| 3   | 5-C   | 442 | GLN  |
| 3   | 5-D   | 81  | ASN  |
| 3   | 5-D   | 91  | ASN  |
| 3   | 5-D   | 137 | GLN  |
| 3   | 5-D   | 211 | ASN  |
| 3   | 5-D   | 266 | HIS  |
| 3   | 5-D   | 289 | HIS  |
| 3   | 5-D   | 311 | ASN  |
| 3   | 5-D   | 312 | ASN  |
| 3   | 5-D   | 320 | ASN  |
| 3   | 5-D   | 325 | ASN  |
| 3   | 5-D   | 355 | ASN  |
| 3   | 5-D   | 385 | ASN  |
| 3   | 5-D   | 389 | ASN  |
| 3   | 5-D   | 418 | ASN  |
| 3   | 5-D   | 420 | GLN  |
| 1   | 6-A   | 115 | GLN  |
| 1   | 6-A   | 185 | GLN  |
| 1   | 6-A   | 274 | ASN  |
| 1   | 6-A   | 376 | GLN  |
| 1   | 6-A   | 417 | ASN  |
| 1   | 6-A   | 421 | HIS  |
| 1   | 6-A   | 424 | GLN  |
| 1   | 6-A   | 433 | HIS  |
| 1   | 6-A   | 434 | ASN  |
| 1   | 6-A   | 457 | ASN  |
| 1   | 6-A   | 565 | ASN  |
| 1   | 6-A   | 571 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6-A   | 633 | HIS  |
| 1   | 6-A   | 637 | ASN  |
| 1   | 6-A   | 686 | ASN  |
| 1   | 6-A   | 770 | ASN  |
| 2   | 6-B   | 222 | HIS  |
| 2   | 6-B   | 245 | ASN  |
| 2   | 6-B   | 322 | HIS  |
| 2   | 6-B   | 367 | ASN  |
| 2   | 6-B   | 452 | GLN  |
| 2   | 6-B   | 466 | GLN  |
| 2   | 6-B   | 469 | HIS  |
| 2   | 6-B   | 521 | GLN  |
| 2   | 6-B   | 527 | HIS  |
| 2   | 6-B   | 534 | ASN  |
| 2   | 6-B   | 588 | ASN  |
| 2   | 6-B   | 608 | ASN  |
| 2   | 6-B   | 728 | HIS  |
| 2   | 6-B   | 734 | ASN  |
| 2   | 6-B   | 806 | ASN  |
| 3   | 6-C   | 16  | HIS  |
| 3   | 6-C   | 103 | ASN  |
| 3   | 6-C   | 219 | ASN  |
| 3   | 6-C   | 281 | HIS  |
| 3   | 6-C   | 303 | ASN  |
| 3   | 6-C   | 317 | ASN  |
| 3   | 6-C   | 340 | GLN  |
| 3   | 6-C   | 379 | ASN  |
| 3   | 6-C   | 405 | ASN  |
| 3   | 6-C   | 408 | ASN  |
| 3   | 6-C   | 420 | GLN  |
| 3   | 6-D   | 24  | GLN  |
| 3   | 6-D   | 29  | HIS  |
| 3   | 6-D   | 103 | ASN  |
| 3   | 6-D   | 115 | ASN  |
| 3   | 6-D   | 226 | HIS  |
| 3   | 6-D   | 266 | HIS  |
| 3   | 6-D   | 303 | ASN  |
| 3   | 6-D   | 312 | ASN  |
| 3   | 6-D   | 385 | ASN  |
| 3   | 6-D   | 431 | GLN  |
| 1   | 7-A   | 55  | GLN  |
| 1   | 7-A   | 79  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 7-A   | 273 | ASN  |
| 1   | 7-A   | 369 | ASN  |
| 1   | 7-A   | 389 | ASN  |
| 1   | 7-A   | 454 | ASN  |
| 1   | 7-A   | 475 | ASN  |
| 1   | 7-A   | 648 | ASN  |
| 1   | 7-A   | 665 | ASN  |
| 1   | 7-A   | 674 | ASN  |
| 1   | 7-A   | 696 | GLN  |
| 1   | 7-A   | 698 | GLN  |
| 2   | 7-B   | 208 | GLN  |
| 2   | 7-B   | 215 | ASN  |
| 2   | 7-B   | 262 | GLN  |
| 2   | 7-B   | 303 | HIS  |
| 2   | 7-B   | 436 | ASN  |
| 2   | 7-B   | 459 | HIS  |
| 2   | 7-B   | 509 | ASN  |
| 2   | 7-B   | 534 | ASN  |
| 2   | 7-B   | 573 | ASN  |
| 2   | 7-B   | 597 | ASN  |
| 2   | 7-B   | 640 | GLN  |
| 2   | 7-B   | 642 | GLN  |
| 2   | 7-B   | 654 | ASN  |
| 2   | 7-B   | 728 | HIS  |
| 2   | 7-B   | 734 | ASN  |
| 3   | 7-C   | 9   | GLN  |
| 3   | 7-C   | 12  | GLN  |
| 3   | 7-C   | 16  | HIS  |
| 3   | 7-C   | 121 | ASN  |
| 3   | 7-C   | 132 | ASN  |
| 3   | 7-C   | 219 | ASN  |
| 3   | 7-C   | 225 | GLN  |
| 3   | 7-C   | 228 | ASN  |
| 3   | 7-C   | 286 | HIS  |
| 3   | 7-C   | 289 | HIS  |
| 3   | 7-C   | 303 | ASN  |
| 3   | 7-C   | 311 | ASN  |
| 3   | 7-C   | 353 | HIS  |
| 3   | 7-C   | 406 | ASN  |
| 3   | 7-C   | 418 | ASN  |
| 3   | 7-D   | 9   | GLN  |
| 3   | 7-D   | 15  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 7-D   | 24  | GLN  |
| 3   | 7-D   | 107 | ASN  |
| 3   | 7-D   | 137 | GLN  |
| 3   | 7-D   | 153 | ASN  |
| 3   | 7-D   | 186 | ASN  |
| 3   | 7-D   | 211 | ASN  |
| 3   | 7-D   | 226 | HIS  |
| 3   | 7-D   | 286 | HIS  |
| 3   | 7-D   | 355 | ASN  |
| 3   | 7-D   | 379 | ASN  |
| 3   | 7-D   | 414 | GLN  |
| 3   | 7-D   | 420 | GLN  |
| 3   | 7-D   | 431 | GLN  |
| 1   | 8-A   | 167 | ASN  |
| 1   | 8-A   | 258 | ASN  |
| 1   | 8-A   | 273 | ASN  |
| 1   | 8-A   | 402 | ASN  |
| 1   | 8-A   | 417 | ASN  |
| 1   | 8-A   | 424 | GLN  |
| 1   | 8-A   | 430 | GLN  |
| 1   | 8-A   | 449 | HIS  |
| 1   | 8-A   | 463 | GLN  |
| 1   | 8-A   | 464 | ASN  |
| 1   | 8-A   | 473 | ASN  |
| 1   | 8-A   | 480 | GLN  |
| 1   | 8-A   | 607 | ASN  |
| 1   | 8-A   | 637 | ASN  |
| 1   | 8-A   | 648 | ASN  |
| 1   | 8-A   | 650 | ASN  |
| 1   | 8-A   | 674 | ASN  |
| 1   | 8-A   | 696 | GLN  |
| 1   | 8-A   | 698 | GLN  |
| 1   | 8-A   | 762 | GLN  |
| 1   | 8-A   | 770 | ASN  |
| 2   | 8-B   | 222 | HIS  |
| 2   | 8-B   | 290 | ASN  |
| 2   | 8-B   | 322 | HIS  |
| 2   | 8-B   | 348 | ASN  |
| 2   | 8-B   | 380 | HIS  |
| 2   | 8-B   | 386 | ASN  |
| 2   | 8-B   | 466 | GLN  |
| 2   | 8-B   | 780 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 8-B   | 808 | ASN  |
| 2   | 8-B   | 815 | GLN  |
| 2   | 8-B   | 832 | ASN  |
| 3   | 8-C   | 116 | GLN  |
| 3   | 8-C   | 137 | GLN  |
| 3   | 8-C   | 229 | GLN  |
| 3   | 8-C   | 286 | HIS  |
| 3   | 8-C   | 368 | ASN  |
| 3   | 8-C   | 442 | GLN  |
| 3   | 8-D   | 15  | ASN  |
| 3   | 8-D   | 29  | HIS  |
| 3   | 8-D   | 81  | ASN  |
| 3   | 8-D   | 211 | ASN  |
| 3   | 8-D   | 225 | GLN  |
| 3   | 8-D   | 281 | HIS  |
| 3   | 8-D   | 289 | HIS  |
| 3   | 8-D   | 317 | ASN  |
| 3   | 8-D   | 408 | ASN  |
| 3   | 8-D   | 431 | GLN  |
| 1   | 9-A   | 65  | ASN  |
| 1   | 9-A   | 167 | ASN  |
| 1   | 9-A   | 178 | ASN  |
| 1   | 9-A   | 289 | GLN  |
| 1   | 9-A   | 379 | ASN  |
| 1   | 9-A   | 421 | HIS  |
| 1   | 9-A   | 423 | GLN  |
| 1   | 9-A   | 449 | HIS  |
| 1   | 9-A   | 455 | ASN  |
| 1   | 9-A   | 464 | ASN  |
| 1   | 9-A   | 485 | GLN  |
| 1   | 9-A   | 633 | HIS  |
| 1   | 9-A   | 638 | HIS  |
| 2   | 9-B   | 206 | GLN  |
| 2   | 9-B   | 222 | HIS  |
| 2   | 9-B   | 322 | HIS  |
| 2   | 9-B   | 423 | ASN  |
| 2   | 9-B   | 458 | ASN  |
| 2   | 9-B   | 459 | HIS  |
| 2   | 9-B   | 469 | HIS  |
| 2   | 9-B   | 497 | ASN  |
| 2   | 9-B   | 530 | ASN  |
| 2   | 9-B   | 539 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 9-B   | 597 | ASN  |
| 2   | 9-B   | 629 | ASN  |
| 2   | 9-B   | 640 | GLN  |
| 2   | 9-B   | 642 | GLN  |
| 2   | 9-B   | 645 | ASN  |
| 2   | 9-B   | 660 | ASN  |
| 2   | 9-B   | 669 | GLN  |
| 2   | 9-B   | 720 | ASN  |
| 2   | 9-B   | 729 | ASN  |
| 2   | 9-B   | 767 | ASN  |
| 3   | 9-C   | 9   | GLN  |
| 3   | 9-C   | 15  | ASN  |
| 3   | 9-C   | 57  | ASN  |
| 3   | 9-C   | 107 | ASN  |
| 3   | 9-C   | 116 | GLN  |
| 3   | 9-C   | 183 | GLN  |
| 3   | 9-C   | 266 | HIS  |
| 3   | 9-C   | 286 | HIS  |
| 3   | 9-C   | 289 | HIS  |
| 3   | 9-C   | 312 | ASN  |
| 3   | 9-C   | 320 | ASN  |
| 3   | 9-C   | 330 | GLN  |
| 3   | 9-C   | 339 | GLN  |
| 3   | 9-C   | 355 | ASN  |
| 3   | 9-D   | 29  | HIS  |
| 3   | 9-D   | 115 | ASN  |
| 3   | 9-D   | 116 | GLN  |
| 3   | 9-D   | 137 | GLN  |
| 3   | 9-D   | 186 | ASN  |
| 3   | 9-D   | 206 | ASN  |
| 3   | 9-D   | 211 | ASN  |
| 3   | 9-D   | 225 | GLN  |
| 3   | 9-D   | 281 | HIS  |
| 3   | 9-D   | 289 | HIS  |
| 3   | 9-D   | 320 | ASN  |
| 3   | 9-D   | 368 | ASN  |
| 3   | 9-D   | 389 | ASN  |
| 1   | 10-A  | 115 | GLN  |
| 1   | 10-A  | 136 | GLN  |
| 1   | 10-A  | 191 | ASN  |
| 1   | 10-A  | 273 | ASN  |
| 1   | 10-A  | 297 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 10-A  | 417 | ASN  |
| 1   | 10-A  | 421 | HIS  |
| 1   | 10-A  | 433 | HIS  |
| 1   | 10-A  | 463 | GLN  |
| 1   | 10-A  | 559 | HIS  |
| 1   | 10-A  | 589 | GLN  |
| 1   | 10-A  | 638 | HIS  |
| 1   | 10-A  | 648 | ASN  |
| 1   | 10-A  | 665 | ASN  |
| 1   | 10-A  | 674 | ASN  |
| 1   | 10-A  | 781 | ASN  |
| 1   | 10-A  | 784 | GLN  |
| 2   | 10-B  | 206 | GLN  |
| 2   | 10-B  | 322 | HIS  |
| 2   | 10-B  | 333 | ASN  |
| 2   | 10-B  | 336 | ASN  |
| 2   | 10-B  | 430 | HIS  |
| 2   | 10-B  | 462 | GLN  |
| 2   | 10-B  | 479 | ASN  |
| 2   | 10-B  | 521 | GLN  |
| 2   | 10-B  | 550 | HIS  |
| 2   | 10-B  | 573 | ASN  |
| 2   | 10-B  | 597 | ASN  |
| 2   | 10-B  | 608 | ASN  |
| 2   | 10-B  | 642 | GLN  |
| 2   | 10-B  | 643 | GLN  |
| 2   | 10-B  | 645 | ASN  |
| 2   | 10-B  | 669 | GLN  |
| 2   | 10-B  | 734 | ASN  |
| 3   | 10-C  | 12  | GLN  |
| 3   | 10-C  | 15  | ASN  |
| 3   | 10-C  | 16  | HIS  |
| 3   | 10-C  | 57  | ASN  |
| 3   | 10-C  | 107 | ASN  |
| 3   | 10-C  | 115 | ASN  |
| 3   | 10-C  | 121 | ASN  |
| 3   | 10-C  | 132 | ASN  |
| 3   | 10-C  | 186 | ASN  |
| 3   | 10-C  | 206 | ASN  |
| 3   | 10-C  | 225 | GLN  |
| 3   | 10-C  | 228 | ASN  |
| 3   | 10-C  | 266 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 10-C  | 281 | HIS  |
| 3   | 10-C  | 289 | HIS  |
| 3   | 10-C  | 303 | ASN  |
| 3   | 10-C  | 325 | ASN  |
| 3   | 10-C  | 330 | GLN  |
| 3   | 10-C  | 339 | GLN  |
| 3   | 10-C  | 355 | ASN  |
| 3   | 10-C  | 392 | ASN  |
| 3   | 10-C  | 408 | ASN  |
| 3   | 10-C  | 414 | GLN  |
| 3   | 10-C  | 418 | ASN  |
| 3   | 10-C  | 431 | GLN  |
| 3   | 10-D  | 9   | GLN  |
| 3   | 10-D  | 16  | HIS  |
| 3   | 10-D  | 137 | GLN  |
| 3   | 10-D  | 225 | GLN  |
| 3   | 10-D  | 266 | HIS  |
| 3   | 10-D  | 320 | ASN  |
| 3   | 10-D  | 325 | ASN  |
| 3   | 10-D  | 330 | GLN  |
| 3   | 10-D  | 353 | HIS  |
| 3   | 10-D  | 366 | GLN  |
| 3   | 10-D  | 418 | ASN  |
| 3   | 10-D  | 420 | GLN  |
| 3   | 10-D  | 431 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

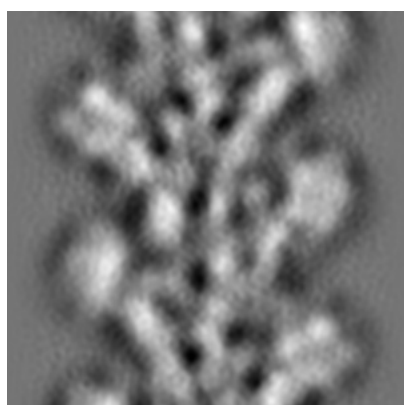
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1731. These allow visual inspection of the internal detail of the map and identification of artifacts.

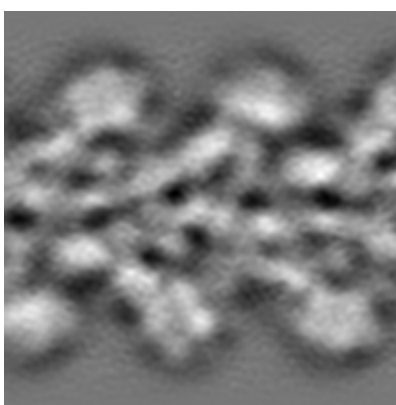
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

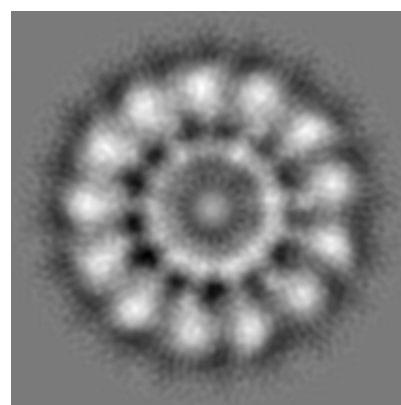
#### 6.1.1 Primary map



X



Y

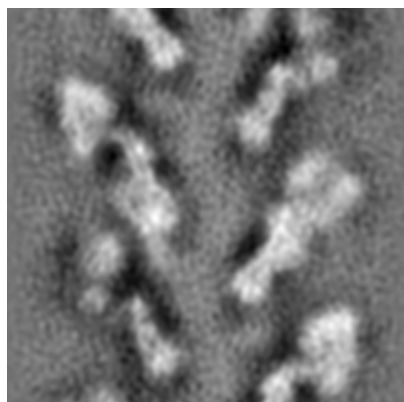


Z

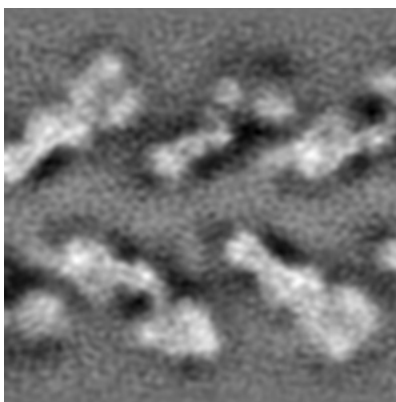
The images above show the map projected in three orthogonal directions.

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

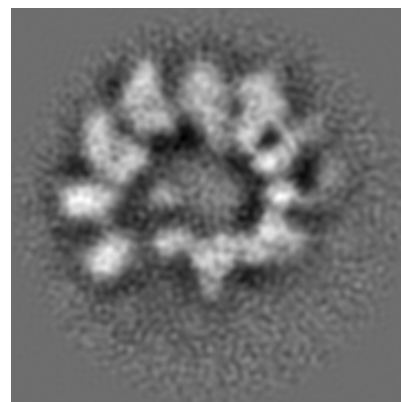
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

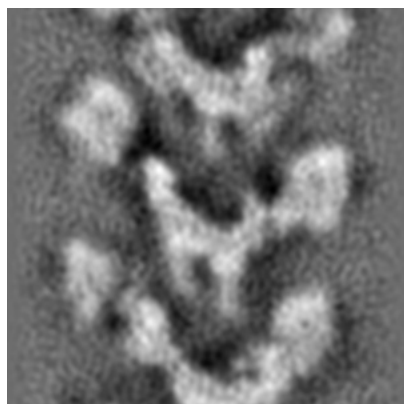


Z Index: 160

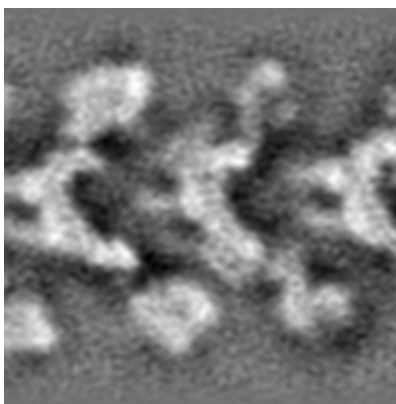
The images above show central slices of the map in three orthogonal directions.

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

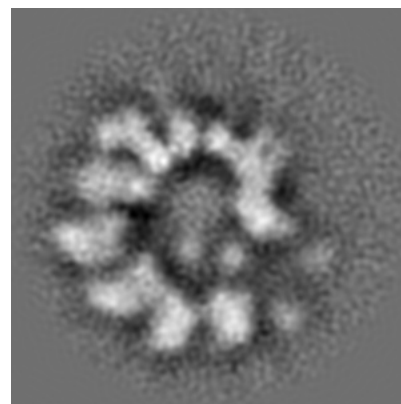
### 6.3.1 Primary map



X Index: 196



Y Index: 124

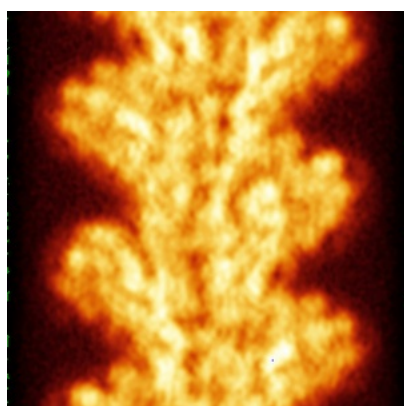


Z Index: 5

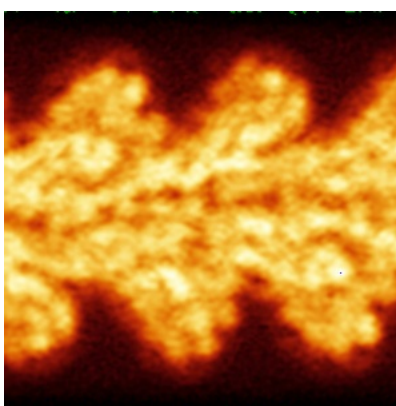
The images above show the largest variance slices of the map in three orthogonal directions.

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

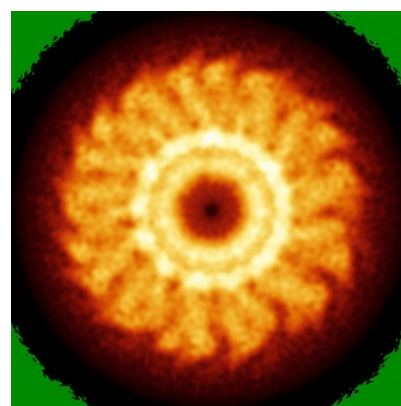
### 6.4.1 Primary map



X



Y

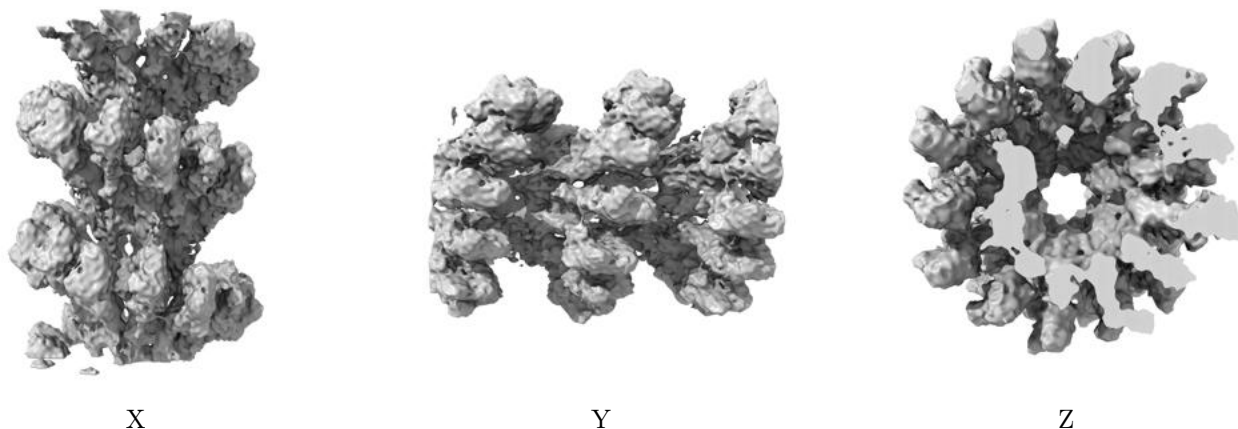


Z

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

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

### 6.5.1 Primary map



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

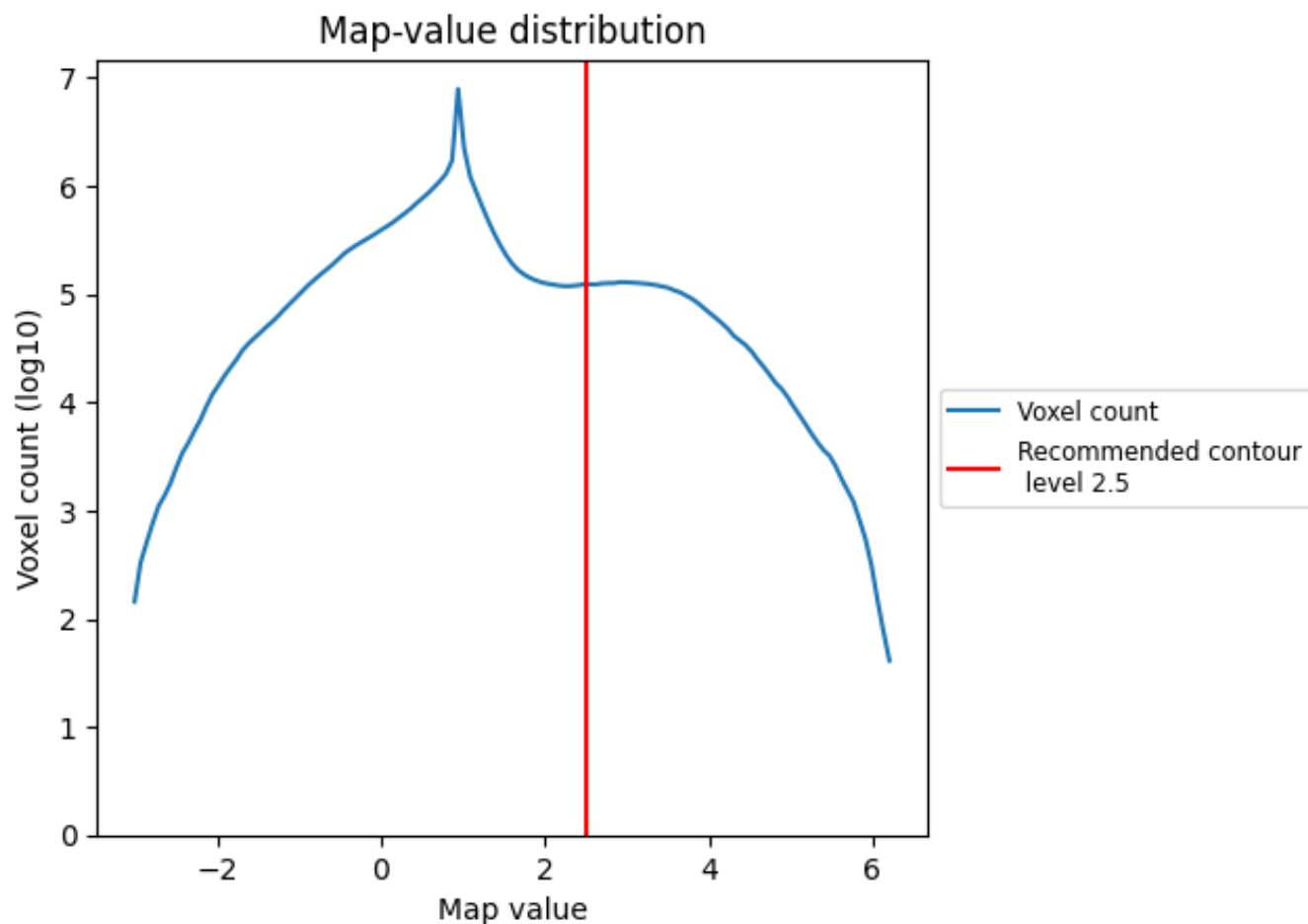
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

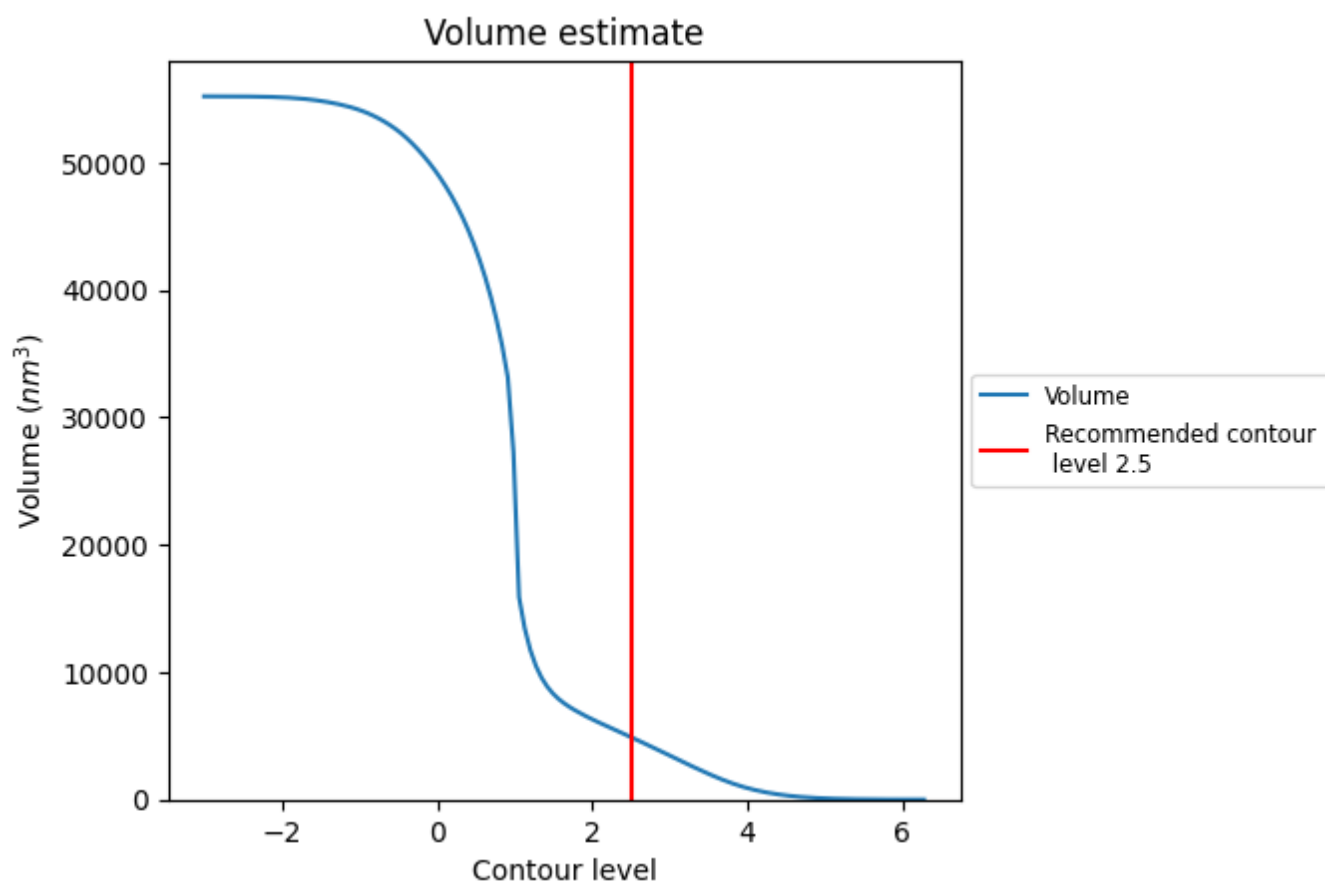
This section contains the results of statistical analysis of the map.

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



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

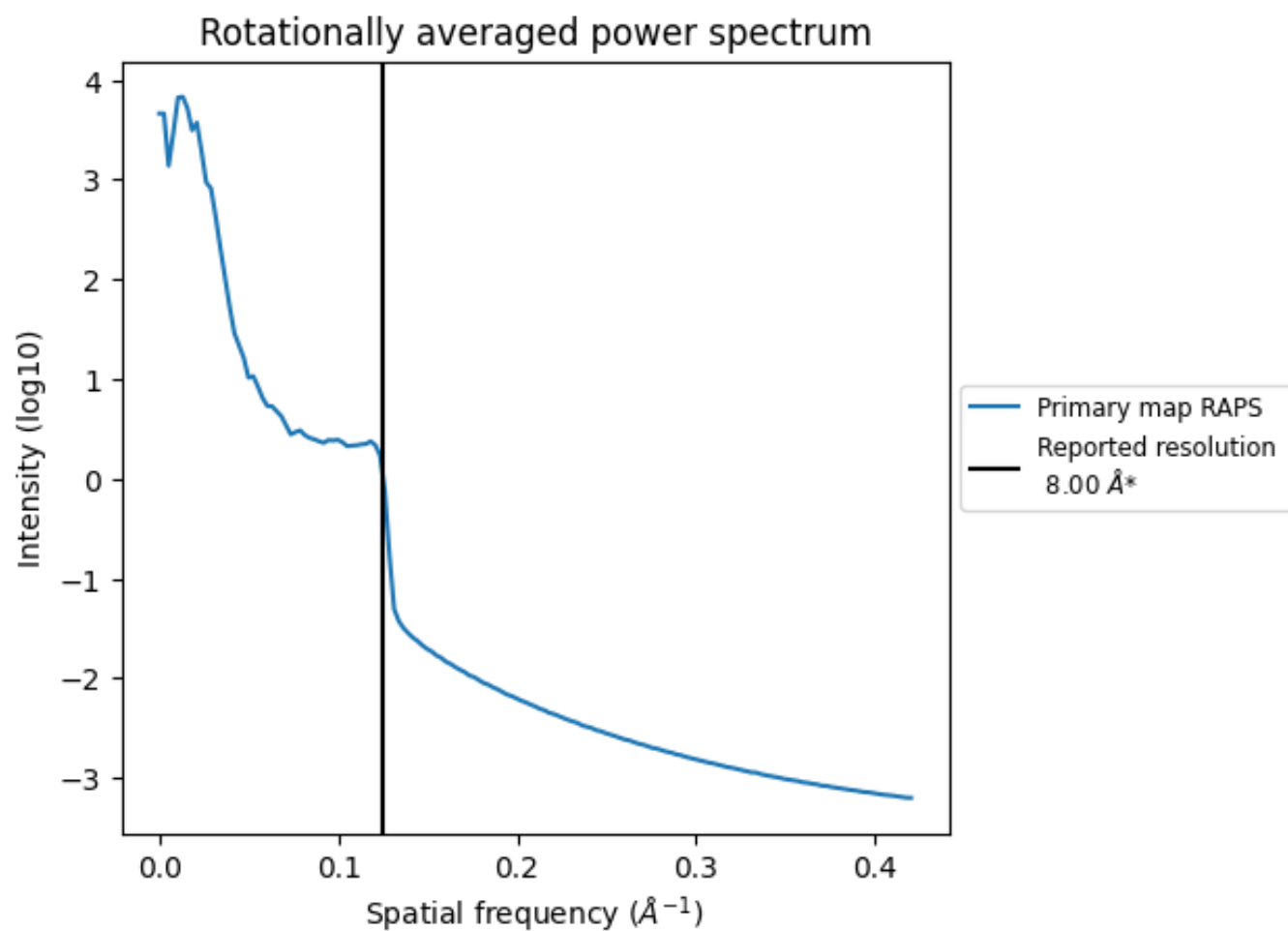
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4902 nm<sup>3</sup>; this corresponds to an approximate mass of 4428 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 0.125 Å<sup>-1</sup>

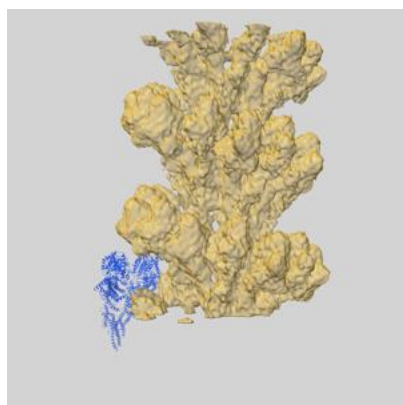
## 8 Fourier-Shell correlation

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

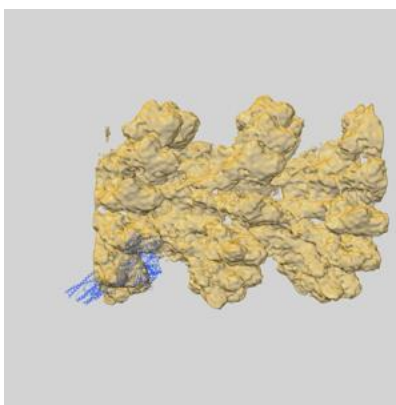
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1731 and PDB model 5FM1. Per-residue inclusion information can be found in section 3 on page 10.

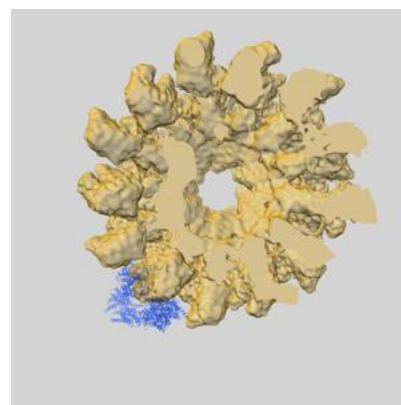
### 9.1 Map-model overlay [i](#)



X



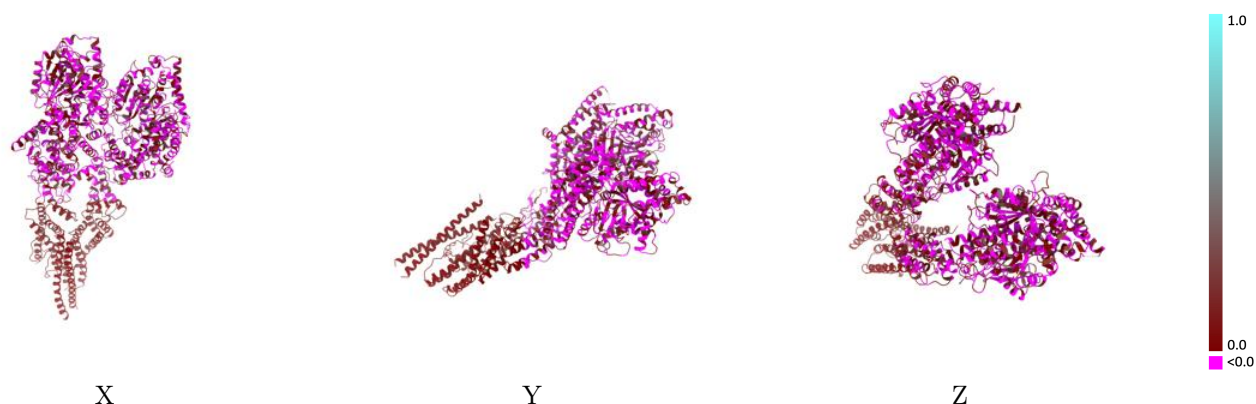
Y



Z

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

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

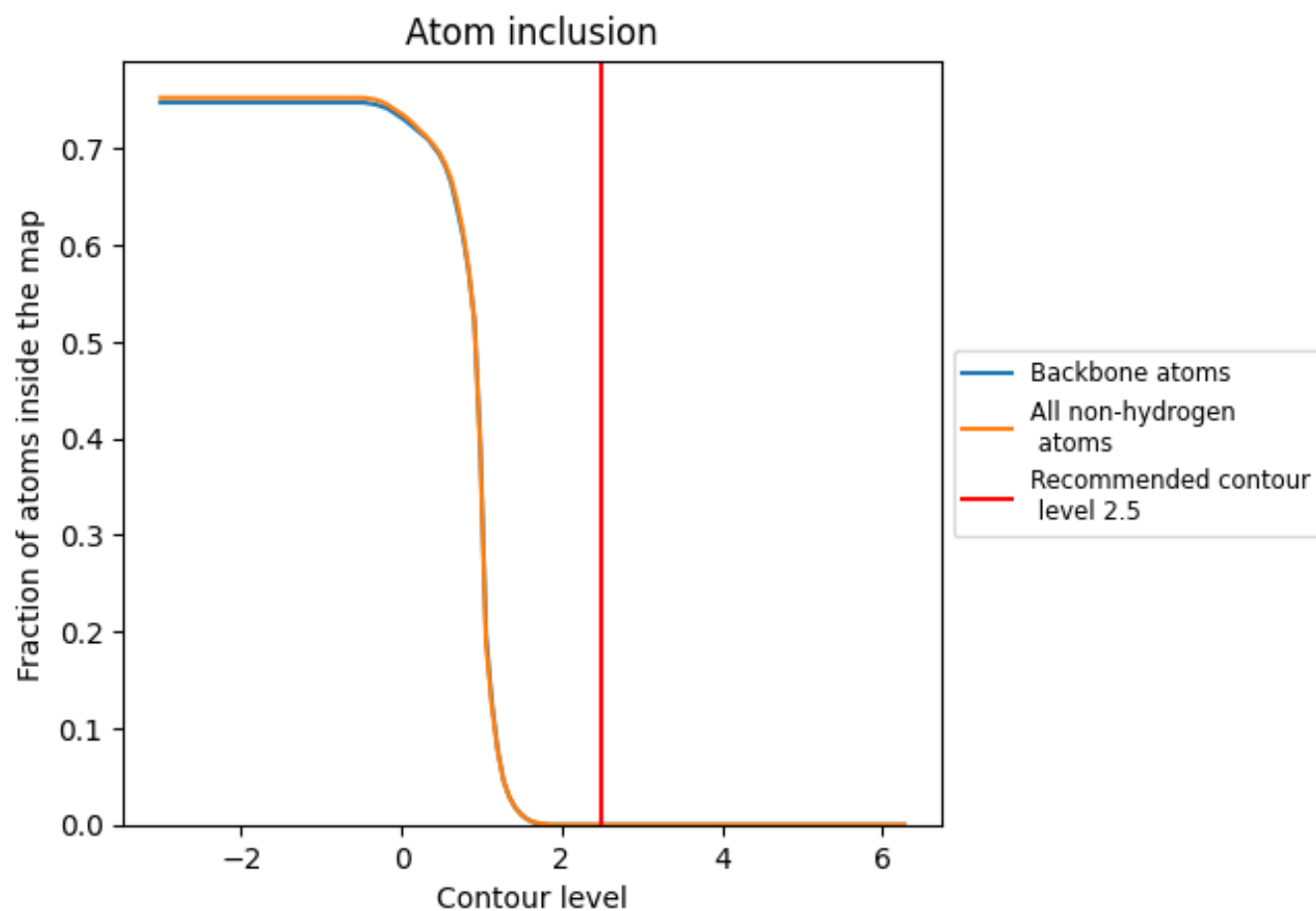


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

| Chain | Atom inclusion     | Q-score             |
|-------|--------------------|---------------------|
| All   | <div></div> 0.0000 | <div></div> 0.0000  |
| A     | <div></div> 0.0000 | <div></div> -0.0000 |
| B     | <div></div> 0.0000 | <div></div> 0.0040  |
| C     | <div></div> 0.0000 | <div></div> -0.0090 |
| D     | <div></div> 0.0000 | <div></div> 0.0060  |
| E     | <div></div> 0.0000 | <div></div> 0.0000  |
| F     | <div></div> 0.0000 | <div></div> 0.0000  |

1.0  
0.0  
-0.0