



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 14, 2026 – 10:19 PM UTC

PDB ID : 1HQI / pdb\_00001hqi  
Title : COMPONENT P2 FROM THE MULTICOMPONENT PHENOL HYDROXYLASE, NMR, 11 STRUCTURES  
Authors : Qian, H.; Sethon, I.  
Deposited on : 1996-09-19

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

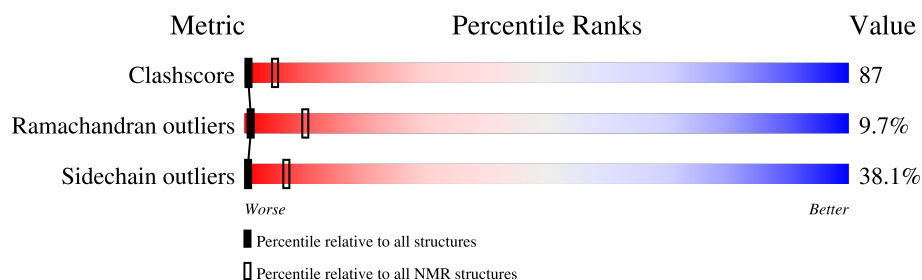
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | A     | 90     | <div> <div>11%</div> <div>59%</div> <div>24%</div> <div>6%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 12 models. Model 9 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:3-A:87 (85)         | 3.22              | 9            |

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 1 single-model cluster was found.

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

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

There is only 1 type of molecule in this entry. The entry contains 1449 atoms, of which 711 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PHENOL HYDROXYLASE P2 PROTEIN.

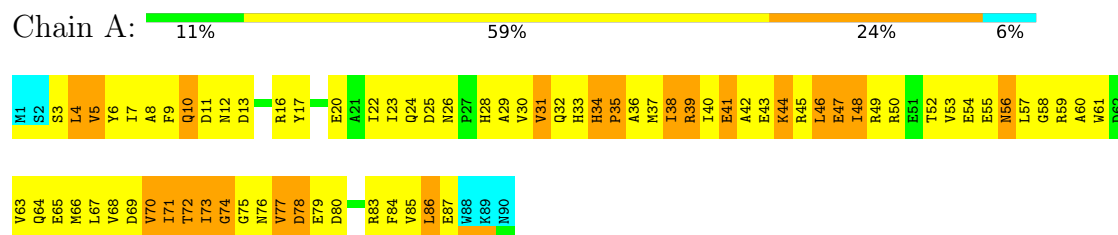
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 90       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1449  | 459 | 711 | 131 | 145 | 3 |       |

## 4 Residue-property plots

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

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

#### • Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN

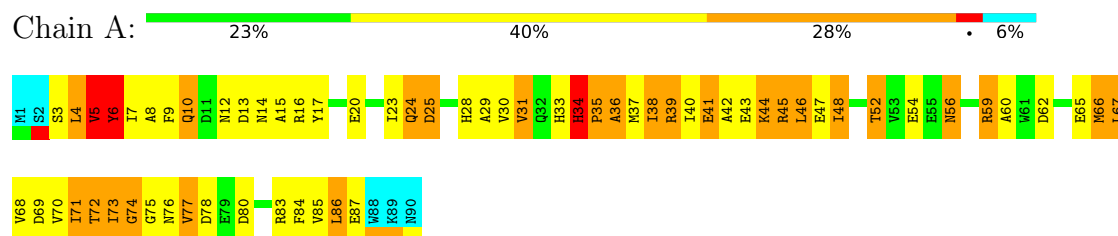


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

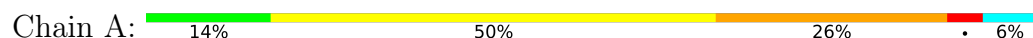
#### 4.2.1 Score per residue for model 1

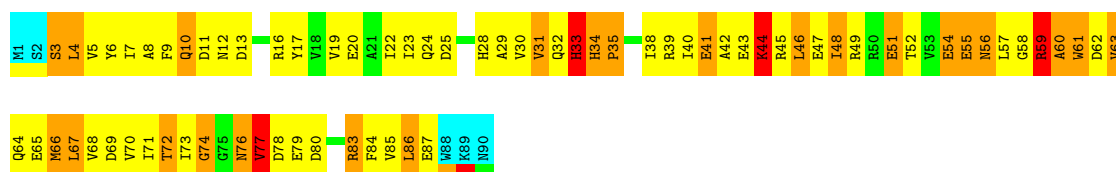
#### • Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN



#### 4.2.2 Score per residue for model 2

#### • Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN

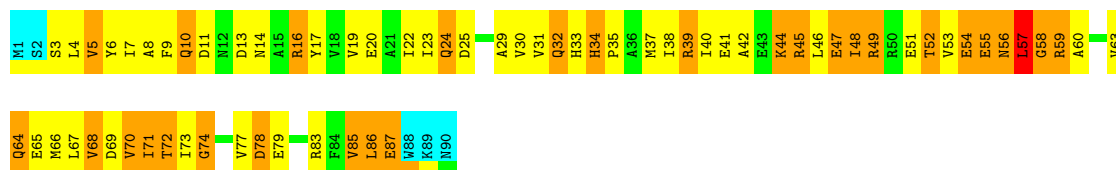




### 4.2.3 Score per residue for model 3

- Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN

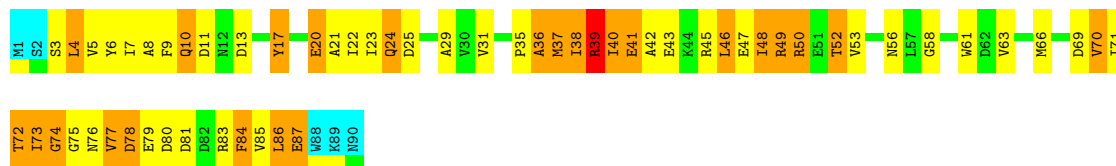
Chain A: 20% 42% 31% 6%



### 4.2.4 Score per residue for model 4

- Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN

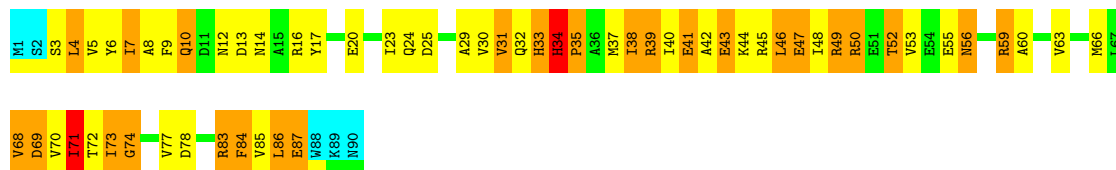
Chain A: 29% 38% 27% 6%



### 4.2.5 Score per residue for model 5

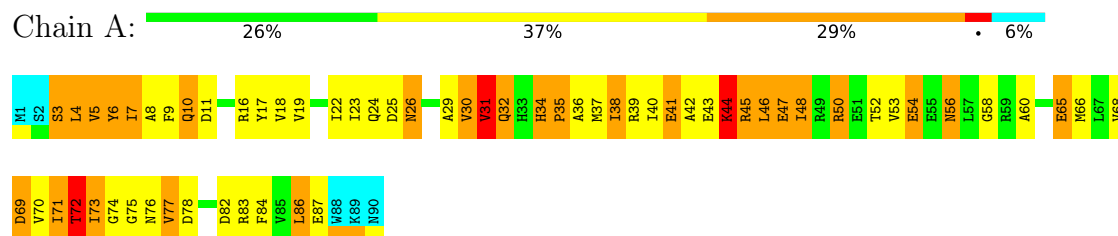
- Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN

Chain A: 28% 37% 28% 6%



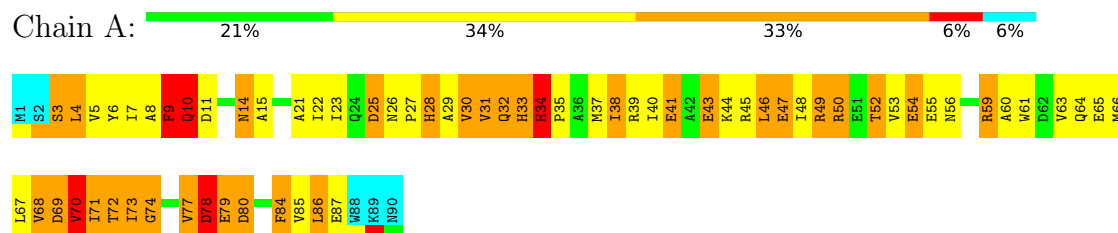
### 4.2.6 Score per residue for model 6

- Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN



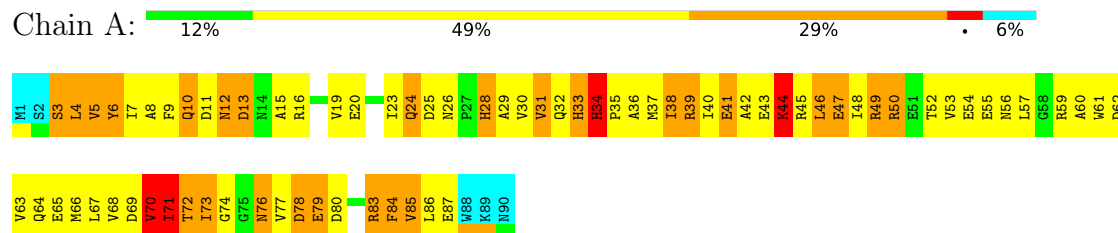
#### 4.2.7 Score per residue for model 7

- Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN



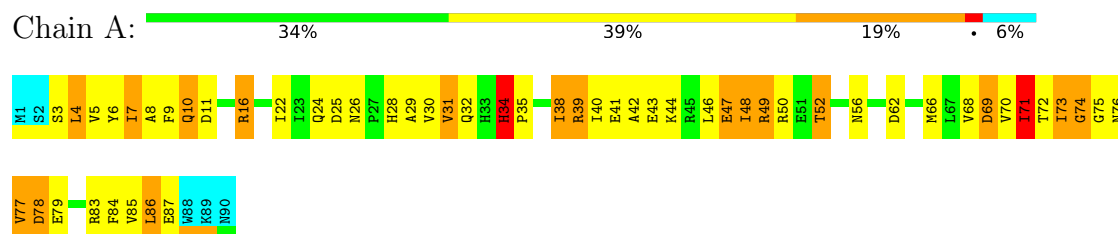
#### 4.2.8 Score per residue for model 8

- Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN



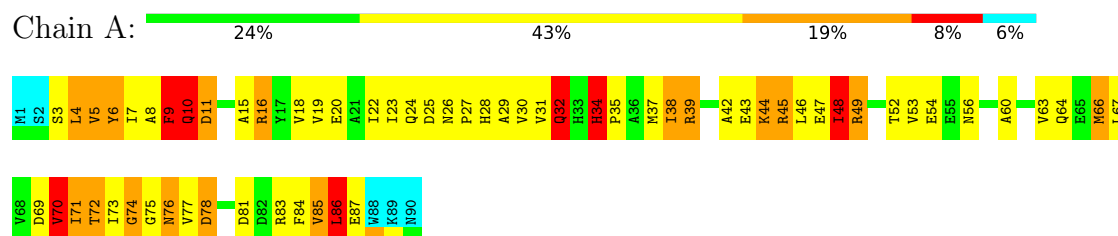
#### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN



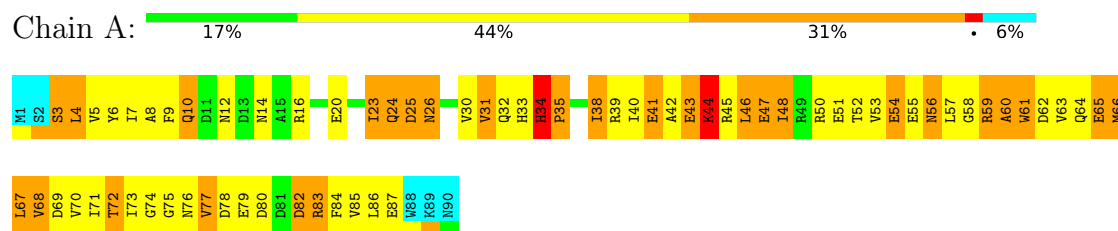
### 4.2.10 Score per residue for model 10

#### • Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN



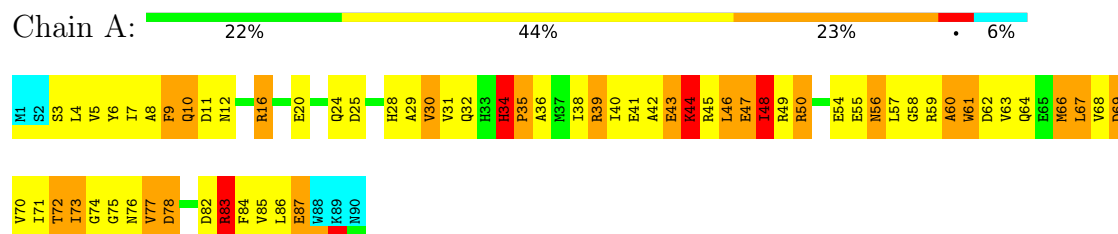
### 4.2.11 Score per residue for model 11

#### • Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN



### 4.2.12 Score per residue for model 12

#### • Molecule 1: PHENOL HYDROXYLASE P2 PROTEIN



## 5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 12 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     |         |

No chemical shift data was provided.

## 6 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.46±0.02    | 0±0/703 ( 0.0± 0.1%) | 1.30±0.03   | 0±0/956 ( 0.0± 0.0%) |
| All | All   | 1.46         | 2/8436 ( 0.0%)       | 1.30        | 4/11472 ( 0.0%)      |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 70  | VAL  | C-O   | -5.11 | 1.18        | 1.24     | 7      | 1     |
| 1   | A     | 44  | LYS  | C-N   | -5.09 | 1.26        | 1.33     | 11     | 1     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
|     |       |     |      |          |       |             |          | Worst  | Total |
| 1   | A     | 9   | PHE  | CA-CB-CG | -8.64 | 105.16      | 113.80   | 10     | 2     |
| 1   | A     | 58  | GLY  | N-CA-C   | -5.56 | 108.55      | 114.67   | 6      | 2     |

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 692   | 666      | 666      | 118±20  |
| All | All   | 8304  | 7992     | 7992     | 1421    |

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 87.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:VAL:HG22  | 1:A:42:ALA:HB3  | 1.08     | 1.21        | 4      | 5     |
| 1:A:9:PHE:CE2   | 1:A:71:ILE:HG22 | 1.07     | 1.84        | 11     | 1     |
| 1:A:9:PHE:CZ    | 1:A:71:ILE:HG23 | 1.00     | 1.92        | 2      | 1     |
| 1:A:45:ARG:C    | 1:A:46:LEU:HD23 | 0.98     | 1.81        | 2      | 5     |
| 1:A:47:GLU:CA   | 1:A:85:VAL:HG12 | 0.98     | 1.88        | 8      | 1     |
| 1:A:9:PHE:CD2   | 1:A:70:VAL:HG22 | 0.98     | 1.93        | 7      | 2     |
| 1:A:9:PHE:CZ    | 1:A:71:ILE:HD13 | 0.96     | 1.94        | 1      | 1     |
| 1:A:48:ILE:HG21 | 1:A:52:THR:HG21 | 0.96     | 1.36        | 5      | 1     |
| 1:A:5:VAL:HG11  | 1:A:46:LEU:HD21 | 0.95     | 1.37        | 6      | 2     |
| 1:A:5:VAL:HG21  | 1:A:87:GLU:CD   | 0.94     | 1.88        | 4      | 1     |
| 1:A:72:THR:O    | 1:A:73:ILE:HD13 | 0.93     | 1.64        | 11     | 2     |
| 1:A:78:ASP:CG   | 1:A:86:LEU:HD23 | 0.92     | 1.87        | 7      | 2     |
| 1:A:9:PHE:CE2   | 1:A:38:ILE:HD11 | 0.91     | 2.00        | 3      | 1     |
| 1:A:9:PHE:CE2   | 1:A:70:VAL:HG13 | 0.91     | 2.00        | 7      | 2     |
| 1:A:65:GLU:O    | 1:A:68:VAL:HG23 | 0.91     | 1.66        | 7      | 3     |
| 1:A:5:VAL:HG22  | 1:A:42:ALA:CB   | 0.91     | 1.94        | 1      | 3     |
| 1:A:37:MET:C    | 1:A:38:ILE:HD13 | 0.89     | 1.92        | 4      | 2     |
| 1:A:9:PHE:CZ    | 1:A:19:VAL:HG21 | 0.89     | 2.01        | 8      | 1     |
| 1:A:48:ILE:CG2  | 1:A:52:THR:HG21 | 0.89     | 1.97        | 5      | 1     |
| 1:A:86:LEU:HD22 | 1:A:87:GLU:N    | 0.88     | 1.83        | 2      | 5     |
| 1:A:47:GLU:HA   | 1:A:85:VAL:HG12 | 0.88     | 1.44        | 8      | 1     |
| 1:A:6:TYR:OH    | 1:A:72:THR:HG21 | 0.87     | 1.68        | 1      | 1     |
| 1:A:45:ARG:O    | 1:A:46:LEU:HD23 | 0.86     | 1.68        | 8      | 6     |
| 1:A:53:VAL:HG22 | 1:A:84:PHE:CD1  | 0.85     | 2.06        | 4      | 1     |
| 1:A:8:ALA:HA    | 1:A:39:ARG:CB   | 0.85     | 2.02        | 4      | 1     |
| 1:A:6:TYR:CE2   | 1:A:73:ILE:HG21 | 0.85     | 2.07        | 6      | 2     |
| 1:A:64:GLN:O    | 1:A:67:LEU:HD22 | 0.85     | 1.72        | 12     | 1     |
| 1:A:18:VAL:O    | 1:A:22:ILE:HD13 | 0.84     | 1.73        | 10     | 1     |
| 1:A:47:GLU:CB   | 1:A:85:VAL:HG23 | 0.84     | 2.03        | 2      | 1     |
| 1:A:4:LEU:HD13  | 1:A:4:LEU:N     | 0.83     | 1.88        | 2      | 2     |
| 1:A:76:ASN:HA   | 1:A:86:LEU:HD23 | 0.83     | 1.46        | 2      | 1     |
| 1:A:48:ILE:HD12 | 1:A:84:PHE:O    | 0.83     | 1.74        | 11     | 1     |
| 1:A:22:ILE:HD11 | 1:A:38:ILE:HG13 | 0.82     | 1.49        | 7      | 1     |
| 1:A:46:LEU:HD12 | 1:A:86:LEU:CD1  | 0.81     | 2.05        | 2      | 4     |
| 1:A:8:ALA:HB3   | 1:A:72:THR:OG1  | 0.81     | 1.75        | 10     | 5     |
| 1:A:7:ILE:HB    | 1:A:72:THR:HG22 | 0.80     | 1.52        | 6      | 2     |
| 1:A:5:VAL:CG2   | 1:A:42:ALA:HB3  | 0.80     | 2.03        | 1      | 4     |
| 1:A:9:PHE:CE1   | 1:A:38:ILE:HD11 | 0.80     | 2.11        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:64:GLN:O    | 1:A:67:LEU:HD23 | 0.79     | 1.76        | 2      | 1     |
| 1:A:25:ASP:O    | 1:A:29:ALA:HB3  | 0.79     | 1.77        | 7      | 2     |
| 1:A:15:ALA:O    | 1:A:19:VAL:HG23 | 0.79     | 1.75        | 10     | 1     |
| 1:A:26:ASN:OD1  | 1:A:31:VAL:HG13 | 0.79     | 1.78        | 7      | 1     |
| 1:A:47:GLU:C    | 1:A:48:ILE:HD12 | 0.79     | 2.02        | 7      | 2     |
| 1:A:33:HIS:HB3  | 1:A:38:ILE:HG22 | 0.79     | 1.55        | 8      | 1     |
| 1:A:5:VAL:HG21  | 1:A:46:LEU:HD11 | 0.78     | 1.54        | 8      | 1     |
| 1:A:46:LEU:HD12 | 1:A:86:LEU:HD12 | 0.78     | 1.55        | 2      | 3     |
| 1:A:77:VAL:HG23 | 1:A:85:VAL:O    | 0.78     | 1.78        | 5      | 1     |
| 1:A:5:VAL:HG23  | 1:A:6:TYR:N     | 0.78     | 1.93        | 1      | 2     |
| 1:A:19:VAL:HA   | 1:A:22:ILE:HD12 | 0.78     | 1.55        | 2      | 2     |
| 1:A:9:PHE:CG    | 1:A:70:VAL:O    | 0.77     | 2.37        | 7      | 2     |
| 1:A:86:LEU:C    | 1:A:86:LEU:HD13 | 0.77     | 2.04        | 12     | 5     |
| 1:A:5:VAL:HB    | 1:A:42:ALA:HB3  | 0.76     | 1.56        | 11     | 3     |
| 1:A:38:ILE:C    | 1:A:38:ILE:HD13 | 0.75     | 2.06        | 7      | 1     |
| 1:A:48:ILE:HG23 | 1:A:49:ARG:N    | 0.75     | 1.96        | 12     | 1     |
| 1:A:4:LEU:HD12  | 1:A:4:LEU:O     | 0.75     | 1.81        | 12     | 3     |
| 1:A:76:ASN:C    | 1:A:86:LEU:HD13 | 0.75     | 2.06        | 8      | 1     |
| 1:A:3:SER:C     | 1:A:4:LEU:HD13  | 0.75     | 2.07        | 11     | 2     |
| 1:A:47:GLU:HA   | 1:A:85:VAL:HG23 | 0.74     | 1.59        | 3      | 3     |
| 1:A:46:LEU:HD12 | 1:A:87:GLU:O    | 0.74     | 1.81        | 9      | 3     |
| 1:A:9:PHE:CD1   | 1:A:70:VAL:O    | 0.74     | 2.40        | 7      | 3     |
| 1:A:71:ILE:HD13 | 1:A:71:ILE:N    | 0.74     | 1.97        | 3      | 1     |
| 1:A:46:LEU:HD12 | 1:A:48:ILE:HD11 | 0.74     | 1.59        | 7      | 1     |
| 1:A:67:LEU:HD12 | 1:A:67:LEU:C    | 0.73     | 2.07        | 2      | 1     |
| 1:A:77:VAL:HG23 | 1:A:84:PHE:CE1  | 0.73     | 2.18        | 1      | 2     |
| 1:A:86:LEU:HD22 | 1:A:87:GLU:H    | 0.73     | 1.41        | 6      | 4     |
| 1:A:24:GLN:HG2  | 1:A:31:VAL:HG23 | 0.73     | 1.60        | 6      | 1     |
| 1:A:48:ILE:HD12 | 1:A:48:ILE:N    | 0.73     | 1.98        | 9      | 2     |
| 1:A:71:ILE:O    | 1:A:72:THR:HG23 | 0.73     | 1.81        | 6      | 2     |
| 1:A:10:GLN:N    | 1:A:70:VAL:HG12 | 0.72     | 1.99        | 4      | 2     |
| 1:A:73:ILE:HD13 | 1:A:73:ILE:C    | 0.72     | 2.10        | 1      | 2     |
| 1:A:46:LEU:CB   | 1:A:86:LEU:HD12 | 0.72     | 2.14        | 7      | 2     |
| 1:A:77:VAL:O    | 1:A:77:VAL:HG13 | 0.71     | 1.84        | 9      | 9     |
| 1:A:9:PHE:CZ    | 1:A:70:VAL:HG13 | 0.71     | 2.20        | 7      | 2     |
| 1:A:67:LEU:HD21 | 1:A:71:ILE:HG21 | 0.71     | 1.61        | 3      | 1     |
| 1:A:9:PHE:CE2   | 1:A:70:VAL:HG22 | 0.71     | 2.20        | 10     | 2     |
| 1:A:5:VAL:HG21  | 1:A:46:LEU:CD1  | 0.70     | 2.15        | 8      | 1     |
| 1:A:39:ARG:O    | 1:A:40:ILE:HD13 | 0.70     | 1.86        | 3      | 1     |
| 1:A:39:ARG:C    | 1:A:40:ILE:HD12 | 0.70     | 2.12        | 6      | 3     |
| 1:A:9:PHE:CB    | 1:A:38:ILE:HG23 | 0.70     | 2.17        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:10:GLN:C    | 1:A:70:VAL:HG23 | 0.70     | 2.12        | 10     | 2     |
| 1:A:48:ILE:HG22 | 1:A:51:GLU:CG   | 0.69     | 2.17        | 3      | 1     |
| 1:A:5:VAL:HG11  | 1:A:87:GLU:HB2  | 0.69     | 1.63        | 4      | 1     |
| 1:A:5:VAL:HG13  | 1:A:75:GLY:HA2  | 0.69     | 1.65        | 9      | 1     |
| 1:A:6:TYR:O     | 1:A:74:GLY:N    | 0.69     | 2.25        | 8      | 12    |
| 1:A:46:LEU:HD23 | 1:A:46:LEU:N    | 0.69     | 2.02        | 2      | 3     |
| 1:A:60:ALA:O    | 1:A:62:ASP:N    | 0.69     | 2.26        | 2      | 3     |
| 1:A:48:ILE:CD1  | 1:A:85:VAL:HG11 | 0.69     | 2.18        | 8      | 1     |
| 1:A:76:ASN:O    | 1:A:86:LEU:HD21 | 0.69     | 1.88        | 9      | 1     |
| 1:A:53:VAL:HG22 | 1:A:84:PHE:CE1  | 0.69     | 2.23        | 4      | 1     |
| 1:A:23:ILE:HG23 | 1:A:29:ALA:CB   | 0.68     | 2.19        | 2      | 3     |
| 1:A:58:GLY:O    | 1:A:59:ARG:CB   | 0.68     | 2.41        | 2      | 2     |
| 1:A:33:HIS:CE1  | 1:A:38:ILE:HG22 | 0.68     | 2.24        | 5      | 1     |
| 1:A:77:VAL:O    | 1:A:85:VAL:O    | 0.67     | 2.12        | 7      | 3     |
| 1:A:7:ILE:HD12  | 1:A:7:ILE:C     | 0.67     | 2.15        | 7      | 3     |
| 1:A:57:LEU:C    | 1:A:57:LEU:HD13 | 0.67     | 2.15        | 3      | 1     |
| 1:A:61:TRP:CZ2  | 1:A:63:VAL:HG21 | 0.67     | 2.24        | 2      | 1     |
| 1:A:9:PHE:HB2   | 1:A:38:ILE:HD12 | 0.67     | 1.65        | 7      | 1     |
| 1:A:47:GLU:N    | 1:A:85:VAL:HG23 | 0.67     | 2.04        | 12     | 1     |
| 1:A:33:HIS:ND1  | 1:A:38:ILE:HG22 | 0.67     | 2.04        | 5      | 1     |
| 1:A:46:LEU:CD1  | 1:A:86:LEU:HD11 | 0.67     | 2.20        | 10     | 1     |
| 1:A:7:ILE:HD11  | 1:A:40:ILE:HD12 | 0.66     | 1.67        | 7      | 1     |
| 1:A:5:VAL:HG21  | 1:A:87:GLU:OE1  | 0.66     | 1.90        | 4      | 1     |
| 1:A:10:GLN:N    | 1:A:70:VAL:HA   | 0.66     | 2.04        | 10     | 2     |
| 1:A:78:ASP:OD2  | 1:A:86:LEU:HD23 | 0.66     | 1.90        | 7      | 1     |
| 1:A:52:THR:HG21 | 1:A:78:ASP:OD2  | 0.66     | 1.90        | 7      | 1     |
| 1:A:6:TYR:CZ    | 1:A:73:ILE:HG21 | 0.65     | 2.25        | 6      | 1     |
| 1:A:47:GLU:H    | 1:A:85:VAL:HG23 | 0.65     | 1.51        | 12     | 1     |
| 1:A:78:ASP:OD1  | 1:A:85:VAL:HG13 | 0.65     | 1.92        | 10     | 2     |
| 1:A:9:PHE:CZ    | 1:A:38:ILE:CG1  | 0.65     | 2.80        | 8      | 1     |
| 1:A:60:ALA:O    | 1:A:61:TRP:C    | 0.65     | 2.38        | 12     | 3     |
| 1:A:86:LEU:HD13 | 1:A:86:LEU:O    | 0.64     | 1.92        | 2      | 2     |
| 1:A:48:ILE:HD12 | 1:A:85:VAL:HG11 | 0.64     | 1.68        | 8      | 1     |
| 1:A:86:LEU:HD22 | 1:A:86:LEU:C    | 0.64     | 2.18        | 2      | 2     |
| 1:A:57:LEU:C    | 1:A:57:LEU:CD1  | 0.64     | 2.70        | 3      | 1     |
| 1:A:7:ILE:HG22  | 1:A:73:ILE:HA   | 0.64     | 1.68        | 1      | 1     |
| 1:A:9:PHE:CD1   | 1:A:9:PHE:N     | 0.64     | 2.66        | 3      | 2     |
| 1:A:46:LEU:CB   | 1:A:86:LEU:CD1  | 0.64     | 2.76        | 3      | 3     |
| 1:A:4:LEU:HD22  | 1:A:4:LEU:O     | 0.64     | 1.92        | 11     | 2     |
| 1:A:70:VAL:C    | 1:A:71:ILE:HD13 | 0.64     | 2.17        | 3      | 1     |
| 1:A:6:TYR:CD1   | 1:A:7:ILE:N     | 0.64     | 2.66        | 6      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:PHE:CE2   | 1:A:70:VAL:CG1  | 0.64     | 2.80        | 7      | 2     |
| 1:A:9:PHE:CE2   | 1:A:38:ILE:CD1  | 0.64     | 2.81        | 3      | 2     |
| 1:A:9:PHE:CE1   | 1:A:70:VAL:O    | 0.64     | 2.51        | 10     | 2     |
| 1:A:9:PHE:CD1   | 1:A:69:ASP:O    | 0.63     | 2.52        | 9      | 2     |
| 1:A:9:PHE:CD2   | 1:A:70:VAL:O    | 0.63     | 2.51        | 10     | 3     |
| 1:A:4:LEU:N     | 1:A:4:LEU:CD1   | 0.63     | 2.61        | 2      | 2     |
| 1:A:8:ALA:O     | 1:A:9:PHE:CD1   | 0.63     | 2.52        | 5      | 3     |
| 1:A:46:LEU:HD13 | 1:A:86:LEU:HD21 | 0.63     | 1.70        | 4      | 1     |
| 1:A:45:ARG:O    | 1:A:46:LEU:HG   | 0.63     | 1.93        | 12     | 2     |
| 1:A:77:VAL:CG2  | 1:A:84:PHE:CZ   | 0.63     | 2.81        | 6      | 1     |
| 1:A:5:VAL:CB    | 1:A:42:ALA:HB3  | 0.63     | 2.23        | 12     | 1     |
| 1:A:46:LEU:CD1  | 1:A:86:LEU:HD21 | 0.63     | 2.24        | 4      | 1     |
| 1:A:53:VAL:HG21 | 1:A:84:PHE:CD1  | 0.63     | 2.28        | 10     | 1     |
| 1:A:5:VAL:CG1   | 1:A:6:TYR:N     | 0.62     | 2.61        | 8      | 2     |
| 1:A:69:ASP:O    | 1:A:70:VAL:O    | 0.62     | 2.16        | 8      | 1     |
| 1:A:23:ILE:HG23 | 1:A:29:ALA:HB1  | 0.62     | 1.71        | 4      | 3     |
| 1:A:76:ASN:O    | 1:A:86:LEU:HD13 | 0.62     | 1.93        | 8      | 1     |
| 1:A:8:ALA:O     | 1:A:71:ILE:HG22 | 0.62     | 1.93        | 8      | 1     |
| 1:A:73:ILE:HG22 | 1:A:74:GLY:H    | 0.62     | 1.54        | 8      | 1     |
| 1:A:86:LEU:HD12 | 1:A:87:GLU:H    | 0.62     | 1.54        | 8      | 3     |
| 1:A:85:VAL:HG13 | 1:A:86:LEU:H    | 0.62     | 1.53        | 8      | 1     |
| 1:A:10:GLN:C    | 1:A:10:GLN:NE2  | 0.62     | 2.58        | 11     | 9     |
| 1:A:70:VAL:O    | 1:A:71:ILE:CG1  | 0.62     | 2.47        | 8      | 3     |
| 1:A:8:ALA:CB    | 1:A:71:ILE:CG2  | 0.61     | 2.77        | 9      | 2     |
| 1:A:76:ASN:C    | 1:A:86:LEU:HD21 | 0.61     | 2.20        | 12     | 2     |
| 1:A:61:TRP:CD1  | 1:A:61:TRP:O    | 0.61     | 2.53        | 4      | 2     |
| 1:A:77:VAL:HG22 | 1:A:84:PHE:CE1  | 0.61     | 2.29        | 5      | 2     |
| 1:A:9:PHE:CE2   | 1:A:71:ILE:HD13 | 0.61     | 2.31        | 1      | 1     |
| 1:A:30:VAL:C    | 1:A:31:VAL:HG22 | 0.61     | 2.20        | 5      | 2     |
| 1:A:10:GLN:HG3  | 1:A:69:ASP:CA   | 0.61     | 2.25        | 8      | 1     |
| 1:A:7:ILE:HD13  | 1:A:7:ILE:N     | 0.61     | 2.11        | 9      | 1     |
| 1:A:46:LEU:CB   | 1:A:86:LEU:O    | 0.61     | 2.49        | 8      | 3     |
| 1:A:73:ILE:HG22 | 1:A:74:GLY:N    | 0.61     | 2.11        | 8      | 1     |
| 1:A:8:ALA:O     | 1:A:72:THR:N    | 0.60     | 2.34        | 8      | 7     |
| 1:A:46:LEU:CD1  | 1:A:86:LEU:CD1  | 0.60     | 2.78        | 2      | 2     |
| 1:A:3:SER:CB    | 1:A:44:LYS:CB   | 0.60     | 2.79        | 11     | 1     |
| 1:A:9:PHE:CZ    | 1:A:71:ILE:HG22 | 0.60     | 2.30        | 11     | 1     |
| 1:A:9:PHE:CE2   | 1:A:39:ARG:CD   | 0.60     | 2.85        | 4      | 1     |
| 1:A:48:ILE:HG22 | 1:A:52:THR:OG1  | 0.60     | 1.97        | 1      | 1     |
| 1:A:46:LEU:CA   | 1:A:86:LEU:O    | 0.60     | 2.49        | 12     | 1     |
| 1:A:70:VAL:O    | 1:A:71:ILE:HG12 | 0.60     | 1.96        | 5      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:PHE:CE1   | 1:A:71:ILE:HG23 | 0.60     | 2.32        | 2      | 2     |
| 1:A:35:PRO:O    | 1:A:36:ALA:HB2  | 0.60     | 1.95        | 4      | 1     |
| 1:A:52:THR:HG21 | 1:A:82:ASP:O    | 0.60     | 1.97        | 11     | 1     |
| 1:A:46:LEU:HB2  | 1:A:87:GLU:O    | 0.59     | 1.97        | 4      | 4     |
| 1:A:7:ILE:HD11  | 1:A:40:ILE:HG21 | 0.59     | 1.74        | 6      | 1     |
| 1:A:71:ILE:HD12 | 1:A:72:THR:H    | 0.59     | 1.57        | 1      | 1     |
| 1:A:9:PHE:CZ    | 1:A:38:ILE:HG13 | 0.59     | 2.32        | 8      | 2     |
| 1:A:47:GLU:HB3  | 1:A:85:VAL:HG23 | 0.59     | 1.74        | 2      | 1     |
| 1:A:72:THR:O    | 1:A:73:ILE:CD1  | 0.59     | 2.50        | 8      | 1     |
| 1:A:8:ALA:O     | 1:A:9:PHE:CG    | 0.59     | 2.56        | 9      | 2     |
| 1:A:78:ASP:CG   | 1:A:84:PHE:CD2  | 0.59     | 2.81        | 4      | 2     |
| 1:A:47:GLU:C    | 1:A:85:VAL:HG12 | 0.59     | 2.21        | 8      | 1     |
| 1:A:8:ALA:C     | 1:A:71:ILE:HG22 | 0.59     | 2.22        | 9      | 1     |
| 1:A:8:ALA:HB3   | 1:A:72:THR:CB   | 0.59     | 2.27        | 10     | 2     |
| 1:A:46:LEU:CD1  | 1:A:86:LEU:HD12 | 0.59     | 2.28        | 11     | 1     |
| 1:A:9:PHE:HB2   | 1:A:71:ILE:N    | 0.59     | 2.13        | 8      | 1     |
| 1:A:72:THR:O    | 1:A:73:ILE:HG12 | 0.59     | 1.97        | 8      | 1     |
| 1:A:9:PHE:CD2   | 1:A:38:ILE:HD11 | 0.59     | 2.32        | 12     | 1     |
| 1:A:6:TYR:CD1   | 1:A:6:TYR:C     | 0.59     | 2.80        | 6      | 3     |
| 1:A:71:ILE:HG22 | 1:A:72:THR:N    | 0.59     | 2.13        | 5      | 2     |
| 1:A:5:VAL:CG2   | 1:A:6:TYR:N     | 0.59     | 2.65        | 10     | 2     |
| 1:A:46:LEU:HD12 | 1:A:86:LEU:HD11 | 0.59     | 1.73        | 10     | 2     |
| 1:A:9:PHE:CB    | 1:A:38:ILE:CG2  | 0.59     | 2.81        | 7      | 1     |
| 1:A:46:LEU:CD2  | 1:A:85:VAL:CG2  | 0.59     | 2.81        | 12     | 1     |
| 1:A:46:LEU:CG   | 1:A:86:LEU:O    | 0.58     | 2.51        | 8      | 2     |
| 1:A:9:PHE:HB3   | 1:A:38:ILE:CG2  | 0.58     | 2.29        | 7      | 1     |
| 1:A:22:ILE:HD11 | 1:A:38:ILE:CG1  | 0.58     | 2.26        | 7      | 1     |
| 1:A:10:GLN:O    | 1:A:69:ASP:C    | 0.58     | 2.46        | 8      | 1     |
| 1:A:72:THR:O    | 1:A:73:ILE:CG1  | 0.58     | 2.52        | 8      | 1     |
| 1:A:77:VAL:C    | 1:A:85:VAL:O    | 0.58     | 2.46        | 2      | 2     |
| 1:A:78:ASP:HA   | 1:A:85:VAL:O    | 0.58     | 1.98        | 2      | 3     |
| 1:A:76:ASN:C    | 1:A:86:LEU:CD2  | 0.58     | 2.76        | 12     | 3     |
| 1:A:77:VAL:CG2  | 1:A:84:PHE:CD1  | 0.58     | 2.86        | 5      | 1     |
| 1:A:5:VAL:HG12  | 1:A:6:TYR:N     | 0.58     | 2.13        | 11     | 2     |
| 1:A:9:PHE:CB    | 1:A:70:VAL:O    | 0.58     | 2.52        | 12     | 3     |
| 1:A:4:LEU:HA    | 1:A:43:GLU:HA   | 0.58     | 1.73        | 12     | 11    |
| 1:A:10:GLN:HB2  | 1:A:70:VAL:HG23 | 0.58     | 1.75        | 6      | 1     |
| 1:A:48:ILE:CG2  | 1:A:53:VAL:CG2  | 0.58     | 2.81        | 8      | 1     |
| 1:A:10:GLN:O    | 1:A:70:VAL:N    | 0.57     | 2.36        | 8      | 2     |
| 1:A:77:VAL:HG22 | 1:A:84:PHE:CZ   | 0.57     | 2.34        | 8      | 1     |
| 1:A:46:LEU:O    | 1:A:85:VAL:CG2  | 0.57     | 2.52        | 10     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:10:GLN:HB3  | 1:A:70:VAL:HG23 | 0.57     | 1.76        | 11     | 3     |
| 1:A:61:TRP:CE2  | 1:A:63:VAL:CG2  | 0.57     | 2.88        | 2      | 1     |
| 1:A:10:GLN:O    | 1:A:70:VAL:CA   | 0.57     | 2.52        | 10     | 2     |
| 1:A:61:TRP:CE2  | 1:A:63:VAL:HG21 | 0.57     | 2.34        | 2      | 1     |
| 1:A:46:LEU:HB3  | 1:A:86:LEU:HD12 | 0.57     | 1.75        | 7      | 1     |
| 1:A:9:PHE:CD2   | 1:A:39:ARG:HG2  | 0.57     | 2.34        | 4      | 1     |
| 1:A:84:PHE:C    | 1:A:84:PHE:CD1  | 0.57     | 2.81        | 8      | 3     |
| 1:A:73:ILE:HG23 | 1:A:74:GLY:N    | 0.57     | 2.15        | 6      | 1     |
| 1:A:78:ASP:OD1  | 1:A:86:LEU:HD23 | 0.57     | 2.00        | 7      | 1     |
| 1:A:43:GLU:O    | 1:A:44:LYS:HB3  | 0.57     | 2.00        | 11     | 1     |
| 1:A:4:LEU:O     | 1:A:4:LEU:HD12  | 0.57     | 2.00        | 1      | 2     |
| 1:A:8:ALA:HA    | 1:A:39:ARG:CG   | 0.57     | 2.30        | 4      | 1     |
| 1:A:46:LEU:N    | 1:A:86:LEU:O    | 0.57     | 2.38        | 12     | 2     |
| 1:A:8:ALA:HB3   | 1:A:71:ILE:HG22 | 0.57     | 1.76        | 5      | 2     |
| 1:A:40:ILE:HG22 | 1:A:41:GLU:N    | 0.57     | 2.14        | 12     | 6     |
| 1:A:86:LEU:HD12 | 1:A:87:GLU:N    | 0.57     | 2.14        | 8      | 2     |
| 1:A:8:ALA:HB1   | 1:A:38:ILE:O    | 0.57     | 2.00        | 5      | 2     |
| 1:A:23:ILE:HD12 | 1:A:24:GLN:N    | 0.57     | 2.15        | 8      | 1     |
| 1:A:34:HIS:CB   | 1:A:35:PRO:CD   | 0.56     | 2.82        | 12     | 9     |
| 1:A:40:ILE:HG22 | 1:A:41:GLU:H    | 0.56     | 1.60        | 4      | 3     |
| 1:A:70:VAL:HG12 | 1:A:71:ILE:H    | 0.56     | 1.60        | 6      | 2     |
| 1:A:45:ARG:O    | 1:A:87:GLU:HB3  | 0.56     | 2.00        | 12     | 1     |
| 1:A:38:ILE:HD13 | 1:A:38:ILE:N    | 0.56     | 2.15        | 8      | 2     |
| 1:A:70:VAL:O    | 1:A:71:ILE:CB   | 0.56     | 2.53        | 9      | 2     |
| 1:A:77:VAL:O    | 1:A:77:VAL:CG1  | 0.56     | 2.52        | 8      | 3     |
| 1:A:72:THR:C    | 1:A:73:ILE:HD13 | 0.56     | 2.23        | 11     | 1     |
| 1:A:9:PHE:CZ    | 1:A:71:ILE:CD1  | 0.56     | 2.82        | 1      | 1     |
| 1:A:46:LEU:CG   | 1:A:87:GLU:O    | 0.56     | 2.54        | 4      | 4     |
| 1:A:9:PHE:C     | 1:A:9:PHE:CD1   | 0.56     | 2.82        | 8      | 2     |
| 1:A:77:VAL:HG22 | 1:A:84:PHE:CD1  | 0.56     | 2.35        | 5      | 1     |
| 1:A:31:VAL:HG13 | 1:A:32:GLN:N    | 0.56     | 2.15        | 6      | 1     |
| 1:A:9:PHE:CZ    | 1:A:70:VAL:O    | 0.56     | 2.59        | 10     | 2     |
| 1:A:5:VAL:HG13  | 1:A:75:GLY:CA   | 0.56     | 2.29        | 9      | 2     |
| 1:A:8:ALA:CB    | 1:A:71:ILE:HG22 | 0.56     | 2.31        | 9      | 1     |
| 1:A:39:ARG:C    | 1:A:40:ILE:CG1  | 0.56     | 2.77        | 4      | 5     |
| 1:A:6:TYR:CZ    | 1:A:73:ILE:HG13 | 0.56     | 2.35        | 8      | 1     |
| 1:A:10:GLN:CB   | 1:A:70:VAL:HG23 | 0.56     | 2.30        | 6      | 3     |
| 1:A:69:ASP:O    | 1:A:71:ILE:N    | 0.56     | 2.39        | 7      | 2     |
| 1:A:7:ILE:HA    | 1:A:73:ILE:HG22 | 0.56     | 1.76        | 6      | 1     |
| 1:A:22:ILE:H    | 1:A:22:ILE:HD12 | 0.56     | 1.61        | 6      | 1     |
| 1:A:10:GLN:CB   | 1:A:70:VAL:HG12 | 0.56     | 2.31        | 12     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:11:ASP:OD1  | 1:A:70:VAL:HG21 | 0.56     | 2.01        | 10     | 1     |
| 1:A:68:VAL:CG1  | 1:A:69:ASP:N    | 0.55     | 2.69        | 12     | 2     |
| 1:A:9:PHE:CE2   | 1:A:70:VAL:O    | 0.55     | 2.58        | 10     | 2     |
| 1:A:45:ARG:C    | 1:A:87:GLU:HA   | 0.55     | 2.26        | 12     | 1     |
| 1:A:38:ILE:CG1  | 1:A:38:ILE:O    | 0.55     | 2.54        | 10     | 2     |
| 1:A:59:ARG:O    | 1:A:60:ALA:O    | 0.55     | 2.23        | 12     | 3     |
| 1:A:46:LEU:CD1  | 1:A:87:GLU:O    | 0.55     | 2.54        | 9      | 2     |
| 1:A:40:ILE:CG2  | 1:A:41:GLU:N    | 0.55     | 2.70        | 6      | 4     |
| 1:A:68:VAL:HG13 | 1:A:69:ASP:N    | 0.55     | 2.16        | 12     | 2     |
| 1:A:67:LEU:HD23 | 1:A:71:ILE:HG12 | 0.55     | 1.77        | 7      | 1     |
| 1:A:9:PHE:CZ    | 1:A:71:ILE:CG2  | 0.55     | 2.81        | 2      | 1     |
| 1:A:26:ASN:ND2  | 1:A:26:ASN:N    | 0.55     | 2.53        | 6      | 2     |
| 1:A:5:VAL:HG21  | 1:A:87:GLU:O    | 0.55     | 2.01        | 11     | 1     |
| 1:A:30:VAL:HG22 | 1:A:31:VAL:N    | 0.55     | 2.16        | 8      | 1     |
| 1:A:45:ARG:O    | 1:A:46:LEU:CG   | 0.55     | 2.53        | 12     | 1     |
| 1:A:6:TYR:O     | 1:A:7:ILE:CG2   | 0.55     | 2.55        | 9      | 9     |
| 1:A:48:ILE:N    | 1:A:48:ILE:CD1  | 0.55     | 2.67        | 9      | 2     |
| 1:A:77:VAL:CG2  | 1:A:84:PHE:CE1  | 0.55     | 2.90        | 6      | 1     |
| 1:A:10:GLN:HB2  | 1:A:70:VAL:HG12 | 0.55     | 1.77        | 12     | 1     |
| 1:A:86:LEU:C    | 1:A:86:LEU:CD1  | 0.55     | 2.77        | 12     | 3     |
| 1:A:4:LEU:CD2   | 1:A:4:LEU:C     | 0.55     | 2.80        | 11     | 2     |
| 1:A:31:VAL:CG2  | 1:A:32:GLN:N    | 0.55     | 2.69        | 10     | 3     |
| 1:A:63:VAL:HG12 | 1:A:63:VAL:O    | 0.55     | 2.01        | 11     | 1     |
| 1:A:77:VAL:O    | 1:A:85:VAL:CG1  | 0.55     | 2.55        | 2      | 1     |
| 1:A:10:GLN:CG   | 1:A:69:ASP:O    | 0.55     | 2.55        | 7      | 1     |
| 1:A:10:GLN:CG   | 1:A:69:ASP:C    | 0.55     | 2.80        | 7      | 1     |
| 1:A:39:ARG:O    | 1:A:40:ILE:CG1  | 0.55     | 2.55        | 12     | 3     |
| 1:A:31:VAL:HG22 | 1:A:32:GLN:N    | 0.55     | 2.16        | 10     | 3     |
| 1:A:46:LEU:HB3  | 1:A:86:LEU:CD1  | 0.55     | 2.31        | 3      | 3     |
| 1:A:72:THR:C    | 1:A:73:ILE:CG1  | 0.55     | 2.79        | 5      | 2     |
| 1:A:9:PHE:C     | 1:A:70:VAL:HG12 | 0.54     | 2.26        | 4      | 1     |
| 1:A:9:PHE:HB3   | 1:A:38:ILE:CG1  | 0.54     | 2.32        | 10     | 1     |
| 1:A:43:GLU:O    | 1:A:44:LYS:CB   | 0.54     | 2.55        | 12     | 3     |
| 1:A:49:ARG:HA   | 1:A:83:ARG:CB   | 0.54     | 2.32        | 2      | 1     |
| 1:A:9:PHE:CE2   | 1:A:39:ARG:NE   | 0.54     | 2.75        | 4      | 1     |
| 1:A:20:GLU:OE2  | 1:A:33:HIS:CD2  | 0.54     | 2.60        | 11     | 1     |
| 1:A:10:GLN:O    | 1:A:69:ASP:CB   | 0.54     | 2.55        | 4      | 2     |
| 1:A:71:ILE:CG2  | 1:A:72:THR:N    | 0.54     | 2.70        | 8      | 1     |
| 1:A:5:VAL:HG13  | 1:A:6:TYR:N     | 0.54     | 2.17        | 8      | 1     |
| 1:A:76:ASN:O    | 1:A:86:LEU:CD2  | 0.54     | 2.55        | 9      | 1     |
| 1:A:9:PHE:CE1   | 1:A:38:ILE:HB   | 0.54     | 2.38        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:38:ILE:CG2  | 1:A:38:ILE:O    | 0.54     | 2.56        | 11     | 1     |
| 1:A:4:LEU:CB    | 1:A:42:ALA:O    | 0.54     | 2.56        | 1      | 4     |
| 1:A:46:LEU:HB2  | 1:A:86:LEU:CD1  | 0.54     | 2.32        | 3      | 2     |
| 1:A:47:GLU:C    | 1:A:48:ILE:CD1  | 0.54     | 2.79        | 7      | 1     |
| 1:A:39:ARG:C    | 1:A:39:ARG:CD   | 0.54     | 2.81        | 9      | 1     |
| 1:A:5:VAL:O     | 1:A:41:GLU:CB   | 0.54     | 2.56        | 11     | 1     |
| 1:A:6:TYR:C     | 1:A:6:TYR:CD1   | 0.54     | 2.85        | 3      | 5     |
| 1:A:53:VAL:CG2  | 1:A:84:PHE:CD1  | 0.54     | 2.87        | 4      | 1     |
| 1:A:46:LEU:HD23 | 1:A:85:VAL:CG2  | 0.54     | 2.32        | 12     | 1     |
| 1:A:56:ASN:O    | 1:A:60:ALA:N    | 0.54     | 2.41        | 10     | 4     |
| 1:A:6:TYR:C     | 1:A:7:ILE:CG2   | 0.54     | 2.81        | 5      | 8     |
| 1:A:30:VAL:C    | 1:A:31:VAL:CG2  | 0.54     | 2.81        | 5      | 4     |
| 1:A:23:ILE:O    | 1:A:27:PRO:CD   | 0.54     | 2.56        | 10     | 2     |
| 1:A:78:ASP:O    | 1:A:85:VAL:HG12 | 0.54     | 2.02        | 10     | 1     |
| 1:A:38:ILE:HD11 | 1:A:40:ILE:HG13 | 0.54     | 1.80        | 7      | 1     |
| 1:A:80:ASP:HB2  | 1:A:85:VAL:HG12 | 0.54     | 1.78        | 7      | 1     |
| 1:A:47:GLU:HG3  | 1:A:85:VAL:HG23 | 0.54     | 1.79        | 9      | 1     |
| 1:A:6:TYR:N     | 1:A:74:GLY:O    | 0.54     | 2.41        | 1      | 1     |
| 1:A:34:HIS:CB   | 1:A:35:PRO:HD3  | 0.54     | 2.33        | 10     | 7     |
| 1:A:48:ILE:HD12 | 1:A:85:VAL:CG1  | 0.54     | 2.33        | 8      | 1     |
| 1:A:30:VAL:HG13 | 1:A:41:GLU:HG3  | 0.54     | 1.80        | 11     | 1     |
| 1:A:3:SER:O     | 1:A:44:LYS:N    | 0.53     | 2.41        | 6      | 7     |
| 1:A:47:GLU:HA   | 1:A:85:VAL:CG1  | 0.53     | 2.26        | 8      | 1     |
| 1:A:46:LEU:HB2  | 1:A:87:GLU:C    | 0.53     | 2.28        | 7      | 3     |
| 1:A:10:GLN:CD   | 1:A:10:GLN:C    | 0.53     | 2.77        | 9      | 1     |
| 1:A:61:TRP:CD1  | 1:A:63:VAL:HG23 | 0.53     | 2.38        | 11     | 1     |
| 1:A:46:LEU:HB2  | 1:A:86:LEU:HD13 | 0.53     | 1.80        | 3      | 1     |
| 1:A:56:ASN:O    | 1:A:59:ARG:N    | 0.53     | 2.42        | 11     | 2     |
| 1:A:85:VAL:HG22 | 1:A:86:LEU:N    | 0.53     | 2.17        | 8      | 2     |
| 1:A:39:ARG:CG   | 1:A:40:ILE:N    | 0.53     | 2.72        | 6      | 1     |
| 1:A:67:LEU:HD12 | 1:A:68:VAL:N    | 0.53     | 2.18        | 2      | 1     |
| 1:A:6:TYR:O     | 1:A:74:GLY:CA   | 0.53     | 2.56        | 6      | 2     |
| 1:A:68:VAL:CG1  | 1:A:69:ASP:OD2  | 0.53     | 2.57        | 6      | 1     |
| 1:A:6:TYR:O     | 1:A:7:ILE:HG23  | 0.53     | 2.03        | 8      | 1     |
| 1:A:43:GLU:O    | 1:A:44:LYS:CG   | 0.53     | 2.56        | 12     | 1     |
| 1:A:46:LEU:HG   | 1:A:86:LEU:O    | 0.53     | 2.04        | 11     | 4     |
| 1:A:46:LEU:HD23 | 1:A:85:VAL:HG22 | 0.53     | 1.78        | 12     | 1     |
| 1:A:10:GLN:O    | 1:A:69:ASP:HA   | 0.53     | 2.04        | 6      | 7     |
| 1:A:78:ASP:OD1  | 1:A:85:VAL:CG1  | 0.53     | 2.57        | 3      | 2     |
| 1:A:4:LEU:HA    | 1:A:43:GLU:CA   | 0.53     | 2.34        | 11     | 2     |
| 1:A:45:ARG:O    | 1:A:46:LEU:CD2  | 0.53     | 2.57        | 5      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:49:ARG:O    | 1:A:53:VAL:CG2  | 0.53     | 2.57        | 8      | 1     |
| 1:A:74:GLY:C    | 1:A:86:LEU:HD21 | 0.53     | 2.29        | 8      | 1     |
| 1:A:48:ILE:CG2  | 1:A:51:GLU:CB   | 0.53     | 2.87        | 2      | 3     |
| 1:A:46:LEU:CB   | 1:A:87:GLU:O    | 0.53     | 2.57        | 10     | 2     |
| 1:A:77:VAL:O    | 1:A:85:VAL:HG13 | 0.53     | 2.04        | 2      | 1     |
| 1:A:73:ILE:O    | 1:A:75:GLY:N    | 0.52     | 2.42        | 1      | 1     |
| 1:A:10:GLN:HB2  | 1:A:69:ASP:O    | 0.52     | 2.04        | 10     | 1     |
| 1:A:66:MET:O    | 1:A:68:VAL:N    | 0.52     | 2.42        | 11     | 3     |
| 1:A:46:LEU:O    | 1:A:85:VAL:HG23 | 0.52     | 2.05        | 10     | 2     |
| 1:A:6:TYR:CE2   | 1:A:73:ILE:HG13 | 0.52     | 2.39        | 8      | 1     |
| 1:A:19:VAL:O    | 1:A:23:ILE:CG1  | 0.52     | 2.57        | 8      | 1     |
| 1:A:38:ILE:HD13 | 1:A:38:ILE:H    | 0.52     | 1.63        | 8      | 1     |
| 1:A:57:LEU:HD12 | 1:A:61:TRP:CE3  | 0.52     | 2.39        | 8      | 1     |
| 1:A:46:LEU:N    | 1:A:46:LEU:CD2  | 0.52     | 2.68        | 2      | 2     |
| 1:A:67:LEU:C    | 1:A:67:LEU:CD1  | 0.52     | 2.79        | 2      | 1     |
| 1:A:48:ILE:HG22 | 1:A:51:GLU:HG3  | 0.52     | 1.81        | 3      | 1     |
| 1:A:46:LEU:CB   | 1:A:86:LEU:HG   | 0.52     | 2.33        | 4      | 2     |
| 1:A:69:ASP:OD1  | 1:A:69:ASP:N    | 0.52     | 2.42        | 5      | 2     |
| 1:A:6:TYR:O     | 1:A:73:ILE:HG23 | 0.52     | 2.04        | 6      | 1     |
| 1:A:67:LEU:O    | 1:A:71:ILE:CG1  | 0.52     | 2.57        | 7      | 1     |
| 1:A:59:ARG:O    | 1:A:59:ARG:CG   | 0.52     | 2.56        | 12     | 1     |
| 1:A:6:TYR:C     | 1:A:7:ILE:HG23  | 0.52     | 2.29        | 11     | 9     |
| 1:A:47:GLU:C    | 1:A:48:ILE:CG1  | 0.52     | 2.82        | 4      | 4     |
| 1:A:8:ALA:O     | 1:A:72:THR:CA   | 0.52     | 2.58        | 6      | 2     |
| 1:A:71:ILE:O    | 1:A:72:THR:CG2  | 0.52     | 2.54        | 6      | 1     |
| 1:A:42:ALA:O    | 1:A:43:GLU:CG   | 0.52     | 2.57        | 10     | 1     |
| 1:A:4:LEU:HD12  | 1:A:4:LEU:C     | 0.52     | 2.30        | 12     | 2     |
| 1:A:9:PHE:CA    | 1:A:71:ILE:HB   | 0.52     | 2.34        | 9      | 2     |
| 1:A:8:ALA:N     | 1:A:72:THR:HA   | 0.52     | 2.20        | 6      | 1     |
| 1:A:9:PHE:HB2   | 1:A:70:VAL:CG1  | 0.52     | 2.34        | 8      | 1     |
| 1:A:53:VAL:HG21 | 1:A:84:PHE:CG   | 0.52     | 2.40        | 10     | 1     |
| 1:A:85:VAL:HG22 | 1:A:86:LEU:H    | 0.52     | 1.65        | 9      | 2     |
| 1:A:8:ALA:HB3   | 1:A:71:ILE:CG2  | 0.52     | 2.35        | 9      | 2     |
| 1:A:78:ASP:OD2  | 1:A:86:LEU:CD2  | 0.52     | 2.57        | 7      | 1     |
| 1:A:49:ARG:HA   | 1:A:83:ARG:CG   | 0.52     | 2.34        | 3      | 2     |
| 1:A:9:PHE:CE2   | 1:A:39:ARG:HG2  | 0.52     | 2.39        | 4      | 1     |
| 1:A:23:ILE:CG2  | 1:A:24:GLN:N    | 0.52     | 2.73        | 11     | 1     |
| 1:A:10:GLN:CB   | 1:A:70:VAL:CG2  | 0.52     | 2.88        | 3      | 1     |
| 1:A:48:ILE:N    | 1:A:84:PHE:O    | 0.52     | 2.43        | 12     | 1     |
| 1:A:3:SER:O     | 1:A:43:GLU:HA   | 0.52     | 2.05        | 12     | 2     |
| 1:A:9:PHE:O     | 1:A:38:ILE:CG1  | 0.52     | 2.58        | 2      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:25:ASP:O    | 1:A:29:ALA:CB   | 0.52     | 2.57        | 10     | 2     |
| 1:A:38:ILE:C    | 1:A:38:ILE:CD1  | 0.52     | 2.77        | 7      | 1     |
| 1:A:52:THR:HG21 | 1:A:78:ASP:CG   | 0.52     | 2.29        | 7      | 1     |
| 1:A:9:PHE:CE1   | 1:A:38:ILE:CD1  | 0.52     | 2.90        | 8      | 1     |
| 1:A:67:LEU:O    | 1:A:69:ASP:N    | 0.51     | 2.43        | 7      | 3     |
| 1:A:72:THR:HG22 | 1:A:73:ILE:H    | 0.51     | 1.65        | 5      | 2     |
| 1:A:11:ASP:N    | 1:A:11:ASP:OD1  | 0.51     | 2.43        | 12     | 1     |
| 1:A:84:PHE:CD1  | 1:A:85:VAL:N    | 0.51     | 2.77        | 1      | 2     |
| 1:A:33:HIS:O    | 1:A:33:HIS:CD2  | 0.51     | 2.63        | 2      | 1     |
| 1:A:26:ASN:OD1  | 1:A:31:VAL:CG1  | 0.51     | 2.57        | 7      | 1     |
| 1:A:8:ALA:O     | 1:A:71:ILE:C    | 0.51     | 2.53        | 8      | 1     |
| 1:A:70:VAL:HG12 | 1:A:71:ILE:N    | 0.51     | 2.21        | 11     | 5     |
| 1:A:67:LEU:O    | 1:A:68:VAL:C    | 0.51     | 2.53        | 8      | 7     |
| 1:A:63:VAL:O    | 1:A:64:GLN:C    | 0.51     | 2.54        | 3      | 5     |
| 1:A:78:ASP:HB3  | 1:A:84:PHE:CE2  | 0.51     | 2.41        | 4      | 2     |
| 1:A:45:ARG:O    | 1:A:46:LEU:CB   | 0.51     | 2.59        | 12     | 1     |
| 1:A:6:TYR:HH    | 1:A:72:THR:HG21 | 0.51     | 1.61        | 1      | 1     |
| 1:A:30:VAL:HG21 | 1:A:41:GLU:HB3  | 0.51     | 1.82        | 6      | 1     |
| 1:A:7:ILE:HG13  | 1:A:40:ILE:HD12 | 0.51     | 1.83        | 8      | 1     |
| 1:A:9:PHE:HB2   | 1:A:70:VAL:HG12 | 0.51     | 1.82        | 8      | 1     |
| 1:A:7:ILE:HD11  | 1:A:40:ILE:CG2  | 0.51     | 2.35        | 6      | 1     |
| 1:A:45:ARG:HA   | 1:A:87:GLU:HB3  | 0.51     | 1.83        | 8      | 1     |
| 1:A:22:ILE:O    | 1:A:26:ASN:ND2  | 0.51     | 2.43        | 9      | 1     |
| 1:A:8:ALA:HB2   | 1:A:39:ARG:HB2  | 0.51     | 1.82        | 11     | 1     |
| 1:A:10:GLN:NE2  | 1:A:11:ASP:O    | 0.51     | 2.44        | 12     | 1     |
| 1:A:71:ILE:HD12 | 1:A:72:THR:N    | 0.51     | 2.21        | 1      | 1     |
| 1:A:56:ASN:O    | 1:A:59:ARG:CB   | 0.51     | 2.59        | 3      | 1     |
| 1:A:52:THR:HB   | 1:A:84:PHE:CD2  | 0.51     | 2.41        | 7      | 2     |
| 1:A:9:PHE:CE2   | 1:A:71:ILE:CD1  | 0.50     | 2.94        | 1      | 1     |
| 1:A:10:GLN:HB2  | 1:A:70:VAL:CG2  | 0.50     | 2.36        | 3      | 2     |
| 1:A:79:GLU:HB3  | 1:A:84:PHE:CD1  | 0.50     | 2.41        | 8      | 1     |
| 1:A:61:TRP:NE1  | 1:A:63:VAL:CG2  | 0.50     | 2.74        | 12     | 1     |
| 1:A:26:ASN:O    | 1:A:27:PRO:C    | 0.50     | 2.54        | 10     | 2     |
| 1:A:39:ARG:HG3  | 1:A:39:ARG:NH1  | 0.50     | 2.22        | 1      | 1     |
| 1:A:33:HIS:CD2  | 1:A:33:HIS:N    | 0.50     | 2.78        | 2      | 1     |
| 1:A:34:HIS:CD2  | 1:A:35:PRO:HD2  | 0.50     | 2.41        | 2      | 2     |
| 1:A:58:GLY:O    | 1:A:59:ARG:HB3  | 0.50     | 2.06        | 12     | 3     |
| 1:A:49:ARG:HG3  | 1:A:49:ARG:NH1  | 0.50     | 2.20        | 3      | 1     |
| 1:A:24:GLN:O    | 1:A:24:GLN:NE2  | 0.50     | 2.44        | 4      | 1     |
| 1:A:71:ILE:HG22 | 1:A:72:THR:OG1  | 0.50     | 2.06        | 5      | 1     |
| 1:A:73:ILE:HG23 | 1:A:74:GLY:H    | 0.50     | 1.65        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:10:GLN:C    | 1:A:10:GLN:CD   | 0.50     | 2.80        | 5      | 2     |
| 1:A:3:SER:HB3   | 1:A:44:LYS:CB   | 0.50     | 2.36        | 11     | 1     |
| 1:A:75:GLY:O    | 1:A:87:GLU:CB   | 0.50     | 2.59        | 4      | 1     |
| 1:A:31:VAL:HG22 | 1:A:32:GLN:H    | 0.50     | 1.66        | 6      | 1     |
| 1:A:10:GLN:CB   | 1:A:69:ASP:O    | 0.50     | 2.60        | 8      | 1     |
| 1:A:8:ALA:HB2   | 1:A:39:ARG:CB   | 0.50     | 2.36        | 11     | 1     |
| 1:A:46:LEU:O    | 1:A:47:GLU:CB   | 0.50     | 2.59        | 12     | 1     |
| 1:A:10:GLN:H    | 1:A:70:VAL:HA   | 0.50     | 1.65        | 7      | 2     |
| 1:A:33:HIS:CB   | 1:A:38:ILE:HG22 | 0.50     | 2.33        | 8      | 1     |
| 1:A:30:VAL:HG22 | 1:A:31:VAL:H    | 0.50     | 1.66        | 12     | 1     |
| 1:A:78:ASP:HB2  | 1:A:84:PHE:CE2  | 0.50     | 2.42        | 2      | 1     |
| 1:A:8:ALA:CB    | 1:A:72:THR:OG1  | 0.50     | 2.55        | 10     | 1     |
| 1:A:83:ARG:CG   | 1:A:84:PHE:N    | 0.50     | 2.75        | 1      | 1     |
| 1:A:9:PHE:CE2   | 1:A:70:VAL:CG2  | 0.50     | 2.95        | 7      | 2     |
| 1:A:8:ALA:C     | 1:A:72:THR:HG1  | 0.50     | 2.12        | 11     | 1     |
| 1:A:73:ILE:C    | 1:A:73:ILE:CD1  | 0.49     | 2.81        | 12     | 2     |
| 1:A:78:ASP:OD1  | 1:A:78:ASP:N    | 0.49     | 2.45        | 12     | 1     |
| 1:A:9:PHE:N     | 1:A:71:ILE:HB   | 0.49     | 2.22        | 5      | 1     |
| 1:A:10:GLN:N    | 1:A:70:VAL:HB   | 0.49     | 2.21        | 3      | 1     |
| 1:A:10:GLN:HG3  | 1:A:69:ASP:HA   | 0.49     | 1.84        | 8      | 1     |
| 1:A:10:GLN:O    | 1:A:70:VAL:HG23 | 0.49     | 2.08        | 10     | 1     |
| 1:A:24:GLN:O    | 1:A:25:ASP:C    | 0.49     | 2.55        | 8      | 8     |
| 1:A:48:ILE:HG22 | 1:A:53:VAL:CG2  | 0.49     | 2.35        | 8      | 1     |
| 1:A:48:ILE:HD13 | 1:A:84:PHE:CD2  | 0.49     | 2.43        | 1      | 2     |
| 1:A:63:VAL:O    | 1:A:65:GLU:N    | 0.49     | 2.46        | 3      | 3     |
| 1:A:30:VAL:CG2  | 1:A:31:VAL:N    | 0.49     | 2.75        | 8      | 1     |
| 1:A:86:LEU:N    | 1:A:86:LEU:HD12 | 0.49     | 2.22        | 3      | 1     |
| 1:A:3:SER:C     | 1:A:44:LYS:O    | 0.49     | 2.56        | 5      | 1     |
| 1:A:9:PHE:CE2   | 1:A:38:ILE:HG13 | 0.49     | 2.43        | 6      | 1     |
| 1:A:47:GLU:CA   | 1:A:85:VAL:HG23 | 0.49     | 2.35        | 3      | 2     |
| 1:A:46:LEU:HG   | 1:A:87:GLU:CG   | 0.49     | 2.37        | 12     | 1     |
| 1:A:45:ARG:CB   | 1:A:87:GLU:HB3  | 0.49     | 2.38        | 1      | 3     |
| 1:A:52:THR:O    | 1:A:53:VAL:C    | 0.49     | 2.56        | 5      | 7     |
| 1:A:46:LEU:HD13 | 1:A:86:LEU:CD2  | 0.49     | 2.37        | 4      | 1     |
| 1:A:11:ASP:N    | 1:A:70:VAL:HG23 | 0.49     | 2.21        | 7      | 2     |
| 1:A:70:VAL:HG22 | 1:A:71:ILE:H    | 0.49     | 1.67        | 12     | 1     |
| 1:A:14:ASN:O    | 1:A:15:ALA:C    | 0.49     | 2.56        | 7      | 2     |
| 1:A:30:VAL:HG12 | 1:A:31:VAL:H    | 0.49     | 1.67        | 1      | 1     |
| 1:A:45:ARG:CG   | 1:A:87:GLU:HB3  | 0.49     | 2.38        | 6      | 2     |
| 1:A:64:GLN:O    | 1:A:67:LEU:CD2  | 0.49     | 2.55        | 2      | 1     |
| 1:A:57:LEU:O    | 1:A:58:GLY:C    | 0.49     | 2.54        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:57:LEU:O    | 1:A:59:ARG:N    | 0.49     | 2.46        | 3      | 1     |
| 1:A:7:ILE:C     | 1:A:7:ILE:CD1   | 0.49     | 2.83        | 7      | 2     |
| 1:A:9:PHE:CE1   | 1:A:71:ILE:HG22 | 0.49     | 2.43        | 7      | 1     |
| 1:A:38:ILE:HD13 | 1:A:39:ARG:N    | 0.48     | 2.22        | 7      | 1     |
| 1:A:78:ASP:CG   | 1:A:86:LEU:CD2  | 0.48     | 2.87        | 4      | 1     |
| 1:A:47:GLU:HB2  | 1:A:80:ASP:OD1  | 0.48     | 2.08        | 8      | 1     |
| 1:A:3:SER:CB    | 1:A:44:LYS:HB3  | 0.48     | 2.37        | 11     | 1     |
| 1:A:3:SER:CB    | 1:A:44:LYS:HA   | 0.48     | 2.38        | 12     | 1     |
| 1:A:5:VAL:HB    | 1:A:74:GLY:HA2  | 0.48     | 1.84        | 1      | 1     |
| 1:A:39:ARG:O    | 1:A:40:ILE:CD1  | 0.48     | 2.61        | 3      | 1     |
| 1:A:69:ASP:O    | 1:A:70:VAL:C    | 0.48     | 2.56        | 3      | 1     |
| 1:A:45:ARG:HA   | 1:A:87:GLU:HA   | 0.48     | 1.85        | 10     | 2     |
| 1:A:71:ILE:C    | 1:A:72:THR:OG1  | 0.48     | 2.56        | 6      | 2     |
| 1:A:48:ILE:CG2  | 1:A:49:ARG:N    | 0.48     | 2.68        | 12     | 1     |
| 1:A:28:HIS:O    | 1:A:29:ALA:C    | 0.48     | 2.56        | 12     | 5     |
| 1:A:67:LEU:O    | 1:A:71:ILE:O    | 0.48     | 2.31        | 10     | 1     |
| 1:A:80:ASP:HB2  | 1:A:85:VAL:CG1  | 0.48     | 2.38        | 2      | 1     |
| 1:A:59:ARG:O    | 1:A:60:ALA:C    | 0.48     | 2.54        | 3      | 2     |
| 1:A:4:LEU:C     | 1:A:87:GLU:OE2  | 0.48     | 2.57        | 5      | 1     |
| 1:A:3:SER:O     | 1:A:43:GLU:C    | 0.48     | 2.57        | 1      | 7     |
| 1:A:3:SER:O     | 1:A:44:LYS:O    | 0.48     | 2.32        | 10     | 3     |
| 1:A:66:MET:O    | 1:A:67:LEU:C    | 0.48     | 2.56        | 2      | 3     |
| 1:A:76:ASN:CA   | 1:A:86:LEU:HD23 | 0.48     | 2.30        | 2      | 1     |
| 1:A:75:GLY:O    | 1:A:87:GLU:HB3  | 0.48     | 2.08        | 4      | 1     |
| 1:A:32:GLN:O    | 1:A:33:HIS:O    | 0.48     | 2.32        | 5      | 1     |
| 1:A:48:ILE:CD1  | 1:A:86:LEU:HD23 | 0.48     | 2.39        | 5      | 1     |
| 1:A:4:LEU:O     | 1:A:87:GLU:CD   | 0.48     | 2.57        | 7      | 1     |
| 1:A:8:ALA:C     | 1:A:72:THR:OG1  | 0.48     | 2.56        | 10     | 2     |
| 1:A:26:ASN:O    | 1:A:29:ALA:O    | 0.48     | 2.31        | 10     | 2     |
| 1:A:16:ARG:HG2  | 1:A:16:ARG:NH1  | 0.48     | 2.24        | 10     | 1     |
| 1:A:59:ARG:O    | 1:A:60:ALA:HB3  | 0.48     | 2.09        | 2      | 2     |
| 1:A:22:ILE:HD12 | 1:A:22:ILE:N    | 0.48     | 2.23        | 6      | 1     |
| 1:A:10:GLN:HG2  | 1:A:69:ASP:O    | 0.48     | 2.08        | 7      | 1     |
| 1:A:48:ILE:O    | 1:A:84:PHE:O    | 0.48     | 2.32        | 7      | 3     |
| 1:A:7:ILE:N     | 1:A:7:ILE:CD1   | 0.48     | 2.76        | 9      | 1     |
| 1:A:78:ASP:HB2  | 1:A:85:VAL:CG1  | 0.48     | 2.39        | 10     | 2     |
| 1:A:45:ARG:C    | 1:A:46:LEU:CD2  | 0.48     | 2.86        | 8      | 1     |
| 1:A:47:GLU:CB   | 1:A:80:ASP:OD1  | 0.48     | 2.62        | 8      | 1     |
| 1:A:46:LEU:O    | 1:A:47:GLU:HB2  | 0.48     | 2.08        | 12     | 1     |
| 1:A:55:GLU:O    | 1:A:58:GLY:N    | 0.48     | 2.47        | 12     | 1     |
| 1:A:6:TYR:O     | 1:A:7:ILE:HG22  | 0.47     | 2.09        | 9      | 6     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:PHE:CD2   | 1:A:39:ARG:CG   | 0.47     | 2.96        | 4      | 1     |
| 1:A:10:GLN:CG   | 1:A:69:ASP:HA   | 0.47     | 2.39        | 8      | 1     |
| 1:A:10:GLN:OE1  | 1:A:11:ASP:O    | 0.47     | 2.31        | 9      | 1     |
| 1:A:6:TYR:OH    | 1:A:72:THR:CG2  | 0.47     | 2.56        | 1      | 1     |
| 1:A:48:ILE:CG2  | 1:A:52:THR:OG1  | 0.47     | 2.62        | 1      | 2     |
| 1:A:59:ARG:HG3  | 1:A:59:ARG:NH1  | 0.47     | 2.23        | 2      | 1     |
| 1:A:39:ARG:C    | 1:A:40:ILE:HG13 | 0.47     | 2.33        | 4      | 5     |
| 1:A:46:LEU:HG   | 1:A:87:GLU:O    | 0.47     | 2.09        | 10     | 1     |
| 1:A:4:LEU:O     | 1:A:4:LEU:CD2   | 0.47     | 2.61        | 11     | 2     |
| 1:A:10:GLN:O    | 1:A:68:VAL:O    | 0.47     | 2.33        | 9      | 2     |
| 1:A:53:VAL:HG22 | 1:A:84:PHE:CD2  | 0.47     | 2.44        | 5      | 1     |
| 1:A:26:ASN:N    | 1:A:27:PRO:HD2  | 0.47     | 2.23        | 10     | 2     |
| 1:A:32:GLN:O    | 1:A:39:ARG:O    | 0.47     | 2.33        | 7      | 1     |
| 1:A:3:SER:HB2   | 1:A:44:LYS:CB   | 0.47     | 2.40        | 12     | 1     |
| 1:A:16:ARG:HG3  | 1:A:16:ARG:NH1  | 0.47     | 2.24        | 12     | 1     |
| 1:A:70:VAL:HG22 | 1:A:71:ILE:N    | 0.47     | 2.24        | 12     | 1     |
| 1:A:5:VAL:HG23  | 1:A:6:TYR:H     | 0.47     | 1.67        | 1      | 1     |
| 1:A:9:PHE:O     | 1:A:38:ILE:HG12 | 0.47     | 2.10        | 5      | 4     |
| 1:A:8:ALA:N     | 1:A:72:THR:HB   | 0.47     | 2.24        | 11     | 3     |
| 1:A:34:HIS:O    | 1:A:35:PRO:O    | 0.47     | 2.32        | 6      | 2     |
| 1:A:50:ARG:NH1  | 1:A:50:ARG:HG2  | 0.47     | 2.24        | 6      | 1     |
| 1:A:70:VAL:C    | 1:A:71:ILE:CG1  | 0.47     | 2.87        | 12     | 1     |
| 1:A:11:ASP:CA   | 1:A:69:ASP:HB3  | 0.47     | 2.40        | 2      | 1     |
| 1:A:9:PHE:HB3   | 1:A:69:ASP:CB   | 0.47     | 2.40        | 9      | 2     |
| 1:A:10:GLN:O    | 1:A:69:ASP:HB3  | 0.47     | 2.09        | 6      | 2     |
| 1:A:65:GLU:O    | 1:A:69:ASP:OD1  | 0.47     | 2.33        | 6      | 1     |
| 1:A:11:ASP:OD1  | 1:A:69:ASP:OD1  | 0.47     | 2.33        | 9      | 1     |
| 1:A:3:SER:C     | 1:A:44:LYS:HB2  | 0.47     | 2.35        | 11     | 1     |
| 1:A:55:GLU:O    | 1:A:56:ASN:C    | 0.47     | 2.56        | 12     | 2     |
| 1:A:78:ASP:CA   | 1:A:85:VAL:O    | 0.47     | 2.62        | 2      | 1     |
| 1:A:50:ARG:HG3  | 1:A:50:ARG:NH1  | 0.47     | 2.24        | 4      | 1     |
| 1:A:26:ASN:C    | 1:A:28:HIS:N    | 0.47     | 2.72        | 10     | 2     |
| 1:A:71:ILE:CG2  | 1:A:72:THR:H    | 0.47     | 2.21        | 8      | 1     |
| 1:A:10:GLN:HB2  | 1:A:70:VAL:O    | 0.47     | 2.10        | 9      | 1     |
| 1:A:54:GLU:O    | 1:A:57:LEU:HB3  | 0.47     | 2.10        | 11     | 2     |
| 1:A:46:LEU:CB   | 1:A:86:LEU:HD13 | 0.47     | 2.39        | 3      | 1     |
| 1:A:23:ILE:CG2  | 1:A:29:ALA:HB1  | 0.47     | 2.40        | 4      | 2     |
| 1:A:18:VAL:O    | 1:A:22:ILE:HD12 | 0.47     | 2.10        | 6      | 1     |
| 1:A:9:PHE:HB2   | 1:A:70:VAL:O    | 0.47     | 2.10        | 4      | 2     |
| 1:A:86:LEU:HD12 | 1:A:87:GLU:O    | 0.47     | 2.10        | 5      | 1     |
| 1:A:30:VAL:HG11 | 1:A:41:GLU:HB2  | 0.47     | 1.87        | 12     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:PHE:CE2   | 1:A:39:ARG:CG   | 0.47     | 2.97        | 4      | 1     |
| 1:A:46:LEU:HD12 | 1:A:86:LEU:CG   | 0.47     | 2.39        | 4      | 1     |
| 1:A:76:ASN:C    | 1:A:77:VAL:CG2  | 0.46     | 2.88        | 2      | 1     |
| 1:A:44:LYS:HD3  | 1:A:45:ARG:CG   | 0.46     | 2.41        | 11     | 1     |
| 1:A:39:ARG:NH1  | 1:A:39:ARG:CG   | 0.46     | 2.78        | 12     | 6     |
| 1:A:10:GLN:HG2  | 1:A:37:MET:HA   | 0.46     | 1.88        | 10     | 1     |
| 1:A:58:GLY:O    | 1:A:59:ARG:HB2  | 0.46     | 2.11        | 2      | 1     |
| 1:A:32:GLN:O    | 1:A:33:HIS:C    | 0.46     | 2.57        | 3      | 1     |
| 1:A:46:LEU:CD1  | 1:A:86:LEU:CD2  | 0.46     | 2.93        | 4      | 1     |
| 1:A:46:LEU:HB2  | 1:A:86:LEU:C    | 0.46     | 2.35        | 4      | 1     |
| 1:A:78:ASP:O    | 1:A:84:PHE:HA   | 0.46     | 2.10        | 7      | 2     |
| 1:A:19:VAL:HA   | 1:A:22:ILE:HD13 | 0.46     | 1.86        | 6      | 1     |
| 1:A:73:ILE:CG2  | 1:A:74:GLY:H    | 0.46     | 2.24        | 8      | 1     |
| 1:A:3:SER:C     | 1:A:4:LEU:CD1   | 0.46     | 2.87        | 11     | 1     |
| 1:A:14:ASN:OD1  | 1:A:14:ASN:O    | 0.46     | 2.33        | 11     | 1     |
| 1:A:4:LEU:HD22  | 1:A:4:LEU:C     | 0.46     | 2.34        | 11     | 2     |
| 1:A:8:ALA:HA    | 1:A:39:ARG:HG3  | 0.46     | 1.85        | 4      | 1     |
| 1:A:5:VAL:HG13  | 1:A:6:TYR:H     | 0.46     | 1.68        | 8      | 1     |
| 1:A:5:VAL:HG12  | 1:A:6:TYR:H     | 0.46     | 1.70        | 12     | 1     |
| 1:A:46:LEU:O    | 1:A:86:LEU:O    | 0.46     | 2.34        | 7      | 2     |
| 1:A:9:PHE:CE1   | 1:A:38:ILE:CB   | 0.46     | 2.98        | 6      | 1     |
| 1:A:24:GLN:CG   | 1:A:31:VAL:HG23 | 0.46     | 2.36        | 6      | 1     |
| 1:A:47:GLU:HG2  | 1:A:85:VAL:HG23 | 0.46     | 1.87        | 1      | 1     |
| 1:A:52:THR:OG1  | 1:A:83:ARG:C    | 0.46     | 2.59        | 2      | 1     |
| 1:A:8:ALA:O     | 1:A:72:THR:OG1  | 0.46     | 2.31        | 4      | 1     |
| 1:A:49:ARG:NH1  | 1:A:49:ARG:CG   | 0.46     | 2.79        | 4      | 5     |
| 1:A:26:ASN:HB2  | 1:A:27:PRO:HD3  | 0.46     | 1.88        | 7      | 2     |
| 1:A:43:GLU:H    | 1:A:46:LEU:HD21 | 0.46     | 1.71        | 11     | 1     |
| 1:A:76:ASN:CB   | 1:A:87:GLU:HB3  | 0.46     | 2.41        | 4      | 1     |
| 1:A:67:LEU:O    | 1:A:71:ILE:HG13 | 0.46     | 2.11        | 7      | 1     |
| 1:A:32:GLN:HB3  | 1:A:38:ILE:CA   | 0.46     | 2.41        | 12     | 1     |
| 1:A:62:ASP:O    | 1:A:62:ASP:CG   | 0.46     | 2.59        | 1      | 3     |
| 1:A:66:MET:O    | 1:A:69:ASP:O    | 0.46     | 2.33        | 1      | 1     |
| 1:A:45:ARG:HA   | 1:A:87:GLU:CG   | 0.46     | 2.40        | 3      | 1     |
| 1:A:56:ASN:O    | 1:A:59:ARG:CA   | 0.46     | 2.64        | 11     | 2     |
| 1:A:83:ARG:O    | 1:A:84:PHE:HB2  | 0.46     | 2.11        | 8      | 1     |
| 1:A:3:SER:O     | 1:A:43:GLU:CA   | 0.46     | 2.64        | 12     | 1     |
| 1:A:7:ILE:HG22  | 1:A:74:GLY:H    | 0.46     | 1.71        | 1      | 1     |
| 1:A:8:ALA:CB    | 1:A:39:ARG:HD2  | 0.46     | 2.41        | 1      | 1     |
| 1:A:86:LEU:CD1  | 1:A:86:LEU:C    | 0.46     | 2.80        | 2      | 1     |
| 1:A:46:LEU:HD13 | 1:A:47:GLU:H    | 0.46     | 1.71        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:48:ILE:HG22 | 1:A:49:ARG:N    | 0.46     | 2.25        | 7      | 1     |
| 1:A:4:LEU:CA    | 1:A:43:GLU:HA   | 0.46     | 2.41        | 10     | 1     |
| 1:A:20:GLU:HG2  | 1:A:33:HIS:CD2  | 0.46     | 2.46        | 11     | 1     |
| 1:A:45:ARG:CB   | 1:A:87:GLU:HA   | 0.46     | 2.41        | 12     | 1     |
| 1:A:43:GLU:O    | 1:A:44:LYS:HB2  | 0.45     | 2.10        | 1      | 4     |
| 1:A:78:ASP:CG   | 1:A:79:GLU:N    | 0.45     | 2.74        | 2      | 1     |
| 1:A:83:ARG:NH1  | 1:A:83:ARG:CG   | 0.45     | 2.79        | 5      | 2     |
| 1:A:16:ARG:NH1  | 1:A:16:ARG:CG   | 0.45     | 2.77        | 9      | 4     |
| 1:A:50:ARG:NH1  | 1:A:50:ARG:CG   | 0.45     | 2.79        | 5      | 5     |
| 1:A:77:VAL:O    | 1:A:77:VAL:HG22 | 0.45     | 2.11        | 7      | 1     |
| 1:A:75:GLY:O    | 1:A:76:ASN:OD1  | 0.45     | 2.33        | 10     | 1     |
| 1:A:61:TRP:NE1  | 1:A:63:VAL:HG21 | 0.45     | 2.26        | 12     | 1     |
| 1:A:35:PRO:O    | 1:A:36:ALA:CB   | 0.45     | 2.60        | 4      | 1     |
| 1:A:39:ARG:O    | 1:A:40:ILE:HG13 | 0.45     | 2.11        | 12     | 3     |
| 1:A:26:ASN:O    | 1:A:28:HIS:N    | 0.45     | 2.49        | 10     | 2     |
| 1:A:9:PHE:O     | 1:A:38:ILE:HB   | 0.45     | 2.11        | 9      | 1     |
| 1:A:32:GLN:HB3  | 1:A:39:ARG:N    | 0.45     | 2.26        | 12     | 1     |
| 1:A:5:VAL:O     | 1:A:6:TYR:CB    | 0.45     | 2.64        | 1      | 1     |
| 1:A:38:ILE:N    | 1:A:38:ILE:CD1  | 0.45     | 2.79        | 4      | 2     |
| 1:A:78:ASP:HB2  | 1:A:85:VAL:HG12 | 0.45     | 1.87        | 10     | 1     |
| 1:A:3:SER:HB2   | 1:A:44:LYS:HB3  | 0.45     | 1.88        | 11     | 1     |
| 1:A:47:GLU:C    | 1:A:85:VAL:HA   | 0.45     | 2.36        | 12     | 1     |
| 1:A:63:VAL:O    | 1:A:63:VAL:HG12 | 0.45     | 2.11        | 12     | 1     |
| 1:A:48:ILE:HB   | 1:A:52:THR:CB   | 0.45     | 2.41        | 5      | 1     |
| 1:A:9:PHE:HA    | 1:A:70:VAL:HB   | 0.45     | 1.89        | 6      | 1     |
| 1:A:10:GLN:HB3  | 1:A:69:ASP:O    | 0.45     | 2.11        | 8      | 1     |
| 1:A:9:PHE:O     | 1:A:38:ILE:CB   | 0.45     | 2.64        | 9      | 1     |
| 1:A:44:LYS:O    | 1:A:45:ARG:HG2  | 0.45     | 2.12        | 12     | 1     |
| 1:A:8:ALA:HB2   | 1:A:39:ARG:HD2  | 0.45     | 1.87        | 1      | 1     |
| 1:A:10:GLN:C    | 1:A:69:ASP:HB2  | 0.45     | 2.37        | 11     | 2     |
| 1:A:57:LEU:C    | 1:A:59:ARG:N    | 0.45     | 2.73        | 3      | 3     |
| 1:A:72:THR:O    | 1:A:73:ILE:HB   | 0.45     | 2.12        | 6      | 1     |
| 1:A:48:ILE:HD13 | 1:A:84:PHE:CE2  | 0.45     | 2.47        | 1      | 1     |
| 1:A:67:LEU:C    | 1:A:69:ASP:N    | 0.45     | 2.75        | 7      | 3     |
| 1:A:9:PHE:HD2   | 1:A:70:VAL:HG22 | 0.45     | 1.57        | 7      | 1     |
| 1:A:30:VAL:CG1  | 1:A:41:GLU:HB2  | 0.45     | 2.40        | 12     | 1     |
| 1:A:35:PRO:O    | 1:A:36:ALA:C    | 0.45     | 2.58        | 12     | 2     |
| 1:A:47:GLU:HG2  | 1:A:85:VAL:CG2  | 0.45     | 2.41        | 1      | 1     |
| 1:A:63:VAL:C    | 1:A:65:GLU:N    | 0.45     | 2.74        | 3      | 4     |
| 1:A:40:ILE:O    | 1:A:41:GLU:HB2  | 0.45     | 2.11        | 5      | 1     |
| 1:A:70:VAL:O    | 1:A:70:VAL:HG13 | 0.45     | 2.12        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:77:VAL:HA   | 1:A:86:LEU:HB3  | 0.45     | 1.87        | 5      | 1     |
| 1:A:4:LEU:HD13  | 1:A:41:GLU:OE2  | 0.45     | 2.11        | 1      | 1     |
| 1:A:10:GLN:HG2  | 1:A:37:MET:CB   | 0.45     | 2.42        | 1      | 1     |
| 1:A:48:ILE:HG21 | 1:A:51:GLU:CB   | 0.45     | 2.41        | 2      | 1     |
| 1:A:23:ILE:CG2  | 1:A:29:ALA:CB   | 0.45     | 2.95        | 5      | 2     |
| 1:A:47:GLU:CA   | 1:A:85:VAL:CG1  | 0.45     | 2.80        | 8      | 1     |
| 1:A:10:GLN:NE2  | 1:A:11:ASP:N    | 0.45     | 2.65        | 9      | 1     |
| 1:A:39:ARG:O    | 1:A:40:ILE:HG12 | 0.45     | 2.11        | 4      | 2     |
| 1:A:85:VAL:HG13 | 1:A:86:LEU:N    | 0.45     | 2.23        | 8      | 1     |
| 1:A:47:GLU:CB   | 1:A:85:VAL:HA   | 0.45     | 2.41        | 12     | 1     |
| 1:A:56:ASN:O    | 1:A:59:ARG:HA   | 0.45     | 2.12        | 11     | 2     |
| 1:A:66:MET:C    | 1:A:68:VAL:N    | 0.45     | 2.75        | 2      | 3     |
| 1:A:11:ASP:OD1  | 1:A:69:ASP:OD2  | 0.45     | 2.35        | 3      | 1     |
| 1:A:8:ALA:HA    | 1:A:39:ARG:HB2  | 0.45     | 1.83        | 4      | 1     |
| 1:A:38:ILE:O    | 1:A:39:ARG:CB   | 0.45     | 2.62        | 4      | 1     |
| 1:A:45:ARG:CG   | 1:A:45:ARG:NH1  | 0.45     | 2.78        | 6      | 1     |
| 1:A:4:LEU:HB2   | 1:A:42:ALA:O    | 0.44     | 2.13        | 2      | 3     |
| 1:A:7:ILE:CG1   | 1:A:40:ILE:HB   | 0.44     | 2.42        | 1      | 1     |
| 1:A:70:VAL:C    | 1:A:71:ILE:HG13 | 0.44     | 2.36        | 12     | 2     |
| 1:A:30:VAL:CG1  | 1:A:41:GLU:HG3  | 0.44     | 2.43        | 3      | 2     |
| 1:A:48:ILE:CG2  | 1:A:51:GLU:HB2  | 0.44     | 2.42        | 11     | 2     |
| 1:A:22:ILE:O    | 1:A:25:ASP:CB   | 0.44     | 2.65        | 4      | 1     |
| 1:A:72:THR:C    | 1:A:73:ILE:HG13 | 0.44     | 2.37        | 5      | 2     |
| 1:A:78:ASP:HB3  | 1:A:84:PHE:CD2  | 0.44     | 2.47        | 7      | 1     |
| 1:A:12:ASN:O    | 1:A:13:ASP:HB2  | 0.44     | 2.12        | 8      | 1     |
| 1:A:74:GLY:HA3  | 1:A:86:LEU:CD1  | 0.44     | 2.42        | 1      | 1     |
| 1:A:63:VAL:HG12 | 1:A:66:MET:HB2  | 0.44     | 1.88        | 2      | 1     |
| 1:A:11:ASP:CB   | 1:A:16:ARG:NH1  | 0.44     | 2.80        | 6      | 1     |
| 1:A:10:GLN:CB   | 1:A:70:VAL:O    | 0.44     | 2.65        | 9      | 1     |
| 1:A:45:ARG:HB3  | 1:A:87:GLU:HA   | 0.44     | 1.87        | 12     | 1     |
| 1:A:73:ILE:HG12 | 1:A:74:GLY:N    | 0.44     | 2.27        | 12     | 1     |
| 1:A:59:ARG:NH1  | 1:A:59:ARG:CG   | 0.44     | 2.78        | 3      | 4     |
| 1:A:80:ASP:C    | 1:A:80:ASP:OD1  | 0.44     | 2.59        | 2      | 1     |
| 1:A:68:VAL:HG13 | 1:A:69:ASP:OD2  | 0.44     | 2.12        | 6      | 1     |
| 1:A:74:GLY:CA   | 1:A:86:LEU:CD2  | 0.44     | 2.96        | 8      | 1     |
| 1:A:69:ASP:OD1  | 1:A:69:ASP:C    | 0.44     | 2.59        | 11     | 1     |
| 1:A:45:ARG:NH1  | 1:A:45:ARG:HG2  | 0.44     | 2.27        | 3      | 2     |
| 1:A:11:ASP:OD2  | 1:A:13:ASP:O    | 0.44     | 2.35        | 4      | 1     |
| 1:A:76:ASN:HB3  | 1:A:87:GLU:OE1  | 0.44     | 2.12        | 4      | 1     |
| 1:A:14:ASN:OD1  | 1:A:17:TYR:CB   | 0.44     | 2.65        | 5      | 1     |
| 1:A:77:VAL:CG2  | 1:A:85:VAL:O    | 0.44     | 2.58        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:6:TYR:HE1   | 1:A:8:ALA:HB2   | 0.44     | 1.72        | 6      | 1     |
| 1:A:65:GLU:O    | 1:A:69:ASP:O    | 0.44     | 2.35        | 6      | 1     |
| 1:A:45:ARG:HB3  | 1:A:87:GLU:CG   | 0.44     | 2.42        | 6      | 2     |
| 1:A:56:ASN:HA   | 1:A:60:ALA:N    | 0.44     | 2.28        | 2      | 2     |
| 1:A:46:LEU:HB2  | 1:A:86:LEU:HG   | 0.44     | 1.89        | 10     | 2     |
| 1:A:78:ASP:N    | 1:A:86:LEU:HB3  | 0.44     | 2.27        | 4      | 1     |
| 1:A:21:ALA:O    | 1:A:25:ASP:N    | 0.44     | 2.51        | 7      | 1     |
| 1:A:69:ASP:C    | 1:A:71:ILE:N    | 0.44     | 2.72        | 7      | 1     |
| 1:A:22:ILE:HG23 | 1:A:26:ASN:ND2  | 0.44     | 2.27        | 10     | 1     |
| 1:A:45:ARG:HG3  | 1:A:45:ARG:NH1  | 0.44     | 2.26        | 10     | 1     |
| 1:A:49:ARG:HB2  | 1:A:83:ARG:CG   | 0.44     | 2.43        | 12     | 1     |
| 1:A:38:ILE:HG13 | 1:A:38:ILE:O    | 0.44     | 2.11        | 3      | 3     |
| 1:A:56:ASN:O    | 1:A:57:LEU:C    | 0.44     | 2.61        | 2      | 2     |
| 1:A:45:ARG:NH1  | 1:A:45:ARG:CG   | 0.44     | 2.79        | 10     | 3     |
| 1:A:70:VAL:CG1  | 1:A:71:ILE:N    | 0.44     | 2.81        | 3      | 1     |
| 1:A:71:ILE:O    | 1:A:72:THR:CB   | 0.44     | 2.64        | 6      | 1     |
| 1:A:76:ASN:CA   | 1:A:86:LEU:HD21 | 0.44     | 2.43        | 12     | 1     |
| 1:A:8:ALA:CB    | 1:A:39:ARG:HA   | 0.44     | 2.42        | 8      | 4     |
| 1:A:9:PHE:O     | 1:A:38:ILE:HG23 | 0.44     | 2.13        | 5      | 1     |
| 1:A:64:GLN:O    | 1:A:71:ILE:HD11 | 0.44     | 2.11        | 7      | 1     |
| 1:A:5:VAL:CG2   | 1:A:46:LEU:HD11 | 0.44     | 2.37        | 8      | 1     |
| 1:A:61:TRP:CD1  | 1:A:63:VAL:CG2  | 0.44     | 3.00        | 11     | 1     |
| 1:A:10:GLN:O    | 1:A:69:ASP:CA   | 0.44     | 2.66        | 4      | 2     |
| 1:A:34:HIS:HB3  | 1:A:35:PRO:HD3  | 0.44     | 1.89        | 6      | 4     |
| 1:A:86:LEU:HD13 | 1:A:87:GLU:H    | 0.44     | 1.73        | 9      | 1     |
| 1:A:44:LYS:O    | 1:A:87:GLU:HB3  | 0.44     | 2.12        | 11     | 1     |
| 1:A:5:VAL:HB    | 1:A:42:ALA:CB   | 0.44     | 2.40        | 12     | 1     |
| 1:A:6:TYR:O     | 1:A:73:ILE:C    | 0.44     | 2.61        | 4      | 2     |
| 1:A:17:TYR:CE2  | 1:A:38:ILE:HG22 | 0.44     | 2.47        | 4      | 1     |
| 1:A:45:ARG:CA   | 1:A:87:GLU:HG3  | 0.44     | 2.43        | 5      | 1     |
| 1:A:36:ALA:O    | 1:A:38:ILE:CD1  | 0.44     | 2.66        | 6      | 1     |
| 1:A:7:ILE:HA    | 1:A:73:ILE:N    | 0.44     | 2.28        | 8      | 1     |
| 1:A:10:GLN:NE2  | 1:A:10:GLN:CA   | 0.43     | 2.80        | 9      | 2     |
| 1:A:39:ARG:HG2  | 1:A:40:ILE:N    | 0.43     | 2.27        | 6      | 1     |
| 1:A:46:LEU:HA   | 1:A:86:LEU:C    | 0.43     | 2.38        | 12     | 1     |
| 1:A:8:ALA:HA    | 1:A:39:ARG:HB3  | 0.43     | 1.86        | 4      | 1     |
| 1:A:9:PHE:C     | 1:A:71:ILE:HG12 | 0.43     | 2.38        | 5      | 1     |
| 1:A:68:VAL:O    | 1:A:71:ILE:O    | 0.43     | 2.36        | 7      | 1     |
| 1:A:20:GLU:HA   | 1:A:23:ILE:CG1  | 0.43     | 2.43        | 8      | 1     |
| 1:A:43:GLU:O    | 1:A:44:LYS:HG2  | 0.43     | 2.13        | 12     | 1     |
| 1:A:10:GLN:HB2  | 1:A:70:VAL:HB   | 0.43     | 1.90        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:30:VAL:O    | 1:A:31:VAL:HG22 | 0.43     | 2.13        | 5      | 2     |
| 1:A:5:VAL:HG13  | 1:A:75:GLY:HA3  | 0.43     | 1.89        | 11     | 1     |
| 1:A:11:ASP:OD2  | 1:A:14:ASN:CB   | 0.43     | 2.65        | 7      | 1     |
| 1:A:48:ILE:HG22 | 1:A:53:VAL:HG23 | 0.43     | 1.90        | 8      | 1     |
| 1:A:9:PHE:N     | 1:A:71:ILE:CG2  | 0.43     | 2.80        | 9      | 1     |
| 1:A:76:ASN:O    | 1:A:86:LEU:HG   | 0.43     | 2.13        | 1      | 1     |
| 1:A:48:ILE:HG22 | 1:A:51:GLU:CB   | 0.43     | 2.43        | 3      | 1     |
| 1:A:7:ILE:O     | 1:A:7:ILE:CG1   | 0.43     | 2.67        | 5      | 1     |
| 1:A:10:GLN:O    | 1:A:70:VAL:HA   | 0.43     | 2.14        | 7      | 2     |
| 1:A:10:GLN:HG3  | 1:A:69:ASP:C    | 0.43     | 2.39        | 7      | 2     |
| 1:A:11:ASP:OD2  | 1:A:13:ASP:CB   | 0.43     | 2.66        | 3      | 1     |
| 1:A:5:VAL:CG1   | 1:A:87:GLU:CG   | 0.43     | 2.96        | 5      | 1     |
| 1:A:10:GLN:OE1  | 1:A:37:MET:HG2  | 0.43     | 2.12        | 10     | 1     |
| 1:A:3:SER:HB3   | 1:A:44:LYS:CD   | 0.43     | 2.43        | 11     | 1     |
| 1:A:30:VAL:HG13 | 1:A:31:VAL:N    | 0.43     | 2.27        | 12     | 1     |
| 1:A:34:HIS:CG   | 1:A:35:PRO:HD2  | 0.43     | 2.49        | 3      | 3     |
| 1:A:20:GLU:O    | 1:A:21:ALA:C    | 0.43     | 2.61        | 4      | 1     |
| 1:A:78:ASP:HA   | 1:A:85:VAL:C    | 0.43     | 2.39        | 4      | 1     |
| 1:A:52:THR:O    | 1:A:55:GLU:N    | 0.43     | 2.52        | 11     | 3     |
| 1:A:66:MET:HE3  | 1:A:73:ILE:HD11 | 0.43     | 1.90        | 5      | 1     |
| 1:A:33:HIS:CE1  | 1:A:38:ILE:HB   | 0.43     | 2.48        | 7      | 1     |
| 1:A:9:PHE:HB2   | 1:A:70:VAL:CA   | 0.43     | 2.44        | 8      | 1     |
| 1:A:47:GLU:HA   | 1:A:85:VAL:N    | 0.43     | 2.28        | 8      | 1     |
| 1:A:62:ASP:OD1  | 1:A:65:GLU:CB   | 0.43     | 2.67        | 1      | 1     |
| 1:A:46:LEU:N    | 1:A:87:GLU:HA   | 0.43     | 2.29        | 3      | 1     |
| 1:A:49:ARG:O    | 1:A:52:THR:OG1  | 0.43     | 2.37        | 7      | 1     |
| 1:A:45:ARG:HA   | 1:A:86:LEU:O    | 0.43     | 2.14        | 10     | 1     |
| 1:A:66:MET:HB3  | 1:A:71:ILE:CD1  | 0.43     | 2.44        | 10     | 1     |
| 1:A:11:ASP:CG   | 1:A:69:ASP:CB   | 0.43     | 2.92        | 12     | 1     |
| 1:A:5:VAL:HA    | 1:A:74:GLY:O    | 0.43     | 2.14        | 2      | 1     |
| 1:A:41:GLU:HG2  | 1:A:42:ALA:N    | 0.43     | 2.28        | 5      | 1     |
| 1:A:74:GLY:C    | 1:A:86:LEU:CD2  | 0.43     | 2.92        | 8      | 1     |
| 1:A:4:LEU:CB    | 1:A:43:GLU:HA   | 0.43     | 2.44        | 9      | 1     |
| 1:A:39:ARG:NH1  | 1:A:39:ARG:HG3  | 0.43     | 2.29        | 9      | 1     |
| 1:A:30:VAL:CG2  | 1:A:41:GLU:OE2  | 0.43     | 2.67        | 11     | 1     |
| 1:A:9:PHE:HA    | 1:A:70:VAL:HG13 | 0.43     | 1.91        | 12     | 1     |
| 1:A:5:VAL:CG2   | 1:A:42:ALA:CB   | 0.42     | 2.84        | 1      | 1     |
| 1:A:54:GLU:O    | 1:A:55:GLU:C    | 0.42     | 2.61        | 3      | 3     |
| 1:A:4:LEU:N     | 1:A:87:GLU:OE2  | 0.42     | 2.52        | 5      | 2     |
| 1:A:52:THR:C    | 1:A:54:GLU:N    | 0.42     | 2.75        | 10     | 3     |
| 1:A:10:GLN:HG2  | 1:A:69:ASP:C    | 0.42     | 2.39        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:PHE:HB2   | 1:A:71:ILE:H    | 0.42     | 1.71        | 8      | 1     |
| 1:A:9:PHE:CB    | 1:A:71:ILE:N    | 0.42     | 2.81        | 8      | 1     |
| 1:A:6:TYR:O     | 1:A:6:TYR:CD1   | 0.42     | 2.72        | 1      | 1     |
| 1:A:24:GLN:C    | 1:A:26:ASN:N    | 0.42     | 2.77        | 6      | 1     |
| 1:A:76:ASN:H    | 1:A:86:LEU:HD21 | 0.42     | 1.74        | 6      | 1     |
| 1:A:11:ASP:CA   | 1:A:70:VAL:HG23 | 0.42     | 2.44        | 10     | 2     |
| 1:A:59:ARG:HG2  | 1:A:60:ALA:N    | 0.42     | 2.27        | 8      | 1     |
| 1:A:70:VAL:O    | 1:A:71:ILE:HB   | 0.42     | 2.14        | 9      | 1     |
| 1:A:10:GLN:CG   | 1:A:37:MET:HG2  | 0.42     | 2.44        | 10     | 1     |
| 1:A:59:ARG:O    | 1:A:59:ARG:HG3  | 0.42     | 2.14        | 11     | 1     |
| 1:A:83:ARG:CG   | 1:A:83:ARG:NH1  | 0.42     | 2.78        | 12     | 1     |
| 1:A:20:GLU:CG   | 1:A:24:GLN:OE1  | 0.42     | 2.68        | 5      | 1     |
| 1:A:9:PHE:HB3   | 1:A:71:ILE:C    | 0.42     | 2.39        | 6      | 1     |
| 1:A:11:ASP:OD2  | 1:A:14:ASN:HB3  | 0.42     | 2.14        | 7      | 1     |
| 1:A:10:GLN:C    | 1:A:70:VAL:HA   | 0.42     | 2.39        | 10     | 1     |
| 1:A:50:ARG:O    | 1:A:51:GLU:C    | 0.42     | 2.62        | 11     | 1     |
| 1:A:82:ASP:O    | 1:A:83:ARG:O    | 0.42     | 2.37        | 12     | 2     |
| 1:A:48:ILE:HG23 | 1:A:50:ARG:H    | 0.42     | 1.74        | 12     | 1     |
| 1:A:49:ARG:HB2  | 1:A:83:ARG:CB   | 0.42     | 2.44        | 12     | 1     |
| 1:A:49:ARG:CB   | 1:A:83:ARG:HA   | 0.42     | 2.44        | 12     | 1     |
| 1:A:6:TYR:HA    | 1:A:41:GLU:HA   | 0.42     | 1.91        | 1      | 1     |
| 1:A:49:ARG:HA   | 1:A:83:ARG:HB2  | 0.42     | 1.90        | 2      | 1     |
| 1:A:45:ARG:NH1  | 1:A:45:ARG:HG3  | 0.42     | 2.29        | 4      | 1     |
| 1:A:39:ARG:NH1  | 1:A:39:ARG:HG2  | 0.42     | 2.28        | 5      | 1     |
| 1:A:9:PHE:HB3   | 1:A:71:ILE:O    | 0.42     | 2.14        | 8      | 2     |
| 1:A:38:ILE:CG1  | 1:A:39:ARG:N    | 0.42     | 2.81        | 7      | 1     |
| 1:A:3:SER:C     | 1:A:44:LYS:N    | 0.42     | 2.77        | 12     | 1     |
| 1:A:6:TYR:HB2   | 1:A:40:ILE:O    | 0.42     | 2.15        | 1      | 1     |
| 1:A:47:GLU:C    | 1:A:48:ILE:HG12 | 0.42     | 2.39        | 4      | 1     |
| 1:A:78:ASP:CA   | 1:A:86:LEU:HB3  | 0.42     | 2.44        | 4      | 1     |
| 1:A:26:ASN:CB   | 1:A:27:PRO:CD   | 0.42     | 2.97        | 7      | 1     |
| 1:A:76:ASN:O    | 1:A:86:LEU:CB   | 0.42     | 2.67        | 10     | 1     |
| 1:A:16:ARG:CG   | 1:A:17:TYR:N    | 0.42     | 2.81        | 2      | 1     |
| 1:A:30:VAL:HG11 | 1:A:41:GLU:HG3  | 0.42     | 1.92        | 3      | 1     |
| 1:A:56:ASN:O    | 1:A:59:ARG:HB2  | 0.42     | 2.14        | 3      | 1     |
| 1:A:9:PHE:HA    | 1:A:70:VAL:O    | 0.42     | 2.15        | 11     | 2     |
| 1:A:43:GLU:O    | 1:A:43:GLU:OE2  | 0.42     | 2.37        | 7      | 1     |
| 1:A:5:VAL:HB    | 1:A:87:GLU:CB   | 0.42     | 2.45        | 10     | 1     |
| 1:A:20:GLU:O    | 1:A:20:GLU:OE1  | 0.42     | 2.37        | 10     | 1     |
| 1:A:42:ALA:C    | 1:A:43:GLU:HG3  | 0.42     | 2.39        | 10     | 1     |
| 1:A:30:VAL:HG12 | 1:A:31:VAL:N    | 0.42     | 2.29        | 6      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:48:ILE:CD1  | 1:A:52:THR:HG21 | 0.42     | 2.45        | 4      | 1     |
| 1:A:45:ARG:O    | 1:A:46:LEU:HD22 | 0.42     | 2.15        | 5      | 1     |
| 1:A:4:LEU:C     | 1:A:5:VAL:CG2   | 0.42     | 2.92        | 9      | 1     |
| 1:A:9:PHE:C     | 1:A:70:VAL:HB   | 0.42     | 2.40        | 6      | 1     |
| 1:A:9:PHE:CD1   | 1:A:38:ILE:HB   | 0.42     | 2.50        | 6      | 1     |
| 1:A:9:PHE:HA    | 1:A:71:ILE:HB   | 0.42     | 1.91        | 9      | 1     |
| 1:A:48:ILE:HG23 | 1:A:49:ARG:H    | 0.42     | 1.67        | 12     | 1     |
| 1:A:67:LEU:CD2  | 1:A:71:ILE:HG21 | 0.42     | 2.41        | 3      | 1     |
| 1:A:86:LEU:CG   | 1:A:87:GLU:N    | 0.42     | 2.82        | 4      | 1     |
| 1:A:4:LEU:O     | 1:A:87:GLU:OE2  | 0.42     | 2.37        | 7      | 1     |
| 1:A:71:ILE:O    | 1:A:72:THR:OG1  | 0.42     | 2.35        | 9      | 1     |
| 1:A:64:GLN:O    | 1:A:67:LEU:HB3  | 0.42     | 2.14        | 10     | 1     |
| 1:A:5:VAL:CG2   | 1:A:87:GLU:O    | 0.42     | 2.68        | 11     | 1     |
| 1:A:35:PRO:O    | 1:A:36:ALA:O    | 0.42     | 2.38        | 1      | 1     |
| 1:A:47:GLU:C    | 1:A:48:ILE:HG13 | 0.42     | 2.39        | 8      | 3     |
| 1:A:7:ILE:HA    | 1:A:72:THR:O    | 0.42     | 2.15        | 2      | 1     |
| 1:A:7:ILE:CA    | 1:A:73:ILE:HG22 | 0.42     | 2.45        | 6      | 1     |
| 1:A:51:GLU:O    | 1:A:54:GLU:HB3  | 0.41     | 2.15        | 2      | 2     |
| 1:A:46:LEU:HB2  | 1:A:86:LEU:O    | 0.41     | 2.12        | 8      | 1     |
| 1:A:10:GLN:N    | 1:A:70:VAL:O    | 0.41     | 2.53        | 9      | 1     |
| 1:A:44:LYS:CD   | 1:A:45:ARG:CG   | 0.41     | 2.98        | 11     | 1     |
| 1:A:34:HIS:CB   | 1:A:35:PRO:HD2  | 0.41     | 2.44        | 2      | 1     |
| 1:A:83:ARG:NH1  | 1:A:83:ARG:HG3  | 0.41     | 2.28        | 2      | 1     |
| 1:A:48:ILE:HG22 | 1:A:51:GLU:CD   | 0.41     | 2.39        | 3      | 1     |
| 1:A:7:ILE:O     | 1:A:39:ARG:HB3  | 0.41     | 2.15        | 4      | 1     |
| 1:A:46:LEU:HG   | 1:A:86:LEU:HD11 | 0.41     | 1.92        | 5      | 1     |
| 1:A:77:VAL:HA   | 1:A:86:LEU:CB   | 0.41     | 2.45        | 5      | 1     |
| 1:A:9:PHE:C     | 1:A:71:ILE:HB   | 0.41     | 2.39        | 9      | 1     |
| 1:A:10:GLN:CD   | 1:A:36:ALA:HB1  | 0.41     | 2.40        | 12     | 1     |
| 1:A:63:VAL:CG1  | 1:A:66:MET:HB2  | 0.41     | 2.45        | 12     | 1     |
| 1:A:7:ILE:O     | 1:A:40:ILE:N    | 0.41     | 2.53        | 8      | 2     |
| 1:A:49:ARG:O    | 1:A:83:ARG:HB2  | 0.41     | 2.16        | 2      | 1     |
| 1:A:71:ILE:N    | 1:A:71:ILE:CD1  | 0.41     | 2.66        | 3      | 1     |
| 1:A:33:HIS:NE2  | 1:A:38:ILE:HB   | 0.41     | 2.29        | 7      | 1     |
| 1:A:67:LEU:O    | 1:A:67:LEU:HG   | 0.41     | 2.15        | 3      | 2     |
| 1:A:61:TRP:O    | 1:A:61:TRP:CG   | 0.41     | 2.72        | 4      | 1     |
| 1:A:85:VAL:O    | 1:A:85:VAL:CG1  | 0.41     | 2.66        | 4      | 1     |
| 1:A:10:GLN:N    | 1:A:71:ILE:HG12 | 0.41     | 2.30        | 5      | 1     |
| 1:A:18:VAL:O    | 1:A:19:VAL:C    | 0.41     | 2.62        | 6      | 1     |
| 1:A:5:VAL:O     | 1:A:41:GLU:HG2  | 0.41     | 2.14        | 9      | 2     |
| 1:A:72:THR:C    | 1:A:73:ILE:HG12 | 0.41     | 2.40        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:11:ASP:OD1  | 1:A:69:ASP:HB3  | 0.41     | 2.15        | 12     | 1     |
| 1:A:76:ASN:O    | 1:A:77:VAL:HB   | 0.41     | 2.15        | 9      | 3     |
| 1:A:14:ASN:OD1  | 1:A:17:TYR:HB3  | 0.41     | 2.15        | 5      | 1     |
| 1:A:72:THR:HG22 | 1:A:73:ILE:N    | 0.41     | 2.29        | 5      | 1     |
| 1:A:9:PHE:HB2   | 1:A:71:ILE:HA   | 0.41     | 1.92        | 6      | 1     |
| 1:A:38:ILE:CD1  | 1:A:39:ARG:N    | 0.41     | 2.84        | 7      | 1     |
| 1:A:3:SER:CB    | 1:A:44:LYS:HB2  | 0.41     | 2.44        | 11     | 1     |
| 1:A:69:ASP:C    | 1:A:70:VAL:O    | 0.41     | 2.63        | 8      | 1     |
| 1:A:7:ILE:O     | 1:A:7:ILE:HG12  | 0.41     | 2.15        | 9      | 1     |
| 1:A:9:PHE:O     | 1:A:38:ILE:HG13 | 0.41     | 2.16        | 9      | 1     |
| 1:A:39:ARG:CD   | 1:A:40:ILE:N    | 0.41     | 2.84        | 9      | 1     |
| 1:A:5:VAL:CG1   | 1:A:75:GLY:HA3  | 0.41     | 2.45        | 11     | 1     |
| 1:A:3:SER:HB3   | 1:A:44:LYS:HA   | 0.41     | 1.92        | 12     | 1     |
| 1:A:57:LEU:C    | 1:A:59:ARG:H    | 0.41     | 2.23        | 12     | 1     |
| 1:A:7:ILE:O     | 1:A:40:ILE:HB   | 0.41     | 2.15        | 5      | 1     |
| 1:A:78:ASP:HB2  | 1:A:87:GLU:CD   | 0.41     | 2.41        | 8      | 1     |
| 1:A:10:GLN:OE1  | 1:A:37:MET:CG   | 0.41     | 2.69        | 10     | 1     |
| 1:A:77:VAL:N    | 1:A:86:LEU:HD23 | 0.41     | 2.30        | 12     | 1     |
| 1:A:16:ARG:O    | 1:A:17:TYR:C    | 0.41     | 2.62        | 1      | 1     |
| 1:A:5:VAL:CG1   | 1:A:87:GLU:HG2  | 0.41     | 2.46        | 5      | 1     |
| 1:A:32:GLN:HA   | 1:A:39:ARG:O    | 0.41     | 2.15        | 6      | 1     |
| 1:A:47:GLU:O    | 1:A:48:ILE:HG13 | 0.41     | 2.15        | 7      | 1     |
| 1:A:86:LEU:CD1  | 1:A:87:GLU:N    | 0.41     | 2.83        | 8      | 1     |
| 1:A:10:GLN:CA   | 1:A:70:VAL:HA   | 0.41     | 2.46        | 10     | 1     |
| 1:A:70:VAL:HG12 | 1:A:71:ILE:HG12 | 0.41     | 1.91        | 10     | 1     |
| 1:A:8:ALA:CB    | 1:A:39:ARG:CB   | 0.41     | 2.98        | 11     | 1     |
| 1:A:47:GLU:HB3  | 1:A:85:VAL:HA   | 0.41     | 1.92        | 12     | 1     |
| 1:A:11:ASP:HA   | 1:A:69:ASP:HB3  | 0.41     | 1.93        | 2      | 1     |
| 1:A:6:TYR:O     | 1:A:74:GLY:HA2  | 0.41     | 2.14        | 6      | 1     |
| 1:A:48:ILE:HD12 | 1:A:85:VAL:CB   | 0.40     | 2.46        | 8      | 1     |
| 1:A:49:ARG:O    | 1:A:53:VAL:HG23 | 0.40     | 2.15        | 8      | 1     |
| 1:A:66:MET:HB2  | 1:A:66:MET:HE2  | 0.40     | 1.81        | 2      | 1     |
| 1:A:17:TYR:CE2  | 1:A:38:ILE:CG2  | 0.40     | 3.05        | 4      | 1     |
| 1:A:5:VAL:O     | 1:A:41:GLU:CG   | 0.40     | 2.69        | 9      | 1     |
| 1:A:42:ALA:C    | 1:A:43:GLU:CG   | 0.40     | 2.94        | 10     | 1     |
| 1:A:52:THR:OG1  | 1:A:83:ARG:O    | 0.40     | 2.39        | 2      | 1     |
| 1:A:48:ILE:CD1  | 1:A:84:PHE:HB3  | 0.40     | 2.46        | 5      | 1     |
| 1:A:9:PHE:CE1   | 1:A:38:ILE:HG21 | 0.40     | 2.50        | 6      | 1     |
| 1:A:6:TYR:CD2   | 1:A:73:ILE:HG21 | 0.40     | 2.50        | 8      | 1     |
| 1:A:11:ASP:CG   | 1:A:16:ARG:CG   | 0.40     | 2.94        | 8      | 1     |
| 1:A:12:ASN:O    | 1:A:13:ASP:CB   | 0.40     | 2.69        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:8:ALA:HB1   | 1:A:71:ILE:CG2  | 0.40     | 2.45        | 9      | 1     |
| 1:A:70:VAL:O    | 1:A:71:ILE:CD1  | 0.40     | 2.69        | 5      | 1     |
| 1:A:16:ARG:HG2  | 1:A:17:TYR:N    | 0.40     | 2.32        | 6      | 1     |
| 1:A:59:ARG:C    | 1:A:61:TRP:N    | 0.40     | 2.77        | 7      | 1     |
| 1:A:6:TYR:CE2   | 1:A:73:ILE:CG2  | 0.40     | 3.04        | 8      | 1     |
| 1:A:11:ASP:HB2  | 1:A:15:ALA:HB3  | 0.40     | 1.92        | 8      | 1     |
| 1:A:67:LEU:HD23 | 1:A:68:VAL:N    | 0.40     | 2.32        | 12     | 1     |
| 1:A:76:ASN:N    | 1:A:86:LEU:HD21 | 0.40     | 2.31        | 12     | 1     |
| 1:A:7:ILE:O     | 1:A:7:ILE:HG13  | 0.40     | 2.16        | 1      | 1     |
| 1:A:17:TYR:O    | 1:A:20:GLU:HB3  | 0.40     | 2.16        | 1      | 1     |
| 1:A:62:ASP:OD1  | 1:A:65:GLU:HB3  | 0.40     | 2.17        | 1      | 1     |
| 1:A:77:VAL:O    | 1:A:79:GLU:N    | 0.40     | 2.54        | 7      | 1     |
| 1:A:9:PHE:CD2   | 1:A:38:ILE:CD1  | 0.40     | 3.05        | 12     | 1     |
| 1:A:44:LYS:CG   | 1:A:45:ARG:N    | 0.40     | 2.84        | 12     | 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     | 85/90 (94%)     | 56±6 (65±7%) | 21±4 (25±5%) | 8±3 (10±3%) | <b>1</b>    | <b>10</b> |
| All | All   | 1020/1080 (94%) | 668 (65%)    | 253 (25%)    | 99 (10%)    | <b>1</b>    | <b>10</b> |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 34  | HIS  | 9              |
| 1   | A     | 74  | GLY  | 8              |
| 1   | A     | 77  | VAL  | 8              |
| 1   | A     | 35  | PRO  | 6              |
| 1   | A     | 44  | LYS  | 5              |
| 1   | A     | 70  | VAL  | 4              |
| 1   | A     | 12  | ASN  | 3              |
| 1   | A     | 36  | ALA  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 60  | ALA  | 3              |
| 1   | A     | 61  | TRP  | 3              |
| 1   | A     | 67  | LEU  | 3              |
| 1   | A     | 68  | VAL  | 3              |
| 1   | A     | 71  | ILE  | 3              |
| 1   | A     | 30  | VAL  | 3              |
| 1   | A     | 83  | ARG  | 3              |
| 1   | A     | 33  | HIS  | 2              |
| 1   | A     | 59  | ARG  | 2              |
| 1   | A     | 73  | ILE  | 2              |
| 1   | A     | 10  | GLN  | 2              |
| 1   | A     | 48  | ILE  | 2              |
| 1   | A     | 5   | VAL  | 1              |
| 1   | A     | 6   | TYR  | 1              |
| 1   | A     | 57  | LEU  | 1              |
| 1   | A     | 58  | GLY  | 1              |
| 1   | A     | 64  | GLN  | 1              |
| 1   | A     | 39  | ARG  | 1              |
| 1   | A     | 40  | ILE  | 1              |
| 1   | A     | 41  | GLU  | 1              |
| 1   | A     | 31  | VAL  | 1              |
| 1   | A     | 72  | THR  | 1              |
| 1   | A     | 75  | GLY  | 1              |
| 1   | A     | 69  | ASP  | 1              |
| 1   | A     | 78  | ASP  | 1              |
| 1   | A     | 13  | ASP  | 1              |
| 1   | A     | 28  | HIS  | 1              |
| 1   | A     | 76  | ASN  | 1              |
| 1   | A     | 84  | PHE  | 1              |
| 1   | A     | 85  | VAL  | 1              |
| 1   | A     | 32  | GLN  | 1              |
| 1   | A     | 86  | LEU  | 1              |
| 1   | A     | 46  | LEU  | 1              |
| 1   | A     | 47  | GLU  | 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     | 75/80 (94%)   | 46±4 (62±5%) | 29±4 (38±5%) | <b>0</b> <b>7</b> |
| All | All   | 900/960 (94%) | 557 (62%)    | 343 (38%)    | <b>0</b> <b>7</b> |

All 66 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     | 10  | GLN  | 12             |
| 1   | A     | 4   | LEU  | 11             |
| 1   | A     | 56  | ASN  | 11             |
| 1   | A     | 66  | MET  | 11             |
| 1   | A     | 78  | ASP  | 11             |
| 1   | A     | 31  | VAL  | 10             |
| 1   | A     | 34  | HIS  | 10             |
| 1   | A     | 72  | THR  | 10             |
| 1   | A     | 38  | ILE  | 9              |
| 1   | A     | 48  | ILE  | 9              |
| 1   | A     | 71  | ILE  | 9              |
| 1   | A     | 73  | ILE  | 9              |
| 1   | A     | 86  | LEU  | 9              |
| 1   | A     | 39  | ARG  | 8              |
| 1   | A     | 46  | LEU  | 8              |
| 1   | A     | 54  | GLU  | 8              |
| 1   | A     | 44  | LYS  | 8              |
| 1   | A     | 41  | GLU  | 7              |
| 1   | A     | 52  | THR  | 7              |
| 1   | A     | 47  | GLU  | 7              |
| 1   | A     | 49  | ARG  | 7              |
| 1   | A     | 50  | ARG  | 7              |
| 1   | A     | 5   | VAL  | 6              |
| 1   | A     | 24  | GLN  | 6              |
| 1   | A     | 3   | SER  | 6              |
| 1   | A     | 83  | ARG  | 6              |
| 1   | A     | 16  | ARG  | 6              |
| 1   | A     | 32  | GLN  | 6              |
| 1   | A     | 79  | GLU  | 6              |
| 1   | A     | 59  | ARG  | 5              |
| 1   | A     | 37  | MET  | 5              |
| 1   | A     | 6   | TYR  | 4              |
| 1   | A     | 25  | ASP  | 4              |
| 1   | A     | 33  | HIS  | 4              |
| 1   | A     | 45  | ARG  | 4              |
| 1   | A     | 80  | ASP  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 20  | GLU  | 4              |
| 1   | A     | 63  | VAL  | 4              |
| 1   | A     | 87  | GLU  | 4              |
| 1   | A     | 70  | VAL  | 4              |
| 1   | A     | 43  | GLU  | 4              |
| 1   | A     | 69  | ASP  | 4              |
| 1   | A     | 13  | ASP  | 3              |
| 1   | A     | 55  | GLU  | 3              |
| 1   | A     | 65  | GLU  | 3              |
| 1   | A     | 84  | PHE  | 3              |
| 1   | A     | 7   | ILE  | 3              |
| 1   | A     | 12  | ASN  | 3              |
| 1   | A     | 26  | ASN  | 3              |
| 1   | A     | 9   | PHE  | 3              |
| 1   | A     | 23  | ILE  | 2              |
| 1   | A     | 30  | VAL  | 2              |
| 1   | A     | 76  | ASN  | 2              |
| 1   | A     | 77  | VAL  | 2              |
| 1   | A     | 14  | ASN  | 2              |
| 1   | A     | 17  | TYR  | 2              |
| 1   | A     | 85  | VAL  | 2              |
| 1   | A     | 81  | ASP  | 2              |
| 1   | A     | 82  | ASP  | 2              |
| 1   | A     | 67  | LEU  | 1              |
| 1   | A     | 51  | GLU  | 1              |
| 1   | A     | 57  | LEU  | 1              |
| 1   | A     | 68  | VAL  | 1              |
| 1   | A     | 28  | HIS  | 1              |
| 1   | A     | 62  | ASP  | 1              |
| 1   | A     | 11  | 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 [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided