



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 06:49 PM UTC

PDB ID : 1TDP / pdb\_00001tdp  
Title : NMR solution structure of the carnobacteriocin B2 immunity protein  
Authors : Sprules, T.; Kawulka, K.E.; Vederas, J.C.  
Deposited on : 2004-05-23

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

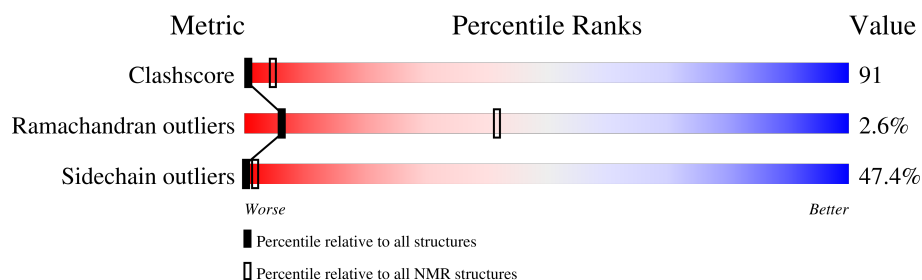
# 1 Overall quality at a glance

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     | 111    | <div> <div>14%</div> <div>41%</div> <div>29%</div> <div>17%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                           |                   |              |
|--------------------------------------|---------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)     | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:1-A:58, A:70-A:103 (92) | 0.75              | 10           |

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 3 clusters and 2 single-model clusters were found.

| Cluster number        | Models                        |
|-----------------------|-------------------------------|
| 1                     | 1, 2, 5, 7, 9, 10, 11, 13, 15 |
| 2                     | 3, 8                          |
| 3                     | 4, 6                          |
| Single-model clusters | 12; 14                        |

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

There is only 1 type of molecule in this entry. The entry contains 1811 atoms, of which 921 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called carnobacteriocin B2 immunity protein.

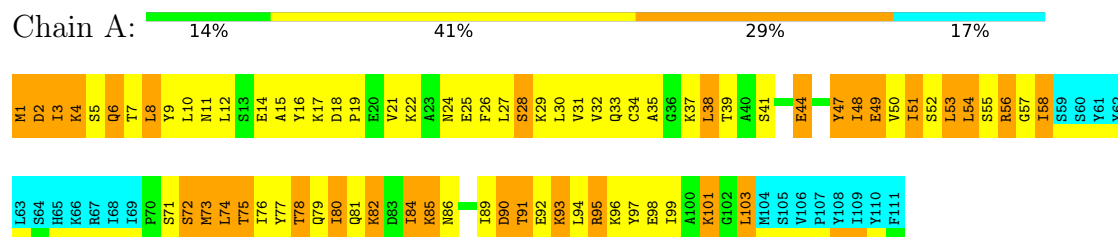
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 111      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1811  | 571 | 921 | 143 | 172 | 4 |       |

## 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: carnobacteriocin B2 immunity protein

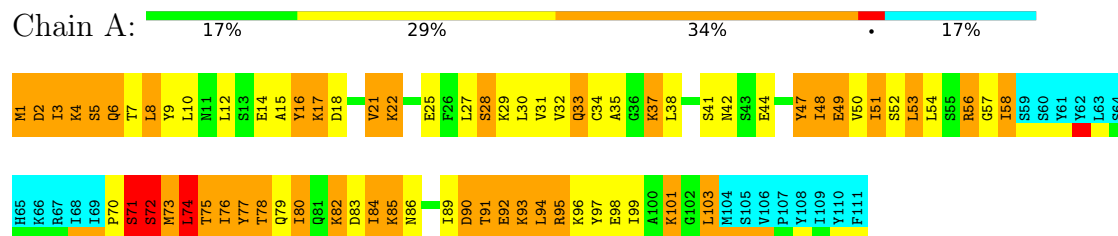


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

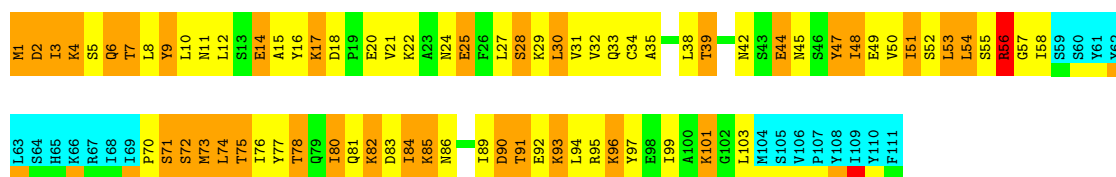
- Molecule 1: carnobacteriocin B2 immunity protein



#### 4.2.2 Score per residue for model 2

- Molecule 1: carnobacteriocin B2 immunity protein





### 4.2.3 Score per residue for model 3

- Molecule 1: carnobacteriocin B2 immunity protein

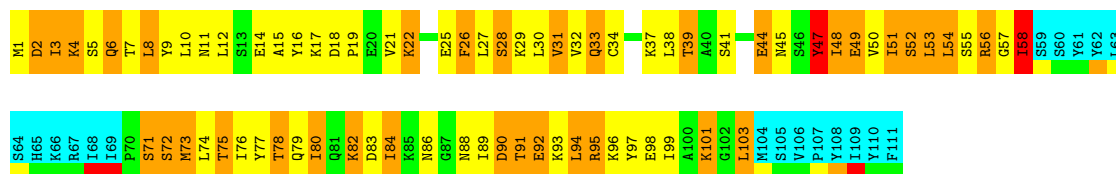
Chain A: 15% 38% 30% 17%



### 4.2.4 Score per residue for model 4

- Molecule 1: carnobacteriocin B2 immunity protein

Chain A: 14% 36% 31% 17%



### 4.2.5 Score per residue for model 5

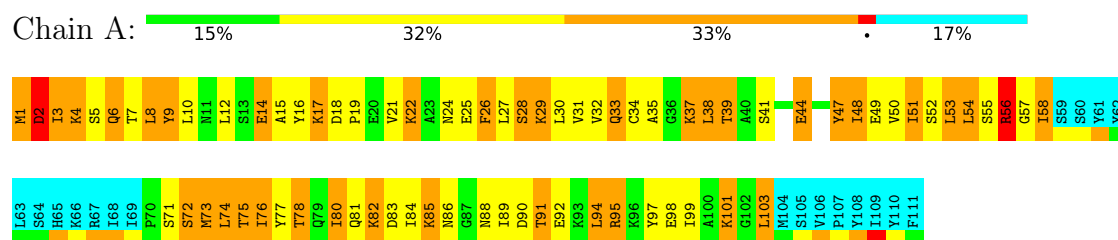
- Molecule 1: carnobacteriocin B2 immunity protein

Chain A: 13% 36% 33% 17%



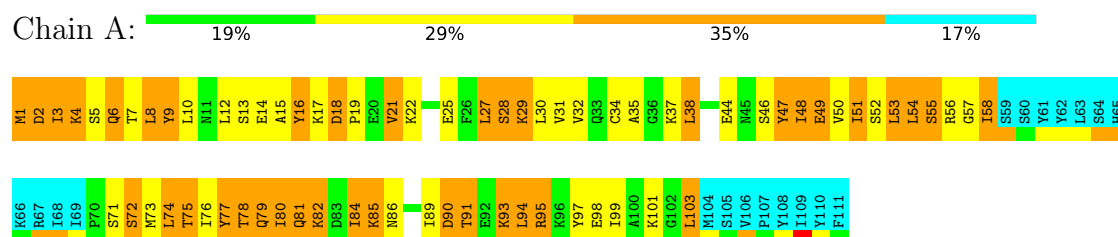
### 4.2.6 Score per residue for model 6

- Molecule 1: carnobacteriocin B2 immunity protein



#### 4.2.7 Score per residue for model 7

- Molecule 1: carnobacteriocin B2 immunity protein



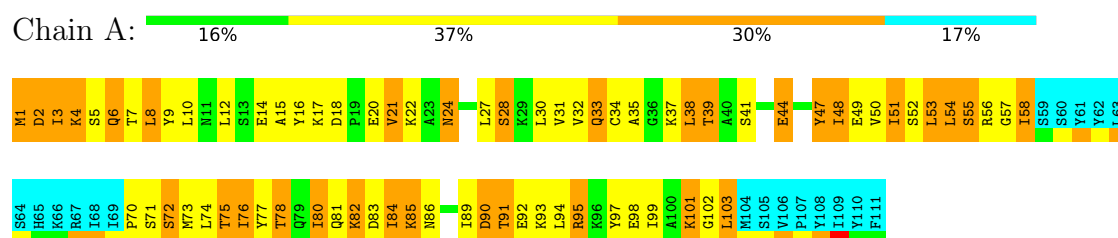
#### 4.2.8 Score per residue for model 8

- Molecule 1: carnobacteriocin B2 immunity protein



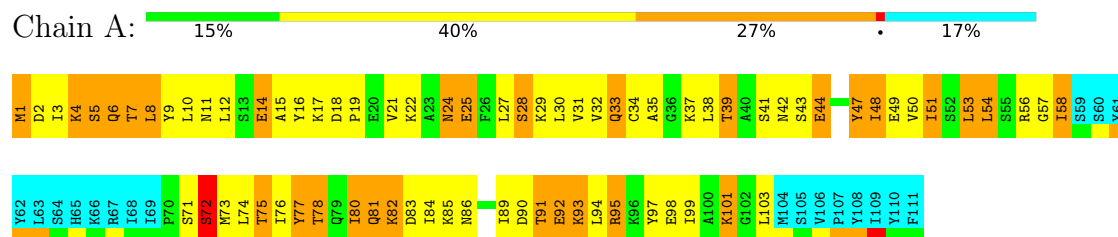
#### 4.2.9 Score per residue for model 9

- Molecule 1: carnobacteriocin B2 immunity protein



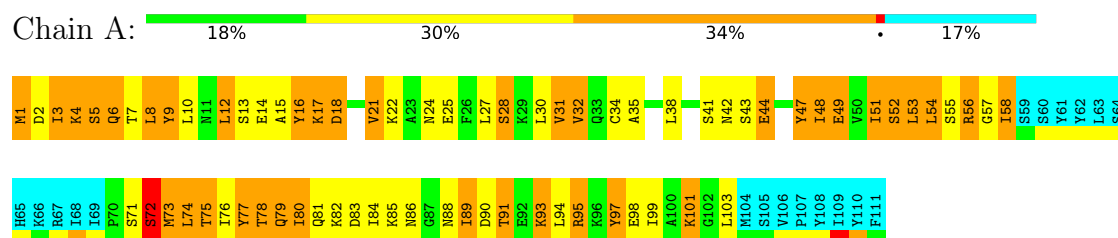
#### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: carnobacteriocin B2 immunity protein



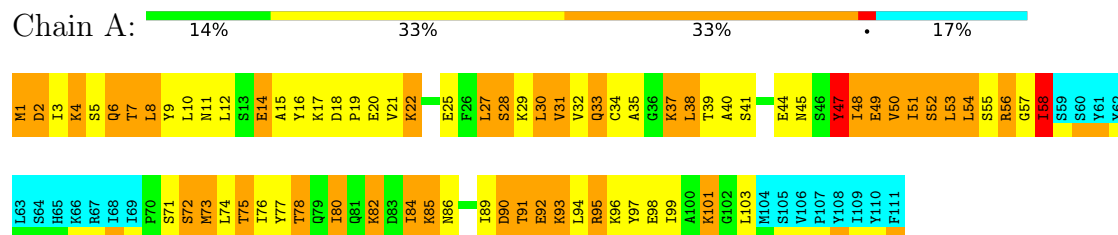
#### 4.2.11 Score per residue for model 11

- Molecule 1: carnobacteriocin B2 immunity protein



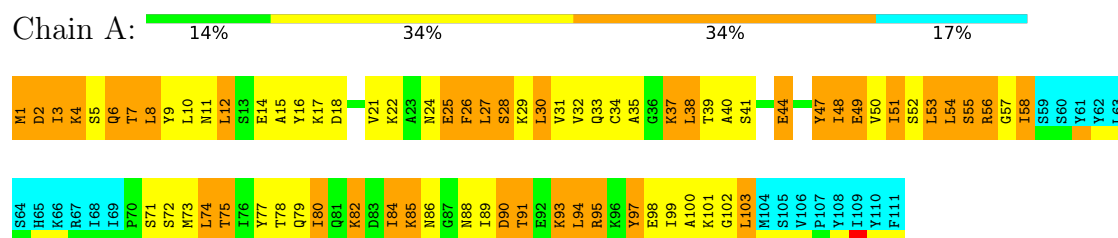
#### 4.2.12 Score per residue for model 12

- Molecule 1: carnobacteriocin B2 immunity protein



#### 4.2.13 Score per residue for model 13

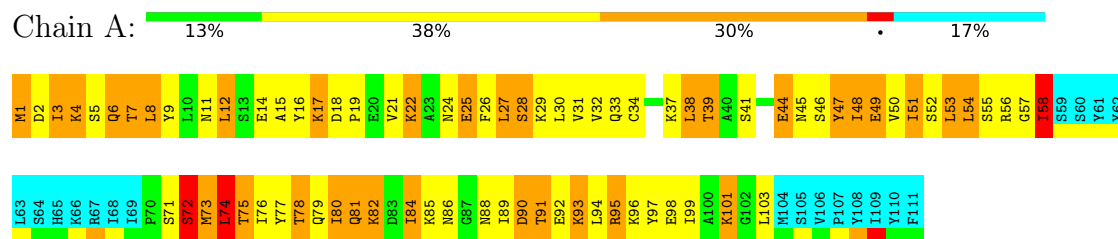
- Molecule 1: carnobacteriocin B2 immunity protein





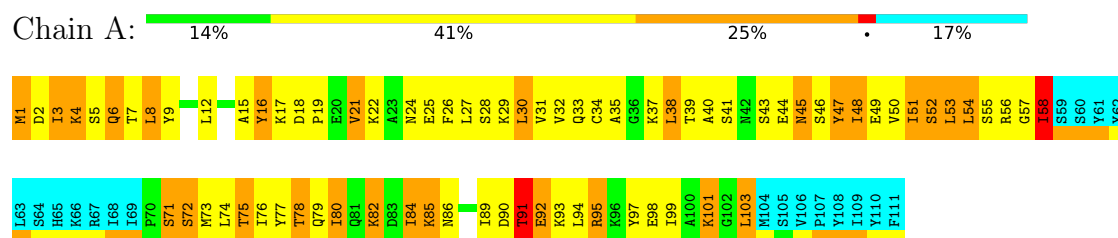
#### 4.2.14 Score per residue for model 14

- Molecule 1: carnobacteriocin B2 immunity protein



#### 4.2.15 Score per residue for model 15

- Molecule 1: carnobacteriocin B2 immunity protein



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CNS           | structure solution | 1.1     |
| CNS           | refinement         | 1.1     |

No chemical shift data was provided.

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 0.61±0.02    | 0±0/730 ( 0.0± 0.0%) | 0.90±0.02   | 1±1/982 ( 0.1± 0.1%) |
| All | All   | 0.61         | 0/10950 ( 0.0%)      | 0.90        | 11/14730 ( 0.1%)     |

There are no bond-length outliers.

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     | 21  | VAL  | N-CA-C  | -7.86 | 105.52      | 112.12   | 6      | 7     |
| 1   | A     | 47  | TYR  | N-CA-C  | -5.26 | 106.37      | 112.89   | 12     | 2     |
| 1   | A     | 89  | ILE  | N-CA-CB | -5.23 | 106.38      | 112.34   | 11     | 1     |
| 1   | A     | 88  | ASN  | N-CA-C  | -5.09 | 106.92      | 113.23   | 8      | 1     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 722   | 753      | 753      | 134±12  |
| All | All   | 10830 | 11295    | 11295    | 2012    |

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 91.

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

| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:51:ILE:HG22 | 1:A:94:LEU:HD21  | 1.07     | 1.25        | 6      | 8     |
| 1:A:95:ARG:O    | 1:A:99:ILE:HG13  | 1.06     | 1.47        | 9      | 8     |
| 1:A:12:LEU:HD22 | 1:A:31:VAL:HG13  | 1.01     | 1.33        | 2      | 5     |
| 1:A:53:LEU:O    | 1:A:57:GLY:HA3   | 1.00     | 1.56        | 7      | 8     |
| 1:A:28:SER:O    | 1:A:32:VAL:HG23  | 0.99     | 1.56        | 11     | 15    |
| 1:A:89:ILE:HG21 | 1:A:94:LEU:HD11  | 0.97     | 1.35        | 9      | 7     |
| 1:A:89:ILE:CG2  | 1:A:94:LEU:HD11  | 0.95     | 1.90        | 9      | 7     |
| 1:A:51:ILE:HD12 | 1:A:80:ILE:HG22  | 0.94     | 1.38        | 12     | 1     |
| 1:A:48:ILE:HG23 | 1:A:94:LEU:HD23  | 0.94     | 1.38        | 9      | 5     |
| 1:A:51:ILE:HG21 | 1:A:94:LEU:HD23  | 0.92     | 1.41        | 12     | 1     |
| 1:A:49:GLU:HA   | 1:A:97:TYR:CE2   | 0.90     | 2.01        | 6      | 15    |
| 1:A:84:ILE:HG23 | 1:A:91:THR:CG2   | 0.90     | 1.95        | 8      | 6     |
| 1:A:12:LEU:HD23 | 1:A:31:VAL:HG12  | 0.90     | 1.40        | 4      | 2     |
| 1:A:9:TYR:CE1   | 1:A:35:ALA:HB1   | 0.90     | 2.01        | 7      | 10    |
| 1:A:51:ILE:CG2  | 1:A:94:LEU:HD21  | 0.89     | 1.97        | 13     | 8     |
| 1:A:12:LEU:HD23 | 1:A:31:VAL:HG13  | 0.88     | 1.45        | 14     | 6     |
| 1:A:73:MET:HE3  | 1:A:73:MET:HA    | 0.87     | 1.47        | 9      | 7     |
| 1:A:1:MET:HE3   | 1:A:9:TYR:CE2    | 0.86     | 2.04        | 2      | 6     |
| 1:A:90:ASP:CB   | 1:A:93:LYS:HE2   | 0.86     | 2.00        | 1      | 2     |
| 1:A:47:TYR:OH   | 1:A:89:ILE:HD13  | 0.85     | 1.70        | 5      | 3     |
| 1:A:58:ILE:HD11 | 1:A:74:LEU:N     | 0.85     | 1.86        | 14     | 1     |
| 1:A:47:TYR:O    | 1:A:51:ILE:HB    | 0.85     | 1.71        | 7      | 15    |
| 1:A:51:ILE:HG21 | 1:A:94:LEU:CD2   | 0.84     | 2.02        | 12     | 3     |
| 1:A:53:LEU:O    | 1:A:57:GLY:CA    | 0.83     | 2.26        | 15     | 10    |
| 1:A:1:MET:HE3   | 1:A:9:TYR:CD2    | 0.83     | 2.08        | 6      | 8     |
| 1:A:15:ALA:O    | 1:A:18:ASP:N     | 0.83     | 2.12        | 3      | 12    |
| 1:A:51:ILE:HD12 | 1:A:80:ILE:CG2   | 0.83     | 2.03        | 12     | 2     |
| 1:A:84:ILE:HG23 | 1:A:91:THR:HG21  | 0.82     | 1.51        | 1      | 7     |
| 1:A:47:TYR:CZ   | 1:A:89:ILE:HD13  | 0.82     | 2.08        | 15     | 2     |
| 1:A:9:TYR:HA    | 1:A:12:LEU:HD23  | 0.82     | 1.51        | 11     | 1     |
| 1:A:52:SER:OG   | 1:A:103:LEU:HD11 | 0.82     | 1.73        | 5      | 2     |
| 1:A:53:LEU:O    | 1:A:57:GLY:N     | 0.82     | 2.11        | 13     | 14    |
| 1:A:12:LEU:HD11 | 1:A:35:ALA:HB2   | 0.82     | 1.50        | 11     | 1     |
| 1:A:12:LEU:CD2  | 1:A:31:VAL:HG13  | 0.82     | 2.04        | 2      | 7     |
| 1:A:27:LEU:O    | 1:A:31:VAL:HG23  | 0.81     | 1.75        | 8      | 10    |
| 1:A:48:ILE:HG23 | 1:A:94:LEU:HG    | 0.81     | 1.52        | 1      | 6     |
| 1:A:1:MET:SD    | 1:A:39:THR:HA    | 0.81     | 2.15        | 10     | 3     |
| 1:A:34:CYS:O    | 1:A:38:LEU:HD12  | 0.81     | 1.75        | 2      | 7     |
| 1:A:1:MET:HE3   | 1:A:9:TYR:CG     | 0.80     | 2.11        | 15     | 4     |
| 1:A:8:LEU:HD11  | 1:A:38:LEU:HD11  | 0.80     | 1.54        | 12     | 3     |
| 1:A:74:LEU:O    | 1:A:78:THR:HB    | 0.79     | 1.77        | 4      | 11    |
| 1:A:54:LEU:C    | 1:A:54:LEU:HD12  | 0.79     | 2.02        | 8      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:50:VAL:HA   | 1:A:53:LEU:HD12  | 0.79     | 1.55        | 7      | 1     |
| 1:A:90:ASP:HB3  | 1:A:93:LYS:CE    | 0.78     | 2.08        | 8      | 1     |
| 1:A:54:LEU:HD12 | 1:A:54:LEU:O     | 0.78     | 1.78        | 8      | 2     |
| 1:A:15:ALA:O    | 1:A:18:ASP:CG    | 0.78     | 2.25        | 3      | 1     |
| 1:A:49:GLU:O    | 1:A:53:LEU:HG    | 0.78     | 1.79        | 9      | 14    |
| 1:A:48:ILE:HD12 | 1:A:94:LEU:HD21  | 0.78     | 1.54        | 8      | 3     |
| 1:A:1:MET:HE3   | 1:A:9:TYR:CB     | 0.78     | 2.09        | 15     | 3     |
| 1:A:51:ILE:HG21 | 1:A:94:LEU:HD11  | 0.77     | 1.56        | 14     | 5     |
| 1:A:58:ILE:HD11 | 1:A:73:MET:C     | 0.77     | 2.05        | 14     | 4     |
| 1:A:34:CYS:O    | 1:A:38:LEU:HD23  | 0.77     | 1.78        | 11     | 5     |
| 1:A:12:LEU:HD22 | 1:A:31:VAL:HG12  | 0.77     | 1.56        | 6      | 1     |
| 1:A:90:ASP:O    | 1:A:94:LEU:HD12  | 0.76     | 1.80        | 15     | 2     |
| 1:A:1:MET:HE2   | 1:A:9:TYR:CG     | 0.76     | 2.15        | 13     | 4     |
| 1:A:1:MET:HE1   | 1:A:38:LEU:HB3   | 0.76     | 1.56        | 15     | 3     |
| 1:A:48:ILE:HG23 | 1:A:94:LEU:CD2   | 0.76     | 2.10        | 2      | 4     |
| 1:A:78:THR:O    | 1:A:82:LYS:HG2   | 0.75     | 1.80        | 15     | 3     |
| 1:A:1:MET:HE3   | 1:A:9:TYR:HB2    | 0.75     | 1.58        | 12     | 3     |
| 1:A:95:ARG:O    | 1:A:99:ILE:HG12  | 0.75     | 1.82        | 14     | 7     |
| 1:A:54:LEU:HD11 | 1:A:80:ILE:CD1   | 0.75     | 2.11        | 14     | 1     |
| 1:A:52:SER:OG   | 1:A:94:LEU:HD23  | 0.74     | 1.83        | 6      | 1     |
| 1:A:28:SER:HA   | 1:A:31:VAL:CG2   | 0.74     | 2.13        | 6      | 2     |
| 1:A:28:SER:HA   | 1:A:31:VAL:HG22  | 0.74     | 1.58        | 6      | 1     |
| 1:A:48:ILE:HD11 | 1:A:89:ILE:HG23  | 0.74     | 1.60        | 10     | 4     |
| 1:A:1:MET:HE2   | 1:A:9:TYR:CD2    | 0.73     | 2.18        | 9      | 4     |
| 1:A:12:LEU:HD11 | 1:A:31:VAL:O     | 0.73     | 1.83        | 11     | 1     |
| 1:A:1:MET:SD    | 1:A:9:TYR:HB2    | 0.73     | 2.23        | 14     | 1     |
| 1:A:51:ILE:CG2  | 1:A:94:LEU:HD11  | 0.73     | 2.14        | 6      | 3     |
| 1:A:95:ARG:O    | 1:A:99:ILE:CG1   | 0.73     | 2.35        | 8      | 13    |
| 1:A:5:SER:HA    | 1:A:8:LEU:HD21   | 0.72     | 1.59        | 4      | 1     |
| 1:A:47:TYR:CD1  | 1:A:48:ILE:HD13  | 0.72     | 2.19        | 7      | 5     |
| 1:A:58:ILE:HD13 | 1:A:73:MET:O     | 0.72     | 1.83        | 11     | 1     |
| 1:A:4:LYS:O     | 1:A:8:LEU:HD21   | 0.72     | 1.84        | 14     | 5     |
| 1:A:12:LEU:HD23 | 1:A:31:VAL:CG1   | 0.72     | 2.14        | 4      | 1     |
| 1:A:75:THR:O    | 1:A:78:THR:HG22  | 0.72     | 1.84        | 6      | 11    |
| 1:A:52:SER:HB3  | 1:A:103:LEU:HD12 | 0.72     | 1.60        | 9      | 1     |
| 1:A:84:ILE:HG22 | 1:A:85:LYS:HD2   | 0.71     | 1.62        | 8      | 1     |
| 1:A:21:VAL:HG13 | 1:A:27:LEU:HB3   | 0.71     | 1.60        | 3      | 1     |
| 1:A:48:ILE:O    | 1:A:51:ILE:HG22  | 0.71     | 1.85        | 11     | 6     |
| 1:A:31:VAL:O    | 1:A:35:ALA:HB2   | 0.71     | 1.86        | 6      | 3     |
| 1:A:16:TYR:O    | 1:A:22:LYS:CD    | 0.71     | 2.39        | 6      | 2     |
| 1:A:12:LEU:HB3  | 1:A:35:ALA:HB2   | 0.71     | 1.63        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:5:SER:HA    | 1:A:8:LEU:HD23  | 0.70     | 1.61        | 12     | 6     |
| 1:A:51:ILE:CG2  | 1:A:94:LEU:HD23 | 0.70     | 2.15        | 12     | 1     |
| 1:A:24:ASN:CG   | 1:A:27:LEU:HD12 | 0.70     | 2.10        | 13     | 2     |
| 1:A:54:LEU:HD11 | 1:A:80:ILE:HD13 | 0.70     | 1.64        | 14     | 1     |
| 1:A:1:MET:SD    | 1:A:9:TYR:CD2   | 0.70     | 2.84        | 10     | 4     |
| 1:A:84:ILE:HG13 | 1:A:91:THR:HG23 | 0.70     | 1.61        | 2      | 6     |
| 1:A:1:MET:CE    | 1:A:9:TYR:CG    | 0.70     | 2.75        | 10     | 7     |
| 1:A:76:ILE:HG22 | 1:A:80:ILE:CD1  | 0.70     | 2.16        | 4      | 4     |
| 1:A:96:LYS:HE2  | 1:A:99:ILE:HD12 | 0.70     | 1.64        | 3      | 1     |
| 1:A:54:LEU:O    | 1:A:58:ILE:HG23 | 0.69     | 1.87        | 15     | 4     |
| 1:A:51:ILE:HG22 | 1:A:94:LEU:CD2  | 0.69     | 2.13        | 6      | 4     |
| 1:A:18:ASP:OD1  | 1:A:21:VAL:HB   | 0.69     | 1.88        | 3      | 1     |
| 1:A:91:THR:O    | 1:A:95:ARG:HB2  | 0.69     | 1.87        | 3      | 3     |
| 1:A:1:MET:HE3   | 1:A:39:THR:N    | 0.69     | 2.03        | 10     | 3     |
| 1:A:96:LYS:CE   | 1:A:99:ILE:HD12 | 0.68     | 2.18        | 3      | 1     |
| 1:A:51:ILE:CG2  | 1:A:94:LEU:CD2  | 0.68     | 2.71        | 15     | 3     |
| 1:A:95:ARG:HD3  | 1:A:99:ILE:HD11 | 0.68     | 1.64        | 11     | 1     |
| 1:A:84:ILE:HG22 | 1:A:85:LYS:N    | 0.68     | 2.04        | 13     | 10    |
| 1:A:38:LEU:O    | 1:A:41:SER:N    | 0.67     | 2.28        | 4      | 10    |
| 1:A:8:LEU:HD11  | 1:A:38:LEU:HD21 | 0.67     | 1.63        | 15     | 2     |
| 1:A:1:MET:HB3   | 1:A:38:LEU:O    | 0.67     | 1.88        | 11     | 5     |
| 1:A:9:TYR:HE1   | 1:A:35:ALA:HB1  | 0.67     | 1.47        | 7      | 13    |
| 1:A:51:ILE:HG21 | 1:A:94:LEU:HD22 | 0.67     | 1.65        | 15     | 2     |
| 1:A:53:LEU:HD21 | 1:A:97:TYR:OH   | 0.67     | 1.89        | 6      | 5     |
| 1:A:47:TYR:O    | 1:A:51:ILE:CB   | 0.67     | 2.43        | 9      | 15    |
| 1:A:58:ILE:HD13 | 1:A:77:TYR:HB2  | 0.67     | 1.66        | 14     | 4     |
| 1:A:80:ILE:O    | 1:A:84:ILE:HB   | 0.67     | 1.90        | 3      | 1     |
| 1:A:51:ILE:HG13 | 1:A:89:ILE:HD12 | 0.67     | 1.66        | 15     | 2     |
| 1:A:90:ASP:HB3  | 1:A:93:LYS:CD   | 0.67     | 2.20        | 8      | 1     |
| 1:A:47:TYR:HA   | 1:A:50:VAL:HG12 | 0.67     | 1.67        | 10     | 11    |
| 1:A:1:MET:CE    | 1:A:9:TYR:CD2   | 0.66     | 2.78        | 9      | 14    |
| 1:A:12:LEU:HD21 | 1:A:35:ALA:HA   | 0.66     | 1.65        | 11     | 1     |
| 1:A:8:LEU:C     | 1:A:8:LEU:HD12  | 0.66     | 2.16        | 3      | 8     |
| 1:A:58:ILE:O    | 1:A:73:MET:HE2  | 0.66     | 1.90        | 12     | 1     |
| 1:A:34:CYS:SG   | 1:A:54:LEU:HD21 | 0.66     | 2.31        | 15     | 1     |
| 1:A:1:MET:SD    | 1:A:38:LEU:HB3  | 0.66     | 2.31        | 14     | 1     |
| 1:A:12:LEU:CD2  | 1:A:31:VAL:HG12 | 0.66     | 2.19        | 6      | 3     |
| 1:A:24:ASN:ND2  | 1:A:27:LEU:HB2  | 0.66     | 2.06        | 9      | 2     |
| 1:A:9:TYR:C     | 1:A:9:TYR:CD1   | 0.66     | 2.73        | 7      | 7     |
| 1:A:44:GLU:O    | 1:A:48:ILE:N    | 0.65     | 2.28        | 6      | 13    |
| 1:A:8:LEU:H     | 1:A:8:LEU:HD13  | 0.65     | 1.50        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:18:ASP:OD2   | 1:A:21:VAL:HG21  | 0.65     | 1.92        | 3      | 1     |
| 1:A:24:ASN:HB3   | 1:A:27:LEU:HD23  | 0.65     | 1.68        | 8      | 1     |
| 1:A:81:GLN:O     | 1:A:85:LYS:HG2   | 0.65     | 1.92        | 8      | 3     |
| 1:A:58:ILE:HB    | 1:A:73:MET:HE2   | 0.65     | 1.68        | 6      | 1     |
| 1:A:74:LEU:HD12  | 1:A:77:TYR:CE2   | 0.65     | 2.27        | 11     | 1     |
| 1:A:54:LEU:HD12  | 1:A:54:LEU:C     | 0.65     | 2.16        | 14     | 1     |
| 1:A:15:ALA:O     | 1:A:18:ASP:HB2   | 0.65     | 1.92        | 11     | 8     |
| 1:A:77:TYR:C     | 1:A:77:TYR:CD1   | 0.65     | 2.75        | 11     | 13    |
| 1:A:9:TYR:HA     | 1:A:12:LEU:HD12  | 0.65     | 1.66        | 8      | 5     |
| 1:A:4:LYS:O      | 1:A:8:LEU:HD11   | 0.65     | 1.92        | 4      | 2     |
| 1:A:90:ASP:CB    | 1:A:93:LYS:CE    | 0.64     | 2.74        | 8      | 5     |
| 1:A:1:MET:CE     | 1:A:38:LEU:HB3   | 0.64     | 2.22        | 15     | 4     |
| 1:A:84:ILE:HD12  | 1:A:89:ILE:CB    | 0.64     | 2.23        | 13     | 9     |
| 1:A:27:LEU:HD22  | 1:A:73:MET:SD    | 0.64     | 2.32        | 13     | 2     |
| 1:A:84:ILE:HD12  | 1:A:89:ILE:HB    | 0.64     | 1.70        | 3      | 8     |
| 1:A:1:MET:HE3    | 1:A:38:LEU:CB    | 0.64     | 2.22        | 13     | 2     |
| 1:A:73:MET:C     | 1:A:74:LEU:HD22  | 0.64     | 2.18        | 12     | 1     |
| 1:A:26:PHE:CZ    | 1:A:27:LEU:HD12  | 0.64     | 2.27        | 5      | 1     |
| 1:A:103:LEU:N    | 1:A:103:LEU:HD23 | 0.63     | 2.08        | 9      | 1     |
| 1:A:37:LYS:HB2   | 1:A:50:VAL:HG21  | 0.63     | 1.68        | 12     | 2     |
| 1:A:9:TYR:O      | 1:A:12:LEU:HB2   | 0.63     | 1.93        | 4      | 13    |
| 1:A:5:SER:O      | 1:A:9:TYR:N      | 0.63     | 2.30        | 10     | 6     |
| 1:A:58:ILE:HG13  | 1:A:73:MET:HE2   | 0.63     | 1.70        | 9      | 4     |
| 1:A:26:PHE:CD2   | 1:A:27:LEU:HD12  | 0.63     | 2.29        | 6      | 1     |
| 1:A:33:GLN:O     | 1:A:37:LYS:HD2   | 0.63     | 1.94        | 6      | 1     |
| 1:A:81:GLN:O     | 1:A:85:LYS:HB2   | 0.63     | 1.94        | 3      | 1     |
| 1:A:98:GLU:HG2   | 1:A:103:LEU:HD21 | 0.63     | 1.69        | 14     | 2     |
| 1:A:49:GLU:HA    | 1:A:97:TYR:CZ    | 0.63     | 2.29        | 7      | 9     |
| 1:A:77:TYR:HA    | 1:A:80:ILE:HD11  | 0.63     | 1.70        | 12     | 1     |
| 1:A:91:THR:O     | 1:A:95:ARG:HB3   | 0.63     | 1.94        | 7      | 6     |
| 1:A:47:TYR:OH    | 1:A:89:ILE:HD11  | 0.63     | 1.93        | 11     | 6     |
| 1:A:2:ASP:O      | 1:A:6:GLN:HB2    | 0.62     | 1.93        | 3      | 11    |
| 1:A:48:ILE:CG2   | 1:A:94:LEU:HG    | 0.62     | 2.24        | 15     | 2     |
| 1:A:1:MET:HG3    | 1:A:5:SER:CB     | 0.62     | 2.23        | 4      | 1     |
| 1:A:98:GLU:HG2   | 1:A:103:LEU:HD12 | 0.62     | 1.69        | 13     | 1     |
| 1:A:92:GLU:O     | 1:A:96:LYS:HG2   | 0.62     | 1.94        | 3      | 5     |
| 1:A:97:TYR:CE1   | 1:A:101:LYS:HD2  | 0.62     | 2.29        | 15     | 5     |
| 1:A:91:THR:HG23  | 1:A:94:LEU:HD12  | 0.62     | 1.71        | 9      | 2     |
| 1:A:103:LEU:HD12 | 1:A:103:LEU:H    | 0.62     | 1.55        | 13     | 1     |
| 1:A:8:LEU:HD13   | 1:A:8:LEU:N      | 0.61     | 2.09        | 4      | 1     |
| 1:A:91:THR:O     | 1:A:95:ARG:CB    | 0.61     | 2.48        | 7      | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:97:TYR:O    | 1:A:101:LYS:HG2  | 0.61     | 1.95        | 1      | 10    |
| 1:A:5:SER:OG    | 1:A:47:TYR:CE2   | 0.61     | 2.53        | 2      | 2     |
| 1:A:58:ILE:CG1  | 1:A:73:MET:HE2   | 0.61     | 2.25        | 10     | 4     |
| 1:A:21:VAL:HG12 | 1:A:28:SER:CB    | 0.61     | 2.26        | 7      | 8     |
| 1:A:15:ALA:O    | 1:A:18:ASP:OD1   | 0.61     | 2.17        | 3      | 1     |
| 1:A:48:ILE:HG23 | 1:A:94:LEU:CG    | 0.61     | 2.25        | 15     | 2     |
| 1:A:94:LEU:C    | 1:A:94:LEU:HD12  | 0.61     | 2.20        | 3      | 1     |
| 1:A:58:ILE:HG21 | 1:A:77:TYR:CD2   | 0.61     | 2.31        | 14     | 3     |
| 1:A:4:LYS:CD    | 1:A:4:LYS:N      | 0.61     | 2.64        | 11     | 1     |
| 1:A:51:ILE:HG21 | 1:A:94:LEU:HD21  | 0.61     | 1.72        | 11     | 1     |
| 1:A:82:LYS:O    | 1:A:86:ASN:CB    | 0.61     | 2.49        | 14     | 15    |
| 1:A:89:ILE:HG22 | 1:A:94:LEU:HD11  | 0.61     | 1.72        | 7      | 4     |
| 1:A:84:ILE:CG1  | 1:A:91:THR:HG23  | 0.60     | 2.26        | 6      | 4     |
| 1:A:9:TYR:HA    | 1:A:38:LEU:HD23  | 0.60     | 1.71        | 6      | 1     |
| 1:A:58:ILE:HG21 | 1:A:77:TYR:HD2   | 0.60     | 1.56        | 12     | 1     |
| 1:A:89:ILE:HG21 | 1:A:94:LEU:HD21  | 0.60     | 1.73        | 12     | 1     |
| 1:A:12:LEU:CD1  | 1:A:31:VAL:O     | 0.60     | 2.49        | 11     | 1     |
| 1:A:1:MET:CE    | 1:A:38:LEU:C     | 0.60     | 2.75        | 14     | 2     |
| 1:A:21:VAL:HG13 | 1:A:27:LEU:HG    | 0.60     | 1.73        | 8      | 1     |
| 1:A:78:THR:O    | 1:A:82:LYS:CE    | 0.60     | 2.49        | 11     | 1     |
| 1:A:46:SER:O    | 1:A:50:VAL:HG23  | 0.60     | 1.95        | 15     | 2     |
| 1:A:48:ILE:HA   | 1:A:94:LEU:HD21  | 0.60     | 1.73        | 15     | 1     |
| 1:A:73:MET:O    | 1:A:74:LEU:HD22  | 0.60     | 1.97        | 12     | 1     |
| 1:A:89:ILE:HG21 | 1:A:94:LEU:CD1   | 0.60     | 2.27        | 1      | 4     |
| 1:A:16:TYR:CE1  | 1:A:32:VAL:CG2   | 0.60     | 2.85        | 6      | 7     |
| 1:A:54:LEU:HD12 | 1:A:80:ILE:HD11  | 0.60     | 1.72        | 4      | 4     |
| 1:A:24:ASN:CB   | 1:A:27:LEU:HD23  | 0.59     | 2.26        | 8      | 1     |
| 1:A:4:LYS:HD2   | 1:A:5:SER:H      | 0.59     | 1.56        | 8      | 3     |
| 1:A:18:ASP:HB3  | 1:A:21:VAL:HG23  | 0.59     | 1.73        | 11     | 1     |
| 1:A:48:ILE:CG1  | 1:A:93:LYS:HE3   | 0.59     | 2.28        | 1      | 2     |
| 1:A:74:LEU:O    | 1:A:74:LEU:HD23  | 0.59     | 1.97        | 8      | 2     |
| 1:A:85:LYS:N    | 1:A:85:LYS:HD2   | 0.59     | 2.12        | 9      | 1     |
| 1:A:73:MET:HA   | 1:A:73:MET:HE2   | 0.59     | 1.73        | 3      | 2     |
| 1:A:70:PRO:O    | 1:A:72:SER:N     | 0.59     | 2.36        | 1      | 1     |
| 1:A:1:MET:HE3   | 1:A:38:LEU:C     | 0.59     | 2.22        | 10     | 3     |
| 1:A:72:SER:O    | 1:A:76:ILE:HD13  | 0.59     | 1.98        | 15     | 5     |
| 1:A:102:GLY:C   | 1:A:103:LEU:HD23 | 0.59     | 2.23        | 9      | 1     |
| 1:A:12:LEU:O    | 1:A:31:VAL:HG11  | 0.59     | 1.97        | 2      | 5     |
| 1:A:48:ILE:CG2  | 1:A:94:LEU:HD23  | 0.59     | 2.23        | 9      | 2     |
| 1:A:50:VAL:O    | 1:A:54:LEU:HB3   | 0.59     | 1.98        | 14     | 1     |
| 1:A:97:TYR:CE1  | 1:A:101:LYS:HG3  | 0.58     | 2.32        | 1      | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:58:ILE:HG21 | 1:A:77:TYR:HB2  | 0.58     | 1.76        | 14     | 2     |
| 1:A:77:TYR:O    | 1:A:80:ILE:HG13 | 0.58     | 1.97        | 12     | 3     |
| 1:A:97:TYR:C    | 1:A:97:TYR:CD1  | 0.58     | 2.80        | 13     | 1     |
| 1:A:5:SER:O     | 1:A:9:TYR:CB    | 0.58     | 2.51        | 3      | 8     |
| 1:A:90:ASP:CB   | 1:A:93:LYS:HD2  | 0.58     | 2.29        | 2      | 4     |
| 1:A:1:MET:SD    | 1:A:38:LEU:O    | 0.58     | 2.61        | 4      | 3     |
| 1:A:47:TYR:C    | 1:A:47:TYR:CD1  | 0.58     | 2.80        | 11     | 5     |
| 1:A:5:SER:HA    | 1:A:8:LEU:CD1   | 0.58     | 2.28        | 13     | 1     |
| 1:A:85:LYS:HD2  | 1:A:85:LYS:N    | 0.58     | 2.13        | 8      | 1     |
| 1:A:77:TYR:O    | 1:A:80:ILE:HB   | 0.58     | 1.98        | 10     | 2     |
| 1:A:98:GLU:HA   | 1:A:101:LYS:HE3 | 0.58     | 1.75        | 4      | 1     |
| 1:A:58:ILE:O    | 1:A:58:ILE:HD13 | 0.57     | 1.99        | 4      | 2     |
| 1:A:4:LYS:CD    | 1:A:4:LYS:H     | 0.57     | 2.10        | 11     | 1     |
| 1:A:12:LEU:HD13 | 1:A:31:VAL:O    | 0.57     | 1.98        | 13     | 1     |
| 1:A:74:LEU:O    | 1:A:78:THR:OG1  | 0.57     | 2.20        | 8      | 3     |
| 1:A:73:MET:HA   | 1:A:73:MET:CE   | 0.57     | 2.28        | 7      | 6     |
| 1:A:34:CYS:O    | 1:A:38:LEU:HD22 | 0.57     | 2.00        | 6      | 1     |
| 1:A:1:MET:CE    | 1:A:39:THR:HA   | 0.57     | 2.30        | 9      | 2     |
| 1:A:1:MET:HE1   | 1:A:39:THR:CA   | 0.57     | 2.29        | 9      | 1     |
| 1:A:14:GLU:HA   | 1:A:17:LYS:CD   | 0.57     | 2.29        | 6      | 4     |
| 1:A:74:LEU:HD13 | 1:A:74:LEU:N    | 0.57     | 2.15        | 7      | 1     |
| 1:A:1:MET:HG3   | 1:A:5:SER:HB2   | 0.57     | 1.76        | 4      | 3     |
| 1:A:84:ILE:HG23 | 1:A:91:THR:HG23 | 0.57     | 1.75        | 9      | 2     |
| 1:A:58:ILE:HA   | 1:A:73:MET:HE2  | 0.57     | 1.76        | 14     | 2     |
| 1:A:77:TYR:HA   | 1:A:80:ILE:HG12 | 0.57     | 1.76        | 15     | 1     |
| 1:A:16:TYR:CD1  | 1:A:32:VAL:CG2  | 0.57     | 2.88        | 5      | 11    |
| 1:A:32:VAL:O    | 1:A:35:ALA:HB3  | 0.57     | 2.00        | 7      | 9     |
| 1:A:54:LEU:O    | 1:A:58:ILE:HG22 | 0.57     | 1.99        | 12     | 3     |
| 1:A:98:GLU:O    | 1:A:102:GLY:N   | 0.57     | 2.37        | 9      | 2     |
| 1:A:47:TYR:OH   | 1:A:89:ILE:CD1  | 0.56     | 2.52        | 9      | 9     |
| 1:A:9:TYR:CE2   | 1:A:39:THR:HG23 | 0.56     | 2.35        | 8      | 3     |
| 1:A:27:LEU:HD21 | 1:A:58:ILE:O    | 0.56     | 2.00        | 14     | 1     |
| 1:A:89:ILE:HG22 | 1:A:90:ASP:N    | 0.56     | 2.15        | 9      | 9     |
| 1:A:1:MET:HE1   | 1:A:39:THR:N    | 0.56     | 2.14        | 9      | 2     |
| 1:A:89:ILE:HG22 | 1:A:94:LEU:HD13 | 0.56     | 1.76        | 15     | 1     |
| 1:A:89:ILE:CG2  | 1:A:94:LEU:CD1  | 0.56     | 2.83        | 1      | 4     |
| 1:A:24:ASN:HB3  | 1:A:27:LEU:HD13 | 0.56     | 1.78        | 11     | 2     |
| 1:A:58:ILE:HD11 | 1:A:73:MET:CE   | 0.56     | 2.29        | 2      | 1     |
| 1:A:16:TYR:HA   | 1:A:21:VAL:HG11 | 0.56     | 1.78        | 10     | 3     |
| 1:A:91:THR:CG2  | 1:A:94:LEU:HD12 | 0.56     | 2.30        | 9      | 3     |
| 1:A:27:LEU:O    | 1:A:31:VAL:HG22 | 0.56     | 2.01        | 11     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:26:PHE:O    | 1:A:27:LEU:C     | 0.56     | 2.48        | 13     | 1     |
| 1:A:9:TYR:O     | 1:A:12:LEU:N     | 0.55     | 2.39        | 13     | 15    |
| 1:A:1:MET:HG2   | 1:A:5:SER:OG     | 0.55     | 2.00        | 13     | 1     |
| 1:A:5:SER:O     | 1:A:9:TYR:HB3    | 0.55     | 1.99        | 3      | 4     |
| 1:A:84:ILE:HD12 | 1:A:89:ILE:CG1   | 0.55     | 2.30        | 6      | 6     |
| 1:A:55:SER:O    | 1:A:56:ARG:CB    | 0.55     | 2.53        | 4      | 3     |
| 1:A:1:MET:HE1   | 1:A:39:THR:HA    | 0.55     | 1.77        | 9      | 1     |
| 1:A:56:ARG:HG2  | 1:A:103:LEU:HD22 | 0.55     | 1.77        | 8      | 1     |
| 1:A:93:LYS:HG2  | 1:A:94:LEU:HD12  | 0.55     | 1.77        | 12     | 1     |
| 1:A:90:ASP:HB2  | 1:A:93:LYS:HE2   | 0.55     | 1.77        | 1      | 3     |
| 1:A:91:THR:CG2  | 1:A:94:LEU:HD21  | 0.55     | 2.32        | 3      | 1     |
| 1:A:8:LEU:N     | 1:A:8:LEU:HD23   | 0.55     | 2.17        | 5      | 2     |
| 1:A:15:ALA:HB3  | 1:A:31:VAL:HG11  | 0.55     | 1.77        | 12     | 1     |
| 1:A:15:ALA:O    | 1:A:18:ASP:CB    | 0.55     | 2.55        | 10     | 11    |
| 1:A:77:TYR:O    | 1:A:80:ILE:CD1   | 0.55     | 2.55        | 8      | 4     |
| 1:A:58:ILE:HG21 | 1:A:77:TYR:HB3   | 0.55     | 1.79        | 11     | 3     |
| 1:A:9:TYR:CB    | 1:A:38:LEU:HD23  | 0.55     | 2.31        | 6      | 1     |
| 1:A:84:ILE:CG2  | 1:A:85:LYS:N     | 0.55     | 2.70        | 13     | 1     |
| 1:A:90:ASP:C    | 1:A:94:LEU:HD12  | 0.55     | 2.26        | 15     | 1     |
| 1:A:51:ILE:CD1  | 1:A:80:ILE:HG22  | 0.55     | 2.25        | 12     | 2     |
| 1:A:26:PHE:O    | 1:A:29:LYS:N     | 0.55     | 2.40        | 13     | 1     |
| 1:A:81:GLN:O    | 1:A:84:ILE:HB    | 0.54     | 2.02        | 10     | 3     |
| 1:A:90:ASP:C    | 1:A:94:LEU:HD13  | 0.54     | 2.26        | 12     | 1     |
| 1:A:17:LYS:C    | 1:A:22:LYS:HD3   | 0.54     | 2.27        | 12     | 12    |
| 1:A:91:THR:HA   | 1:A:94:LEU:HB2   | 0.54     | 1.80        | 14     | 11    |
| 1:A:51:ILE:HD11 | 1:A:80:ILE:HG22  | 0.54     | 1.79        | 13     | 1     |
| 1:A:73:MET:HE3  | 1:A:73:MET:CA    | 0.54     | 2.29        | 9      | 2     |
| 1:A:48:ILE:CD1  | 1:A:89:ILE:HG23  | 0.54     | 2.30        | 10     | 1     |
| 1:A:58:ILE:HD13 | 1:A:77:TYR:HB3   | 0.54     | 1.79        | 10     | 2     |
| 1:A:25:GLU:O    | 1:A:29:LYS:HB3   | 0.54     | 2.02        | 6      | 5     |
| 1:A:93:LYS:HG2  | 1:A:94:LEU:N     | 0.54     | 2.16        | 13     | 5     |
| 1:A:103:LEU:H   | 1:A:103:LEU:HD23 | 0.54     | 1.63        | 11     | 3     |
| 1:A:58:ILE:HG21 | 1:A:77:TYR:CB    | 0.54     | 2.32        | 10     | 2     |
| 1:A:54:LEU:HD21 | 1:A:80:ILE:HD11  | 0.54     | 1.79        | 14     | 1     |
| 1:A:16:TYR:CD1  | 1:A:28:SER:CB    | 0.54     | 2.91        | 2      | 13    |
| 1:A:2:ASP:O     | 1:A:6:GLN:N      | 0.54     | 2.40        | 15     | 7     |
| 1:A:2:ASP:CB    | 1:A:4:LYS:HE2    | 0.54     | 2.33        | 12     | 5     |
| 1:A:47:TYR:CE1  | 1:A:89:ILE:HD12  | 0.54     | 2.38        | 14     | 2     |
| 1:A:77:TYR:CA   | 1:A:80:ILE:HG12  | 0.54     | 2.33        | 15     | 1     |
| 1:A:8:LEU:HA    | 1:A:11:ASN:ND2   | 0.54     | 2.18        | 4      | 1     |
| 1:A:48:ILE:HG13 | 1:A:94:LEU:HD23  | 0.54     | 1.79        | 7      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:89:ILE:HG22 | 1:A:94:LEU:CD1   | 0.54     | 2.32        | 15     | 3     |
| 1:A:47:TYR:CZ   | 1:A:51:ILE:CG1   | 0.53     | 2.91        | 14     | 3     |
| 1:A:76:ILE:O    | 1:A:80:ILE:HD12  | 0.53     | 2.03        | 14     | 4     |
| 1:A:28:SER:CA   | 1:A:31:VAL:HG22  | 0.53     | 2.31        | 6      | 1     |
| 1:A:48:ILE:CD1  | 1:A:94:LEU:HD11  | 0.53     | 2.34        | 11     | 2     |
| 1:A:20:GLU:HB2  | 1:A:70:PRO:HB3   | 0.53     | 1.80        | 2      | 3     |
| 1:A:9:TYR:CA    | 1:A:38:LEU:HD23  | 0.53     | 2.33        | 6      | 1     |
| 1:A:98:GLU:CG   | 1:A:103:LEU:HD12 | 0.53     | 2.32        | 13     | 1     |
| 1:A:14:GLU:HA   | 1:A:17:LYS:HD3   | 0.53     | 1.79        | 14     | 4     |
| 1:A:78:THR:O    | 1:A:82:LYS:CG    | 0.53     | 2.56        | 15     | 2     |
| 1:A:80:ILE:HG12 | 1:A:81:GLN:N     | 0.53     | 2.18        | 3      | 1     |
| 1:A:1:MET:HE3   | 1:A:38:LEU:HB2   | 0.53     | 1.80        | 13     | 3     |
| 1:A:52:SER:HB2  | 1:A:94:LEU:HD23  | 0.53     | 1.79        | 4      | 1     |
| 1:A:1:MET:HG3   | 1:A:38:LEU:O     | 0.53     | 2.03        | 10     | 2     |
| 1:A:12:LEU:HD21 | 1:A:76:ILE:HG21  | 0.53     | 1.80        | 5      | 1     |
| 1:A:72:SER:O    | 1:A:74:LEU:N     | 0.53     | 2.42        | 13     | 1     |
| 1:A:54:LEU:C    | 1:A:54:LEU:CD1   | 0.53     | 2.74        | 8      | 1     |
| 1:A:89:ILE:HG21 | 1:A:94:LEU:HD12  | 0.53     | 1.78        | 10     | 1     |
| 1:A:1:MET:HE2   | 1:A:39:THR:HA    | 0.53     | 1.81        | 14     | 1     |
| 1:A:54:LEU:HD21 | 1:A:80:ILE:CG1   | 0.53     | 2.33        | 14     | 1     |
| 1:A:5:SER:HA    | 1:A:8:LEU:CD2    | 0.53     | 2.34        | 4      | 2     |
| 1:A:48:ILE:HD12 | 1:A:94:LEU:CD2   | 0.53     | 2.34        | 7      | 1     |
| 1:A:58:ILE:HG21 | 1:A:77:TYR:CG    | 0.53     | 2.39        | 14     | 1     |
| 1:A:1:MET:HE1   | 1:A:9:TYR:CD1    | 0.52     | 2.40        | 10     | 2     |
| 1:A:3:ILE:CD1   | 1:A:3:ILE:N      | 0.52     | 2.73        | 3      | 5     |
| 1:A:89:ILE:CG2  | 1:A:94:LEU:HD12  | 0.52     | 2.35        | 10     | 1     |
| 1:A:28:SER:HA   | 1:A:31:VAL:HG23  | 0.52     | 1.82        | 11     | 2     |
| 1:A:1:MET:HE1   | 1:A:35:ALA:O     | 0.52     | 2.03        | 13     | 1     |
| 1:A:55:SER:CB   | 1:A:80:ILE:HG21  | 0.52     | 2.34        | 15     | 2     |
| 1:A:91:THR:HA   | 1:A:94:LEU:HG    | 0.52     | 1.80        | 7      | 1     |
| 1:A:79:GLN:HA   | 1:A:82:LYS:CG    | 0.52     | 2.35        | 11     | 2     |
| 1:A:33:GLN:CG   | 1:A:34:CYS:N     | 0.52     | 2.72        | 6      | 3     |
| 1:A:1:MET:HE1   | 1:A:9:TYR:CG     | 0.52     | 2.39        | 5      | 2     |
| 1:A:4:LYS:O     | 1:A:8:LEU:CG     | 0.52     | 2.57        | 8      | 2     |
| 1:A:16:TYR:HD1  | 1:A:28:SER:CB    | 0.52     | 2.17        | 4      | 10    |
| 1:A:16:TYR:CE1  | 1:A:28:SER:CB    | 0.52     | 2.93        | 6      | 1     |
| 1:A:91:THR:HA   | 1:A:94:LEU:HD12  | 0.52     | 1.80        | 9      | 2     |
| 1:A:1:MET:CG    | 1:A:5:SER:CB     | 0.52     | 2.87        | 15     | 2     |
| 1:A:52:SER:OG   | 1:A:103:LEU:HD22 | 0.52     | 2.04        | 1      | 2     |
| 1:A:46:SER:HA   | 1:A:49:GLU:CG    | 0.52     | 2.35        | 7      | 1     |
| 1:A:100:ALA:HB3 | 1:A:101:LYS:HD2  | 0.52     | 1.82        | 13     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:16:TYR:CD1  | 1:A:28:SER:HB2   | 0.52     | 2.39        | 12     | 7     |
| 1:A:9:TYR:HE2   | 1:A:39:THR:HG23  | 0.52     | 1.63        | 6      | 3     |
| 1:A:48:ILE:O    | 1:A:94:LEU:HD21  | 0.52     | 2.05        | 2      | 1     |
| 1:A:52:SER:OG   | 1:A:53:LEU:HD23  | 0.52     | 2.05        | 3      | 1     |
| 1:A:25:GLU:O    | 1:A:29:LYS:HG3   | 0.52     | 2.05        | 4      | 2     |
| 1:A:84:ILE:CG2  | 1:A:91:THR:HG21  | 0.52     | 2.31        | 4      | 6     |
| 1:A:55:SER:O    | 1:A:77:TYR:CE2   | 0.52     | 2.63        | 15     | 4     |
| 1:A:71:SER:C    | 1:A:73:MET:H     | 0.52     | 2.13        | 9      | 14    |
| 1:A:12:LEU:HD13 | 1:A:31:VAL:HG13  | 0.52     | 1.81        | 5      | 1     |
| 1:A:53:LEU:HD21 | 1:A:97:TYR:HH    | 0.52     | 1.65        | 5      | 1     |
| 1:A:4:LYS:HD2   | 1:A:5:SER:N      | 0.52     | 2.19        | 10     | 2     |
| 1:A:58:ILE:HG12 | 1:A:58:ILE:O     | 0.52     | 2.04        | 9      | 1     |
| 1:A:8:LEU:HD11  | 1:A:38:LEU:CD1   | 0.52     | 2.32        | 12     | 1     |
| 1:A:97:TYR:CZ   | 1:A:101:LYS:NZ   | 0.52     | 2.76        | 4      | 1     |
| 1:A:24:ASN:ND2  | 1:A:27:LEU:HD22  | 0.52     | 2.20        | 15     | 1     |
| 1:A:16:TYR:HE1  | 1:A:28:SER:HG    | 0.51     | 1.47        | 3      | 4     |
| 1:A:84:ILE:HG22 | 1:A:85:LYS:CD    | 0.51     | 2.33        | 8      | 1     |
| 1:A:1:MET:SD    | 1:A:39:THR:CA    | 0.51     | 2.97        | 10     | 2     |
| 1:A:48:ILE:HG12 | 1:A:93:LYS:CD    | 0.51     | 2.35        | 1      | 1     |
| 1:A:83:ASP:CB   | 1:A:89:ILE:HD12  | 0.51     | 2.36        | 10     | 2     |
| 1:A:1:MET:HG2   | 1:A:5:SER:O      | 0.51     | 2.05        | 4      | 1     |
| 1:A:5:SER:CA    | 1:A:8:LEU:HD21   | 0.51     | 2.31        | 4      | 1     |
| 1:A:90:ASP:HB3  | 1:A:93:LYS:HD2   | 0.51     | 1.81        | 8      | 1     |
| 1:A:95:ARG:CD   | 1:A:99:ILE:HD11  | 0.51     | 2.36        | 11     | 1     |
| 1:A:38:LEU:HD13 | 1:A:47:TYR:CD2   | 0.51     | 2.40        | 1      | 1     |
| 1:A:47:TYR:O    | 1:A:51:ILE:N     | 0.51     | 2.43        | 11     | 9     |
| 1:A:33:GLN:HG3  | 1:A:34:CYS:N     | 0.51     | 2.19        | 1      | 4     |
| 1:A:90:ASP:HB2  | 1:A:93:LYS:CE    | 0.51     | 2.36        | 12     | 5     |
| 1:A:9:TYR:CZ    | 1:A:35:ALA:O     | 0.51     | 2.64        | 6      | 1     |
| 1:A:48:ILE:HG12 | 1:A:93:LYS:HD3   | 0.51     | 1.81        | 13     | 2     |
| 1:A:15:ALA:HB2  | 1:A:76:ILE:HD11  | 0.51     | 1.81        | 9      | 1     |
| 1:A:81:GLN:HA   | 1:A:84:ILE:HG12  | 0.51     | 1.83        | 10     | 2     |
| 1:A:18:ASP:O    | 1:A:21:VAL:N     | 0.51     | 2.41        | 4      | 4     |
| 1:A:48:ILE:HG13 | 1:A:93:LYS:CG    | 0.51     | 2.35        | 5      | 3     |
| 1:A:97:TYR:O    | 1:A:101:LYS:CG   | 0.51     | 2.59        | 9      | 6     |
| 1:A:98:GLU:HA   | 1:A:103:LEU:HD12 | 0.51     | 1.80        | 8      | 1     |
| 1:A:12:LEU:CD1  | 1:A:38:LEU:HD22  | 0.51     | 2.36        | 14     | 1     |
| 1:A:15:ALA:HB1  | 1:A:72:SER:HB3   | 0.51     | 1.82        | 3      | 1     |
| 1:A:58:ILE:HG13 | 1:A:73:MET:CE    | 0.51     | 2.36        | 4      | 2     |
| 1:A:84:ILE:HD12 | 1:A:89:ILE:HG13  | 0.51     | 1.82        | 5      | 1     |
| 1:A:80:ILE:HD13 | 1:A:80:ILE:N     | 0.51     | 2.20        | 15     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:16:TYR:CD1  | 1:A:32:VAL:HG22 | 0.51     | 2.41        | 5      | 3     |
| 1:A:55:SER:HB2  | 1:A:80:ILE:HG21 | 0.51     | 1.81        | 15     | 1     |
| 1:A:44:GLU:O    | 1:A:48:ILE:CG1  | 0.50     | 2.59        | 8      | 11    |
| 1:A:70:PRO:O    | 1:A:71:SER:C    | 0.50     | 2.53        | 1      | 1     |
| 1:A:78:THR:CG2  | 1:A:79:GLN:N    | 0.50     | 2.73        | 11     | 4     |
| 1:A:24:ASN:ND2  | 1:A:27:LEU:CB   | 0.50     | 2.74        | 5      | 2     |
| 1:A:21:VAL:O    | 1:A:24:ASN:ND2  | 0.50     | 2.45        | 9      | 1     |
| 1:A:5:SER:HB3   | 1:A:38:LEU:HD12 | 0.50     | 1.84        | 1      | 1     |
| 1:A:50:VAL:O    | 1:A:54:LEU:HD23 | 0.50     | 2.06        | 13     | 6     |
| 1:A:50:VAL:CA   | 1:A:53:LEU:HD12 | 0.50     | 2.33        | 7      | 1     |
| 1:A:10:LEU:O    | 1:A:14:GLU:HG3  | 0.50     | 2.06        | 1      | 3     |
| 1:A:15:ALA:HB1  | 1:A:72:SER:CB   | 0.50     | 2.37        | 8      | 1     |
| 1:A:1:MET:SD    | 1:A:9:TYR:CE2   | 0.50     | 3.05        | 13     | 2     |
| 1:A:12:LEU:HD13 | 1:A:35:ALA:HA   | 0.50     | 1.84        | 10     | 1     |
| 1:A:91:THR:CG2  | 1:A:94:LEU:CD2  | 0.50     | 2.90        | 3      | 1     |
| 1:A:77:TYR:O    | 1:A:77:TYR:CD1  | 0.50     | 2.64        | 12     | 2     |
| 1:A:11:ASN:OD1  | 1:A:11:ASN:C    | 0.50     | 2.53        | 4      | 1     |
| 1:A:81:GLN:HA   | 1:A:84:ILE:CG1  | 0.50     | 2.37        | 10     | 1     |
| 1:A:37:LYS:HB3  | 1:A:50:VAL:HG21 | 0.50     | 1.83        | 14     | 1     |
| 1:A:27:LEU:N    | 1:A:27:LEU:HD12 | 0.50     | 2.21        | 10     | 3     |
| 1:A:48:ILE:O    | 1:A:52:SER:N    | 0.50     | 2.45        | 4      | 4     |
| 1:A:58:ILE:O    | 1:A:58:ILE:CG1  | 0.50     | 2.60        | 8      | 2     |
| 1:A:22:LYS:HA   | 1:A:22:LYS:HE2  | 0.50     | 1.81        | 8      | 1     |
| 1:A:18:ASP:O    | 1:A:22:LYS:HG2  | 0.50     | 2.07        | 9      | 9     |
| 1:A:90:ASP:O    | 1:A:94:LEU:N    | 0.50     | 2.38        | 8      | 1     |
| 1:A:89:ILE:CG2  | 1:A:90:ASP:N    | 0.50     | 2.75        | 8      | 6     |
| 1:A:85:LYS:N    | 1:A:85:LYS:CD   | 0.50     | 2.74        | 9      | 2     |
| 1:A:58:ILE:CD1  | 1:A:73:MET:C    | 0.49     | 2.84        | 7      | 1     |
| 1:A:2:ASP:HB2   | 1:A:4:LYS:CE    | 0.49     | 2.37        | 9      | 1     |
| 1:A:12:LEU:CD1  | 1:A:38:LEU:HD13 | 0.49     | 2.36        | 10     | 1     |
| 1:A:1:MET:CG    | 1:A:5:SER:HB2   | 0.49     | 2.37        | 14     | 2     |
| 1:A:22:LYS:HB3  | 1:A:22:LYS:NZ   | 0.49     | 2.22        | 8      | 1     |
| 1:A:48:ILE:CG1  | 1:A:93:LYS:CE   | 0.49     | 2.89        | 1      | 1     |
| 1:A:47:TYR:CE1  | 1:A:51:ILE:HG13 | 0.49     | 2.42        | 6      | 2     |
| 1:A:84:ILE:CG2  | 1:A:91:THR:CG2  | 0.49     | 2.88        | 10     | 2     |
| 1:A:82:LYS:O    | 1:A:86:ASN:HB2  | 0.49     | 2.06        | 2      | 9     |
| 1:A:90:ASP:HB3  | 1:A:93:LYS:HB2  | 0.49     | 1.83        | 8      | 1     |
| 1:A:101:LYS:HD2 | 1:A:101:LYS:N   | 0.49     | 2.22        | 13     | 1     |
| 1:A:3:ILE:HA    | 1:A:6:GLN:HB2   | 0.49     | 1.84        | 9      | 11    |
| 1:A:52:SER:CB   | 1:A:97:TYR:CE2  | 0.49     | 2.96        | 13     | 5     |
| 1:A:4:LYS:O     | 1:A:8:LEU:CD2   | 0.49     | 2.61        | 8      | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:8:LEU:HD22  | 1:A:83:ASP:OD2  | 0.49     | 2.07        | 1      | 1     |
| 1:A:90:ASP:HB3  | 1:A:93:LYS:HE2  | 0.49     | 1.78        | 1      | 2     |
| 1:A:38:LEU:N    | 1:A:38:LEU:HD13 | 0.49     | 2.22        | 6      | 1     |
| 1:A:51:ILE:CD1  | 1:A:80:ILE:CG2  | 0.49     | 2.86        | 12     | 2     |
| 1:A:4:LYS:HG2   | 1:A:88:ASN:HB3  | 0.49     | 1.84        | 6      | 1     |
| 1:A:52:SER:HB3  | 1:A:97:TYR:CE2  | 0.49     | 2.42        | 8      | 3     |
| 1:A:4:LYS:CE    | 1:A:5:SER:N     | 0.49     | 2.76        | 2      | 2     |
| 1:A:48:ILE:HG23 | 1:A:94:LEU:CB   | 0.49     | 2.37        | 3      | 1     |
| 1:A:77:TYR:CD1  | 1:A:77:TYR:C    | 0.49     | 2.91        | 12     | 2     |
| 1:A:84:ILE:CD1  | 1:A:89:ILE:HG21 | 0.49     | 2.37        | 8      | 1     |
| 1:A:48:ILE:HD11 | 1:A:89:ILE:CG2  | 0.49     | 2.38        | 3      | 1     |
| 1:A:97:TYR:CE1  | 1:A:101:LYS:CD  | 0.49     | 2.96        | 15     | 3     |
| 1:A:16:TYR:CE1  | 1:A:28:SER:HB2  | 0.48     | 2.42        | 6      | 1     |
| 1:A:79:GLN:HA   | 1:A:82:LYS:HG2  | 0.48     | 1.85        | 1      | 2     |
| 1:A:4:LYS:HG2   | 1:A:5:SER:N     | 0.48     | 2.22        | 4      | 2     |
| 1:A:51:ILE:HD12 | 1:A:80:ILE:HG21 | 0.48     | 1.85        | 8      | 1     |
| 1:A:9:TYR:HB2   | 1:A:38:LEU:HD23 | 0.48     | 1.84        | 6      | 1     |
| 1:A:47:TYR:CE1  | 1:A:48:ILE:CD1  | 0.48     | 2.96        | 7      | 2     |
| 1:A:89:ILE:O    | 1:A:91:THR:N    | 0.48     | 2.46        | 3      | 1     |
| 1:A:47:TYR:CZ   | 1:A:51:ILE:HG13 | 0.48     | 2.44        | 6      | 3     |
| 1:A:1:MET:CE    | 1:A:38:LEU:CB   | 0.48     | 2.91        | 10     | 1     |
| 1:A:24:ASN:CB   | 1:A:27:LEU:HD13 | 0.48     | 2.38        | 11     | 1     |
| 1:A:24:ASN:CB   | 1:A:27:LEU:HD12 | 0.48     | 2.38        | 13     | 1     |
| 1:A:26:PHE:CD1  | 1:A:26:PHE:C    | 0.48     | 2.92        | 6      | 1     |
| 1:A:28:SER:O    | 1:A:31:VAL:CG2  | 0.48     | 2.62        | 6      | 1     |
| 1:A:91:THR:HA   | 1:A:94:LEU:CD1  | 0.48     | 2.39        | 7      | 2     |
| 1:A:80:ILE:O    | 1:A:84:ILE:HD13 | 0.48     | 2.08        | 15     | 2     |
| 1:A:21:VAL:HG12 | 1:A:28:SER:HB3  | 0.48     | 1.85        | 8      | 4     |
| 1:A:18:ASP:CG   | 1:A:21:VAL:HB   | 0.48     | 2.32        | 3      | 1     |
| 1:A:1:MET:HA    | 1:A:41:SER:HB3  | 0.48     | 1.84        | 3      | 2     |
| 1:A:10:LEU:O    | 1:A:14:GLU:HG2  | 0.48     | 2.09        | 4      | 1     |
| 1:A:58:ILE:HD13 | 1:A:77:TYR:H    | 0.48     | 1.69        | 14     | 1     |
| 1:A:80:ILE:HG22 | 1:A:81:GLN:N    | 0.48     | 2.24        | 11     | 6     |
| 1:A:84:ILE:HD12 | 1:A:89:ILE:CD1  | 0.48     | 2.38        | 2      | 2     |
| 1:A:11:ASN:O    | 1:A:15:ALA:N    | 0.48     | 2.47        | 14     | 5     |
| 1:A:74:LEU:O    | 1:A:78:THR:CB   | 0.48     | 2.61        | 3      | 2     |
| 1:A:1:MET:HE1   | 1:A:38:LEU:C    | 0.48     | 2.34        | 4      | 1     |
| 1:A:54:LEU:HD21 | 1:A:80:ILE:CD1  | 0.48     | 2.39        | 14     | 1     |
| 1:A:1:MET:HG2   | 1:A:6:GLN:HG3   | 0.47     | 1.86        | 2      | 1     |
| 1:A:39:THR:C    | 1:A:41:SER:H    | 0.47     | 2.17        | 13     | 2     |
| 1:A:77:TYR:O    | 1:A:80:ILE:CG1  | 0.47     | 2.62        | 12     | 3     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:26:PHE:O    | 1:A:30:LEU:HB2   | 0.47     | 2.08        | 15     | 1     |
| 1:A:90:ASP:C    | 1:A:92:GLU:N     | 0.47     | 2.71        | 15     | 6     |
| 1:A:24:ASN:OD1  | 1:A:27:LEU:HD13  | 0.47     | 2.09        | 10     | 1     |
| 1:A:33:GLN:O    | 1:A:37:LYS:HG2   | 0.47     | 2.09        | 4      | 3     |
| 1:A:90:ASP:C    | 1:A:94:LEU:CD1   | 0.47     | 2.87        | 12     | 2     |
| 1:A:48:ILE:CG1  | 1:A:93:LYS:CG    | 0.47     | 2.92        | 13     | 2     |
| 1:A:48:ILE:HD12 | 1:A:94:LEU:HD11  | 0.47     | 1.85        | 1      | 1     |
| 1:A:14:GLU:O    | 1:A:17:LYS:HG2   | 0.47     | 2.09        | 3      | 4     |
| 1:A:75:THR:CG2  | 1:A:76:ILE:N     | 0.47     | 2.78        | 4      | 3     |
| 1:A:21:VAL:HG13 | 1:A:27:LEU:CG    | 0.47     | 2.39        | 8      | 1     |
| 1:A:8:LEU:HD12  | 1:A:8:LEU:O      | 0.47     | 2.09        | 10     | 3     |
| 1:A:52:SER:CB   | 1:A:97:TYR:HE2   | 0.47     | 2.22        | 14     | 2     |
| 1:A:44:GLU:O    | 1:A:48:ILE:HD13  | 0.47     | 2.10        | 14     | 5     |
| 1:A:58:ILE:HG13 | 1:A:73:MET:HE1   | 0.47     | 1.86        | 3      | 1     |
| 1:A:98:GLU:OE2  | 1:A:103:LEU:HD13 | 0.47     | 2.09        | 7      | 1     |
| 1:A:52:SER:CB   | 1:A:103:LEU:HD12 | 0.47     | 2.38        | 9      | 1     |
| 1:A:54:LEU:HB3  | 1:A:80:ILE:HG12  | 0.47     | 1.86        | 10     | 1     |
| 1:A:12:LEU:O    | 1:A:31:VAL:CG1   | 0.47     | 2.62        | 2      | 10    |
| 1:A:27:LEU:HD22 | 1:A:73:MET:CG    | 0.47     | 2.39        | 1      | 1     |
| 1:A:75:THR:C    | 1:A:78:THR:HG22  | 0.47     | 2.34        | 5      | 3     |
| 1:A:90:ASP:CB   | 1:A:93:LYS:HE3   | 0.47     | 2.39        | 8      | 3     |
| 1:A:97:TYR:CZ   | 1:A:101:LYS:HE2  | 0.47     | 2.45        | 4      | 1     |
| 1:A:1:MET:HE1   | 1:A:9:TYR:CD2    | 0.47     | 2.44        | 5      | 2     |
| 1:A:50:VAL:O    | 1:A:54:LEU:N     | 0.47     | 2.47        | 14     | 2     |
| 1:A:75:THR:HG22 | 1:A:76:ILE:HD12  | 0.47     | 1.86        | 7      | 2     |
| 1:A:12:LEU:CD1  | 1:A:35:ALA:HB2   | 0.47     | 2.30        | 11     | 1     |
| 1:A:10:LEU:O    | 1:A:14:GLU:CG    | 0.47     | 2.63        | 13     | 8     |
| 1:A:18:ASP:HB3  | 1:A:21:VAL:CG2   | 0.47     | 2.40        | 12     | 6     |
| 1:A:25:GLU:O    | 1:A:29:LYS:CG    | 0.47     | 2.63        | 12     | 4     |
| 1:A:73:MET:CE   | 1:A:73:MET:HA    | 0.47     | 2.40        | 2      | 1     |
| 1:A:48:ILE:HG23 | 1:A:94:LEU:HB2   | 0.47     | 1.86        | 3      | 1     |
| 1:A:8:LEU:O     | 1:A:11:ASN:OD1   | 0.47     | 2.33        | 4      | 1     |
| 1:A:14:GLU:O    | 1:A:17:LYS:CG    | 0.47     | 2.62        | 4      | 3     |
| 1:A:34:CYS:HA   | 1:A:37:LYS:HG2   | 0.47     | 1.87        | 4      | 2     |
| 1:A:8:LEU:HD13  | 1:A:80:ILE:HD11  | 0.47     | 1.86        | 10     | 1     |
| 1:A:91:THR:HA   | 1:A:94:LEU:HD13  | 0.47     | 1.87        | 12     | 2     |
| 1:A:5:SER:HA    | 1:A:8:LEU:HD11   | 0.47     | 1.86        | 13     | 2     |
| 1:A:1:MET:HG2   | 1:A:9:TYR:HD2    | 0.47     | 1.70        | 3      | 1     |
| 1:A:8:LEU:O     | 1:A:12:LEU:HG    | 0.47     | 2.10        | 4      | 1     |
| 1:A:90:ASP:HB2  | 1:A:93:LYS:HE3   | 0.47     | 1.87        | 15     | 2     |
| 1:A:78:THR:O    | 1:A:82:LYS:HE2   | 0.47     | 2.07        | 11     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:1:MET:CG    | 1:A:5:SER:HB3   | 0.47     | 2.40        | 15     | 2     |
| 1:A:7:THR:O     | 1:A:11:ASN:N    | 0.47     | 2.47        | 14     | 5     |
| 1:A:8:LEU:C     | 1:A:8:LEU:CD1   | 0.47     | 2.88        | 11     | 3     |
| 1:A:4:LYS:N     | 1:A:4:LYS:HD3   | 0.46     | 2.24        | 11     | 3     |
| 1:A:91:THR:HG23 | 1:A:94:LEU:HD21 | 0.46     | 1.87        | 3      | 1     |
| 1:A:1:MET:HG3   | 1:A:39:THR:HA   | 0.46     | 1.87        | 5      | 1     |
| 1:A:24:ASN:ND2  | 1:A:24:ASN:O    | 0.46     | 2.47        | 5      | 1     |
| 1:A:37:LYS:N    | 1:A:37:LYS:CD   | 0.46     | 2.78        | 1      | 1     |
| 1:A:54:LEU:HD13 | 1:A:80:ILE:HD11 | 0.46     | 1.86        | 1      | 1     |
| 1:A:52:SER:HB2  | 1:A:97:TYR:CE2  | 0.46     | 2.46        | 12     | 1     |
| 1:A:90:ASP:O    | 1:A:94:LEU:CD1  | 0.46     | 2.63        | 12     | 1     |
| 1:A:97:TYR:CE1  | 1:A:101:LYS:CG  | 0.46     | 2.99        | 1      | 4     |
| 1:A:72:SER:O    | 1:A:76:ILE:CD1  | 0.46     | 2.64        | 15     | 6     |
| 1:A:20:GLU:CB   | 1:A:70:PRO:HB3  | 0.46     | 2.41        | 9      | 1     |
| 1:A:84:ILE:CG2  | 1:A:85:LYS:HE2  | 0.46     | 2.41        | 10     | 1     |
| 1:A:82:LYS:O    | 1:A:86:ASN:N    | 0.46     | 2.46        | 13     | 2     |
| 1:A:1:MET:HE2   | 1:A:38:LEU:O    | 0.46     | 2.10        | 14     | 1     |
| 1:A:53:LEU:HD23 | 1:A:53:LEU:N    | 0.46     | 2.25        | 2      | 9     |
| 1:A:14:GLU:O    | 1:A:17:LYS:CE   | 0.46     | 2.63        | 3      | 1     |
| 1:A:91:THR:HG23 | 1:A:94:LEU:CD2  | 0.46     | 2.41        | 3      | 1     |
| 1:A:47:TYR:CD1  | 1:A:48:ILE:CD1  | 0.46     | 2.96        | 7      | 1     |
| 1:A:47:TYR:HD1  | 1:A:48:ILE:HD13 | 0.46     | 1.69        | 12     | 1     |
| 1:A:76:ILE:O    | 1:A:79:GLN:N    | 0.46     | 2.48        | 15     | 3     |
| 1:A:45:ASN:O    | 1:A:49:GLU:HG3  | 0.46     | 2.11        | 15     | 1     |
| 1:A:4:LYS:HE3   | 1:A:5:SER:N     | 0.46     | 2.26        | 2      | 2     |
| 1:A:44:GLU:HG3  | 1:A:93:LYS:CE   | 0.46     | 2.41        | 5      | 1     |
| 1:A:91:THR:HA   | 1:A:94:LEU:CG   | 0.46     | 2.41        | 7      | 2     |
| 1:A:80:ILE:O    | 1:A:84:ILE:HG12 | 0.46     | 2.11        | 10     | 1     |
| 1:A:77:TYR:CA   | 1:A:80:ILE:HD11 | 0.46     | 2.38        | 12     | 1     |
| 1:A:1:MET:HB3   | 1:A:6:GLN:HA    | 0.46     | 1.88        | 14     | 1     |
| 1:A:7:THR:O     | 1:A:11:ASN:ND2  | 0.46     | 2.48        | 14     | 1     |
| 1:A:3:ILE:N     | 1:A:3:ILE:HD13  | 0.46     | 2.26        | 2      | 3     |
| 1:A:17:LYS:C    | 1:A:22:LYS:HD2  | 0.46     | 2.35        | 8      | 1     |
| 1:A:1:MET:HE2   | 1:A:38:LEU:C    | 0.46     | 2.35        | 14     | 1     |
| 1:A:88:ASN:C    | 1:A:89:ILE:HD13 | 0.46     | 2.36        | 14     | 4     |
| 1:A:58:ILE:HD11 | 1:A:73:MET:HB3  | 0.46     | 1.87        | 8      | 2     |
| 1:A:58:ILE:CG2  | 1:A:77:TYR:CD2  | 0.46     | 2.99        | 14     | 2     |
| 1:A:52:SER:HB2  | 1:A:97:TYR:OH   | 0.46     | 2.10        | 12     | 1     |
| 1:A:51:ILE:HG21 | 1:A:94:LEU:CD1  | 0.46     | 2.36        | 14     | 1     |
| 1:A:1:MET:HE2   | 1:A:9:TYR:HD2   | 0.46     | 1.68        | 3      | 1     |
| 1:A:2:ASP:O     | 1:A:6:GLN:CB    | 0.46     | 2.64        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:18:ASP:CG   | 1:A:21:VAL:CG2  | 0.46     | 2.89        | 3      | 1     |
| 1:A:38:LEU:N    | 1:A:38:LEU:CD1  | 0.46     | 2.78        | 6      | 1     |
| 1:A:14:GLU:C    | 1:A:17:LYS:HG2  | 0.45     | 2.36        | 4      | 1     |
| 1:A:14:GLU:HA   | 1:A:17:LYS:HD2  | 0.45     | 1.87        | 7      | 2     |
| 1:A:16:TYR:CE1  | 1:A:32:VAL:HG22 | 0.45     | 2.45        | 6      | 2     |
| 1:A:31:VAL:O    | 1:A:35:ALA:N    | 0.45     | 2.48        | 11     | 1     |
| 1:A:12:LEU:HD22 | 1:A:31:VAL:CG1  | 0.45     | 2.24        | 2      | 1     |
| 1:A:47:TYR:CE1  | 1:A:51:ILE:CG1  | 0.45     | 2.99        | 11     | 2     |
| 1:A:47:TYR:OH   | 1:A:89:ILE:HD12 | 0.45     | 2.11        | 9      | 1     |
| 1:A:48:ILE:HG12 | 1:A:93:LYS:CE   | 0.45     | 2.42        | 1      | 1     |
| 1:A:91:THR:O    | 1:A:95:ARG:N    | 0.45     | 2.50        | 7      | 6     |
| 1:A:58:ILE:CG1  | 1:A:73:MET:CE   | 0.45     | 2.95        | 2      | 3     |
| 1:A:1:MET:O     | 1:A:5:SER:HB2   | 0.45     | 2.11        | 4      | 1     |
| 1:A:26:PHE:CD2  | 1:A:27:LEU:CD1  | 0.45     | 2.99        | 6      | 1     |
| 1:A:78:THR:O    | 1:A:82:LYS:HD3  | 0.45     | 2.12        | 6      | 2     |
| 1:A:52:SER:OG   | 1:A:97:TYR:CE2  | 0.45     | 2.70        | 8      | 1     |
| 1:A:26:PHE:CE2  | 1:A:30:LEU:CD1  | 0.45     | 2.99        | 3      | 1     |
| 1:A:75:THR:O    | 1:A:79:GLN:CG   | 0.45     | 2.65        | 3      | 3     |
| 1:A:51:ILE:HG22 | 1:A:94:LEU:HD22 | 0.45     | 1.89        | 8      | 1     |
| 1:A:97:TYR:CZ   | 1:A:101:LYS:CE  | 0.45     | 3.00        | 4      | 1     |
| 1:A:26:PHE:O    | 1:A:30:LEU:N    | 0.45     | 2.47        | 13     | 1     |
| 1:A:51:ILE:CG2  | 1:A:94:LEU:HD22 | 0.45     | 2.38        | 15     | 1     |
| 1:A:3:ILE:N     | 1:A:3:ILE:CD1   | 0.45     | 2.79        | 1      | 5     |
| 1:A:83:ASP:CB   | 1:A:89:ILE:HG12 | 0.45     | 2.41        | 6      | 4     |
| 1:A:2:ASP:CB    | 1:A:4:LYS:HE3   | 0.45     | 2.41        | 7      | 1     |
| 1:A:26:PHE:C    | 1:A:26:PHE:CD1  | 0.45     | 2.95        | 8      | 1     |
| 1:A:72:SER:OG   | 1:A:73:MET:N    | 0.45     | 2.48        | 13     | 1     |
| 1:A:1:MET:HG2   | 1:A:5:SER:HB2   | 0.45     | 1.88        | 14     | 1     |
| 1:A:8:LEU:O     | 1:A:12:LEU:N    | 0.45     | 2.50        | 14     | 1     |
| 1:A:93:LYS:NZ   | 1:A:93:LYS:HB3  | 0.45     | 2.26        | 2      | 1     |
| 1:A:33:GLN:O    | 1:A:37:LYS:HD3  | 0.45     | 2.12        | 13     | 2     |
| 1:A:82:LYS:O    | 1:A:86:ASN:CG   | 0.45     | 2.60        | 15     | 2     |
| 1:A:1:MET:CG    | 1:A:39:THR:HA   | 0.45     | 2.42        | 5      | 1     |
| 1:A:81:GLN:O    | 1:A:85:LYS:CG   | 0.45     | 2.64        | 8      | 1     |
| 1:A:1:MET:HE1   | 1:A:9:TYR:CE1   | 0.45     | 2.47        | 10     | 1     |
| 1:A:1:MET:HG2   | 1:A:5:SER:C     | 0.45     | 2.37        | 14     | 3     |
| 1:A:84:ILE:CD1  | 1:A:89:ILE:HG13 | 0.44     | 2.42        | 9      | 4     |
| 1:A:90:ASP:CA   | 1:A:93:LYS:HE2  | 0.44     | 2.40        | 1      | 1     |
| 1:A:33:GLN:O    | 1:A:37:LYS:N    | 0.44     | 2.51        | 5      | 1     |
| 1:A:101:LYS:HB3 | 1:A:103:LEU:HG  | 0.44     | 1.89        | 7      | 2     |
| 1:A:103:LEU:N   | 1:A:103:LEU:CD2 | 0.44     | 2.76        | 9      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:45:ASN:O    | 1:A:49:GLU:CG   | 0.44     | 2.65        | 12     | 1     |
| 1:A:47:TYR:OH   | 1:A:89:ILE:CG1  | 0.44     | 2.65        | 10     | 3     |
| 1:A:18:ASP:N    | 1:A:18:ASP:OD1  | 0.44     | 2.49        | 3      | 1     |
| 1:A:76:ILE:HG22 | 1:A:77:TYR:N    | 0.44     | 2.25        | 8      | 1     |
| 1:A:24:ASN:CG   | 1:A:27:LEU:HB2  | 0.44     | 2.37        | 9      | 1     |
| 1:A:12:LEU:HD12 | 1:A:12:LEU:C    | 0.44     | 2.38        | 11     | 1     |
| 1:A:54:LEU:HD13 | 1:A:76:ILE:CG2  | 0.44     | 2.43        | 12     | 1     |
| 1:A:48:ILE:HD11 | 1:A:93:LYS:NZ   | 0.44     | 2.27        | 1      | 1     |
| 1:A:8:LEU:CD1   | 1:A:38:LEU:CD2  | 0.44     | 2.96        | 2      | 1     |
| 1:A:58:ILE:HD13 | 1:A:77:TYR:CB   | 0.44     | 2.39        | 12     | 3     |
| 1:A:4:LYS:HE2   | 1:A:5:SER:OG    | 0.44     | 2.12        | 2      | 1     |
| 1:A:19:PRO:HA   | 1:A:22:LYS:HG2  | 0.44     | 1.89        | 12     | 8     |
| 1:A:5:SER:HA    | 1:A:8:LEU:HG    | 0.44     | 1.88        | 5      | 1     |
| 1:A:48:ILE:HG23 | 1:A:94:LEU:HA   | 0.44     | 1.87        | 3      | 1     |
| 1:A:83:ASP:CB   | 1:A:89:ILE:CD1  | 0.44     | 2.95        | 2      | 2     |
| 1:A:52:SER:HB3  | 1:A:97:TYR:CD2  | 0.44     | 2.47        | 8      | 1     |
| 1:A:48:ILE:HG13 | 1:A:94:LEU:HG   | 0.44     | 1.89        | 15     | 1     |
| 1:A:94:LEU:O    | 1:A:98:GLU:CG   | 0.44     | 2.66        | 10     | 3     |
| 1:A:4:LYS:CE    | 1:A:5:SER:H     | 0.44     | 2.26        | 15     | 1     |
| 1:A:20:GLU:HB2  | 1:A:70:PRO:CB   | 0.44     | 2.42        | 8      | 1     |
| 1:A:97:TYR:CD1  | 1:A:101:LYS:HD3 | 0.44     | 2.47        | 13     | 1     |
| 1:A:94:LEU:O    | 1:A:98:GLU:N    | 0.44     | 2.48        | 5      | 3     |
| 1:A:5:SER:O     | 1:A:8:LEU:HG    | 0.44     | 2.13        | 14     | 1     |
| 1:A:47:TYR:CZ   | 1:A:51:ILE:HG12 | 0.44     | 2.48        | 14     | 1     |
| 1:A:48:ILE:CG1  | 1:A:93:LYS:HD3  | 0.43     | 2.43        | 2      | 3     |
| 1:A:47:TYR:CE1  | 1:A:48:ILE:HD13 | 0.43     | 2.47        | 5      | 1     |
| 1:A:50:VAL:HG22 | 1:A:54:LEU:CD2  | 0.43     | 2.43        | 5      | 1     |
| 1:A:2:ASP:HB3   | 1:A:4:LYS:HE2   | 0.43     | 1.89        | 14     | 4     |
| 1:A:16:TYR:O    | 1:A:22:LYS:HD3  | 0.43     | 2.12        | 6      | 1     |
| 1:A:97:TYR:CZ   | 1:A:101:LYS:HD2 | 0.43     | 2.48        | 15     | 3     |
| 1:A:52:SER:HB2  | 1:A:97:TYR:HE2  | 0.43     | 1.72        | 9      | 1     |
| 1:A:84:ILE:HG22 | 1:A:85:LYS:HE2  | 0.43     | 1.90        | 10     | 1     |
| 1:A:25:GLU:O    | 1:A:29:LYS:CB   | 0.43     | 2.66        | 6      | 1     |
| 1:A:44:GLU:HG2  | 1:A:93:LYS:NZ   | 0.43     | 2.28        | 10     | 1     |
| 1:A:84:ILE:HD13 | 1:A:89:ILE:CD1  | 0.43     | 2.42        | 10     | 1     |
| 1:A:96:LYS:HE3  | 1:A:99:ILE:HD12 | 0.43     | 1.90        | 12     | 1     |
| 1:A:34:CYS:SG   | 1:A:54:LEU:HD11 | 0.43     | 2.53        | 1      | 1     |
| 1:A:33:GLN:O    | 1:A:37:LYS:NZ   | 0.43     | 2.47        | 6      | 1     |
| 1:A:9:TYR:CE1   | 1:A:35:ALA:CB   | 0.43     | 2.91        | 7      | 1     |
| 1:A:44:GLU:CG   | 1:A:93:LYS:CE   | 0.43     | 2.96        | 10     | 1     |
| 1:A:94:LEU:O    | 1:A:98:GLU:CB   | 0.43     | 2.66        | 10     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:12:LEU:HD11 | 1:A:35:ALA:CB   | 0.43     | 2.33        | 11     | 1     |
| 1:A:58:ILE:HD12 | 1:A:73:MET:HA   | 0.43     | 1.89        | 13     | 1     |
| 1:A:77:TYR:O    | 1:A:80:ILE:HD11 | 0.43     | 2.14        | 13     | 2     |
| 1:A:22:LYS:HA   | 1:A:22:LYS:CE   | 0.43     | 2.44        | 8      | 1     |
| 1:A:58:ILE:C    | 1:A:73:MET:HE2  | 0.43     | 2.38        | 12     | 1     |
| 1:A:77:TYR:CD1  | 1:A:77:TYR:O    | 0.43     | 2.72        | 15     | 1     |
| 1:A:79:GLN:CA   | 1:A:82:LYS:HG2  | 0.43     | 2.43        | 1      | 1     |
| 1:A:84:ILE:CD1  | 1:A:89:ILE:CG1  | 0.43     | 2.97        | 1      | 5     |
| 1:A:48:ILE:O    | 1:A:94:LEU:CD2  | 0.43     | 2.66        | 2      | 1     |
| 1:A:96:LYS:CE   | 1:A:99:ILE:CD1  | 0.43     | 2.95        | 3      | 1     |
| 1:A:98:GLU:CG   | 1:A:103:LEU:CD1 | 0.43     | 2.97        | 4      | 1     |
| 1:A:2:ASP:HB3   | 1:A:4:LYS:HE3   | 0.43     | 1.89        | 7      | 1     |
| 1:A:97:TYR:CE1  | 1:A:101:LYS:HE2 | 0.43     | 2.49        | 4      | 1     |
| 1:A:16:TYR:O    | 1:A:22:LYS:HD2  | 0.43     | 2.11        | 6      | 1     |
| 1:A:76:ILE:CG2  | 1:A:80:ILE:CD1  | 0.43     | 2.97        | 6      | 1     |
| 1:A:95:ARG:O    | 1:A:99:ILE:CD1  | 0.43     | 2.67        | 15     | 4     |
| 1:A:44:GLU:O    | 1:A:48:ILE:HG12 | 0.43     | 2.13        | 7      | 1     |
| 1:A:90:ASP:O    | 1:A:93:LYS:N    | 0.43     | 2.52        | 7      | 4     |
| 1:A:80:ILE:O    | 1:A:84:ILE:CG1  | 0.43     | 2.67        | 8      | 1     |
| 1:A:16:TYR:O    | 1:A:22:LYS:CE   | 0.43     | 2.67        | 15     | 1     |
| 1:A:52:SER:HB3  | 1:A:97:TYR:OH   | 0.43     | 2.13        | 15     | 1     |
| 1:A:90:ASP:O    | 1:A:92:GLU:N    | 0.43     | 2.52        | 15     | 1     |
| 1:A:27:LEU:N    | 1:A:27:LEU:CD1  | 0.43     | 2.82        | 10     | 1     |
| 1:A:82:LYS:O    | 1:A:86:ASN:HB3  | 0.43     | 2.14        | 15     | 2     |
| 1:A:4:LYS:CE    | 1:A:5:SER:OG    | 0.43     | 2.67        | 5      | 3     |
| 1:A:58:ILE:HD11 | 1:A:73:MET:HE2  | 0.43     | 1.90        | 2      | 1     |
| 1:A:85:LYS:HA   | 1:A:85:LYS:CE   | 0.43     | 2.44        | 2      | 2     |
| 1:A:1:MET:CE    | 1:A:38:LEU:HB2  | 0.43     | 2.44        | 5      | 3     |
| 1:A:1:MET:HG2   | 1:A:5:SER:CB    | 0.43     | 2.44        | 12     | 2     |
| 1:A:73:MET:HA   | 1:A:73:MET:HE3  | 0.42     | 1.91        | 5      | 1     |
| 1:A:7:THR:O     | 1:A:11:ASN:HB2  | 0.42     | 2.14        | 14     | 2     |
| 1:A:1:MET:SD    | 1:A:6:GLN:CG    | 0.42     | 3.07        | 3      | 3     |
| 1:A:55:SER:O    | 1:A:77:TYR:CD1  | 0.42     | 2.72        | 5      | 1     |
| 1:A:75:THR:O    | 1:A:79:GLN:N    | 0.42     | 2.51        | 13     | 2     |
| 1:A:76:ILE:O    | 1:A:80:ILE:HD13 | 0.42     | 2.14        | 10     | 1     |
| 1:A:9:TYR:OH    | 1:A:39:THR:HG23 | 0.42     | 2.13        | 14     | 1     |
| 1:A:77:TYR:HA   | 1:A:80:ILE:CD1  | 0.42     | 2.44        | 3      | 1     |
| 1:A:20:GLU:CB   | 1:A:70:PRO:HG3  | 0.42     | 2.44        | 5      | 1     |
| 1:A:90:ASP:HB3  | 1:A:93:LYS:HD3  | 0.42     | 1.90        | 9      | 1     |
| 1:A:15:ALA:C    | 1:A:17:LYS:N    | 0.42     | 2.75        | 3      | 2     |
| 1:A:2:ASP:CB    | 1:A:4:LYS:CD    | 0.42     | 2.97        | 15     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:8:LEU:N     | 1:A:8:LEU:CD1    | 0.42     | 2.79        | 4      | 1     |
| 1:A:13:SER:O    | 1:A:17:LYS:HG3   | 0.42     | 2.14        | 7      | 1     |
| 1:A:37:LYS:CB   | 1:A:50:VAL:HG21  | 0.42     | 2.44        | 14     | 2     |
| 1:A:30:LEU:O    | 1:A:34:CYS:CB    | 0.42     | 2.67        | 15     | 1     |
| 1:A:46:SER:O    | 1:A:50:VAL:CG2   | 0.42     | 2.65        | 15     | 1     |
| 1:A:50:VAL:HA   | 1:A:53:LEU:HG    | 0.42     | 1.91        | 15     | 1     |
| 1:A:51:ILE:HD13 | 1:A:51:ILE:HA    | 0.42     | 1.71        | 12     | 3     |
| 1:A:5:SER:O     | 1:A:9:TYR:HB2    | 0.42     | 2.14        | 4      | 2     |
| 1:A:52:SER:CB   | 1:A:94:LEU:HD23  | 0.42     | 2.44        | 4      | 1     |
| 1:A:48:ILE:HA   | 1:A:51:ILE:HB    | 0.42     | 1.91        | 1      | 2     |
| 1:A:25:GLU:O    | 1:A:29:LYS:CE    | 0.42     | 2.67        | 13     | 1     |
| 1:A:94:LEU:HD12 | 1:A:94:LEU:O     | 0.42     | 2.14        | 3      | 1     |
| 1:A:71:SER:O    | 1:A:73:MET:N     | 0.42     | 2.50        | 4      | 1     |
| 1:A:103:LEU:H   | 1:A:103:LEU:HD12 | 0.42     | 1.75        | 6      | 1     |
| 1:A:27:LEU:HD11 | 1:A:73:MET:SD    | 0.42     | 2.55        | 8      | 1     |
| 1:A:47:TYR:CE1  | 1:A:89:ILE:HG12  | 0.42     | 2.50        | 10     | 1     |
| 1:A:33:GLN:OE1  | 1:A:37:LYS:CG    | 0.42     | 2.67        | 12     | 1     |
| 1:A:101:LYS:N   | 1:A:101:LYS:CD   | 0.42     | 2.83        | 13     | 1     |
| 1:A:7:THR:O     | 1:A:11:ASN:CB    | 0.42     | 2.68        | 3      | 4     |
| 1:A:8:LEU:N     | 1:A:8:LEU:HD22   | 0.42     | 2.30        | 4      | 1     |
| 1:A:58:ILE:O    | 1:A:58:ILE:CD1   | 0.42     | 2.67        | 4      | 1     |
| 1:A:1:MET:HE1   | 1:A:38:LEU:CB    | 0.42     | 2.41        | 12     | 1     |
| 1:A:71:SER:C    | 1:A:73:MET:N     | 0.42     | 2.78        | 12     | 7     |
| 1:A:26:PHE:CG   | 1:A:27:LEU:N     | 0.42     | 2.87        | 5      | 1     |
| 1:A:16:TYR:HB2  | 1:A:31:VAL:CG1   | 0.42     | 2.45        | 14     | 1     |
| 1:A:58:ILE:HG12 | 1:A:73:MET:HE2   | 0.41     | 1.91        | 5      | 1     |
| 1:A:2:ASP:CB    | 1:A:4:LYS:CE     | 0.41     | 2.98        | 6      | 3     |
| 1:A:22:LYS:NZ   | 1:A:22:LYS:CB    | 0.41     | 2.83        | 8      | 1     |
| 1:A:84:ILE:HD13 | 1:A:89:ILE:CG1   | 0.41     | 2.45        | 9      | 1     |
| 1:A:26:PHE:CE1  | 1:A:30:LEU:CD1   | 0.41     | 3.03        | 14     | 1     |
| 1:A:55:SER:C    | 1:A:77:TYR:CE2   | 0.41     | 2.98        | 2      | 2     |
| 1:A:1:MET:SD    | 1:A:1:MET:N      | 0.41     | 2.91        | 3      | 1     |
| 1:A:11:ASN:OD1  | 1:A:12:LEU:N     | 0.41     | 2.53        | 4      | 1     |
| 1:A:16:TYR:CG   | 1:A:32:VAL:HG22  | 0.41     | 2.50        | 4      | 1     |
| 1:A:2:ASP:CB    | 1:A:4:LYS:NZ     | 0.41     | 2.83        | 7      | 1     |
| 1:A:18:ASP:CG   | 1:A:72:SER:CB    | 0.41     | 2.93        | 7      | 1     |
| 1:A:97:TYR:CZ   | 1:A:101:LYS:HG3  | 0.41     | 2.50        | 10     | 1     |
| 1:A:1:MET:HE2   | 1:A:39:THR:CA    | 0.41     | 2.44        | 14     | 1     |
| 1:A:84:ILE:HG13 | 1:A:91:THR:CG2   | 0.41     | 2.44        | 12     | 2     |
| 1:A:9:TYR:CE1   | 1:A:35:ALA:O     | 0.41     | 2.74        | 8      | 2     |
| 1:A:1:MET:CG    | 1:A:5:SER:C      | 0.41     | 2.94        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:49:GLU:OE1  | 1:A:97:TYR:CE1  | 0.41     | 2.74        | 9      | 1     |
| 1:A:8:LEU:HD11  | 1:A:38:LEU:CD2  | 0.41     | 2.45        | 10     | 1     |
| 1:A:1:MET:SD    | 1:A:38:LEU:C    | 0.41     | 3.03        | 12     | 1     |
| 1:A:52:SER:OG   | 1:A:103:LEU:CD1 | 0.41     | 2.69        | 14     | 1     |
| 1:A:48:ILE:CD1  | 1:A:94:LEU:CD2  | 0.41     | 2.99        | 7      | 1     |
| 1:A:58:ILE:CD1  | 1:A:73:MET:O    | 0.41     | 2.68        | 7      | 1     |
| 1:A:44:GLU:CG   | 1:A:93:LYS:NZ   | 0.41     | 2.83        | 11     | 2     |
| 1:A:76:ILE:O    | 1:A:80:ILE:HG12 | 0.41     | 2.16        | 15     | 2     |
| 1:A:97:TYR:O    | 1:A:101:LYS:HD3 | 0.41     | 2.15        | 13     | 1     |
| 1:A:90:ASP:CA   | 1:A:93:LYS:CE   | 0.41     | 2.98        | 8      | 1     |
| 1:A:21:VAL:HA   | 1:A:24:ASN:ND2  | 0.41     | 2.30        | 9      | 1     |
| 1:A:44:GLU:HA   | 1:A:47:TYR:CD1  | 0.41     | 2.49        | 9      | 1     |
| 1:A:49:GLU:C    | 1:A:53:LEU:HG   | 0.41     | 2.40        | 9      | 1     |
| 1:A:47:TYR:O    | 1:A:51:ILE:CG1  | 0.41     | 2.68        | 15     | 3     |
| 1:A:55:SER:O    | 1:A:56:ARG:HB3  | 0.41     | 2.15        | 6      | 1     |
| 1:A:22:LYS:HE2  | 1:A:22:LYS:CA   | 0.41     | 2.46        | 8      | 1     |
| 1:A:72:SER:O    | 1:A:73:MET:SD   | 0.41     | 2.78        | 8      | 1     |
| 1:A:81:GLN:HA   | 1:A:84:ILE:HB   | 0.41     | 1.92        | 8      | 1     |
| 1:A:58:ILE:CD1  | 1:A:77:TYR:HB2  | 0.41     | 2.45        | 15     | 1     |
| 1:A:41:SER:C    | 1:A:43:SER:N    | 0.41     | 2.77        | 15     | 2     |
| 1:A:80:ILE:O    | 1:A:84:ILE:CB   | 0.41     | 2.64        | 3      | 1     |
| 1:A:47:TYR:CD1  | 1:A:47:TYR:C    | 0.41     | 2.98        | 8      | 1     |
| 1:A:1:MET:CE    | 1:A:39:THR:N    | 0.41     | 2.83        | 9      | 1     |
| 1:A:30:LEU:O    | 1:A:34:CYS:HB2  | 0.41     | 2.16        | 14     | 1     |
| 1:A:4:LYS:O     | 1:A:8:LEU:HG    | 0.41     | 2.16        | 1      | 1     |
| 1:A:83:ASP:HB3  | 1:A:89:ILE:CD1  | 0.41     | 2.45        | 2      | 1     |
| 1:A:1:MET:SD    | 1:A:5:SER:HB3   | 0.41     | 2.55        | 4      | 1     |
| 1:A:26:PHE:O    | 1:A:29:LYS:HG2  | 0.41     | 2.16        | 5      | 1     |
| 1:A:9:TYR:CD1   | 1:A:9:TYR:C     | 0.41     | 2.96        | 9      | 1     |
| 1:A:84:ILE:HD13 | 1:A:84:ILE:N    | 0.41     | 2.30        | 9      | 1     |
| 1:A:57:GLY:O    | 1:A:58:ILE:C    | 0.41     | 2.64        | 14     | 1     |
| 1:A:50:VAL:O    | 1:A:54:LEU:CG   | 0.41     | 2.69        | 5      | 3     |
| 1:A:12:LEU:O    | 1:A:31:VAL:HG12 | 0.41     | 2.15        | 3      | 1     |
| 1:A:11:ASN:ND2  | 1:A:76:ILE:HG13 | 0.41     | 2.31        | 4      | 1     |
| 1:A:1:MET:HG3   | 1:A:39:THR:CA   | 0.41     | 2.46        | 5      | 1     |
| 1:A:28:SER:O    | 1:A:32:VAL:N    | 0.41     | 2.52        | 8      | 1     |
| 1:A:55:SER:HA   | 1:A:77:TYR:CE2  | 0.41     | 2.51        | 13     | 1     |
| 1:A:52:SER:OG   | 1:A:94:LEU:HD22 | 0.41     | 2.16        | 2      | 1     |
| 1:A:48:ILE:HD11 | 1:A:90:ASP:HB2  | 0.41     | 1.93        | 8      | 1     |
| 1:A:90:ASP:CB   | 1:A:93:LYS:HD3  | 0.41     | 2.45        | 11     | 1     |
| 1:A:2:ASP:HB3   | 1:A:4:LYS:CD    | 0.41     | 2.46        | 15     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:37:LYS:N    | 1:A:37:LYS:HD3   | 0.40     | 2.31        | 1      | 1     |
| 1:A:16:TYR:CE1  | 1:A:28:SER:OG    | 0.40     | 2.73        | 3      | 1     |
| 1:A:25:GLU:O    | 1:A:29:LYS:HD3   | 0.40     | 2.16        | 3      | 1     |
| 1:A:15:ALA:CB   | 1:A:72:SER:HB2   | 0.40     | 2.46        | 4      | 1     |
| 1:A:81:GLN:CA   | 1:A:84:ILE:HG12  | 0.40     | 2.45        | 10     | 1     |
| 1:A:47:TYR:CE1  | 1:A:51:ILE:HG12  | 0.40     | 2.50        | 11     | 1     |
| 1:A:91:THR:N    | 1:A:94:LEU:HD13  | 0.40     | 2.31        | 12     | 1     |
| 1:A:48:ILE:HG12 | 1:A:93:LYS:CG    | 0.40     | 2.46        | 13     | 1     |
| 1:A:56:ARG:N    | 1:A:77:TYR:CE2   | 0.40     | 2.88        | 13     | 1     |
| 1:A:29:LYS:CG   | 1:A:30:LEU:N     | 0.40     | 2.84        | 15     | 1     |
| 1:A:2:ASP:OD1   | 1:A:2:ASP:N      | 0.40     | 2.54        | 9      | 1     |
| 1:A:44:GLU:HG3  | 1:A:93:LYS:NZ    | 0.40     | 2.30        | 9      | 1     |
| 1:A:48:ILE:O    | 1:A:51:ILE:CG2   | 0.40     | 2.65        | 11     | 1     |
| 1:A:38:LEU:C    | 1:A:40:ALA:N     | 0.40     | 2.80        | 12     | 2     |
| 1:A:89:ILE:HG21 | 1:A:94:LEU:CD2   | 0.40     | 2.43        | 12     | 1     |
| 1:A:1:MET:SD    | 1:A:41:SER:HB2   | 0.40     | 2.55        | 15     | 1     |
| 1:A:52:SER:OG   | 1:A:103:LEU:HD21 | 0.40     | 2.16        | 15     | 1     |
| 1:A:48:ILE:CD1  | 1:A:89:ILE:CG2   | 0.40     | 2.99        | 3      | 1     |
| 1:A:21:VAL:HG13 | 1:A:24:ASN:HD21  | 0.40     | 1.77        | 5      | 1     |
| 1:A:84:ILE:HD12 | 1:A:89:ILE:CG2   | 0.40     | 2.46        | 8      | 1     |
| 1:A:90:ASP:OD2  | 1:A:93:LYS:HD2   | 0.40     | 2.16        | 8      | 1     |
| 1:A:52:SER:OG   | 1:A:97:TYR:CD2   | 0.40     | 2.74        | 9      | 1     |
| 1:A:2:ASP:HB2   | 1:A:4:LYS:NZ     | 0.40     | 2.31        | 13     | 1     |
| 1:A:28:SER:C    | 1:A:32:VAL:HG23  | 0.40     | 2.38        | 14     | 1     |
| 1:A:48:ILE:HG23 | 1:A:94:LEU:CA    | 0.40     | 2.47        | 3      | 1     |
| 1:A:1:MET:CB    | 1:A:38:LEU:O     | 0.40     | 2.69        | 6      | 1     |
| 1:A:90:ASP:C    | 1:A:92:GLU:H     | 0.40     | 2.23        | 15     | 1     |
| 1:A:1:MET:HG2   | 1:A:9:TYR:CD2    | 0.40     | 2.51        | 3      | 1     |
| 1:A:8:LEU:H     | 1:A:8:LEU:HD22   | 0.40     | 1.76        | 4      | 1     |
| 1:A:1:MET:HE2   | 1:A:1:MET:HB2    | 0.40     | 1.79        | 12     | 1     |
| 1:A:12:LEU:HD12 | 1:A:38:LEU:HG    | 0.40     | 1.93        | 12     | 1     |
| 1:A:27:LEU:O    | 1:A:31:VAL:CG2   | 0.40     | 2.69        | 13     | 1     |
| 1:A:48:ILE:HG13 | 1:A:93:LYS:HG2   | 0.40     | 1.93        | 14     | 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     | 91/111 (82%)    | 77±2 (85±2%) | 11±2 (12±2%) | 2±1 (3±1%) | 6           | 42 |
| All | All   | 1365/1665 (82%) | 1162 (85%)   | 167 (12%)    | 36 (3%)    | 6           | 42 |

All 13 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     | 72  | SER  | 14             |
| 1   | A     | 56  | ARG  | 4              |
| 1   | A     | 58  | ILE  | 4              |
| 1   | A     | 74  | LEU  | 3              |
| 1   | A     | 2   | ASP  | 2              |
| 1   | A     | 40  | ALA  | 2              |
| 1   | A     | 71  | SER  | 1              |
| 1   | A     | 55  | SER  | 1              |
| 1   | A     | 57  | GLY  | 1              |
| 1   | A     | 76  | ILE  | 1              |
| 1   | A     | 32  | VAL  | 1              |
| 1   | A     | 27  | LEU  | 1              |
| 1   | A     | 91  | THR  | 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     | 83/102 (81%)    | 44±3 (53±4%) | 39±3 (47±4%) | 0           | 2 |
| All | All   | 1245/1530 (81%) | 655 (53%)    | 590 (47%)    | 0           | 2 |

All 67 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     | 3   | ILE  | 15             |
| 1   | A     | 4   | LYS  | 15             |
| 1   | A     | 6   | GLN  | 15             |
| 1   | A     | 7   | THR  | 15             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 47  | TYR  | 15             |
| 1   | A     | 48  | ILE  | 15             |
| 1   | A     | 51  | ILE  | 15             |
| 1   | A     | 53  | LEU  | 15             |
| 1   | A     | 80  | ILE  | 15             |
| 1   | A     | 91  | THR  | 15             |
| 1   | A     | 8   | LEU  | 14             |
| 1   | A     | 28  | SER  | 14             |
| 1   | A     | 30  | LEU  | 14             |
| 1   | A     | 75  | THR  | 14             |
| 1   | A     | 82  | LYS  | 14             |
| 1   | A     | 95  | ARG  | 14             |
| 1   | A     | 54  | LEU  | 14             |
| 1   | A     | 1   | MET  | 13             |
| 1   | A     | 58  | ILE  | 13             |
| 1   | A     | 78  | THR  | 12             |
| 1   | A     | 84  | ILE  | 12             |
| 1   | A     | 93  | LYS  | 12             |
| 1   | A     | 103 | LEU  | 12             |
| 1   | A     | 33  | GLN  | 11             |
| 1   | A     | 101 | LYS  | 11             |
| 1   | A     | 2   | ASP  | 10             |
| 1   | A     | 49  | GLU  | 10             |
| 1   | A     | 85  | LYS  | 10             |
| 1   | A     | 39  | THR  | 10             |
| 1   | A     | 44  | GLU  | 10             |
| 1   | A     | 56  | ARG  | 9              |
| 1   | A     | 73  | MET  | 9              |
| 1   | A     | 90  | ASP  | 9              |
| 1   | A     | 38  | LEU  | 9              |
| 1   | A     | 17  | LYS  | 8              |
| 1   | A     | 74  | LEU  | 8              |
| 1   | A     | 92  | GLU  | 8              |
| 1   | A     | 55  | SER  | 8              |
| 1   | A     | 22  | LYS  | 7              |
| 1   | A     | 37  | LYS  | 7              |
| 1   | A     | 94  | LEU  | 7              |
| 1   | A     | 27  | LEU  | 7              |
| 1   | A     | 71  | SER  | 6              |
| 1   | A     | 72  | SER  | 6              |
| 1   | A     | 25  | GLU  | 6              |
| 1   | A     | 16  | TYR  | 5              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 42  | ASN  | 5              |
| 1   | A     | 77  | TYR  | 5              |
| 1   | A     | 9   | TYR  | 5              |
| 1   | A     | 24  | ASN  | 5              |
| 1   | A     | 45  | ASN  | 5              |
| 1   | A     | 79  | GLN  | 5              |
| 1   | A     | 52  | SER  | 5              |
| 1   | A     | 5   | SER  | 4              |
| 1   | A     | 76  | ILE  | 4              |
| 1   | A     | 14  | GLU  | 4              |
| 1   | A     | 12  | LEU  | 4              |
| 1   | A     | 81  | GLN  | 4              |
| 1   | A     | 96  | LYS  | 3              |
| 1   | A     | 18  | ASP  | 3              |
| 1   | A     | 29  | LYS  | 3              |
| 1   | A     | 26  | PHE  | 3              |
| 1   | A     | 31  | VAL  | 3              |
| 1   | A     | 97  | TYR  | 3              |
| 1   | A     | 43  | SER  | 2              |
| 1   | A     | 13  | SER  | 1              |
| 1   | A     | 50  | VAL  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided