



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 12:26 AM UTC

PDB ID : 1Z3K / pdb\_00001z3k  
Title : Structural Insight into the Binding Diversity between the Tyr-Phosphorylated Human EphrinBs and Nck2 SH2 Domain  
Authors : Ran, X.; Song, J.  
Deposited on : 2005-03-14

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

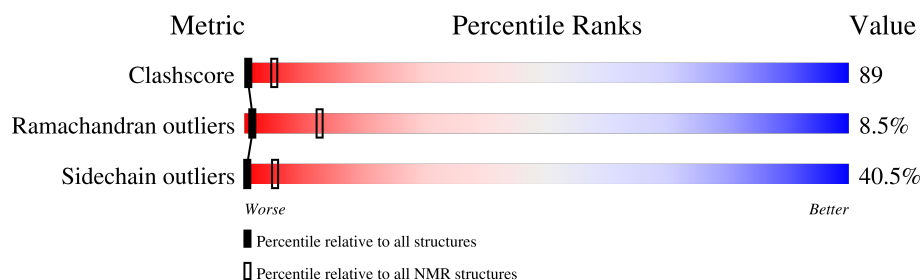
# 1 Overall quality at a glance

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     | 98     | <div> <div></div> <div>20%</div> <div>48%</div> <div>27%</div> <div>5%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 6 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:4, A:8-A:98 (93) | 1.30              | 6            |

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

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

There is only 1 type of molecule in this entry. The entry contains 1589 atoms, of which 784 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytoplasmic protein NCK2.

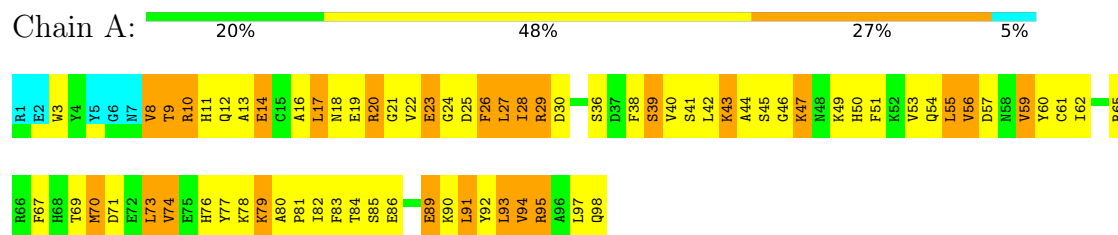
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 98       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1589  | 506 | 784 | 145 | 151 | 3 |       |

## 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: Cytoplasmic protein NCK2

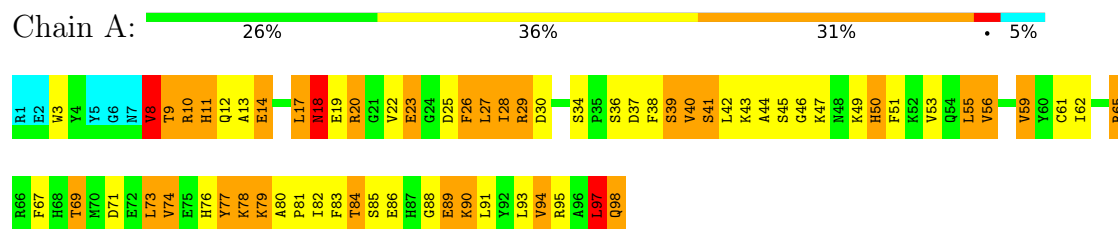


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

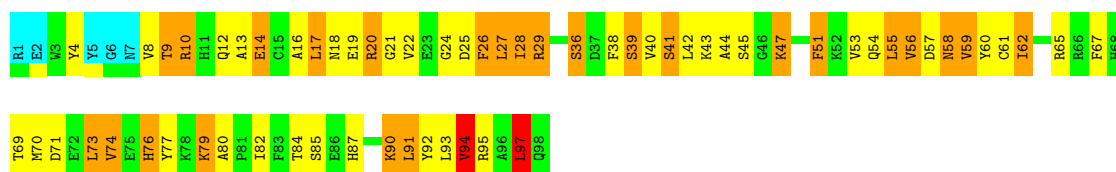
- Molecule 1: Cytoplasmic protein NCK2



#### 4.2.2 Score per residue for model 2

- Molecule 1: Cytoplasmic protein NCK2

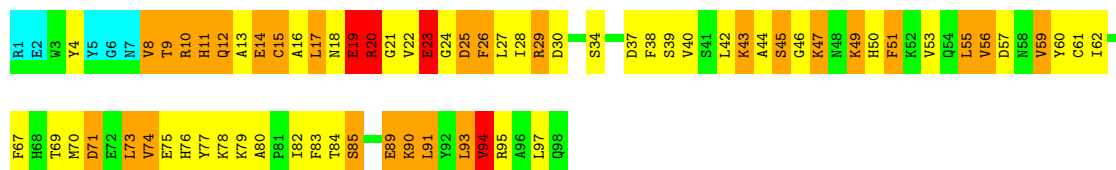




#### 4.2.3 Score per residue for model 3

- Molecule 1: Cytoplasmic protein NCK2

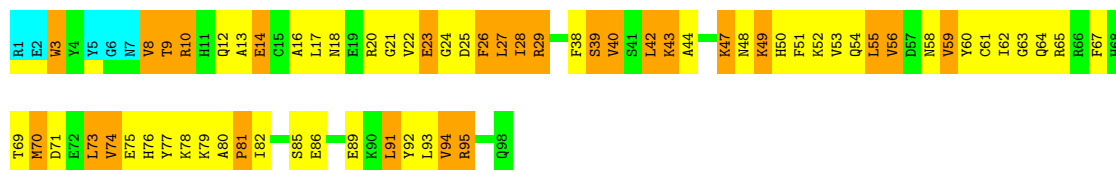
Chain A: 24% 39% 28% 5%



#### 4.2.4 Score per residue for model 4

- Molecule 1: Cytoplasmic protein NCK2

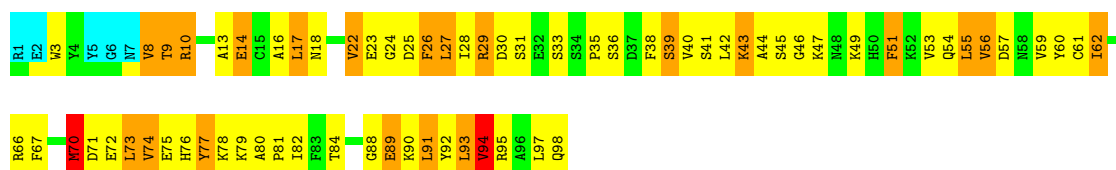
Chain A: 28% 41% 27% 5%



#### 4.2.5 Score per residue for model 5

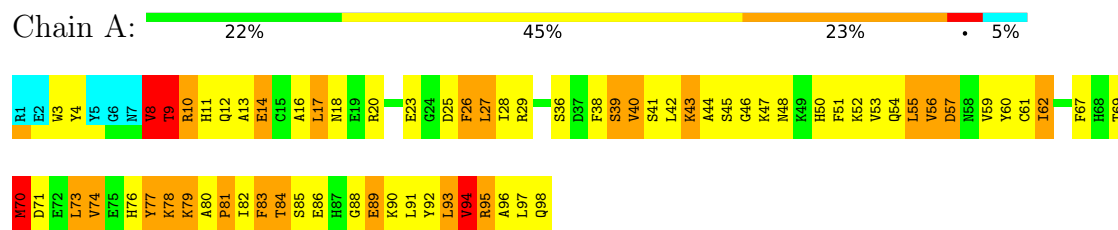
- Molecule 1: Cytoplasmic protein NCK2

Chain A: 24% 47% 21% 5%



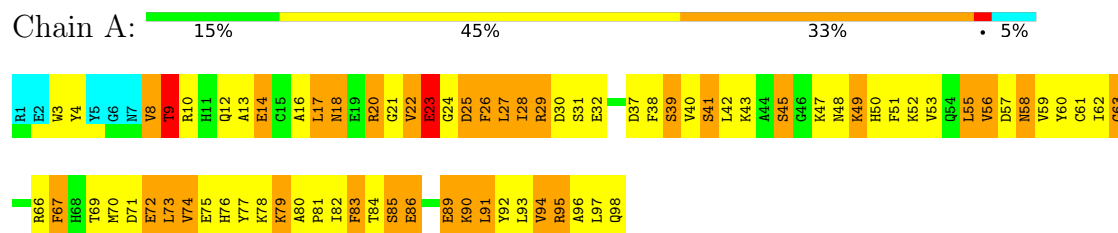
#### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Cytoplasmic protein NCK2



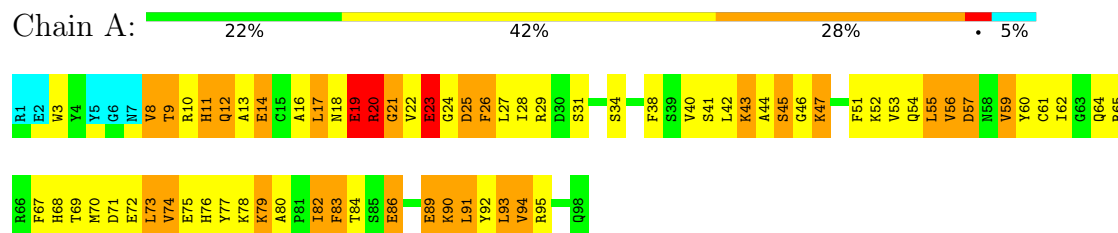
#### 4.2.7 Score per residue for model 7

- Molecule 1: Cytoplasmic protein NCK2



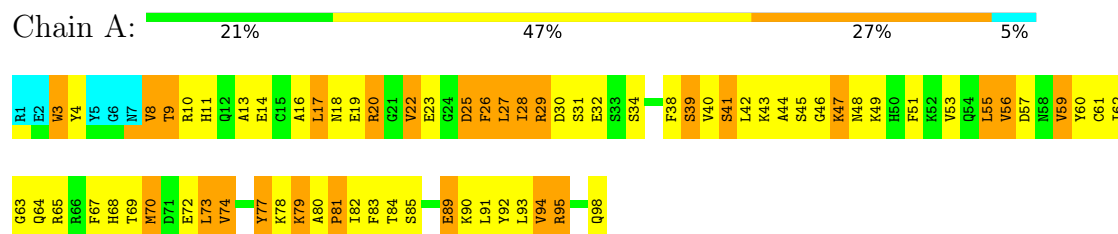
#### 4.2.8 Score per residue for model 8

- Molecule 1: Cytoplasmic protein NCK2



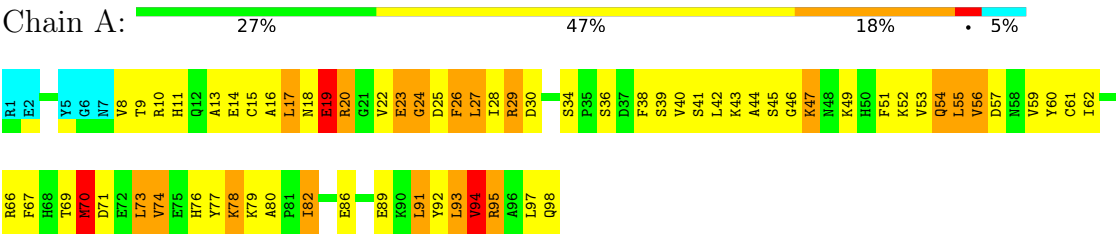
#### 4.2.9 Score per residue for model 9

- Molecule 1: Cytoplasmic protein NCK2



4.2.10 Score per residue for model 10

● Molecule 1: Cytoplasmic protein NCK2





## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures accepted by CNS program with the lowest energy*.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                       |
|-----|-------|--------------|----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                  |
| 1   | A     | 0.37±0.01    | 0±0/778 ( 0.0± 0.0%) | 0.66±0.01   | 0±0/1045 ( 0.0± 0.0%) |
| All | All   | 0.37         | 0/7780 ( 0.0%)       | 0.66        | 1/10450 ( 0.0%)       |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 81  | PRO  | N-CA-C | -5.03 | 109.44      | 114.68   | 5      | 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     | 761   | 745      | 740      | 133±13  |
| All | All   | 7610  | 7450     | 7400     | 1334    |

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 89.

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

| Atom-1          | Atom-2       | Clash(Å) | Distance(Å) | Models |       |
|-----------------|--------------|----------|-------------|--------|-------|
|                 |              |          |             | Worst  | Total |
| 1:A:82:ILE:HG23 | 1:A:91:LEU:O | 1.21     | 1.35        | 3      | 10    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:28:ILE:HG21 | 1:A:74:VAL:HG21 | 1.07     | 1.18        | 10     | 6     |
| 1:A:53:VAL:HG22 | 1:A:62:ILE:HG23 | 0.98     | 1.32        | 4      | 5     |
| 1:A:55:LEU:HD13 | 1:A:55:LEU:O    | 0.96     | 1.59        | 2      | 7     |
| 1:A:53:VAL:HG12 | 1:A:70:MET:HE2  | 0.95     | 1.38        | 4      | 2     |
| 1:A:9:THR:HG23  | 1:A:27:LEU:HD12 | 0.94     | 1.37        | 2      | 1     |
| 1:A:26:PHE:CD2  | 1:A:94:VAL:HG12 | 0.94     | 1.97        | 4      | 1     |
| 1:A:26:PHE:CG   | 1:A:42:LEU:HD13 | 0.92     | 1.98        | 9      | 9     |
| 1:A:9:THR:O     | 1:A:11:HIS:N    | 0.91     | 2.03        | 3      | 1     |
| 1:A:26:PHE:CD1  | 1:A:40:VAL:HG22 | 0.91     | 2.00        | 10     | 8     |
| 1:A:26:PHE:CE1  | 1:A:40:VAL:HG22 | 0.91     | 2.01        | 7      | 8     |
| 1:A:17:LEU:HD13 | 1:A:43:LYS:CG   | 0.88     | 1.99        | 7      | 2     |
| 1:A:28:ILE:HD11 | 1:A:74:VAL:HG11 | 0.88     | 1.42        | 9      | 1     |
| 1:A:80:ALA:CB   | 1:A:82:ILE:HD12 | 0.85     | 2.02        | 5      | 3     |
| 1:A:22:VAL:HG23 | 1:A:43:LYS:CE   | 0.85     | 2.02        | 7      | 1     |
| 1:A:82:ILE:CG2  | 1:A:91:LEU:O    | 0.85     | 2.23        | 3      | 10    |
| 1:A:26:PHE:CD2  | 1:A:42:LEU:HD22 | 0.83     | 2.08        | 7      | 8     |
| 1:A:25:ASP:O    | 1:A:42:LEU:HD12 | 0.83     | 1.73        | 2      | 9     |
| 1:A:9:THR:HA    | 1:A:13:ALA:HB2  | 0.83     | 1.48        | 1      | 3     |
| 1:A:26:PHE:CD2  | 1:A:42:LEU:HD13 | 0.83     | 2.09        | 5      | 8     |
| 1:A:26:PHE:CG   | 1:A:93:LEU:HD23 | 0.83     | 2.08        | 7      | 4     |
| 1:A:26:PHE:CB   | 1:A:42:LEU:HD13 | 0.82     | 2.03        | 2      | 9     |
| 1:A:77:TYR:HB3  | 1:A:82:ILE:HD12 | 0.82     | 1.50        | 10     | 3     |
| 1:A:9:THR:CG2   | 1:A:13:ALA:HB2  | 0.82     | 2.04        | 7      | 2     |
| 1:A:55:LEU:C    | 1:A:55:LEU:HD22 | 0.82     | 2.00        | 9      | 7     |
| 1:A:9:THR:HG23  | 1:A:27:LEU:CD1  | 0.82     | 2.03        | 2      | 1     |
| 1:A:9:THR:HG22  | 1:A:13:ALA:HB2  | 0.82     | 1.51        | 7      | 2     |
| 1:A:42:LEU:HD23 | 1:A:51:PHE:CZ   | 0.82     | 2.08        | 4      | 1     |
| 1:A:9:THR:HG23  | 1:A:29:ARG:HD3  | 0.82     | 1.51        | 10     | 2     |
| 1:A:13:ALA:HA   | 1:A:27:LEU:HD11 | 0.81     | 1.52        | 9      | 8     |
| 1:A:82:ILE:HD11 | 1:A:93:LEU:HG   | 0.81     | 1.51        | 4      | 6     |
| 1:A:28:ILE:CG2  | 1:A:74:VAL:HG21 | 0.81     | 2.04        | 10     | 3     |
| 1:A:67:PHE:CE2  | 1:A:73:LEU:HD23 | 0.81     | 2.10        | 7      | 1     |
| 1:A:27:LEU:C    | 1:A:40:VAL:HG23 | 0.81     | 2.01        | 10     | 7     |
| 1:A:26:PHE:CE2  | 1:A:93:LEU:HD23 | 0.81     | 2.11        | 8      | 6     |
| 1:A:55:LEU:HD11 | 1:A:60:TYR:CE1  | 0.81     | 2.11        | 5      | 1     |
| 1:A:22:VAL:HG23 | 1:A:43:LYS:NZ   | 0.80     | 1.90        | 7      | 1     |
| 1:A:77:TYR:HB3  | 1:A:82:ILE:HD13 | 0.80     | 1.53        | 8      | 3     |
| 1:A:14:GLU:O    | 1:A:18:ASN:N    | 0.80     | 2.13        | 3      | 10    |
| 1:A:16:ALA:C    | 1:A:17:LEU:HD23 | 0.79     | 2.01        | 6      | 7     |
| 1:A:53:VAL:CG1  | 1:A:70:MET:HE2  | 0.79     | 2.08        | 4      | 1     |
| 1:A:9:THR:HA    | 1:A:27:LEU:HD12 | 0.79     | 1.53        | 7      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:8:VAL:O     | 1:A:27:LEU:HD12 | 0.78     | 1.79        | 1      | 3     |
| 1:A:26:PHE:CD2  | 1:A:93:LEU:HD23 | 0.78     | 2.12        | 10     | 9     |
| 1:A:53:VAL:HG13 | 1:A:62:ILE:CD1  | 0.78     | 2.08        | 5      | 4     |
| 1:A:42:LEU:HD23 | 1:A:91:LEU:CD2  | 0.78     | 2.09        | 2      | 2     |
| 1:A:62:ILE:HD11 | 1:A:70:MET:HE2  | 0.78     | 1.56        | 6      | 1     |
| 1:A:42:LEU:HD23 | 1:A:91:LEU:HD23 | 0.77     | 1.57        | 2      | 1     |
| 1:A:61:CYS:O    | 1:A:62:ILE:HD13 | 0.77     | 1.80        | 8      | 3     |
| 1:A:26:PHE:CD1  | 1:A:42:LEU:CD1  | 0.77     | 2.68        | 4      | 1     |
| 1:A:8:VAL:HA    | 1:A:12:GLN:CB   | 0.76     | 2.10        | 3      | 1     |
| 1:A:53:VAL:HG13 | 1:A:62:ILE:HD13 | 0.76     | 1.56        | 1      | 6     |
| 1:A:62:ILE:HD13 | 1:A:73:LEU:HD21 | 0.76     | 1.56        | 4      | 1     |
| 1:A:9:THR:OG1   | 1:A:27:LEU:HD12 | 0.76     | 1.80        | 8      | 2     |
| 1:A:22:VAL:HG23 | 1:A:43:LYS:HE3  | 0.75     | 1.57        | 7      | 1     |
| 1:A:62:ILE:HG21 | 1:A:81:PRO:HD3  | 0.74     | 1.59        | 9      | 2     |
| 1:A:36:SER:OG   | 1:A:55:LEU:HD12 | 0.74     | 1.82        | 5      | 1     |
| 1:A:17:LEU:HD22 | 1:A:25:ASP:CG   | 0.74     | 2.07        | 10     | 2     |
| 1:A:26:PHE:CB   | 1:A:93:LEU:HA   | 0.74     | 2.13        | 6      | 5     |
| 1:A:82:ILE:HG23 | 1:A:91:LEU:C    | 0.74     | 2.07        | 1      | 3     |
| 1:A:9:THR:CG2   | 1:A:27:LEU:HD12 | 0.74     | 2.12        | 2      | 1     |
| 1:A:51:PHE:CZ   | 1:A:62:ILE:HG22 | 0.74     | 2.17        | 5      | 3     |
| 1:A:17:LEU:HD22 | 1:A:25:ASP:HB3  | 0.73     | 1.60        | 5      | 3     |
| 1:A:26:PHE:C    | 1:A:27:LEU:HD23 | 0.73     | 2.07        | 7      | 5     |
| 1:A:24:GLY:O    | 1:A:94:VAL:HG21 | 0.73     | 1.83        | 7      | 2     |
| 1:A:82:ILE:HD11 | 1:A:93:LEU:CD1  | 0.73     | 2.12        | 3      | 6     |
| 1:A:83:PHE:HB3  | 1:A:91:LEU:HD12 | 0.73     | 1.59        | 1      | 3     |
| 1:A:27:LEU:HD12 | 1:A:27:LEU:O    | 0.72     | 1.84        | 3      | 1     |
| 1:A:80:ALA:HB3  | 1:A:82:ILE:HG13 | 0.72     | 1.61        | 10     | 1     |
| 1:A:73:LEU:HD13 | 1:A:74:VAL:N    | 0.72     | 1.98        | 9      | 8     |
| 1:A:9:THR:CA    | 1:A:27:LEU:HD12 | 0.71     | 2.16        | 7      | 3     |
| 1:A:42:LEU:CD2  | 1:A:91:LEU:HD23 | 0.71     | 2.14        | 8      | 1     |
| 1:A:17:LEU:HD13 | 1:A:43:LYS:HG3  | 0.71     | 1.61        | 2      | 2     |
| 1:A:8:VAL:HA    | 1:A:12:GLN:HB2  | 0.70     | 1.62        | 3      | 2     |
| 1:A:26:PHE:HB2  | 1:A:42:LEU:HD13 | 0.70     | 1.61        | 2      | 9     |
| 1:A:74:VAL:HG12 | 1:A:93:LEU:HB3  | 0.70     | 1.62        | 6      | 1     |
| 1:A:62:ILE:CD1  | 1:A:73:LEU:HD21 | 0.70     | 2.16        | 7      | 2     |
| 1:A:84:THR:HG23 | 1:A:90:LYS:HG2  | 0.70     | 1.62        | 7      | 3     |
| 1:A:9:THR:HB    | 1:A:29:ARG:HD3  | 0.70     | 1.63        | 7      | 5     |
| 1:A:9:THR:CG2   | 1:A:29:ARG:HD3  | 0.70     | 2.15        | 10     | 2     |
| 1:A:13:ALA:CA   | 1:A:27:LEU:HD11 | 0.69     | 2.16        | 5      | 6     |
| 1:A:82:ILE:HG12 | 1:A:92:TYR:HA   | 0.69     | 1.63        | 5      | 4     |
| 1:A:28:ILE:HD12 | 1:A:40:VAL:CG1  | 0.69     | 2.17        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:42:LEU:HD23 | 1:A:91:LEU:HB3  | 0.69     | 1.64        | 1      | 4     |
| 1:A:77:TYR:CB   | 1:A:82:ILE:HD12 | 0.69     | 2.16        | 10     | 3     |
| 1:A:51:PHE:CE1  | 1:A:62:ILE:HG22 | 0.69     | 2.23        | 5      | 1     |
| 1:A:17:LEU:HD13 | 1:A:43:LYS:HG2  | 0.69     | 1.62        | 7      | 2     |
| 1:A:17:LEU:HD23 | 1:A:17:LEU:N    | 0.69     | 2.02        | 10     | 8     |
| 1:A:26:PHE:CD1  | 1:A:42:LEU:HD11 | 0.69     | 2.23        | 4      | 1     |
| 1:A:74:VAL:HG12 | 1:A:93:LEU:CB   | 0.69     | 2.18        | 6      | 1     |
| 1:A:80:ALA:HB3  | 1:A:82:ILE:HD12 | 0.68     | 1.65        | 3      | 4     |
| 1:A:74:VAL:HG13 | 1:A:93:LEU:HB3  | 0.68     | 1.63        | 1      | 7     |
| 1:A:8:VAL:O     | 1:A:9:THR:OG1   | 0.68     | 2.10        | 3      | 1     |
| 1:A:9:THR:HG23  | 1:A:13:ALA:HB2  | 0.68     | 1.64        | 4      | 4     |
| 1:A:62:ILE:HD12 | 1:A:73:LEU:HD21 | 0.68     | 1.64        | 7      | 1     |
| 1:A:36:SER:CB   | 1:A:55:LEU:HD12 | 0.68     | 2.19        | 2      | 1     |
| 1:A:53:VAL:HG13 | 1:A:61:CYS:O    | 0.68     | 1.88        | 10     | 1     |
| 1:A:40:VAL:HG21 | 1:A:93:LEU:CD2  | 0.68     | 2.19        | 1      | 2     |
| 1:A:73:LEU:HD22 | 1:A:80:ALA:HB2  | 0.68     | 1.64        | 4      | 2     |
| 1:A:28:ILE:HA   | 1:A:39:SER:O    | 0.67     | 1.89        | 9      | 8     |
| 1:A:84:THR:HG23 | 1:A:90:LYS:CG   | 0.67     | 2.19        | 8      | 3     |
| 1:A:94:VAL:HG22 | 1:A:95:ARG:N    | 0.67     | 2.05        | 10     | 8     |
| 1:A:27:LEU:O    | 1:A:40:VAL:HG23 | 0.67     | 1.89        | 7      | 6     |
| 1:A:9:THR:HA    | 1:A:13:ALA:CB   | 0.66     | 2.18        | 1      | 2     |
| 1:A:74:VAL:HG13 | 1:A:93:LEU:HD22 | 0.66     | 1.67        | 4      | 2     |
| 1:A:44:ALA:HB2  | 1:A:49:LYS:CG   | 0.66     | 2.20        | 9      | 1     |
| 1:A:28:ILE:HG23 | 1:A:40:VAL:HB   | 0.66     | 1.68        | 9      | 4     |
| 1:A:82:ILE:HD11 | 1:A:93:LEU:CG   | 0.66     | 2.20        | 8      | 6     |
| 1:A:55:LEU:HD23 | 1:A:59:VAL:O    | 0.66     | 1.90        | 7      | 2     |
| 1:A:80:ALA:HB1  | 1:A:93:LEU:HD11 | 0.66     | 1.67        | 9      | 2     |
| 1:A:83:PHE:CB   | 1:A:91:LEU:HD12 | 0.66     | 2.21        | 6      | 1     |
| 1:A:26:PHE:CE1  | 1:A:40:VAL:HG23 | 0.65     | 2.26        | 6      | 1     |
| 1:A:8:VAL:HG12  | 1:A:12:GLN:HB3  | 0.65     | 1.68        | 8      | 1     |
| 1:A:84:THR:HG23 | 1:A:89:GLU:C    | 0.65     | 2.16        | 6      | 2     |
| 1:A:13:ALA:O    | 1:A:17:LEU:HG   | 0.65     | 1.91        | 2      | 8     |
| 1:A:61:CYS:C    | 1:A:62:ILE:HD13 | 0.65     | 2.17        | 2      | 3     |
| 1:A:9:THR:HB    | 1:A:29:ARG:CD   | 0.65     | 2.20        | 2      | 6     |
| 1:A:17:LEU:HD12 | 1:A:43:LYS:CE   | 0.65     | 2.21        | 5      | 1     |
| 1:A:82:ILE:HD13 | 1:A:92:TYR:HA   | 0.65     | 1.67        | 10     | 1     |
| 1:A:13:ALA:CB   | 1:A:27:LEU:HD11 | 0.65     | 2.22        | 10     | 2     |
| 1:A:73:LEU:O    | 1:A:77:TYR:N    | 0.65     | 2.30        | 2      | 9     |
| 1:A:38:PHE:CD2  | 1:A:70:MET:HE3  | 0.65     | 2.27        | 9      | 1     |
| 1:A:26:PHE:CD1  | 1:A:40:VAL:CG2  | 0.65     | 2.80        | 9      | 8     |
| 1:A:67:PHE:CD2  | 1:A:73:LEU:HD23 | 0.64     | 2.27        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:40:VAL:HG13 | 1:A:51:PHE:HB3  | 0.64     | 1.69        | 8      | 1     |
| 1:A:89:GLU:HG3  | 1:A:89:GLU:O    | 0.64     | 1.91        | 8      | 2     |
| 1:A:24:GLY:O    | 1:A:94:VAL:HG11 | 0.64     | 1.93        | 10     | 1     |
| 1:A:82:ILE:CD1  | 1:A:93:LEU:HG   | 0.63     | 2.22        | 4      | 2     |
| 1:A:56:VAL:O    | 1:A:59:VAL:HG22 | 0.63     | 1.92        | 5      | 2     |
| 1:A:24:GLY:HA2  | 1:A:26:PHE:CE1  | 0.63     | 2.28        | 4      | 1     |
| 1:A:54:GLN:O    | 1:A:61:CYS:HB2  | 0.63     | 1.94        | 4      | 1     |
| 1:A:43:LYS:HA   | 1:A:43:LYS:HE2  | 0.62     | 1.71        | 1      | 1     |
| 1:A:73:LEU:O    | 1:A:77:TYR:HA   | 0.62     | 1.94        | 9      | 10    |
| 1:A:22:VAL:O    | 1:A:23:GLU:O    | 0.62     | 2.17        | 10     | 1     |
| 1:A:76:HIS:CG   | 1:A:76:HIS:O    | 0.62     | 2.51        | 2      | 1     |
| 1:A:9:THR:HB    | 1:A:29:ARG:CG   | 0.62     | 2.24        | 9      | 6     |
| 1:A:9:THR:HG23  | 1:A:29:ARG:CD   | 0.62     | 2.23        | 3      | 1     |
| 1:A:51:PHE:CE2  | 1:A:62:ILE:HG22 | 0.62     | 2.29        | 2      | 1     |
| 1:A:74:VAL:CG1  | 1:A:93:LEU:HB3  | 0.62     | 2.24        | 4      | 7     |
| 1:A:82:ILE:HD12 | 1:A:91:LEU:O    | 0.61     | 1.94        | 1      | 1     |
| 1:A:8:VAL:HG11  | 1:A:96:ALA:HB2  | 0.61     | 1.70        | 7      | 1     |
| 1:A:26:PHE:CZ   | 1:A:42:LEU:HB2  | 0.61     | 2.29        | 1      | 9     |
| 1:A:8:VAL:HG13  | 1:A:12:GLN:CD   | 0.61     | 2.21        | 4      | 1     |
| 1:A:25:ASP:C    | 1:A:42:LEU:HD12 | 0.61     | 2.20        | 1      | 9     |
| 1:A:26:PHE:HB3  | 1:A:93:LEU:HA   | 0.61     | 1.72        | 6      | 2     |
| 1:A:28:ILE:CG1  | 1:A:40:VAL:HG12 | 0.61     | 2.26        | 6      | 1     |
| 1:A:9:THR:HB    | 1:A:29:ARG:HG2  | 0.61     | 1.72        | 9      | 1     |
| 1:A:28:ILE:HG21 | 1:A:74:VAL:CG2  | 0.60     | 2.12        | 10     | 2     |
| 1:A:17:LEU:HD21 | 1:A:27:LEU:CD2  | 0.60     | 2.26        | 8      | 3     |
| 1:A:94:VAL:HG13 | 1:A:95:ARG:H    | 0.60     | 1.57        | 1      | 8     |
| 1:A:80:ALA:C    | 1:A:82:ILE:H    | 0.60     | 2.04        | 1      | 10    |
| 1:A:80:ALA:HB3  | 1:A:82:ILE:HG12 | 0.60     | 1.73        | 4      | 2     |
| 1:A:26:PHE:CG   | 1:A:42:LEU:HD11 | 0.59     | 2.32        | 4      | 1     |
| 1:A:12:GLN:CD   | 1:A:27:LEU:HD13 | 0.59     | 2.22        | 8      | 1     |
| 1:A:54:GLN:O    | 1:A:61:CYS:CB   | 0.59     | 2.50        | 4      | 1     |
| 1:A:9:THR:O     | 1:A:10:ARG:HB3  | 0.59     | 1.97        | 5      | 5     |
| 1:A:17:LEU:HB3  | 1:A:43:LYS:CE   | 0.59     | 2.27        | 2      | 2     |
| 1:A:19:GLU:O    | 1:A:20:ARG:HB2  | 0.59     | 1.97        | 2      | 1     |
| 1:A:22:VAL:HG12 | 1:A:23:GLU:HG2  | 0.59     | 1.74        | 8      | 2     |
| 1:A:17:LEU:HD22 | 1:A:25:ASP:OD1  | 0.59     | 1.97        | 9      | 2     |
| 1:A:17:LEU:HD21 | 1:A:25:ASP:HB3  | 0.59     | 1.74        | 4      | 1     |
| 1:A:82:ILE:HA   | 1:A:91:LEU:O    | 0.59     | 1.98        | 10     | 3     |
| 1:A:88:GLY:O    | 1:A:89:GLU:CB   | 0.59     | 2.51        | 5      | 1     |
| 1:A:77:TYR:CB   | 1:A:82:ILE:HD13 | 0.58     | 2.27        | 3      | 3     |
| 1:A:8:VAL:HA    | 1:A:29:ARG:HB3  | 0.58     | 1.73        | 9      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:69:THR:HG21 | 1:A:78:LYS:HB2  | 0.58     | 1.74        | 10     | 2     |
| 1:A:82:ILE:HG12 | 1:A:91:LEU:O    | 0.58     | 1.98        | 7      | 3     |
| 1:A:19:GLU:O    | 1:A:20:ARG:CB   | 0.58     | 2.51        | 2      | 6     |
| 1:A:53:VAL:HG13 | 1:A:62:ILE:HG12 | 0.58     | 1.75        | 6      | 4     |
| 1:A:13:ALA:HB2  | 1:A:27:LEU:HD11 | 0.58     | 1.74        | 10     | 1     |
| 1:A:36:SER:HB2  | 1:A:55:LEU:HD12 | 0.58     | 1.74        | 2      | 1     |
| 1:A:73:LEU:HD13 | 1:A:73:LEU:C    | 0.58     | 2.24        | 7      | 5     |
| 1:A:88:GLY:O    | 1:A:89:GLU:HB2  | 0.58     | 1.97        | 5      | 3     |
| 1:A:42:LEU:HD23 | 1:A:51:PHE:CE2  | 0.58     | 2.33        | 4      | 1     |
| 1:A:17:LEU:HD12 | 1:A:43:LYS:HE3  | 0.58     | 1.74        | 5      | 1     |
| 1:A:26:PHE:CD2  | 1:A:93:LEU:HA   | 0.57     | 2.34        | 7      | 7     |
| 1:A:44:ALA:HB3  | 1:A:47:LYS:O    | 0.57     | 1.99        | 8      | 4     |
| 1:A:27:LEU:O    | 1:A:40:VAL:HA   | 0.57     | 1.99        | 9      | 6     |
| 1:A:70:MET:O    | 1:A:73:LEU:HD11 | 0.57     | 2.00        | 3      | 1     |
| 1:A:94:VAL:HG13 | 1:A:95:ARG:N    | 0.57     | 2.15        | 4      | 4     |
| 1:A:9:THR:C     | 1:A:29:ARG:HD3  | 0.57     | 2.24        | 6      | 2     |
| 1:A:82:ILE:HG21 | 1:A:92:TYR:CD1  | 0.57     | 2.35        | 6      | 1     |
| 1:A:80:ALA:HB3  | 1:A:82:ILE:CG1  | 0.57     | 2.30        | 10     | 1     |
| 1:A:22:VAL:HG23 | 1:A:25:ASP:OD2  | 0.57     | 1.98        | 9      | 1     |
| 1:A:38:PHE:CE1  | 1:A:70:MET:HE2  | 0.57     | 2.35        | 5      | 1     |
| 1:A:73:LEU:O    | 1:A:77:TYR:CA   | 0.57     | 2.52        | 2      | 8     |
| 1:A:97:LEU:HD12 | 1:A:98:GLN:N    | 0.57     | 2.14        | 1      | 1     |
| 1:A:80:ALA:HB1  | 1:A:82:ILE:HD12 | 0.56     | 1.74        | 5      | 1     |
| 1:A:26:PHE:CE1  | 1:A:42:LEU:HB2  | 0.56     | 2.36        | 9      | 9     |
| 1:A:26:PHE:CE2  | 1:A:42:LEU:HD22 | 0.56     | 2.34        | 1      | 8     |
| 1:A:74:VAL:HG13 | 1:A:93:LEU:CB   | 0.56     | 2.30        | 9      | 5     |
| 1:A:62:ILE:HD13 | 1:A:73:LEU:CD2  | 0.56     | 2.30        | 4      | 1     |
| 1:A:80:ALA:O    | 1:A:82:ILE:N    | 0.56     | 2.39        | 1      | 4     |
| 1:A:62:ILE:HD11 | 1:A:69:THR:O    | 0.56     | 2.00        | 10     | 2     |
| 1:A:8:VAL:O     | 1:A:27:LEU:HD13 | 0.56     | 2.01        | 10     | 1     |
| 1:A:56:VAL:O    | 1:A:59:VAL:N    | 0.56     | 2.39        | 1      | 10    |
| 1:A:27:LEU:HD23 | 1:A:27:LEU:N    | 0.56     | 2.16        | 7      | 4     |
| 1:A:26:PHE:CE2  | 1:A:93:LEU:CD2  | 0.56     | 2.89        | 5      | 6     |
| 1:A:9:THR:HG22  | 1:A:27:LEU:CD1  | 0.56     | 2.31        | 10     | 1     |
| 1:A:26:PHE:CE2  | 1:A:42:LEU:HB2  | 0.55     | 2.36        | 7      | 9     |
| 1:A:80:ALA:HB1  | 1:A:93:LEU:HD12 | 0.55     | 1.77        | 1      | 1     |
| 1:A:42:LEU:CD2  | 1:A:91:LEU:HD22 | 0.55     | 2.32        | 10     | 1     |
| 1:A:9:THR:CB    | 1:A:29:ARG:HD3  | 0.55     | 2.32        | 9      | 4     |
| 1:A:12:GLN:HG3  | 1:A:27:LEU:CD1  | 0.55     | 2.31        | 8      | 1     |
| 1:A:40:VAL:CG1  | 1:A:51:PHE:CD1  | 0.55     | 2.89        | 8      | 1     |
| 1:A:23:GLU:O    | 1:A:25:ASP:N    | 0.55     | 2.39        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:THR:CG2   | 1:A:10:ARG:N    | 0.55     | 2.69        | 5      | 4     |
| 1:A:77:TYR:CG   | 1:A:92:TYR:CD1  | 0.55     | 2.94        | 6      | 1     |
| 1:A:8:VAL:CG1   | 1:A:96:ALA:HB2  | 0.55     | 2.31        | 7      | 1     |
| 1:A:84:THR:HG23 | 1:A:90:LYS:N    | 0.55     | 2.16        | 6      | 2     |
| 1:A:17:LEU:HD13 | 1:A:43:LYS:HE2  | 0.55     | 1.78        | 6      | 1     |
| 1:A:56:VAL:N    | 1:A:59:VAL:O    | 0.55     | 2.40        | 2      | 5     |
| 1:A:53:VAL:CG2  | 1:A:62:ILE:HG23 | 0.54     | 2.20        | 4      | 2     |
| 1:A:84:THR:OG1  | 1:A:90:LYS:HG3  | 0.54     | 2.02        | 6      | 2     |
| 1:A:97:LEU:HD23 | 1:A:97:LEU:N    | 0.54     | 2.17        | 2      | 1     |
| 1:A:28:ILE:N    | 1:A:40:VAL:HG23 | 0.54     | 2.16        | 5      | 4     |
| 1:A:60:TYR:CB   | 1:A:69:THR:O    | 0.54     | 2.55        | 8      | 6     |
| 1:A:17:LEU:HB3  | 1:A:43:LYS:HD2  | 0.54     | 1.79        | 4      | 1     |
| 1:A:62:ILE:HD11 | 1:A:70:MET:CE   | 0.54     | 2.31        | 6      | 1     |
| 1:A:24:GLY:CA   | 1:A:26:PHE:CE1  | 0.54     | 2.90        | 4      | 1     |
| 1:A:22:VAL:HG22 | 1:A:43:LYS:NZ   | 0.54     | 2.18        | 2      | 1     |
| 1:A:28:ILE:CD1  | 1:A:74:VAL:HG11 | 0.54     | 2.26        | 9      | 1     |
| 1:A:17:LEU:HD22 | 1:A:43:LYS:HE2  | 0.54     | 1.78        | 7      | 1     |
| 1:A:28:ILE:HB   | 1:A:40:VAL:HG12 | 0.54     | 1.80        | 6      | 1     |
| 1:A:82:ILE:CG1  | 1:A:91:LEU:O    | 0.54     | 2.56        | 7      | 2     |
| 1:A:42:LEU:CD2  | 1:A:91:LEU:CD2  | 0.54     | 2.84        | 8      | 3     |
| 1:A:82:ILE:HG21 | 1:A:92:TYR:CD2  | 0.54     | 2.38        | 5      | 1     |
| 1:A:14:GLU:O    | 1:A:18:ASN:HB2  | 0.54     | 2.02        | 4      | 3     |
| 1:A:38:PHE:CE2  | 1:A:70:MET:HE3  | 0.54     | 2.37        | 9      | 1     |
| 1:A:55:LEU:C    | 1:A:55:LEU:CD2  | 0.53     | 2.80        | 1      | 5     |
| 1:A:14:GLU:O    | 1:A:18:ASN:HB3  | 0.53     | 2.04        | 6      | 1     |
| 1:A:82:ILE:HG21 | 1:A:92:TYR:CE1  | 0.53     | 2.38        | 6      | 1     |
| 1:A:28:ILE:HD11 | 1:A:38:PHE:HB3  | 0.53     | 1.81        | 8      | 1     |
| 1:A:17:LEU:HD22 | 1:A:25:ASP:CB   | 0.53     | 2.33        | 10     | 2     |
| 1:A:62:ILE:CD1  | 1:A:70:MET:HE2  | 0.53     | 2.30        | 6      | 1     |
| 1:A:26:PHE:CD1  | 1:A:42:LEU:HB2  | 0.53     | 2.39        | 2      | 3     |
| 1:A:60:TYR:HB2  | 1:A:69:THR:O    | 0.53     | 2.04        | 10     | 2     |
| 1:A:53:VAL:CG1  | 1:A:70:MET:CG   | 0.53     | 2.87        | 6      | 2     |
| 1:A:9:THR:OG1   | 1:A:27:LEU:CD1  | 0.53     | 2.55        | 8      | 2     |
| 1:A:28:ILE:CB   | 1:A:74:VAL:HG21 | 0.53     | 2.33        | 4      | 1     |
| 1:A:42:LEU:CD2  | 1:A:91:LEU:HD13 | 0.53     | 2.33        | 5      | 1     |
| 1:A:17:LEU:HD13 | 1:A:43:LYS:HD2  | 0.52     | 1.79        | 4      | 1     |
| 1:A:8:VAL:HA    | 1:A:12:GLN:HB3  | 0.52     | 1.81        | 3      | 1     |
| 1:A:8:VAL:HG12  | 1:A:13:ALA:HA   | 0.52     | 1.81        | 3      | 1     |
| 1:A:73:LEU:CD2  | 1:A:80:ALA:HB2  | 0.52     | 2.33        | 4      | 2     |
| 1:A:17:LEU:O    | 1:A:20:ARG:N    | 0.52     | 2.43        | 9      | 3     |
| 1:A:42:LEU:HD21 | 1:A:91:LEU:HD22 | 0.52     | 1.80        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:55:LEU:HD22 | 1:A:56:VAL:N    | 0.52     | 2.19        | 6      | 5     |
| 1:A:77:TYR:CE1  | 1:A:92:TYR:CE2  | 0.52     | 2.97        | 8      | 2     |
| 1:A:28:ILE:HD12 | 1:A:40:VAL:HG12 | 0.52     | 1.81        | 6      | 1     |
| 1:A:26:PHE:CD2  | 1:A:93:LEU:CD2  | 0.52     | 2.93        | 7      | 3     |
| 1:A:8:VAL:CA    | 1:A:12:GLN:HB2  | 0.52     | 2.33        | 3      | 1     |
| 1:A:53:VAL:CG2  | 1:A:62:ILE:HD13 | 0.52     | 2.34        | 6      | 1     |
| 1:A:82:ILE:HG23 | 1:A:92:TYR:HA   | 0.52     | 1.81        | 4      | 1     |
| 1:A:28:ILE:HB   | 1:A:40:VAL:HB   | 0.51     | 1.81        | 10     | 4     |
| 1:A:29:ARG:HG2  | 1:A:39:SER:O    | 0.51     | 2.04        | 4      | 1     |
| 1:A:85:SER:O    | 1:A:86:GLU:C    | 0.51     | 2.53        | 6      | 2     |
| 1:A:28:ILE:HG12 | 1:A:40:VAL:HB   | 0.51     | 1.81        | 4      | 1     |
| 1:A:28:ILE:HD12 | 1:A:74:VAL:CG2  | 0.51     | 2.36        | 1      | 3     |
| 1:A:67:PHE:CG   | 1:A:79:LYS:CB   | 0.51     | 2.94        | 5      | 2     |
| 1:A:73:LEU:HD12 | 1:A:73:LEU:N    | 0.51     | 2.21        | 2      | 8     |
| 1:A:77:TYR:HB3  | 1:A:82:ILE:CD1  | 0.51     | 2.31        | 9      | 2     |
| 1:A:49:LYS:HE2  | 1:A:91:LEU:HD11 | 0.51     | 1.81        | 4      | 1     |
| 1:A:53:VAL:HG22 | 1:A:62:ILE:HG12 | 0.51     | 1.80        | 7      | 2     |
| 1:A:67:PHE:N    | 1:A:67:PHE:CD1  | 0.51     | 2.78        | 7      | 1     |
| 1:A:83:PHE:HB2  | 1:A:91:LEU:HD12 | 0.51     | 1.83        | 7      | 1     |
| 1:A:70:MET:HE3  | 1:A:73:LEU:HG   | 0.51     | 1.81        | 6      | 1     |
| 1:A:28:ILE:CD1  | 1:A:74:VAL:CG2  | 0.51     | 2.88        | 2      | 3     |
| 1:A:14:GLU:O    | 1:A:18:ASN:CB   | 0.51     | 2.59        | 6      | 3     |
| 1:A:42:LEU:HD22 | 1:A:91:LEU:CD2  | 0.51     | 2.35        | 8      | 1     |
| 1:A:82:ILE:HG23 | 1:A:92:TYR:CD1  | 0.51     | 2.40        | 8      | 1     |
| 1:A:28:ILE:CB   | 1:A:40:VAL:HB   | 0.50     | 2.37        | 10     | 4     |
| 1:A:25:ASP:C    | 1:A:26:PHE:CD1  | 0.50     | 2.90        | 4      | 1     |
| 1:A:57:ASP:O    | 1:A:57:ASP:CG   | 0.50     | 2.54        | 7      | 1     |
| 1:A:82:ILE:HD11 | 1:A:93:LEU:HB2  | 0.50     | 1.82        | 7      | 1     |
| 1:A:94:VAL:HG22 | 1:A:95:ARG:H    | 0.50     | 1.66        | 4      | 1     |
| 1:A:80:ALA:C    | 1:A:82:ILE:N    | 0.50     | 2.70        | 1      | 8     |
| 1:A:9:THR:CB    | 1:A:27:LEU:HD12 | 0.50     | 2.36        | 2      | 1     |
| 1:A:8:VAL:O     | 1:A:9:THR:CB    | 0.50     | 2.59        | 3      | 1     |
| 1:A:82:ILE:HG22 | 1:A:91:LEU:O    | 0.50     | 2.01        | 4      | 1     |
| 1:A:28:ILE:CB   | 1:A:40:VAL:HG12 | 0.50     | 2.36        | 6      | 1     |
| 1:A:55:LEU:HD23 | 1:A:59:VAL:C    | 0.50     | 2.32        | 7      | 1     |
| 1:A:96:ALA:C    | 1:A:97:LEU:HD22 | 0.50     | 2.32        | 6      | 1     |
| 1:A:13:ALA:HB2  | 1:A:27:LEU:CD1  | 0.50     | 2.36        | 10     | 1     |
| 1:A:28:ILE:HD13 | 1:A:40:VAL:HG11 | 0.50     | 1.81        | 7      | 3     |
| 1:A:17:LEU:CB   | 1:A:43:LYS:NZ   | 0.50     | 2.75        | 2      | 1     |
| 1:A:44:ALA:N    | 1:A:47:LYS:O    | 0.50     | 2.44        | 4      | 3     |
| 1:A:26:PHE:CE1  | 1:A:40:VAL:CG2  | 0.50     | 2.95        | 6      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:17:LEU:HD22 | 1:A:25:ASP:HB2  | 0.50     | 1.84        | 10     | 1     |
| 1:A:28:ILE:HB   | 1:A:74:VAL:HG11 | 0.49     | 1.84        | 4      | 1     |
| 1:A:17:LEU:N    | 1:A:17:LEU:CD2  | 0.49     | 2.74        | 10     | 3     |
| 1:A:53:VAL:HG11 | 1:A:70:MET:CG   | 0.49     | 2.36        | 6      | 1     |
| 1:A:9:THR:N     | 1:A:29:ARG:HD2  | 0.49     | 2.22        | 6      | 3     |
| 1:A:55:LEU:O    | 1:A:55:LEU:CD1  | 0.49     | 2.55        | 9      | 7     |
| 1:A:22:VAL:O    | 1:A:23:GLU:C    | 0.49     | 2.54        | 7      | 2     |
| 1:A:67:PHE:CE2  | 1:A:79:LYS:O    | 0.49     | 2.65        | 7      | 2     |
| 1:A:26:PHE:CZ   | 1:A:93:LEU:HD23 | 0.49     | 2.41        | 9      | 2     |
| 1:A:67:PHE:CD2  | 1:A:79:LYS:CB   | 0.49     | 2.95        | 10     | 1     |
| 1:A:8:VAL:O     | 1:A:9:THR:O     | 0.49     | 2.30        | 4      | 3     |
| 1:A:28:ILE:HA   | 1:A:40:VAL:HB   | 0.49     | 1.82        | 4      | 1     |
| 1:A:94:VAL:HG23 | 1:A:95:ARG:N    | 0.49     | 2.22        | 7      | 1     |
| 1:A:69:THR:OG1  | 1:A:73:LEU:HB3  | 0.49     | 2.06        | 9      | 1     |
| 1:A:17:LEU:HD13 | 1:A:43:LYS:CE   | 0.49     | 2.37        | 6      | 1     |
| 1:A:28:ILE:HD12 | 1:A:74:VAL:HG22 | 0.49     | 1.83        | 7      | 3     |
| 1:A:10:ARG:O    | 1:A:14:GLU:CG   | 0.49     | 2.61        | 3      | 3     |
| 1:A:53:VAL:HG13 | 1:A:62:ILE:HD12 | 0.49     | 1.82        | 5      | 1     |
| 1:A:17:LEU:HB2  | 1:A:43:LYS:HD3  | 0.49     | 1.85        | 2      | 1     |
| 1:A:22:VAL:HG11 | 1:A:25:ASP:OD2  | 0.49     | 2.07        | 4      | 1     |
| 1:A:73:LEU:HD12 | 1:A:73:LEU:H    | 0.49     | 1.67        | 9      | 6     |
| 1:A:8:VAL:O     | 1:A:29:ARG:HD2  | 0.49     | 2.07        | 7      | 1     |
| 1:A:11:HIS:O    | 1:A:14:GLU:HG3  | 0.49     | 2.07        | 1      | 3     |
| 1:A:42:LEU:CD2  | 1:A:91:LEU:HB3  | 0.49     | 2.37        | 9      | 3     |
| 1:A:42:LEU:CB   | 1:A:51:PHE:CE1  | 0.49     | 2.96        | 4      | 1     |
| 1:A:67:PHE:CG   | 1:A:79:LYS:HB3  | 0.49     | 2.43        | 4      | 4     |
| 1:A:26:PHE:HE1  | 1:A:40:VAL:HG23 | 0.49     | 1.64        | 6      | 1     |
| 1:A:53:VAL:HG22 | 1:A:62:ILE:CG1  | 0.49     | 2.37        | 7      | 2     |
| 1:A:17:LEU:CD2  | 1:A:25:ASP:CB   | 0.49     | 2.91        | 4      | 1     |
| 1:A:26:PHE:CD1  | 1:A:41:SER:C    | 0.48     | 2.91        | 1      | 4     |
| 1:A:28:ILE:CD1  | 1:A:74:VAL:HG22 | 0.48     | 2.38        | 1      | 3     |
| 1:A:51:PHE:CZ   | 1:A:62:ILE:CG2  | 0.48     | 2.96        | 8      | 3     |
| 1:A:58:ASN:O    | 1:A:58:ASN:CG   | 0.48     | 2.56        | 2      | 1     |
| 1:A:55:LEU:HD11 | 1:A:60:TYR:HE1  | 0.48     | 1.64        | 5      | 1     |
| 1:A:91:LEU:CD2  | 1:A:91:LEU:C    | 0.48     | 2.86        | 8      | 1     |
| 1:A:67:PHE:CD2  | 1:A:79:LYS:O    | 0.48     | 2.67        | 2      | 7     |
| 1:A:60:TYR:CD1  | 1:A:70:MET:HB3  | 0.48     | 2.43        | 5      | 1     |
| 1:A:97:LEU:HD22 | 1:A:97:LEU:N    | 0.48     | 2.23        | 6      | 1     |
| 1:A:69:THR:CG2  | 1:A:73:LEU:HB3  | 0.48     | 2.38        | 9      | 2     |
| 1:A:9:THR:HG23  | 1:A:10:ARG:N    | 0.48     | 2.24        | 1      | 1     |
| 1:A:17:LEU:HA   | 1:A:43:LYS:HZ1  | 0.48     | 1.67        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:21:GLY:HA2  | 1:A:43:LYS:HB2  | 0.48     | 1.84        | 3      | 2     |
| 1:A:28:ILE:CD1  | 1:A:40:VAL:CG1  | 0.48     | 2.91        | 4      | 1     |
| 1:A:17:LEU:C    | 1:A:19:GLU:H    | 0.48     | 2.17        | 10     | 2     |
| 1:A:76:HIS:C    | 1:A:77:TYR:CD1  | 0.48     | 2.92        | 8      | 4     |
| 1:A:14:GLU:O    | 1:A:18:ASN:HA   | 0.48     | 2.09        | 8      | 2     |
| 1:A:90:LYS:CB   | 1:A:92:TYR:CE2  | 0.48     | 2.96        | 6      | 1     |
| 1:A:21:GLY:H    | 1:A:43:LYS:CD   | 0.48     | 2.21        | 7      | 1     |
| 1:A:42:LEU:HD22 | 1:A:91:LEU:HD23 | 0.48     | 1.83        | 8      | 1     |
| 1:A:28:ILE:CD1  | 1:A:40:VAL:HG12 | 0.48     | 2.39        | 6      | 1     |
| 1:A:67:PHE:CZ   | 1:A:80:ALA:HA   | 0.48     | 2.44        | 7      | 1     |
| 1:A:51:PHE:CE2  | 1:A:62:ILE:CG2  | 0.48     | 2.97        | 2      | 1     |
| 1:A:24:GLY:C    | 1:A:26:PHE:CE1  | 0.48     | 2.92        | 4      | 1     |
| 1:A:59:VAL:HG13 | 1:A:60:TYR:N    | 0.48     | 2.23        | 9      | 1     |
| 1:A:67:PHE:CD1  | 1:A:79:LYS:HG2  | 0.48     | 2.44        | 10     | 1     |
| 1:A:51:PHE:CD1  | 1:A:51:PHE:N    | 0.48     | 2.81        | 3      | 1     |
| 1:A:38:PHE:CE1  | 1:A:70:MET:CE   | 0.48     | 2.97        | 5      | 1     |
| 1:A:85:SER:HB3  | 1:A:88:GLY:HA3  | 0.48     | 1.86        | 6      | 1     |
| 1:A:8:VAL:O     | 1:A:12:GLN:HB2  | 0.47     | 2.07        | 6      | 1     |
| 1:A:53:VAL:HG22 | 1:A:62:ILE:HD13 | 0.47     | 1.85        | 6      | 1     |
| 1:A:22:VAL:HG23 | 1:A:43:LYS:HZ2  | 0.47     | 1.68        | 7      | 1     |
| 1:A:9:THR:O     | 1:A:10:ARG:CB   | 0.47     | 2.62        | 8      | 2     |
| 1:A:73:LEU:C    | 1:A:73:LEU:CD1  | 0.47     | 2.87        | 7      | 4     |
| 1:A:74:VAL:CG1  | 1:A:93:LEU:CB   | 0.47     | 2.92        | 10     | 2     |
| 1:A:3:TRP:O     | 1:A:8:VAL:HG21  | 0.47     | 2.10        | 1      | 1     |
| 1:A:94:VAL:HG21 | 1:A:97:LEU:HD11 | 0.47     | 1.87        | 5      | 1     |
| 1:A:82:ILE:CD1  | 1:A:93:LEU:CD1  | 0.47     | 2.91        | 8      | 1     |
| 1:A:60:TYR:CD1  | 1:A:60:TYR:N    | 0.47     | 2.81        | 10     | 1     |
| 1:A:73:LEU:CD1  | 1:A:74:VAL:HG22 | 0.47     | 2.40        | 6      | 4     |
| 1:A:16:ALA:HB3  | 1:A:27:LEU:CD2  | 0.47     | 2.40        | 3      | 1     |
| 1:A:22:VAL:HG12 | 1:A:23:GLU:N    | 0.47     | 2.25        | 4      | 1     |
| 1:A:74:VAL:HA   | 1:A:93:LEU:HD13 | 0.47     | 1.86        | 10     | 2     |
| 1:A:38:PHE:O    | 1:A:53:VAL:N    | 0.47     | 2.46        | 7      | 1     |
| 1:A:80:ALA:CB   | 1:A:93:LEU:HD11 | 0.47     | 2.40        | 9      | 1     |
| 1:A:24:GLY:CA   | 1:A:26:PHE:CZ   | 0.47     | 2.98        | 4      | 1     |
| 1:A:82:ILE:CB   | 1:A:91:LEU:O    | 0.47     | 2.63        | 5      | 3     |
| 1:A:26:PHE:CD2  | 1:A:42:LEU:HB2  | 0.47     | 2.45        | 7      | 3     |
| 1:A:60:TYR:O    | 1:A:67:PHE:O    | 0.47     | 2.33        | 2      | 2     |
| 1:A:8:VAL:HG12  | 1:A:13:ALA:CA   | 0.47     | 2.40        | 3      | 1     |
| 1:A:8:VAL:CA    | 1:A:29:ARG:HB3  | 0.47     | 2.40        | 5      | 1     |
| 1:A:82:ILE:HD11 | 1:A:93:LEU:CB   | 0.47     | 2.40        | 7      | 1     |
| 1:A:9:THR:OG1   | 1:A:29:ARG:NE   | 0.47     | 2.48        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:55:LEU:HA   | 1:A:59:VAL:O    | 0.47     | 2.09        | 7      | 1     |
| 1:A:89:GLU:O    | 1:A:89:GLU:CG   | 0.47     | 2.62        | 7      | 1     |
| 1:A:73:LEU:CD1  | 1:A:74:VAL:N    | 0.46     | 2.78        | 4      | 6     |
| 1:A:22:VAL:N    | 1:A:43:LYS:HE3  | 0.46     | 2.26        | 7      | 2     |
| 1:A:9:THR:C     | 1:A:29:ARG:CD   | 0.46     | 2.88        | 4      | 3     |
| 1:A:26:PHE:CD1  | 1:A:41:SER:O    | 0.46     | 2.68        | 6      | 3     |
| 1:A:53:VAL:HA   | 1:A:61:CYS:O    | 0.46     | 2.10        | 6      | 5     |
| 1:A:57:ASP:O    | 1:A:59:VAL:HG23 | 0.46     | 2.09        | 7      | 1     |
| 1:A:44:ALA:HB2  | 1:A:49:LYS:HG3  | 0.46     | 1.85        | 9      | 1     |
| 1:A:25:ASP:C    | 1:A:42:LEU:CD1  | 0.46     | 2.89        | 1      | 2     |
| 1:A:43:LYS:HA   | 1:A:43:LYS:CE   | 0.46     | 2.41        | 1      | 1     |
| 1:A:94:VAL:CG2  | 1:A:95:ARG:N    | 0.46     | 2.74        | 10     | 3     |
| 1:A:67:PHE:CD1  | 1:A:79:LYS:HB3  | 0.46     | 2.46        | 6      | 4     |
| 1:A:17:LEU:HD21 | 1:A:25:ASP:CB   | 0.46     | 2.40        | 4      | 1     |
| 1:A:26:PHE:CG   | 1:A:42:LEU:HB2  | 0.46     | 2.46        | 2      | 1     |
| 1:A:62:ILE:CD1  | 1:A:73:LEU:CD2  | 0.46     | 2.93        | 4      | 1     |
| 1:A:59:VAL:HG12 | 1:A:60:TYR:N    | 0.46     | 2.25        | 7      | 1     |
| 1:A:84:THR:HA   | 1:A:89:GLU:O    | 0.46     | 2.11        | 1      | 1     |
| 1:A:77:TYR:CD2  | 1:A:77:TYR:O    | 0.46     | 2.68        | 2      | 3     |
| 1:A:42:LEU:HD23 | 1:A:49:LYS:HE2  | 0.46     | 1.88        | 3      | 1     |
| 1:A:22:VAL:O    | 1:A:24:GLY:N    | 0.46     | 2.48        | 8      | 3     |
| 1:A:3:TRP:CD1   | 1:A:3:TRP:O     | 0.46     | 2.69        | 7      | 2     |
| 1:A:4:TYR:O     | 1:A:4:TYR:CG    | 0.46     | 2.68        | 6      | 1     |
| 1:A:69:THR:HG23 | 1:A:73:LEU:HB3  | 0.46     | 1.88        | 7      | 1     |
| 1:A:8:VAL:O     | 1:A:27:LEU:HB2  | 0.46     | 2.11        | 9      | 1     |
| 1:A:44:ALA:HB2  | 1:A:49:LYS:NZ   | 0.46     | 2.26        | 3      | 1     |
| 1:A:54:GLN:O    | 1:A:61:CYS:N    | 0.46     | 2.48        | 4      | 1     |
| 1:A:40:VAL:CG1  | 1:A:51:PHE:HB3  | 0.46     | 2.40        | 5      | 2     |
| 1:A:51:PHE:CE1  | 1:A:62:ILE:CG2  | 0.46     | 2.99        | 8      | 1     |
| 1:A:9:THR:OG1   | 1:A:29:ARG:HD3  | 0.46     | 2.10        | 10     | 1     |
| 1:A:24:GLY:O    | 1:A:94:VAL:CG1  | 0.46     | 2.62        | 10     | 1     |
| 1:A:21:GLY:CA   | 1:A:43:LYS:HE3  | 0.46     | 2.41        | 2      | 1     |
| 1:A:9:THR:HG22  | 1:A:10:ARG:N    | 0.46     | 2.26        | 4      | 1     |
| 1:A:10:ARG:CG   | 1:A:11:HIS:N    | 0.46     | 2.78        | 9      | 3     |
| 1:A:84:THR:HG23 | 1:A:90:LYS:HG3  | 0.46     | 1.87        | 8      | 1     |
| 1:A:9:THR:N     | 1:A:29:ARG:CD   | 0.46     | 2.79        | 9      | 1     |
| 1:A:40:VAL:O    | 1:A:51:PHE:CB   | 0.46     | 2.64        | 10     | 1     |
| 1:A:3:TRP:CD1   | 1:A:3:TRP:N     | 0.45     | 2.84        | 1      | 2     |
| 1:A:69:THR:CG2  | 1:A:73:LEU:N    | 0.45     | 2.79        | 1      | 1     |
| 1:A:53:VAL:HG22 | 1:A:62:ILE:CD1  | 0.45     | 2.42        | 6      | 1     |
| 1:A:62:ILE:CD1  | 1:A:70:MET:CE   | 0.45     | 2.93        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:57:ASP:O    | 1:A:58:ASN:OD1  | 0.45     | 2.33        | 7      | 1     |
| 1:A:66:ARG:C    | 1:A:67:PHE:CD1  | 0.45     | 2.95        | 7      | 1     |
| 1:A:76:HIS:C    | 1:A:77:TYR:CG   | 0.45     | 2.94        | 6      | 4     |
| 1:A:67:PHE:CZ   | 1:A:79:LYS:O    | 0.45     | 2.69        | 7      | 1     |
| 1:A:44:ALA:O    | 1:A:46:GLY:N    | 0.45     | 2.50        | 10     | 7     |
| 1:A:82:ILE:CG2  | 1:A:92:TYR:HA   | 0.45     | 2.41        | 4      | 1     |
| 1:A:12:GLN:HG3  | 1:A:13:ALA:N    | 0.45     | 2.26        | 8      | 1     |
| 1:A:43:LYS:NZ   | 1:A:48:ASN:CB   | 0.45     | 2.80        | 6      | 1     |
| 1:A:70:MET:HE2  | 1:A:73:LEU:HD21 | 0.45     | 1.88        | 6      | 1     |
| 1:A:83:PHE:CE1  | 1:A:84:THR:O    | 0.45     | 2.70        | 1      | 1     |
| 1:A:77:TYR:HB2  | 1:A:80:ALA:HB3  | 0.45     | 1.88        | 2      | 1     |
| 1:A:8:VAL:C     | 1:A:29:ARG:CD   | 0.45     | 2.90        | 3      | 1     |
| 1:A:58:ASN:O    | 1:A:58:ASN:ND2  | 0.45     | 2.50        | 7      | 1     |
| 1:A:26:PHE:H    | 1:A:94:VAL:HG23 | 0.45     | 1.72        | 2      | 1     |
| 1:A:49:LYS:HD2  | 1:A:91:LEU:HD11 | 0.45     | 1.89        | 3      | 1     |
| 1:A:16:ALA:O    | 1:A:22:VAL:HG21 | 0.45     | 2.11        | 4      | 1     |
| 1:A:17:LEU:HD12 | 1:A:43:LYS:HE2  | 0.45     | 1.89        | 5      | 1     |
| 1:A:70:MET:O    | 1:A:70:MET:HE3  | 0.45     | 2.12        | 10     | 1     |
| 1:A:21:GLY:H    | 1:A:43:LYS:CE   | 0.45     | 2.24        | 2      | 1     |
| 1:A:70:MET:O    | 1:A:71:ASP:CB   | 0.45     | 2.65        | 7      | 5     |
| 1:A:17:LEU:HD21 | 1:A:27:LEU:HD21 | 0.45     | 1.88        | 5      | 1     |
| 1:A:9:THR:HG22  | 1:A:13:ALA:CB   | 0.45     | 2.34        | 7      | 1     |
| 1:A:17:LEU:O    | 1:A:18:ASN:C    | 0.45     | 2.59        | 1      | 2     |
| 1:A:26:PHE:CG   | 1:A:42:LEU:CD1  | 0.45     | 2.90        | 8      | 5     |
| 1:A:42:LEU:HB3  | 1:A:51:PHE:CE1  | 0.45     | 2.47        | 4      | 1     |
| 1:A:9:THR:CG2   | 1:A:13:ALA:CB   | 0.45     | 2.94        | 6      | 1     |
| 1:A:85:SER:HB3  | 1:A:89:GLU:CD   | 0.45     | 2.37        | 7      | 1     |
| 1:A:12:GLN:O    | 1:A:16:ALA:N    | 0.45     | 2.49        | 2      | 4     |
| 1:A:73:LEU:CD1  | 1:A:74:VAL:CG2  | 0.45     | 2.95        | 5      | 2     |
| 1:A:55:LEU:HD13 | 1:A:55:LEU:C    | 0.45     | 2.31        | 10     | 2     |
| 1:A:62:ILE:HG21 | 1:A:81:PRO:CD   | 0.45     | 2.42        | 6      | 1     |
| 1:A:77:TYR:CG   | 1:A:82:ILE:CD1  | 0.45     | 3.00        | 9      | 1     |
| 1:A:17:LEU:HB3  | 1:A:43:LYS:NZ   | 0.44     | 2.27        | 2      | 1     |
| 1:A:44:ALA:HB3  | 1:A:47:LYS:CE   | 0.44     | 2.42        | 2      | 1     |
| 1:A:77:TYR:CB   | 1:A:82:ILE:CD1  | 0.44     | 2.93        | 10     | 3     |
| 1:A:9:THR:H     | 1:A:13:ALA:N    | 0.44     | 2.10        | 3      | 1     |
| 1:A:26:PHE:HB2  | 1:A:42:LEU:CD1  | 0.44     | 2.42        | 5      | 1     |
| 1:A:9:THR:HG23  | 1:A:27:LEU:HG   | 0.44     | 1.90        | 7      | 1     |
| 1:A:83:PHE:O    | 1:A:91:LEU:N    | 0.44     | 2.49        | 1      | 3     |
| 1:A:14:GLU:C    | 1:A:16:ALA:N    | 0.44     | 2.74        | 3      | 2     |
| 1:A:43:LYS:CD   | 1:A:43:LYS:C    | 0.44     | 2.90        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:26:PHE:O    | 1:A:95:ARG:HA   | 0.44     | 2.12        | 4      | 1     |
| 1:A:38:PHE:CE1  | 1:A:71:ASP:CG   | 0.44     | 2.95        | 4      | 2     |
| 1:A:72:GLU:O    | 1:A:75:GLU:CG   | 0.44     | 2.65        | 7      | 1     |
| 1:A:8:VAL:HG13  | 1:A:12:GLN:NE2  | 0.44     | 2.27        | 4      | 1     |
| 1:A:9:THR:HG22  | 1:A:29:ARG:HD3  | 0.44     | 1.89        | 5      | 3     |
| 1:A:77:TYR:CD2  | 1:A:92:TYR:CE1  | 0.44     | 3.06        | 6      | 1     |
| 1:A:22:VAL:O    | 1:A:22:VAL:HG23 | 0.44     | 2.11        | 10     | 1     |
| 1:A:29:ARG:N    | 1:A:39:SER:O    | 0.44     | 2.49        | 2      | 1     |
| 1:A:56:VAL:O    | 1:A:57:ASP:C    | 0.44     | 2.61        | 5      | 7     |
| 1:A:43:LYS:CD   | 1:A:44:ALA:N    | 0.44     | 2.81        | 3      | 1     |
| 1:A:28:ILE:CG2  | 1:A:74:VAL:HG11 | 0.44     | 2.43        | 6      | 1     |
| 1:A:60:TYR:O    | 1:A:67:PHE:N    | 0.44     | 2.48        | 7      | 1     |
| 1:A:28:ILE:HD11 | 1:A:93:LEU:HD22 | 0.44     | 1.90        | 1      | 1     |
| 1:A:8:VAL:O     | 1:A:9:THR:HG23  | 0.44     | 2.12        | 3      | 1     |
| 1:A:8:VAL:CA    | 1:A:29:ARG:HD2  | 0.44     | 2.43        | 3      | 1     |
| 1:A:12:GLN:CG   | 1:A:27:LEU:CD1  | 0.44     | 2.95        | 8      | 1     |
| 1:A:9:THR:C     | 1:A:11:HIS:H    | 0.44     | 2.20        | 10     | 1     |
| 1:A:44:ALA:HB2  | 1:A:49:LYS:HZ1  | 0.44     | 1.73        | 3      | 1     |
| 1:A:53:VAL:HG12 | 1:A:70:MET:CE   | 0.44     | 2.28        | 4      | 1     |
| 1:A:3:TRP:HB3   | 1:A:96:ALA:HB3  | 0.44     | 1.90        | 6      | 1     |
| 1:A:69:THR:O    | 1:A:70:MET:HB2  | 0.44     | 2.12        | 6      | 1     |
| 1:A:24:GLY:O    | 1:A:94:VAL:CG2  | 0.44     | 2.63        | 7      | 1     |
| 1:A:8:VAL:CG1   | 1:A:12:GLN:HB3  | 0.44     | 2.42        | 8      | 1     |
| 1:A:4:TYR:CD1   | 1:A:4:TYR:O     | 0.44     | 2.71        | 3      | 1     |
| 1:A:26:PHE:CB   | 1:A:42:LEU:CD1  | 0.44     | 2.96        | 5      | 6     |
| 1:A:85:SER:N    | 1:A:89:GLU:O    | 0.44     | 2.51        | 3      | 2     |
| 1:A:17:LEU:CD2  | 1:A:25:ASP:HB3  | 0.44     | 2.42        | 4      | 1     |
| 1:A:26:PHE:CD2  | 1:A:92:TYR:O    | 0.44     | 2.71        | 4      | 1     |
| 1:A:9:THR:HG23  | 1:A:13:ALA:CB   | 0.43     | 2.40        | 4      | 1     |
| 1:A:38:PHE:CE2  | 1:A:71:ASP:CG   | 0.43     | 2.96        | 5      | 2     |
| 1:A:40:VAL:O    | 1:A:51:PHE:HB3  | 0.43     | 2.13        | 8      | 1     |
| 1:A:10:ARG:HG3  | 1:A:11:HIS:CE1  | 0.43     | 2.48        | 1      | 1     |
| 1:A:42:LEU:O    | 1:A:43:LYS:HE2  | 0.43     | 2.13        | 1      | 1     |
| 1:A:9:THR:C     | 1:A:11:HIS:N    | 0.43     | 2.73        | 3      | 1     |
| 1:A:53:VAL:HG11 | 1:A:70:MET:HG3  | 0.43     | 1.90        | 4      | 2     |
| 1:A:56:VAL:O    | 1:A:59:VAL:CG2  | 0.43     | 2.63        | 5      | 1     |
| 1:A:56:VAL:CG1  | 1:A:57:ASP:OD1  | 0.43     | 2.66        | 7      | 1     |
| 1:A:38:PHE:HB2  | 1:A:53:VAL:HB   | 0.43     | 1.89        | 4      | 1     |
| 1:A:76:HIS:O    | 1:A:77:TYR:C    | 0.43     | 2.62        | 1      | 1     |
| 1:A:22:VAL:H    | 1:A:43:LYS:HE3  | 0.43     | 1.74        | 2      | 1     |
| 1:A:26:PHE:CD1  | 1:A:42:LEU:HD12 | 0.43     | 2.45        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:40:VAL:HG12 | 1:A:51:PHE:CD1  | 0.43     | 2.48        | 8      | 1     |
| 1:A:28:ILE:CG2  | 1:A:40:VAL:HB   | 0.43     | 2.40        | 9      | 1     |
| 1:A:73:LEU:C    | 1:A:73:LEU:HD13 | 0.43     | 2.39        | 2      | 1     |
| 1:A:26:PHE:CE2  | 1:A:92:TYR:HB2  | 0.43     | 2.49        | 4      | 1     |
| 1:A:84:THR:HG23 | 1:A:89:GLU:O    | 0.43     | 2.12        | 5      | 1     |
| 1:A:60:TYR:CD1  | 1:A:70:MET:HB2  | 0.43     | 2.48        | 7      | 1     |
| 1:A:54:GLN:O    | 1:A:61:CYS:HB3  | 0.43     | 2.12        | 10     | 1     |
| 1:A:73:LEU:HD13 | 1:A:74:VAL:HG22 | 0.43     | 1.91        | 6      | 1     |
| 1:A:22:VAL:CG2  | 1:A:43:LYS:HE3  | 0.43     | 2.39        | 7      | 1     |
| 1:A:14:GLU:O    | 1:A:18:ASN:CA   | 0.43     | 2.67        | 8      | 2     |
| 1:A:28:ILE:HB   | 1:A:74:VAL:HG21 | 0.43     | 1.91        | 4      | 1     |
| 1:A:76:HIS:O    | 1:A:77:TYR:CD1  | 0.43     | 2.72        | 4      | 1     |
| 1:A:3:TRP:CD2   | 1:A:3:TRP:O     | 0.43     | 2.72        | 9      | 1     |
| 1:A:26:PHE:CE1  | 1:A:41:SER:C    | 0.43     | 2.97        | 1      | 2     |
| 1:A:84:THR:HA   | 1:A:90:LYS:HA   | 0.43     | 1.91        | 1      | 1     |
| 1:A:11:HIS:CD2  | 1:A:11:HIS:C    | 0.43     | 2.96        | 3      | 1     |
| 1:A:12:GLN:O    | 1:A:15:CYS:N    | 0.43     | 2.51        | 3      | 1     |
| 1:A:73:LEU:HD12 | 1:A:74:VAL:N    | 0.43     | 2.29        | 3      | 1     |
| 1:A:66:ARG:O    | 1:A:67:PHE:CD1  | 0.43     | 2.72        | 5      | 1     |
| 1:A:60:TYR:CB   | 1:A:70:MET:SD   | 0.43     | 3.07        | 6      | 1     |
| 1:A:56:VAL:HG12 | 1:A:59:VAL:HG12 | 0.43     | 1.90        | 1      | 2     |
| 1:A:73:LEU:CD1  | 1:A:73:LEU:C    | 0.43     | 2.92        | 8      | 3     |
| 1:A:28:ILE:HG13 | 1:A:93:LEU:HD22 | 0.43     | 1.90        | 4      | 1     |
| 1:A:53:VAL:HG22 | 1:A:62:ILE:CG2  | 0.43     | 2.23        | 4      | 1     |
| 1:A:83:PHE:O    | 1:A:91:LEU:HG   | 0.43     | 2.14        | 6      | 1     |
| 1:A:70:MET:O    | 1:A:70:MET:HE2  | 0.43     | 2.14        | 8      | 1     |
| 1:A:62:ILE:HD12 | 1:A:67:PHE:CD2  | 0.43     | 2.49        | 9      | 1     |
| 1:A:8:VAL:CB    | 1:A:29:ARG:HD2  | 0.42     | 2.44        | 3      | 1     |
| 1:A:38:PHE:CE2  | 1:A:71:ASP:HB2  | 0.42     | 2.49        | 3      | 1     |
| 1:A:9:THR:OG1   | 1:A:29:ARG:CD   | 0.42     | 2.67        | 10     | 1     |
| 1:A:28:ILE:HG12 | 1:A:40:VAL:CB   | 0.42     | 2.44        | 4      | 1     |
| 1:A:21:GLY:H    | 1:A:43:LYS:HD2  | 0.42     | 1.73        | 7      | 1     |
| 1:A:17:LEU:CD1  | 1:A:43:LYS:CG   | 0.42     | 2.97        | 2      | 1     |
| 1:A:56:VAL:O    | 1:A:59:VAL:HB   | 0.42     | 2.13        | 2      | 1     |
| 1:A:62:ILE:O    | 1:A:64:GLN:N    | 0.42     | 2.51        | 9      | 1     |
| 1:A:19:GLU:O    | 1:A:20:ARG:HB3  | 0.42     | 2.15        | 3      | 1     |
| 1:A:22:VAL:C    | 1:A:23:GLU:CG   | 0.42     | 2.92        | 3      | 1     |
| 1:A:26:PHE:CG   | 1:A:92:TYR:O    | 0.42     | 2.72        | 4      | 1     |
| 1:A:27:LEU:O    | 1:A:40:VAL:CB   | 0.42     | 2.67        | 4      | 1     |
| 1:A:84:THR:HG23 | 1:A:90:LYS:CA   | 0.42     | 2.44        | 6      | 1     |
| 1:A:62:ILE:HB   | 1:A:67:PHE:CZ   | 0.42     | 2.49        | 7      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:88:GLY:O    | 1:A:89:GLU:CD   | 0.42     | 2.63        | 5      | 1     |
| 1:A:8:VAL:HG23  | 1:A:29:ARG:HD2  | 0.42     | 1.92        | 3      | 1     |
| 1:A:10:ARG:HB2  | 1:A:29:ARG:NE   | 0.42     | 2.29        | 4      | 1     |
| 1:A:8:VAL:C     | 1:A:29:ARG:HG2  | 0.42     | 2.40        | 9      | 1     |
| 1:A:90:LYS:O    | 1:A:92:TYR:CD2  | 0.42     | 2.72        | 9      | 1     |
| 1:A:17:LEU:HD13 | 1:A:43:LYS:CD   | 0.42     | 2.45        | 4      | 1     |
| 1:A:9:THR:CB    | 1:A:29:ARG:CD   | 0.42     | 2.96        | 8      | 1     |
| 1:A:17:LEU:C    | 1:A:19:GLU:N    | 0.42     | 2.77        | 10     | 1     |
| 1:A:84:THR:HG21 | 1:A:90:LYS:HE2  | 0.42     | 1.92        | 2      | 1     |
| 1:A:9:THR:O     | 1:A:29:ARG:CD   | 0.42     | 2.68        | 6      | 1     |
| 1:A:26:PHE:CG   | 1:A:93:LEU:HA   | 0.42     | 2.50        | 6      | 1     |
| 1:A:8:VAL:CG1   | 1:A:96:ALA:CB   | 0.42     | 2.98        | 7      | 1     |
| 1:A:73:LEU:N    | 1:A:73:LEU:CD1  | 0.42     | 2.82        | 9      | 1     |
| 1:A:38:PHE:CZ   | 1:A:71:ASP:CG   | 0.42     | 2.97        | 10     | 1     |
| 1:A:8:VAL:C     | 1:A:29:ARG:HB3  | 0.42     | 2.40        | 5      | 1     |
| 1:A:43:LYS:HA   | 1:A:43:LYS:HD3  | 0.42     | 1.68        | 5      | 1     |
| 1:A:49:LYS:N    | 1:A:49:LYS:HD2  | 0.42     | 2.29        | 7      | 1     |
| 1:A:28:ILE:HD13 | 1:A:40:VAL:CG1  | 0.42     | 2.44        | 7      | 2     |
| 1:A:9:THR:H     | 1:A:13:ALA:H    | 0.41     | 1.56        | 3      | 1     |
| 1:A:74:VAL:O    | 1:A:93:LEU:O    | 0.41     | 2.38        | 4      | 1     |
| 1:A:37:ASP:C    | 1:A:38:PHE:CD1  | 0.41     | 2.98        | 7      | 1     |
| 1:A:80:ALA:HB1  | 1:A:93:LEU:CD1  | 0.41     | 2.42        | 9      | 1     |
| 1:A:67:PHE:CD2  | 1:A:79:LYS:HB3  | 0.41     | 2.49        | 10     | 1     |
| 1:A:50:HIS:O    | 1:A:51:PHE:CD1  | 0.41     | 2.73        | 6      | 2     |
| 1:A:51:PHE:CD2  | 1:A:81:PRO:HG2  | 0.41     | 2.50        | 4      | 1     |
| 1:A:30:ASP:OD2  | 1:A:38:PHE:CZ   | 0.41     | 2.74        | 10     | 1     |
| 1:A:30:ASP:OD1  | 1:A:38:PHE:CZ   | 0.41     | 2.74        | 7      | 1     |
| 1:A:70:MET:O    | 1:A:70:MET:CE   | 0.41     | 2.68        | 10     | 1     |
| 1:A:9:THR:C     | 1:A:29:ARG:HD2  | 0.41     | 2.40        | 4      | 1     |
| 1:A:90:LYS:HB2  | 1:A:92:TYR:CD2  | 0.41     | 2.50        | 6      | 1     |
| 1:A:60:TYR:CD2  | 1:A:69:THR:O    | 0.41     | 2.73        | 7      | 1     |
| 1:A:38:PHE:CE2  | 1:A:71:ASP:OD2  | 0.41     | 2.74        | 2      | 1     |
| 1:A:30:ASP:HA   | 1:A:38:PHE:CD1  | 0.41     | 2.50        | 3      | 1     |
| 1:A:38:PHE:CD2  | 1:A:71:ASP:OD1  | 0.41     | 2.73        | 3      | 1     |
| 1:A:28:ILE:CD1  | 1:A:40:VAL:HG11 | 0.41     | 2.46        | 4      | 1     |
| 1:A:53:VAL:CG2  | 1:A:62:ILE:CD1  | 0.41     | 2.99        | 6      | 1     |
| 1:A:73:LEU:H    | 1:A:73:LEU:HD12 | 0.41     | 1.75        | 10     | 1     |
| 1:A:38:PHE:CG   | 1:A:71:ASP:OD1  | 0.41     | 2.74        | 1      | 1     |
| 1:A:27:LEU:O    | 1:A:40:VAL:HB   | 0.41     | 2.16        | 4      | 1     |
| 1:A:44:ALA:HB2  | 1:A:91:LEU:CD2  | 0.41     | 2.46        | 4      | 1     |
| 1:A:10:ARG:HG2  | 1:A:11:HIS:N    | 0.41     | 2.31        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:83:PHE:CD1  | 1:A:84:THR:N    | 0.41     | 2.89        | 9      | 1     |
| 1:A:9:THR:HG23  | 1:A:10:ARG:H    | 0.41     | 1.74        | 5      | 1     |
| 1:A:60:TYR:CB   | 1:A:70:MET:HB2  | 0.41     | 2.46        | 6      | 1     |
| 1:A:41:SER:OG   | 1:A:50:HIS:CE1  | 0.41     | 2.74        | 7      | 1     |
| 1:A:51:PHE:CG   | 1:A:63:GLY:HA3  | 0.41     | 2.51        | 7      | 1     |
| 1:A:9:THR:O     | 1:A:10:ARG:HG2  | 0.41     | 2.16        | 8      | 1     |
| 1:A:28:ILE:CG1  | 1:A:40:VAL:HB   | 0.41     | 2.46        | 9      | 1     |
| 1:A:38:PHE:CD1  | 1:A:71:ASP:OD2  | 0.41     | 2.73        | 1      | 2     |
| 1:A:40:VAL:HG21 | 1:A:93:LEU:HD22 | 0.41     | 1.92        | 1      | 1     |
| 1:A:59:VAL:CG1  | 1:A:60:TYR:N    | 0.41     | 2.84        | 4      | 1     |
| 1:A:42:LEU:CD2  | 1:A:91:LEU:CD1  | 0.41     | 2.99        | 5      | 1     |
| 1:A:10:ARG:HB3  | 1:A:29:ARG:HD2  | 0.41     | 1.92        | 7      | 1     |
| 1:A:94:VAL:HG23 | 1:A:95:ARG:H    | 0.41     | 1.74        | 7      | 1     |
| 1:A:49:LYS:HB3  | 1:A:51:PHE:CZ   | 0.41     | 2.51        | 9      | 1     |
| 1:A:17:LEU:HD21 | 1:A:27:LEU:HD23 | 0.41     | 1.92        | 10     | 1     |
| 1:A:49:LYS:HB2  | 1:A:51:PHE:CZ   | 0.41     | 2.51        | 3      | 1     |
| 1:A:30:ASP:CG   | 1:A:38:PHE:CE2  | 0.41     | 2.99        | 5      | 1     |
| 1:A:8:VAL:O     | 1:A:12:GLN:OE1  | 0.41     | 2.39        | 6      | 1     |
| 1:A:57:ASP:OD1  | 1:A:57:ASP:O    | 0.41     | 2.39        | 6      | 1     |
| 1:A:67:PHE:CD1  | 1:A:79:LYS:CB   | 0.41     | 3.04        | 6      | 1     |
| 1:A:21:GLY:N    | 1:A:43:LYS:NZ   | 0.41     | 2.68        | 7      | 1     |
| 1:A:68:HIS:O    | 1:A:68:HIS:CG   | 0.41     | 2.72        | 8      | 1     |
| 1:A:65:ARG:HB3  | 1:A:67:PHE:CZ   | 0.40     | 2.51        | 1      | 1     |
| 1:A:60:TYR:HB3  | 1:A:70:MET:CB   | 0.40     | 2.47        | 4      | 1     |
| 1:A:51:PHE:CE1  | 1:A:62:ILE:HG23 | 0.40     | 2.50        | 8      | 1     |
| 1:A:30:ASP:OD1  | 1:A:38:PHE:CE1  | 0.40     | 2.74        | 1      | 1     |
| 1:A:30:ASP:CG   | 1:A:38:PHE:CE1  | 0.40     | 2.99        | 10     | 1     |
| 1:A:22:VAL:HG22 | 1:A:43:LYS:CE   | 0.40     | 2.46        | 2      | 1     |
| 1:A:38:PHE:CD2  | 1:A:71:ASP:OD2  | 0.40     | 2.74        | 2      | 1     |
| 1:A:8:VAL:O     | 1:A:29:ARG:CD   | 0.40     | 2.69        | 3      | 1     |
| 1:A:38:PHE:CD2  | 1:A:70:MET:HG2  | 0.40     | 2.51        | 3      | 1     |
| 1:A:8:VAL:C     | 1:A:9:THR:O     | 0.40     | 2.64        | 4      | 1     |
| 1:A:70:MET:CE   | 1:A:73:LEU:HG   | 0.40     | 2.46        | 6      | 1     |
| 1:A:8:VAL:O     | 1:A:29:ARG:CG   | 0.40     | 2.69        | 7      | 1     |
| 1:A:85:SER:O    | 1:A:89:GLU:HG3  | 0.40     | 2.16        | 7      | 1     |
| 1:A:9:THR:HA    | 1:A:13:ALA:H    | 0.40     | 1.77        | 10     | 1     |
| 1:A:13:ALA:O    | 1:A:17:LEU:CB   | 0.40     | 2.69        | 4      | 1     |
| 1:A:67:PHE:CG   | 1:A:79:LYS:HB2  | 0.40     | 2.51        | 6      | 1     |
| 1:A:76:HIS:O    | 1:A:77:TYR:CD2  | 0.40     | 2.74        | 6      | 1     |
| 1:A:3:TRP:O     | 1:A:3:TRP:CE3   | 0.40     | 2.74        | 9      | 1     |
| 1:A:59:VAL:CG1  | 1:A:66:ARG:HB3  | 0.40     | 2.46        | 10     | 1     |

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| Atom-1         | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|----------------|----------------|----------|-------------|--------|-------|
|                |                |          |             | Worst  | Total |
| 1:A:9:THR:OG1  | 1:A:13:ALA:HB2 | 0.40     | 2.17        | 1      | 1     |
| 1:A:84:THR:CG2 | 1:A:90:LYS:HE2 | 0.40     | 2.46        | 2      | 1     |
| 1:A:26:PHE:HB3 | 1:A:42:LEU:CD1 | 0.40     | 2.46        | 4      | 1     |
| 1:A:26:PHE:CD2 | 1:A:42:LEU:CD2 | 0.40     | 2.96        | 7      | 1     |
| 1:A:9:THR:O    | 1:A:29:ARG:HD2 | 0.40     | 2.17        | 8      | 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     | 92/98 (94%)   | 68±2 (74±2%) | 16±2 (18±3%) | 8±2 (8±2%) | <b>1</b>    | <b>12</b> |
| All | All   | 920/980 (94%) | 679 (74%)    | 163 (18%)    | 78 (8%)    | <b>1</b>    | <b>12</b> |

All 21 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     | 94  | VAL  | 10             |
| 1   | A     | 23  | GLU  | 9              |
| 1   | A     | 45  | SER  | 8              |
| 1   | A     | 20  | ARG  | 7              |
| 1   | A     | 78  | LYS  | 7              |
| 1   | A     | 81  | PRO  | 5              |
| 1   | A     | 9   | THR  | 5              |
| 1   | A     | 70  | MET  | 4              |
| 1   | A     | 8   | VAL  | 3              |
| 1   | A     | 97  | LEU  | 3              |
| 1   | A     | 19  | GLU  | 3              |
| 1   | A     | 63  | GLY  | 3              |
| 1   | A     | 21  | GLY  | 2              |
| 1   | A     | 86  | GLU  | 2              |
| 1   | A     | 18  | ASN  | 1              |
| 1   | A     | 10  | ARG  | 1              |
| 1   | A     | 35  | PRO  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 89  | GLU  | 1              |
| 1   | A     | 57  | ASP  | 1              |
| 1   | A     | 3   | TRP  | 1              |
| 1   | A     | 24  | GLY  | 1              |

### 6.3.2 Protein sidechains [i](#)

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     | 83/87 (95%)   | 49±4 (60±4%) | 34±4 (40±4%) | 0           | 5 |
| All | All   | 830/870 (95%) | 494 (60%)    | 336 (40%)    | 0           | 5 |

All 76 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     | 26  | PHE  | 10             |
| 1   | A     | 47  | LYS  | 10             |
| 1   | A     | 55  | LEU  | 10             |
| 1   | A     | 56  | VAL  | 10             |
| 1   | A     | 73  | LEU  | 10             |
| 1   | A     | 74  | VAL  | 10             |
| 1   | A     | 17  | LEU  | 9              |
| 1   | A     | 8   | VAL  | 8              |
| 1   | A     | 14  | GLU  | 8              |
| 1   | A     | 27  | LEU  | 8              |
| 1   | A     | 29  | ARG  | 8              |
| 1   | A     | 89  | GLU  | 8              |
| 1   | A     | 39  | SER  | 7              |
| 1   | A     | 91  | LEU  | 7              |
| 1   | A     | 43  | LYS  | 7              |
| 1   | A     | 9   | THR  | 6              |
| 1   | A     | 49  | LYS  | 6              |
| 1   | A     | 59  | VAL  | 6              |
| 1   | A     | 79  | LYS  | 6              |
| 1   | A     | 90  | LYS  | 6              |
| 1   | A     | 98  | GLN  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 95  | ARG  | 6              |
| 1   | A     | 10  | ARG  | 5              |
| 1   | A     | 28  | ILE  | 5              |
| 1   | A     | 34  | SER  | 5              |
| 1   | A     | 41  | SER  | 5              |
| 1   | A     | 65  | ARG  | 5              |
| 1   | A     | 54  | GLN  | 5              |
| 1   | A     | 70  | MET  | 5              |
| 1   | A     | 94  | VAL  | 5              |
| 1   | A     | 93  | LEU  | 5              |
| 1   | A     | 52  | LYS  | 5              |
| 1   | A     | 22  | VAL  | 4              |
| 1   | A     | 23  | GLU  | 4              |
| 1   | A     | 36  | SER  | 4              |
| 1   | A     | 77  | TYR  | 4              |
| 1   | A     | 97  | LEU  | 4              |
| 1   | A     | 45  | SER  | 4              |
| 1   | A     | 85  | SER  | 4              |
| 1   | A     | 25  | ASP  | 4              |
| 1   | A     | 75  | GLU  | 4              |
| 1   | A     | 83  | PHE  | 4              |
| 1   | A     | 86  | GLU  | 4              |
| 1   | A     | 31  | SER  | 4              |
| 1   | A     | 72  | GLU  | 4              |
| 1   | A     | 11  | HIS  | 3              |
| 1   | A     | 40  | VAL  | 3              |
| 1   | A     | 50  | HIS  | 3              |
| 1   | A     | 78  | LYS  | 3              |
| 1   | A     | 4   | TYR  | 3              |
| 1   | A     | 51  | PHE  | 3              |
| 1   | A     | 58  | ASN  | 3              |
| 1   | A     | 62  | ILE  | 3              |
| 1   | A     | 19  | GLU  | 3              |
| 1   | A     | 20  | ARG  | 3              |
| 1   | A     | 48  | ASN  | 3              |
| 1   | A     | 18  | ASN  | 2              |
| 1   | A     | 37  | ASP  | 2              |
| 1   | A     | 84  | THR  | 2              |
| 1   | A     | 12  | GLN  | 2              |
| 1   | A     | 15  | CYS  | 2              |
| 1   | A     | 3   | TRP  | 2              |
| 1   | A     | 64  | GLN  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 32  | GLU  | 2              |
| 1   | A     | 82  | ILE  | 2              |
| 1   | A     | 69  | THR  | 1              |
| 1   | A     | 76  | HIS  | 1              |
| 1   | A     | 87  | HIS  | 1              |
| 1   | A     | 71  | ASP  | 1              |
| 1   | A     | 42  | LEU  | 1              |
| 1   | A     | 33  | SER  | 1              |
| 1   | A     | 38  | PHE  | 1              |
| 1   | A     | 67  | PHE  | 1              |
| 1   | A     | 57  | ASP  | 1              |
| 1   | A     | 30  | ASP  | 1              |
| 1   | A     | 68  | HIS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided