



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 05:37 AM UTC

PDB ID : 2HQI / pdb\_00002hqi  
Title : NMR SOLUTION STRUCTURE OF THE OXIDIZED FORM OF MERP, 14  
STRUCTURES  
Authors : Qian, H.; Sahlman, L.; Eriksson, P.O.; Hambreus, C.; Edlund, U.; Sethson, I.  
Deposited on : 1998-03-31

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                                                             |

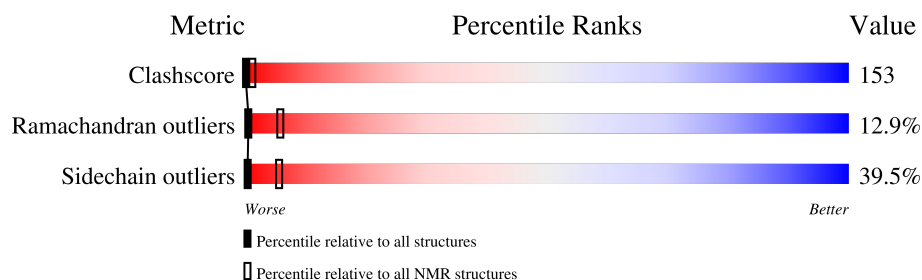
# 1 Overall quality at a glance

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     | 72     |                  |

## 2 Ensemble composition and analysis

This entry contains 14 models. Model 4 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:3-A:72 (70)         | 0.63              | 4            |

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 and 1 single-model cluster was found.

| Cluster number        | Models                  |
|-----------------------|-------------------------|
| 1                     | 2, 3, 4, 5, 7, 8, 9, 14 |
| 2                     | 1, 6, 10, 12, 13        |
| Single-model clusters | 11                      |

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1072 atoms, of which 550 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MERCURIC TRANSPORT PROTEIN.

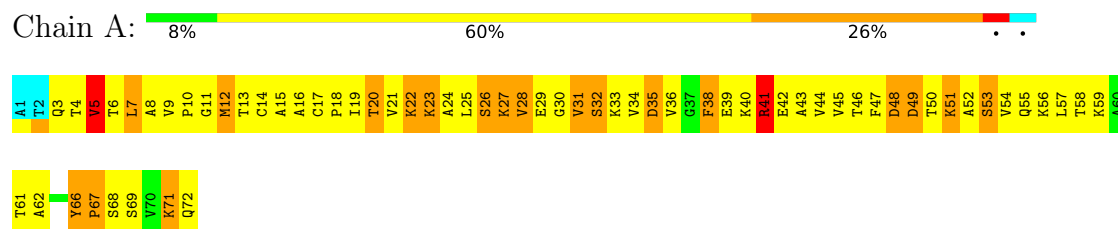
| Mol | Chain | Residues | Atoms |     |     |    |     |   | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|-------|
| 1   | A     | 72       | Total | C   | H   | N  | O   | S | 0     |
|     |       |          | 1072  | 327 | 550 | 87 | 105 | 3 |       |

## 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: MERCURIC TRANSPORT PROTEIN

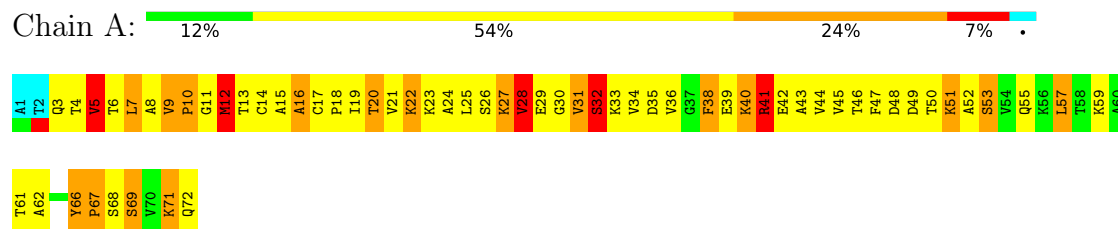


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: MERCURIC TRANSPORT PROTEIN



#### 4.2.2 Score per residue for model 2

- Molecule 1: MERCURIC TRANSPORT PROTEIN

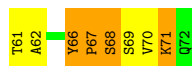




### 4.2.3 Score per residue for model 3

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 10% 53% 28% 7% .



### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 7% 56% 29% 6% .



### 4.2.5 Score per residue for model 5

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 11% 42% 39% 6% .



### 4.2.6 Score per residue for model 6

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 7% 57% 28% 6% .





#### 4.2.7 Score per residue for model 7

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 12% 46% 33% 6% .



#### 4.2.8 Score per residue for model 8

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 14% 56% 22% 6% .



#### 4.2.9 Score per residue for model 9

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 10% 54% 28% 6% .



#### 4.2.10 Score per residue for model 10

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 8% 56% 26% 7% .

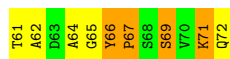




#### 4.2.11 Score per residue for model 11

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 12% 54% 26% . .



#### 4.2.12 Score per residue for model 12

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 14% 50% 28% 6% .



#### 4.2.13 Score per residue for model 13

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 8% 53% 29% 7% .



#### 4.2.14 Score per residue for model 14

- Molecule 1: MERCURIC TRANSPORT PROTEIN

Chain A: 14% 51% 24% 8% .





|     |     |
|-----|-----|
| T61 | Y66 |
| AG2 | P67 |
| D63 | SG8 |
|     | SG9 |
|     | V70 |
|     | K71 |
|     | Q72 |

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *SA*.

Of the 20 calculated structures, 14 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR        | refinement         | 3.8     |
| X-PLOR        | structure solution |         |

No chemical shift data was provided.

## 6 Model quality [i](#)

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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     | 510   | 536      | 534      | 159±14  |
| All | All   | 7140  | 7504     | 7476     | 2230    |

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 153.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:VAL:CG2   | 1:A:43:ALA:HB2  | 1.00     | 1.87        | 9      | 7     |
| 1:A:24:ALA:O    | 1:A:28:VAL:HG23 | 1.00     | 1.56        | 10     | 6     |
| 1:A:57:LEU:O    | 1:A:61:THR:HG23 | 0.97     | 1.60        | 10     | 10    |
| 1:A:9:VAL:HG22  | 1:A:43:ALA:HB2  | 0.92     | 1.42        | 5      | 6     |
| 1:A:28:VAL:HG11 | 1:A:57:LEU:HA   | 0.91     | 1.42        | 14     | 3     |
| 1:A:9:VAL:HG21  | 1:A:18:PRO:HB3  | 0.91     | 1.41        | 3      | 2     |
| 1:A:7:LEU:HD22  | 1:A:25:LEU:CD2  | 0.91     | 1.96        | 4      | 4     |
| 1:A:25:LEU:CD1  | 1:A:36:VAL:HG21 | 0.91     | 1.96        | 9      | 10    |
| 1:A:8:ALA:HB3   | 1:A:69:SER:OG   | 0.90     | 1.66        | 4      | 1     |
| 1:A:29:GLU:HB2  | 1:A:52:ALA:HB2  | 0.89     | 1.42        | 8      | 8     |
| 1:A:7:LEU:HD13  | 1:A:45:VAL:CG2  | 0.89     | 1.97        | 2      | 8     |
| 1:A:28:VAL:HG21 | 1:A:57:LEU:HA   | 0.89     | 1.44        | 6      | 10    |
| 1:A:6:THR:HG23  | 1:A:44:VAL:HG22 | 0.88     | 1.45        | 10     | 8     |
| 1:A:29:GLU:HB3  | 1:A:52:ALA:HB2  | 0.87     | 1.46        | 12     | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:28:VAL:HG21 | 1:A:57:LEU:CB   | 0.87     | 2.00        | 2      | 5     |
| 1:A:58:THR:HG22 | 1:A:68:SER:O    | 0.86     | 1.70        | 8      | 1     |
| 1:A:9:VAL:HG23  | 1:A:43:ALA:HB2  | 0.86     | 1.48        | 9      | 2     |
| 1:A:29:GLU:CB   | 1:A:52:ALA:HB2  | 0.86     | 2.01        | 10     | 7     |
| 1:A:57:LEU:HD12 | 1:A:58:THR:N    | 0.85     | 1.85        | 3      | 7     |
| 1:A:7:LEU:HD13  | 1:A:45:VAL:HG22 | 0.84     | 1.46        | 12     | 7     |
| 1:A:25:LEU:C    | 1:A:31:VAL:HG11 | 0.84     | 1.96        | 14     | 1     |
| 1:A:47:PHE:CZ   | 1:A:54:VAL:HG23 | 0.84     | 2.06        | 2      | 3     |
| 1:A:47:PHE:CE1  | 1:A:54:VAL:HG23 | 0.83     | 2.09        | 2      | 3     |
| 1:A:16:ALA:HB1  | 1:A:19:ILE:HD12 | 0.82     | 1.49        | 7      | 2     |
| 1:A:36:VAL:HG22 | 1:A:43:ALA:CA   | 0.82     | 2.03        | 4      | 11    |
| 1:A:26:SER:CA   | 1:A:34:VAL:HG21 | 0.81     | 2.06        | 2      | 3     |
| 1:A:9:VAL:HG23  | 1:A:21:VAL:HG21 | 0.80     | 1.52        | 8      | 2     |
| 1:A:25:LEU:O    | 1:A:28:VAL:HG12 | 0.80     | 1.76        | 11     | 4     |
| 1:A:47:PHE:CD2  | 1:A:57:LEU:HD21 | 0.78     | 2.14        | 4      | 3     |
| 1:A:58:THR:HG22 | 1:A:68:SER:OG   | 0.78     | 1.79        | 6      | 1     |
| 1:A:7:LEU:HD22  | 1:A:25:LEU:HD21 | 0.77     | 1.54        | 2      | 4     |
| 1:A:25:LEU:HD21 | 1:A:68:SER:CB   | 0.77     | 2.07        | 8      | 2     |
| 1:A:28:VAL:HG21 | 1:A:57:LEU:CA   | 0.77     | 2.08        | 4      | 9     |
| 1:A:9:VAL:HG12  | 1:A:21:VAL:HG11 | 0.77     | 1.56        | 3      | 1     |
| 1:A:25:LEU:HD21 | 1:A:68:SER:HB2  | 0.77     | 1.54        | 8      | 1     |
| 1:A:28:VAL:HG11 | 1:A:57:LEU:CB   | 0.76     | 2.10        | 4      | 7     |
| 1:A:25:LEU:HD13 | 1:A:36:VAL:HG21 | 0.75     | 1.58        | 13     | 7     |
| 1:A:26:SER:O    | 1:A:31:VAL:HG21 | 0.75     | 1.81        | 9      | 7     |
| 1:A:36:VAL:HG22 | 1:A:43:ALA:HA   | 0.75     | 1.57        | 4      | 11    |
| 1:A:6:THR:CG2   | 1:A:44:VAL:HG22 | 0.75     | 2.12        | 7      | 4     |
| 1:A:4:THR:O     | 1:A:4:THR:HG23  | 0.75     | 1.82        | 13     | 14    |
| 1:A:26:SER:CB   | 1:A:34:VAL:HG21 | 0.75     | 2.11        | 2      | 3     |
| 1:A:16:ALA:HB1  | 1:A:19:ILE:CD1  | 0.74     | 2.11        | 7      | 1     |
| 1:A:57:LEU:HD12 | 1:A:57:LEU:C    | 0.74     | 2.06        | 13     | 3     |
| 1:A:28:VAL:O    | 1:A:31:VAL:HG23 | 0.74     | 1.83        | 9      | 8     |
| 1:A:4:THR:O     | 1:A:5:VAL:HG13  | 0.74     | 1.83        | 8      | 3     |
| 1:A:28:VAL:HG11 | 1:A:57:LEU:HB2  | 0.74     | 1.60        | 4      | 7     |
| 1:A:9:VAL:HG11  | 1:A:18:PRO:HB3  | 0.74     | 1.59        | 14     | 7     |
| 1:A:34:VAL:HG13 | 1:A:34:VAL:O    | 0.73     | 1.83        | 5      | 8     |
| 1:A:9:VAL:HB    | 1:A:21:VAL:HG11 | 0.73     | 1.61        | 2      | 3     |
| 1:A:28:VAL:HG11 | 1:A:57:LEU:CA   | 0.73     | 2.14        | 14     | 1     |
| 1:A:24:ALA:HB1  | 1:A:61:THR:HB   | 0.73     | 1.60        | 5      | 4     |
| 1:A:46:THR:O    | 1:A:46:THR:HG23 | 0.72     | 1.85        | 6      | 4     |
| 1:A:9:VAL:HG12  | 1:A:18:PRO:HB3  | 0.71     | 1.61        | 12     | 2     |
| 1:A:24:ALA:HB1  | 1:A:61:THR:HG22 | 0.71     | 1.63        | 9      | 10    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:28:VAL:HG11 | 1:A:57:LEU:HB3  | 0.70     | 1.64        | 6      | 2     |
| 1:A:7:LEU:CD2   | 1:A:25:LEU:HD22 | 0.70     | 2.15        | 8      | 1     |
| 1:A:48:ASP:OD1  | 1:A:50:THR:HG23 | 0.70     | 1.86        | 10     | 1     |
| 1:A:25:LEU:HD12 | 1:A:36:VAL:HG21 | 0.70     | 1.64        | 2      | 7     |
| 1:A:6:THR:HG23  | 1:A:44:VAL:CG2  | 0.69     | 2.16        | 14     | 1     |
| 1:A:7:LEU:O     | 1:A:43:ALA:HB3  | 0.69     | 1.87        | 5      | 6     |
| 1:A:7:LEU:HD22  | 1:A:25:LEU:HD22 | 0.69     | 1.64        | 4      | 4     |
| 1:A:7:LEU:HD23  | 1:A:69:SER:O    | 0.67     | 1.89        | 5      | 6     |
| 1:A:9:VAL:HG13  | 1:A:21:VAL:HG11 | 0.67     | 1.65        | 6      | 7     |
| 1:A:47:PHE:CD1  | 1:A:57:LEU:CD1  | 0.67     | 2.78        | 12     | 3     |
| 1:A:12:MET:C    | 1:A:13:THR:HG22 | 0.67     | 2.15        | 13     | 3     |
| 1:A:47:PHE:CE1  | 1:A:57:LEU:CD1  | 0.66     | 2.78        | 10     | 3     |
| 1:A:9:VAL:CG1   | 1:A:43:ALA:HB2  | 0.66     | 2.19        | 2      | 3     |
| 1:A:9:VAL:CG1   | 1:A:21:VAL:HG11 | 0.66     | 2.19        | 3      | 1     |
| 1:A:14:CYS:O    | 1:A:15:ALA:HB3  | 0.66     | 1.90        | 8      | 3     |
| 1:A:15:ALA:O    | 1:A:16:ALA:HB3  | 0.66     | 1.91        | 13     | 5     |
| 1:A:47:PHE:CG   | 1:A:47:PHE:O    | 0.66     | 2.49        | 6      | 9     |
| 1:A:14:CYS:O    | 1:A:15:ALA:HB2  | 0.66     | 1.91        | 13     | 4     |
| 1:A:26:SER:HA   | 1:A:31:VAL:HG13 | 0.65     | 1.67        | 13     | 6     |
| 1:A:9:VAL:HG23  | 1:A:43:ALA:CB   | 0.65     | 2.20        | 9      | 1     |
| 1:A:8:ALA:HB2   | 1:A:71:LYS:CD   | 0.65     | 2.21        | 11     | 1     |
| 1:A:62:ALA:HB2  | 1:A:67:PRO:HB3  | 0.65     | 1.67        | 11     | 14    |
| 1:A:12:MET:HE2  | 1:A:41:ARG:NH2  | 0.65     | 2.07        | 5      | 1     |
| 1:A:3:GLN:CD    | 1:A:54:VAL:HG22 | 0.65     | 2.17        | 10     | 1     |
| 1:A:36:VAL:HG22 | 1:A:43:ALA:C    | 0.65     | 2.17        | 14     | 10    |
| 1:A:47:PHE:CD2  | 1:A:57:LEU:CD2  | 0.65     | 2.80        | 5      | 6     |
| 1:A:3:GLN:CB    | 1:A:47:PHE:CE2  | 0.64     | 2.80        | 10     | 4     |
| 1:A:25:LEU:HD22 | 1:A:45:VAL:HG21 | 0.64     | 1.67        | 10     | 5     |
| 1:A:47:PHE:CG   | 1:A:57:LEU:CD2  | 0.64     | 2.80        | 11     | 5     |
| 1:A:15:ALA:O    | 1:A:16:ALA:HB2  | 0.64     | 1.91        | 5      | 5     |
| 1:A:9:VAL:HG12  | 1:A:21:VAL:CG1  | 0.64     | 2.22        | 3      | 1     |
| 1:A:47:PHE:CZ   | 1:A:54:VAL:N    | 0.64     | 2.65        | 4      | 4     |
| 1:A:19:ILE:CG1  | 1:A:38:PHE:CG   | 0.64     | 2.81        | 9      | 3     |
| 1:A:21:VAL:HG23 | 1:A:66:TYR:HB3  | 0.64     | 1.68        | 8      | 6     |
| 1:A:9:VAL:HG23  | 1:A:21:VAL:HG11 | 0.64     | 1.68        | 4      | 1     |
| 1:A:28:VAL:HG21 | 1:A:57:LEU:HB2  | 0.64     | 1.69        | 4      | 4     |
| 1:A:4:THR:HB    | 1:A:46:THR:HG23 | 0.64     | 1.69        | 3      | 7     |
| 1:A:7:LEU:CD1   | 1:A:45:VAL:HG22 | 0.64     | 2.22        | 12     | 3     |
| 1:A:47:PHE:CD1  | 1:A:48:ASP:N    | 0.63     | 2.66        | 13     | 4     |
| 1:A:4:THR:CB    | 1:A:46:THR:HG23 | 0.63     | 2.24        | 3      | 6     |
| 1:A:47:PHE:CE1  | 1:A:54:VAL:CG2  | 0.63     | 2.81        | 14     | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:36:VAL:HG13 | 1:A:43:ALA:HA   | 0.63     | 1.70        | 14     | 11    |
| 1:A:54:VAL:O    | 1:A:58:THR:HG23 | 0.63     | 1.93        | 11     | 2     |
| 1:A:25:LEU:HD13 | 1:A:45:VAL:HG11 | 0.63     | 1.69        | 9      | 6     |
| 1:A:8:ALA:HB2   | 1:A:71:LYS:HD3  | 0.63     | 1.69        | 11     | 1     |
| 1:A:47:PHE:CD1  | 1:A:57:LEU:HD11 | 0.62     | 2.29        | 10     | 3     |
| 1:A:9:VAL:CB    | 1:A:21:VAL:HG11 | 0.62     | 2.23        | 2      | 3     |
| 1:A:3:GLN:CG    | 1:A:47:PHE:CE2  | 0.62     | 2.83        | 13     | 5     |
| 1:A:19:ILE:CG1  | 1:A:38:PHE:CD2  | 0.62     | 2.83        | 7      | 1     |
| 1:A:66:TYR:CD1  | 1:A:66:TYR:N    | 0.61     | 2.64        | 6      | 7     |
| 1:A:3:GLN:CG    | 1:A:47:PHE:CZ   | 0.61     | 2.83        | 10     | 3     |
| 1:A:36:VAL:CG2  | 1:A:43:ALA:CB   | 0.61     | 2.77        | 10     | 2     |
| 1:A:36:VAL:CG2  | 1:A:45:VAL:CG1  | 0.61     | 2.79        | 8      | 8     |
| 1:A:44:VAL:O    | 1:A:45:VAL:HG13 | 0.61     | 1.95        | 5      | 4     |
| 1:A:47:PHE:CZ   | 1:A:57:LEU:HD21 | 0.61     | 2.31        | 6      | 1     |
| 1:A:8:ALA:HB2   | 1:A:71:LYS:HG3  | 0.61     | 1.71        | 4      | 1     |
| 1:A:12:MET:HE2  | 1:A:41:ARG:HB2  | 0.60     | 1.73        | 3      | 1     |
| 1:A:47:PHE:CE2  | 1:A:57:LEU:HD21 | 0.60     | 2.31        | 13     | 4     |
| 1:A:21:VAL:HG23 | 1:A:66:TYR:CB   | 0.60     | 2.27        | 2      | 6     |
| 1:A:57:LEU:CD1  | 1:A:58:THR:N    | 0.60     | 2.63        | 13     | 6     |
| 1:A:47:PHE:CZ   | 1:A:53:SER:C    | 0.60     | 2.80        | 5      | 2     |
| 1:A:47:PHE:CE2  | 1:A:57:LEU:CD2  | 0.60     | 2.84        | 13     | 3     |
| 1:A:26:SER:N    | 1:A:31:VAL:HG11 | 0.60     | 2.12        | 14     | 1     |
| 1:A:25:LEU:HD13 | 1:A:45:VAL:HG21 | 0.60     | 1.74        | 5      | 1     |
| 1:A:12:MET:CG   | 1:A:41:ARG:CB   | 0.59     | 2.80        | 7      | 2     |
| 1:A:19:ILE:HD12 | 1:A:38:PHE:CD2  | 0.59     | 2.31        | 10     | 2     |
| 1:A:11:GLY:O    | 1:A:13:THR:N    | 0.59     | 2.35        | 4      | 10    |
| 1:A:48:ASP:O    | 1:A:49:ASP:C    | 0.59     | 2.46        | 6      | 6     |
| 1:A:25:LEU:HD11 | 1:A:43:ALA:HB1  | 0.59     | 1.75        | 5      | 7     |
| 1:A:7:LEU:CD2   | 1:A:25:LEU:CD2  | 0.59     | 2.80        | 8      | 1     |
| 1:A:17:CYS:N    | 1:A:18:PRO:CD   | 0.59     | 2.66        | 6      | 12    |
| 1:A:4:THR:CA    | 1:A:46:THR:HG23 | 0.59     | 2.28        | 5      | 6     |
| 1:A:17:CYS:SG   | 1:A:66:TYR:CD1  | 0.58     | 2.96        | 10     | 5     |
| 1:A:64:ALA:O    | 1:A:66:TYR:CE1  | 0.58     | 2.56        | 13     | 2     |
| 1:A:8:ALA:HB3   | 1:A:69:SER:HB3  | 0.58     | 1.73        | 1      | 2     |
| 1:A:21:VAL:HG22 | 1:A:67:PRO:O    | 0.58     | 1.99        | 8      | 3     |
| 1:A:33:LYS:N    | 1:A:46:THR:CG2  | 0.58     | 2.67        | 8      | 3     |
| 1:A:20:THR:OG1  | 1:A:66:TYR:CD2  | 0.58     | 2.56        | 4      | 7     |
| 1:A:15:ALA:O    | 1:A:38:PHE:CE1  | 0.58     | 2.56        | 7      | 1     |
| 1:A:4:THR:O     | 1:A:4:THR:CG2   | 0.58     | 2.51        | 10     | 13    |
| 1:A:9:VAL:HB    | 1:A:43:ALA:HB2  | 0.58     | 1.75        | 4      | 1     |
| 1:A:21:VAL:HG21 | 1:A:67:PRO:O    | 0.58     | 1.97        | 10     | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:3:GLN:CB    | 1:A:47:PHE:CZ   | 0.58     | 2.87        | 12     | 3     |
| 1:A:19:ILE:N    | 1:A:38:PHE:CB   | 0.58     | 2.67        | 10     | 10    |
| 1:A:21:VAL:O    | 1:A:25:LEU:HD12 | 0.58     | 1.99        | 12     | 1     |
| 1:A:20:THR:OG1  | 1:A:66:TYR:CG   | 0.58     | 2.57        | 13     | 4     |
| 1:A:38:PHE:O    | 1:A:38:PHE:CD1  | 0.58     | 2.57        | 4      | 6     |
| 1:A:25:LEU:O    | 1:A:28:VAL:HG23 | 0.58     | 1.99        | 14     | 1     |
| 1:A:3:GLN:HB3   | 1:A:47:PHE:CE2  | 0.58     | 2.34        | 1      | 4     |
| 1:A:4:THR:C     | 1:A:5:VAL:CG2   | 0.58     | 2.77        | 12     | 10    |
| 1:A:7:LEU:CD1   | 1:A:45:VAL:CG2  | 0.58     | 2.81        | 2      | 1     |
| 1:A:19:ILE:CG2  | 1:A:20:THR:N    | 0.58     | 2.66        | 10     | 4     |
| 1:A:47:PHE:O    | 1:A:47:PHE:CD2  | 0.57     | 2.57        | 6      | 4     |
| 1:A:9:VAL:CG1   | 1:A:42:GLU:C    | 0.57     | 2.77        | 2      | 2     |
| 1:A:21:VAL:HG13 | 1:A:67:PRO:O    | 0.57     | 1.99        | 8      | 4     |
| 1:A:7:LEU:CB    | 1:A:69:SER:O    | 0.57     | 2.52        | 9      | 9     |
| 1:A:47:PHE:O    | 1:A:47:PHE:CD1  | 0.57     | 2.56        | 9      | 5     |
| 1:A:15:ALA:O    | 1:A:38:PHE:CZ   | 0.57     | 2.57        | 11     | 3     |
| 1:A:26:SER:C    | 1:A:31:VAL:HG21 | 0.57     | 2.24        | 2      | 5     |
| 1:A:28:VAL:CG2  | 1:A:57:LEU:CB   | 0.57     | 2.80        | 4      | 3     |
| 1:A:17:CYS:SG   | 1:A:66:TYR:CE1  | 0.57     | 2.98        | 4      | 4     |
| 1:A:9:VAL:CG2   | 1:A:43:ALA:CB   | 0.57     | 2.83        | 10     | 4     |
| 1:A:19:ILE:HG13 | 1:A:38:PHE:CD2  | 0.57     | 2.35        | 7      | 1     |
| 1:A:3:GLN:HB3   | 1:A:47:PHE:CD2  | 0.57     | 2.35        | 13     | 4     |
| 1:A:21:VAL:O    | 1:A:24:ALA:HB3  | 0.57     | 2.00        | 2      | 7     |
| 1:A:54:VAL:HA   | 1:A:57:LEU:HD21 | 0.57     | 1.76        | 9      | 3     |
| 1:A:35:ASP:O    | 1:A:44:VAL:N    | 0.57     | 2.37        | 11     | 13    |
| 1:A:19:ILE:HG13 | 1:A:38:PHE:CG   | 0.57     | 2.35        | 9      | 5     |
| 1:A:17:CYS:HA   | 1:A:66:TYR:CG   | 0.57     | 2.35        | 7      | 3     |
| 1:A:47:PHE:CE1  | 1:A:57:LEU:HD23 | 0.57     | 2.35        | 8      | 1     |
| 1:A:38:PHE:CD1  | 1:A:39:GLU:N    | 0.57     | 2.73        | 3      | 1     |
| 1:A:14:CYS:O    | 1:A:38:PHE:CE1  | 0.57     | 2.57        | 4      | 1     |
| 1:A:40:LYS:O    | 1:A:41:ARG:CB   | 0.57     | 2.53        | 12     | 6     |
| 1:A:13:THR:OG1  | 1:A:14:CYS:N    | 0.56     | 2.38        | 5      | 1     |
| 1:A:49:ASP:CG   | 1:A:50:THR:N    | 0.56     | 2.63        | 6      | 1     |
| 1:A:6:THR:O     | 1:A:71:LYS:N    | 0.56     | 2.39        | 13     | 13    |
| 1:A:9:VAL:HG12  | 1:A:43:ALA:N    | 0.56     | 2.15        | 1      | 2     |
| 1:A:22:LYS:CB   | 1:A:36:VAL:HB   | 0.56     | 2.31        | 13     | 11    |
| 1:A:23:LYS:O    | 1:A:27:LYS:CG   | 0.56     | 2.54        | 14     | 10    |
| 1:A:4:THR:O     | 1:A:5:VAL:HG22  | 0.56     | 2.01        | 12     | 10    |
| 1:A:7:LEU:HD23  | 1:A:25:LEU:CD2  | 0.56     | 2.30        | 8      | 1     |
| 1:A:47:PHE:O    | 1:A:47:PHE:CG   | 0.56     | 2.59        | 9      | 1     |
| 1:A:7:LEU:N     | 1:A:43:ALA:O    | 0.56     | 2.38        | 4      | 14    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:35:ASP:N    | 1:A:44:VAL:O    | 0.56     | 2.39        | 12     | 13    |
| 1:A:4:THR:O     | 1:A:5:VAL:CG1   | 0.56     | 2.54        | 2      | 4     |
| 1:A:38:PHE:CD1  | 1:A:38:PHE:C    | 0.56     | 2.83        | 12     | 4     |
| 1:A:12:MET:O    | 1:A:13:THR:CG2  | 0.56     | 2.54        | 3      | 2     |
| 1:A:19:ILE:HD12 | 1:A:38:PHE:HD2  | 0.56     | 1.60        | 6      | 1     |
| 1:A:27:LYS:CD   | 1:A:27:LYS:C    | 0.56     | 2.78        | 1      | 1     |
| 1:A:7:LEU:O     | 1:A:43:ALA:N    | 0.56     | 2.39        | 3      | 4     |
| 1:A:31:VAL:O    | 1:A:31:VAL:HG22 | 0.55     | 2.01        | 11     | 1     |
| 1:A:3:GLN:O     | 1:A:47:PHE:N    | 0.55     | 2.39        | 10     | 4     |
| 1:A:23:LYS:O    | 1:A:27:LYS:N    | 0.55     | 2.40        | 13     | 11    |
| 1:A:41:ARG:O    | 1:A:41:ARG:CG   | 0.55     | 2.54        | 5      | 6     |
| 1:A:25:LEU:HD13 | 1:A:45:VAL:CG2  | 0.55     | 2.31        | 5      | 1     |
| 1:A:58:THR:O    | 1:A:61:THR:CG2  | 0.55     | 2.54        | 6      | 3     |
| 1:A:57:LEU:C    | 1:A:57:LEU:CD1  | 0.55     | 2.79        | 13     | 3     |
| 1:A:28:VAL:HG13 | 1:A:29:GLU:N    | 0.55     | 2.15        | 5      | 8     |
| 1:A:49:ASP:O    | 1:A:50:THR:C    | 0.55     | 2.49        | 6      | 5     |
| 1:A:14:CYS:O    | 1:A:15:ALA:CB   | 0.55     | 2.55        | 9      | 7     |
| 1:A:24:ALA:HB1  | 1:A:61:THR:CB   | 0.55     | 2.31        | 13     | 2     |
| 1:A:35:ASP:O    | 1:A:44:VAL:CB   | 0.55     | 2.54        | 5      | 1     |
| 1:A:30:GLY:O    | 1:A:32:SER:N    | 0.55     | 2.39        | 14     | 4     |
| 1:A:36:VAL:HG23 | 1:A:45:VAL:CG1  | 0.55     | 2.32        | 12     | 6     |
| 1:A:19:ILE:HG12 | 1:A:38:PHE:CD1  | 0.55     | 2.37        | 9      | 2     |
| 1:A:3:GLN:HG2   | 1:A:47:PHE:CZ   | 0.55     | 2.37        | 10     | 2     |
| 1:A:30:GLY:O    | 1:A:31:VAL:C    | 0.54     | 2.50        | 5      | 11    |
| 1:A:24:ALA:HB1  | 1:A:61:THR:CG2  | 0.54     | 2.32        | 13     | 6     |
| 1:A:17:CYS:CB   | 1:A:66:TYR:CD1  | 0.54     | 2.90        | 4      | 4     |
| 1:A:29:GLU:CG   | 1:A:51:LYS:CB   | 0.54     | 2.84        | 14     | 2     |
| 1:A:9:VAL:CG2   | 1:A:42:GLU:C    | 0.54     | 2.80        | 13     | 2     |
| 1:A:7:LEU:CB    | 1:A:43:ALA:O    | 0.54     | 2.55        | 1      | 4     |
| 1:A:36:VAL:CG2  | 1:A:43:ALA:HA   | 0.54     | 2.33        | 14     | 13    |
| 1:A:55:GLN:O    | 1:A:59:LYS:CB   | 0.54     | 2.55        | 1      | 4     |
| 1:A:3:GLN:HG2   | 1:A:47:PHE:CE2  | 0.54     | 2.37        | 13     | 3     |
| 1:A:53:SER:OG   | 1:A:54:VAL:N    | 0.54     | 2.41        | 8      | 9     |
| 1:A:26:SER:C    | 1:A:31:VAL:CG2  | 0.54     | 2.80        | 10     | 5     |
| 1:A:48:ASP:O    | 1:A:48:ASP:CG   | 0.54     | 2.51        | 6      | 6     |
| 1:A:17:CYS:HB3  | 1:A:66:TYR:CD1  | 0.54     | 2.38        | 6      | 5     |
| 1:A:58:THR:O    | 1:A:61:THR:HG22 | 0.54     | 2.03        | 5      | 3     |
| 1:A:33:LYS:O    | 1:A:45:VAL:HG13 | 0.54     | 2.02        | 11     | 1     |
| 1:A:39:GLU:O    | 1:A:40:LYS:CG   | 0.54     | 2.56        | 3      | 1     |
| 1:A:25:LEU:C    | 1:A:31:VAL:CG1  | 0.54     | 2.79        | 14     | 1     |
| 1:A:3:GLN:HG3   | 1:A:47:PHE:CZ   | 0.54     | 2.37        | 12     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:25:LEU:O    | 1:A:57:LEU:CD2  | 0.54     | 2.56        | 12     | 2     |
| 1:A:38:PHE:O    | 1:A:39:GLU:C    | 0.54     | 2.51        | 1      | 14    |
| 1:A:20:THR:HB   | 1:A:66:TYR:CD1  | 0.54     | 2.37        | 13     | 3     |
| 1:A:48:ASP:OD1  | 1:A:49:ASP:N    | 0.54     | 2.40        | 3      | 3     |
| 1:A:32:SER:CB   | 1:A:46:THR:O    | 0.54     | 2.55        | 13     | 6     |
| 1:A:36:VAL:HG13 | 1:A:43:ALA:CA   | 0.54     | 2.33        | 3      | 8     |
| 1:A:15:ALA:O    | 1:A:16:ALA:CB   | 0.54     | 2.56        | 5      | 5     |
| 1:A:7:LEU:CG    | 1:A:69:SER:O    | 0.54     | 2.56        | 14     | 10    |
| 1:A:44:VAL:O    | 1:A:45:VAL:CG1  | 0.54     | 2.56        | 14     | 10    |
| 1:A:8:ALA:HB3   | 1:A:69:SER:HB2  | 0.54     | 1.78        | 12     | 4     |
| 1:A:48:ASP:O    | 1:A:50:THR:N    | 0.54     | 2.41        | 2      | 10    |
| 1:A:20:THR:HB   | 1:A:66:TYR:CD2  | 0.54     | 2.38        | 1      | 2     |
| 1:A:28:VAL:HG12 | 1:A:29:GLU:H    | 0.54     | 1.63        | 10     | 6     |
| 1:A:11:GLY:O    | 1:A:12:MET:O    | 0.54     | 2.26        | 8      | 2     |
| 1:A:26:SER:HB2  | 1:A:31:VAL:HG23 | 0.54     | 1.79        | 7      | 1     |
| 1:A:7:LEU:HB2   | 1:A:43:ALA:O    | 0.54     | 2.03        | 3      | 12    |
| 1:A:54:VAL:CG1  | 1:A:55:GLN:N    | 0.54     | 2.71        | 4      | 3     |
| 1:A:47:PHE:CZ   | 1:A:53:SER:HA   | 0.54     | 2.38        | 4      | 1     |
| 1:A:3:GLN:CD    | 1:A:54:VAL:CG2  | 0.54     | 2.81        | 10     | 1     |
| 1:A:47:PHE:C    | 1:A:47:PHE:CD1  | 0.53     | 2.86        | 3      | 2     |
| 1:A:26:SER:C    | 1:A:31:VAL:HG22 | 0.53     | 2.28        | 10     | 1     |
| 1:A:8:ALA:N     | 1:A:69:SER:O    | 0.53     | 2.41        | 4      | 4     |
| 1:A:21:VAL:CG1  | 1:A:67:PRO:O    | 0.53     | 2.56        | 11     | 8     |
| 1:A:26:SER:N    | 1:A:34:VAL:HG21 | 0.53     | 2.18        | 9      | 3     |
| 1:A:17:CYS:CB   | 1:A:18:PRO:CD   | 0.53     | 2.86        | 5      | 2     |
| 1:A:4:THR:CB    | 1:A:46:THR:OG1  | 0.53     | 2.56        | 8      | 4     |
| 1:A:9:VAL:CG1   | 1:A:21:VAL:CG1  | 0.53     | 2.86        | 3      | 1     |
| 1:A:7:LEU:CA    | 1:A:69:SER:O    | 0.53     | 2.56        | 7      | 9     |
| 1:A:50:THR:O    | 1:A:51:LYS:CG   | 0.53     | 2.56        | 6      | 3     |
| 1:A:34:VAL:O    | 1:A:34:VAL:CG1  | 0.53     | 2.56        | 5      | 4     |
| 1:A:17:CYS:O    | 1:A:66:TYR:CB   | 0.53     | 2.56        | 12     | 4     |
| 1:A:21:VAL:CG2  | 1:A:67:PRO:O    | 0.53     | 2.56        | 2      | 12    |
| 1:A:46:THR:O    | 1:A:46:THR:CG2  | 0.53     | 2.56        | 6      | 2     |
| 1:A:7:LEU:CD2   | 1:A:69:SER:O    | 0.53     | 2.57        | 3      | 5     |
| 1:A:8:ALA:O     | 1:A:69:SER:N    | 0.53     | 2.42        | 1      | 7     |
| 1:A:17:CYS:O    | 1:A:66:TYR:CD2  | 0.53     | 2.62        | 3      | 3     |
| 1:A:29:GLU:CG   | 1:A:51:LYS:HB3  | 0.53     | 2.34        | 14     | 7     |
| 1:A:26:SER:HA   | 1:A:31:VAL:CG2  | 0.53     | 2.34        | 11     | 5     |
| 1:A:9:VAL:CG1   | 1:A:18:PRO:HB3  | 0.53     | 2.34        | 13     | 9     |
| 1:A:24:ALA:O    | 1:A:28:VAL:CG2  | 0.53     | 2.57        | 14     | 3     |
| 1:A:19:ILE:N    | 1:A:38:PHE:HB3  | 0.53     | 2.19        | 5      | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:26:SER:CA   | 1:A:31:VAL:HG13 | 0.53     | 2.33        | 13     | 2     |
| 1:A:40:LYS:O    | 1:A:41:ARG:CG   | 0.53     | 2.57        | 13     | 3     |
| 1:A:21:VAL:HG22 | 1:A:66:TYR:O    | 0.53     | 2.04        | 5      | 1     |
| 1:A:49:ASP:OD1  | 1:A:52:ALA:N    | 0.53     | 2.42        | 6      | 1     |
| 1:A:11:GLY:CA   | 1:A:14:CYS:SG   | 0.53     | 2.97        | 7      | 1     |
| 1:A:36:VAL:CG2  | 1:A:43:ALA:HB2  | 0.53     | 2.34        | 11     | 1     |
| 1:A:12:MET:O    | 1:A:13:THR:CB   | 0.53     | 2.57        | 13     | 1     |
| 1:A:53:SER:O    | 1:A:57:LEU:HD23 | 0.52     | 2.04        | 4      | 1     |
| 1:A:36:VAL:CB   | 1:A:43:ALA:HA   | 0.52     | 2.34        | 11     | 3     |
| 1:A:40:LYS:O    | 1:A:41:ARG:C    | 0.52     | 2.49        | 3      | 1     |
| 1:A:26:SER:O    | 1:A:31:VAL:CB   | 0.52     | 2.57        | 4      | 4     |
| 1:A:32:SER:N    | 1:A:46:THR:O    | 0.52     | 2.42        | 4      | 2     |
| 1:A:34:VAL:HA   | 1:A:45:VAL:HG12 | 0.52     | 1.82        | 12     | 3     |
| 1:A:3:GLN:HG2   | 1:A:47:PHE:CD2  | 0.52     | 2.40        | 13     | 1     |
| 1:A:23:LYS:O    | 1:A:27:LYS:CB   | 0.52     | 2.58        | 3      | 8     |
| 1:A:25:LEU:HD13 | 1:A:45:VAL:CG1  | 0.52     | 2.35        | 3      | 4     |
| 1:A:53:SER:O    | 1:A:57:LEU:CD2  | 0.52     | 2.57        | 4      | 1     |
| 1:A:36:VAL:CG2  | 1:A:45:VAL:HG13 | 0.52     | 2.35        | 13     | 5     |
| 1:A:40:LYS:O    | 1:A:41:ARG:CD   | 0.52     | 2.57        | 3      | 2     |
| 1:A:50:THR:O    | 1:A:51:LYS:CB   | 0.52     | 2.57        | 3      | 3     |
| 1:A:4:THR:C     | 1:A:5:VAL:HG13  | 0.52     | 2.30        | 2      | 3     |
| 1:A:11:GLY:O    | 1:A:14:CYS:N    | 0.52     | 2.42        | 1      | 1     |
| 1:A:17:CYS:N    | 1:A:18:PRO:HD2  | 0.52     | 2.20        | 13     | 11    |
| 1:A:31:VAL:HG12 | 1:A:31:VAL:O    | 0.52     | 2.04        | 2      | 1     |
| 1:A:40:LYS:C    | 1:A:41:ARG:CG   | 0.52     | 2.80        | 13     | 5     |
| 1:A:28:VAL:CG1  | 1:A:57:LEU:CB   | 0.52     | 2.88        | 4      | 1     |
| 1:A:26:SER:OG   | 1:A:34:VAL:CG2  | 0.52     | 2.58        | 5      | 1     |
| 1:A:61:THR:OG1  | 1:A:66:TYR:O    | 0.52     | 2.28        | 12     | 2     |
| 1:A:21:VAL:HG11 | 1:A:68:SER:OG   | 0.52     | 2.05        | 10     | 2     |
| 1:A:19:ILE:HD12 | 1:A:38:PHE:CD1  | 0.51     | 2.40        | 5      | 1     |
| 1:A:16:ALA:CB   | 1:A:19:ILE:HD12 | 0.51     | 2.30        | 7      | 1     |
| 1:A:44:VAL:C    | 1:A:45:VAL:HG13 | 0.51     | 2.31        | 14     | 9     |
| 1:A:17:CYS:HA   | 1:A:66:TYR:CD2  | 0.51     | 2.41        | 6      | 3     |
| 1:A:14:CYS:O    | 1:A:16:ALA:N    | 0.51     | 2.43        | 2      | 3     |
| 1:A:23:LYS:O    | 1:A:27:LYS:HB3  | 0.51     | 2.06        | 13     | 11    |
| 1:A:21:VAL:CG1  | 1:A:68:SER:OG   | 0.51     | 2.59        | 13     | 2     |
| 1:A:26:SER:HB3  | 1:A:34:VAL:HG11 | 0.51     | 1.82        | 2      | 1     |
| 1:A:12:MET:O    | 1:A:13:THR:C    | 0.51     | 2.53        | 3      | 2     |
| 1:A:65:GLY:C    | 1:A:66:TYR:CD1  | 0.51     | 2.89        | 10     | 4     |
| 1:A:25:LEU:CD1  | 1:A:43:ALA:HB1  | 0.51     | 2.36        | 4      | 4     |
| 1:A:17:CYS:HB2  | 1:A:18:PRO:CD   | 0.51     | 2.36        | 5      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:3:GLN:HB2   | 1:A:47:PHE:CZ   | 0.51     | 2.41        | 12     | 3     |
| 1:A:27:LYS:NZ   | 1:A:27:LYS:O    | 0.51     | 2.43        | 4      | 1     |
| 1:A:21:VAL:CG2  | 1:A:66:TYR:C    | 0.51     | 2.84        | 5      | 1     |
| 1:A:9:VAL:HB    | 1:A:21:VAL:CG1  | 0.51     | 2.34        | 2      | 2     |
| 1:A:22:LYS:HA   | 1:A:36:VAL:HB   | 0.51     | 1.82        | 14     | 11    |
| 1:A:24:ALA:HA   | 1:A:27:LYS:HG2  | 0.51     | 1.83        | 10     | 1     |
| 1:A:30:GLY:O    | 1:A:48:ASP:N    | 0.51     | 2.43        | 10     | 5     |
| 1:A:28:VAL:O    | 1:A:31:VAL:CG2  | 0.51     | 2.58        | 13     | 3     |
| 1:A:9:VAL:HG22  | 1:A:41:ARG:CA   | 0.51     | 2.36        | 3      | 1     |
| 1:A:36:VAL:HG13 | 1:A:43:ALA:CB   | 0.51     | 2.36        | 3      | 1     |
| 1:A:26:SER:CA   | 1:A:31:VAL:CG2  | 0.51     | 2.89        | 7      | 5     |
| 1:A:48:ASP:OD1  | 1:A:50:THR:N    | 0.51     | 2.43        | 10     | 1     |
| 1:A:8:ALA:HB3   | 1:A:69:SER:CB   | 0.51     | 2.36        | 1      | 1     |
| 1:A:20:THR:CB   | 1:A:66:TYR:CD1  | 0.51     | 2.94        | 13     | 1     |
| 1:A:13:THR:O    | 1:A:14:CYS:C    | 0.50     | 2.55        | 4      | 5     |
| 1:A:9:VAL:HG22  | 1:A:43:ALA:CB   | 0.50     | 2.36        | 10     | 2     |
| 1:A:49:ASP:O    | 1:A:51:LYS:N    | 0.50     | 2.44        | 6      | 2     |
| 1:A:9:VAL:CG1   | 1:A:21:VAL:HG21 | 0.50     | 2.36        | 11     | 3     |
| 1:A:23:LYS:O    | 1:A:24:ALA:C    | 0.50     | 2.54        | 8      | 5     |
| 1:A:47:PHE:CE1  | 1:A:53:SER:HA   | 0.50     | 2.41        | 4      | 1     |
| 1:A:47:PHE:CG   | 1:A:57:LEU:HD13 | 0.50     | 2.41        | 7      | 1     |
| 1:A:47:PHE:CD1  | 1:A:57:LEU:CD2  | 0.50     | 2.94        | 11     | 2     |
| 1:A:20:THR:O    | 1:A:21:VAL:C    | 0.50     | 2.55        | 8      | 13    |
| 1:A:28:VAL:CG1  | 1:A:57:LEU:HB2  | 0.50     | 2.35        | 4      | 3     |
| 1:A:47:PHE:CZ   | 1:A:54:VAL:HB   | 0.50     | 2.41        | 9      | 1     |
| 1:A:9:VAL:HG13  | 1:A:21:VAL:CG1  | 0.50     | 2.37        | 13     | 2     |
| 1:A:35:ASP:O    | 1:A:44:VAL:O    | 0.50     | 2.30        | 5      | 3     |
| 1:A:54:VAL:O    | 1:A:58:THR:CG2  | 0.50     | 2.58        | 11     | 1     |
| 1:A:33:LYS:N    | 1:A:46:THR:HG23 | 0.50     | 2.22        | 9      | 3     |
| 1:A:29:GLU:N    | 1:A:29:GLU:CD   | 0.50     | 2.69        | 9      | 2     |
| 1:A:33:LYS:O    | 1:A:46:THR:N    | 0.50     | 2.42        | 12     | 2     |
| 1:A:18:PRO:CG   | 1:A:38:PHE:HB2  | 0.50     | 2.37        | 11     | 12    |
| 1:A:7:LEU:O     | 1:A:43:ALA:O    | 0.50     | 2.30        | 3      | 1     |
| 1:A:25:LEU:HB3  | 1:A:45:VAL:HG21 | 0.50     | 1.82        | 10     | 1     |
| 1:A:24:ALA:CB   | 1:A:61:THR:HG22 | 0.50     | 2.36        | 7      | 1     |
| 1:A:29:GLU:N    | 1:A:29:GLU:OE1  | 0.50     | 2.45        | 9      | 1     |
| 1:A:3:GLN:HG3   | 1:A:47:PHE:CE2  | 0.50     | 2.41        | 1      | 2     |
| 1:A:22:LYS:CD   | 1:A:36:VAL:O    | 0.50     | 2.60        | 3      | 5     |
| 1:A:17:CYS:CA   | 1:A:66:TYR:CG   | 0.50     | 2.95        | 7      | 2     |
| 1:A:12:MET:CG   | 1:A:41:ARG:HB3  | 0.50     | 2.37        | 7      | 1     |
| 1:A:10:PRO:O    | 1:A:11:GLY:C    | 0.49     | 2.55        | 13     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:49:ASP:CG   | 1:A:49:ASP:O    | 0.49     | 2.56        | 3      | 3     |
| 1:A:16:ALA:HA   | 1:A:38:PHE:CD1  | 0.49     | 2.43        | 10     | 4     |
| 1:A:71:LYS:O    | 1:A:72:GLN:CB   | 0.49     | 2.58        | 2      | 2     |
| 1:A:12:MET:HG3  | 1:A:41:ARG:CB   | 0.49     | 2.37        | 7      | 1     |
| 1:A:33:LYS:HB3  | 1:A:46:THR:CB   | 0.49     | 2.36        | 14     | 1     |
| 1:A:14:CYS:O    | 1:A:15:ALA:C    | 0.49     | 2.56        | 7      | 4     |
| 1:A:30:GLY:O    | 1:A:47:PHE:CA   | 0.49     | 2.61        | 10     | 3     |
| 1:A:55:GLN:O    | 1:A:59:LYS:N    | 0.49     | 2.43        | 12     | 4     |
| 1:A:47:PHE:CG   | 1:A:57:LEU:HD22 | 0.49     | 2.41        | 6      | 4     |
| 1:A:7:LEU:O     | 1:A:43:ALA:CB   | 0.49     | 2.60        | 5      | 1     |
| 1:A:17:CYS:HB3  | 1:A:66:TYR:CG   | 0.49     | 2.42        | 6      | 1     |
| 1:A:13:THR:O    | 1:A:13:THR:OG1  | 0.49     | 2.30        | 13     | 2     |
| 1:A:38:PHE:C    | 1:A:40:LYS:N    | 0.49     | 2.70        | 9      | 13    |
| 1:A:55:GLN:O    | 1:A:59:LYS:CG   | 0.49     | 2.60        | 14     | 2     |
| 1:A:20:THR:CB   | 1:A:66:TYR:CD2  | 0.49     | 2.96        | 1      | 1     |
| 1:A:9:VAL:CG2   | 1:A:41:ARG:HA   | 0.49     | 2.38        | 3      | 1     |
| 1:A:19:ILE:HG12 | 1:A:38:PHE:CG   | 0.49     | 2.42        | 1      | 2     |
| 1:A:38:PHE:O    | 1:A:40:LYS:N    | 0.49     | 2.46        | 1      | 13    |
| 1:A:40:LYS:O    | 1:A:41:ARG:HB3  | 0.49     | 2.08        | 12     | 12    |
| 1:A:48:ASP:OD2  | 1:A:50:THR:OG1  | 0.49     | 2.31        | 3      | 5     |
| 1:A:19:ILE:N    | 1:A:38:PHE:HB2  | 0.49     | 2.22        | 11     | 6     |
| 1:A:9:VAL:HG11  | 1:A:18:PRO:CB   | 0.49     | 2.37        | 10     | 3     |
| 1:A:9:VAL:CG2   | 1:A:43:ALA:N    | 0.49     | 2.75        | 10     | 2     |
| 1:A:30:GLY:O    | 1:A:47:PHE:HA   | 0.49     | 2.08        | 13     | 4     |
| 1:A:4:THR:HB    | 1:A:46:THR:OG1  | 0.49     | 2.08        | 2      | 4     |
| 1:A:4:THR:HA    | 1:A:46:THR:CB   | 0.49     | 2.37        | 9      | 3     |
| 1:A:26:SER:CB   | 1:A:34:VAL:HB   | 0.49     | 2.37        | 3      | 5     |
| 1:A:49:ASP:OD1  | 1:A:49:ASP:O    | 0.49     | 2.31        | 11     | 3     |
| 1:A:47:PHE:CD1  | 1:A:57:LEU:HD23 | 0.49     | 2.42        | 8      | 1     |
| 1:A:6:THR:O     | 1:A:71:LYS:CA   | 0.49     | 2.60        | 11     | 1     |
| 1:A:25:LEU:O    | 1:A:57:LEU:HD23 | 0.49     | 2.08        | 12     | 1     |
| 1:A:7:LEU:HG    | 1:A:69:SER:O    | 0.49     | 2.07        | 4      | 8     |
| 1:A:9:VAL:HG13  | 1:A:43:ALA:HB2  | 0.49     | 1.82        | 3      | 1     |
| 1:A:19:ILE:CG1  | 1:A:38:PHE:HB3  | 0.49     | 2.38        | 7      | 5     |
| 1:A:3:GLN:N     | 1:A:47:PHE:O    | 0.49     | 2.44        | 10     | 6     |
| 1:A:40:LYS:O    | 1:A:41:ARG:NE   | 0.49     | 2.46        | 12     | 1     |
| 1:A:9:VAL:CG2   | 1:A:18:PRO:HB3  | 0.48     | 2.38        | 1      | 4     |
| 1:A:11:GLY:O    | 1:A:12:MET:C    | 0.48     | 2.56        | 11     | 5     |
| 1:A:49:ASP:C    | 1:A:51:LYS:N    | 0.48     | 2.68        | 6      | 5     |
| 1:A:49:ASP:OD1  | 1:A:52:ALA:O    | 0.48     | 2.32        | 9      | 5     |
| 1:A:21:VAL:HG22 | 1:A:66:TYR:C    | 0.48     | 2.33        | 5      | 2     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:54:VAL:O   | 1:A:58:THR:OG1  | 0.48     | 2.28        | 11     | 4     |
| 1:A:9:VAL:HG21 | 1:A:36:VAL:HG13 | 0.48     | 1.85        | 12     | 1     |
| 1:A:22:LYS:HA  | 1:A:36:VAL:CB   | 0.48     | 2.38        | 14     | 9     |
| 1:A:13:THR:O   | 1:A:14:CYS:O    | 0.48     | 2.31        | 5      | 3     |
| 1:A:9:VAL:HG23 | 1:A:43:ALA:N    | 0.48     | 2.23        | 10     | 2     |
| 1:A:25:LEU:CD1 | 1:A:45:VAL:HG11 | 0.48     | 2.37        | 2      | 2     |
| 1:A:25:LEU:O   | 1:A:31:VAL:CG2  | 0.48     | 2.61        | 2      | 1     |
| 1:A:58:THR:O   | 1:A:59:LYS:C    | 0.48     | 2.56        | 11     | 7     |
| 1:A:9:VAL:HG22 | 1:A:41:ARG:HA   | 0.48     | 1.84        | 3      | 1     |
| 1:A:17:CYS:CB  | 1:A:18:PRO:HD3  | 0.48     | 2.39        | 10     | 2     |
| 1:A:26:SER:N   | 1:A:31:VAL:CG1  | 0.48     | 2.77        | 14     | 1     |
| 1:A:19:ILE:CG1 | 1:A:38:PHE:CD1  | 0.48     | 2.97        | 2      | 2     |
| 1:A:28:VAL:CG2 | 1:A:57:LEU:HA   | 0.48     | 2.36        | 11     | 7     |
| 1:A:24:ALA:HA  | 1:A:27:LYS:CG   | 0.48     | 2.38        | 5      | 4     |
| 1:A:58:THR:HA  | 1:A:61:THR:CG2  | 0.48     | 2.38        | 12     | 3     |
| 1:A:38:PHE:CD1 | 1:A:38:PHE:O    | 0.48     | 2.65        | 14     | 1     |
| 1:A:18:PRO:O   | 1:A:19:ILE:C    | 0.48     | 2.55        | 9      | 7     |
| 1:A:48:ASP:OD1 | 1:A:50:THR:OG1  | 0.48     | 2.32        | 8      | 6     |
| 1:A:16:ALA:O   | 1:A:19:ILE:HG22 | 0.48     | 2.08        | 5      | 2     |
| 1:A:49:ASP:O   | 1:A:49:ASP:CG   | 0.48     | 2.57        | 11     | 2     |
| 1:A:21:VAL:O   | 1:A:22:LYS:C    | 0.48     | 2.56        | 13     | 13    |
| 1:A:4:THR:CA   | 1:A:46:THR:OG1  | 0.48     | 2.61        | 8      | 1     |
| 1:A:33:LYS:HB2 | 1:A:46:THR:HG22 | 0.48     | 1.85        | 8      | 1     |
| 1:A:4:THR:C    | 1:A:5:VAL:HG22  | 0.48     | 2.33        | 9      | 6     |
| 1:A:12:MET:CG  | 1:A:41:ARG:HB2  | 0.48     | 2.38        | 10     | 1     |
| 1:A:6:THR:O    | 1:A:71:LYS:CB   | 0.48     | 2.62        | 13     | 2     |
| 1:A:25:LEU:O   | 1:A:27:LYS:N    | 0.48     | 2.46        | 14     | 1     |
| 1:A:4:THR:HB   | 1:A:46:THR:CG2  | 0.48     | 2.39        | 4      | 5     |
| 1:A:12:MET:CA  | 1:A:41:ARG:HB3  | 0.48     | 2.39        | 3      | 1     |
| 1:A:7:LEU:C    | 1:A:43:ALA:HB3  | 0.48     | 2.34        | 5      | 1     |
| 1:A:12:MET:HA  | 1:A:41:ARG:CG   | 0.48     | 2.39        | 3      | 1     |
| 1:A:24:ALA:CB  | 1:A:61:THR:HB   | 0.48     | 2.38        | 6      | 3     |
| 1:A:35:ASP:C   | 1:A:44:VAL:O    | 0.48     | 2.57        | 5      | 2     |
| 1:A:49:ASP:CG  | 1:A:52:ALA:O    | 0.48     | 2.57        | 6      | 2     |
| 1:A:22:LYS:HA  | 1:A:36:VAL:CG1  | 0.48     | 2.39        | 11     | 5     |
| 1:A:47:PHE:CD1 | 1:A:47:PHE:C    | 0.48     | 2.91        | 12     | 5     |
| 1:A:25:LEU:O   | 1:A:31:VAL:HG22 | 0.48     | 2.09        | 2      | 5     |
| 1:A:57:LEU:HG  | 1:A:58:THR:N    | 0.48     | 2.23        | 8      | 2     |
| 1:A:36:VAL:HB  | 1:A:43:ALA:CA   | 0.48     | 2.39        | 11     | 2     |
| 1:A:48:ASP:OD1 | 1:A:48:ASP:C    | 0.47     | 2.56        | 4      | 5     |
| 1:A:12:MET:C   | 1:A:13:THR:CG2  | 0.47     | 2.87        | 8      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:16:ALA:HA   | 1:A:38:PHE:CG   | 0.47     | 2.44        | 14     | 2     |
| 1:A:54:VAL:HG22 | 1:A:70:VAL:HG21 | 0.47     | 1.85        | 8      | 1     |
| 1:A:29:GLU:HG3  | 1:A:51:LYS:CB   | 0.47     | 2.39        | 14     | 1     |
| 1:A:17:CYS:O    | 1:A:20:THR:OG1  | 0.47     | 2.32        | 1      | 5     |
| 1:A:33:LYS:CB   | 1:A:46:THR:HB   | 0.47     | 2.39        | 14     | 2     |
| 1:A:9:VAL:HG21  | 1:A:43:ALA:HB2  | 0.47     | 1.86        | 10     | 1     |
| 1:A:48:ASP:O    | 1:A:48:ASP:OD2  | 0.47     | 2.33        | 2      | 4     |
| 1:A:4:THR:OG1   | 1:A:46:THR:OG1  | 0.47     | 2.29        | 7      | 2     |
| 1:A:16:ALA:HA   | 1:A:38:PHE:CE1  | 0.47     | 2.44        | 10     | 2     |
| 1:A:17:CYS:HA   | 1:A:66:TYR:CD1  | 0.47     | 2.43        | 10     | 2     |
| 1:A:53:SER:O    | 1:A:54:VAL:C    | 0.47     | 2.57        | 7      | 1     |
| 1:A:47:PHE:CZ   | 1:A:57:LEU:HD23 | 0.47     | 2.44        | 13     | 2     |
| 1:A:9:VAL:O     | 1:A:10:PRO:O    | 0.47     | 2.33        | 2      | 3     |
| 1:A:18:PRO:HB2  | 1:A:38:PHE:HA   | 0.47     | 1.86        | 11     | 11    |
| 1:A:27:LYS:O    | 1:A:27:LYS:CE   | 0.47     | 2.62        | 4      | 1     |
| 1:A:29:GLU:OE1  | 1:A:51:LYS:CB   | 0.47     | 2.63        | 8      | 1     |
| 1:A:48:ASP:OD1  | 1:A:50:THR:CG2  | 0.47     | 2.62        | 10     | 2     |
| 1:A:25:LEU:CB   | 1:A:31:VAL:HG11 | 0.47     | 2.40        | 14     | 1     |
| 1:A:17:CYS:HB2  | 1:A:18:PRO:HD3  | 0.47     | 1.84        | 5      | 2     |
| 1:A:26:SER:CB   | 1:A:31:VAL:CG2  | 0.47     | 2.92        | 7      | 1     |
| 1:A:36:VAL:HG22 | 1:A:44:VAL:N    | 0.47     | 2.24        | 14     | 3     |
| 1:A:61:THR:O    | 1:A:66:TYR:O    | 0.47     | 2.33        | 4      | 10    |
| 1:A:4:THR:C     | 1:A:5:VAL:CG1   | 0.47     | 2.88        | 7      | 2     |
| 1:A:44:VAL:C    | 1:A:45:VAL:CG1  | 0.47     | 2.87        | 7      | 8     |
| 1:A:12:MET:HE2  | 1:A:41:ARG:CB   | 0.47     | 2.40        | 3      | 1     |
| 1:A:47:PHE:HB2  | 1:A:57:LEU:HD11 | 0.47     | 1.85        | 7      | 1     |
| 1:A:47:PHE:CE2  | 1:A:53:SER:HA   | 0.47     | 2.45        | 7      | 1     |
| 1:A:9:VAL:O     | 1:A:10:PRO:C    | 0.47     | 2.57        | 12     | 1     |
| 1:A:25:LEU:O    | 1:A:31:VAL:HG21 | 0.47     | 2.10        | 14     | 1     |
| 1:A:48:ASP:O    | 1:A:48:ASP:OD1  | 0.47     | 2.33        | 14     | 1     |
| 1:A:9:VAL:HG12  | 1:A:43:ALA:CB   | 0.47     | 2.40        | 2      | 1     |
| 1:A:6:THR:O     | 1:A:71:LYS:C    | 0.47     | 2.57        | 11     | 1     |
| 1:A:3:GLN:O     | 1:A:46:THR:HA   | 0.47     | 2.09        | 13     | 4     |
| 1:A:36:VAL:HG23 | 1:A:45:VAL:HG13 | 0.47     | 1.87        | 1      | 1     |
| 1:A:58:THR:HG22 | 1:A:68:SER:HB3  | 0.47     | 1.87        | 3      | 1     |
| 1:A:9:VAL:CG2   | 1:A:42:GLU:N    | 0.47     | 2.78        | 13     | 1     |
| 1:A:29:GLU:HB2  | 1:A:52:ALA:CB   | 0.47     | 2.36        | 5      | 6     |
| 1:A:33:LYS:CB   | 1:A:46:THR:HG22 | 0.47     | 2.40        | 6      | 1     |
| 1:A:32:SER:C    | 1:A:33:LYS:HG3  | 0.47     | 2.34        | 8      | 1     |
| 1:A:62:ALA:CB   | 1:A:67:PRO:HB3  | 0.46     | 2.41        | 5      | 11    |
| 1:A:29:GLU:HB3  | 1:A:51:LYS:C    | 0.46     | 2.34        | 11     | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:30:GLY:HA3  | 1:A:48:ASP:O    | 0.46     | 2.10        | 5      | 6     |
| 1:A:9:VAL:HG12  | 1:A:42:GLU:N    | 0.46     | 2.25        | 4      | 1     |
| 1:A:4:THR:HG1   | 1:A:46:THR:CB   | 0.46     | 2.22        | 6      | 1     |
| 1:A:67:PRO:O    | 1:A:68:SER:CB   | 0.46     | 2.63        | 8      | 1     |
| 1:A:3:GLN:O     | 1:A:47:PHE:O    | 0.46     | 2.33        | 10     | 1     |
| 1:A:29:GLU:OE1  | 1:A:29:GLU:N    | 0.46     | 2.48        | 13     | 1     |
| 1:A:12:MET:HG2  | 1:A:41:ARG:CB   | 0.46     | 2.40        | 7      | 3     |
| 1:A:49:ASP:O    | 1:A:49:ASP:OD1  | 0.46     | 2.33        | 2      | 2     |
| 1:A:57:LEU:CD1  | 1:A:58:THR:HG23 | 0.46     | 2.41        | 5      | 3     |
| 1:A:16:ALA:HB1  | 1:A:19:ILE:HG21 | 0.46     | 1.87        | 5      | 1     |
| 1:A:18:PRO:C    | 1:A:20:THR:N    | 0.46     | 2.71        | 3      | 3     |
| 1:A:41:ARG:O    | 1:A:41:ARG:HG2  | 0.46     | 2.11        | 5      | 6     |
| 1:A:29:GLU:HB3  | 1:A:51:LYS:CB   | 0.46     | 2.40        | 2      | 3     |
| 1:A:47:PHE:CE1  | 1:A:57:LEU:HD13 | 0.46     | 2.45        | 1      | 2     |
| 1:A:9:VAL:CG2   | 1:A:21:VAL:HG11 | 0.46     | 2.38        | 4      | 2     |
| 1:A:41:ARG:NH1  | 1:A:41:ARG:CG   | 0.46     | 2.78        | 7      | 2     |
| 1:A:11:GLY:C    | 1:A:12:MET:CG   | 0.46     | 2.87        | 1      | 2     |
| 1:A:61:THR:OG1  | 1:A:67:PRO:HA   | 0.46     | 2.10        | 2      | 8     |
| 1:A:22:LYS:HD3  | 1:A:36:VAL:O    | 0.46     | 2.10        | 3      | 1     |
| 1:A:23:LYS:HG3  | 1:A:24:ALA:N    | 0.46     | 2.24        | 14     | 2     |
| 1:A:24:ALA:CA   | 1:A:27:LYS:HG2  | 0.46     | 2.41        | 10     | 1     |
| 1:A:33:LYS:CB   | 1:A:46:THR:CB   | 0.46     | 2.93        | 14     | 1     |
| 1:A:20:THR:OG1  | 1:A:66:TYR:CD1  | 0.46     | 2.68        | 2      | 1     |
| 1:A:33:LYS:HG3  | 1:A:46:THR:CB   | 0.46     | 2.40        | 5      | 1     |
| 1:A:38:PHE:O    | 1:A:38:PHE:CG   | 0.46     | 2.68        | 7      | 5     |
| 1:A:6:THR:O     | 1:A:71:LYS:O    | 0.46     | 2.33        | 8      | 1     |
| 1:A:7:LEU:O     | 1:A:43:ALA:C    | 0.46     | 2.59        | 3      | 1     |
| 1:A:9:VAL:O     | 1:A:12:MET:HE3  | 0.46     | 2.11        | 3      | 1     |
| 1:A:14:CYS:O    | 1:A:14:CYS:SG   | 0.46     | 2.73        | 9      | 2     |
| 1:A:25:LEU:O    | 1:A:28:VAL:CG1  | 0.46     | 2.59        | 11     | 1     |
| 1:A:18:PRO:CB   | 1:A:38:PHE:HB2  | 0.46     | 2.41        | 9      | 4     |
| 1:A:32:SER:HB2  | 1:A:46:THR:O    | 0.46     | 2.11        | 4      | 5     |
| 1:A:62:ALA:CA   | 1:A:67:PRO:HB3  | 0.46     | 2.41        | 9      | 7     |
| 1:A:4:THR:OG1   | 1:A:46:THR:HB   | 0.46     | 2.11        | 9      | 4     |
| 1:A:7:LEU:O     | 1:A:43:ALA:CA   | 0.46     | 2.64        | 3      | 1     |
| 1:A:40:LYS:C    | 1:A:41:ARG:HG3  | 0.46     | 2.36        | 8      | 3     |
| 1:A:28:VAL:HB   | 1:A:57:LEU:CD2  | 0.46     | 2.41        | 7      | 3     |
| 1:A:54:VAL:O    | 1:A:55:GLN:C    | 0.46     | 2.56        | 7      | 1     |
| 1:A:25:LEU:HD22 | 1:A:45:VAL:CG2  | 0.46     | 2.40        | 10     | 1     |
| 1:A:30:GLY:O    | 1:A:31:VAL:O    | 0.46     | 2.34        | 13     | 3     |
| 1:A:40:LYS:O    | 1:A:41:ARG:HD2  | 0.46     | 2.11        | 3      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:41:ARG:O    | 1:A:42:GLU:CG   | 0.46     | 2.64        | 10     | 1     |
| 1:A:30:GLY:HA2  | 1:A:50:THR:CB   | 0.45     | 2.41        | 11     | 5     |
| 1:A:20:THR:HB   | 1:A:66:TYR:CG   | 0.45     | 2.45        | 8      | 1     |
| 1:A:26:SER:HB2  | 1:A:34:VAL:HB   | 0.45     | 1.89        | 10     | 1     |
| 1:A:53:SER:O    | 1:A:57:LEU:HD12 | 0.45     | 2.11        | 12     | 3     |
| 1:A:9:VAL:CG1   | 1:A:42:GLU:N    | 0.45     | 2.79        | 4      | 1     |
| 1:A:36:VAL:CG2  | 1:A:37:GLY:N    | 0.45     | 2.79        | 11     | 2     |
| 1:A:25:LEU:O    | 1:A:26:SER:C    | 0.45     | 2.58        | 14     | 1     |
| 1:A:12:MET:N    | 1:A:18:PRO:HG3  | 0.45     | 2.26        | 13     | 3     |
| 1:A:26:SER:O    | 1:A:31:VAL:HB   | 0.45     | 2.12        | 4      | 3     |
| 1:A:26:SER:HB3  | 1:A:34:VAL:CG2  | 0.45     | 2.41        | 11     | 1     |
| 1:A:47:PHE:CB   | 1:A:57:LEU:CD1  | 0.45     | 2.94        | 7      | 1     |
| 1:A:48:ASP:OD1  | 1:A:50:THR:HG22 | 0.45     | 2.11        | 13     | 1     |
| 1:A:36:VAL:HB   | 1:A:43:ALA:HA   | 0.45     | 1.89        | 11     | 3     |
| 1:A:23:LYS:O    | 1:A:27:LYS:HG2  | 0.45     | 2.12        | 8      | 4     |
| 1:A:33:LYS:HG3  | 1:A:46:THR:HG21 | 0.45     | 1.89        | 8      | 1     |
| 1:A:7:LEU:HA    | 1:A:69:SER:O    | 0.45     | 2.11        | 14     | 7     |
| 1:A:58:THR:C    | 1:A:61:THR:HG22 | 0.45     | 2.37        | 12     | 2     |
| 1:A:34:VAL:HG23 | 1:A:45:VAL:HG12 | 0.45     | 1.89        | 1      | 1     |
| 1:A:41:ARG:CG   | 1:A:41:ARG:NH1  | 0.45     | 2.78        | 10     | 2     |
| 1:A:67:PRO:C    | 1:A:68:SER:OG   | 0.45     | 2.56        | 8      | 1     |
| 1:A:11:GLY:HA3  | 1:A:17:CYS:CB   | 0.45     | 2.42        | 10     | 1     |
| 1:A:34:VAL:O    | 1:A:34:VAL:HG22 | 0.45     | 2.11        | 14     | 1     |
| 1:A:58:THR:O    | 1:A:61:THR:N    | 0.45     | 2.50        | 11     | 2     |
| 1:A:22:LYS:CA   | 1:A:36:VAL:HB   | 0.45     | 2.42        | 8      | 6     |
| 1:A:12:MET:HB3  | 1:A:41:ARG:CB   | 0.45     | 2.41        | 14     | 1     |
| 1:A:12:MET:HA   | 1:A:41:ARG:CB   | 0.45     | 2.42        | 10     | 2     |
| 1:A:54:VAL:HG21 | 1:A:70:VAL:HG12 | 0.45     | 1.88        | 3      | 1     |
| 1:A:7:LEU:HD23  | 1:A:68:SER:CB   | 0.45     | 2.42        | 4      | 1     |
| 1:A:22:LYS:CG   | 1:A:36:VAL:HB   | 0.45     | 2.42        | 12     | 4     |
| 1:A:36:VAL:CG1  | 1:A:43:ALA:HA   | 0.45     | 2.42        | 1      | 3     |
| 1:A:47:PHE:CE1  | 1:A:57:LEU:HD21 | 0.45     | 2.47        | 6      | 1     |
| 1:A:9:VAL:HG12  | 1:A:11:GLY:H    | 0.45     | 1.72        | 14     | 1     |
| 1:A:21:VAL:CG1  | 1:A:68:SER:HB3  | 0.44     | 2.43        | 8      | 1     |
| 1:A:16:ALA:HA   | 1:A:38:PHE:CD2  | 0.44     | 2.48        | 4      | 1     |
| 1:A:33:LYS:N    | 1:A:46:THR:HB   | 0.44     | 2.28        | 4      | 2     |
| 1:A:12:MET:HG2  | 1:A:41:ARG:CD   | 0.44     | 2.43        | 9      | 1     |
| 1:A:47:PHE:CZ   | 1:A:57:LEU:HD13 | 0.44     | 2.47        | 10     | 1     |
| 1:A:4:THR:HA    | 1:A:46:THR:HA   | 0.44     | 1.90        | 12     | 4     |
| 1:A:17:CYS:O    | 1:A:66:TYR:HB3  | 0.44     | 2.13        | 6      | 7     |
| 1:A:26:SER:HB2  | 1:A:31:VAL:CG2  | 0.44     | 2.42        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:VAL:HG12  | 1:A:6:THR:H     | 0.44     | 1.72        | 3      | 1     |
| 1:A:61:THR:CB   | 1:A:67:PRO:HA   | 0.44     | 2.43        | 10     | 1     |
| 1:A:3:GLN:OE1   | 1:A:3:GLN:C     | 0.44     | 2.60        | 12     | 1     |
| 1:A:29:GLU:C    | 1:A:52:ALA:CB   | 0.44     | 2.91        | 12     | 1     |
| 1:A:33:LYS:CB   | 1:A:46:THR:OG1  | 0.44     | 2.66        | 14     | 1     |
| 1:A:9:VAL:O     | 1:A:9:VAL:HG22  | 0.44     | 2.11        | 2      | 1     |
| 1:A:22:LYS:CG   | 1:A:36:VAL:HG13 | 0.44     | 2.42        | 5      | 3     |
| 1:A:32:SER:C    | 1:A:33:LYS:CG   | 0.44     | 2.90        | 8      | 1     |
| 1:A:9:VAL:HG13  | 1:A:21:VAL:HG21 | 0.44     | 1.90        | 14     | 1     |
| 1:A:53:SER:O    | 1:A:57:LEU:HG   | 0.44     | 2.13        | 2      | 3     |
| 1:A:69:SER:OG   | 1:A:70:VAL:N    | 0.44     | 2.51        | 6      | 1     |
| 1:A:36:VAL:HG12 | 1:A:37:GLY:N    | 0.44     | 2.27        | 8      | 5     |
| 1:A:28:VAL:HG22 | 1:A:29:GLU:H    | 0.44     | 1.73        | 11     | 4     |
| 1:A:42:GLU:O    | 1:A:42:GLU:CG   | 0.44     | 2.65        | 3      | 1     |
| 1:A:29:GLU:HG2  | 1:A:51:LYS:CB   | 0.44     | 2.42        | 11     | 1     |
| 1:A:9:VAL:CG1   | 1:A:43:ALA:N    | 0.44     | 2.81        | 2      | 2     |
| 1:A:33:LYS:H    | 1:A:46:THR:HG23 | 0.44     | 1.73        | 9      | 2     |
| 1:A:48:ASP:C    | 1:A:50:THR:N    | 0.44     | 2.76        | 14     | 5     |
| 1:A:30:GLY:CA   | 1:A:48:ASP:O    | 0.44     | 2.66        | 5      | 2     |
| 1:A:47:PHE:CZ   | 1:A:53:SER:CA   | 0.44     | 3.01        | 4      | 1     |
| 1:A:7:LEU:HB3   | 1:A:69:SER:O    | 0.44     | 2.13        | 7      | 2     |
| 1:A:36:VAL:HG21 | 1:A:43:ALA:CB   | 0.44     | 2.43        | 10     | 1     |
| 1:A:49:ASP:HB2  | 1:A:52:ALA:C    | 0.44     | 2.37        | 6      | 1     |
| 1:A:32:SER:HB3  | 1:A:46:THR:O    | 0.44     | 2.13        | 13     | 1     |
| 1:A:35:ASP:O    | 1:A:44:VAL:HB   | 0.43     | 2.12        | 5      | 3     |
| 1:A:57:LEU:HD11 | 1:A:58:THR:HG23 | 0.43     | 1.90        | 5      | 1     |
| 1:A:25:LEU:C    | 1:A:27:LYS:N    | 0.43     | 2.75        | 14     | 1     |
| 1:A:22:LYS:HA   | 1:A:36:VAL:HG11 | 0.43     | 1.90        | 1      | 3     |
| 1:A:38:PHE:C    | 1:A:38:PHE:CD1  | 0.43     | 2.95        | 2      | 1     |
| 1:A:57:LEU:CG   | 1:A:58:THR:N    | 0.43     | 2.81        | 13     | 2     |
| 1:A:12:MET:O    | 1:A:13:THR:HG22 | 0.43     | 2.12        | 3      | 1     |
| 1:A:71:LYS:O    | 1:A:72:GLN:HB3  | 0.43     | 2.12        | 5      | 1     |
| 1:A:35:ASP:C    | 1:A:35:ASP:OD1  | 0.43     | 2.60        | 10     | 1     |
| 1:A:33:LYS:HB3  | 1:A:46:THR:N    | 0.43     | 2.28        | 14     | 1     |
| 1:A:28:VAL:CG2  | 1:A:57:LEU:HB2  | 0.43     | 2.41        | 4      | 1     |
| 1:A:34:VAL:HA   | 1:A:45:VAL:CG1  | 0.43     | 2.42        | 12     | 1     |
| 1:A:29:GLU:OE1  | 1:A:51:LYS:HB2  | 0.43     | 2.13        | 2      | 2     |
| 1:A:53:SER:O    | 1:A:57:LEU:CG   | 0.43     | 2.66        | 4      | 1     |
| 1:A:7:LEU:HB2   | 1:A:43:ALA:HB3  | 0.43     | 1.91        | 12     | 1     |
| 1:A:18:PRO:HG2  | 1:A:38:PHE:CB   | 0.43     | 2.43        | 13     | 1     |
| 1:A:14:CYS:C    | 1:A:16:ALA:N    | 0.43     | 2.75        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:22:LYS:HD2  | 1:A:36:VAL:O    | 0.43     | 2.13        | 6      | 3     |
| 1:A:35:ASP:HB2  | 1:A:44:VAL:O    | 0.43     | 2.14        | 8      | 1     |
| 1:A:31:VAL:HG12 | 1:A:32:SER:N    | 0.43     | 2.27        | 10     | 1     |
| 1:A:19:ILE:CA   | 1:A:38:PHE:HB3  | 0.43     | 2.44        | 10     | 2     |
| 1:A:17:CYS:C    | 1:A:66:TYR:HB3  | 0.43     | 2.39        | 7      | 1     |
| 1:A:26:SER:HB2  | 1:A:34:VAL:CG2  | 0.43     | 2.43        | 10     | 2     |
| 1:A:12:MET:CB   | 1:A:41:ARG:HB3  | 0.43     | 2.44        | 10     | 1     |
| 1:A:29:GLU:C    | 1:A:52:ALA:HB2  | 0.43     | 2.39        | 12     | 1     |
| 1:A:18:PRO:HG2  | 1:A:38:PHE:HB2  | 0.43     | 1.91        | 3      | 2     |
| 1:A:61:THR:HG23 | 1:A:67:PRO:HA   | 0.43     | 1.90        | 12     | 2     |
| 1:A:58:THR:CG2  | 1:A:68:SER:O    | 0.43     | 2.57        | 8      | 1     |
| 1:A:70:VAL:HG12 | 1:A:71:LYS:N    | 0.43     | 2.28        | 8      | 1     |
| 1:A:9:VAL:HG23  | 1:A:41:ARG:C    | 0.43     | 2.38        | 13     | 1     |
| 1:A:48:ASP:CG   | 1:A:50:THR:OG1  | 0.43     | 2.62        | 14     | 1     |
| 1:A:7:LEU:CA    | 1:A:43:ALA:O    | 0.43     | 2.67        | 3      | 1     |
| 1:A:47:PHE:CG   | 1:A:57:LEU:CD1  | 0.43     | 3.02        | 7      | 1     |
| 1:A:55:GLN:O    | 1:A:59:LYS:HB3  | 0.42     | 2.14        | 1      | 2     |
| 1:A:4:THR:CB    | 1:A:46:THR:CG2  | 0.42     | 2.97        | 4      | 3     |
| 1:A:7:LEU:CD2   | 1:A:25:LEU:HD21 | 0.42     | 2.39        | 4      | 1     |
| 1:A:9:VAL:CG1   | 1:A:41:ARG:C    | 0.42     | 2.92        | 4      | 1     |
| 1:A:26:SER:HB3  | 1:A:34:VAL:HG21 | 0.42     | 1.91        | 11     | 2     |
| 1:A:26:SER:HB2  | 1:A:34:VAL:CB   | 0.42     | 2.44        | 9      | 2     |
| 1:A:9:VAL:HG13  | 1:A:21:VAL:CB   | 0.42     | 2.44        | 12     | 1     |
| 1:A:62:ALA:HA   | 1:A:67:PRO:CG   | 0.42     | 2.44        | 14     | 1     |
| 1:A:21:VAL:CG2  | 1:A:66:TYR:HB2  | 0.42     | 2.44        | 3      | 1     |
| 1:A:23:LYS:CG   | 1:A:24:ALA:N    | 0.42     | 2.81        | 7      | 2     |
| 1:A:12:MET:O    | 1:A:13:THR:HB   | 0.42     | 2.14        | 13     | 1     |
| 1:A:29:GLU:CG   | 1:A:51:LYS:HB2  | 0.42     | 2.44        | 14     | 1     |
| 1:A:9:VAL:HG12  | 1:A:42:GLU:CA   | 0.42     | 2.45        | 4      | 1     |
| 1:A:17:CYS:CB   | 1:A:66:TYR:CG   | 0.42     | 3.03        | 6      | 1     |
| 1:A:55:GLN:O    | 1:A:59:LYS:HG3  | 0.42     | 2.14        | 6      | 1     |
| 1:A:3:GLN:CB    | 1:A:47:PHE:CD2  | 0.42     | 3.02        | 13     | 1     |
| 1:A:47:PHE:CD1  | 1:A:57:LEU:HD13 | 0.42     | 2.50        | 1      | 1     |
| 1:A:40:LYS:O    | 1:A:41:ARG:HG2  | 0.42     | 2.13        | 4      | 1     |
| 1:A:6:THR:HG22  | 1:A:7:LEU:N     | 0.42     | 2.30        | 5      | 1     |
| 1:A:26:SER:HA   | 1:A:31:VAL:HB   | 0.42     | 1.92        | 14     | 1     |
| 1:A:9:VAL:HG22  | 1:A:18:PRO:HB3  | 0.42     | 1.91        | 2      | 1     |
| 1:A:10:PRO:O    | 1:A:12:MET:HG3  | 0.42     | 2.14        | 3      | 1     |
| 1:A:21:VAL:CG2  | 1:A:66:TYR:CB   | 0.42     | 2.97        | 3      | 1     |
| 1:A:9:VAL:HG23  | 1:A:42:GLU:C    | 0.42     | 2.39        | 10     | 1     |
| 1:A:22:LYS:CB   | 1:A:36:VAL:HG13 | 0.42     | 2.45        | 11     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:11:GLY:O    | 1:A:12:MET:HB2  | 0.42     | 2.14        | 13     | 1     |
| 1:A:36:VAL:HG23 | 1:A:43:ALA:HA   | 0.42     | 1.91        | 10     | 1     |
| 1:A:63:ASP:O    | 1:A:63:ASP:OD1  | 0.42     | 2.37        | 10     | 1     |
| 1:A:20:THR:O    | 1:A:23:LYS:HG2  | 0.42     | 2.15        | 14     | 1     |
| 1:A:9:VAL:O     | 1:A:12:MET:CE   | 0.42     | 2.68        | 3      | 1     |
| 1:A:18:PRO:HG2  | 1:A:38:PHE:HA   | 0.42     | 1.90        | 7      | 1     |
| 1:A:19:ILE:HG23 | 1:A:20:THR:N    | 0.42     | 2.30        | 11     | 2     |
| 1:A:33:LYS:O    | 1:A:45:VAL:HB   | 0.42     | 2.14        | 12     | 2     |
| 1:A:19:ILE:HG12 | 1:A:38:PHE:HB3  | 0.42     | 1.92        | 1      | 1     |
| 1:A:7:LEU:HD23  | 1:A:69:SER:C    | 0.42     | 2.37        | 5      | 1     |
| 1:A:24:ALA:O    | 1:A:28:VAL:HB   | 0.42     | 2.15        | 5      | 1     |
| 1:A:12:MET:HG2  | 1:A:41:ARG:CG   | 0.42     | 2.45        | 7      | 1     |
| 1:A:24:ALA:HA   | 1:A:27:LYS:CD   | 0.42     | 2.45        | 10     | 2     |
| 1:A:6:THR:HA    | 1:A:44:VAL:HG13 | 0.42     | 1.91        | 10     | 1     |
| 1:A:45:VAL:HG12 | 1:A:46:THR:N    | 0.42     | 2.30        | 11     | 1     |
| 1:A:33:LYS:HB3  | 1:A:46:THR:HG22 | 0.41     | 1.90        | 6      | 1     |
| 1:A:26:SER:HB2  | 1:A:34:VAL:HG21 | 0.41     | 1.91        | 9      | 1     |
| 1:A:47:PHE:CE2  | 1:A:57:LEU:HD13 | 0.41     | 2.50        | 10     | 1     |
| 1:A:7:LEU:HD23  | 1:A:68:SER:OG   | 0.41     | 2.14        | 4      | 1     |
| 1:A:4:THR:OG1   | 1:A:46:THR:CB   | 0.41     | 2.68        | 6      | 1     |
| 1:A:17:CYS:O    | 1:A:66:TYR:CG   | 0.41     | 2.73        | 10     | 1     |
| 1:A:11:GLY:O    | 1:A:18:PRO:HD3  | 0.41     | 2.15        | 14     | 1     |
| 1:A:26:SER:HA   | 1:A:34:VAL:HG21 | 0.41     | 1.85        | 2      | 2     |
| 1:A:4:THR:HA    | 1:A:46:THR:OG1  | 0.41     | 2.15        | 8      | 1     |
| 1:A:26:SER:HA   | 1:A:31:VAL:HG23 | 0.41     | 1.91        | 11     | 2     |
| 1:A:26:SER:HA   | 1:A:31:VAL:CG1  | 0.41     | 2.46        | 9      | 2     |
| 1:A:3:GLN:NE2   | 1:A:54:VAL:CG2  | 0.41     | 2.83        | 10     | 1     |
| 1:A:3:GLN:HB2   | 1:A:47:PHE:CE1  | 0.41     | 2.49        | 12     | 1     |
| 1:A:31:VAL:CG2  | 1:A:32:SER:N    | 0.41     | 2.83        | 12     | 1     |
| 1:A:49:ASP:OD1  | 1:A:49:ASP:N    | 0.41     | 2.53        | 10     | 1     |
| 1:A:22:LYS:O    | 1:A:25:LEU:HD12 | 0.41     | 2.14        | 13     | 1     |
| 1:A:33:LYS:HB3  | 1:A:46:THR:OG1  | 0.41     | 2.16        | 14     | 1     |
| 1:A:65:GLY:O    | 1:A:67:PRO:HD3  | 0.41     | 2.16        | 6      | 4     |
| 1:A:18:PRO:CD   | 1:A:38:PHE:HB2  | 0.41     | 2.46        | 4      | 1     |
| 1:A:31:VAL:O    | 1:A:31:VAL:HG12 | 0.41     | 2.15        | 9      | 1     |
| 1:A:26:SER:CB   | 1:A:31:VAL:HG23 | 0.41     | 2.43        | 7      | 1     |
| 1:A:59:LYS:O    | 1:A:60:ALA:C    | 0.41     | 2.63        | 4      | 1     |
| 1:A:3:GLN:OE1   | 1:A:47:PHE:CZ   | 0.41     | 2.73        | 10     | 1     |
| 1:A:13:THR:C    | 1:A:15:ALA:N    | 0.41     | 2.75        | 10     | 1     |
| 1:A:22:LYS:O    | 1:A:23:LYS:C    | 0.41     | 2.63        | 10     | 1     |
| 1:A:49:ASP:HA   | 1:A:52:ALA:O    | 0.41     | 2.15        | 12     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:30:GLY:C    | 1:A:47:PHE:HA   | 0.41     | 2.40        | 14     | 1     |
| 1:A:19:ILE:HG13 | 1:A:38:PHE:HB3  | 0.41     | 1.91        | 3      | 1     |
| 1:A:28:VAL:CG1  | 1:A:29:GLU:N    | 0.41     | 2.84        | 5      | 1     |
| 1:A:55:GLN:O    | 1:A:59:LYS:HB2  | 0.41     | 2.16        | 5      | 3     |
| 1:A:65:GLY:C    | 1:A:67:PRO:HD3  | 0.41     | 2.41        | 5      | 1     |
| 1:A:47:PHE:HZ   | 1:A:54:VAL:HG23 | 0.41     | 1.76        | 6      | 1     |
| 1:A:53:SER:N    | 1:A:56:LYS:HB2  | 0.41     | 2.31        | 11     | 1     |
| 1:A:40:LYS:C    | 1:A:41:ARG:HG2  | 0.41     | 2.39        | 12     | 1     |
| 1:A:29:GLU:HG3  | 1:A:51:LYS:HB2  | 0.41     | 1.92        | 14     | 1     |
| 1:A:21:VAL:HG23 | 1:A:66:TYR:HB2  | 0.41     | 1.92        | 3      | 1     |
| 1:A:29:GLU:OE1  | 1:A:51:LYS:O    | 0.41     | 2.39        | 5      | 1     |
| 1:A:35:ASP:O    | 1:A:44:VAL:CA   | 0.41     | 2.69        | 5      | 1     |
| 1:A:33:LYS:CG   | 1:A:46:THR:HG21 | 0.41     | 2.46        | 8      | 1     |
| 1:A:57:LEU:HD12 | 1:A:57:LEU:O    | 0.41     | 2.16        | 8      | 1     |
| 1:A:10:PRO:HD2  | 1:A:67:PRO:O    | 0.41     | 2.16        | 9      | 1     |
| 1:A:54:VAL:HA   | 1:A:57:LEU:CD2  | 0.41     | 2.45        | 9      | 1     |
| 1:A:47:PHE:CG   | 1:A:57:LEU:HD23 | 0.41     | 2.49        | 11     | 1     |
| 1:A:19:ILE:CG1  | 1:A:38:PHE:CB   | 0.41     | 2.98        | 12     | 1     |
| 1:A:47:PHE:CD1  | 1:A:54:VAL:HG23 | 0.41     | 2.51        | 14     | 1     |
| 1:A:27:LYS:HE3  | 1:A:27:LYS:C    | 0.40     | 2.41        | 4      | 1     |
| 1:A:66:TYR:N    | 1:A:67:PRO:HD3  | 0.40     | 2.30        | 5      | 1     |
| 1:A:23:LYS:C    | 1:A:27:LYS:HD2  | 0.40     | 2.40        | 10     | 1     |
| 1:A:9:VAL:HG21  | 1:A:42:GLU:C    | 0.40     | 2.41        | 13     | 1     |
| 1:A:40:LYS:O    | 1:A:42:GLU:N    | 0.40     | 2.55        | 3      | 1     |
| 1:A:17:CYS:HB3  | 1:A:66:TYR:CB   | 0.40     | 2.46        | 6      | 1     |
| 1:A:20:THR:OG1  | 1:A:66:TYR:CE2  | 0.40     | 2.74        | 8      | 1     |
| 1:A:12:MET:HB3  | 1:A:41:ARG:HB3  | 0.40     | 1.93        | 14     | 1     |
| 1:A:24:ALA:O    | 1:A:27:LYS:HG3  | 0.40     | 2.16        | 2      | 1     |
| 1:A:54:VAL:O    | 1:A:57:LEU:HG   | 0.40     | 2.16        | 14     | 2     |
| 1:A:33:LYS:HB2  | 1:A:46:THR:CB   | 0.40     | 2.45        | 5      | 1     |
| 1:A:35:ASP:O    | 1:A:44:VAL:HG23 | 0.40     | 2.16        | 5      | 1     |
| 1:A:3:GLN:OE1   | 1:A:47:PHE:CE1  | 0.40     | 2.75        | 10     | 1     |
| 1:A:46:THR:O    | 1:A:46:THR:HG22 | 0.40     | 2.15        | 12     | 1     |
| 1:A:48:ASP:OD1  | 1:A:48:ASP:O    | 0.40     | 2.40        | 12     | 1     |
| 1:A:26:SER:O    | 1:A:31:VAL:CG2  | 0.40     | 2.69        | 3      | 1     |
| 1:A:15:ALA:O    | 1:A:38:PHE:CE2  | 0.40     | 2.74        | 4      | 1     |
| 1:A:58:THR:HA   | 1:A:61:THR:HG22 | 0.40     | 1.93        | 6      | 1     |
| 1:A:27:LYS:O    | 1:A:27:LYS:HG3  | 0.40     | 2.15        | 7      | 1     |
| 1:A:40:LYS:C    | 1:A:41:ARG:CD   | 0.40     | 2.95        | 9      | 1     |
| 1:A:58:THR:HA   | 1:A:61:THR:OG1  | 0.40     | 2.17        | 10     | 1     |
| 1:A:11:GLY:HA3  | 1:A:18:PRO:CD   | 0.40     | 2.46        | 13     | 1     |

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| Atom-1          | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|-----------------|----------------|----------|-------------|--------|-------|
|                 |                |          |             | Worst  | Total |
| 1:A:49:ASP:OD1  | 1:A:49:ASP:C   | 0.40     | 2.64        | 3      | 1     |
| 1:A:36:VAL:HG23 | 1:A:42:GLU:O   | 0.40     | 2.17        | 5      | 1     |
| 1:A:18:PRO:HB2  | 1:A:38:PHE:CA  | 0.40     | 2.47        | 9      | 1     |
| 1:A:24:ALA:O    | 1:A:27:LYS:HG2 | 0.40     | 2.17        | 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     | 69/72 (96%)    | 46±1 (67±2%) | 14±2 (20±3%) | 9±2 (13±2%) | 0           | 6 |
| All | All   | 966/1008 (96%) | 647 (67%)    | 194 (20%)    | 125 (13%)   | 0           | 6 |

All 19 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     | 5   | VAL  | 14             |
| 1   | A     | 41  | ARG  | 14             |
| 1   | A     | 67  | PRO  | 14             |
| 1   | A     | 31  | VAL  | 12             |
| 1   | A     | 12  | MET  | 11             |
| 1   | A     | 16  | ALA  | 8              |
| 1   | A     | 28  | VAL  | 7              |
| 1   | A     | 49  | ASP  | 7              |
| 1   | A     | 51  | LYS  | 7              |
| 1   | A     | 32  | SER  | 6              |
| 1   | A     | 10  | PRO  | 5              |
| 1   | A     | 15  | ALA  | 5              |
| 1   | A     | 45  | VAL  | 4              |
| 1   | A     | 14  | CYS  | 3              |
| 1   | A     | 13  | THR  | 3              |
| 1   | A     | 52  | ALA  | 2              |
| 1   | A     | 50  | THR  | 1              |
| 1   | A     | 68  | SER  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 26  | SER  | 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     | 57/58 (98%)   | 34±2 (61±4%) | 22±2 (39±4%) | 0 6         |
| All | All   | 798/812 (98%) | 483 (61%)    | 315 (39%)    | 0 6         |

All 45 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     | 38  | PHE  | 14             |
| 1   | A     | 20  | THR  | 13             |
| 1   | A     | 32  | SER  | 13             |
| 1   | A     | 41  | ARG  | 12             |
| 1   | A     | 53  | SER  | 12             |
| 1   | A     | 66  | TYR  | 12             |
| 1   | A     | 71  | LYS  | 12             |
| 1   | A     | 26  | SER  | 12             |
| 1   | A     | 5   | VAL  | 11             |
| 1   | A     | 28  | VAL  | 11             |
| 1   | A     | 3   | GLN  | 11             |
| 1   | A     | 12  | MET  | 10             |
| 1   | A     | 27  | LYS  | 10             |
| 1   | A     | 68  | SER  | 9              |
| 1   | A     | 48  | ASP  | 9              |
| 1   | A     | 7   | LEU  | 8              |
| 1   | A     | 22  | LYS  | 8              |
| 1   | A     | 51  | LYS  | 8              |
| 1   | A     | 23  | LYS  | 8              |
| 1   | A     | 35  | ASP  | 8              |
| 1   | A     | 33  | LYS  | 7              |
| 1   | A     | 40  | LYS  | 7              |
| 1   | A     | 57  | LEU  | 7              |
| 1   | A     | 69  | SER  | 7              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 56  | LYS  | 7              |
| 1   | A     | 72  | GLN  | 6              |
| 1   | A     | 55  | GLN  | 6              |
| 1   | A     | 19  | ILE  | 6              |
| 1   | A     | 9   | VAL  | 5              |
| 1   | A     | 13  | THR  | 5              |
| 1   | A     | 31  | VAL  | 5              |
| 1   | A     | 59  | LYS  | 4              |
| 1   | A     | 63  | ASP  | 4              |
| 1   | A     | 25  | LEU  | 4              |
| 1   | A     | 29  | GLU  | 4              |
| 1   | A     | 54  | VAL  | 3              |
| 1   | A     | 36  | VAL  | 3              |
| 1   | A     | 39  | GLU  | 3              |
| 1   | A     | 44  | VAL  | 2              |
| 1   | A     | 47  | PHE  | 2              |
| 1   | A     | 50  | THR  | 2              |
| 1   | A     | 6   | THR  | 2              |
| 1   | A     | 42  | GLU  | 1              |
| 1   | A     | 49  | ASP  | 1              |
| 1   | A     | 58  | THR  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry ⓘ

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