



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 20, 2018 – 03:15 am GMT

PDB ID : 1PMR  
Title : LIPOYL DOMAIN FROM THE DIHYDROLIPOYL SUCCINYLTRANSFERASE COMPONENT OF THE 2-OXOGLUTARATE DEHYDROGENASE MULTIENZYME COMPLEX OF ESCHERICHIA COLI, NMR, 25 STRUCTURES  
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Deposited on : 1997-07-24

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.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk30686  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

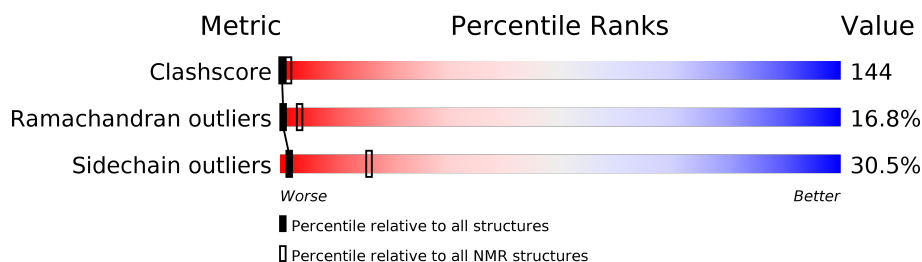
# 1 Overall quality at a glance

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            | 136279                      | 12091                     |
| Ramachandran outliers | 132675                      | 10835                     |
| Sidechain outliers    | 132484                      | 10811                     |

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     | 80     |                  |

## 2 Ensemble composition and analysis

This entry contains 25 models. Model 24 is the overall representative, medoid model (most similar to other models). The authors have identified model 21 as representative.

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:2-A:9, A:17-A:77 (69) | 0.35              | 24           |

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 4 clusters and 3 single-model clusters were found.

| Cluster number        | Models                                     |
|-----------------------|--|
| 1                     | 4, 5, 6, 7, 10, 12, 16, 18, 19, 22, 23, 24 |
| 2                     | 2, 3, 11, 20, 21                           |
| 3                     | 1, 9, 25                                   |
| 4                     | 13, 15                                     |
| Single-model clusters | 8; 14; 17                                  |

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

There is only 1 type of molecule in this entry. The entry contains 1201 atoms, of which 602 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DIHYDROLIPOYL SUCCINYLTRANSFERASE.

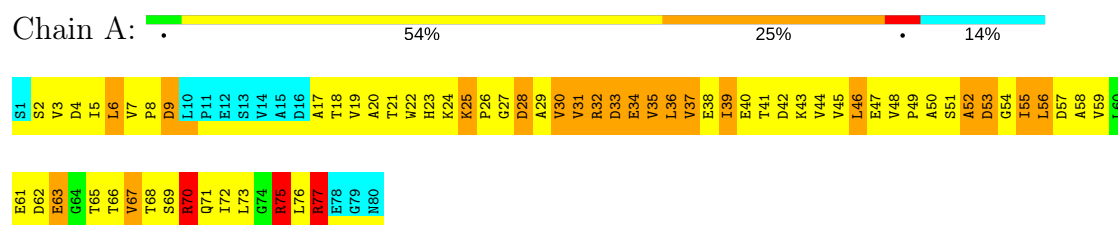
| Mol | Chain | Residues | Atoms |     |     |     |     | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|-------|
| 1   | A     | 80       | Total | C   | H   | N   | O   | 0     |
|     |       |          | 1201  | 371 | 602 | 100 | 128 |       |

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

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

These plots are provided for all protein, RNA and DNA 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: DIHYDROLIPOYL SUCCINYLTRANSFERASE

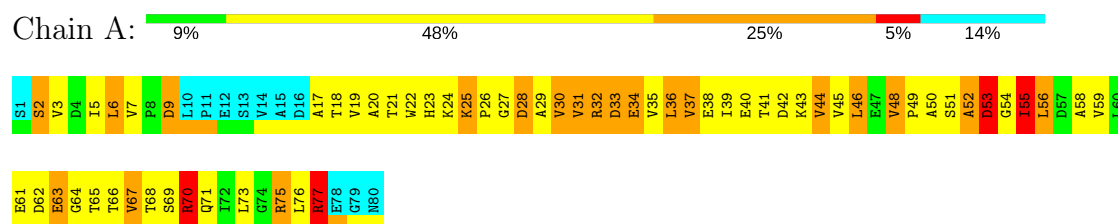


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

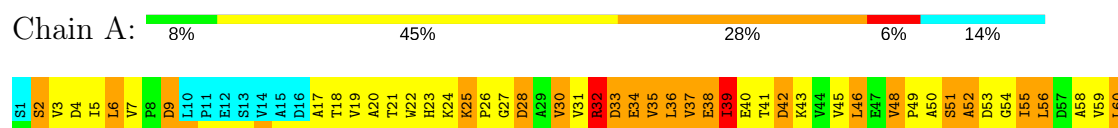
#### 4.2.1 Score per residue for model 1

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE



#### 4.2.2 Score per residue for model 2

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE





### 4.2.3 Score per residue for model 3

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 9% 43% 29% 6% 14%



### 4.2.4 Score per residue for model 4

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

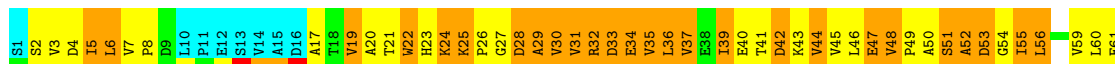
Chain A: 9% 49% 21% 8% 14%



### 4.2.5 Score per residue for model 5

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 11% 35% 39% 14%



### 4.2.6 Score per residue for model 6

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 8% 50% 24% 5% 14%





#### 4.2.7 Score per residue for model 7

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 8% 43% 30% 6% 14%



#### 4.2.8 Score per residue for model 8

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

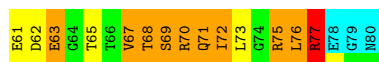
Chain A: 6% 48% 30% 14%



#### 4.2.9 Score per residue for model 9

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 13% 38% 34% 14%



#### 4.2.10 Score per residue for model 10

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 9% 41% 31% 5% 14%





#### 4.2.11 Score per residue for model 11

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 9% 40% 35% 14%



#### 4.2.12 Score per residue for model 12

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 9% 44% 24% 10% 14%



#### 4.2.13 Score per residue for model 13

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 11% 36% 31% 8% 14%



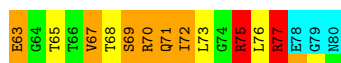
#### 4.2.14 Score per residue for model 14

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 10% 40% 31% 5% 14%







#### 4.2.15 Score per residue for model 15

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

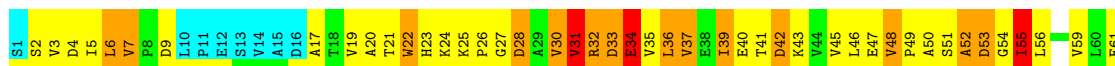
Chain A: 9% 44% 24% 10% 14%



#### 4.2.16 Score per residue for model 16

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 13% 45% 24% 5% 14%



#### 4.2.17 Score per residue for model 17

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 5% 46% 28% 8% 14%



#### 4.2.18 Score per residue for model 18

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 9% 43% 30% 5% 14%





#### 4.2.19 Score per residue for model 19

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 9% 45% 26% 6% 14%



#### 4.2.20 Score per residue for model 20

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 6% 43% 33% 5% 14%



#### 4.2.21 Score per residue for model 21

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 6% 45% 30% 5% 14%



#### 4.2.22 Score per residue for model 22

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 5% 45% 33% 14%





#### 4.2.23 Score per residue for model 23

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 9% 49% 21% 8% 14%



#### 4.2.24 Score per residue for model 24 (medoid)

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 9% 40% 33% 5% 14%



#### 4.2.25 Score per residue for model 25

- Molecule 1: DIHYDROLIPOYL SUCCINYLTRANSFERASE

Chain A: 6% 53% 23% 5% 14%



## 5 Refinement protocol and experimental data overview

Of the 72 calculated structures, 25 were deposited, based on the following criterion: ?.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| X-PLOR        | refinement     | 3.1     |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

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

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 3.8±0.4   |
| All | All   | 0         | 96        |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 75  | ARG  | Sidechain | 25             |
| 1   | A     | 70  | ARG  | Sidechain | 24             |
| 1   | A     | 32  | ARG  | Sidechain | 24             |
| 1   | A     | 77  | ARG  | Sidechain | 23             |

### 6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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     | 521   | 533      | 533      | 152±8   |
| All | All   | 13025 | 13325    | 13325    | 3807    |

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:34:GLU:CG   | 1:A:50:ALA:HB3  | 1.03     | 1.84        | 13     | 9     |
| 1:A:7:VAL:HG21  | 1:A:39:ILE:HD13 | 1.03     | 1.31        | 3      | 5     |
| 1:A:37:VAL:HG21 | 1:A:73:LEU:HD21 | 1.01     | 1.33        | 14     | 5     |
| 1:A:56:LEU:HD12 | 1:A:76:LEU:CD1  | 1.01     | 1.84        | 22     | 3     |
| 1:A:3:VAL:HG12  | 1:A:5:ILE:CD1   | 1.00     | 1.84        | 6      | 2     |
| 1:A:34:GLU:CB   | 1:A:50:ALA:HB3  | 1.00     | 1.86        | 12     | 22    |
| 1:A:37:VAL:HG11 | 1:A:73:LEU:CD1  | 0.99     | 1.87        | 19     | 16    |
| 1:A:7:VAL:CG2   | 1:A:73:LEU:HD21 | 0.99     | 1.86        | 5      | 11    |
| 1:A:34:GLU:OE1  | 1:A:35:VAL:HG12 | 0.99     | 1.57        | 25     | 7     |
| 1:A:34:GLU:HB3  | 1:A:50:ALA:HB3  | 0.99     | 1.32        | 6      | 22    |
| 1:A:7:VAL:HG21  | 1:A:67:VAL:HG21 | 0.99     | 1.35        | 10     | 17    |
| 1:A:5:ILE:CG1   | 1:A:48:VAL:HG22 | 0.98     | 1.87        | 11     | 15    |
| 1:A:68:THR:HG22 | 1:A:71:GLN:CG   | 0.98     | 1.88        | 14     | 10    |
| 1:A:37:VAL:HG12 | 1:A:48:VAL:HG12 | 0.97     | 1.36        | 15     | 9     |
| 1:A:3:VAL:HG21  | 1:A:34:GLU:OE2  | 0.95     | 1.61        | 3      | 2     |
| 1:A:68:THR:HG22 | 1:A:71:GLN:HG3  | 0.95     | 1.38        | 14     | 8     |
| 1:A:7:VAL:HG23  | 1:A:73:LEU:HD21 | 0.94     | 1.35        | 5      | 8     |
| 1:A:7:VAL:CG1   | 1:A:46:LEU:HD12 | 0.93     | 1.93        | 12     | 5     |
| 1:A:22:TRP:HA   | 1:A:37:VAL:HG23 | 0.93     | 1.40        | 22     | 25    |
| 1:A:19:VAL:HG12 | 1:A:63:GLU:OE1  | 0.92     | 1.63        | 20     | 4     |
| 1:A:56:LEU:HD12 | 1:A:76:LEU:CD2  | 0.92     | 1.94        | 21     | 4     |
| 1:A:3:VAL:HG21  | 1:A:34:GLU:OE1  | 0.92     | 1.64        | 16     | 9     |
| 1:A:56:LEU:HD12 | 1:A:76:LEU:HD22 | 0.92     | 1.41        | 5      | 4     |
| 1:A:37:VAL:HG11 | 1:A:73:LEU:HD22 | 0.90     | 1.41        | 14     | 4     |
| 1:A:7:VAL:HG13  | 1:A:46:LEU:HD12 | 0.90     | 1.41        | 12     | 4     |
| 1:A:3:VAL:HG12  | 1:A:5:ILE:HG23  | 0.90     | 1.40        | 18     | 1     |
| 1:A:30:VAL:HG21 | 1:A:34:GLU:HA   | 0.90     | 1.44        | 6      | 23    |
| 1:A:5:ILE:HG12  | 1:A:48:VAL:HG22 | 0.89     | 1.43        | 3      | 19    |
| 1:A:9:ASP:HB2   | 1:A:46:LEU:HD13 | 0.88     | 1.42        | 15     | 10    |
| 1:A:19:VAL:CG1  | 1:A:73:LEU:HD11 | 0.88     | 1.98        | 14     | 4     |
| 1:A:17:ALA:HB2  | 1:A:41:THR:HG23 | 0.87     | 1.46        | 17     | 1     |
| 1:A:3:VAL:HG23  | 1:A:77:ARG:O    | 0.87     | 1.68        | 15     | 3     |
| 1:A:24:LYS:O    | 1:A:56:LEU:HD22 | 0.86     | 1.69        | 2      | 5     |
| 1:A:39:ILE:O    | 1:A:45:VAL:HG13 | 0.86     | 1.71        | 20     | 19    |
| 1:A:9:ASP:CB    | 1:A:46:LEU:HD13 | 0.86     | 2.01        | 7      | 11    |
| 1:A:9:ASP:HB3   | 1:A:46:LEU:HD22 | 0.85     | 1.49        | 9      | 5     |
| 1:A:34:GLU:OE2  | 1:A:35:VAL:HG12 | 0.84     | 1.73        | 16     | 7     |
| 1:A:37:VAL:HG12 | 1:A:48:VAL:HB   | 0.84     | 1.49        | 12     | 19    |
| 1:A:39:ILE:HD11 | 1:A:67:VAL:HG11 | 0.84     | 1.47        | 15     | 5     |
| 1:A:56:LEU:HD12 | 1:A:76:LEU:HG   | 0.84     | 1.48        | 2      | 9     |
| 1:A:3:VAL:HG12  | 1:A:5:ILE:HD12  | 0.83     | 1.49        | 6      | 1     |
| 1:A:24:LYS:CB   | 1:A:56:LEU:HD23 | 0.83     | 2.03        | 11     | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:34:GLU:HG3  | 1:A:50:ALA:HB3  | 0.83     | 1.49        | 13     | 2     |
| 1:A:5:ILE:HG13  | 1:A:48:VAL:HG21 | 0.83     | 1.51        | 6      | 3     |
| 1:A:9:ASP:CG    | 1:A:46:LEU:HD22 | 0.82     | 1.95        | 15     | 4     |
| 1:A:5:ILE:HG21  | 1:A:48:VAL:HG22 | 0.82     | 1.49        | 6      | 1     |
| 1:A:30:VAL:HG12 | 1:A:53:ASP:O    | 0.82     | 1.74        | 18     | 9     |
| 1:A:3:VAL:HG12  | 1:A:5:ILE:CG2   | 0.81     | 2.05        | 18     | 1     |
| 1:A:39:ILE:HD11 | 1:A:67:VAL:CG1  | 0.81     | 2.06        | 25     | 5     |
| 1:A:19:VAL:CG2  | 1:A:73:LEU:HD11 | 0.81     | 2.05        | 21     | 4     |
| 1:A:21:THR:HG23 | 1:A:63:GLU:OE1  | 0.81     | 1.73        | 9      | 5     |
| 1:A:34:GLU:OE2  | 1:A:76:LEU:HD23 | 0.81     | 1.76        | 18     | 1     |
| 1:A:3:VAL:HG21  | 1:A:34:GLU:CD   | 0.80     | 1.96        | 6      | 3     |
| 1:A:39:ILE:HD11 | 1:A:67:VAL:HG21 | 0.80     | 1.50        | 11     | 1     |
| 1:A:56:LEU:HD11 | 1:A:59:VAL:HG21 | 0.80     | 1.52        | 3      | 5     |
| 1:A:6:LEU:HD22  | 1:A:70:ARG:HG2  | 0.80     | 1.51        | 3      | 4     |
| 1:A:34:GLU:CD   | 1:A:50:ALA:HB3  | 0.80     | 1.95        | 13     | 6     |
| 1:A:7:VAL:HG21  | 1:A:67:VAL:CG2  | 0.80     | 2.07        | 17     | 8     |
| 1:A:48:VAL:HG13 | 1:A:48:VAL:O    | 0.80     | 1.77        | 6      | 7     |
| 1:A:46:LEU:N    | 1:A:46:LEU:HD13 | 0.80     | 1.92        | 21     | 6     |
| 1:A:5:ILE:HG21  | 1:A:22:TRP:CZ2  | 0.80     | 2.12        | 8      | 1     |
| 1:A:76:LEU:HD12 | 1:A:76:LEU:N    | 0.80     | 1.92        | 19     | 9     |
| 1:A:37:VAL:HG21 | 1:A:73:LEU:CD2  | 0.79     | 2.07        | 15     | 5     |
| 1:A:5:ILE:HG13  | 1:A:48:VAL:HG22 | 0.79     | 1.54        | 11     | 8     |
| 1:A:46:LEU:HD13 | 1:A:46:LEU:N    | 0.79     | 1.89        | 2      | 2     |
| 1:A:48:VAL:O    | 1:A:48:VAL:HG12 | 0.79     | 1.78        | 10     | 8     |
| 1:A:56:LEU:CD2  | 1:A:59:VAL:HG22 | 0.79     | 2.07        | 24     | 1     |
| 1:A:7:VAL:HG21  | 1:A:39:ILE:CD1  | 0.79     | 2.07        | 3      | 2     |
| 1:A:30:VAL:HG12 | 1:A:34:GLU:OE2  | 0.79     | 1.77        | 12     | 2     |
| 1:A:37:VAL:HG11 | 1:A:73:LEU:HD12 | 0.78     | 1.53        | 11     | 2     |
| 1:A:56:LEU:HD11 | 1:A:59:VAL:CG2  | 0.78     | 2.07        | 11     | 15    |
| 1:A:58:ALA:HB3  | 1:A:75:ARG:HG3  | 0.78     | 1.56        | 22     | 4     |
| 1:A:19:VAL:HG11 | 1:A:73:LEU:HD11 | 0.78     | 1.54        | 14     | 2     |
| 1:A:56:LEU:HD21 | 1:A:59:VAL:HG21 | 0.78     | 1.55        | 7      | 7     |
| 1:A:56:LEU:HD12 | 1:A:76:LEU:HD21 | 0.78     | 1.56        | 21     | 3     |
| 1:A:48:VAL:HG12 | 1:A:48:VAL:O    | 0.78     | 1.78        | 19     | 2     |
| 1:A:68:THR:HG22 | 1:A:71:GLN:HG2  | 0.78     | 1.56        | 6      | 8     |
| 1:A:3:VAL:O     | 1:A:5:ILE:HD13  | 0.78     | 1.79        | 6      | 1     |
| 1:A:20:ALA:HB3  | 1:A:38:GLU:O    | 0.77     | 1.79        | 10     | 14    |
| 1:A:5:ILE:HG23  | 1:A:48:VAL:HG21 | 0.77     | 1.56        | 17     | 3     |
| 1:A:58:ALA:HB3  | 1:A:75:ARG:O    | 0.77     | 1.79        | 8      | 7     |
| 1:A:60:LEU:HD12 | 1:A:74:GLY:HA2  | 0.77     | 1.54        | 5      | 2     |
| 1:A:39:ILE:O    | 1:A:45:VAL:HG22 | 0.77     | 1.79        | 1      | 8     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:22:TRP:CZ3  | 1:A:76:LEU:HD11 | 0.77     | 2.14        | 10     | 1     |
| 1:A:37:VAL:HG12 | 1:A:48:VAL:CG1  | 0.77     | 2.10        | 20     | 15    |
| 1:A:56:LEU:HD12 | 1:A:76:LEU:HD11 | 0.77     | 1.57        | 22     | 2     |
| 1:A:37:VAL:HG11 | 1:A:73:LEU:CD2  | 0.77     | 2.09        | 14     | 3     |
| 1:A:27:GLY:HA2  | 1:A:55:ILE:HG23 | 0.77     | 1.57        | 19     | 11    |
| 1:A:75:ARG:C    | 1:A:76:LEU:HD12 | 0.76     | 2.00        | 25     | 14    |
| 1:A:5:ILE:HG12  | 1:A:48:VAL:HG11 | 0.76     | 1.56        | 8      | 1     |
| 1:A:48:VAL:HG21 | 1:A:73:LEU:CD1  | 0.76     | 2.10        | 12     | 11    |
| 1:A:18:THR:HG23 | 1:A:65:THR:O    | 0.76     | 1.79        | 2      | 3     |
| 1:A:48:VAL:O    | 1:A:48:VAL:HG13 | 0.76     | 1.79        | 17     | 8     |
| 1:A:30:VAL:HG11 | 1:A:34:GLU:CB   | 0.75     | 2.09        | 5      | 15    |
| 1:A:56:LEU:CD1  | 1:A:59:VAL:HG22 | 0.75     | 2.10        | 10     | 6     |
| 1:A:56:LEU:HD22 | 1:A:59:VAL:HG22 | 0.75     | 1.54        | 24     | 1     |
| 1:A:30:VAL:HG21 | 1:A:33:ASP:O    | 0.75     | 1.81        | 18     | 17    |
| 1:A:19:VAL:HG12 | 1:A:63:GLU:CD   | 0.75     | 2.02        | 24     | 4     |
| 1:A:31:VAL:HG22 | 1:A:32:ARG:N    | 0.75     | 1.96        | 21     | 4     |
| 1:A:30:VAL:HG13 | 1:A:31:VAL:N    | 0.75     | 1.97        | 12     | 19    |
| 1:A:34:GLU:CD   | 1:A:35:VAL:HG12 | 0.75     | 2.02        | 17     | 12    |
| 1:A:34:GLU:HG2  | 1:A:50:ALA:HB3  | 0.75     | 1.58        | 20     | 3     |
| 1:A:38:GLU:OE1  | 1:A:45:VAL:HG11 | 0.74     | 1.81        | 22     | 2     |
| 1:A:75:ARG:C    | 1:A:76:LEU:HD23 | 0.74     | 2.03        | 17     | 6     |
| 1:A:39:ILE:HG23 | 1:A:40:GLU:N    | 0.74     | 1.96        | 7      | 25    |
| 1:A:5:ILE:HG12  | 1:A:48:VAL:HG13 | 0.74     | 1.58        | 9      | 10    |
| 1:A:56:LEU:HD11 | 1:A:59:VAL:HG22 | 0.74     | 1.59        | 5      | 10    |
| 1:A:6:LEU:HD12  | 1:A:6:LEU:N     | 0.73     | 1.98        | 5      | 11    |
| 1:A:5:ILE:CB    | 1:A:48:VAL:HG21 | 0.73     | 2.12        | 18     | 2     |
| 1:A:48:VAL:HG21 | 1:A:73:LEU:HD12 | 0.73     | 1.58        | 19     | 8     |
| 1:A:34:GLU:HG3  | 1:A:35:VAL:HG12 | 0.73     | 1.60        | 20     | 3     |
| 1:A:6:LEU:N     | 1:A:6:LEU:HD12  | 0.73     | 1.98        | 2      | 9     |
| 1:A:56:LEU:HD22 | 1:A:76:LEU:HG   | 0.73     | 1.59        | 3      | 4     |
| 1:A:76:LEU:N    | 1:A:76:LEU:HD12 | 0.73     | 1.99        | 13     | 5     |
| 1:A:24:LYS:HB3  | 1:A:56:LEU:HD23 | 0.73     | 1.60        | 13     | 4     |
| 1:A:59:VAL:O    | 1:A:59:VAL:HG13 | 0.72     | 1.83        | 9      | 1     |
| 1:A:27:GLY:CA   | 1:A:55:ILE:HG23 | 0.72     | 2.15        | 24     | 15    |
| 1:A:46:LEU:HD23 | 1:A:46:LEU:N    | 0.72     | 1.98        | 7      | 2     |
| 1:A:6:LEU:HD12  | 1:A:6:LEU:H     | 0.72     | 1.45        | 19     | 10    |
| 1:A:68:THR:HG23 | 1:A:69:SER:N    | 0.72     | 2.00        | 3      | 13    |
| 1:A:19:VAL:HG22 | 1:A:39:ILE:HD11 | 0.72     | 1.62        | 4      | 10    |
| 1:A:3:VAL:HG12  | 1:A:3:VAL:O     | 0.72     | 1.85        | 3      | 12    |
| 1:A:37:VAL:HG12 | 1:A:48:VAL:CG2  | 0.72     | 2.14        | 22     | 9     |
| 1:A:7:VAL:HG12  | 1:A:46:LEU:HD12 | 0.71     | 1.62        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:6:LEU:O     | 1:A:48:VAL:HG23 | 0.71     | 1.84        | 11     | 2     |
| 1:A:22:TRP:HZ3  | 1:A:35:VAL:HG11 | 0.71     | 1.45        | 9      | 16    |
| 1:A:46:LEU:N    | 1:A:46:LEU:HD23 | 0.71     | 2.00        | 6      | 3     |
| 1:A:6:LEU:H     | 1:A:6:LEU:HD12  | 0.71     | 1.46        | 8      | 11    |
| 1:A:48:VAL:CG1  | 1:A:48:VAL:O    | 0.71     | 2.39        | 21     | 11    |
| 1:A:3:VAL:O     | 1:A:3:VAL:HG12  | 0.70     | 1.85        | 10     | 7     |
| 1:A:48:VAL:O    | 1:A:48:VAL:CG1  | 0.70     | 2.39        | 25     | 13    |
| 1:A:6:LEU:HD22  | 1:A:70:ARG:CG   | 0.70     | 2.16        | 14     | 2     |
| 1:A:46:LEU:N    | 1:A:46:LEU:HD22 | 0.70     | 2.01        | 4      | 2     |
| 1:A:46:LEU:HD22 | 1:A:46:LEU:N    | 0.70     | 2.01        | 23     | 3     |
| 1:A:41:THR:HB   | 1:A:44:VAL:HG23 | 0.70     | 1.64        | 1      | 1     |
| 1:A:51:SER:O    | 1:A:52:ALA:HB2  | 0.70     | 1.86        | 13     | 18    |
| 1:A:19:VAL:CG1  | 1:A:73:LEU:HD21 | 0.69     | 2.16        | 21     | 2     |
| 1:A:28:ASP:O    | 1:A:29:ALA:HB2  | 0.69     | 1.88        | 24     | 13    |
| 1:A:7:VAL:O     | 1:A:7:VAL:HG12  | 0.69     | 1.85        | 5      | 7     |
| 1:A:22:TRP:CZ3  | 1:A:35:VAL:HG11 | 0.69     | 2.21        | 25     | 16    |
| 1:A:37:VAL:HG12 | 1:A:48:VAL:CB   | 0.69     | 2.17        | 9      | 20    |
| 1:A:75:ARG:O    | 1:A:76:LEU:HD23 | 0.69     | 1.88        | 7      | 4     |
| 1:A:7:VAL:CG2   | 1:A:39:ILE:HD13 | 0.69     | 2.17        | 8      | 8     |
| 1:A:41:THR:HG22 | 1:A:41:THR:O    | 0.69     | 1.86        | 13     | 1     |
| 1:A:7:VAL:HG12  | 1:A:7:VAL:O     | 0.69     | 1.87        | 9      | 7     |
| 1:A:5:ILE:CG1   | 1:A:48:VAL:HG13 | 0.69     | 2.18        | 7      | 5     |
| 1:A:56:LEU:HD23 | 1:A:76:LEU:HD22 | 0.69     | 1.64        | 24     | 1     |
| 1:A:5:ILE:CG1   | 1:A:48:VAL:HG11 | 0.69     | 2.18        | 8      | 1     |
| 1:A:9:ASP:OD1   | 1:A:46:LEU:HD22 | 0.69     | 1.88        | 15     | 1     |
| 1:A:41:THR:O    | 1:A:41:THR:HG22 | 0.68     | 1.87        | 10     | 4     |
| 1:A:39:ILE:HD11 | 1:A:67:VAL:CG2  | 0.68     | 2.18        | 11     | 4     |
| 1:A:30:VAL:HG11 | 1:A:34:GLU:CG   | 0.68     | 2.18        | 5      | 1     |
| 1:A:5:ILE:HG21  | 1:A:48:VAL:CG2  | 0.68     | 2.18        | 6      | 1     |
| 1:A:56:LEU:HD12 | 1:A:76:LEU:HD13 | 0.68     | 1.64        | 6      | 3     |
| 1:A:51:SER:O    | 1:A:52:ALA:HB3  | 0.68     | 1.89        | 16     | 7     |
| 1:A:39:ILE:HD11 | 1:A:67:VAL:HG13 | 0.68     | 1.64        | 25     | 2     |
| 1:A:5:ILE:CG1   | 1:A:48:VAL:HG21 | 0.68     | 2.18        | 6      | 5     |
| 1:A:9:ASP:HB3   | 1:A:46:LEU:HD13 | 0.68     | 1.65        | 6      | 3     |
| 1:A:22:TRP:CE2  | 1:A:73:LEU:HD23 | 0.68     | 2.24        | 15     | 5     |
| 1:A:51:SER:O    | 1:A:52:ALA:CB   | 0.68     | 2.42        | 12     | 25    |
| 1:A:24:LYS:HB2  | 1:A:56:LEU:HD23 | 0.68     | 1.66        | 11     | 2     |
| 1:A:17:ALA:HB2  | 1:A:41:THR:OG1  | 0.67     | 1.90        | 15     | 1     |
| 1:A:30:VAL:HG13 | 1:A:52:ALA:HA   | 0.67     | 1.66        | 25     | 5     |
| 1:A:19:VAL:HG22 | 1:A:73:LEU:HD11 | 0.67     | 1.66        | 21     | 3     |
| 1:A:72:ILE:HG23 | 1:A:72:ILE:O    | 0.67     | 1.89        | 14     | 14    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:30:VAL:HG11 | 1:A:34:GLU:HG2  | 0.67     | 1.64        | 5      | 1     |
| 1:A:5:ILE:HD13  | 1:A:48:VAL:HG21 | 0.67     | 1.67        | 8      | 1     |
| 1:A:6:LEU:HD23  | 1:A:71:GLN:O    | 0.67     | 1.89        | 13     | 1     |
| 1:A:56:LEU:HD22 | 1:A:76:LEU:CD2  | 0.67     | 2.20        | 11     | 2     |
| 1:A:34:GLU:HB3  | 1:A:50:ALA:CB   | 0.67     | 2.20        | 20     | 15    |
| 1:A:37:VAL:CG1  | 1:A:48:VAL:HG12 | 0.66     | 2.17        | 15     | 7     |
| 1:A:56:LEU:CD1  | 1:A:76:LEU:HD21 | 0.66     | 2.20        | 21     | 3     |
| 1:A:41:THR:HG21 | 1:A:46:LEU:HD21 | 0.66     | 1.66        | 2      | 2     |
| 1:A:5:ILE:HB    | 1:A:48:VAL:HG21 | 0.66     | 1.65        | 18     | 2     |
| 1:A:76:LEU:N    | 1:A:76:LEU:HD23 | 0.66     | 2.06        | 17     | 2     |
| 1:A:39:ILE:O    | 1:A:45:VAL:HG23 | 0.65     | 1.91        | 3      | 3     |
| 1:A:58:ALA:HB3  | 1:A:75:ARG:HG2  | 0.65     | 1.67        | 20     | 3     |
| 1:A:41:THR:HG22 | 1:A:44:VAL:O    | 0.65     | 1.90        | 8      | 2     |
| 1:A:17:ALA:HB2  | 1:A:41:THR:HG22 | 0.65     | 1.66        | 22     | 1     |
| 1:A:19:VAL:HG21 | 1:A:73:LEU:CD1  | 0.65     | 2.21        | 15     | 2     |
| 1:A:24:LYS:HB3  | 1:A:56:LEU:HD13 | 0.65     | 1.68        | 22     | 8     |
| 1:A:54:GLY:O    | 1:A:76:LEU:HD23 | 0.65     | 1.91        | 8      | 6     |
| 1:A:22:TRP:CA   | 1:A:37:VAL:HG23 | 0.64     | 2.22        | 1      | 24    |
| 1:A:7:VAL:HG22  | 1:A:73:LEU:HD11 | 0.64     | 1.69        | 16     | 1     |
| 1:A:76:LEU:CD1  | 1:A:76:LEU:N    | 0.64     | 2.61        | 2      | 10    |
| 1:A:52:ALA:O    | 1:A:53:ASP:CB   | 0.64     | 2.46        | 9      | 10    |
| 1:A:48:VAL:HG21 | 1:A:73:LEU:HD11 | 0.64     | 1.68        | 12     | 4     |
| 1:A:30:VAL:HG11 | 1:A:34:GLU:CA   | 0.64     | 2.23        | 16     | 16    |
| 1:A:76:LEU:N    | 1:A:76:LEU:CD1  | 0.64     | 2.61        | 3      | 6     |
| 1:A:31:VAL:O    | 1:A:52:ALA:HB2  | 0.63     | 1.93        | 16     | 6     |
| 1:A:24:LYS:CB   | 1:A:56:LEU:HD13 | 0.63     | 2.23        | 22     | 2     |
| 1:A:37:VAL:HG11 | 1:A:73:LEU:HD13 | 0.63     | 1.69        | 1      | 5     |
| 1:A:5:ILE:HG23  | 1:A:73:LEU:HD22 | 0.63     | 1.69        | 16     | 1     |
| 1:A:7:VAL:HG23  | 1:A:73:LEU:CD2  | 0.62     | 2.18        | 5      | 1     |
| 1:A:55:ILE:HD12 | 1:A:77:ARG:HD3  | 0.62     | 1.70        | 5      | 1     |
| 1:A:6:LEU:O     | 1:A:7:VAL:HG23  | 0.62     | 1.93        | 25     | 1     |
| 1:A:9:ASP:OD2   | 1:A:46:LEU:HD12 | 0.62     | 1.94        | 17     | 1     |
| 1:A:45:VAL:O    | 1:A:45:VAL:HG13 | 0.62     | 1.95        | 15     | 1     |
| 1:A:56:LEU:CD1  | 1:A:76:LEU:HD22 | 0.62     | 2.23        | 14     | 3     |
| 1:A:19:VAL:HG13 | 1:A:73:LEU:HD21 | 0.62     | 1.71        | 21     | 2     |
| 1:A:60:LEU:HD21 | 1:A:74:GLY:HA2  | 0.62     | 1.71        | 17     | 1     |
| 1:A:21:THR:O    | 1:A:21:THR:HG23 | 0.62     | 1.94        | 2      | 1     |
| 1:A:3:VAL:CG1   | 1:A:5:ILE:CD1   | 0.61     | 2.78        | 15     | 1     |
| 1:A:56:LEU:CD1  | 1:A:59:VAL:CG2  | 0.61     | 2.78        | 13     | 15    |
| 1:A:24:LYS:HG2  | 1:A:56:LEU:HD23 | 0.61     | 1.70        | 18     | 1     |
| 1:A:25:LYS:CB   | 1:A:26:PRO:HD2  | 0.61     | 2.25        | 20     | 25    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:ILE:CG1   | 1:A:48:VAL:CG2  | 0.61     | 2.78        | 5      | 11    |
| 1:A:7:VAL:CG2   | 1:A:67:VAL:HG21 | 0.61     | 2.21        | 22     | 5     |
| 1:A:72:ILE:O    | 1:A:72:ILE:HG23 | 0.61     | 1.94        | 12     | 8     |
| 1:A:30:VAL:CG1  | 1:A:53:ASP:O    | 0.61     | 2.48        | 3      | 8     |
| 1:A:36:LEU:HD12 | 1:A:36:LEU:N    | 0.60     | 2.12        | 3      | 2     |
| 1:A:36:LEU:HD12 | 1:A:36:LEU:H    | 0.60     | 1.56        | 3      | 1     |
| 1:A:44:VAL:HG12 | 1:A:46:LEU:CD2  | 0.60     | 2.26        | 17     | 1     |
| 1:A:3:VAL:HG21  | 1:A:54:GLY:HA2  | 0.60     | 1.73        | 20     | 3     |
| 1:A:42:ASP:O    | 1:A:43:LYS:CB   | 0.60     | 2.50        | 21     | 24    |
| 1:A:30:VAL:HG11 | 1:A:34:GLU:HA   | 0.60     | 1.73        | 12     | 7     |
| 1:A:22:TRP:CD1  | 1:A:63:GLU:OE2  | 0.60     | 2.55        | 20     | 4     |
| 1:A:3:VAL:CG1   | 1:A:5:ILE:HD13  | 0.60     | 2.27        | 20     | 2     |
| 1:A:25:LYS:CB   | 1:A:26:PRO:CD   | 0.60     | 2.80        | 25     | 25    |
| 1:A:32:ARG:O    | 1:A:33:ASP:CB   | 0.60     | 2.50        | 13     | 17    |
| 1:A:7:VAL:N     | 1:A:8:PRO:HD3   | 0.60     | 2.11        | 22     | 17    |
| 1:A:25:LYS:CB   | 1:A:28:ASP:OD1  | 0.60     | 2.50        | 22     | 19    |
| 1:A:30:VAL:CG1  | 1:A:31:VAL:N    | 0.60     | 2.65        | 9      | 12    |
| 1:A:67:VAL:CG2  | 1:A:68:THR:N    | 0.59     | 2.65        | 20     | 23    |
| 1:A:46:LEU:CD2  | 1:A:46:LEU:N    | 0.59     | 2.65        | 5      | 4     |
| 1:A:30:VAL:CG1  | 1:A:34:GLU:OE2  | 0.59     | 2.49        | 12     | 2     |
| 1:A:9:ASP:CB    | 1:A:46:LEU:HD22 | 0.59     | 2.25        | 9      | 5     |
| 1:A:56:LEU:CD1  | 1:A:76:LEU:CD2  | 0.59     | 2.80        | 25     | 3     |
| 1:A:46:LEU:HD22 | 1:A:46:LEU:H    | 0.59     | 1.55        | 1      | 6     |
| 1:A:3:VAL:CG1   | 1:A:5:ILE:CG2   | 0.59     | 2.81        | 18     | 1     |
| 1:A:46:LEU:N    | 1:A:46:LEU:CD1  | 0.59     | 2.65        | 19     | 2     |
| 1:A:34:GLU:CD   | 1:A:50:ALA:CB   | 0.59     | 2.71        | 9      | 4     |
| 1:A:19:VAL:HG21 | 1:A:73:LEU:HD11 | 0.59     | 1.73        | 15     | 2     |
| 1:A:22:TRP:HE3  | 1:A:35:VAL:HG21 | 0.59     | 1.57        | 13     | 5     |
| 1:A:41:THR:O    | 1:A:42:ASP:CB   | 0.59     | 2.50        | 4      | 9     |
| 1:A:56:LEU:HG   | 1:A:59:VAL:HG23 | 0.59     | 1.72        | 4      | 4     |
| 1:A:46:LEU:H    | 1:A:46:LEU:HD22 | 0.59     | 1.57        | 2      | 2     |
| 1:A:37:VAL:CG1  | 1:A:48:VAL:CG1  | 0.58     | 2.81        | 13     | 9     |
| 1:A:3:VAL:HB    | 1:A:76:LEU:HD23 | 0.58     | 1.74        | 6      | 2     |
| 1:A:6:LEU:HD13  | 1:A:8:PRO:CG    | 0.58     | 2.28        | 22     | 6     |
| 1:A:76:LEU:CD2  | 1:A:76:LEU:N    | 0.58     | 2.67        | 22     | 2     |
| 1:A:6:LEU:CD1   | 1:A:6:LEU:N     | 0.58     | 2.66        | 6      | 7     |
| 1:A:19:VAL:HG21 | 1:A:61:GLU:O    | 0.58     | 1.98        | 13     | 2     |
| 1:A:46:LEU:CD1  | 1:A:46:LEU:N    | 0.58     | 2.65        | 13     | 4     |
| 1:A:5:ILE:HG21  | 1:A:73:LEU:HD12 | 0.58     | 1.75        | 17     | 1     |
| 1:A:39:ILE:CG2  | 1:A:40:GLU:N    | 0.58     | 2.66        | 15     | 25    |
| 1:A:22:TRP:O    | 1:A:23:HIS:CD2  | 0.58     | 2.57        | 17     | 15    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:ILE:CD1   | 1:A:48:VAL:HG21 | 0.58     | 2.28        | 8      | 1     |
| 1:A:5:ILE:CG2   | 1:A:48:VAL:HG21 | 0.58     | 2.27        | 17     | 1     |
| 1:A:56:LEU:CG   | 1:A:59:VAL:CG2  | 0.58     | 2.81        | 6      | 10    |
| 1:A:5:ILE:HG21  | 1:A:22:TRP:CH2  | 0.58     | 2.33        | 8      | 2     |
| 1:A:44:VAL:HG12 | 1:A:46:LEU:HD23 | 0.58     | 1.75        | 17     | 1     |
| 1:A:5:ILE:CB    | 1:A:48:VAL:CG2  | 0.58     | 2.82        | 6      | 1     |
| 1:A:41:THR:OG1  | 1:A:44:VAL:HG13 | 0.58     | 1.99        | 18     | 1     |
| 1:A:5:ILE:HG22  | 1:A:74:GLY:O    | 0.57     | 1.99        | 8      | 1     |
| 1:A:35:VAL:HG22 | 1:A:36:LEU:N    | 0.57     | 2.14        | 19     | 19    |
| 1:A:3:VAL:HG13  | 1:A:5:ILE:HD13  | 0.57     | 1.76        | 20     | 1     |
| 1:A:22:TRP:CE2  | 1:A:59:VAL:CG1  | 0.57     | 2.88        | 13     | 1     |
| 1:A:17:ALA:HB1  | 1:A:40:GLU:O    | 0.57     | 1.99        | 4      | 15    |
| 1:A:30:VAL:HG12 | 1:A:53:ASP:N    | 0.57     | 2.14        | 6      | 9     |
| 1:A:54:GLY:O    | 1:A:56:LEU:N    | 0.57     | 2.37        | 13     | 19    |
| 1:A:28:ASP:O    | 1:A:29:ALA:CB   | 0.57     | 2.53        | 24     | 12    |
| 1:A:25:LYS:HB3  | 1:A:26:PRO:HD2  | 0.57     | 1.77        | 5      | 21    |
| 1:A:37:VAL:CG1  | 1:A:48:VAL:CG2  | 0.57     | 2.83        | 22     | 3     |
| 1:A:59:VAL:HG12 | 1:A:62:ASP:OD1  | 0.57     | 1.99        | 19     | 1     |
| 1:A:27:GLY:HA2  | 1:A:55:ILE:HG22 | 0.57     | 1.77        | 12     | 10    |
| 1:A:56:LEU:HD12 | 1:A:76:LEU:CG   | 0.57     | 2.26        | 1      | 6     |
| 1:A:28:ASP:O    | 1:A:55:ILE:CG1  | 0.57     | 2.53        | 6      | 4     |
| 1:A:76:LEU:N    | 1:A:76:LEU:HD22 | 0.57     | 2.14        | 6      | 1     |
| 1:A:22:TRP:NE1  | 1:A:73:LEU:CD2  | 0.57     | 2.67        | 15     | 1     |
| 1:A:68:THR:CG2  | 1:A:71:GLN:CG   | 0.57     | 2.81        | 20     | 2     |
| 1:A:30:VAL:CG1  | 1:A:34:GLU:OE1  | 0.57     | 2.53        | 20     | 1     |
| 1:A:24:LYS:CA   | 1:A:28:ASP:OD2  | 0.57     | 2.53        | 19     | 1     |
| 1:A:76:LEU:N    | 1:A:76:LEU:CD2  | 0.57     | 2.67        | 6      | 1     |
| 1:A:6:LEU:HD13  | 1:A:8:PRO:HG3   | 0.56     | 1.76        | 22     | 9     |
| 1:A:5:ILE:HG21  | 1:A:22:TRP:HZ2  | 0.56     | 1.53        | 8      | 1     |
| 1:A:7:VAL:HG22  | 1:A:39:ILE:HD13 | 0.56     | 1.77        | 8      | 2     |
| 1:A:76:LEU:HD22 | 1:A:76:LEU:N    | 0.56     | 2.15        | 22     | 1     |
| 1:A:22:TRP:CZ2  | 1:A:59:VAL:HG23 | 0.56     | 2.35        | 9      | 1     |
| 1:A:31:VAL:CG2  | 1:A:32:ARG:N    | 0.56     | 2.67        | 8      | 2     |
| 1:A:3:VAL:O     | 1:A:76:LEU:HD23 | 0.56     | 1.99        | 6      | 2     |
| 1:A:6:LEU:N     | 1:A:6:LEU:CD1   | 0.56     | 2.67        | 19     | 13    |
| 1:A:41:THR:HG21 | 1:A:46:LEU:HD11 | 0.56     | 1.77        | 22     | 1     |
| 1:A:34:GLU:OE1  | 1:A:54:GLY:CA   | 0.56     | 2.54        | 5      | 3     |
| 1:A:69:SER:O    | 1:A:70:ARG:CB   | 0.56     | 2.54        | 22     | 13    |
| 1:A:24:LYS:CD   | 1:A:28:ASP:HB2  | 0.56     | 2.30        | 2      | 10    |
| 1:A:60:LEU:HD11 | 1:A:72:ILE:HG23 | 0.56     | 1.77        | 22     | 1     |
| 1:A:21:THR:HG23 | 1:A:63:GLU:OE2  | 0.55     | 2.01        | 15     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:35:VAL:CG2  | 1:A:36:LEU:N    | 0.55     | 2.68        | 15     | 20    |
| 1:A:31:VAL:O    | 1:A:52:ALA:CA   | 0.55     | 2.54        | 16     | 6     |
| 1:A:17:ALA:CB   | 1:A:40:GLU:O    | 0.55     | 2.54        | 13     | 13    |
| 1:A:6:LEU:HD13  | 1:A:8:PRO:CD    | 0.55     | 2.30        | 8      | 3     |
| 1:A:25:LYS:N    | 1:A:28:ASP:OD1  | 0.55     | 2.39        | 19     | 3     |
| 1:A:30:VAL:CG2  | 1:A:33:ASP:O    | 0.55     | 2.54        | 4      | 11    |
| 1:A:22:TRP:N    | 1:A:63:GLU:OE2  | 0.55     | 2.39        | 24     | 4     |
| 1:A:30:VAL:HG21 | 1:A:34:GLU:CA   | 0.55     | 2.27        | 6      | 4     |
| 1:A:24:LYS:HB2  | 1:A:56:LEU:CD2  | 0.55     | 2.32        | 17     | 3     |
| 1:A:3:VAL:HG12  | 1:A:5:ILE:HD13  | 0.55     | 1.79        | 15     | 1     |
| 1:A:36:LEU:O    | 1:A:37:VAL:O    | 0.55     | 2.25        | 25     | 25    |
| 1:A:22:TRP:O    | 1:A:23:HIS:CG   | 0.55     | 2.59        | 17     | 6     |
| 1:A:56:LEU:CD2  | 1:A:76:LEU:CD2  | 0.55     | 2.84        | 11     | 2     |
| 1:A:23:HIS:HB2  | 1:A:35:VAL:HG23 | 0.55     | 1.76        | 3      | 14    |
| 1:A:17:ALA:C    | 1:A:67:VAL:HG13 | 0.55     | 2.21        | 8      | 4     |
| 1:A:34:GLU:OE2  | 1:A:52:ALA:O    | 0.55     | 2.25        | 5      | 2     |
| 1:A:56:LEU:CD2  | 1:A:59:VAL:HG21 | 0.55     | 2.31        | 6      | 5     |
| 1:A:62:ASP:O    | 1:A:63:GLU:C    | 0.55     | 2.45        | 25     | 25    |
| 1:A:3:VAL:HG11  | 1:A:76:LEU:HD22 | 0.55     | 1.79        | 20     | 1     |
| 1:A:5:ILE:O     | 1:A:5:ILE:HG23  | 0.55     | 2.02        | 8      | 1     |
| 1:A:5:ILE:CG2   | 1:A:48:VAL:CG2  | 0.55     | 2.85        | 6      | 1     |
| 1:A:72:ILE:O    | 1:A:72:ILE:CG2  | 0.55     | 2.55        | 15     | 4     |
| 1:A:34:GLU:HB2  | 1:A:50:ALA:HB3  | 0.55     | 1.77        | 21     | 11    |
| 1:A:34:GLU:OE2  | 1:A:54:GLY:CA   | 0.55     | 2.55        | 4      | 9     |
| 1:A:65:THR:HG22 | 1:A:66:THR:N    | 0.55     | 2.16        | 7      | 5     |
| 1:A:34:GLU:CG   | 1:A:54:GLY:HA3  | 0.55     | 2.31        | 10     | 14    |
| 1:A:20:ALA:CB   | 1:A:38:GLU:O    | 0.55     | 2.55        | 2      | 11    |
| 1:A:7:VAL:CG2   | 1:A:73:LEU:HD11 | 0.55     | 2.32        | 16     | 1     |
| 1:A:56:LEU:HD13 | 1:A:59:VAL:CG2  | 0.55     | 2.32        | 18     | 1     |
| 1:A:19:VAL:CG2  | 1:A:73:LEU:CD1  | 0.54     | 2.84        | 15     | 3     |
| 1:A:23:HIS:CE1  | 1:A:37:VAL:HA   | 0.54     | 2.37        | 14     | 24    |
| 1:A:25:LYS:CG   | 1:A:26:PRO:HD2  | 0.54     | 2.33        | 10     | 13    |
| 1:A:72:ILE:CG2  | 1:A:72:ILE:O    | 0.54     | 2.54        | 9      | 6     |
| 1:A:70:ARG:O    | 1:A:70:ARG:CG   | 0.54     | 2.55        | 16     | 1     |
| 1:A:58:ALA:CB   | 1:A:75:ARG:NE   | 0.54     | 2.70        | 22     | 1     |
| 1:A:34:GLU:OE2  | 1:A:54:GLY:N    | 0.54     | 2.40        | 12     | 3     |
| 1:A:3:VAL:CG2   | 1:A:34:GLU:OE1  | 0.54     | 2.55        | 6      | 4     |
| 1:A:34:GLU:OE1  | 1:A:50:ALA:CB   | 0.54     | 2.55        | 16     | 3     |
| 1:A:7:VAL:CG2   | 1:A:67:VAL:CG2  | 0.54     | 2.84        | 19     | 5     |
| 1:A:24:LYS:CD   | 1:A:28:ASP:CB   | 0.54     | 2.86        | 15     | 4     |
| 1:A:27:GLY:CA   | 1:A:55:ILE:CG2  | 0.54     | 2.86        | 11     | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:21:THR:HA   | 1:A:63:GLU:CB   | 0.54     | 2.32        | 16     | 13    |
| 1:A:28:ASP:O    | 1:A:55:ILE:CD1  | 0.54     | 2.55        | 13     | 1     |
| 1:A:58:ALA:HB3  | 1:A:75:ARG:CG   | 0.54     | 2.28        | 22     | 2     |
| 1:A:55:ILE:HD12 | 1:A:77:ARG:CD   | 0.54     | 2.33        | 5      | 1     |
| 1:A:27:GLY:HA2  | 1:A:55:ILE:CG2  | 0.54     | 2.33        | 19     | 21    |
| 1:A:25:LYS:CG   | 1:A:28:ASP:OD1  | 0.54     | 2.56        | 6      | 4     |
| 1:A:20:ALA:N    | 1:A:63:GLU:OE1  | 0.54     | 2.41        | 17     | 4     |
| 1:A:46:LEU:N    | 1:A:46:LEU:CD2  | 0.54     | 2.71        | 4      | 5     |
| 1:A:3:VAL:O     | 1:A:3:VAL:CG1   | 0.54     | 2.56        | 24     | 3     |
| 1:A:39:ILE:CD1  | 1:A:67:VAL:HG21 | 0.54     | 2.29        | 11     | 2     |
| 1:A:34:GLU:CD   | 1:A:54:GLY:CA   | 0.54     | 2.76        | 24     | 15    |
| 1:A:6:LEU:CB    | 1:A:71:GLN:O    | 0.54     | 2.55        | 8      | 4     |
| 1:A:25:LYS:O    | 1:A:56:LEU:CB   | 0.54     | 2.56        | 7      | 7     |
| 1:A:30:VAL:HG11 | 1:A:34:GLU:HB2  | 0.54     | 1.77        | 4      | 4     |
| 1:A:24:LYS:CB   | 1:A:56:LEU:CD2  | 0.54     | 2.84        | 3      | 3     |
| 1:A:34:GLU:OE2  | 1:A:35:VAL:CG1  | 0.53     | 2.56        | 24     | 6     |
| 1:A:31:VAL:O    | 1:A:52:ALA:CB   | 0.53     | 2.57        | 9      | 5     |
| 1:A:70:ARG:CG   | 1:A:70:ARG:O    | 0.53     | 2.55        | 19     | 1     |
| 1:A:54:GLY:O    | 1:A:55:ILE:C    | 0.53     | 2.47        | 3      | 18    |
| 1:A:56:LEU:CD1  | 1:A:76:LEU:HD11 | 0.53     | 2.33        | 6      | 2     |
| 1:A:2:SER:CB    | 1:A:76:LEU:O    | 0.53     | 2.57        | 19     | 3     |
| 1:A:25:LYS:CG   | 1:A:28:ASP:OD2  | 0.53     | 2.56        | 7      | 4     |
| 1:A:44:VAL:HG12 | 1:A:45:VAL:N    | 0.53     | 2.19        | 12     | 2     |
| 1:A:3:VAL:CG1   | 1:A:3:VAL:O     | 0.53     | 2.56        | 3      | 7     |
| 1:A:53:ASP:O    | 1:A:55:ILE:N    | 0.53     | 2.41        | 7      | 5     |
| 1:A:19:VAL:HG22 | 1:A:39:ILE:CD1  | 0.53     | 2.34        | 12     | 1     |
| 1:A:56:LEU:CD2  | 1:A:76:LEU:HD21 | 0.53     | 2.33        | 11     | 1     |
| 1:A:18:THR:O    | 1:A:40:GLU:N    | 0.53     | 2.41        | 15     | 7     |
| 1:A:27:GLY:O    | 1:A:28:ASP:O    | 0.53     | 2.26        | 6      | 19    |
| 1:A:61:GLU:CG   | 1:A:73:LEU:O    | 0.53     | 2.56        | 9      | 4     |
| 1:A:55:ILE:O    | 1:A:57:ASP:N    | 0.53     | 2.41        | 14     | 12    |
| 1:A:41:THR:OG1  | 1:A:46:LEU:CD2  | 0.53     | 2.56        | 1      | 2     |
| 1:A:17:ALA:CA   | 1:A:40:GLU:O    | 0.53     | 2.56        | 4      | 15    |
| 1:A:34:GLU:OE1  | 1:A:35:VAL:N    | 0.53     | 2.42        | 7      | 2     |
| 1:A:5:ILE:HG21  | 1:A:48:VAL:HG11 | 0.53     | 1.79        | 12     | 8     |
| 1:A:30:VAL:CB   | 1:A:53:ASP:O    | 0.53     | 2.56        | 5      | 6     |
| 1:A:3:VAL:O     | 1:A:5:ILE:CD1   | 0.53     | 2.55        | 6      | 1     |
| 1:A:7:VAL:N     | 1:A:8:PRO:CD    | 0.53     | 2.72        | 22     | 14    |
| 1:A:37:VAL:CG2  | 1:A:63:GLU:OE2  | 0.53     | 2.57        | 24     | 4     |
| 1:A:36:LEU:HD23 | 1:A:49:PRO:HB3  | 0.53     | 1.79        | 8      | 3     |
| 1:A:24:LYS:CB   | 1:A:56:LEU:HD21 | 0.53     | 2.33        | 16     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:3:VAL:CG2   | 1:A:34:GLU:OE2  | 0.53     | 2.55        | 5      | 1     |
| 1:A:6:LEU:HD22  | 1:A:70:ARG:CD   | 0.53     | 2.34        | 14     | 1     |
| 1:A:39:ILE:O    | 1:A:45:VAL:CG1  | 0.53     | 2.57        | 2      | 7     |
| 1:A:6:LEU:O     | 1:A:7:VAL:CG2   | 0.53     | 2.56        | 25     | 1     |
| 1:A:57:ASP:CB   | 1:A:76:LEU:O    | 0.53     | 2.57        | 22     | 2     |
| 1:A:22:TRP:CE2  | 1:A:59:VAL:CG2  | 0.53     | 2.92        | 9      | 1     |
| 1:A:61:GLU:O    | 1:A:73:LEU:CD1  | 0.53     | 2.57        | 15     | 1     |
| 1:A:55:ILE:CD1  | 1:A:55:ILE:N    | 0.53     | 2.71        | 13     | 1     |
| 1:A:39:ILE:O    | 1:A:45:VAL:CG2  | 0.53     | 2.57        | 19     | 2     |
| 1:A:21:THR:N    | 1:A:63:GLU:OE1  | 0.53     | 2.42        | 20     | 3     |
| 1:A:21:THR:O    | 1:A:21:THR:CG2  | 0.53     | 2.56        | 2      | 1     |
| 1:A:34:GLU:OE1  | 1:A:54:GLY:N    | 0.53     | 2.42        | 5      | 3     |
| 1:A:41:THR:HG23 | 1:A:44:VAL:O    | 0.53     | 2.04        | 11     | 1     |
| 1:A:17:ALA:CB   | 1:A:41:THR:OG1  | 0.53     | 2.57        | 15     | 1     |
| 1:A:25:LYS:CA   | 1:A:28:ASP:OD1  | 0.53     | 2.57        | 25     | 2     |
| 1:A:34:GLU:CD   | 1:A:54:GLY:N    | 0.53     | 2.61        | 19     | 2     |
| 1:A:34:GLU:HG2  | 1:A:35:VAL:HG12 | 0.53     | 1.80        | 3      | 1     |
| 1:A:3:VAL:CG1   | 1:A:5:ILE:HD12  | 0.53     | 2.31        | 6      | 1     |
| 1:A:56:LEU:HD22 | 1:A:76:LEU:HD23 | 0.53     | 1.81        | 16     | 1     |
| 1:A:41:THR:OG1  | 1:A:44:VAL:CG1  | 0.53     | 2.57        | 18     | 1     |
| 1:A:44:VAL:CG2  | 1:A:45:VAL:N    | 0.52     | 2.72        | 21     | 1     |
| 1:A:25:LYS:O    | 1:A:56:LEU:HB2  | 0.52     | 2.04        | 11     | 24    |
| 1:A:53:ASP:CB   | 1:A:77:ARG:O    | 0.52     | 2.56        | 16     | 7     |
| 1:A:6:LEU:HA    | 1:A:72:ILE:HA   | 0.52     | 1.81        | 18     | 17    |
| 1:A:61:GLU:OE1  | 1:A:67:VAL:CG1  | 0.52     | 2.57        | 2      | 1     |
| 1:A:24:LYS:CD   | 1:A:34:GLU:OE2  | 0.52     | 2.57        | 8      | 2     |
| 1:A:24:LYS:CG   | 1:A:54:GLY:O    | 0.52     | 2.57        | 9      | 1     |
| 1:A:30:VAL:CG1  | 1:A:52:ALA:HA   | 0.52     | 2.34        | 20     | 5     |
| 1:A:24:LYS:HB3  | 1:A:56:LEU:CD2  | 0.52     | 2.33        | 10     | 3     |
| 1:A:40:GLU:HA   | 1:A:45:VAL:HG22 | 0.52     | 1.80        | 14     | 2     |
| 1:A:44:VAL:HG22 | 1:A:45:VAL:N    | 0.52     | 2.19        | 21     | 1     |
| 1:A:6:LEU:O     | 1:A:48:VAL:CG2  | 0.52     | 2.57        | 11     | 1     |
| 1:A:56:LEU:HG   | 1:A:59:VAL:CG2  | 0.52     | 2.34        | 6      | 14    |
| 1:A:7:VAL:O     | 1:A:69:SER:O    | 0.52     | 2.28        | 3      | 8     |
| 1:A:5:ILE:HB    | 1:A:48:VAL:CG2  | 0.52     | 2.35        | 18     | 2     |
| 1:A:5:ILE:CG2   | 1:A:73:LEU:HB3  | 0.52     | 2.35        | 15     | 1     |
| 1:A:35:VAL:O    | 1:A:48:VAL:O    | 0.52     | 2.26        | 19     | 19    |
| 1:A:30:VAL:CB   | 1:A:34:GLU:HB3  | 0.52     | 2.34        | 13     | 1     |
| 1:A:44:VAL:CG1  | 1:A:46:LEU:CD2  | 0.52     | 2.87        | 17     | 1     |
| 1:A:56:LEU:HD21 | 1:A:59:VAL:CG2  | 0.52     | 2.30        | 7      | 1     |
| 1:A:5:ILE:CD1   | 1:A:74:GLY:O    | 0.52     | 2.57        | 18     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:ILE:HG13  | 1:A:48:VAL:CG2  | 0.52     | 2.34        | 5      | 9     |
| 1:A:5:ILE:CD1   | 1:A:5:ILE:C     | 0.52     | 2.78        | 8      | 1     |
| 1:A:5:ILE:HD13  | 1:A:48:VAL:CG2  | 0.52     | 2.35        | 8      | 1     |
| 1:A:5:ILE:O     | 1:A:72:ILE:CG1  | 0.52     | 2.58        | 17     | 1     |
| 1:A:22:TRP:CZ2  | 1:A:59:VAL:HG13 | 0.52     | 2.39        | 13     | 1     |
| 1:A:31:VAL:HG13 | 1:A:32:ARG:H    | 0.52     | 1.65        | 10     | 7     |
| 1:A:22:TRP:CZ2  | 1:A:73:LEU:HB3  | 0.52     | 2.40        | 11     | 1     |
| 1:A:41:THR:HG22 | 1:A:42:ASP:N    | 0.52     | 2.20        | 19     | 2     |
| 1:A:3:VAL:HG13  | 1:A:5:ILE:CD1   | 0.52     | 2.34        | 20     | 3     |
| 1:A:32:ARG:O    | 1:A:33:ASP:CG   | 0.52     | 2.47        | 25     | 25    |
| 1:A:34:GLU:O    | 1:A:35:VAL:O    | 0.52     | 2.27        | 4      | 11    |
| 1:A:39:ILE:CG1  | 1:A:67:VAL:HG11 | 0.52     | 2.34        | 19     | 4     |
| 1:A:61:GLU:N    | 1:A:73:LEU:O    | 0.52     | 2.43        | 24     | 9     |
| 1:A:25:LYS:HB3  | 1:A:26:PRO:CD   | 0.52     | 2.35        | 7      | 6     |
| 1:A:30:VAL:HB   | 1:A:53:ASP:O    | 0.52     | 2.04        | 5      | 5     |
| 1:A:5:ILE:CG1   | 1:A:22:TRP:CH2  | 0.52     | 2.93        | 8      | 1     |
| 1:A:65:THR:CG2  | 1:A:66:THR:N    | 0.52     | 2.73        | 7      | 3     |
| 1:A:61:GLU:O    | 1:A:73:LEU:HD11 | 0.51     | 2.05        | 15     | 1     |
| 1:A:52:ALA:O    | 1:A:53:ASP:HB2  | 0.51     | 2.05        | 5      | 16    |
| 1:A:41:THR:CG2  | 1:A:44:VAL:HB   | 0.51     | 2.36        | 4      | 3     |
| 1:A:17:ALA:N    | 1:A:67:VAL:O    | 0.51     | 2.43        | 1      | 2     |
| 1:A:5:ILE:HG23  | 1:A:73:LEU:HG   | 0.51     | 1.82        | 24     | 1     |
| 1:A:22:TRP:CZ2  | 1:A:73:LEU:HD23 | 0.51     | 2.39        | 14     | 4     |
| 1:A:32:ARG:CD   | 1:A:32:ARG:O    | 0.51     | 2.59        | 2      | 1     |
| 1:A:56:LEU:HD12 | 1:A:59:VAL:CG2  | 0.51     | 2.35        | 16     | 1     |
| 1:A:24:LYS:HD2  | 1:A:28:ASP:CB   | 0.51     | 2.36        | 15     | 1     |
| 1:A:5:ILE:HG13  | 1:A:22:TRP:CH2  | 0.51     | 2.41        | 8      | 1     |
| 1:A:59:VAL:CG1  | 1:A:62:ASP:OD1  | 0.51     | 2.57        | 19     | 1     |
| 1:A:30:VAL:HG12 | 1:A:52:ALA:C    | 0.51     | 2.26        | 6      | 9     |
| 1:A:34:GLU:HB3  | 1:A:50:ALA:CA   | 0.51     | 2.35        | 20     | 2     |
| 1:A:25:LYS:HB2  | 1:A:28:ASP:OD1  | 0.51     | 2.06        | 25     | 20    |
| 1:A:7:VAL:O     | 1:A:7:VAL:CG1   | 0.51     | 2.58        | 9      | 3     |
| 1:A:6:LEU:CA    | 1:A:71:GLN:O    | 0.51     | 2.59        | 6      | 3     |
| 1:A:39:ILE:HG23 | 1:A:40:GLU:H    | 0.50     | 1.64        | 13     | 16    |
| 1:A:4:ASP:OD2   | 1:A:72:ILE:HD11 | 0.50     | 2.06        | 10     | 1     |
| 1:A:30:VAL:HG11 | 1:A:34:GLU:N    | 0.50     | 2.21        | 9      | 1     |
| 1:A:35:VAL:O    | 1:A:49:PRO:HA   | 0.50     | 2.07        | 13     | 24    |
| 1:A:24:LYS:HD3  | 1:A:28:ASP:CB   | 0.50     | 2.36        | 2      | 1     |
| 1:A:36:LEU:CD1  | 1:A:36:LEU:N    | 0.50     | 2.74        | 3      | 1     |
| 1:A:4:ASP:OD1   | 1:A:4:ASP:N     | 0.50     | 2.43        | 9      | 1     |
| 1:A:34:GLU:HG2  | 1:A:50:ALA:CB   | 0.50     | 2.35        | 20     | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:61:GLU:OE2  | 1:A:71:GLN:NE2  | 0.50     | 2.45        | 22     | 1     |
| 1:A:5:ILE:HG12  | 1:A:48:VAL:CG2  | 0.50     | 2.37        | 24     | 8     |
| 1:A:3:VAL:CG1   | 1:A:76:LEU:HD22 | 0.50     | 2.37        | 20     | 1     |
| 1:A:30:VAL:CG1  | 1:A:34:GLU:HG2  | 0.50     | 2.34        | 5      | 2     |
| 1:A:30:VAL:CG1  | 1:A:52:ALA:CA   | 0.50     | 2.90        | 25     | 3     |
| 1:A:24:LYS:CG   | 1:A:35:VAL:HB   | 0.50     | 2.37        | 19     | 5     |
| 1:A:31:VAL:HG23 | 1:A:32:ARG:N    | 0.50     | 2.20        | 8      | 1     |
| 1:A:41:THR:OG1  | 1:A:46:LEU:HD21 | 0.50     | 2.07        | 12     | 2     |
| 1:A:17:ALA:HB2  | 1:A:41:THR:CG2  | 0.50     | 2.31        | 17     | 1     |
| 1:A:25:LYS:HG3  | 1:A:26:PRO:CD   | 0.50     | 2.37        | 24     | 2     |
| 1:A:37:VAL:HG11 | 1:A:73:LEU:HD11 | 0.50     | 1.78        | 11     | 1     |
| 1:A:69:SER:C    | 1:A:70:ARG:CG   | 0.49     | 2.80        | 24     | 1     |
| 1:A:56:LEU:CD1  | 1:A:59:VAL:HG21 | 0.49     | 2.37        | 18     | 1     |
| 1:A:9:ASP:HB3   | 1:A:46:LEU:CD2  | 0.49     | 2.36        | 25     | 2     |
| 1:A:5:ILE:HD13  | 1:A:5:ILE:N     | 0.49     | 2.22        | 6      | 1     |
| 1:A:24:LYS:CG   | 1:A:56:LEU:HD21 | 0.49     | 2.37        | 16     | 1     |
| 1:A:22:TRP:C    | 1:A:23:HIS:CG   | 0.49     | 2.86        | 17     | 15    |
| 1:A:34:GLU:O    | 1:A:35:VAL:C    | 0.49     | 2.50        | 13     | 8     |
| 1:A:56:LEU:HD22 | 1:A:76:LEU:CG   | 0.49     | 2.38        | 11     | 2     |
| 1:A:7:VAL:O     | 1:A:69:SER:CA   | 0.49     | 2.61        | 25     | 2     |
| 1:A:18:THR:HA   | 1:A:67:VAL:CG1  | 0.49     | 2.38        | 12     | 6     |
| 1:A:17:ALA:HB3  | 1:A:67:VAL:HG22 | 0.49     | 1.83        | 8      | 2     |
| 1:A:55:ILE:HB   | 1:A:77:ARG:CB   | 0.49     | 2.37        | 17     | 19    |
| 1:A:69:SER:O    | 1:A:71:GLN:N    | 0.49     | 2.45        | 7      | 1     |
| 1:A:5:ILE:HG22  | 1:A:73:LEU:HB3  | 0.49     | 1.84        | 15     | 1     |
| 1:A:22:TRP:CE2  | 1:A:59:VAL:HG11 | 0.49     | 2.43        | 13     | 1     |
| 1:A:41:THR:CG2  | 1:A:41:THR:O    | 0.49     | 2.59        | 13     | 2     |
| 1:A:24:LYS:CE   | 1:A:35:VAL:HB   | 0.49     | 2.36        | 2      | 11    |
| 1:A:17:ALA:HA   | 1:A:40:GLU:O    | 0.49     | 2.08        | 4      | 23    |
| 1:A:58:ALA:CB   | 1:A:75:ARG:O    | 0.49     | 2.57        | 8      | 2     |
| 1:A:5:ILE:O     | 1:A:5:ILE:CG2   | 0.49     | 2.61        | 8      | 1     |
| 1:A:5:ILE:CD1   | 1:A:6:LEU:N     | 0.49     | 2.76        | 8      | 1     |
| 1:A:69:SER:O    | 1:A:70:ARG:CG   | 0.49     | 2.61        | 17     | 2     |
| 1:A:56:LEU:CD2  | 1:A:59:VAL:CG2  | 0.49     | 2.91        | 7      | 1     |
| 1:A:37:VAL:CG1  | 1:A:48:VAL:HB   | 0.48     | 2.35        | 11     | 8     |
| 1:A:41:THR:O    | 1:A:42:ASP:HB2  | 0.48     | 2.07        | 8      | 4     |
| 1:A:6:LEU:HD13  | 1:A:8:PRO:HD3   | 0.48     | 1.83        | 8      | 1     |
| 1:A:56:LEU:HD22 | 1:A:76:LEU:HD22 | 0.48     | 1.85        | 10     | 1     |
| 1:A:68:THR:CG2  | 1:A:71:GLN:HG2  | 0.48     | 2.38        | 15     | 3     |
| 1:A:61:GLU:HA   | 1:A:65:THR:CB   | 0.48     | 2.38        | 8      | 2     |
| 1:A:5:ILE:HD12  | 1:A:48:VAL:CG2  | 0.48     | 2.38        | 17     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:22:TRP:CE2  | 1:A:73:LEU:CD2  | 0.48     | 2.96        | 15     | 2     |
| 1:A:34:GLU:OE2  | 1:A:54:GLY:HA3  | 0.48     | 2.09        | 4      | 4     |
| 1:A:69:SER:O    | 1:A:70:ARG:HB2  | 0.48     | 2.08        | 16     | 12    |
| 1:A:38:GLU:HB3  | 1:A:45:VAL:HG11 | 0.48     | 1.85        | 8      | 3     |
| 1:A:42:ASP:O    | 1:A:43:LYS:HB3  | 0.48     | 2.09        | 22     | 19    |
| 1:A:56:LEU:CD2  | 1:A:76:LEU:HD13 | 0.48     | 2.38        | 10     | 1     |
| 1:A:24:LYS:NZ   | 1:A:28:ASP:CB   | 0.48     | 2.76        | 22     | 1     |
| 1:A:18:THR:CA   | 1:A:67:VAL:CG1  | 0.48     | 2.91        | 22     | 3     |
| 1:A:47:GLU:CG   | 1:A:48:VAL:N    | 0.48     | 2.76        | 17     | 1     |
| 1:A:59:VAL:CB   | 1:A:62:ASP:OD1  | 0.48     | 2.62        | 19     | 1     |
| 1:A:68:THR:CG2  | 1:A:71:GLN:HG3  | 0.48     | 2.38        | 20     | 1     |
| 1:A:34:GLU:HG3  | 1:A:35:VAL:N    | 0.48     | 2.23        | 4      | 3     |
| 1:A:24:LYS:CE   | 1:A:24:LYS:HA   | 0.48     | 2.38        | 8      | 1     |
| 1:A:8:PRO:CA    | 1:A:70:ARG:HG2  | 0.48     | 2.39        | 11     | 1     |
| 1:A:62:ASP:O    | 1:A:63:GLU:O    | 0.48     | 2.32        | 24     | 7     |
| 1:A:71:GLN:O    | 1:A:72:ILE:C    | 0.48     | 2.52        | 7      | 6     |
| 1:A:41:THR:OG1  | 1:A:42:ASP:N    | 0.48     | 2.46        | 2      | 2     |
| 1:A:23:HIS:O    | 1:A:24:LYS:NZ   | 0.48     | 2.47        | 24     | 1     |
| 1:A:22:TRP:NE1  | 1:A:59:VAL:HG11 | 0.48     | 2.23        | 13     | 2     |
| 1:A:76:LEU:N    | 1:A:76:LEU:HD13 | 0.48     | 2.24        | 20     | 1     |
| 1:A:59:VAL:O    | 1:A:62:ASP:OD1  | 0.48     | 2.31        | 19     | 2     |
| 1:A:5:ILE:CD1   | 1:A:48:VAL:HG13 | 0.48     | 2.39        | 7      | 2     |
| 1:A:31:VAL:O    | 1:A:52:ALA:HA   | 0.48     | 2.08        | 15     | 14    |
| 1:A:58:ALA:O    | 1:A:75:ARG:O    | 0.48     | 2.31        | 11     | 9     |
| 1:A:63:GLU:N    | 1:A:63:GLU:CD   | 0.48     | 2.67        | 2      | 1     |
| 1:A:7:VAL:HG22  | 1:A:73:LEU:CD1  | 0.48     | 2.37        | 16     | 1     |
| 1:A:31:VAL:O    | 1:A:51:SER:O    | 0.47     | 2.32        | 15     | 4     |
| 1:A:25:LYS:HG3  | 1:A:28:ASP:OD2  | 0.47     | 2.08        | 11     | 6     |
| 1:A:3:VAL:CB    | 1:A:76:LEU:HD23 | 0.47     | 2.38        | 22     | 1     |
| 1:A:19:VAL:HG22 | 1:A:73:LEU:CD1  | 0.47     | 2.39        | 22     | 2     |
| 1:A:30:VAL:HG11 | 1:A:33:ASP:C    | 0.47     | 2.28        | 9      | 1     |
| 1:A:25:LYS:HD2  | 1:A:25:LYS:N    | 0.47     | 2.24        | 13     | 1     |
| 1:A:24:LYS:HD2  | 1:A:34:GLU:OE2  | 0.47     | 2.09        | 18     | 6     |
| 1:A:30:VAL:HG11 | 1:A:34:GLU:HB3  | 0.47     | 1.84        | 5      | 1     |
| 1:A:34:GLU:OE1  | 1:A:52:ALA:O    | 0.47     | 2.31        | 6      | 4     |
| 1:A:22:TRP:CE2  | 1:A:59:VAL:HG21 | 0.47     | 2.44        | 9      | 1     |
| 1:A:44:VAL:HG12 | 1:A:45:VAL:H    | 0.47     | 1.68        | 6      | 1     |
| 1:A:53:ASP:HB3  | 1:A:77:ARG:O    | 0.47     | 2.09        | 4      | 15    |
| 1:A:24:LYS:CE   | 1:A:28:ASP:HB2  | 0.47     | 2.39        | 20     | 4     |
| 1:A:3:VAL:CG2   | 1:A:54:GLY:HA2  | 0.47     | 2.39        | 20     | 2     |
| 1:A:51:SER:OG   | 1:A:51:SER:O    | 0.47     | 2.32        | 8      | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:56:LEU:HA   | 1:A:76:LEU:HD13 | 0.47     | 1.86        | 6      | 2     |
| 1:A:36:LEU:O    | 1:A:47:GLU:OE1  | 0.47     | 2.33        | 21     | 1     |
| 1:A:24:LYS:CD   | 1:A:35:VAL:HB   | 0.47     | 2.40        | 11     | 3     |
| 1:A:3:VAL:CG2   | 1:A:34:GLU:CD   | 0.47     | 2.83        | 5      | 1     |
| 1:A:54:GLY:CA   | 1:A:76:LEU:HD23 | 0.47     | 2.39        | 20     | 1     |
| 1:A:39:ILE:HG22 | 1:A:46:LEU:HG   | 0.47     | 1.86        | 22     | 1     |
| 1:A:25:LYS:HG3  | 1:A:26:PRO:HD2  | 0.47     | 1.87        | 24     | 2     |
| 1:A:30:VAL:HG22 | 1:A:31:VAL:H    | 0.47     | 1.68        | 18     | 2     |
| 1:A:9:ASP:CB    | 1:A:46:LEU:HG   | 0.47     | 2.39        | 2      | 12    |
| 1:A:3:VAL:HB    | 1:A:76:LEU:CG   | 0.47     | 2.40        | 14     | 5     |
| 1:A:68:THR:CG2  | 1:A:69:SER:N    | 0.47     | 2.78        | 24     | 3     |
| 1:A:34:GLU:HG3  | 1:A:54:GLY:CA   | 0.47     | 2.40        | 7      | 1     |
| 1:A:20:ALA:N    | 1:A:38:GLU:O    | 0.47     | 2.47        | 1      | 2     |
| 1:A:20:ALA:O    | 1:A:21:THR:OG1  | 0.47     | 2.33        | 18     | 13    |
| 1:A:34:GLU:OE2  | 1:A:53:ASP:C    | 0.47     | 2.54        | 12     | 2     |
| 1:A:73:LEU:N    | 1:A:73:LEU:HD23 | 0.47     | 2.25        | 6      | 1     |
| 1:A:34:GLU:CD   | 1:A:54:GLY:HA2  | 0.46     | 2.31        | 6      | 12    |
| 1:A:61:GLU:OE2  | 1:A:72:ILE:O    | 0.46     | 2.33        | 18     | 3     |
| 1:A:6:LEU:HA    | 1:A:71:GLN:O    | 0.46     | 2.10        | 6      | 6     |
| 1:A:61:GLU:O    | 1:A:62:ASP:C    | 0.46     | 2.53        | 14     | 17    |
| 1:A:24:LYS:HA   | 1:A:24:LYS:CE   | 0.46     | 2.40        | 3      | 2     |
| 1:A:18:THR:O    | 1:A:39:ILE:HA   | 0.46     | 2.11        | 11     | 6     |
| 1:A:28:ASP:O    | 1:A:55:ILE:HG13 | 0.46     | 2.10        | 19     | 3     |
| 1:A:36:LEU:H    | 1:A:36:LEU:HD12 | 0.46     | 1.70        | 14     | 1     |
| 1:A:24:LYS:HG2  | 1:A:56:LEU:CD2  | 0.46     | 2.40        | 18     | 1     |
| 1:A:19:VAL:CG1  | 1:A:63:GLU:HA   | 0.46     | 2.39        | 15     | 12    |
| 1:A:25:LYS:HB3  | 1:A:28:ASP:OD1  | 0.46     | 2.10        | 18     | 7     |
| 1:A:24:LYS:HD3  | 1:A:54:GLY:O    | 0.46     | 2.11        | 13     | 3     |
| 1:A:69:SER:O    | 1:A:69:SER:OG   | 0.46     | 2.34        | 10     | 1     |
| 1:A:19:VAL:HG23 | 1:A:67:VAL:HG11 | 0.46     | 1.87        | 11     | 1     |
| 1:A:41:THR:CB   | 1:A:44:VAL:O    | 0.46     | 2.63        | 3      | 1     |
| 1:A:66:THR:HG22 | 1:A:67:VAL:N    | 0.46     | 2.25        | 16     | 1     |
| 1:A:34:GLU:HG3  | 1:A:50:ALA:CB   | 0.46     | 2.37        | 5      | 2     |
| 1:A:37:VAL:O    | 1:A:47:GLU:HA   | 0.46     | 2.11        | 5      | 8     |
| 1:A:61:GLU:CB   | 1:A:73:LEU:O    | 0.46     | 2.63        | 17     | 8     |
| 1:A:18:THR:N    | 1:A:67:VAL:HG13 | 0.46     | 2.26        | 22     | 5     |
| 1:A:59:VAL:O    | 1:A:62:ASP:OD2  | 0.46     | 2.34        | 22     | 1     |
| 1:A:5:ILE:HG21  | 1:A:48:VAL:CG1  | 0.46     | 2.40        | 19     | 3     |
| 1:A:67:VAL:HG23 | 1:A:71:GLN:HB2  | 0.46     | 1.88        | 3      | 1     |
| 1:A:23:HIS:ND1  | 1:A:36:LEU:HD12 | 0.46     | 2.26        | 9      | 1     |
| 1:A:7:VAL:C     | 1:A:69:SER:O    | 0.46     | 2.54        | 9      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:67:VAL:HG23 | 1:A:68:THR:N    | 0.46     | 2.26        | 6      | 21    |
| 1:A:34:GLU:OE1  | 1:A:54:GLY:HA2  | 0.46     | 2.11        | 13     | 3     |
| 1:A:54:GLY:HA2  | 1:A:76:LEU:HD23 | 0.46     | 1.88        | 20     | 2     |
| 1:A:34:GLU:CG   | 1:A:35:VAL:N    | 0.46     | 2.79        | 4      | 2     |
| 1:A:7:VAL:CG1   | 1:A:7:VAL:O     | 0.46     | 2.61        | 15     | 2     |
| 1:A:25:LYS:C    | 1:A:28:ASP:OD1  | 0.46     | 2.54        | 25     | 3     |
| 1:A:60:LEU:HD12 | 1:A:61:GLU:CG   | 0.46     | 2.41        | 22     | 1     |
| 1:A:71:GLN:O    | 1:A:72:ILE:HB   | 0.46     | 2.11        | 15     | 4     |
| 1:A:6:LEU:HB3   | 1:A:71:GLN:O    | 0.46     | 2.11        | 1      | 1     |
| 1:A:61:GLU:CG   | 1:A:73:LEU:HA   | 0.46     | 2.41        | 1      | 7     |
| 1:A:20:ALA:C    | 1:A:63:GLU:OE1  | 0.46     | 2.54        | 24     | 4     |
| 1:A:5:ILE:O     | 1:A:72:ILE:HG13 | 0.46     | 2.11        | 17     | 5     |
| 1:A:62:ASP:O    | 1:A:65:THR:OG1  | 0.46     | 2.33        | 24     | 2     |
| 1:A:28:ASP:O    | 1:A:55:ILE:HG12 | 0.46     | 2.11        | 6      | 5     |
| 1:A:7:VAL:HG11  | 1:A:67:VAL:HG21 | 0.46     | 1.87        | 4      | 2     |
| 1:A:5:ILE:CG2   | 1:A:73:LEU:HD12 | 0.46     | 2.41        | 17     | 2     |
| 1:A:3:VAL:HB    | 1:A:76:LEU:CD2  | 0.46     | 2.40        | 6      | 2     |
| 1:A:60:LEU:CD2  | 1:A:74:GLY:HA2  | 0.46     | 2.40        | 17     | 1     |
| 1:A:56:LEU:HD21 | 1:A:59:VAL:HG11 | 0.46     | 1.88        | 9      | 1     |
| 1:A:21:THR:HA   | 1:A:63:GLU:HB3  | 0.45     | 1.88        | 21     | 14    |
| 1:A:6:LEU:CA    | 1:A:72:ILE:HA   | 0.45     | 2.41        | 4      | 4     |
| 1:A:34:GLU:OE2  | 1:A:52:ALA:C    | 0.45     | 2.54        | 12     | 2     |
| 1:A:61:GLU:CG   | 1:A:72:ILE:O    | 0.45     | 2.64        | 14     | 1     |
| 1:A:34:GLU:HG3  | 1:A:53:ASP:O    | 0.45     | 2.11        | 18     | 2     |
| 1:A:30:VAL:HG12 | 1:A:52:ALA:HA   | 0.45     | 1.87        | 4      | 2     |
| 1:A:19:VAL:HA   | 1:A:39:ILE:HG13 | 0.45     | 1.89        | 11     | 6     |
| 1:A:2:SER:HA    | 1:A:77:ARG:CA   | 0.45     | 2.42        | 25     | 5     |
| 1:A:24:LYS:HG2  | 1:A:35:VAL:HB   | 0.45     | 1.88        | 17     | 5     |
| 1:A:7:VAL:CG1   | 1:A:69:SER:HA   | 0.45     | 2.42        | 2      | 1     |
| 1:A:61:GLU:OE2  | 1:A:72:ILE:C    | 0.45     | 2.55        | 5      | 1     |
| 1:A:24:LYS:HE2  | 1:A:34:GLU:OE2  | 0.45     | 2.11        | 24     | 1     |
| 1:A:20:ALA:O    | 1:A:63:GLU:HB2  | 0.45     | 2.11        | 10     | 3     |
| 1:A:24:LYS:NZ   | 1:A:54:GLY:O    | 0.45     | 2.50        | 20     | 1     |
| 1:A:34:GLU:CD   | 1:A:54:GLY:HA3  | 0.45     | 2.32        | 10     | 6     |
| 1:A:25:LYS:HE3  | 1:A:25:LYS:CA   | 0.45     | 2.41        | 8      | 1     |
| 1:A:70:ARG:O    | 1:A:71:GLN:O    | 0.45     | 2.33        | 9      | 1     |
| 1:A:5:ILE:CD1   | 1:A:5:ILE:H     | 0.45     | 2.24        | 18     | 1     |
| 1:A:41:THR:O    | 1:A:42:ASP:O    | 0.45     | 2.34        | 13     | 1     |
| 1:A:25:LYS:HG3  | 1:A:28:ASP:OD1  | 0.45     | 2.12        | 8      | 6     |
| 1:A:3:VAL:HG21  | 1:A:54:GLY:CA   | 0.45     | 2.42        | 20     | 1     |
| 1:A:42:ASP:O    | 1:A:43:LYS:HB2  | 0.45     | 2.12        | 4      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:37:VAL:HG23 | 1:A:63:GLU:OE2  | 0.45     | 2.11        | 17     | 1     |
| 1:A:56:LEU:CD2  | 1:A:76:LEU:HD23 | 0.45     | 2.41        | 16     | 1     |
| 1:A:73:LEU:HD13 | 1:A:73:LEU:N    | 0.45     | 2.25        | 16     | 1     |
| 1:A:19:VAL:O    | 1:A:20:ALA:C    | 0.45     | 2.53        | 1      | 5     |
| 1:A:41:THR:CG2  | 1:A:44:VAL:CB   | 0.45     | 2.94        | 4      | 2     |
| 1:A:5:ILE:HG12  | 1:A:48:VAL:CG1  | 0.45     | 2.41        | 7      | 10    |
| 1:A:2:SER:HB3   | 1:A:76:LEU:O    | 0.45     | 2.11        | 19     | 4     |
| 1:A:70:ARG:HG2  | 1:A:70:ARG:O    | 0.45     | 2.12        | 16     | 2     |
| 1:A:3:VAL:O     | 1:A:75:ARG:HA   | 0.45     | 2.12        | 3      | 5     |
| 1:A:17:ALA:CB   | 1:A:41:THR:HA   | 0.45     | 2.42        | 22     | 1     |
| 1:A:34:GLU:OE2  | 1:A:76:LEU:CD2  | 0.45     | 2.57        | 18     | 1     |
| 1:A:30:VAL:HG12 | 1:A:52:ALA:CA   | 0.45     | 2.42        | 13     | 3     |
| 1:A:61:GLU:HG3  | 1:A:73:LEU:O    | 0.45     | 2.12        | 9      | 12    |
| 1:A:23:HIS:CE1  | 1:A:36:LEU:O    | 0.45     | 2.70        | 25     | 9     |
| 1:A:6:LEU:CD1   | 1:A:8:PRO:HG3   | 0.45     | 2.42        | 12     | 2     |
| 1:A:7:VAL:O     | 1:A:68:THR:O    | 0.45     | 2.35        | 16     | 3     |
| 1:A:61:GLU:CB   | 1:A:73:LEU:HA   | 0.45     | 2.42        | 17     | 2     |
| 1:A:20:ALA:O    | 1:A:63:GLU:CB   | 0.45     | 2.65        | 19     | 2     |
| 1:A:22:TRP:CZ2  | 1:A:73:LEU:HD12 | 0.45     | 2.47        | 8      | 1     |
| 1:A:61:GLU:HB2  | 1:A:73:LEU:CA   | 0.45     | 2.42        | 17     | 1     |
| 1:A:56:LEU:CD2  | 1:A:76:LEU:HG   | 0.45     | 2.42        | 18     | 1     |
| 1:A:7:VAL:HG21  | 1:A:39:ILE:HD12 | 0.44     | 1.90        | 7      | 1     |
| 1:A:34:GLU:OE1  | 1:A:53:ASP:C    | 0.44     | 2.56        | 6      | 1     |
| 1:A:5:ILE:N     | 1:A:5:ILE:HD13  | 0.44     | 2.26        | 18     | 1     |
| 1:A:39:ILE:HG12 | 1:A:67:VAL:HG11 | 0.44     | 1.87        | 4      | 2     |
| 1:A:32:ARG:HD3  | 1:A:32:ARG:O    | 0.44     | 2.12        | 2      | 1     |
| 1:A:24:LYS:O    | 1:A:56:LEU:HD12 | 0.44     | 2.12        | 24     | 1     |
| 1:A:51:SER:O    | 1:A:51:SER:OG   | 0.44     | 2.34        | 7      | 3     |
| 1:A:61:GLU:HG3  | 1:A:72:ILE:O    | 0.44     | 2.11        | 14     | 5     |
| 1:A:30:VAL:CG1  | 1:A:52:ALA:C    | 0.44     | 2.86        | 25     | 1     |
| 1:A:34:GLU:OE1  | 1:A:35:VAL:CG1  | 0.44     | 2.48        | 25     | 1     |
| 1:A:34:GLU:CG   | 1:A:35:VAL:HG12 | 0.44     | 2.42        | 4      | 2     |
| 1:A:30:VAL:HB   | 1:A:34:GLU:OE1  | 0.44     | 2.12        | 4      | 2     |
| 1:A:30:VAL:CG2  | 1:A:34:GLU:HA   | 0.44     | 2.34        | 10     | 2     |
| 1:A:7:VAL:HB    | 1:A:67:VAL:CG2  | 0.44     | 2.42        | 24     | 1     |
| 1:A:76:LEU:HD23 | 1:A:76:LEU:N    | 0.44     | 2.26        | 14     | 1     |
| 1:A:30:VAL:HG21 | 1:A:34:GLU:HB3  | 0.44     | 1.87        | 13     | 1     |
| 1:A:19:VAL:HG23 | 1:A:65:THR:O    | 0.44     | 2.12        | 20     | 1     |
| 1:A:7:VAL:O     | 1:A:69:SER:C    | 0.44     | 2.55        | 25     | 4     |
| 1:A:52:ALA:O    | 1:A:53:ASP:CG   | 0.44     | 2.55        | 5      | 1     |
| 1:A:54:GLY:O    | 1:A:76:LEU:HD12 | 0.44     | 2.11        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:61:GLU:HB2  | 1:A:73:LEU:O    | 0.44     | 2.12        | 9      | 11    |
| 1:A:64:GLY:O    | 1:A:65:THR:C    | 0.44     | 2.56        | 25     | 2     |
| 1:A:44:VAL:CG1  | 1:A:45:VAL:N    | 0.44     | 2.79        | 12     | 2     |
| 1:A:59:VAL:HB   | 1:A:62:ASP:OD1  | 0.44     | 2.12        | 19     | 2     |
| 1:A:61:GLU:HB2  | 1:A:73:LEU:HA   | 0.44     | 1.90        | 10     | 3     |
| 1:A:41:THR:O    | 1:A:41:THR:CG2  | 0.44     | 2.65        | 7      | 1     |
| 1:A:25:LYS:HG2  | 1:A:28:ASP:OD1  | 0.44     | 2.13        | 16     | 1     |
| 1:A:41:THR:OG1  | 1:A:44:VAL:O    | 0.44     | 2.34        | 18     | 1     |
| 1:A:24:LYS:CA   | 1:A:24:LYS:HE2  | 0.44     | 2.42        | 1      | 3     |
| 1:A:72:ILE:HG12 | 1:A:74:GLY:N    | 0.44     | 2.28        | 8      | 2     |
| 1:A:5:ILE:HG13  | 1:A:22:TRP:CZ2  | 0.44     | 2.47        | 8      | 1     |
| 1:A:24:LYS:HD2  | 1:A:35:VAL:CG1  | 0.44     | 2.42        | 19     | 1     |
| 1:A:3:VAL:CG2   | 1:A:76:LEU:HB2  | 0.44     | 2.43        | 12     | 4     |
| 1:A:24:LYS:HE2  | 1:A:24:LYS:CA   | 0.44     | 2.43        | 5      | 1     |
| 1:A:7:VAL:CG1   | 1:A:46:LEU:CD1  | 0.44     | 2.82        | 12     | 1     |
| 1:A:24:LYS:CE   | 1:A:34:GLU:OE2  | 0.44     | 2.66        | 24     | 1     |
| 1:A:47:GLU:O    | 1:A:48:VAL:HG23 | 0.44     | 2.12        | 14     | 1     |
| 1:A:59:VAL:CG1  | 1:A:59:VAL:O    | 0.44     | 2.56        | 9      | 1     |
| 1:A:9:ASP:O     | 1:A:41:THR:HG21 | 0.44     | 2.13        | 18     | 1     |
| 1:A:36:LEU:O    | 1:A:37:VAL:C    | 0.44     | 2.56        | 17     | 21    |
| 1:A:24:LYS:HG2  | 1:A:54:GLY:O    | 0.44     | 2.12        | 9      | 4     |
| 1:A:68:THR:HG23 | 1:A:70:ARG:N    | 0.44     | 2.28        | 20     | 1     |
| 1:A:57:ASP:HB3  | 1:A:76:LEU:O    | 0.44     | 2.13        | 20     | 2     |
| 1:A:55:ILE:CD1  | 1:A:55:ILE:H    | 0.44     | 2.26        | 13     | 1     |
| 1:A:3:VAL:HB    | 1:A:76:LEU:HB2  | 0.44     | 1.90        | 25     | 11    |
| 1:A:32:ARG:O    | 1:A:33:ASP:OD1  | 0.44     | 2.36        | 25     | 2     |
| 1:A:7:VAL:CB    | 1:A:67:VAL:HG21 | 0.44     | 2.42        | 24     | 1     |
| 1:A:7:VAL:HB    | 1:A:69:SER:O    | 0.43     | 2.13        | 15     | 2     |
| 1:A:69:SER:OG   | 1:A:69:SER:O    | 0.43     | 2.36        | 22     | 1     |
| 1:A:7:VAL:O     | 1:A:69:SER:HA   | 0.43     | 2.13        | 25     | 6     |
| 1:A:6:LEU:HB3   | 1:A:72:ILE:N    | 0.43     | 2.28        | 21     | 2     |
| 1:A:28:ASP:O    | 1:A:55:ILE:HD12 | 0.43     | 2.13        | 13     | 1     |
| 1:A:58:ALA:O    | 1:A:75:ARG:N    | 0.43     | 2.51        | 2      | 3     |
| 1:A:55:ILE:O    | 1:A:56:LEU:C    | 0.43     | 2.56        | 11     | 4     |
| 1:A:8:PRO:HB3   | 1:A:70:ARG:CG   | 0.43     | 2.43        | 7      | 2     |
| 1:A:34:GLU:CG   | 1:A:54:GLY:CA   | 0.43     | 2.96        | 7      | 2     |
| 1:A:53:ASP:HB2  | 1:A:77:ARG:O    | 0.43     | 2.13        | 7      | 1     |
| 1:A:53:ASP:OD1  | 1:A:77:ARG:CB   | 0.43     | 2.66        | 3      | 1     |
| 1:A:39:ILE:CD1  | 1:A:73:LEU:HD21 | 0.43     | 2.43        | 19     | 1     |
| 1:A:59:VAL:C    | 1:A:62:ASP:OD1  | 0.43     | 2.57        | 19     | 1     |
| 1:A:34:GLU:OE2  | 1:A:54:GLY:HA2  | 0.43     | 2.13        | 22     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:56:LEU:HA   | 1:A:76:LEU:CD1  | 0.43     | 2.43        | 22     | 2     |
| 1:A:24:LYS:HB2  | 1:A:56:LEU:HD13 | 0.43     | 1.90        | 19     | 1     |
| 1:A:19:VAL:HG23 | 1:A:67:VAL:CG1  | 0.43     | 2.43        | 11     | 1     |
| 1:A:60:LEU:O    | 1:A:61:GLU:OE2  | 0.43     | 2.37        | 11     | 1     |
| 1:A:40:GLU:HG2  | 1:A:45:VAL:HG22 | 0.43     | 1.89        | 9      | 1     |
| 1:A:4:ASP:OD2   | 1:A:75:ARG:HB3  | 0.43     | 2.13        | 6      | 2     |
| 1:A:68:THR:OG1  | 1:A:71:GLN:HG3  | 0.43     | 2.14        | 9      | 2     |
| 1:A:7:VAL:HB    | 1:A:68:THR:O    | 0.43     | 2.13        | 2      | 1     |
| 1:A:2:SER:HA    | 1:A:77:ARG:O    | 0.43     | 2.13        | 22     | 1     |
| 1:A:21:THR:HG23 | 1:A:63:GLU:CD   | 0.43     | 2.34        | 14     | 1     |
| 1:A:24:LYS:HD3  | 1:A:56:LEU:CD2  | 0.43     | 2.44        | 16     | 1     |
| 1:A:37:VAL:O    | 1:A:47:GLU:HB2  | 0.43     | 2.14        | 15     | 4     |
| 1:A:39:ILE:HD11 | 1:A:67:VAL:HG22 | 0.43     | 1.89        | 1      | 2     |
| 1:A:47:GLU:CG   | 1:A:49:PRO:HD3  | 0.43     | 2.44        | 22     | 6     |
| 1:A:61:GLU:HG2  | 1:A:65:THR:HG21 | 0.43     | 1.91        | 8      | 1     |
| 1:A:52:ALA:C    | 1:A:53:ASP:OD1  | 0.43     | 2.57        | 7      | 1     |
| 1:A:68:THR:HG23 | 1:A:69:SER:H    | 0.43     | 1.74        | 15     | 3     |
| 1:A:34:GLU:OE1  | 1:A:54:GLY:HA3  | 0.43     | 2.14        | 20     | 2     |
| 1:A:39:ILE:CD1  | 1:A:67:VAL:CG2  | 0.43     | 2.97        | 1      | 2     |
| 1:A:41:THR:HG21 | 1:A:44:VAL:HB   | 0.43     | 1.89        | 4      | 2     |
| 1:A:5:ILE:O     | 1:A:72:ILE:HA   | 0.43     | 2.14        | 22     | 7     |
| 1:A:30:VAL:HG21 | 1:A:33:ASP:C    | 0.43     | 2.34        | 10     | 2     |
| 1:A:39:ILE:CG2  | 1:A:46:LEU:HG   | 0.43     | 2.44        | 22     | 2     |
| 1:A:37:VAL:CG2  | 1:A:73:LEU:HD21 | 0.43     | 2.24        | 14     | 1     |
| 1:A:53:ASP:OD2  | 1:A:77:ARG:C    | 0.43     | 2.57        | 9      | 1     |
| 1:A:39:ILE:CD1  | 1:A:67:VAL:HG22 | 0.43     | 2.44        | 1      | 1     |
| 1:A:61:GLU:HA   | 1:A:65:THR:OG1  | 0.43     | 2.14        | 25     | 1     |
| 1:A:70:ARG:CD   | 1:A:70:ARG:O    | 0.43     | 2.66        | 19     | 1     |
| 1:A:29:ALA:HA   | 1:A:53:ASP:O    | 0.42     | 2.14        | 1      | 4     |
| 1:A:5:ILE:CD1   | 1:A:48:VAL:CG2  | 0.42     | 2.97        | 17     | 2     |
| 1:A:27:GLY:CA   | 1:A:55:ILE:HG22 | 0.42     | 2.44        | 12     | 1     |
| 1:A:53:ASP:CG   | 1:A:77:ARG:O    | 0.42     | 2.56        | 18     | 3     |
| 1:A:68:THR:N    | 1:A:71:GLN:HG3  | 0.42     | 2.29        | 4      | 5     |
| 1:A:18:THR:CA   | 1:A:67:VAL:HG13 | 0.42     | 2.44        | 21     | 1     |
| 1:A:25:LYS:HG2  | 1:A:28:ASP:OD2  | 0.42     | 2.14        | 25     | 2     |
| 1:A:6:LEU:HB3   | 1:A:72:ILE:HA   | 0.42     | 1.91        | 4      | 4     |
| 1:A:5:ILE:C     | 1:A:5:ILE:HD12  | 0.42     | 2.34        | 8      | 1     |
| 1:A:19:VAL:N    | 1:A:39:ILE:HG13 | 0.42     | 2.29        | 24     | 1     |
| 1:A:25:LYS:N    | 1:A:28:ASP:OD2  | 0.42     | 2.52        | 19     | 1     |
| 1:A:19:VAL:HA   | 1:A:39:ILE:CD1  | 0.42     | 2.44        | 20     | 3     |
| 1:A:3:VAL:CB    | 1:A:76:LEU:HD22 | 0.42     | 2.44        | 20     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:6:LEU:C     | 1:A:8:PRO:HD3   | 0.42     | 2.35        | 12     | 7     |
| 1:A:5:ILE:HG22  | 1:A:73:LEU:HG   | 0.42     | 1.91        | 17     | 1     |
| 1:A:6:LEU:HB2   | 1:A:71:GLN:O    | 0.42     | 2.14        | 12     | 1     |
| 1:A:30:VAL:HG13 | 1:A:31:VAL:H    | 0.42     | 1.73        | 9      | 1     |
| 1:A:27:GLY:C    | 1:A:55:ILE:HG23 | 0.42     | 2.35        | 22     | 3     |
| 1:A:9:ASP:CB    | 1:A:46:LEU:CD1  | 0.42     | 2.95        | 25     | 2     |
| 1:A:5:ILE:CD1   | 1:A:48:VAL:CB   | 0.42     | 2.98        | 8      | 1     |
| 1:A:24:LYS:HB3  | 1:A:56:LEU:CD1  | 0.42     | 2.44        | 24     | 1     |
| 1:A:34:GLU:CD   | 1:A:35:VAL:N    | 0.42     | 2.72        | 7      | 1     |
| 1:A:24:LYS:CE   | 1:A:28:ASP:OD2  | 0.42     | 2.67        | 19     | 1     |
| 1:A:68:THR:CB   | 1:A:71:GLN:HG3  | 0.42     | 2.44        | 13     | 1     |
| 1:A:32:ARG:O    | 1:A:33:ASP:HB2  | 0.42     | 2.14        | 17     | 5     |
| 1:A:25:LYS:CG   | 1:A:26:PRO:CD   | 0.42     | 2.98        | 3      | 5     |
| 1:A:24:LYS:NZ   | 1:A:28:ASP:HB2  | 0.42     | 2.29        | 22     | 1     |
| 1:A:55:ILE:HB   | 1:A:77:ARG:HB2  | 0.42     | 1.92        | 14     | 2     |
| 1:A:53:ASP:C    | 1:A:55:ILE:N    | 0.42     | 2.73        | 24     | 3     |
| 1:A:53:ASP:OD1  | 1:A:77:ARG:HB3  | 0.42     | 2.14        | 3      | 2     |
| 1:A:24:LYS:CB   | 1:A:28:ASP:OD2  | 0.42     | 2.68        | 19     | 1     |
| 1:A:19:VAL:HG21 | 1:A:61:GLU:HB3  | 0.42     | 1.92        | 1      | 1     |
| 1:A:25:LYS:HB2  | 1:A:28:ASP:CG   | 0.42     | 2.35        | 24     | 4     |
| 1:A:17:ALA:O    | 1:A:66:THR:HG23 | 0.42     | 2.13        | 2      | 1     |
| 1:A:72:ILE:O    | 1:A:73:LEU:C    | 0.42     | 2.58        | 6      | 4     |
| 1:A:7:VAL:CB    | 1:A:67:VAL:CG2  | 0.42     | 2.97        | 22     | 1     |
| 1:A:7:VAL:CG2   | 1:A:73:LEU:CD1  | 0.42     | 2.98        | 16     | 1     |
| 1:A:24:LYS:HD2  | 1:A:28:ASP:HB2  | 0.42     | 1.90        | 15     | 1     |
| 1:A:18:THR:C    | 1:A:39:ILE:HG12 | 0.42     | 2.35        | 1      | 3     |
| 1:A:56:LEU:CG   | 1:A:59:VAL:HG21 | 0.42     | 2.45        | 20     | 2     |
| 1:A:24:LYS:HE2  | 1:A:28:ASP:HB2  | 0.42     | 1.90        | 6      | 2     |
| 1:A:6:LEU:CB    | 1:A:72:ILE:HA   | 0.42     | 2.45        | 4      | 2     |
| 1:A:34:GLU:HG3  | 1:A:54:GLY:HA3  | 0.42     | 1.91        | 2      | 2     |
| 1:A:73:LEU:HD23 | 1:A:73:LEU:N    | 0.42     | 2.29        | 8      | 1     |
| 1:A:61:GLU:OE1  | 1:A:61:GLU:HA   | 0.42     | 2.14        | 14     | 1     |
| 1:A:20:ALA:C    | 1:A:63:GLU:HB3  | 0.42     | 2.35        | 13     | 2     |
| 1:A:22:TRP:CE3  | 1:A:35:VAL:HG21 | 0.42     | 2.45        | 13     | 2     |
| 1:A:22:TRP:NE1  | 1:A:59:VAL:CG1  | 0.42     | 2.82        | 13     | 1     |
| 1:A:42:ASP:O    | 1:A:42:ASP:CG   | 0.42     | 2.57        | 16     | 2     |
| 1:A:60:LEU:HD12 | 1:A:61:GLU:HG3  | 0.42     | 1.91        | 22     | 1     |
| 1:A:56:LEU:CD1  | 1:A:76:LEU:HG   | 0.42     | 2.42        | 12     | 1     |
| 1:A:30:VAL:CG2  | 1:A:34:GLU:HB3  | 0.42     | 2.44        | 13     | 1     |
| 1:A:53:ASP:O    | 1:A:54:GLY:C    | 0.42     | 2.56        | 7      | 2     |
| 1:A:31:VAL:HG13 | 1:A:32:ARG:N    | 0.42     | 2.30        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:3:VAL:HB    | 1:A:76:LEU:HG   | 0.41     | 1.92        | 24     | 2     |
| 1:A:24:LYS:NZ   | 1:A:35:VAL:HB   | 0.41     | 2.30        | 12     | 2     |
| 1:A:3:VAL:HB    | 1:A:76:LEU:CB   | 0.41     | 2.45        | 7      | 1     |
| 1:A:18:THR:O    | 1:A:39:ILE:HG13 | 0.41     | 2.15        | 15     | 1     |
| 1:A:30:VAL:HB   | 1:A:34:GLU:CD   | 0.41     | 2.36        | 20     | 1     |
| 1:A:37:VAL:CG2  | 1:A:73:LEU:CD2  | 0.41     | 2.94        | 14     | 1     |
| 1:A:9:ASP:HB3   | 1:A:46:LEU:HG   | 0.41     | 1.91        | 14     | 1     |
| 1:A:53:ASP:OD1  | 1:A:77:ARG:CG   | 0.41     | 2.68        | 3      | 1     |
| 1:A:56:LEU:HA   | 1:A:56:LEU:HD12 | 0.41     | 1.71        | 4      | 1     |
| 1:A:56:LEU:HD12 | 1:A:56:LEU:HA   | 0.41     | 1.71        | 23     | 1     |
| 1:A:37:VAL:HG22 | 1:A:38:GLU:N    | 0.41     | 2.30        | 19     | 1     |
| 1:A:5:ILE:N     | 1:A:5:ILE:CD1   | 0.41     | 2.83        | 18     | 1     |
| 1:A:30:VAL:HB   | 1:A:34:GLU:OE2  | 0.41     | 2.16        | 20     | 1     |
| 1:A:6:LEU:CD1   | 1:A:8:PRO:HD3   | 0.41     | 2.45        | 25     | 1     |
| 1:A:24:LYS:HE3  | 1:A:28:ASP:HB2  | 0.41     | 1.93        | 11     | 1     |
| 1:A:25:LYS:N    | 1:A:28:ASP:CG   | 0.41     | 2.74        | 19     | 1     |
| 1:A:21:THR:CA   | 1:A:63:GLU:HB3  | 0.41     | 2.46        | 13     | 1     |
| 1:A:41:THR:CG2  | 1:A:46:LEU:HD11 | 0.41     | 2.43        | 22     | 1     |
| 1:A:58:ALA:HB3  | 1:A:75:ARG:CD   | 0.41     | 2.45        | 22     | 1     |
| 1:A:8:PRO:HA    | 1:A:70:ARG:CG   | 0.41     | 2.45        | 11     | 1     |
| 1:A:9:ASP:OD2   | 1:A:46:LEU:HG   | 0.41     | 2.16        | 16     | 1     |
| 1:A:69:SER:O    | 1:A:70:ARG:HG3  | 0.41     | 2.15        | 1      | 4     |
| 1:A:21:THR:O    | 1:A:23:HIS:CE1  | 0.41     | 2.74        | 3      | 1     |
| 1:A:9:ASP:OD2   | 1:A:46:LEU:HD22 | 0.41     | 2.16        | 3      | 1     |
| 1:A:25:LYS:HE2  | 1:A:25:LYS:CA   | 0.41     | 2.46        | 1      | 2     |
| 1:A:6:LEU:HB3   | 1:A:70:ARG:O    | 0.41     | 2.16        | 10     | 1     |
| 1:A:40:GLU:HA   | 1:A:40:GLU:OE1  | 0.41     | 2.16        | 2      | 1     |
| 1:A:20:ALA:C    | 1:A:21:THR:OG1  | 0.41     | 2.59        | 15     | 1     |
| 1:A:53:ASP:OD2  | 1:A:77:ARG:HB3  | 0.41     | 2.16        | 4      | 2     |
| 1:A:61:GLU:OE1  | 1:A:66:THR:O    | 0.41     | 2.39        | 8      | 1     |
| 1:A:24:LYS:CD   | 1:A:54:GLY:O    | 0.41     | 2.69        | 13     | 1     |
| 1:A:41:THR:O    | 1:A:42:ASP:HB3  | 0.41     | 2.15        | 1      | 1     |
| 1:A:18:THR:CG2  | 1:A:65:THR:O    | 0.41     | 2.61        | 2      | 1     |
| 1:A:41:THR:CG2  | 1:A:46:LEU:HD21 | 0.41     | 2.42        | 2      | 1     |
| 1:A:52:ALA:O    | 1:A:53:ASP:OD2  | 0.41     | 2.38        | 5      | 1     |
| 1:A:18:THR:O    | 1:A:19:VAL:C    | 0.41     | 2.58        | 24     | 1     |
| 1:A:69:SER:O    | 1:A:70:ARG:HG2  | 0.41     | 2.16        | 24     | 1     |
| 1:A:68:THR:OG1  | 1:A:69:SER:N    | 0.41     | 2.51        | 7      | 1     |
| 1:A:24:LYS:HB3  | 1:A:28:ASP:OD2  | 0.41     | 2.16        | 19     | 1     |
| 1:A:5:ILE:CG2   | 1:A:73:LEU:HB2  | 0.41     | 2.45        | 19     | 1     |
| 1:A:24:LYS:HE2  | 1:A:54:GLY:O    | 0.41     | 2.16        | 6      | 1     |

*Continued on next page...*

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:ILE:HD13  | 1:A:74:GLY:O    | 0.41     | 2.15        | 18     | 1     |
| 1:A:19:VAL:O    | 1:A:63:GLU:HA   | 0.41     | 2.16        | 1      | 2     |
| 1:A:53:ASP:HB3  | 1:A:77:ARG:HG3  | 0.41     | 1.91        | 25     | 1     |
| 1:A:24:LYS:HD2  | 1:A:54:GLY:O    | 0.41     | 2.16        | 9      | 2     |
| 1:A:23:HIS:CE1  | 1:A:37:VAL:CA   | 0.40     | 3.04        | 13     | 1     |
| 1:A:53:ASP:CB   | 1:A:77:ARG:C    | 0.40     | 2.90        | 4      | 2     |
| 1:A:21:THR:HA   | 1:A:63:GLU:HG3  | 0.40     | 1.92        | 17     | 1     |
| 1:A:37:VAL:CG1  | 1:A:73:LEU:CD2  | 0.40     | 2.93        | 14     | 1     |
| 1:A:24:LYS:HE3  | 1:A:28:ASP:OD2  | 0.40     | 2.16        | 19     | 1     |
| 1:A:39:ILE:CD1  | 1:A:67:VAL:HG11 | 0.40     | 2.42        | 13     | 1     |
| 1:A:19:VAL:HA   | 1:A:39:ILE:HA   | 0.40     | 1.94        | 25     | 1     |
| 1:A:61:GLU:OE1  | 1:A:67:VAL:HB   | 0.40     | 2.17        | 2      | 1     |
| 1:A:17:ALA:HB1  | 1:A:39:ILE:HG23 | 0.40     | 1.92        | 5      | 1     |
| 1:A:21:THR:HG22 | 1:A:22:TRP:O    | 0.40     | 2.16        | 22     | 1     |
| 1:A:24:LYS:HE3  | 1:A:34:GLU:OE2  | 0.40     | 2.16        | 21     | 1     |
| 1:A:53:ASP:OD2  | 1:A:77:ARG:O    | 0.40     | 2.38        | 9      | 1     |
| 1:A:56:LEU:HD13 | 1:A:59:VAL:HG21 | 0.40     | 1.91        | 18     | 1     |
| 1:A:53:ASP:HB3  | 1:A:77:ARG:C    | 0.40     | 2.37        | 4      | 3     |
| 1:A:34:GLU:CG   | 1:A:50:ALA:CB   | 0.40     | 2.92        | 5      | 1     |
| 1:A:69:SER:C    | 1:A:70:ARG:HG2  | 0.40     | 2.36        | 24     | 1     |
| 1:A:73:LEU:CD1  | 1:A:73:LEU:N    | 0.40     | 2.84        | 16     | 1     |
| 1:A:56:LEU:HD22 | 1:A:56:LEU:HA   | 0.40     | 1.72        | 13     | 1     |
| 1:A:35:VAL:C    | 1:A:36:LEU:HG   | 0.40     | 2.37        | 7      | 1     |
| 1:A:19:VAL:HG12 | 1:A:63:GLU:OE2  | 0.40     | 2.16        | 3      | 1     |
| 1:A:28:ASP:O    | 1:A:55:ILE:HA   | 0.40     | 2.16        | 4      | 2     |
| 1:A:3:VAL:HB    | 1:A:76:LEU:HD22 | 0.40     | 1.94        | 12     | 1     |
| 1:A:56:LEU:HD12 | 1:A:59:VAL:HG21 | 0.40     | 1.94        | 16     | 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     | 69/80 (86%)     | 32±3 (46±4%) | 26±3 (38±4%) | 12±1 (17±2%) | 0           | 3 |
| All | All   | 1725/2000 (86%) | 789 (46%)    | 647 (38%)    | 289 (17%)    | 0           | 3 |

All 25 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     | 37  | VAL  | 25             |
| 1   | A     | 28  | ASP  | 25             |
| 1   | A     | 33  | ASP  | 25             |
| 1   | A     | 52  | ALA  | 24             |
| 1   | A     | 55  | ILE  | 20             |
| 1   | A     | 56  | LEU  | 19             |
| 1   | A     | 35  | VAL  | 18             |
| 1   | A     | 70  | ARG  | 17             |
| 1   | A     | 31  | VAL  | 17             |
| 1   | A     | 53  | ASP  | 14             |
| 1   | A     | 29  | ALA  | 13             |
| 1   | A     | 39  | ILE  | 12             |
| 1   | A     | 72  | ILE  | 12             |
| 1   | A     | 63  | GLU  | 10             |
| 1   | A     | 22  | TRP  | 9              |
| 1   | A     | 69  | SER  | 8              |
| 1   | A     | 42  | ASP  | 8              |
| 1   | A     | 71  | GLN  | 3              |
| 1   | A     | 54  | GLY  | 3              |
| 1   | A     | 43  | LYS  | 2              |
| 1   | A     | 30  | VAL  | 1              |
| 1   | A     | 34  | GLU  | 1              |
| 1   | A     | 76  | LEU  | 1              |
| 1   | A     | 19  | VAL  | 1              |
| 1   | A     | 62  | ASP  | 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     | 59/68 (87%)     | 41±2 (69±4%) | 18±2 (31±4%) | 1           | 16 |
| All | All   | 1475/1700 (87%) | 1025 (69%)   | 450 (31%)    | 1           | 16 |

All 43 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     | 36  | LEU  | 25             |
| 1   | A     | 30  | VAL  | 25             |
| 1   | A     | 6   | LEU  | 25             |
| 1   | A     | 67  | VAL  | 25             |
| 1   | A     | 25  | LYS  | 21             |
| 1   | A     | 39  | ILE  | 21             |
| 1   | A     | 4   | ASP  | 19             |
| 1   | A     | 63  | GLU  | 18             |
| 1   | A     | 34  | GLU  | 17             |
| 1   | A     | 46  | LEU  | 16             |
| 1   | A     | 77  | ARG  | 16             |
| 1   | A     | 9   | ASP  | 15             |
| 1   | A     | 31  | VAL  | 15             |
| 1   | A     | 75  | ARG  | 14             |
| 1   | A     | 2   | SER  | 13             |
| 1   | A     | 48  | VAL  | 11             |
| 1   | A     | 66  | THR  | 11             |
| 1   | A     | 53  | ASP  | 11             |
| 1   | A     | 5   | ILE  | 10             |
| 1   | A     | 32  | ARG  | 10             |
| 1   | A     | 55  | ILE  | 9              |
| 1   | A     | 68  | THR  | 9              |
| 1   | A     | 24  | LYS  | 9              |
| 1   | A     | 43  | LYS  | 9              |
| 1   | A     | 41  | THR  | 8              |
| 1   | A     | 56  | LEU  | 7              |
| 1   | A     | 70  | ARG  | 7              |
| 1   | A     | 65  | THR  | 7              |
| 1   | A     | 71  | GLN  | 5              |
| 1   | A     | 51  | SER  | 5              |
| 1   | A     | 47  | GLU  | 4              |
| 1   | A     | 59  | VAL  | 4              |
| 1   | A     | 60  | LEU  | 4              |
| 1   | A     | 40  | GLU  | 4              |
| 1   | A     | 62  | ASP  | 4              |
| 1   | A     | 69  | SER  | 4              |
| 1   | A     | 21  | THR  | 3              |
| 1   | A     | 73  | LEU  | 2              |
| 1   | A     | 44  | VAL  | 2              |
| 1   | A     | 76  | LEU  | 2              |
| 1   | A     | 38  | GLU  | 2              |
| 1   | A     | 7   | VAL  | 1              |
| 1   | A     | 28  | ASP  | 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 carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 6.7 Other polymers ⓘ

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided