



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 04:07 AM UTC

PDB ID : 1PNB / pdb\_00001pnb  
Title : STRUCTURE OF NAPIN BNIB, NMR, 10 STRUCTURES  
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Deposited on : 1996-09-17

This is a Full wwPDB NMR Structure 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/NMRValidationReportHelp>

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:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI                      | : | v_1n_11_5_13_A (Berjanski et al., 2005)                          |
| PANAV                          | : | Wang et al. (2010)                                               |
| wwPDB-ShiftChecker             | : | v1.2                                                             |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

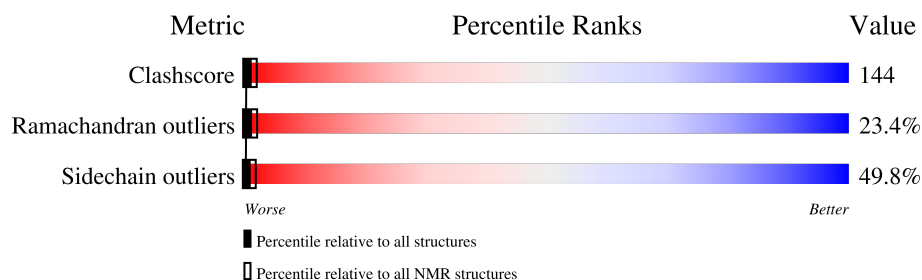
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 31     |                  |
| 2   | B     | 75     |                  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues |                         |                   |              |
|--------------------------------------|-------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)   | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:1-A:27, B:9-B:70 (89) | 2.41              | 1            |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

| Cluster number | Models              |
|----------------|---------------------|
| 1              | 1, 2, 4, 5, 7, 8, 9 |
| 2              | 3, 6, 10            |

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 852 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NAPIN BNIB.

| Mol | Chain | Residues | Atoms |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|----|----|---|-------|
| 1   | A     | 31       | Total | C   | N  | O  | S | 0     |
|     |       |          | 266   | 164 | 54 | 46 | 2 |       |

- Molecule 2 is a protein called NAPIN BNIB.

| Mol | Chain | Residues | Atoms |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|-------|
| 2   | B     | 75       | Total | C   | N   | O   | S | 0     |
|     |       |          | 586   | 365 | 107 | 107 | 7 |       |

There is a discrepancy between the modelled and reference sequences:

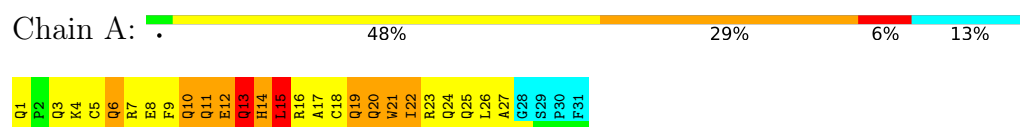
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 6       | GLN      | GLU    | conflict | UNP P24565 |

## 4 Residue-property plots [i](#)

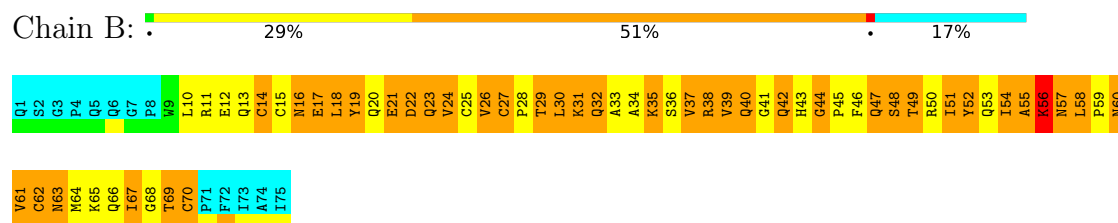
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

#### • Molecule 1: NAPIN BNIB



#### • Molecule 2: NAPIN BNIB

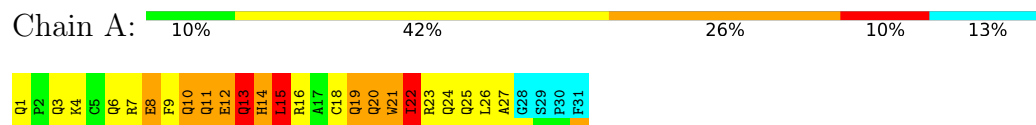


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

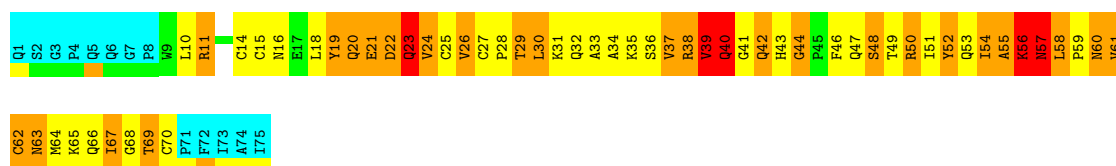
#### 4.2.1 Score per residue for model 1 (medoid)

#### • Molecule 1: NAPIN BNIB



#### • Molecule 2: NAPIN BNIB





#### 4.2.2 Score per residue for model 2

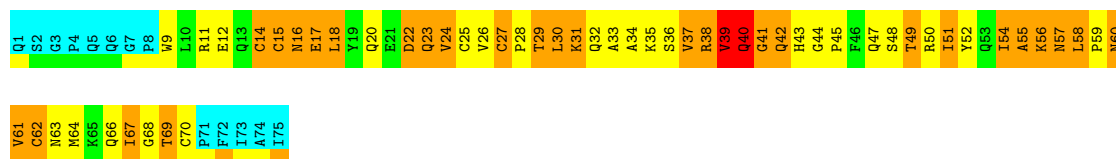
- Molecule 1: NAPIN BNIB

Chain A: 6% 39% 29% 13% 13%



- Molecule 2: NAPIN BNIB

Chain B: 9% 33% 37% 17%



#### 4.2.3 Score per residue for model 3

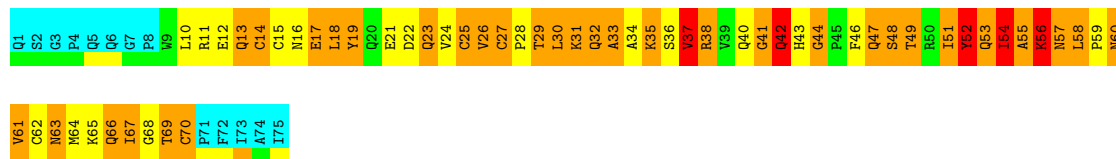
- Molecule 1: NAPIN BNIB

Chain A: 10% 29% 32% 16% 13%



- Molecule 2: NAPIN BNIB

Chain B: 7% 25% 44% 7% 17%



#### 4.2.4 Score per residue for model 4

- Molecule 1: NAPIN BNIB

Chain A: 32% 45% 6% 13%



- Molecule 2: NAPIN BNIB



#### 4.2.5 Score per residue for model 5

- Molecule 1: NAPIN BNIB



- Molecule 2: NAPIN BNIB

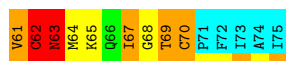


#### 4.2.6 Score per residue for model 6

- Molecule 1: NAPIN BNIB

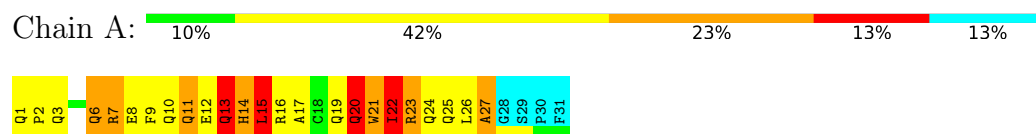


- Molecule 2: NAPIN BNIB

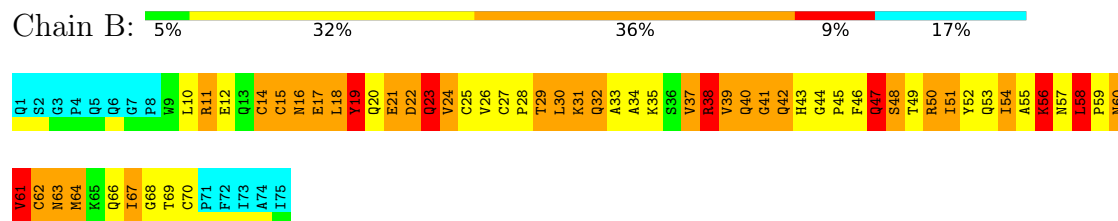


### 4.2.7 Score per residue for model 7

- Molecule 1: NAPIN BNIB

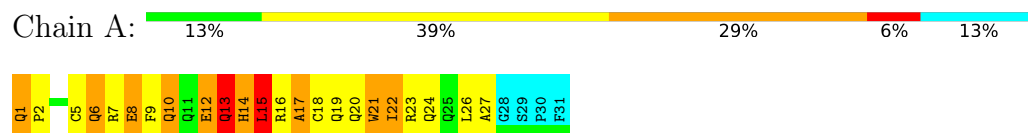


- Molecule 2: NAPIN BNIB

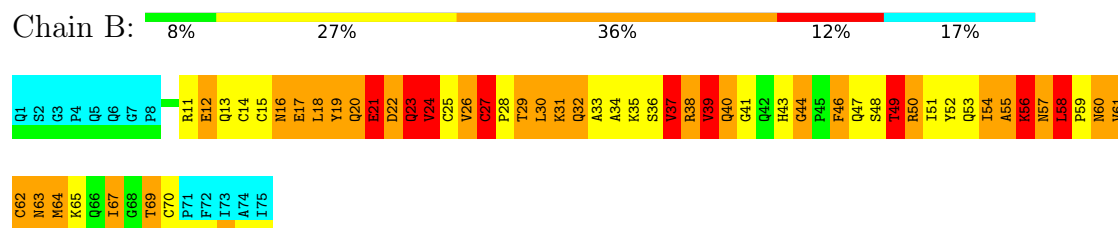


### 4.2.8 Score per residue for model 8

- Molecule 1: NAPIN BNIB

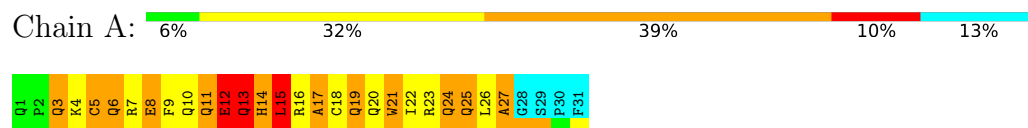


- Molecule 2: NAPIN BNIB



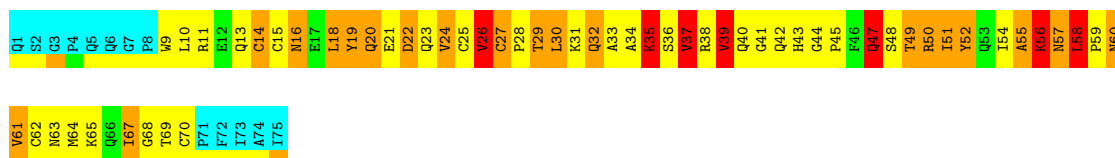
### 4.2.9 Score per residue for model 9

- Molecule 1: NAPIN BNIB



- Molecule 2: NAPIN BNIB

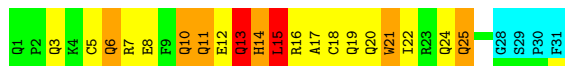




#### 4.2.10 Score per residue for model 10

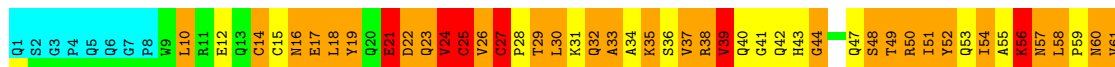
- Molecule 1: NAPIN BNIB

Chain A: 23% 39% 19% 6% 13%



- Molecule 2: NAPIN BNIB

Chain B: 9% 23% 43% 8% 17%



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 10 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|----------------|---------|
| DIANA         | refinement     |         |

No chemical shift data was provided.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 0.74±0.00    | 0±0/243 ( 0.0± 0.0%) | 1.01±0.01   | 0±0/326 ( 0.0± 0.0%) |
| 2   | B     | 0.69±0.01    | 0±0/501 ( 0.0± 0.0%) | 1.09±0.02   | 0±0/679 ( 0.0± 0.0%) |
| All | All   | 0.71         | 0/7440 ( 0.0%)       | 1.06        | 1/10050 ( 0.0%)      |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 2   | B     | 44  | GLY  | O-C-N | 9.58 | 124.52      | 121.07   | 6      | 1     |

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 238   | 0        | 230      | 64±9    |
| 2   | B     | 492   | 0        | 484      | 164±11  |
| All | All   | 7300  | 0        | 7140     | 2074    |

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 144.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:21:TRP:CZ2  | 2:B:56:LYS:O    | 1.30     | 1.84        | 3      | 5     |
| 2:B:27:CYS:H    | 2:B:28:PRO:CD   | 1.25     | 1.43        | 10     | 6     |
| 2:B:54:ILE:O    | 2:B:55:ALA:O    | 1.22     | 1.54        | 5      | 4     |
| 2:B:25:CYS:O    | 2:B:26:VAL:HG23 | 1.21     | 1.31        | 10     | 1     |
| 2:B:30:LEU:HD12 | 2:B:30:LEU:C    | 1.08     | 1.72        | 2      | 2     |
| 2:B:54:ILE:HG13 | 2:B:55:ALA:H    | 1.08     | 1.02        | 3      | 4     |
| 1:A:21:TRP:CH2  | 2:B:56:LYS:O    | 1.07     | 2.07        | 3      | 5     |
| 2:B:18:LEU:HD13 | 2:B:26:VAL:HG11 | 1.07     | 1.22        | 7      | 1     |
| 2:B:27:CYS:N    | 2:B:28:PRO:CD   | 1.06     | 2.17        | 9      | 10    |
| 2:B:19:TYR:CE1  | 2:B:64:MET:HE1  | 1.05     | 1.86        | 4      | 1     |
| 2:B:58:LEU:HB2  | 2:B:59:PRO:C    | 1.05     | 1.77        | 1      | 10    |
| 1:A:16:ARG:O    | 1:A:19:GLN:N    | 1.04     | 1.89        | 4      | 7     |
| 1:A:21:TRP:O    | 1:A:21:TRP:CE3  | 1.04     | 2.09        | 9      | 1     |
| 2:B:27:CYS:H    | 2:B:28:PRO:HD3  | 1.03     | 0.90        | 10     | 6     |
| 1:A:22:ILE:CG2  | 2:B:37:VAL:HG11 | 1.03     | 1.83        | 5      | 1     |
| 1:A:21:TRP:CD1  | 2:B:61:VAL:HG21 | 1.01     | 1.89        | 9      | 2     |
| 2:B:25:CYS:O    | 2:B:29:THR:HG23 | 1.00     | 1.55        | 7      | 2     |
| 1:A:13:GLN:O    | 1:A:14:HIS:O    | 1.00     | 1.80        | 7      | 6     |
| 1:A:21:TRP:HE3  | 1:A:21:TRP:C    | 1.00     | 1.63        | 9      | 1     |
| 2:B:54:ILE:CG1  | 2:B:55:ALA:H    | 1.00     | 1.69        | 3      | 5     |
| 2:B:30:LEU:H    | 2:B:30:LEU:HD22 | 1.00     | 1.09        | 4      | 2     |
| 2:B:44:GLY:N    | 2:B:45:PRO:CD   | 0.98     | 2.26        | 9      | 5     |
| 1:A:21:TRP:CZ3  | 2:B:57:ASN:O    | 0.96     | 2.19        | 6      | 3     |
| 2:B:27:CYS:N    | 2:B:28:PRO:HD3  | 0.96     | 1.75        | 8      | 6     |
| 1:A:21:TRP:CE3  | 1:A:21:TRP:C    | 0.96     | 2.43        | 9      | 3     |
| 2:B:47:GLN:O    | 2:B:51:ILE:HG22 | 0.95     | 1.61        | 7      | 5     |
| 2:B:69:THR:O    | 2:B:70:CYS:SG   | 0.95     | 2.24        | 2      | 7     |
| 1:A:21:TRP:CE3  | 2:B:58:LEU:HD23 | 0.94     | 1.96        | 1      | 7     |
| 2:B:43:HIS:C    | 2:B:45:PRO:HD2  | 0.94     | 1.87        | 9      | 2     |
| 2:B:25:CYS:O    | 2:B:26:VAL:CG2  | 0.94     | 2.15        | 10     | 1     |
| 1:A:22:ILE:HD13 | 1:A:23:ARG:N    | 0.92     | 1.78        | 3      | 1     |
| 2:B:27:CYS:HA   | 2:B:30:LEU:HD21 | 0.91     | 1.42        | 6      | 4     |
| 1:A:15:LEU:HD12 | 2:B:17:GLU:HG2  | 0.91     | 1.42        | 6      | 1     |
| 1:A:21:TRP:CZ2  | 2:B:70:CYS:C    | 0.91     | 2.48        | 9      | 1     |
| 1:A:21:TRP:O    | 1:A:21:TRP:HE3  | 0.91     | 1.43        | 9      | 1     |
| 2:B:30:LEU:N    | 2:B:30:LEU:CD2  | 0.91     | 2.34        | 1      | 3     |
| 1:A:26:LEU:HD11 | 2:B:34:ALA:O    | 0.90     | 1.65        | 3      | 2     |
| 2:B:18:LEU:HD12 | 2:B:18:LEU:C    | 0.90     | 1.91        | 7      | 9     |
| 2:B:54:ILE:HG13 | 2:B:55:ALA:N    | 0.90     | 1.80        | 3      | 3     |
| 2:B:51:ILE:O    | 2:B:55:ALA:N    | 0.90     | 2.04        | 9      | 2     |
| 2:B:30:LEU:N    | 2:B:30:LEU:HD22 | 0.90     | 1.81        | 1      | 5     |
| 1:A:21:TRP:CE2  | 2:B:56:LYS:O    | 0.89     | 2.25        | 1      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:58:LEU:N    | 2:B:59:PRO:HA   | 0.89     | 1.82        | 4      | 10    |
| 2:B:57:ASN:O    | 2:B:61:VAL:HG23 | 0.89     | 1.68        | 8      | 4     |
| 1:A:19:GLN:HA   | 1:A:22:ILE:CG2  | 0.89     | 1.98        | 6      | 4     |
| 1:A:9:PHE:CE2   | 1:A:14:HIS:CE1  | 0.89     | 2.61        | 7      | 1     |
| 2:B:61:VAL:HG12 | 2:B:62:CYS:SG   | 0.88     | 2.08        | 8      | 2     |
| 1:A:18:CYS:O    | 1:A:22:ILE:HG22 | 0.88     | 1.67        | 6      | 2     |
| 2:B:58:LEU:HG   | 2:B:61:VAL:HG23 | 0.88     | 1.44        | 5      | 7     |
| 2:B:58:LEU:CB   | 2:B:59:PRO:C    | 0.88     | 2.46        | 5      | 10    |
| 2:B:58:LEU:HD12 | 2:B:60:ASN:CB   | 0.87     | 1.99        | 5      | 10    |
| 2:B:19:TYR:CZ   | 2:B:64:MET:HE1  | 0.87     | 2.04        | 4      | 1     |
| 1:A:21:TRP:CE3  | 2:B:58:LEU:CD2  | 0.87     | 2.56        | 7      | 8     |
| 2:B:30:LEU:HG   | 2:B:70:CYS:HB3  | 0.87     | 1.42        | 6      | 1     |
| 1:A:21:TRP:HZ2  | 2:B:56:LYS:HG2  | 0.86     | 1.30        | 3      | 1     |
| 2:B:55:ALA:HB3  | 2:B:69:THR:HG23 | 0.86     | 1.46        | 8      | 1     |
| 2:B:54:ILE:HG23 | 2:B:55:ALA:H    | 0.86     | 1.29        | 8      | 1     |
| 2:B:57:ASN:ND2  | 2:B:61:VAL:HB   | 0.86     | 1.86        | 5      | 3     |
| 1:A:22:ILE:O    | 1:A:22:ILE:HD12 | 0.86     | 1.70        | 6      | 1     |
| 1:A:19:GLN:HA   | 1:A:22:ILE:HD12 | 0.85     | 1.47        | 3      | 2     |
| 2:B:57:ASN:O    | 2:B:58:LEU:HD23 | 0.85     | 1.72        | 5      | 6     |
| 2:B:30:LEU:HD13 | 2:B:30:LEU:H    | 0.85     | 1.32        | 6      | 2     |
| 1:A:21:TRP:O    | 2:B:58:LEU:CD2  | 0.85     | 2.25        | 9      | 3     |
| 2:B:57:ASN:OD1  | 2:B:61:VAL:HG11 | 0.85     | 1.70        | 6      | 2     |
| 2:B:35:LYS:O    | 2:B:39:VAL:HG22 | 0.84     | 1.71        | 5      | 3     |
| 1:A:9:PHE:CE1   | 1:A:14:HIS:CG   | 0.84     | 2.65        | 2      | 1     |
| 1:A:21:TRP:CZ2  | 2:B:70:CYS:O    | 0.84     | 2.31        | 9      | 2     |
| 2:B:54:ILE:CG1  | 2:B:55:ALA:N    | 0.84     | 2.35        | 3      | 6     |
| 2:B:34:ALA:HB3  | 2:B:52:TYR:CE1  | 0.84     | 2.07        | 1      | 2     |
| 1:A:9:PHE:CD2   | 1:A:14:HIS:CE1  | 0.84     | 2.65        | 7      | 1     |
| 2:B:48:SER:O    | 2:B:52:TYR:N    | 0.83     | 2.11        | 2      | 7     |
| 2:B:56:LYS:O    | 2:B:58:LEU:N    | 0.83     | 2.11        | 5      | 4     |
| 2:B:30:LEU:C    | 2:B:30:LEU:CD1  | 0.83     | 2.50        | 2      | 2     |
| 1:A:21:TRP:NE1  | 2:B:70:CYS:O    | 0.83     | 2.12        | 8      | 1     |
| 1:A:21:TRP:CD1  | 2:B:58:LEU:O    | 0.83     | 2.32        | 2      | 2     |
| 1:A:22:ILE:HG22 | 2:B:37:VAL:HG11 | 0.83     | 1.48        | 5      | 1     |
| 2:B:30:LEU:HG   | 2:B:70:CYS:CB   | 0.83     | 2.03        | 6      | 2     |
| 2:B:23:GLN:HA   | 2:B:26:VAL:HB   | 0.82     | 1.49        | 7      | 4     |
| 2:B:57:ASN:HB2  | 2:B:69:THR:HG22 | 0.82     | 1.50        | 3      | 2     |
| 1:A:21:TRP:CZ2  | 2:B:30:LEU:HD23 | 0.82     | 2.10        | 10     | 1     |
| 1:A:9:PHE:CD1   | 1:A:14:HIS:CD2  | 0.82     | 2.68        | 2      | 1     |
| 2:B:33:ALA:O    | 2:B:37:VAL:HG23 | 0.82     | 1.74        | 5      | 4     |
| 2:B:57:ASN:HA   | 2:B:69:THR:O    | 0.82     | 1.73        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:26:VAL:HG12 | 2:B:27:CYS:N    | 0.81     | 1.90        | 4      | 8     |
| 1:A:26:LEU:HD23 | 2:B:46:PHE:CZ   | 0.81     | 2.11        | 1      | 1     |
| 2:B:33:ALA:O    | 2:B:37:VAL:N    | 0.81     | 2.14        | 5      | 4     |
| 2:B:38:ARG:O    | 2:B:40:GLN:N    | 0.81     | 2.14        | 9      | 2     |
| 1:A:26:LEU:HD11 | 2:B:38:ARG:CD   | 0.81     | 2.06        | 9      | 1     |
| 2:B:39:VAL:HG23 | 2:B:39:VAL:O    | 0.80     | 1.75        | 9      | 2     |
| 2:B:55:ALA:CB   | 2:B:69:THR:O    | 0.80     | 2.29        | 3      | 1     |
| 2:B:37:VAL:HG12 | 2:B:38:ARG:N    | 0.80     | 1.88        | 5      | 6     |
| 2:B:51:ILE:HD13 | 2:B:52:TYR:N    | 0.80     | 1.90        | 10     | 1     |
| 1:A:22:ILE:C    | 1:A:22:ILE:HD12 | 0.80     | 2.01        | 8      | 2     |
| 1:A:15:LEU:HD12 | 2:B:17:GLU:CG   | 0.80     | 2.06        | 6      | 2     |
| 2:B:58:LEU:HD12 | 2:B:60:ASN:HB2  | 0.80     | 1.51        | 5      | 9     |
| 2:B:55:ALA:C    | 2:B:56:LYS:HG3  | 0.79     | 2.01        | 2      | 3     |
| 2:B:62:CYS:HB3  | 2:B:64:MET:HE2  | 0.79     | 1.53        | 9      | 2     |
| 2:B:61:VAL:HG13 | 2:B:62:CYS:H    | 0.79     | 1.37        | 6      | 1     |
| 2:B:38:ARG:O    | 2:B:39:VAL:O    | 0.79     | 2.01        | 5      | 5     |
| 2:B:57:ASN:O    | 2:B:58:LEU:HG   | 0.79     | 1.78        | 10     | 5     |
| 2:B:30:LEU:HD23 | 2:B:70:CYS:HB2  | 0.79     | 1.51        | 9      | 1     |
| 2:B:55:ALA:HB1  | 2:B:69:THR:O    | 0.79     | 1.77        | 3      | 1     |
| 1:A:22:ILE:HG21 | 2:B:37:VAL:HG21 | 0.79     | 1.54        | 9      | 2     |
| 2:B:25:CYS:O    | 2:B:29:THR:OG1  | 0.78     | 2.00        | 5      | 4     |
| 2:B:43:HIS:CD2  | 2:B:46:PHE:CE2  | 0.78     | 2.71        | 8      | 1     |
| 2:B:30:LEU:HB2  | 2:B:70:CYS:CB   | 0.78     | 2.08        | 1      | 2     |
| 1:A:15:LEU:HD13 | 1:A:15:LEU:H    | 0.78     | 1.37        | 6      | 8     |
| 2:B:27:CYS:CA   | 2:B:30:LEU:HD21 | 0.78     | 2.08        | 6      | 3     |
| 2:B:61:VAL:HG13 | 2:B:62:CYS:N    | 0.78     | 1.94        | 6      | 1     |
| 1:A:21:TRP:CE2  | 2:B:57:ASN:O    | 0.78     | 2.36        | 9      | 2     |
| 1:A:19:GLN:CA   | 1:A:22:ILE:CG2  | 0.78     | 2.62        | 6      | 1     |
| 2:B:58:LEU:HB2  | 2:B:60:ASN:N    | 0.78     | 1.92        | 5      | 10    |
| 2:B:60:ASN:O    | 2:B:62:CYS:N    | 0.77     | 2.17        | 1      | 3     |
| 2:B:39:VAL:HG21 | 2:B:43:HIS:CG   | 0.77     | 2.13        | 6      | 1     |
| 2:B:25:CYS:HB3  | 2:B:29:THR:HG23 | 0.77     | 1.56        | 4      | 1     |
| 2:B:39:VAL:HG21 | 2:B:43:HIS:CD2  | 0.77     | 2.14        | 6      | 1     |
| 2:B:30:LEU:CD2  | 2:B:30:LEU:H    | 0.77     | 1.93        | 1      | 2     |
| 1:A:15:LEU:N    | 1:A:15:LEU:HD22 | 0.77     | 1.95        | 5      | 7     |
| 2:B:51:ILE:HD13 | 2:B:51:ILE:C    | 0.77     | 2.04        | 10     | 1     |
| 2:B:38:ARG:O    | 2:B:39:VAL:C    | 0.77     | 2.28        | 10     | 8     |
| 2:B:62:CYS:O    | 2:B:63:ASN:CB   | 0.77     | 2.33        | 3      | 7     |
| 2:B:26:VAL:N    | 2:B:28:PRO:HD2  | 0.76     | 1.94        | 3      | 6     |
| 2:B:60:ASN:O    | 2:B:61:VAL:C    | 0.76     | 2.28        | 7      | 10    |
| 2:B:25:CYS:O    | 2:B:29:THR:CG2  | 0.76     | 2.33        | 7      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:43:HIS:C    | 2:B:45:PRO:CD   | 0.76     | 2.59        | 9      | 1     |
| 1:A:13:GLN:O    | 1:A:14:HIS:C    | 0.76     | 2.29        | 3      | 10    |
| 1:A:15:LEU:O    | 1:A:19:GLN:HB3  | 0.76     | 1.79        | 2      | 1     |
| 2:B:55:ALA:C    | 2:B:56:LYS:CG   | 0.76     | 2.59        | 2      | 7     |
| 2:B:37:VAL:CG1  | 2:B:38:ARG:N    | 0.76     | 2.49        | 9      | 6     |
| 2:B:26:VAL:C    | 2:B:28:PRO:HD2  | 0.76     | 2.06        | 1      | 6     |
| 2:B:26:VAL:HG12 | 2:B:70:CYS:CB   | 0.75     | 2.09        | 2      | 1     |
| 1:A:21:TRP:HE3  | 1:A:22:ILE:N    | 0.75     | 1.77        | 5      | 1     |
| 2:B:58:LEU:H    | 2:B:59:PRO:HA   | 0.75     | 1.38        | 9      | 9     |
| 2:B:61:VAL:HG12 | 2:B:62:CYS:N    | 0.75     | 1.96        | 2      | 7     |
| 1:A:22:ILE:HD12 | 1:A:22:ILE:C    | 0.75     | 2.03        | 6      | 1     |
| 2:B:55:ALA:O    | 2:B:56:LYS:CD   | 0.75     | 2.34        | 5      | 5     |
| 2:B:54:ILE:O    | 2:B:55:ALA:C    | 0.75     | 2.29        | 1      | 4     |
| 1:A:26:LEU:N    | 1:A:26:LEU:HD23 | 0.75     | 1.95        | 2      | 3     |
| 2:B:30:LEU:HG   | 2:B:70:CYS:O    | 0.74     | 1.81        | 4      | 2     |
| 2:B:26:VAL:O    | 2:B:30:LEU:CD2  | 0.74     | 2.36        | 1      | 1     |
| 2:B:26:VAL:HG12 | 2:B:70:CYS:HB2  | 0.74     | 1.58        | 2      | 1     |
| 2:B:54:ILE:C    | 2:B:54:ILE:HD13 | 0.74     | 2.07        | 8      | 1     |
| 2:B:44:GLY:N    | 2:B:45:PRO:HD3  | 0.74     | 1.98        | 9      | 1     |
| 2:B:39:VAL:O    | 2:B:40:GLN:C    | 0.74     | 2.31        | 4      | 5     |
| 2:B:57:ASN:CG   | 2:B:61:VAL:HB   | 0.74     | 2.07        | 6      | 3     |
| 2:B:54:ILE:HG23 | 2:B:55:ALA:N    | 0.74     | 1.97        | 8      | 1     |
| 2:B:56:LYS:O    | 2:B:57:ASN:C    | 0.74     | 2.30        | 5      | 6     |
| 1:A:21:TRP:CE3  | 1:A:22:ILE:HG23 | 0.74     | 2.18        | 4      | 1     |
| 1:A:21:TRP:O    | 2:B:58:LEU:HD21 | 0.74     | 1.83        | 9      | 3     |
| 2:B:27:CYS:O    | 2:B:30:LEU:CD2  | 0.73     | 2.36        | 6      | 2     |
| 2:B:54:ILE:C    | 2:B:55:ALA:O    | 0.73     | 2.31        | 5      | 4     |
| 2:B:27:CYS:N    | 2:B:28:PRO:HD2  | 0.73     | 1.98        | 4      | 9     |
| 2:B:25:CYS:HA   | 2:B:28:PRO:HG2  | 0.73     | 1.60        | 7      | 6     |
| 2:B:48:SER:HA   | 2:B:51:ILE:HG23 | 0.73     | 1.60        | 10     | 4     |
| 2:B:26:VAL:O    | 2:B:30:LEU:HD23 | 0.73     | 1.84        | 1      | 1     |
| 1:A:21:TRP:CE3  | 2:B:57:ASN:O    | 0.73     | 2.41        | 6      | 3     |
| 2:B:18:LEU:CD1  | 2:B:26:VAL:HG11 | 0.72     | 2.11        | 7      | 1     |
| 2:B:30:LEU:H    | 2:B:30:LEU:CD2  | 0.72     | 1.89        | 4      | 2     |
| 1:A:19:GLN:HA   | 1:A:22:ILE:CG1  | 0.72     | 2.14        | 4      | 2     |
| 2:B:33:ALA:C    | 2:B:37:VAL:HG23 | 0.72     | 2.09        | 3      | 2     |
| 2:B:37:VAL:O    | 2:B:38:ARG:C    | 0.72     | 2.33        | 2      | 5     |
| 1:A:21:TRP:CZ2  | 2:B:56:LYS:HG2  | 0.71     | 2.18        | 3      | 1     |
| 1:A:20:GLN:O    | 1:A:24:GLN:N    | 0.71     | 2.24        | 7      | 6     |
| 2:B:30:LEU:HD22 | 2:B:31:LYS:N    | 0.71     | 1.99        | 3      | 1     |
| 2:B:23:GLN:O    | 2:B:26:VAL:HG23 | 0.71     | 1.86        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:PHE:CE1   | 1:A:14:HIS:CD2  | 0.71     | 2.79        | 2      | 2     |
| 1:A:26:LEU:HD11 | 2:B:37:VAL:C    | 0.71     | 2.11        | 2      | 1     |
| 2:B:57:ASN:O    | 2:B:58:LEU:CD2  | 0.71     | 2.39        | 8      | 6     |
| 2:B:23:GLN:HA   | 2:B:26:VAL:CG2  | 0.71     | 2.15        | 2      | 4     |
| 2:B:30:LEU:HD12 | 2:B:30:LEU:O    | 0.71     | 1.85        | 2      | 1     |
| 2:B:58:LEU:N    | 2:B:59:PRO:CA   | 0.70     | 2.54        | 4      | 10    |
| 2:B:27:CYS:SG   | 2:B:55:ALA:HB2  | 0.70     | 2.26        | 3      | 1     |
| 2:B:33:ALA:C    | 2:B:37:VAL:CG2  | 0.70     | 2.64        | 3      | 1     |
| 2:B:15:CYS:O    | 2:B:18:LEU:N    | 0.70     | 2.25        | 3      | 7     |
| 1:A:9:PHE:CZ    | 2:B:33:ALA:HB2  | 0.70     | 2.20        | 3      | 7     |
| 2:B:58:LEU:CD1  | 2:B:60:ASN:HB2  | 0.70     | 2.17        | 5      | 9     |
| 2:B:58:LEU:CB   | 2:B:60:ASN:HB2  | 0.70     | 2.17        | 8      | 10    |
| 1:A:9:PHE:CD1   | 1:A:9:PHE:C     | 0.70     | 2.70        | 3      | 1     |
| 2:B:36:SER:O    | 2:B:39:VAL:HG22 | 0.69     | 1.87        | 1      | 2     |
| 2:B:16:ASN:O    | 2:B:20:GLN:N    | 0.69     | 2.20        | 9      | 1     |
| 2:B:30:LEU:CB   | 2:B:70:CYS:C    | 0.69     | 2.65        | 1      | 3     |
| 2:B:43:HIS:CD2  | 2:B:46:PHE:CD1  | 0.69     | 2.79        | 1      | 1     |
| 2:B:30:LEU:HD22 | 2:B:30:LEU:N    | 0.69     | 1.94        | 4      | 1     |
| 2:B:35:LYS:CE   | 2:B:46:PHE:CE2  | 0.69     | 2.75        | 5      | 1     |
| 2:B:15:CYS:O    | 2:B:19:TYR:N    | 0.69     | 2.24        | 7      | 3     |
| 1:A:9:PHE:CE2   | 2:B:29:THR:O    | 0.69     | 2.45        | 2      | 1     |
| 2:B:30:LEU:CB   | 2:B:70:CYS:O    | 0.69     | 2.40        | 4      | 1     |
| 2:B:30:LEU:HD11 | 2:B:70:CYS:HB2  | 0.69     | 1.64        | 6      | 1     |
| 2:B:26:VAL:CG1  | 2:B:27:CYS:N    | 0.69     | 2.56        | 9      | 7     |
| 2:B:54:ILE:HD12 | 2:B:55:ALA:N    | 0.69     | 2.02        | 2      | 5     |
| 2:B:57:ASN:O    | 2:B:58:LEU:CG   | 0.69     | 2.40        | 8      | 6     |
| 2:B:37:VAL:HG12 | 2:B:38:ARG:H    | 0.69     | 1.45        | 9      | 6     |
| 2:B:56:LYS:HA   | 2:B:70:CYS:C    | 0.68     | 2.13        | 4      | 1     |
| 2:B:57:ASN:HD21 | 2:B:63:ASN:N    | 0.68     | 1.85        | 4      | 1     |
| 2:B:48:SER:O    | 2:B:52:TYR:CD1  | 0.68     | 2.46        | 7      | 3     |
| 2:B:57:ASN:ND2  | 2:B:70:CYS:O    | 0.68     | 2.26        | 3      | 1     |
| 1:A:21:TRP:CZ3  | 2:B:57:ASN:C    | 0.68     | 2.71        | 6      | 1     |
| 1:A:22:ILE:HD12 | 1:A:23:ARG:N    | 0.68     | 2.02        | 9      | 4     |
| 2:B:18:LEU:HD12 | 2:B:19:TYR:N    | 0.68     | 2.02        | 1      | 3     |
| 2:B:18:LEU:HD21 | 2:B:69:THR:CG2  | 0.68     | 2.19        | 7      | 1     |
| 1:A:21:TRP:O    | 1:A:23:ARG:N    | 0.68     | 2.26        | 3      | 4     |
| 2:B:23:GLN:O    | 2:B:25:CYS:N    | 0.68     | 2.26        | 10     | 4     |
| 2:B:36:SER:O    | 2:B:37:VAL:C    | 0.68     | 2.36        | 3      | 7     |
| 2:B:54:ILE:CG2  | 2:B:55:ALA:H    | 0.68     | 2.02        | 8      | 1     |
| 1:A:15:LEU:HD23 | 1:A:18:CYS:SG   | 0.68     | 2.28        | 5      | 2     |
| 1:A:26:LEU:HD22 | 2:B:43:HIS:CG   | 0.68     | 2.23        | 7      | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:57:ASN:N    | 2:B:69:THR:OG1  | 0.67     | 2.28        | 8      | 3     |
| 2:B:51:ILE:HA   | 2:B:54:ILE:HD11 | 0.67     | 1.66        | 1      | 2     |
| 2:B:18:LEU:HD12 | 2:B:18:LEU:O    | 0.67     | 1.90        | 10     | 5     |
| 2:B:22:ASP:HB3  | 2:B:24:VAL:HG22 | 0.67     | 1.66        | 4      | 1     |
| 2:B:17:GLU:HG3  | 2:B:18:LEU:N    | 0.67     | 2.04        | 10     | 4     |
| 2:B:56:LYS:O    | 2:B:70:CYS:HA   | 0.67     | 1.89        | 7      | 1     |
| 1:A:15:LEU:N    | 1:A:15:LEU:HD13 | 0.67     | 2.04        | 4      | 4     |
| 1:A:26:LEU:HD11 | 2:B:38:ARG:HD2  | 0.67     | 1.66        | 9      | 1     |
| 2:B:47:GLN:C    | 2:B:51:ILE:HG22 | 0.67     | 2.14        | 1      | 2     |
| 2:B:27:CYS:HA   | 2:B:30:LEU:CD2  | 0.67     | 2.20        | 9      | 3     |
| 2:B:55:ALA:O    | 2:B:56:LYS:CG   | 0.67     | 2.43        | 5      | 3     |
| 1:A:21:TRP:O    | 1:A:22:ILE:C    | 0.67     | 2.38        | 3      | 7     |
| 2:B:31:LYS:HA   | 2:B:52:TYR:CE2  | 0.67     | 2.24        | 10     | 2     |
| 2:B:57:ASN:CG   | 2:B:61:VAL:CB   | 0.67     | 2.67        | 6      | 1     |
| 1:A:26:LEU:HD21 | 2:B:37:VAL:HG12 | 0.67     | 1.65        | 1      | 3     |
| 2:B:54:ILE:CD1  | 2:B:55:ALA:N    | 0.67     | 2.57        | 3      | 5     |
| 2:B:57:ASN:O    | 2:B:61:VAL:CG2  | 0.66     | 2.42        | 4      | 3     |
| 1:A:26:LEU:HD11 | 2:B:34:ALA:C    | 0.66     | 2.15        | 6      | 1     |
| 2:B:51:ILE:O    | 2:B:54:ILE:CG1  | 0.66     | 2.43        | 10     | 1     |
| 1:A:21:TRP:CE2  | 2:B:70:CYS:O    | 0.66     | 2.48        | 9      | 1     |
| 2:B:22:ASP:C    | 2:B:24:VAL:H    | 0.66     | 1.98        | 10     | 7     |
| 2:B:30:LEU:HD22 | 2:B:30:LEU:H    | 0.66     | 1.47        | 9      | 2     |
| 1:A:21:TRP:CH2  | 2:B:70:CYS:O    | 0.66     | 2.49        | 1      | 1     |
| 1:A:21:TRP:CE3  | 2:B:58:LEU:HD22 | 0.66     | 2.24        | 7      | 2     |
| 2:B:18:LEU:CD2  | 2:B:70:CYS:O    | 0.66     | 2.44        | 7      | 1     |
| 2:B:62:CYS:SG   | 2:B:64:MET:HE2  | 0.66     | 2.30        | 4      | 2     |
| 2:B:62:CYS:CB   | 2:B:64:MET:HE2  | 0.66     | 2.20        | 9      | 2     |
| 1:A:15:LEU:H    | 1:A:15:LEU:HD22 | 0.66     | 1.51        | 7      | 2     |
| 2:B:48:SER:OG   | 2:B:52:TYR:CE1  | 0.66     | 2.48        | 9      | 1     |
| 1:A:21:TRP:HE1  | 2:B:55:ALA:CB   | 0.66     | 2.04        | 4      | 2     |
| 1:A:21:TRP:CZ3  | 1:A:22:ILE:HG22 | 0.65     | 2.26        | 1      | 1     |
| 1:A:18:CYS:O    | 1:A:21:TRP:N    | 0.65     | 2.30        | 9      | 3     |
| 2:B:30:LEU:CG   | 2:B:70:CYS:CB   | 0.65     | 2.74        | 6      | 1     |
| 2:B:30:LEU:CG   | 2:B:70:CYS:O    | 0.65     | 2.45        | 4      | 2     |
| 2:B:51:ILE:HA   | 2:B:54:ILE:CG1  | 0.65     | 2.22        | 7      | 2     |
| 1:A:26:LEU:HD12 | 2:B:38:ARG:HB3  | 0.65     | 1.69        | 3      | 1     |
| 2:B:54:ILE:C    | 2:B:54:ILE:CD1  | 0.65     | 2.70        | 8      | 1     |
| 2:B:57:ASN:CB   | 2:B:69:THR:OG1  | 0.65     | 2.43        | 2      | 3     |
| 2:B:51:ILE:HD11 | 2:B:55:ALA:O    | 0.64     | 1.92        | 2      | 1     |
| 2:B:30:LEU:HB2  | 2:B:70:CYS:C    | 0.64     | 2.17        | 4      | 3     |
| 1:A:22:ILE:HG23 | 2:B:37:VAL:HG11 | 0.64     | 1.66        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:51:ILE:HD12 | 2:B:54:ILE:HD11 | 0.64     | 1.68        | 1      | 1     |
| 2:B:30:LEU:CD1  | 2:B:70:CYS:HB2  | 0.64     | 2.22        | 6      | 1     |
| 2:B:18:LEU:HD21 | 2:B:69:THR:HG22 | 0.64     | 1.70        | 7      | 1     |
| 2:B:23:GLN:O    | 2:B:24:VAL:C    | 0.64     | 2.40        | 10     | 6     |
| 2:B:44:GLY:N    | 2:B:45:PRO:HD2  | 0.64     | 2.07        | 5      | 3     |
| 1:A:18:CYS:O    | 1:A:20:GLN:N    | 0.64     | 2.31        | 6      | 4     |
| 1:A:19:GLN:O    | 1:A:23:ARG:CB   | 0.64     | 2.45        | 5      | 5     |
| 2:B:18:LEU:C    | 2:B:18:LEU:CD1  | 0.64     | 2.71        | 8      | 6     |
| 2:B:25:CYS:C    | 2:B:28:PRO:HD2  | 0.64     | 2.18        | 7      | 5     |
| 2:B:57:ASN:CG   | 2:B:69:THR:OG1  | 0.64     | 2.41        | 2      | 4     |
| 1:A:21:TRP:HZ2  | 2:B:56:LYS:CG   | 0.64     | 2.04        | 3      | 1     |
| 2:B:57:ASN:OD1  | 2:B:61:VAL:HB   | 0.64     | 1.93        | 7      | 1     |
| 2:B:33:ALA:CA   | 2:B:37:VAL:HG23 | 0.64     | 2.22        | 3      | 1     |
| 2:B:39:VAL:O    | 2:B:39:VAL:CG2  | 0.64     | 2.45        | 9      | 4     |
| 2:B:44:GLY:O    | 2:B:46:PHE:CE1  | 0.63     | 2.51        | 7      | 2     |
| 2:B:56:LYS:O    | 2:B:69:THR:HB   | 0.63     | 1.94        | 4      | 1     |
| 1:A:26:LEU:HD13 | 2:B:43:HIS:HB2  | 0.63     | 1.68        | 7      | 1     |
| 2:B:18:LEU:HD13 | 2:B:26:VAL:O    | 0.63     | 1.93        | 9      | 1     |
| 2:B:58:LEU:HD12 | 2:B:60:ASN:HB3  | 0.63     | 1.70        | 1      | 8     |
| 2:B:26:VAL:C    | 2:B:29:THR:OG1  | 0.63     | 2.42        | 2      | 2     |
| 2:B:64:MET:HE3  | 2:B:67:ILE:CD1  | 0.63     | 2.23        | 4      | 1     |
| 2:B:39:VAL:O    | 2:B:39:VAL:HG23 | 0.63     | 1.93        | 1      | 2     |
| 1:A:21:TRP:CG   | 2:B:58:LEU:O    | 0.63     | 2.51        | 2      | 1     |
| 1:A:21:TRP:HB3  | 2:B:58:LEU:CD2  | 0.63     | 2.24        | 3      | 2     |
| 2:B:30:LEU:CD2  | 2:B:70:CYS:HB2  | 0.63     | 2.24        | 9      | 2     |
| 1:A:26:LEU:HD11 | 2:B:38:ARG:HD3  | 0.63     | 1.71        | 9      | 1     |
| 2:B:30:LEU:O    | 2:B:33:ALA:HB3  | 0.63     | 1.94        | 10     | 2     |
| 1:A:19:GLN:CA   | 1:A:22:ILE:HG23 | 0.63     | 2.23        | 3      | 1     |
| 2:B:40:GLN:C    | 2:B:42:GLN:H    | 0.63     | 2.01        | 3      | 1     |
| 2:B:60:ASN:O    | 2:B:61:VAL:O    | 0.63     | 2.16        | 6      | 2     |
| 2:B:18:LEU:HD11 | 2:B:23:GLN:HB3  | 0.63     | 1.70        | 10     | 1     |
| 2:B:26:VAL:O    | 2:B:29:THR:OG1  | 0.63     | 2.17        | 1      | 4     |
| 1:A:22:ILE:CG2  | 2:B:37:VAL:CG1  | 0.63     | 2.70        | 5      | 1     |
| 2:B:57:ASN:CA   | 2:B:69:THR:OG1  | 0.63     | 2.47        | 10     | 3     |
| 1:A:12:GLU:CG   | 1:A:13:GLN:H    | 0.63     | 2.07        | 9      | 1     |
| 2:B:64:MET:O    | 2:B:64:MET:HG3  | 0.63     | 1.94        | 2      | 2     |
| 2:B:69:THR:OG1  | 2:B:70:CYS:N    | 0.63     | 2.30        | 8      | 2     |
| 2:B:30:LEU:HB2  | 2:B:70:CYS:HB2  | 0.62     | 1.70        | 9      | 2     |
| 1:A:21:TRP:CZ2  | 2:B:57:ASN:O    | 0.62     | 2.52        | 9      | 1     |
| 1:A:17:ALA:HB3  | 2:B:14:CYS:SG   | 0.62     | 2.35        | 3      | 1     |
| 2:B:57:ASN:OD1  | 2:B:63:ASN:HA   | 0.62     | 1.94        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:39:VAL:CG2  | 2:B:43:HIS:CG   | 0.62     | 2.82        | 6      | 1     |
| 1:A:21:TRP:HH2  | 2:B:30:LEU:HD12 | 0.62     | 1.54        | 1      | 1     |
| 2:B:54:ILE:CD1  | 2:B:55:ALA:H    | 0.62     | 2.07        | 2      | 4     |
| 2:B:27:CYS:O    | 2:B:30:LEU:CD1  | 0.62     | 2.48        | 3      | 1     |
| 2:B:39:VAL:CG2  | 2:B:39:VAL:O    | 0.62     | 2.47        | 10     | 1     |
| 2:B:43:HIS:O    | 2:B:44:GLY:C    | 0.62     | 2.41        | 4      | 5     |
| 1:A:26:LEU:HD21 | 2:B:38:ARG:HG3  | 0.62     | 1.72        | 9      | 1     |
| 2:B:55:ALA:HB3  | 2:B:70:CYS:SG   | 0.62     | 2.34        | 2      | 1     |
| 2:B:69:THR:C    | 2:B:70:CYS:SG   | 0.62     | 2.82        | 3      | 3     |
| 2:B:56:LYS:HA   | 2:B:70:CYS:CA   | 0.62     | 2.24        | 4      | 1     |
| 2:B:43:HIS:O    | 2:B:46:PHE:CE1  | 0.62     | 2.52        | 3      | 1     |
| 1:A:18:CYS:C    | 1:A:22:ILE:HG22 | 0.62     | 2.19        | 6      | 1     |
| 2:B:26:VAL:HG12 | 2:B:27:CYS:H    | 0.61     | 1.53        | 9      | 7     |
| 2:B:31:LYS:O    | 2:B:52:TYR:CZ   | 0.61     | 2.53        | 5      | 2     |
| 1:A:14:HIS:O    | 1:A:15:LEU:C    | 0.61     | 2.43        | 9      | 7     |
| 2:B:57:ASN:HD22 | 2:B:61:VAL:HG21 | 0.61     | 1.55        | 2      | 2     |
| 2:B:67:ILE:HG22 | 2:B:68:GLY:N    | 0.61     | 2.10        | 2      | 8     |
| 1:A:21:TRP:CE3  | 1:A:22:ILE:N    | 0.61     | 2.66        | 5      | 3     |
| 2:B:35:LYS:CE   | 2:B:46:PHE:CD2  | 0.61     | 2.83        | 5      | 1     |
| 1:A:21:TRP:CZ2  | 2:B:57:ASN:HA   | 0.61     | 2.30        | 9      | 1     |
| 1:A:14:HIS:O    | 1:A:15:LEU:O    | 0.61     | 2.19        | 9      | 7     |
| 1:A:18:CYS:SG   | 2:B:61:VAL:HG22 | 0.61     | 2.36        | 10     | 2     |
| 2:B:35:LYS:O    | 2:B:39:VAL:HG23 | 0.61     | 1.95        | 6      | 1     |
| 2:B:61:VAL:HG11 | 2:B:69:THR:HG22 | 0.61     | 1.73        | 7      | 1     |
| 1:A:21:TRP:HA   | 2:B:58:LEU:HD21 | 0.61     | 1.73        | 9      | 1     |
| 2:B:59:PRO:O    | 2:B:60:ASN:CB   | 0.61     | 2.48        | 3      | 10    |
| 2:B:33:ALA:O    | 2:B:37:VAL:CG2  | 0.61     | 2.48        | 5      | 2     |
| 1:A:18:CYS:O    | 1:A:22:ILE:CG2  | 0.61     | 2.48        | 3      | 1     |
| 2:B:22:ASP:O    | 2:B:26:VAL:HG23 | 0.61     | 1.96        | 7      | 2     |
| 2:B:22:ASP:OD1  | 2:B:23:GLN:N    | 0.61     | 2.34        | 4      | 1     |
| 1:A:21:TRP:CD1  | 2:B:61:VAL:CG2  | 0.61     | 2.81        | 5      | 1     |
| 2:B:14:CYS:O    | 2:B:18:LEU:HD23 | 0.61     | 1.94        | 5      | 1     |
| 1:A:22:ILE:C    | 1:A:22:ILE:CD1  | 0.61     | 2.72        | 6      | 3     |
| 2:B:44:GLY:O    | 2:B:46:PHE:CZ   | 0.61     | 2.54        | 3      | 1     |
| 2:B:67:ILE:CG2  | 2:B:68:GLY:N    | 0.60     | 2.64        | 10     | 8     |
| 1:A:21:TRP:CZ2  | 2:B:56:LYS:HB2  | 0.60     | 2.31        | 2      | 1     |
| 2:B:29:THR:O    | 2:B:32:GLN:N    | 0.60     | 2.30        | 5      | 2     |
| 1:A:6:GLN:O     | 1:A:9:PHE:CB    | 0.60     | 2.50        | 7      | 1     |
| 2:B:22:ASP:C    | 2:B:24:VAL:N    | 0.60     | 2.57        | 10     | 9     |
| 2:B:18:LEU:O    | 2:B:21:GLU:N    | 0.60     | 2.31        | 7      | 2     |
| 2:B:57:ASN:OD1  | 2:B:61:VAL:CG1  | 0.60     | 2.49        | 6      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:54:ILE:O    | 2:B:55:ALA:HB2  | 0.60     | 1.97        | 3      | 2     |
| 1:A:22:ILE:HG21 | 2:B:34:ALA:HA   | 0.60     | 1.72        | 5      | 1     |
| 2:B:37:VAL:O    | 2:B:38:ARG:O    | 0.60     | 2.19        | 8      | 1     |
| 2:B:35:LYS:O    | 2:B:39:VAL:CG2  | 0.60     | 2.50        | 5      | 4     |
| 2:B:63:ASN:O    | 2:B:65:LYS:N    | 0.60     | 2.34        | 5      | 1     |
| 2:B:51:ILE:HG23 | 2:B:56:LYS:HE3  | 0.60     | 1.73        | 8      | 1     |
| 2:B:51:ILE:HA   | 2:B:54:ILE:CD1  | 0.60     | 2.27        | 1      | 2     |
| 1:A:19:GLN:O    | 1:A:23:ARG:HB2  | 0.60     | 1.97        | 5      | 1     |
| 1:A:8:GLU:O     | 1:A:12:GLU:CD   | 0.60     | 2.44        | 9      | 1     |
| 2:B:27:CYS:SG   | 2:B:69:THR:C    | 0.60     | 2.85        | 9      | 1     |
| 2:B:27:CYS:SG   | 2:B:55:ALA:CB   | 0.60     | 2.89        | 3      | 1     |
| 2:B:56:LYS:HB2  | 2:B:69:THR:C    | 0.60     | 2.22        | 4      | 1     |
| 2:B:57:ASN:HB2  | 2:B:69:THR:OG1  | 0.60     | 1.97        | 2      | 1     |
| 2:B:57:ASN:OD1  | 2:B:63:ASN:N    | 0.60     | 2.34        | 5      | 2     |
| 1:A:16:ARG:HA   | 1:A:19:GLN:HB2  | 0.59     | 1.74        | 3      | 1     |
| 2:B:48:SER:HB3  | 2:B:52:TYR:CE1  | 0.59     | 2.31        | 3      | 3     |
| 1:A:26:LEU:CD2  | 2:B:43:HIS:ND1  | 0.59     | 2.65        | 4      | 2     |
| 2:B:26:VAL:HG12 | 2:B:28:PRO:HD3  | 0.59     | 1.72        | 10     | 1     |
| 2:B:30:LEU:CD1  | 2:B:70:CYS:HB3  | 0.59     | 2.26        | 8      | 1     |
| 2:B:32:GLN:O    | 2:B:35:LYS:N    | 0.59     | 2.35        | 9      | 1     |
| 2:B:57:ASN:CG   | 2:B:69:THR:CB   | 0.59     | 2.75        | 10     | 1     |
| 1:A:20:GLN:O    | 1:A:24:GLN:CB   | 0.59     | 2.50        | 5      | 3     |
| 1:A:18:CYS:C    | 1:A:22:ILE:CG2  | 0.59     | 2.75        | 3      | 2     |
| 2:B:64:MET:CG   | 2:B:64:MET:O    | 0.59     | 2.51        | 6      | 1     |
| 2:B:64:MET:HE3  | 2:B:67:ILE:CG1  | 0.59     | 2.28        | 4      | 1     |
| 1:A:9:PHE:HZ    | 2:B:33:ALA:HB2  | 0.59     | 1.57        | 2      | 2     |
| 1:A:16:ARG:O    | 1:A:17:ALA:C    | 0.59     | 2.46        | 4      | 9     |
| 2:B:22:ASP:OD2  | 2:B:24:VAL:HG13 | 0.59     | 1.97        | 4      | 1     |
| 2:B:25:CYS:C    | 2:B:29:THR:OG1  | 0.59     | 2.46        | 1      | 3     |
| 2:B:57:ASN:O    | 2:B:61:VAL:CB   | 0.59     | 2.51        | 4      | 2     |
| 2:B:51:ILE:O    | 2:B:54:ILE:HG23 | 0.59     | 1.98        | 10     | 1     |
| 2:B:39:VAL:O    | 2:B:40:GLN:O    | 0.59     | 2.21        | 4      | 5     |
| 2:B:69:THR:HG23 | 2:B:70:CYS:SG   | 0.59     | 2.38        | 5      | 1     |
| 2:B:57:ASN:CG   | 2:B:69:THR:HG1  | 0.59     | 2.06        | 2      | 1     |
| 2:B:29:THR:O    | 2:B:30:LEU:C    | 0.59     | 2.46        | 5      | 6     |
| 2:B:30:LEU:HD13 | 2:B:30:LEU:N    | 0.59     | 2.12        | 6      | 2     |
| 2:B:48:SER:HB3  | 2:B:52:TYR:CD1  | 0.58     | 2.33        | 3      | 2     |
| 1:A:26:LEU:HD22 | 2:B:43:HIS:ND1  | 0.58     | 2.13        | 7      | 2     |
| 1:A:15:LEU:O    | 1:A:19:GLN:CG   | 0.58     | 2.51        | 3      | 1     |
| 2:B:31:LYS:HA   | 2:B:52:TYR:CD2  | 0.58     | 2.33        | 6      | 2     |
| 1:A:15:LEU:HD22 | 1:A:15:LEU:H    | 0.58     | 1.55        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:21:TRP:HE3  | 1:A:22:ILE:CA   | 0.58     | 2.10        | 5      | 1     |
| 1:A:21:TRP:CD2  | 1:A:22:ILE:N    | 0.58     | 2.71        | 7      | 3     |
| 2:B:40:GLN:N    | 2:B:43:HIS:O    | 0.58     | 2.36        | 9      | 2     |
| 2:B:30:LEU:O    | 2:B:34:ALA:N    | 0.58     | 2.33        | 5      | 1     |
| 2:B:52:TYR:O    | 2:B:55:ALA:N    | 0.58     | 2.37        | 5      | 1     |
| 1:A:19:GLN:CA   | 1:A:22:ILE:HD12 | 0.58     | 2.28        | 10     | 1     |
| 2:B:17:GLU:C    | 2:B:17:GLU:CD   | 0.58     | 2.72        | 3      | 5     |
| 2:B:27:CYS:O    | 2:B:30:LEU:HD11 | 0.58     | 1.99        | 3      | 1     |
| 2:B:30:LEU:CD1  | 2:B:30:LEU:N    | 0.58     | 2.66        | 3      | 2     |
| 2:B:57:ASN:CB   | 2:B:69:THR:HG22 | 0.58     | 2.25        | 6      | 1     |
| 2:B:24:VAL:HG13 | 2:B:25:CYS:SG   | 0.58     | 2.39        | 7      | 1     |
| 1:A:19:GLN:HA   | 1:A:22:ILE:HG23 | 0.58     | 1.76        | 3      | 2     |
| 1:A:21:TRP:CZ3  | 1:A:22:ILE:CG2  | 0.57     | 2.88        | 4      | 2     |
| 2:B:30:LEU:H    | 2:B:30:LEU:HD23 | 0.57     | 1.58        | 1      | 1     |
| 2:B:30:LEU:O    | 2:B:33:ALA:N    | 0.57     | 2.37        | 4      | 4     |
| 2:B:61:VAL:CG1  | 2:B:62:CYS:N    | 0.57     | 2.66        | 7      | 6     |
| 2:B:57:ASN:OD1  | 2:B:63:ASN:CA   | 0.57     | 2.52        | 5      | 1     |
| 1:A:9:PHE:CD2   | 1:A:14:HIS:NE2  | 0.57     | 2.72        | 7      | 1     |
| 1:A:21:TRP:HZ2  | 2:B:30:LEU:HD23 | 0.57     | 1.53        | 10     | 1     |
| 2:B:30:LEU:HD23 | 2:B:55:ALA:HA   | 0.57     | 1.76        | 2      | 1     |
| 2:B:69:THR:HG23 | 2:B:70:CYS:N    | 0.57     | 2.14        | 5      | 1     |
| 2:B:56:LYS:HA   | 2:B:69:THR:HG23 | 0.57     | 1.77        | 9      | 2     |
| 2:B:40:GLN:O    | 2:B:43:HIS:N    | 0.57     | 2.28        | 7      | 1     |
| 2:B:25:CYS:C    | 2:B:29:THR:HG1  | 0.57     | 2.06        | 1      | 3     |
| 2:B:41:GLY:C    | 2:B:42:GLN:CG   | 0.57     | 2.78        | 3      | 1     |
| 1:A:21:TRP:CZ2  | 2:B:30:LEU:CD2  | 0.57     | 2.87        | 10     | 1     |
| 1:A:21:TRP:CH2  | 2:B:30:LEU:HD23 | 0.57     | 2.34        | 10     | 1     |
| 2:B:47:GLN:O    | 2:B:51:ILE:CG2  | 0.57     | 2.52        | 10     | 1     |
| 2:B:24:VAL:CG2  | 2:B:25:CYS:N    | 0.57     | 2.67        | 9      | 1     |
| 2:B:34:ALA:HB3  | 2:B:52:TYR:OH   | 0.57     | 1.99        | 10     | 1     |
| 1:A:26:LEU:CD2  | 2:B:46:PHE:CZ   | 0.57     | 2.86        | 1      | 1     |
| 2:B:48:SER:O    | 2:B:52:TYR:CB   | 0.57     | 2.51        | 8      | 6     |
| 2:B:33:ALA:O    | 2:B:36:SER:N    | 0.57     | 2.37        | 4      | 1     |
| 2:B:63:ASN:CG   | 2:B:63:ASN:O    | 0.57     | 2.47        | 1      | 1     |
| 1:A:21:TRP:CZ2  | 2:B:57:ASN:CA   | 0.57     | 2.87        | 9      | 1     |
| 2:B:30:LEU:CD2  | 2:B:56:LYS:HG3  | 0.57     | 2.30        | 2      | 1     |
| 2:B:30:LEU:HA   | 2:B:33:ALA:HB3  | 0.57     | 1.76        | 6      | 4     |
| 1:A:16:ARG:HA   | 1:A:19:GLN:HB3  | 0.57     | 1.77        | 10     | 2     |
| 2:B:30:LEU:N    | 2:B:30:LEU:HD13 | 0.57     | 2.14        | 3      | 2     |
| 1:A:21:TRP:CD2  | 2:B:58:LEU:CD2  | 0.57     | 2.88        | 5      | 1     |
| 2:B:14:CYS:O    | 2:B:18:LEU:CD2  | 0.57     | 2.52        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:10:GLN:O    | 1:A:14:HIS:CD2  | 0.56     | 2.58        | 6      | 1     |
| 2:B:69:THR:O    | 2:B:70:CYS:C    | 0.56     | 2.48        | 5      | 1     |
| 2:B:22:ASP:O    | 2:B:24:VAL:N    | 0.56     | 2.38        | 10     | 7     |
| 2:B:64:MET:HE3  | 2:B:67:ILE:HD11 | 0.56     | 1.78        | 4      | 1     |
| 2:B:30:LEU:HD11 | 2:B:70:CYS:HB3  | 0.56     | 1.75        | 8      | 1     |
| 1:A:26:LEU:CD2  | 2:B:43:HIS:CG   | 0.56     | 2.89        | 4      | 1     |
| 2:B:37:VAL:O    | 2:B:39:VAL:N    | 0.56     | 2.39        | 2      | 1     |
| 1:A:14:HIS:H    | 1:A:14:HIS:CD2  | 0.56     | 2.17        | 5      | 3     |
| 2:B:62:CYS:C    | 2:B:63:ASN:CG   | 0.56     | 2.74        | 8      | 2     |
| 1:A:21:TRP:CZ2  | 2:B:56:LYS:CG   | 0.56     | 2.87        | 3      | 1     |
| 2:B:64:MET:HE3  | 2:B:67:ILE:HG13 | 0.56     | 1.78        | 4      | 1     |
| 2:B:35:LYS:HE3  | 2:B:46:PHE:CE2  | 0.56     | 2.35        | 5      | 1     |
| 1:A:15:LEU:O    | 1:A:19:GLN:CB   | 0.56     | 2.54        | 3      | 1     |
| 2:B:30:LEU:CG   | 2:B:70:CYS:HB3  | 0.56     | 2.24        | 6      | 1     |
| 1:A:16:ARG:O    | 1:A:19:GLN:CB   | 0.56     | 2.53        | 4      | 3     |
| 2:B:57:ASN:ND2  | 2:B:63:ASN:N    | 0.56     | 2.53        | 4      | 1     |
| 2:B:53:GLN:O    | 2:B:54:ILE:C    | 0.56     | 2.49        | 1      | 4     |
| 2:B:48:SER:O    | 2:B:52:TYR:CG   | 0.56     | 2.58        | 10     | 3     |
| 1:A:15:LEU:O    | 1:A:19:GLN:HB2  | 0.55     | 2.01        | 3      | 1     |
| 2:B:27:CYS:O    | 2:B:31:LYS:HD2  | 0.55     | 2.02        | 5      | 1     |
| 2:B:33:ALA:O    | 2:B:34:ALA:C    | 0.55     | 2.49        | 3      | 3     |
| 1:A:8:GLU:O     | 1:A:11:GLN:N    | 0.55     | 2.39        | 6      | 2     |
| 1:A:21:TRP:O    | 1:A:24:GLN:N    | 0.55     | 2.39        | 4      | 3     |
| 2:B:57:ASN:ND2  | 2:B:61:VAL:CG1  | 0.55     | 2.69        | 3      | 1     |
| 1:A:21:TRP:NE1  | 2:B:55:ALA:CB   | 0.55     | 2.69        | 4      | 2     |
| 1:A:22:ILE:O    | 1:A:25:GLN:N    | 0.55     | 2.39        | 9      | 2     |
| 1:A:22:ILE:CG2  | 2:B:34:ALA:N    | 0.55     | 2.70        | 10     | 1     |
| 2:B:23:GLN:C    | 2:B:25:CYS:N    | 0.55     | 2.64        | 10     | 4     |
| 2:B:36:SER:O    | 2:B:39:VAL:CG2  | 0.55     | 2.54        | 1      | 1     |
| 2:B:62:CYS:O    | 2:B:63:ASN:CG   | 0.55     | 2.50        | 7      | 3     |
| 2:B:26:VAL:CG1  | 2:B:28:PRO:HD3  | 0.55     | 2.30        | 10     | 1     |
| 1:A:4:LYS:O     | 1:A:8:GLU:N     | 0.55     | 2.34        | 9      | 2     |
| 2:B:33:ALA:HB1  | 2:B:37:VAL:CG2  | 0.55     | 2.32        | 3      | 1     |
| 2:B:55:ALA:O    | 2:B:56:LYS:HD3  | 0.55     | 2.02        | 3      | 1     |
| 2:B:62:CYS:O    | 2:B:63:ASN:HB3  | 0.55     | 2.00        | 3      | 1     |
| 1:A:22:ILE:HG22 | 2:B:37:VAL:CG1  | 0.55     | 2.30        | 5      | 1     |
| 1:A:26:LEU:CD1  | 2:B:38:ARG:HD2  | 0.55     | 2.30        | 9      | 1     |
| 2:B:24:VAL:CG1  | 2:B:25:CYS:SG   | 0.55     | 2.95        | 7      | 2     |
| 2:B:27:CYS:C    | 2:B:30:LEU:CD2  | 0.55     | 2.80        | 6      | 3     |
| 2:B:43:HIS:CD2  | 2:B:43:HIS:O    | 0.55     | 2.60        | 8      | 1     |
| 2:B:58:LEU:HB2  | 2:B:60:ASN:HB2  | 0.55     | 1.78        | 8      | 8     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:PHE:CZ    | 1:A:14:HIS:CE1  | 0.55     | 2.95        | 2      | 1     |
| 2:B:17:GLU:CD   | 2:B:17:GLU:O    | 0.55     | 2.49        | 3      | 2     |
| 2:B:43:HIS:CA   | 2:B:45:PRO:HD2  | 0.55     | 2.31        | 9      | 1     |
| 1:A:22:ILE:CG2  | 2:B:33:ALA:C    | 0.55     | 2.80        | 10     | 1     |
| 1:A:19:GLN:HA   | 1:A:22:ILE:HG12 | 0.55     | 1.78        | 1      | 2     |
| 2:B:48:SER:HA   | 2:B:51:ILE:CG2  | 0.55     | 2.32        | 7      | 5     |
| 2:B:56:LYS:C    | 2:B:58:LEU:N    | 0.55     | 2.63        | 6      | 4     |
| 1:A:24:GLN:O    | 1:A:27:ALA:N    | 0.55     | 2.40        | 7      | 3     |
| 2:B:34:ALA:O    | 2:B:37:VAL:HB   | 0.54     | 2.02        | 5      | 2     |
| 1:A:22:ILE:HD13 | 1:A:22:ILE:C    | 0.54     | 2.27        | 3      | 1     |
| 2:B:35:LYS:HE2  | 2:B:46:PHE:CE2  | 0.54     | 2.36        | 5      | 1     |
| 1:A:21:TRP:HH2  | 2:B:70:CYS:O    | 0.54     | 1.83        | 1      | 1     |
| 2:B:25:CYS:O    | 2:B:26:VAL:C    | 0.54     | 2.51        | 8      | 2     |
| 1:A:21:TRP:CZ2  | 2:B:57:ASN:C    | 0.54     | 2.85        | 9      | 1     |
| 2:B:51:ILE:C    | 2:B:51:ILE:CD1  | 0.54     | 2.75        | 10     | 1     |
| 2:B:34:ALA:O    | 2:B:35:LYS:C    | 0.54     | 2.51        | 9      | 7     |
| 2:B:31:LYS:O    | 2:B:52:TYR:CE2  | 0.54     | 2.61        | 6      | 1     |
| 2:B:57:ASN:CG   | 2:B:61:VAL:CG1  | 0.54     | 2.81        | 6      | 1     |
| 1:A:15:LEU:H    | 1:A:15:LEU:HD13 | 0.54     | 1.61        | 1      | 2     |
| 1:A:21:TRP:CH2  | 1:A:22:ILE:HG12 | 0.54     | 2.37        | 7      | 2     |
| 1:A:8:GLU:O     | 1:A:12:GLU:N    | 0.54     | 2.26        | 6      | 1     |
| 2:B:25:CYS:O    | 2:B:26:VAL:CB   | 0.54     | 2.56        | 10     | 1     |
| 1:A:18:CYS:O    | 1:A:19:GLN:C    | 0.54     | 2.50        | 4      | 7     |
| 1:A:18:CYS:C    | 1:A:20:GLN:N    | 0.54     | 2.62        | 6      | 5     |
| 2:B:61:VAL:CG1  | 2:B:64:MET:HE3  | 0.54     | 2.32        | 2      | 1     |
| 2:B:56:LYS:O    | 2:B:70:CYS:N    | 0.54     | 2.41        | 4      | 1     |
| 2:B:56:LYS:C    | 2:B:69:THR:HB   | 0.54     | 2.28        | 4      | 1     |
| 2:B:57:ASN:O    | 2:B:61:VAL:HB   | 0.54     | 2.02        | 4      | 2     |
| 2:B:62:CYS:O    | 2:B:63:ASN:ND2  | 0.54     | 2.41        | 6      | 1     |
| 2:B:57:ASN:ND2  | 2:B:70:CYS:H    | 0.54     | 2.00        | 3      | 1     |
| 2:B:62:CYS:O    | 2:B:63:ASN:HB2  | 0.54     | 2.03        | 6      | 6     |
| 2:B:30:LEU:CD2  | 2:B:55:ALA:HA   | 0.54     | 2.33        | 2      | 1     |
| 2:B:62:CYS:SG   | 2:B:64:MET:CG   | 0.54     | 2.96        | 8      | 1     |
| 2:B:69:THR:HG23 | 2:B:70:CYS:H    | 0.53     | 1.63        | 5      | 1     |
| 1:A:21:TRP:CD2  | 2:B:57:ASN:O    | 0.53     | 2.61        | 9      | 1     |
| 2:B:57:ASN:ND2  | 2:B:62:CYS:H    | 0.53     | 2.00        | 10     | 1     |
| 1:A:20:GLN:O    | 1:A:21:TRP:C    | 0.53     | 2.51        | 5      | 2     |
| 2:B:30:LEU:CD1  | 2:B:30:LEU:H    | 0.53     | 2.04        | 6      | 2     |
| 1:A:22:ILE:HG13 | 2:B:37:VAL:HG21 | 0.53     | 1.80        | 6      | 1     |
| 2:B:34:ALA:O    | 2:B:37:VAL:N    | 0.53     | 2.41        | 6      | 1     |
| 1:A:18:CYS:N    | 2:B:14:CYS:SG   | 0.53     | 2.81        | 9      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:16:ARG:C    | 1:A:18:CYS:N    | 0.53     | 2.65        | 5      | 6     |
| 2:B:40:GLN:O    | 2:B:42:GLN:N    | 0.53     | 2.39        | 3      | 4     |
| 1:A:10:GLN:O    | 1:A:14:HIS:NE2  | 0.53     | 2.41        | 6      | 1     |
| 2:B:30:LEU:HG   | 2:B:70:CYS:CA   | 0.53     | 2.33        | 8      | 1     |
| 2:B:38:ARG:C    | 2:B:40:GLN:N    | 0.53     | 2.67        | 9      | 1     |
| 2:B:15:CYS:SG   | 2:B:19:TYR:CD1  | 0.53     | 3.01        | 10     | 1     |
| 1:A:7:ARG:O     | 1:A:11:GLN:N    | 0.53     | 2.39        | 1      | 3     |
| 2:B:64:MET:C    | 2:B:66:GLN:H    | 0.53     | 2.12        | 10     | 4     |
| 1:A:26:LEU:CD1  | 2:B:34:ALA:O    | 0.53     | 2.56        | 6      | 1     |
| 2:B:25:CYS:HA   | 2:B:28:PRO:CG   | 0.53     | 2.34        | 7      | 2     |
| 2:B:41:GLY:C    | 2:B:43:HIS:N    | 0.53     | 2.66        | 5      | 2     |
| 1:A:23:ARG:HA   | 2:B:37:VAL:HG11 | 0.53     | 1.81        | 6      | 1     |
| 1:A:9:PHE:CE2   | 1:A:14:HIS:ND1  | 0.53     | 2.77        | 7      | 1     |
| 1:A:22:ILE:CG2  | 2:B:33:ALA:HB1  | 0.53     | 2.34        | 10     | 1     |
| 2:B:48:SER:O    | 2:B:49:THR:C    | 0.52     | 2.52        | 8      | 7     |
| 2:B:55:ALA:O    | 2:B:56:LYS:HG2  | 0.52     | 2.04        | 2      | 1     |
| 2:B:15:CYS:HB2  | 2:B:61:VAL:HG13 | 0.52     | 1.81        | 9      | 2     |
| 2:B:33:ALA:O    | 2:B:37:VAL:HB   | 0.52     | 2.04        | 9      | 4     |
| 2:B:64:MET:O    | 2:B:64:MET:CG   | 0.52     | 2.57        | 2      | 1     |
| 1:A:2:PRO:O     | 1:A:6:GLN:CG    | 0.52     | 2.57        | 2      | 2     |
| 1:A:26:LEU:N    | 1:A:26:LEU:CD2  | 0.52     | 2.67        | 2      | 2     |
| 2:B:57:ASN:O    | 2:B:58:LEU:CB   | 0.52     | 2.57        | 4      | 2     |
| 2:B:51:ILE:O    | 2:B:52:TYR:C    | 0.52     | 2.52        | 6      | 8     |
| 1:A:22:ILE:CD1  | 1:A:23:ARG:N    | 0.52     | 2.73        | 9      | 2     |
| 1:A:9:PHE:CE2   | 2:B:33:ALA:HB2  | 0.52     | 2.40        | 4      | 1     |
| 2:B:22:ASP:CB   | 2:B:24:VAL:HG22 | 0.52     | 2.35        | 4      | 1     |
| 2:B:34:ALA:HA   | 2:B:37:VAL:HB   | 0.52     | 1.81        | 9      | 2     |
| 1:A:25:GLN:HG3  | 2:B:51:ILE:HD11 | 0.52     | 1.82        | 7      | 1     |
| 1:A:17:ALA:C    | 1:A:19:GLN:N    | 0.52     | 2.63        | 8      | 1     |
| 2:B:24:VAL:HG23 | 2:B:25:CYS:SG   | 0.52     | 2.44        | 3      | 2     |
| 1:A:22:ILE:CG1  | 1:A:23:ARG:N    | 0.52     | 2.73        | 8      | 2     |
| 2:B:40:GLN:CD   | 2:B:41:GLY:N    | 0.52     | 2.68        | 9      | 2     |
| 1:A:9:PHE:CE1   | 2:B:29:THR:O    | 0.52     | 2.62        | 4      | 1     |
| 2:B:56:LYS:O    | 2:B:69:THR:CB   | 0.52     | 2.57        | 4      | 1     |
| 1:A:21:TRP:CD2  | 2:B:58:LEU:HD21 | 0.52     | 2.40        | 5      | 1     |
| 2:B:35:LYS:O    | 2:B:39:VAL:CG1  | 0.52     | 2.57        | 8      | 1     |
| 2:B:27:CYS:SG   | 2:B:69:THR:O    | 0.52     | 2.68        | 1      | 1     |
| 2:B:58:LEU:CB   | 2:B:59:PRO:O    | 0.52     | 2.58        | 6      | 7     |
| 2:B:26:VAL:N    | 2:B:28:PRO:CD   | 0.52     | 2.72        | 3      | 2     |
| 2:B:30:LEU:HD13 | 2:B:31:LYS:H    | 0.52     | 1.64        | 3      | 1     |
| 1:A:19:GLN:HA   | 1:A:22:ILE:CD1  | 0.52     | 2.35        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:41:GLY:C    | 2:B:43:HIS:H    | 0.52     | 2.13        | 9      | 2     |
| 2:B:51:ILE:O    | 2:B:54:ILE:N    | 0.52     | 2.43        | 9      | 3     |
| 1:A:25:GLN:OE1  | 2:B:51:ILE:HD13 | 0.52     | 2.05        | 7      | 1     |
| 1:A:16:ARG:O    | 1:A:18:CYS:N    | 0.52     | 2.43        | 9      | 5     |
| 1:A:7:ARG:O     | 1:A:11:GLN:CG   | 0.52     | 2.58        | 6      | 1     |
| 1:A:15:LEU:HD12 | 2:B:17:GLU:CD   | 0.52     | 2.29        | 6      | 1     |
| 1:A:24:GLN:O    | 1:A:27:ALA:HB3  | 0.52     | 2.04        | 8      | 3     |
| 2:B:15:CYS:SG   | 2:B:16:ASN:N    | 0.52     | 2.83        | 7      | 1     |
| 1:A:21:TRP:CE3  | 2:B:58:LEU:HD21 | 0.52     | 2.39        | 8      | 1     |
| 1:A:21:TRP:C    | 1:A:23:ARG:N    | 0.52     | 2.66        | 3      | 4     |
| 2:B:61:VAL:CG1  | 2:B:62:CYS:SG   | 0.52     | 2.92        | 8      | 1     |
| 1:A:8:GLU:O     | 1:A:12:GLU:CG   | 0.51     | 2.58        | 8      | 3     |
| 1:A:15:LEU:N    | 1:A:15:LEU:CD2  | 0.51     | 2.66        | 5      | 4     |
| 2:B:31:LYS:CG   | 2:B:32:GLN:N    | 0.51     | 2.73        | 3      | 1     |
| 2:B:31:LYS:HB2  | 2:B:52:TYR:CD2  | 0.51     | 2.40        | 7      | 1     |
| 2:B:34:ALA:O    | 2:B:38:ARG:N    | 0.51     | 2.43        | 7      | 1     |
| 2:B:27:CYS:O    | 2:B:31:LYS:CE   | 0.51     | 2.58        | 8      | 1     |
| 1:A:19:GLN:CA   | 1:A:22:ILE:CG1  | 0.51     | 2.87        | 4      | 2     |
| 1:A:14:HIS:CD2  | 1:A:14:HIS:N    | 0.51     | 2.78        | 5      | 3     |
| 2:B:57:ASN:HA   | 2:B:69:THR:C    | 0.51     | 2.29        | 7      | 1     |
| 2:B:26:VAL:CG1  | 2:B:70:CYS:O    | 0.51     | 2.59        | 2      | 1     |
| 2:B:64:MET:C    | 2:B:66:GLN:N    | 0.51     | 2.67        | 10     | 4     |
| 1:A:22:ILE:HG13 | 1:A:23:ARG:N    | 0.51     | 2.20        | 8      | 1     |
| 2:B:38:ARG:HB3  | 2:B:43:HIS:CD2  | 0.51     | 2.40        | 9      | 1     |
| 1:A:21:TRP:CD2  | 2:B:58:LEU:HD23 | 0.51     | 2.40        | 4      | 2     |
| 2:B:40:GLN:C    | 2:B:42:GLN:N    | 0.51     | 2.68        | 3      | 1     |
| 1:A:10:GLN:HA   | 1:A:14:HIS:CD2  | 0.51     | 2.40        | 4      | 5     |
| 2:B:46:PHE:CE2  | 2:B:51:ILE:HG12 | 0.51     | 2.41        | 1      | 1     |
| 1:A:22:ILE:HD11 | 2:B:30:LEU:HD13 | 0.51     | 1.83        | 2      | 1     |
| 1:A:19:GLN:CA   | 1:A:22:ILE:HG22 | 0.51     | 2.36        | 6      | 1     |
| 2:B:61:VAL:CG1  | 2:B:62:CYS:H    | 0.51     | 2.09        | 6      | 1     |
| 2:B:47:GLN:O    | 2:B:51:ILE:N    | 0.51     | 2.44        | 1      | 1     |
| 1:A:4:LYS:O     | 1:A:8:GLU:CG    | 0.51     | 2.58        | 3      | 2     |
| 2:B:18:LEU:CD2  | 2:B:69:THR:HG22 | 0.51     | 2.36        | 7      | 1     |
| 1:A:19:GLN:O    | 1:A:22:ILE:HG22 | 0.51     | 2.06        | 7      | 2     |
| 2:B:40:GLN:CG   | 2:B:41:GLY:N    | 0.51     | 2.74        | 10     | 3     |
| 2:B:48:SER:HB3  | 2:B:52:TYR:CD2  | 0.51     | 2.41        | 6      | 1     |
| 1:A:24:GLN:O    | 1:A:25:GLN:C    | 0.51     | 2.53        | 2      | 6     |
| 1:A:26:LEU:HD21 | 2:B:37:VAL:CG1  | 0.51     | 2.36        | 2      | 2     |
| 2:B:43:HIS:O    | 2:B:45:PRO:O    | 0.51     | 2.29        | 4      | 1     |
| 2:B:64:MET:O    | 2:B:68:GLY:O    | 0.51     | 2.28        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:30:LEU:H    | 2:B:30:LEU:HD13 | 0.51     | 1.66        | 8      | 2     |
| 2:B:12:GLU:CG   | 2:B:16:ASN:ND2  | 0.50     | 2.74        | 3      | 2     |
| 1:A:21:TRP:O    | 1:A:25:GLN:N    | 0.50     | 2.35        | 1      | 3     |
| 2:B:30:LEU:HD12 | 2:B:31:LYS:N    | 0.50     | 2.17        | 2      | 1     |
| 2:B:59:PRO:O    | 2:B:60:ASN:HB2  | 0.50     | 2.06        | 3      | 1     |
| 1:A:15:LEU:H    | 1:A:15:LEU:CD1  | 0.50     | 2.16        | 8      | 3     |
| 2:B:51:ILE:CD1  | 2:B:55:ALA:O    | 0.50     | 2.59        | 2      | 1     |
| 1:A:21:TRP:CZ3  | 1:A:22:ILE:HG23 | 0.50     | 2.41        | 4      | 1     |
| 2:B:18:LEU:HD13 | 2:B:26:VAL:CG1  | 0.50     | 2.16        | 7      | 1     |
| 1:A:18:CYS:HB3  | 1:A:22:ILE:CG2  | 0.50     | 2.37        | 1      | 1     |
| 2:B:15:CYS:HB2  | 2:B:61:VAL:HG12 | 0.50     | 1.84        | 1      | 1     |
| 2:B:55:ALA:O    | 2:B:56:LYS:CB   | 0.50     | 2.58        | 1      | 3     |
| 1:A:5:CYS:SG    | 2:B:24:VAL:CG2  | 0.50     | 3.00        | 9      | 2     |
| 2:B:57:ASN:ND2  | 2:B:60:ASN:H    | 0.50     | 2.03        | 4      | 1     |
| 1:A:21:TRP:CE2  | 2:B:56:LYS:HB2  | 0.50     | 2.41        | 2      | 1     |
| 2:B:57:ASN:HA   | 2:B:70:CYS:HA   | 0.50     | 1.84        | 5      | 1     |
| 1:A:15:LEU:HD22 | 1:A:15:LEU:N    | 0.50     | 2.20        | 7      | 1     |
| 1:A:21:TRP:CE3  | 1:A:22:ILE:CG2  | 0.50     | 2.95        | 1      | 2     |
| 2:B:50:ARG:O    | 2:B:51:ILE:C    | 0.50     | 2.55        | 10     | 5     |
| 1:A:14:HIS:C    | 1:A:15:LEU:O    | 0.50     | 2.55        | 2      | 6     |
| 1:A:11:GLN:C    | 1:A:11:GLN:CD   | 0.50     | 2.79        | 3      | 1     |
| 1:A:22:ILE:HD12 | 1:A:26:LEU:HG   | 0.50     | 1.83        | 5      | 1     |
| 1:A:13:GLN:C    | 1:A:14:HIS:O    | 0.50     | 2.52        | 7      | 1     |
| 2:B:51:ILE:CA   | 2:B:54:ILE:CG1  | 0.50     | 2.90        | 7      | 2     |
| 1:A:26:LEU:HD23 | 2:B:43:HIS:ND1  | 0.50     | 2.20        | 4      | 1     |
| 1:A:22:ILE:CG2  | 1:A:23:ARG:N    | 0.50     | 2.74        | 5      | 3     |
| 1:A:19:GLN:HA   | 1:A:22:ILE:HD11 | 0.50     | 1.83        | 4      | 1     |
| 2:B:42:GLN:C    | 2:B:44:GLY:H    | 0.50     | 2.15        | 3      | 1     |
| 2:B:10:LEU:HD13 | 2:B:10:LEU:N    | 0.50     | 2.22        | 10     | 2     |
| 1:A:3:GLN:O     | 1:A:4:LYS:C     | 0.49     | 2.55        | 9      | 3     |
| 2:B:57:ASN:CG   | 2:B:61:VAL:HG11 | 0.49     | 2.31        | 6      | 1     |
| 2:B:34:ALA:CB   | 2:B:52:TYR:CE1  | 0.49     | 2.91        | 1      | 1     |
| 2:B:26:VAL:CG1  | 2:B:70:CYS:C    | 0.49     | 2.85        | 2      | 1     |
| 2:B:40:GLN:C    | 2:B:40:GLN:CD   | 0.49     | 2.80        | 8      | 1     |
| 1:A:21:TRP:CZ2  | 2:B:56:LYS:HD3  | 0.49     | 2.42        | 2      | 1     |
| 2:B:57:ASN:ND2  | 2:B:60:ASN:C    | 0.49     | 2.70        | 4      | 1     |
| 2:B:38:ARG:HH21 | 2:B:51:ILE:HG21 | 0.49     | 1.67        | 8      | 1     |
| 1:A:19:GLN:C    | 1:A:22:ILE:HG13 | 0.49     | 2.32        | 1      | 2     |
| 2:B:30:LEU:O    | 2:B:31:LYS:C    | 0.49     | 2.56        | 5      | 9     |
| 2:B:65:LYS:O    | 2:B:65:LYS:CG   | 0.49     | 2.60        | 5      | 1     |
| 2:B:48:SER:O    | 2:B:52:TYR:HB2  | 0.49     | 2.08        | 6      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:32:GLN:O    | 2:B:35:LYS:HB3  | 0.49     | 2.07        | 7      | 1     |
| 2:B:43:HIS:O    | 2:B:44:GLY:O    | 0.49     | 2.29        | 8      | 3     |
| 1:A:19:GLN:O    | 1:A:20:GLN:C    | 0.49     | 2.56        | 2      | 3     |
| 2:B:19:TYR:CZ   | 2:B:64:MET:CE   | 0.49     | 2.89        | 4      | 1     |
| 2:B:43:HIS:CD2  | 2:B:45:PRO:O    | 0.49     | 2.66        | 4      | 2     |
| 2:B:23:GLN:O    | 2:B:26:VAL:N    | 0.49     | 2.46        | 5      | 3     |
| 1:A:8:GLU:CD    | 2:B:21:GLU:CD   | 0.49     | 2.81        | 6      | 1     |
| 2:B:57:ASN:OD1  | 2:B:61:VAL:CB   | 0.49     | 2.60        | 7      | 1     |
| 2:B:65:LYS:CG   | 2:B:65:LYS:O    | 0.49     | 2.60        | 8      | 1     |
| 2:B:39:VAL:O    | 2:B:39:VAL:HG12 | 0.49     | 2.07        | 2      | 1     |
| 2:B:18:LEU:O    | 2:B:19:TYR:C    | 0.49     | 2.55        | 7      | 3     |
| 2:B:55:ALA:HB3  | 2:B:69:THR:O    | 0.49     | 2.06        | 3      | 1     |
| 1:A:15:LEU:HD23 | 1:A:18:CYS:HB2  | 0.49     | 1.84        | 5      | 1     |
| 2:B:57:ASN:H    | 2:B:69:THR:C    | 0.49     | 2.15        | 6      | 1     |
| 1:A:22:ILE:CG2  | 2:B:37:VAL:HG21 | 0.49     | 2.37        | 10     | 1     |
| 2:B:26:VAL:C    | 2:B:28:PRO:CD   | 0.49     | 2.85        | 9      | 3     |
| 2:B:46:PHE:CZ   | 2:B:51:ILE:HG12 | 0.49     | 2.43        | 1      | 1     |
| 2:B:27:CYS:O    | 2:B:31:LYS:CD   | 0.49     | 2.60        | 5      | 1     |
| 2:B:27:CYS:CA   | 2:B:30:LEU:CD2  | 0.49     | 2.90        | 5      | 2     |
| 1:A:9:PHE:CD2   | 2:B:32:GLN:HB3  | 0.49     | 2.42        | 7      | 1     |
| 2:B:46:PHE:C    | 2:B:48:SER:N    | 0.49     | 2.66        | 6      | 1     |
| 1:A:15:LEU:H    | 1:A:15:LEU:CD2  | 0.49     | 2.15        | 7      | 3     |
| 2:B:15:CYS:O    | 2:B:16:ASN:C    | 0.49     | 2.56        | 7      | 7     |
| 1:A:21:TRP:O    | 1:A:25:GLN:HB2  | 0.49     | 2.06        | 7      | 2     |
| 2:B:33:ALA:O    | 2:B:37:VAL:CB   | 0.49     | 2.61        | 3      | 4     |
| 2:B:21:GLU:CB   | 2:B:25:CYS:SG   | 0.49     | 3.01        | 9      | 1     |
| 1:A:1:GLN:CG    | 1:A:1:GLN:O     | 0.48     | 2.60        | 1      | 1     |
| 2:B:57:ASN:ND2  | 2:B:61:VAL:HG21 | 0.48     | 2.22        | 2      | 2     |
| 2:B:52:TYR:O    | 2:B:53:GLN:C    | 0.48     | 2.56        | 8      | 5     |
| 2:B:50:ARG:O    | 2:B:53:GLN:N    | 0.48     | 2.46        | 7      | 1     |
| 1:A:21:TRP:CG   | 1:A:22:ILE:N    | 0.48     | 2.81        | 4      | 4     |
| 2:B:48:SER:O    | 2:B:50:ARG:N    | 0.48     | 2.46        | 8      | 2     |
| 2:B:11:ARG:CZ   | 2:B:12:GLU:OE1  | 0.48     | 2.61        | 8      | 1     |
| 1:A:10:GLN:O    | 1:A:11:GLN:C    | 0.48     | 2.57        | 10     | 7     |
| 1:A:21:TRP:CH2  | 2:B:30:LEU:HD12 | 0.48     | 2.39        | 1      | 1     |
| 2:B:27:CYS:HA   | 2:B:70:CYS:HB3  | 0.48     | 1.85        | 2      | 1     |
| 2:B:30:LEU:HD23 | 2:B:55:ALA:CA   | 0.48     | 2.38        | 2      | 1     |
| 1:A:22:ILE:HG22 | 2:B:37:VAL:HG21 | 0.48     | 1.83        | 5      | 1     |
| 1:A:12:GLU:CG   | 1:A:13:GLN:N    | 0.48     | 2.76        | 9      | 1     |
| 2:B:58:LEU:H    | 2:B:59:PRO:CA   | 0.48     | 2.16        | 9      | 4     |
| 2:B:25:CYS:CB   | 2:B:29:THR:HG23 | 0.48     | 2.35        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:14:HIS:CD2  | 1:A:14:HIS:H    | 0.48     | 2.26        | 6      | 1     |
| 2:B:14:CYS:O    | 2:B:17:GLU:HB3  | 0.48     | 2.09        | 10     | 1     |
| 1:A:19:GLN:O    | 1:A:23:ARG:N    | 0.48     | 2.45        | 8      | 1     |
| 1:A:7:ARG:O     | 1:A:11:GLN:CB   | 0.48     | 2.62        | 6      | 1     |
| 2:B:35:LYS:O    | 2:B:39:VAL:O    | 0.48     | 2.31        | 6      | 1     |
| 1:A:21:TRP:CZ3  | 1:A:22:ILE:HG12 | 0.48     | 2.44        | 2      | 3     |
| 1:A:15:LEU:HD23 | 1:A:18:CYS:CB   | 0.48     | 2.39        | 5      | 1     |
| 1:A:26:LEU:HD22 | 2:B:43:HIS:CE1  | 0.48     | 2.43        | 8      | 1     |
| 1:A:3:GLN:O     | 1:A:7:ARG:N     | 0.48     | 2.45        | 6      | 2     |
| 1:A:22:ILE:O    | 1:A:25:GLN:CB   | 0.48     | 2.62        | 9      | 1     |
| 1:A:25:GLN:OE1  | 2:B:54:ILE:HD11 | 0.48     | 2.09        | 10     | 1     |
| 2:B:28:PRO:O    | 2:B:31:LYS:HG2  | 0.48     | 2.09        | 2      | 1     |
| 1:A:25:GLN:CD   | 2:B:51:ILE:CD1  | 0.48     | 2.87        | 7      | 1     |
| 1:A:19:GLN:N    | 1:A:22:ILE:HD12 | 0.48     | 2.24        | 10     | 1     |
| 1:A:7:ARG:O     | 1:A:8:GLU:C     | 0.47     | 2.57        | 7      | 8     |
| 1:A:21:TRP:HE3  | 2:B:58:LEU:CD2  | 0.47     | 2.19        | 1      | 2     |
| 1:A:18:CYS:O    | 1:A:21:TRP:CB   | 0.47     | 2.62        | 5      | 2     |
| 1:A:21:TRP:CA   | 2:B:58:LEU:HD21 | 0.47     | 2.39        | 9      | 1     |
| 1:A:15:LEU:CD2  | 1:A:18:CYS:SG   | 0.47     | 3.02        | 5      | 1     |
| 1:A:15:LEU:N    | 1:A:15:LEU:CD1  | 0.47     | 2.74        | 8      | 1     |
| 1:A:17:ALA:O    | 1:A:19:GLN:N    | 0.47     | 2.47        | 8      | 1     |
| 2:B:38:ARG:NH1  | 2:B:46:PHE:CZ   | 0.47     | 2.82        | 8      | 1     |
| 2:B:19:TYR:OH   | 2:B:67:ILE:CD1  | 0.47     | 2.62        | 10     | 1     |
| 2:B:48:SER:O    | 2:B:52:TYR:HB3  | 0.47     | 2.09        | 2      | 1     |
| 2:B:43:HIS:O    | 2:B:46:PHE:CD1  | 0.47     | 2.66        | 3      | 1     |
| 2:B:36:SER:O    | 2:B:37:VAL:O    | 0.47     | 2.31        | 5      | 1     |
| 1:A:8:GLU:OE2   | 2:B:21:GLU:CD   | 0.47     | 2.58        | 6      | 1     |
| 2:B:23:GLN:N    | 2:B:23:GLN:CD   | 0.47     | 2.71        | 7      | 1     |
| 2:B:31:LYS:O    | 2:B:52:TYR:CE1  | 0.47     | 2.67        | 9      | 1     |
| 2:B:62:CYS:O    | 2:B:63:ASN:C    | 0.47     | 2.57        | 2      | 1     |
| 1:A:22:ILE:O    | 1:A:23:ARG:C    | 0.47     | 2.58        | 9      | 3     |
| 2:B:43:HIS:CD2  | 2:B:46:PHE:CD2  | 0.47     | 3.01        | 8      | 1     |
| 2:B:59:PRO:O    | 2:B:60:ASN:CG   | 0.47     | 2.57        | 9      | 9     |
| 1:A:15:LEU:CD1  | 1:A:15:LEU:H    | 0.47     | 2.19        | 3      | 2     |
| 2:B:57:ASN:ND2  | 2:B:69:THR:CB   | 0.47     | 2.78        | 8      | 1     |
| 2:B:19:TYR:O    | 2:B:20:GLN:C    | 0.47     | 2.58        | 9      | 5     |
| 2:B:56:LYS:HA   | 2:B:69:THR:CG2  | 0.47     | 2.39        | 1      | 2     |
| 1:A:9:PHE:CD1   | 1:A:14:HIS:NE2  | 0.47     | 2.83        | 2      | 1     |
| 2:B:15:CYS:SG   | 2:B:61:VAL:O    | 0.47     | 2.72        | 2      | 1     |
| 1:A:23:ARG:O    | 1:A:24:GLN:C    | 0.47     | 2.57        | 2      | 3     |
| 1:A:21:TRP:CZ2  | 2:B:56:LYS:CB   | 0.47     | 2.98        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:CYS:O     | 1:A:6:GLN:C     | 0.47     | 2.57        | 9      | 3     |
| 1:A:8:GLU:O     | 1:A:9:PHE:C     | 0.47     | 2.56        | 9      | 3     |
| 2:B:22:ASP:C    | 2:B:26:VAL:HG23 | 0.47     | 2.34        | 9      | 1     |
| 2:B:21:GLU:OE2  | 2:B:22:ASP:CG   | 0.47     | 2.58        | 1      | 1     |
| 2:B:26:VAL:CA   | 2:B:28:PRO:HD2  | 0.47     | 2.40        | 4      | 3     |
| 1:A:6:GLN:OE1   | 2:B:32:GLN:NE2  | 0.47     | 2.48        | 5      | 1     |
| 1:A:21:TRP:CD1  | 1:A:25:GLN:HB2  | 0.47     | 2.45        | 6      | 1     |
| 2:B:27:CYS:HA   | 2:B:70:CYS:CB   | 0.47     | 2.37        | 7      | 1     |
| 2:B:30:LEU:CB   | 2:B:70:CYS:HB2  | 0.47     | 2.38        | 9      | 1     |
| 2:B:23:GLN:HA   | 2:B:26:VAL:CB   | 0.47     | 2.39        | 2      | 1     |
| 2:B:61:VAL:HG12 | 2:B:62:CYS:H    | 0.47     | 1.65        | 8      | 4     |
| 2:B:53:GLN:O    | 2:B:55:ALA:O    | 0.47     | 2.33        | 7      | 2     |
| 2:B:26:VAL:CB   | 2:B:28:PRO:HD3  | 0.47     | 2.40        | 10     | 1     |
| 1:A:21:TRP:CZ2  | 2:B:56:LYS:C    | 0.47     | 2.92        | 6      | 1     |
| 2:B:57:ASN:CG   | 2:B:69:THR:HA   | 0.46     | 2.35        | 2      | 1     |
| 2:B:62:CYS:C    | 2:B:64:MET:N    | 0.46     | 2.72        | 2      | 1     |
| 1:A:8:GLU:O     | 1:A:11:GLN:HG2  | 0.46     | 2.10        | 5      | 1     |
| 2:B:15:CYS:HA   | 2:B:18:LEU:HD21 | 0.46     | 1.87        | 5      | 1     |
| 2:B:24:VAL:C    | 2:B:26:VAL:H    | 0.46     | 2.18        | 6      | 1     |
| 1:A:21:TRP:CG   | 2:B:61:VAL:HG21 | 0.46     | 2.41        | 9      | 1     |
| 1:A:24:GLN:CG   | 2:B:58:LEU:HD13 | 0.46     | 2.41        | 9      | 1     |
| 1:A:19:GLN:O    | 1:A:23:ARG:HB3  | 0.46     | 2.10        | 6      | 3     |
| 1:A:21:TRP:HB3  | 2:B:58:LEU:HD22 | 0.46     | 1.85        | 1      | 2     |
| 1:A:26:LEU:HD11 | 2:B:37:VAL:CG1  | 0.46     | 2.40        | 2      | 1     |
| 2:B:26:VAL:C    | 2:B:70:CYS:HB3  | 0.46     | 2.35        | 2      | 1     |
| 2:B:35:LYS:HE2  | 2:B:46:PHE:CD2  | 0.46     | 2.44        | 5      | 1     |
| 2:B:15:CYS:HB2  | 2:B:61:VAL:CG1  | 0.46     | 2.39        | 9      | 1     |
| 1:A:22:ILE:O    | 1:A:22:ILE:CD1  | 0.46     | 2.54        | 6      | 1     |
| 2:B:31:LYS:HA   | 2:B:52:TYR:CZ   | 0.46     | 2.45        | 6      | 1     |
| 1:A:4:LYS:O     | 1:A:8:GLU:CD    | 0.46     | 2.59        | 9      | 1     |
| 2:B:48:SER:HB3  | 2:B:52:TYR:CZ   | 0.46     | 2.44        | 10     | 1     |
| 1:A:26:LEU:HD11 | 2:B:37:VAL:O    | 0.46     | 2.10        | 2      | 1     |
| 1:A:5:CYS:O     | 1:A:8:GLU:N     | 0.46     | 2.48        | 9      | 2     |
| 1:A:12:GLU:O    | 1:A:13:GLN:CG   | 0.46     | 2.63        | 8      | 3     |
| 2:B:55:ALA:CB   | 2:B:69:THR:HG23 | 0.46     | 2.29        | 8      | 1     |
| 1:A:25:GLN:O    | 1:A:26:LEU:C    | 0.46     | 2.59        | 1      | 2     |
| 2:B:17:GLU:O    | 2:B:17:GLU:OE1  | 0.46     | 2.34        | 10     | 1     |
| 1:A:9:PHE:CE1   | 1:A:14:HIS:ND1  | 0.46     | 2.83        | 2      | 1     |
| 2:B:31:LYS:O    | 2:B:52:TYR:OH   | 0.46     | 2.18        | 3      | 2     |
| 2:B:48:SER:CB   | 2:B:52:TYR:CD1  | 0.46     | 2.99        | 3      | 1     |
| 2:B:52:TYR:HA   | 2:B:56:LYS:NZ   | 0.46     | 2.25        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:38:ARG:HG2  | 2:B:39:VAL:N    | 0.46     | 2.26        | 4      | 1     |
| 2:B:62:CYS:SG   | 2:B:67:ILE:HG21 | 0.46     | 2.51        | 3      | 1     |
| 2:B:58:LEU:CB   | 2:B:59:PRO:CA   | 0.46     | 2.94        | 5      | 1     |
| 2:B:25:CYS:C    | 2:B:28:PRO:CD   | 0.46     | 2.89        | 8      | 1     |
| 2:B:26:VAL:H    | 2:B:28:PRO:HD2  | 0.46     | 1.70        | 1      | 1     |
| 2:B:57:ASN:ND2  | 2:B:60:ASN:N    | 0.46     | 2.64        | 4      | 1     |
| 2:B:49:THR:HA   | 2:B:52:TYR:CD2  | 0.46     | 2.45        | 5      | 1     |
| 2:B:17:GLU:CD   | 2:B:17:GLU:C    | 0.46     | 2.84        | 6      | 1     |
| 1:A:8:GLU:O     | 1:A:12:GLU:HG2  | 0.46     | 2.10        | 9      | 1     |
| 1:A:18:CYS:O    | 1:A:22:ILE:HG23 | 0.46     | 2.10        | 1      | 2     |
| 2:B:62:CYS:HB2  | 2:B:64:MET:HE3  | 0.46     | 1.88        | 1      | 1     |
| 1:A:23:ARG:HA   | 2:B:37:VAL:CG1  | 0.46     | 2.41        | 3      | 1     |
| 2:B:54:ILE:O    | 2:B:55:ALA:CB   | 0.46     | 2.63        | 3      | 1     |
| 2:B:58:LEU:CG   | 2:B:61:VAL:HG23 | 0.46     | 2.35        | 10     | 2     |
| 2:B:32:GLN:O    | 2:B:33:ALA:C    | 0.46     | 2.58        | 9      | 2     |
| 2:B:58:LEU:HB3  | 2:B:59:PRO:O    | 0.46     | 2.11        | 5      | 3     |
| 2:B:62:CYS:HB2  | 2:B:64:MET:CE   | 0.45     | 2.41        | 2      | 1     |
| 1:A:5:CYS:SG    | 2:B:24:VAL:C    | 0.45     | 2.99        | 4      | 1     |
| 2:B:10:LEU:O    | 2:B:13:GLN:N    | 0.45     | 2.49        | 4      | 1     |
| 1:A:21:TRP:HE3  | 2:B:58:LEU:HD23 | 0.45     | 1.66        | 6      | 1     |
| 1:A:19:GLN:HG3  | 1:A:20:GLN:N    | 0.45     | 2.24        | 7      | 1     |
| 2:B:46:PHE:CZ   | 2:B:51:ILE:CD1  | 0.45     | 3.00        | 1      | 1     |
| 1:A:21:TRP:CE3  | 1:A:22:ILE:CA   | 0.45     | 2.98        | 5      | 1     |
| 2:B:30:LEU:HB3  | 2:B:70:CYS:C    | 0.45     | 2.35        | 1      | 1     |
| 2:B:30:LEU:HB2  | 2:B:70:CYS:HB3  | 0.45     | 1.82        | 1      | 1     |
| 2:B:67:ILE:HG22 | 2:B:68:GLY:H    | 0.45     | 1.70        | 2      | 3     |
| 1:A:21:TRP:HH2  | 2:B:70:CYS:C    | 0.45     | 2.19        | 6      | 1     |
| 2:B:31:LYS:HG2  | 2:B:52:TYR:CG   | 0.45     | 2.47        | 6      | 1     |
| 2:B:39:VAL:CG2  | 2:B:43:HIS:CD2  | 0.45     | 2.94        | 6      | 1     |
| 1:A:16:ARG:O    | 1:A:19:GLN:HG2  | 0.45     | 2.12        | 10     | 1     |
| 2:B:17:GLU:O    | 2:B:21:GLU:HB2  | 0.45     | 2.11        | 10     | 1     |
| 2:B:34:ALA:HB3  | 2:B:52:TYR:CZ   | 0.45     | 2.46        | 10     | 1     |
| 2:B:19:TYR:CE1  | 2:B:64:MET:SD   | 0.45     | 3.10        | 8      | 3     |
| 1:A:21:TRP:CH2  | 2:B:30:LEU:CD2  | 0.45     | 3.00        | 10     | 1     |
| 2:B:48:SER:OG   | 2:B:56:LYS:NZ   | 0.45     | 2.50        | 2      | 1     |
| 2:B:27:CYS:O    | 2:B:30:LEU:HD22 | 0.45     | 2.10        | 6      | 2     |
| 2:B:13:GLN:O    | 2:B:17:GLU:N    | 0.45     | 2.46        | 5      | 2     |
| 2:B:23:GLN:HA   | 2:B:26:VAL:HG23 | 0.45     | 1.89        | 5      | 1     |
| 1:A:1:GLN:N     | 1:A:1:GLN:CD    | 0.45     | 2.75        | 6      | 1     |
| 2:B:20:GLN:C    | 2:B:20:GLN:OE1  | 0.45     | 2.60        | 4      | 1     |
| 2:B:59:PRO:O    | 2:B:60:ASN:ND2  | 0.45     | 2.49        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:34:ALA:O    | 2:B:37:VAL:HG12 | 0.45     | 2.12        | 9      | 1     |
| 1:A:6:GLN:O     | 1:A:9:PHE:HB2   | 0.45     | 2.12        | 7      | 1     |
| 2:B:32:GLN:O    | 2:B:35:LYS:CB   | 0.45     | 2.65        | 9      | 1     |
| 1:A:21:TRP:CD1  | 1:A:25:GLN:HG2  | 0.45     | 2.47        | 2      | 1     |
| 2:B:57:ASN:ND2  | 2:B:61:VAL:HG11 | 0.45     | 2.26        | 3      | 1     |
| 2:B:23:GLN:O    | 2:B:26:VAL:HB   | 0.45     | 2.12        | 5      | 1     |
| 2:B:63:ASN:O    | 2:B:63:ASN:ND2  | 0.44     | 2.50        | 1      | 1     |
| 2:B:61:VAL:HG12 | 2:B:64:MET:HE3  | 0.44     | 1.88        | 2      | 1     |
| 2:B:18:LEU:O    | 2:B:20:GLN:N    | 0.44     | 2.50        | 7      | 1     |
| 2:B:38:ARG:HA   | 2:B:38:ARG:NE   | 0.44     | 2.26        | 9      | 1     |
| 1:A:5:CYS:SG    | 2:B:24:VAL:HG23 | 0.44     | 2.52        | 3      | 1     |
| 2:B:58:LEU:HB3  | 2:B:60:ASN:HB2  | 0.44     | 1.89        | 4      | 2     |
| 2:B:25:CYS:HB3  | 2:B:29:THR:OG1  | 0.44     | 2.12        | 6      | 1     |
| 2:B:44:GLY:H    | 2:B:45:PRO:HD3  | 0.44     | 1.69        | 9      | 1     |
| 2:B:16:ASN:O    | 2:B:20:GLN:HB2  | 0.44     | 2.12        | 1      | 1     |
| 2:B:47:GLN:O    | 2:B:48:SER:C    | 0.44     | 2.59        | 9      | 2     |
| 2:B:24:VAL:HG12 | 2:B:25:CYS:SG   | 0.44     | 2.51        | 2      | 1     |
| 2:B:24:VAL:O    | 2:B:28:PRO:HG2  | 0.44     | 2.12        | 4      | 1     |
| 2:B:51:ILE:HD12 | 2:B:54:ILE:HB   | 0.44     | 1.87        | 5      | 1     |
| 2:B:51:ILE:O    | 2:B:54:ILE:HG12 | 0.44     | 2.12        | 6      | 1     |
| 2:B:62:CYS:SG   | 2:B:64:MET:SD   | 0.44     | 3.16        | 8      | 1     |
| 1:A:15:LEU:HB2  | 1:A:18:CYS:SG   | 0.44     | 2.52        | 8      | 1     |
| 2:B:10:LEU:O    | 2:B:11:ARG:C    | 0.44     | 2.60        | 1      | 4     |
| 2:B:46:PHE:CZ   | 2:B:51:ILE:HD13 | 0.44     | 2.48        | 1      | 1     |
| 1:A:9:PHE:CE1   | 1:A:14:HIS:CE1  | 0.44     | 3.05        | 2      | 1     |
| 2:B:38:ARG:CD   | 2:B:39:VAL:N    | 0.44     | 2.81        | 7      | 1     |
| 2:B:19:TYR:OH   | 2:B:64:MET:SD   | 0.44     | 2.74        | 8      | 2     |
| 2:B:47:GLN:O    | 2:B:50:ARG:N    | 0.44     | 2.50        | 1      | 1     |
| 1:A:19:GLN:C    | 1:A:22:ILE:HG22 | 0.44     | 2.37        | 6      | 1     |
| 1:A:5:CYS:SG    | 2:B:24:VAL:HG13 | 0.44     | 2.53        | 8      | 1     |
| 1:A:26:LEU:CD1  | 2:B:37:VAL:O    | 0.44     | 2.66        | 2      | 1     |
| 2:B:57:ASN:ND2  | 2:B:61:VAL:CB   | 0.44     | 2.71        | 5      | 2     |
| 2:B:29:THR:C    | 2:B:31:LYS:N    | 0.44     | 2.76        | 6      | 2     |
| 2:B:18:LEU:CD2  | 2:B:69:THR:CG2  | 0.44     | 2.93        | 7      | 1     |
| 2:B:60:ASN:N    | 2:B:63:ASN:OD1  | 0.44     | 2.50        | 9      | 1     |
| 2:B:50:ARG:C    | 2:B:52:TYR:N    | 0.44     | 2.76        | 10     | 3     |
| 1:A:8:GLU:CD    | 1:A:11:GLN:OE1  | 0.44     | 2.61        | 2      | 1     |
| 2:B:51:ILE:O    | 2:B:53:GLN:N    | 0.44     | 2.50        | 6      | 2     |
| 2:B:46:PHE:C    | 2:B:48:SER:H    | 0.44     | 2.19        | 6      | 1     |
| 1:A:21:TRP:CB   | 2:B:58:LEU:CD2  | 0.44     | 2.95        | 4      | 2     |
| 2:B:35:LYS:HA   | 2:B:39:VAL:CG2  | 0.44     | 2.42        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:30:LEU:O    | 2:B:33:ALA:CB   | 0.43     | 2.65        | 10     | 2     |
| 2:B:55:ALA:O    | 2:B:56:LYS:HB3  | 0.43     | 2.13        | 3      | 2     |
| 2:B:13:GLN:HA   | 2:B:16:ASN:HB2  | 0.43     | 1.89        | 3      | 1     |
| 2:B:51:ILE:C    | 2:B:53:GLN:N    | 0.43     | 2.76        | 3      | 2     |
| 2:B:34:ALA:C    | 2:B:36:SER:N    | 0.43     | 2.75        | 8      | 2     |
| 1:A:7:ARG:O     | 1:A:11:GLN:HB3  | 0.43     | 2.13        | 7      | 1     |
| 2:B:27:CYS:HA   | 2:B:70:CYS:HB2  | 0.43     | 1.89        | 7      | 1     |
| 1:A:26:LEU:O    | 1:A:27:ALA:C    | 0.43     | 2.61        | 8      | 2     |
| 2:B:25:CYS:SG   | 2:B:29:THR:HG23 | 0.43     | 2.52        | 10     | 1     |
| 1:A:19:GLN:HA   | 1:A:22:ILE:HG22 | 0.43     | 1.90        | 2      | 1     |
| 2:B:18:LEU:CD1  | 2:B:23:GLN:HG3  | 0.43     | 2.43        | 2      | 1     |
| 2:B:35:LYS:HG3  | 2:B:39:VAL:HG21 | 0.43     | 1.89        | 5      | 1     |
| 2:B:11:ARG:O    | 2:B:14:CYS:N    | 0.43     | 2.50        | 6      | 1     |
| 1:A:25:GLN:OE1  | 2:B:51:ILE:CD1  | 0.43     | 2.65        | 7      | 1     |
| 2:B:30:LEU:CG   | 2:B:70:CYS:HB2  | 0.43     | 2.43        | 9      | 2     |
| 2:B:31:LYS:HG2  | 2:B:52:TYR:CB   | 0.43     | 2.43        | 6      | 1     |
| 2:B:57:ASN:OD1  | 2:B:61:VAL:HG21 | 0.43     | 2.12        | 6      | 1     |
| 2:B:62:CYS:C    | 2:B:63:ASN:ND2  | 0.43     | 2.76        | 8      | 1     |
| 2:B:33:ALA:HB1  | 2:B:37:VAL:HG21 | 0.43     | 1.90        | 3      | 1     |
| 2:B:46:PHE:O    | 2:B:49:THR:HB   | 0.43     | 2.12        | 6      | 1     |
| 2:B:48:SER:C    | 2:B:50:ARG:N    | 0.43     | 2.73        | 8      | 2     |
| 1:A:18:CYS:O    | 1:A:22:ILE:HG13 | 0.43     | 2.13        | 10     | 1     |
| 2:B:26:VAL:O    | 2:B:70:CYS:HB3  | 0.43     | 2.13        | 2      | 1     |
| 2:B:55:ALA:CB   | 2:B:70:CYS:SG   | 0.43     | 3.06        | 2      | 1     |
| 1:A:5:CYS:SG    | 2:B:24:VAL:HB   | 0.43     | 2.53        | 3      | 1     |
| 1:A:5:CYS:SG    | 2:B:24:VAL:CG1  | 0.43     | 3.07        | 8      | 1     |
| 1:A:20:GLN:O    | 1:A:24:GLN:HB3  | 0.43     | 2.13        | 8      | 1     |
| 2:B:57:ASN:HA   | 2:B:69:THR:OG1  | 0.43     | 2.13        | 8      | 1     |
| 1:A:18:CYS:SG   | 2:B:61:VAL:CG2  | 0.43     | 3.05        | 10     | 1     |
| 2:B:20:GLN:O    | 2:B:21:GLU:O    | 0.43     | 2.36        | 4      | 2     |
| 2:B:52:TYR:O    | 2:B:55:ALA:CB   | 0.43     | 2.66        | 5      | 1     |
| 1:A:9:PHE:CZ    | 1:A:14:HIS:ND1  | 0.43     | 2.87        | 2      | 1     |
| 1:A:23:ARG:C    | 1:A:25:GLN:N    | 0.43     | 2.74        | 2      | 1     |
| 2:B:27:CYS:C    | 2:B:30:LEU:HD21 | 0.43     | 2.35        | 6      | 1     |
| 2:B:35:LYS:O    | 2:B:39:VAL:C    | 0.43     | 2.61        | 6      | 1     |
| 1:A:17:ALA:O    | 1:A:18:CYS:C    | 0.43     | 2.60        | 8      | 1     |
| 1:A:26:LEU:HD11 | 2:B:37:VAL:HG12 | 0.43     | 1.91        | 2      | 1     |
| 1:A:9:PHE:CG    | 1:A:10:GLN:N    | 0.43     | 2.86        | 3      | 1     |
| 2:B:15:CYS:CB   | 2:B:61:VAL:O    | 0.43     | 2.67        | 3      | 1     |
| 1:A:24:GLN:C    | 1:A:24:GLN:OE1  | 0.43     | 2.61        | 5      | 1     |
| 2:B:27:CYS:SG   | 2:B:69:THR:N    | 0.43     | 2.92        | 9      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:15:CYS:C    | 2:B:17:GLU:N    | 0.43     | 2.75        | 3      | 3     |
| 2:B:50:ARG:O    | 2:B:54:ILE:HG13 | 0.43     | 2.14        | 7      | 1     |
| 1:A:24:GLN:CB   | 2:B:58:LEU:HD13 | 0.43     | 2.42        | 9      | 1     |
| 2:B:21:GLU:HB3  | 2:B:25:CYS:SG   | 0.43     | 2.53        | 9      | 1     |
| 2:B:34:ALA:HA   | 2:B:37:VAL:CG1  | 0.43     | 2.44        | 9      | 1     |
| 1:A:22:ILE:HG23 | 2:B:33:ALA:CB   | 0.43     | 2.44        | 10     | 1     |
| 2:B:38:ARG:CG   | 2:B:39:VAL:N    | 0.43     | 2.81        | 10     | 1     |
| 2:B:57:ASN:O    | 2:B:61:VAL:N    | 0.43     | 2.52        | 4      | 1     |
| 2:B:31:LYS:HG2  | 2:B:52:TYR:CD2  | 0.43     | 2.49        | 6      | 1     |
| 1:A:16:ARG:O    | 1:A:19:GLN:HG3  | 0.43     | 2.14        | 7      | 1     |
| 2:B:19:TYR:OH   | 2:B:67:ILE:HD12 | 0.43     | 2.13        | 10     | 1     |
| 2:B:29:THR:C    | 2:B:30:LEU:HD22 | 0.42     | 2.38        | 1      | 1     |
| 1:A:5:CYS:SG    | 2:B:25:CYS:N    | 0.42     | 2.92        | 4      | 1     |
| 1:A:21:TRP:C    | 2:B:58:LEU:HD21 | 0.42     | 2.38        | 8      | 3     |
| 2:B:24:VAL:O    | 2:B:25:CYS:O    | 0.42     | 2.37        | 10     | 1     |
| 2:B:16:ASN:O    | 2:B:20:GLN:CB   | 0.42     | 2.67        | 1      | 1     |
| 2:B:26:VAL:CA   | 2:B:29:THR:OG1  | 0.42     | 2.68        | 2      | 2     |
| 2:B:56:LYS:HB2  | 2:B:69:THR:HB   | 0.42     | 1.91        | 4      | 1     |
| 1:A:9:PHE:CZ    | 2:B:33:ALA:CB   | 0.42     | 3.00        | 6      | 1     |
| 2:B:34:ALA:HA   | 2:B:37:VAL:CB   | 0.42     | 2.44        | 9      | 1     |
| 2:B:34:ALA:HB3  | 2:B:52:TYR:CD1  | 0.42     | 2.48        | 1      | 1     |
| 2:B:60:ASN:C    | 2:B:62:CYS:N    | 0.42     | 2.76        | 1      | 1     |
| 2:B:31:LYS:HA   | 2:B:52:TYR:CE1  | 0.42     | 2.50        | 2      | 1     |
| 2:B:46:PHE:O    | 2:B:48:SER:N    | 0.42     | 2.53        | 6      | 1     |
| 1:A:1:GLN:H2    | 1:A:2:PRO:HD3   | 0.42     | 1.74        | 7      | 1     |
| 1:A:24:GLN:OE1  | 2:B:60:ASN:CG   | 0.42     | 2.63        | 8      | 1     |
| 2:B:31:LYS:O    | 2:B:35:LYS:CB   | 0.42     | 2.67        | 10     | 1     |
| 1:A:7:ARG:C     | 1:A:9:PHE:N     | 0.42     | 2.78        | 7      | 1     |
| 2:B:18:LEU:C    | 2:B:20:GLN:N    | 0.42     | 2.76        | 7      | 1     |
| 1:A:1:GLN:OE1   | 1:A:1:GLN:N     | 0.42     | 2.50        | 8      | 1     |
| 2:B:48:SER:CB   | 2:B:52:TYR:CE1  | 0.42     | 3.03        | 9      | 2     |
| 2:B:12:GLU:O    | 2:B:16:ASN:N    | 0.42     | 2.46        | 8      | 3     |
| 2:B:35:LYS:NZ   | 2:B:46:PHE:CD2  | 0.42     | 2.87        | 5      | 1     |
| 2:B:50:ARG:O    | 2:B:54:ILE:N    | 0.42     | 2.52        | 7      | 1     |
| 1:A:21:TRP:CD1  | 2:B:61:VAL:HG22 | 0.42     | 2.49        | 8      | 1     |
| 2:B:15:CYS:CB   | 2:B:62:CYS:HA   | 0.42     | 2.44        | 10     | 1     |
| 2:B:11:ARG:O    | 2:B:12:GLU:C    | 0.42     | 2.62        | 7      | 3     |
| 2:B:57:ASN:ND2  | 2:B:63:ASN:H    | 0.42     | 2.12        | 4      | 1     |
| 1:A:1:GLN:CD    | 1:A:1:GLN:H3    | 0.42     | 2.22        | 6      | 1     |
| 2:B:31:LYS:HA   | 2:B:52:TYR:CG   | 0.42     | 2.49        | 6      | 1     |
| 1:A:22:ILE:HG21 | 2:B:37:VAL:CG2  | 0.42     | 2.45        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:62:CYS:O    | 2:B:64:MET:N    | 0.42     | 2.52        | 2      | 1     |
| 2:B:55:ALA:C    | 2:B:56:LYS:HD3  | 0.42     | 2.40        | 3      | 1     |
| 2:B:64:MET:HE2  | 2:B:64:MET:HB3  | 0.42     | 1.74        | 7      | 1     |
| 2:B:51:ILE:O    | 2:B:54:ILE:CG2  | 0.42     | 2.66        | 10     | 1     |
| 2:B:23:GLN:CA   | 2:B:26:VAL:HB   | 0.42     | 2.44        | 2      | 1     |
| 2:B:30:LEU:C    | 2:B:32:GLN:N    | 0.42     | 2.76        | 4      | 1     |
| 2:B:65:LYS:O    | 2:B:65:LYS:HG3  | 0.42     | 2.13        | 5      | 1     |
| 2:B:57:ASN:CG   | 2:B:69:THR:HB   | 0.42     | 2.39        | 8      | 2     |
| 2:B:58:LEU:CG   | 2:B:60:ASN:HB2  | 0.42     | 2.45        | 8      | 1     |
| 2:B:24:VAL:CG2  | 2:B:25:CYS:SG   | 0.42     | 3.08        | 9      | 1     |
| 1:A:16:ARG:O    | 1:A:19:GLN:HB3  | 0.42     | 2.13        | 4      | 1     |
| 2:B:15:CYS:O    | 2:B:19:TYR:HB2  | 0.42     | 2.15        | 5      | 1     |
| 2:B:43:HIS:NE2  | 2:B:46:PHE:CE2  | 0.42     | 2.88        | 8      | 1     |
| 2:B:57:ASN:HA   | 2:B:57:ASN:HD22 | 0.42     | 1.41        | 8      | 1     |
| 2:B:21:GLU:HG2  | 2:B:24:VAL:HG21 | 0.42     | 1.90        | 9      | 1     |
| 1:A:16:ARG:O    | 1:A:19:GLN:HB2  | 0.42     | 2.15        | 6      | 3     |
| 2:B:26:VAL:CG1  | 2:B:68:GLY:CA   | 0.42     | 2.97        | 4      | 1     |
| 2:B:30:LEU:HB2  | 2:B:70:CYS:O    | 0.42     | 2.11        | 4      | 1     |
| 2:B:57:ASN:N    | 2:B:70:CYS:N    | 0.42     | 2.68        | 6      | 1     |
| 2:B:30:LEU:H    | 2:B:30:LEU:CD1  | 0.42     | 2.27        | 9      | 1     |
| 1:A:6:GLN:HA    | 2:B:32:GLN:NE2  | 0.42     | 2.30        | 10     | 1     |
| 2:B:15:CYS:HB2  | 2:B:61:VAL:C    | 0.41     | 2.39        | 3      | 1     |
| 2:B:63:ASN:O    | 2:B:63:ASN:CG   | 0.41     | 2.63        | 3      | 1     |
| 2:B:36:SER:O    | 2:B:39:VAL:HG23 | 0.41     | 2.14        | 4      | 1     |
| 2:B:58:LEU:CD1  | 2:B:60:ASN:CB   | 0.41     | 2.94        | 4      | 1     |
| 1:A:16:ARG:HA   | 1:A:19:GLN:CG   | 0.41     | 2.46        | 2      | 1     |
| 2:B:12:GLU:HG2  | 2:B:16:ASN:ND2  | 0.41     | 2.29        | 3      | 1     |
| 2:B:26:VAL:HG13 | 2:B:70:CYS:O    | 0.41     | 2.15        | 5      | 1     |
| 2:B:35:LYS:CD   | 2:B:52:TYR:OH   | 0.41     | 2.68        | 5      | 1     |
| 1:A:8:GLU:C     | 1:A:10:GLN:N    | 0.41     | 2.75        | 6      | 1     |
| 2:B:46:PHE:O    | 2:B:49:THR:N    | 0.41     | 2.51        | 6      | 1     |
| 2:B:46:PHE:O    | 2:B:47:GLN:CG   | 0.41     | 2.68        | 7      | 1     |
| 2:B:38:ARG:NE   | 2:B:48:SER:HB3  | 0.41     | 2.31        | 8      | 1     |
| 1:A:11:GLN:HG3  | 1:A:12:GLU:N    | 0.41     | 2.30        | 3      | 1     |
| 2:B:19:TYR:OH   | 2:B:64:MET:HE3  | 0.41     | 2.14        | 3      | 1     |
| 2:B:33:ALA:O    | 2:B:35:LYS:N    | 0.41     | 2.53        | 3      | 1     |
| 1:A:9:PHE:CE2   | 2:B:29:THR:HG22 | 0.41     | 2.51        | 5      | 1     |
| 2:B:51:ILE:O    | 2:B:54:ILE:HG13 | 0.41     | 2.15        | 10     | 1     |
| 1:A:21:TRP:CD2  | 2:B:58:LEU:HA   | 0.41     | 2.50        | 2      | 1     |
| 2:B:42:GLN:O    | 2:B:42:GLN:NE2  | 0.41     | 2.54        | 2      | 1     |
| 2:B:33:ALA:C    | 2:B:35:LYS:N    | 0.41     | 2.77        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:25:CYS:HB3  | 2:B:29:THR:CG2  | 0.41     | 2.45        | 6      | 1     |
| 2:B:58:LEU:HG   | 2:B:61:VAL:H    | 0.41     | 1.75        | 10     | 2     |
| 2:B:27:CYS:O    | 2:B:30:LEU:HD23 | 0.41     | 2.15        | 8      | 1     |
| 2:B:26:VAL:O    | 2:B:70:CYS:SG   | 0.41     | 2.78        | 10     | 1     |
| 1:A:6:GLN:O     | 1:A:7:ARG:C     | 0.41     | 2.62        | 6      | 1     |
| 1:A:25:GLN:NE2  | 2:B:54:ILE:CD1  | 0.41     | 2.83        | 1      | 1     |
| 2:B:18:LEU:CD1  | 2:B:19:TYR:N    | 0.41     | 2.80        | 1      | 1     |
| 2:B:21:GLU:OE2  | 2:B:22:ASP:OD2  | 0.41     | 2.37        | 1      | 1     |
| 1:A:23:ARG:O    | 1:A:25:GLN:N    | 0.41     | 2.53        | 2      | 1     |
| 2:B:30:LEU:HD22 | 2:B:30:LEU:C    | 0.41     | 2.41        | 3      | 1     |
| 1:A:19:GLN:HA   | 1:A:22:ILE:HG21 | 0.41     | 1.83        | 6      | 1     |
| 1:A:26:LEU:HD12 | 2:B:38:ARG:CB   | 0.41     | 2.41        | 3      | 1     |
| 2:B:26:VAL:CG1  | 2:B:68:GLY:HA3  | 0.41     | 2.46        | 4      | 1     |
| 2:B:64:MET:CB   | 2:B:67:ILE:HD11 | 0.41     | 2.45        | 4      | 1     |
| 2:B:22:ASP:O    | 2:B:23:GLN:C    | 0.41     | 2.64        | 1      | 1     |
| 2:B:42:GLN:C    | 2:B:44:GLY:N    | 0.41     | 2.77        | 3      | 1     |
| 2:B:61:VAL:CG1  | 2:B:69:THR:HG22 | 0.41     | 2.45        | 7      | 1     |
| 2:B:48:SER:HA   | 2:B:51:ILE:HG22 | 0.41     | 1.92        | 8      | 1     |
| 2:B:54:ILE:CG2  | 2:B:55:ALA:N    | 0.41     | 2.66        | 8      | 1     |
| 1:A:18:CYS:CB   | 1:A:22:ILE:CG2  | 0.41     | 2.99        | 1      | 1     |
| 2:B:50:ARG:O    | 2:B:52:TYR:N    | 0.41     | 2.54        | 7      | 2     |
| 2:B:23:GLN:O    | 2:B:23:GLN:CD   | 0.41     | 2.63        | 3      | 1     |
| 2:B:48:SER:O    | 2:B:51:ILE:N    | 0.41     | 2.53        | 3      | 1     |
| 2:B:66:GLN:O    | 2:B:66:GLN:OE1  | 0.41     | 2.38        | 3      | 1     |
| 1:A:8:GLU:O     | 1:A:10:GLN:N    | 0.41     | 2.54        | 6      | 1     |
| 1:A:8:GLU:CD    | 2:B:21:GLU:CG   | 0.41     | 2.93        | 6      | 1     |
| 1:A:21:TRP:CH2  | 2:B:57:ASN:HA   | 0.41     | 2.51        | 6      | 1     |
| 1:A:15:LEU:CD1  | 1:A:15:LEU:N    | 0.41     | 2.78        | 7      | 1     |
| 2:B:66:GLN:CG   | 2:B:67:ILE:N    | 0.41     | 2.83        | 7      | 1     |
| 2:B:31:LYS:HG3  | 2:B:52:TYR:CE1  | 0.41     | 2.50        | 8      | 1     |
| 1:A:25:GLN:O    | 1:A:25:GLN:NE2  | 0.41     | 2.54        | 10     | 1     |
| 2:B:54:ILE:O    | 2:B:56:LYS:HD3  | 0.41     | 2.16        | 10     | 1     |
| 2:B:16:ASN:O    | 2:B:20:GLN:CG   | 0.41     | 2.69        | 1      | 1     |
| 1:A:19:GLN:C    | 1:A:22:ILE:HG23 | 0.41     | 2.41        | 3      | 1     |
| 2:B:40:GLN:CD   | 2:B:40:GLN:C    | 0.41     | 2.88        | 9      | 1     |
| 2:B:41:GLY:O    | 2:B:43:HIS:N    | 0.41     | 2.54        | 9      | 1     |
| 2:B:48:SER:CA   | 2:B:51:ILE:HG23 | 0.41     | 2.46        | 9      | 1     |
| 2:B:17:GLU:O    | 2:B:17:GLU:OE2  | 0.40     | 2.39        | 3      | 1     |
| 2:B:23:GLN:O    | 2:B:26:VAL:CG2  | 0.40     | 2.65        | 4      | 1     |
| 2:B:57:ASN:HB2  | 2:B:69:THR:CG2  | 0.40     | 2.34        | 6      | 1     |
| 2:B:18:LEU:HD13 | 2:B:26:VAL:HG22 | 0.40     | 1.94        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:34:ALA:CA   | 2:B:37:VAL:HB   | 0.40     | 2.47        | 3      | 1     |
| 2:B:26:VAL:CG1  | 2:B:68:GLY:N    | 0.40     | 2.84        | 4      | 1     |
| 2:B:51:ILE:HA   | 2:B:54:ILE:HB   | 0.40     | 1.93        | 4      | 1     |
| 2:B:15:CYS:HB2  | 2:B:62:CYS:CA   | 0.40     | 2.46        | 10     | 1     |
| 2:B:40:GLN:HG2  | 2:B:41:GLY:N    | 0.40     | 2.31        | 10     | 1     |
| 2:B:48:SER:CA   | 2:B:51:ILE:HG22 | 0.40     | 2.46        | 1      | 1     |
| 2:B:62:CYS:HB2  | 2:B:64:MET:HE2  | 0.40     | 1.92        | 2      | 1     |
| 2:B:57:ASN:CB   | 2:B:61:VAL:CG1  | 0.40     | 2.98        | 6      | 1     |
| 2:B:59:PRO:O    | 2:B:60:ASN:OD1  | 0.40     | 2.38        | 8      | 1     |
| 2:B:57:ASN:ND2  | 2:B:70:CYS:C    | 0.40     | 2.79        | 3      | 1     |
| 1:A:24:GLN:C    | 1:A:26:LEU:N    | 0.40     | 2.79        | 4      | 1     |
| 2:B:52:TYR:C    | 2:B:54:ILE:N    | 0.40     | 2.79        | 5      | 1     |
| 1:A:21:TRP:O    | 2:B:58:LEU:HD22 | 0.40     | 2.14        | 8      | 1     |
| 2:B:15:CYS:HB2  | 2:B:62:CYS:N    | 0.40     | 2.32        | 10     | 1     |
| 1:A:21:TRP:NE1  | 2:B:61:VAL:HG21 | 0.40     | 2.28        | 5      | 1     |
| 2:B:61:VAL:HG11 | 2:B:69:THR:O    | 0.40     | 2.16        | 7      | 1     |
| 2:B:30:LEU:HD21 | 2:B:70:CYS:SG   | 0.40     | 2.56        | 8      | 1     |
| 1:A:26:LEU:O    | 1:A:27:ALA:O    | 0.40     | 2.40        | 9      | 1     |
| 1:A:22:ILE:HG22 | 2:B:34:ALA:HA   | 0.40     | 1.93        | 10     | 1     |
| 2:B:30:LEU:HD21 | 2:B:56:LYS:CA   | 0.40     | 2.46        | 10     | 1     |

## 6.3 Torsion angles

### 6.3.1 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 NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed       | Favoured     | Allowed      | Outliers     | Percentiles |   |
|-----|-------|----------------|--------------|--------------|--------------|-------------|---|
| 1   | A     | 26/31 (84%)    | 12±2 (45±9%) | 8±2 (32±8%)  | 6±2 (23±6%)  | 0           | 1 |
| 2   | B     | 62/75 (83%)    | 30±2 (48±3%) | 18±2 (29±3%) | 14±2 (23±2%) | 0           | 1 |
| All | All   | 880/1060 (83%) | 412 (47%)    | 262 (30%)    | 206 (23%)    | 0           | 1 |

All 42 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 13  | GLN  | 10             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 14  | HIS  | 10             |
| 1   | A     | 15  | LEU  | 10             |
| 2   | B     | 37  | VAL  | 10             |
| 2   | B     | 58  | LEU  | 10             |
| 2   | B     | 60  | ASN  | 10             |
| 2   | B     | 61  | VAL  | 10             |
| 2   | B     | 56  | LYS  | 9              |
| 2   | B     | 39  | VAL  | 8              |
| 2   | B     | 40  | GLN  | 7              |
| 2   | B     | 55  | ALA  | 7              |
| 1   | A     | 12  | GLU  | 6              |
| 1   | A     | 22  | ILE  | 6              |
| 2   | B     | 23  | GLN  | 6              |
| 2   | B     | 54  | ILE  | 6              |
| 2   | B     | 47  | GLN  | 6              |
| 1   | A     | 27  | ALA  | 5              |
| 2   | B     | 38  | ARG  | 5              |
| 2   | B     | 41  | GLY  | 5              |
| 2   | B     | 44  | GLY  | 5              |
| 2   | B     | 63  | ASN  | 5              |
| 2   | B     | 26  | VAL  | 5              |
| 1   | A     | 19  | GLN  | 4              |
| 1   | A     | 20  | GLN  | 4              |
| 2   | B     | 57  | ASN  | 4              |
| 1   | A     | 17  | ALA  | 4              |
| 2   | B     | 24  | VAL  | 4              |
| 2   | B     | 27  | CYS  | 4              |
| 2   | B     | 52  | TYR  | 3              |
| 2   | B     | 21  | GLU  | 3              |
| 2   | B     | 33  | ALA  | 2              |
| 2   | B     | 35  | LYS  | 2              |
| 2   | B     | 67  | ILE  | 2              |
| 2   | B     | 42  | GLN  | 1              |
| 1   | A     | 21  | TRP  | 1              |
| 2   | B     | 64  | MET  | 1              |
| 2   | B     | 70  | CYS  | 1              |
| 1   | A     | 8   | GLU  | 1              |
| 2   | B     | 62  | CYS  | 1              |
| 2   | B     | 19  | TYR  | 1              |
| 2   | B     | 49  | THR  | 1              |
| 2   | B     | 25  | CYS  | 1              |

### 6.3.2 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 NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed      | Rotameric    | Outliers     | Percentiles |   |
|-----|-------|---------------|--------------|--------------|-------------|---|
| 1   | A     | 25/28 (89%)   | 13±2 (53±8%) | 12±2 (47±8%) | 0           | 2 |
| 2   | B     | 56/66 (85%)   | 28±3 (49±5%) | 28±3 (51±5%) | 0           | 1 |
| All | All   | 810/940 (86%) | 407 (50%)    | 403 (50%)    | 0           | 1 |

All 73 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 6   | GLN  | 10             |
| 1   | A     | 13  | GLN  | 10             |
| 1   | A     | 15  | LEU  | 10             |
| 2   | B     | 29  | THR  | 10             |
| 2   | B     | 30  | LEU  | 10             |
| 2   | B     | 32  | GLN  | 10             |
| 2   | B     | 49  | THR  | 10             |
| 2   | B     | 56  | LYS  | 10             |
| 2   | B     | 67  | ILE  | 10             |
| 1   | A     | 3   | GLN  | 9              |
| 2   | B     | 14  | CYS  | 9              |
| 2   | B     | 19  | TYR  | 9              |
| 2   | B     | 42  | GLN  | 9              |
| 2   | B     | 18  | LEU  | 9              |
| 1   | A     | 10  | GLN  | 8              |
| 1   | A     | 11  | GLN  | 8              |
| 1   | A     | 21  | TRP  | 8              |
| 2   | B     | 22  | ASP  | 8              |
| 2   | B     | 24  | VAL  | 8              |
| 2   | B     | 16  | ASN  | 8              |
| 1   | A     | 22  | ILE  | 7              |
| 2   | B     | 39  | VAL  | 7              |
| 2   | B     | 50  | ARG  | 7              |
| 2   | B     | 52  | TYR  | 7              |
| 2   | B     | 57  | ASN  | 7              |
| 2   | B     | 69  | THR  | 7              |
| 1   | A     | 20  | GLN  | 7              |
| 2   | B     | 17  | GLU  | 7              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 51  | ILE  | 7              |
| 2   | B     | 11  | ARG  | 6              |
| 2   | B     | 26  | VAL  | 6              |
| 2   | B     | 62  | CYS  | 6              |
| 2   | B     | 27  | CYS  | 6              |
| 2   | B     | 31  | LYS  | 6              |
| 2   | B     | 47  | GLN  | 6              |
| 1   | A     | 4   | LYS  | 5              |
| 2   | B     | 21  | GLU  | 5              |
| 2   | B     | 23  | GLN  | 5              |
| 2   | B     | 48  | SER  | 5              |
| 2   | B     | 38  | ARG  | 5              |
| 2   | B     | 10  | LEU  | 5              |
| 2   | B     | 58  | LEU  | 5              |
| 2   | B     | 20  | GLN  | 4              |
| 2   | B     | 40  | GLN  | 4              |
| 2   | B     | 65  | LYS  | 4              |
| 2   | B     | 66  | GLN  | 4              |
| 1   | A     | 12  | GLU  | 4              |
| 1   | A     | 19  | GLN  | 4              |
| 1   | A     | 5   | CYS  | 4              |
| 2   | B     | 37  | VAL  | 4              |
| 2   | B     | 70  | CYS  | 4              |
| 1   | A     | 25  | GLN  | 4              |
| 1   | A     | 8   | GLU  | 3              |
| 1   | A     | 23  | ARG  | 3              |
| 1   | A     | 24  | GLN  | 3              |
| 2   | B     | 12  | GLU  | 3              |
| 1   | A     | 9   | PHE  | 3              |
| 1   | A     | 14  | HIS  | 3              |
| 2   | B     | 54  | ILE  | 3              |
| 2   | B     | 35  | LYS  | 3              |
| 2   | B     | 63  | ASN  | 3              |
| 1   | A     | 26  | LEU  | 2              |
| 2   | B     | 15  | CYS  | 2              |
| 2   | B     | 13  | GLN  | 2              |
| 2   | B     | 25  | CYS  | 2              |
| 1   | A     | 1   | GLN  | 2              |
| 2   | B     | 36  | SER  | 2              |
| 2   | B     | 64  | MET  | 2              |
| 2   | B     | 53  | GLN  | 1              |
| 2   | B     | 43  | HIS  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 7   | ARG  | 1              |
| 2   | B     | 61  | VAL  | 1              |
| 2   | B     | 46  | PHE  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided