



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:06 pm GMT

PDB ID : 1NSH  
Title : Solution Structure of Rabbit apo-S100A11 (19 models)  
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Deposited on : 2003-01-27

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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| Cyrange                        | : | Kirchner and Güntert (2011)  |
| NmrClust                       | : | Kelley et al. (1996)   |
| MolProbity                     | : | 4.02b-467  |
| Percentile statistics          | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| RCI                            | : | v_1n_11_5_13_A (Berjanski et al., 2005)                            |
| PANAV                          | : | Wang et al. (2010)   |
| ShiftChecker                   | : | trunk28760   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | recalc28949  |

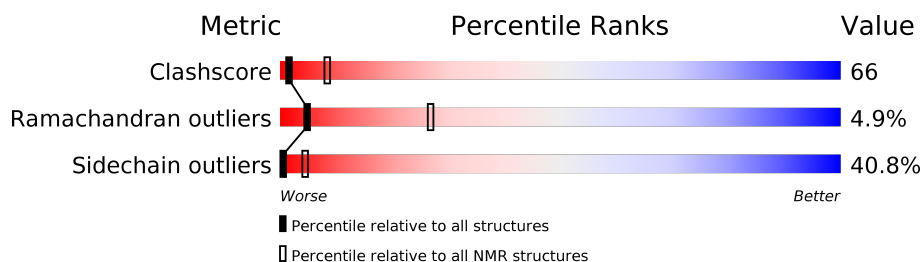
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

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            | 125131                      | 11601                     |
| Ramachandran outliers | 121729                      | 10391                     |
| Sidechain outliers    | 121581                      | 10367                     |

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     | 101    |                  |
| 1   | B     | 101    |                  |

## 2 Ensemble composition and analysis

This entry contains 19 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:4-A:22, A:28-A:47, A:55-A:60, A:70-A:92, B:4-B:22, B:28-B:47, B:55-B:60, B:70-B:92 (136) | 0.42              | 7            |

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 2 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 3172 atoms, of which 1586 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calgizzarin.

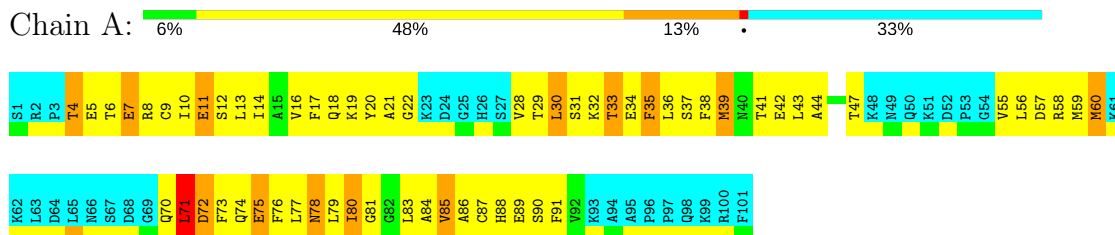
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 101      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1586  | 502 | 793 | 135 | 151 | 5 |       |
| 1   | B     | 101      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1586  | 502 | 793 | 135 | 151 | 5 |       |

## 4 Residue-property plots

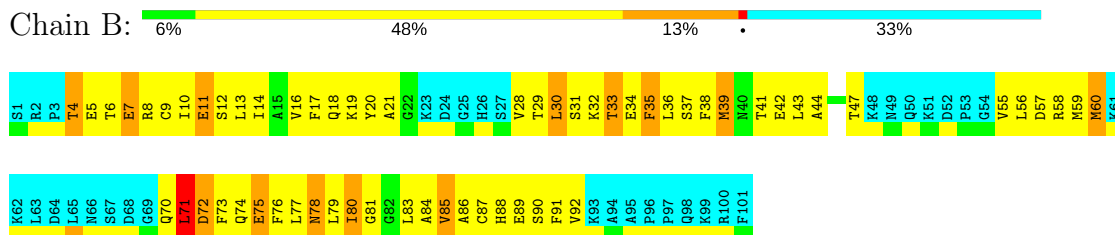
### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Calgizzarin



- Molecule 1: Calgizzarin

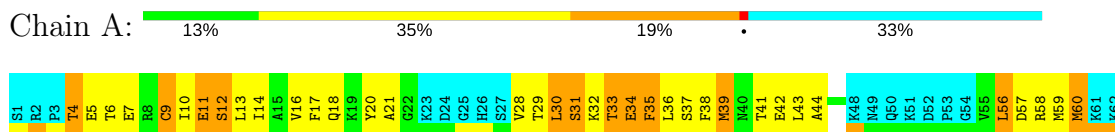


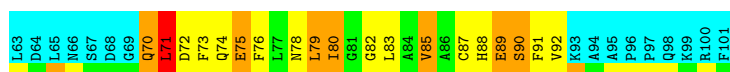
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

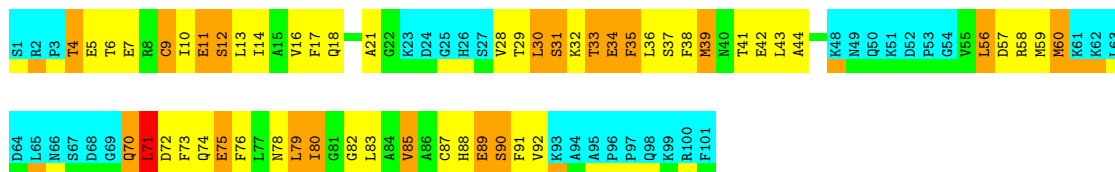
- Molecule 1: Calgizzarin





### • Molecule 1: Calgizzarin

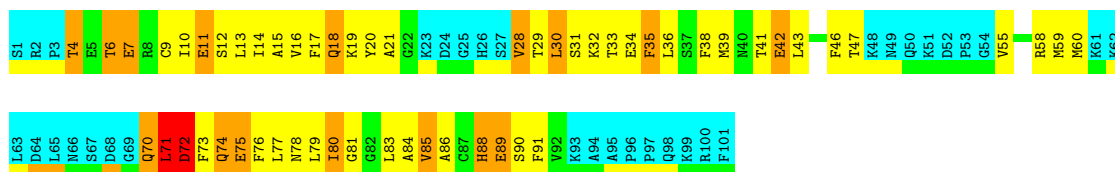
Chain B: 14% 34% 19% • 33%



## 4.2.2 Score per residue for model 2

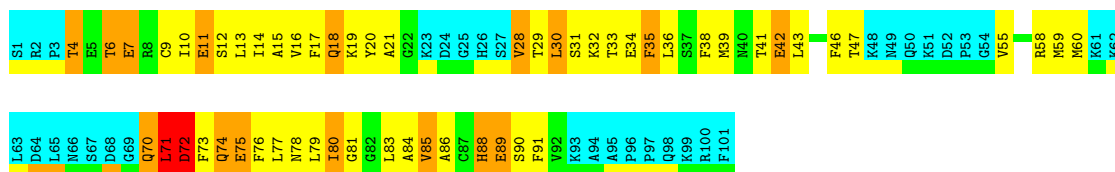
### • Molecule 1: Calgizzarin

Chain A: 12% 38% 16% • 33%



### • Molecule 1: Calgizzarin

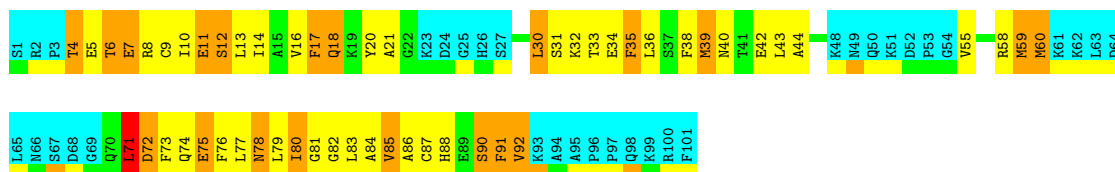
Chain B: 12% 38% 16% • 33%



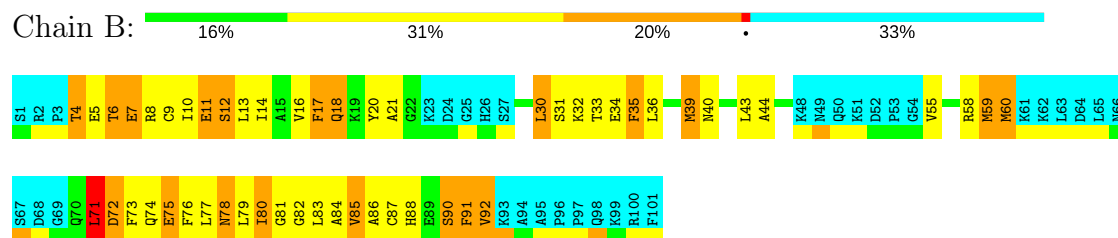
## 4.2.3 Score per residue for model 3

### • Molecule 1: Calgizzarin

Chain A: 14% 33% 20% • 33%

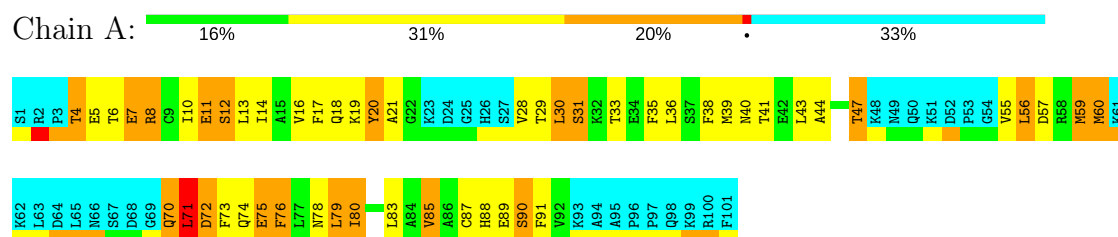


### • Molecule 1: Calgizzarin

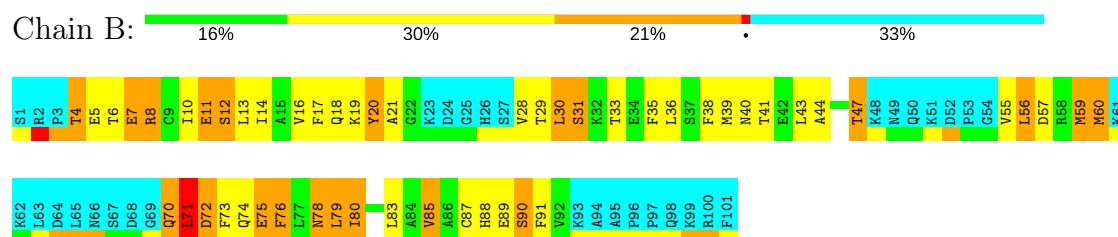


#### 4.2.4 Score per residue for model 4

- Molecule 1: Calgizzarin

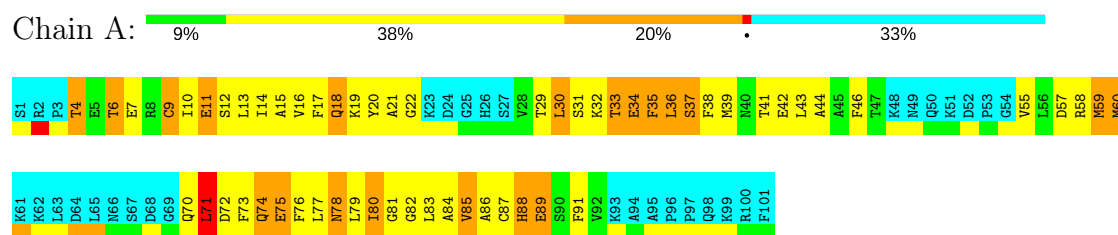


- Molecule 1: Calgizzarin

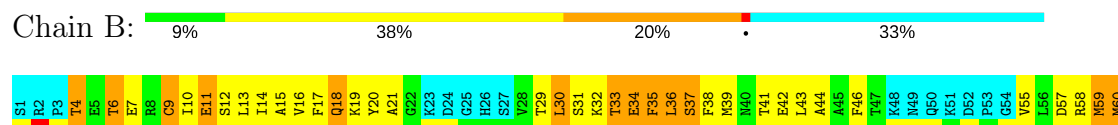


#### 4.2.5 Score per residue for model 5

- Molecule 1: Calgizzarin



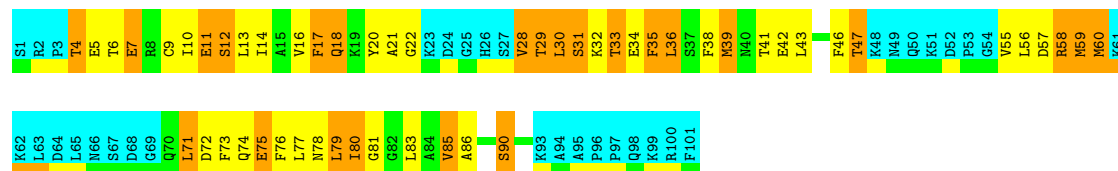
- Molecule 1: Calgizzarin



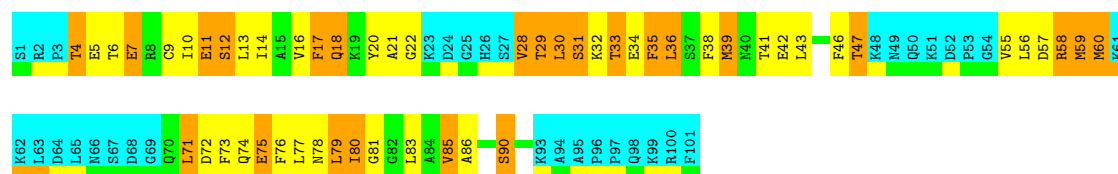


#### 4.2.6 Score per residue for model 6

- Molecule 1: Calgizzarin

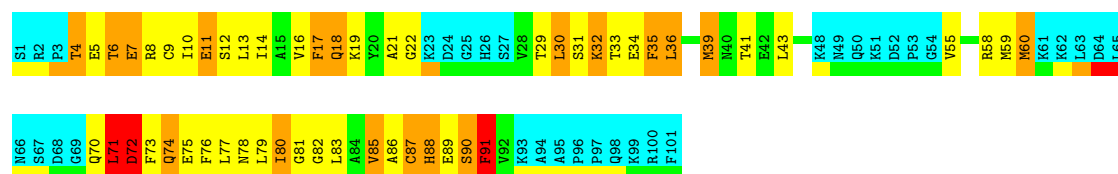


- Molecule 1: Calgizzarin

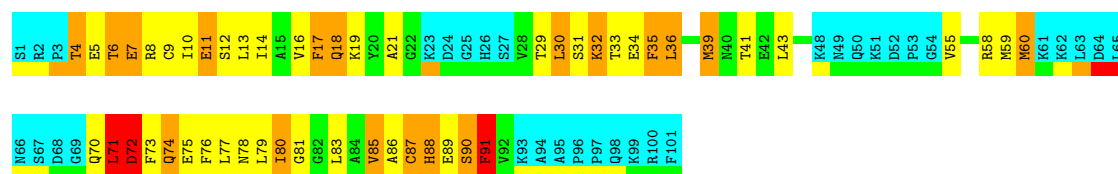


#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Calgizzarin



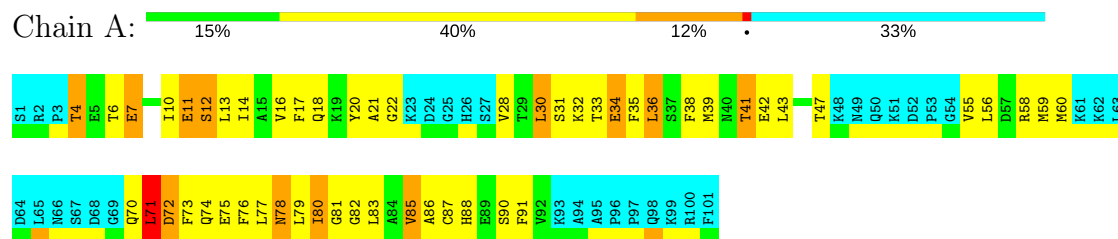
- Molecule 1: Calgizzarin



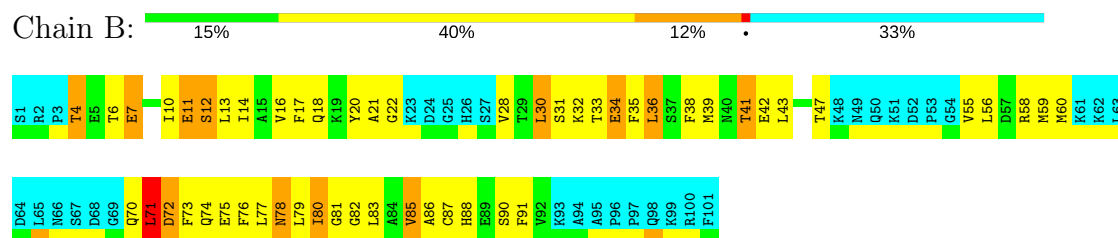


### 4.2.8 Score per residue for model 8

#### • Molecule 1: Calgizzarin

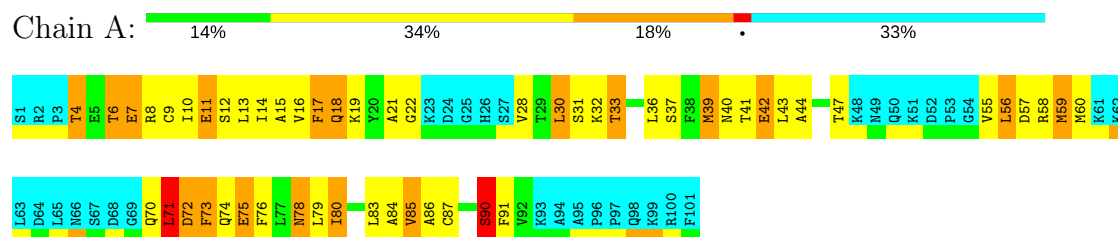


#### • Molecule 1: Calgizzarin

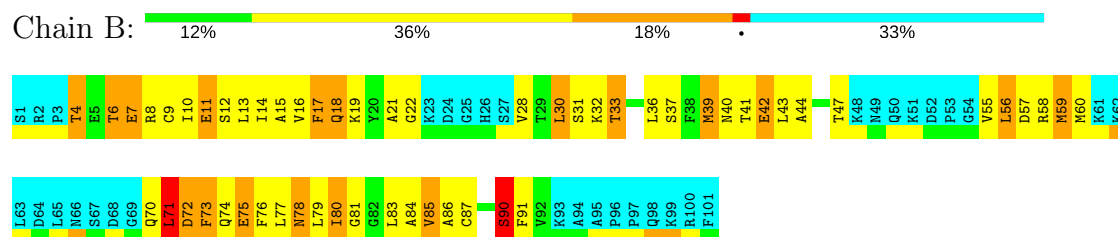


### 4.2.9 Score per residue for model 9

#### • Molecule 1: Calgizzarin

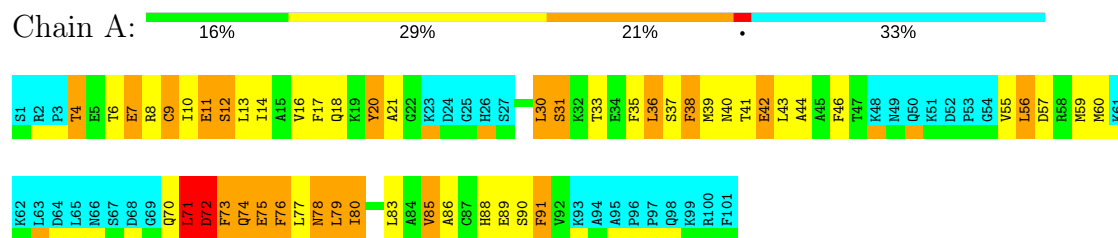


#### • Molecule 1: Calgizzarin

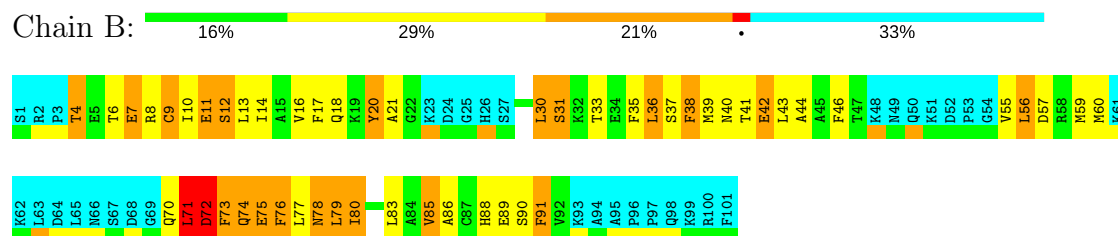


### 4.2.10 Score per residue for model 10

#### • Molecule 1: Calgizzarin

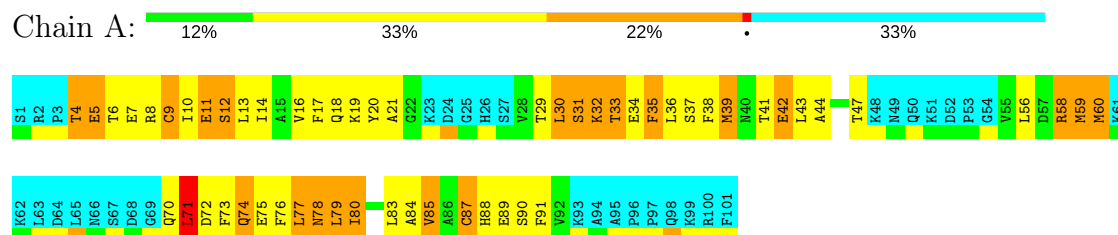


• Molecule 1: Calgizzarin

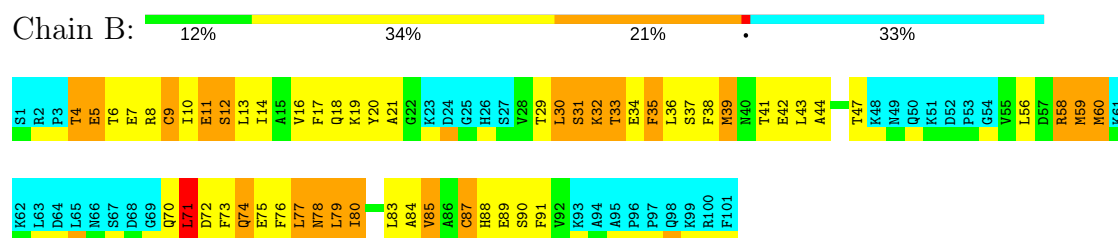


#### 4.2.11 Score per residue for model 11

• Molecule 1: Calgizzarin

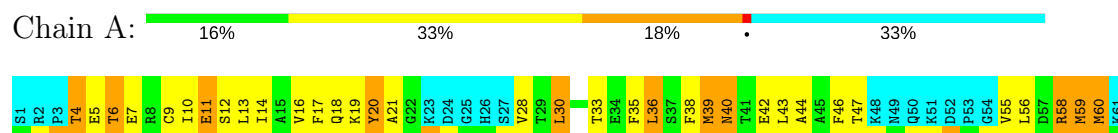


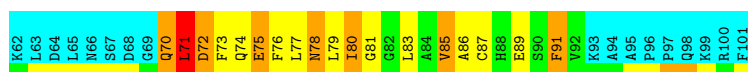
• Molecule 1: Calgizzarin



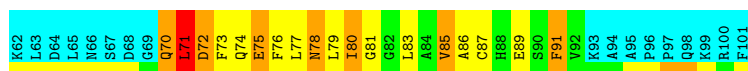
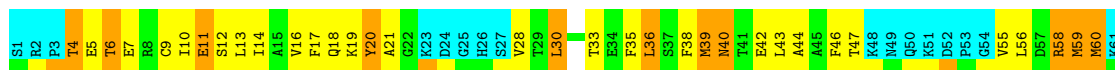
#### 4.2.12 Score per residue for model 12

• Molecule 1: Calgizzarin





• Molecule 1: Calgizzarin

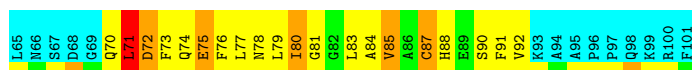


#### 4.2.13 Score per residue for model 13

• Molecule 1: Calgizzarin

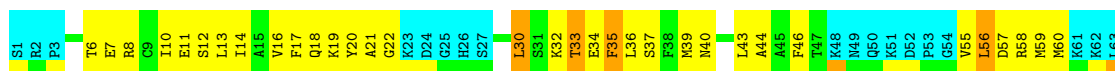


• Molecule 1: Calgizzarin

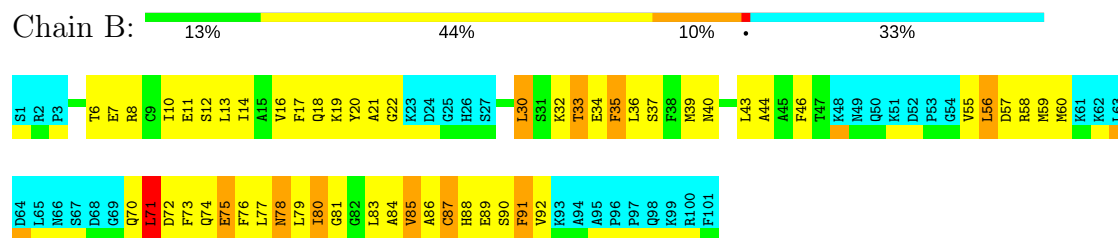


#### 4.2.14 Score per residue for model 14

• Molecule 1: Calgizzarin

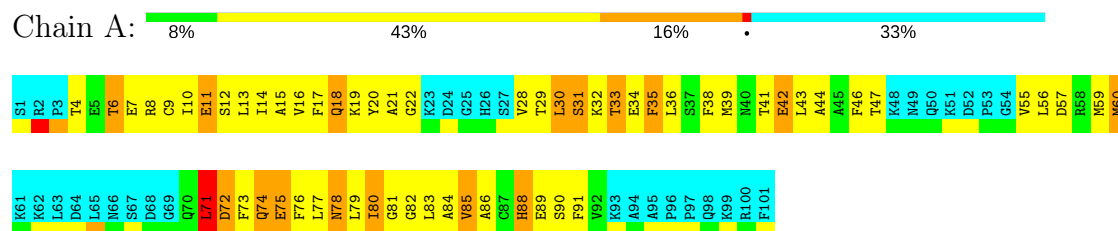


• Molecule 1: Calgizzarin

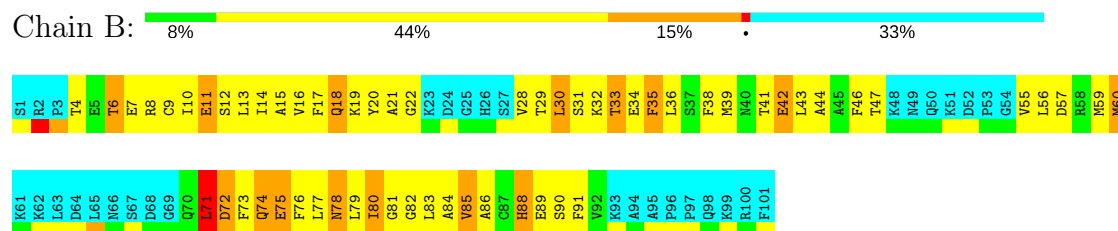


#### 4.2.15 Score per residue for model 15

- Molecule 1: Calgizzarin

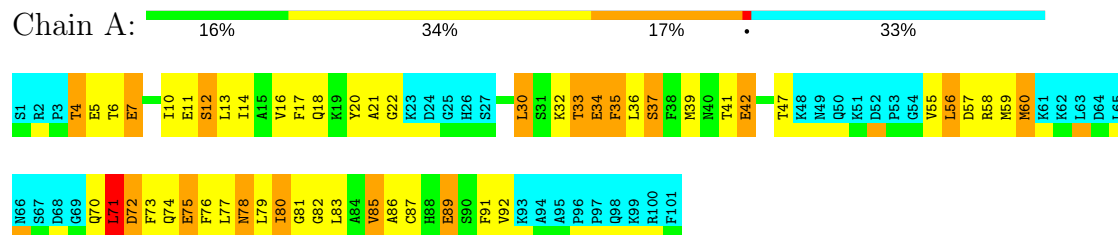


- Molecule 1: Calgizzarin

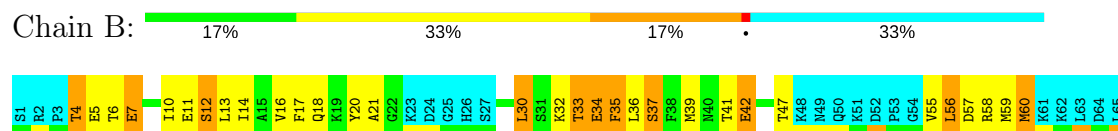


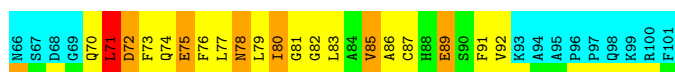
#### 4.2.16 Score per residue for model 16

- Molecule 1: Calgizzarin



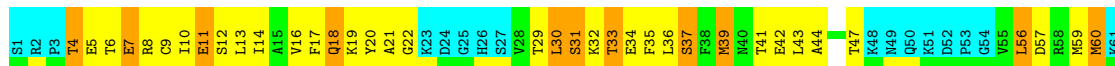
- Molecule 1: Calgizzarin



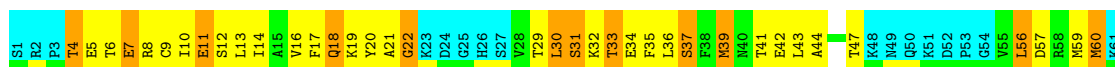


#### 4.2.17 Score per residue for model 17

- Molecule 1: Calgizzarin

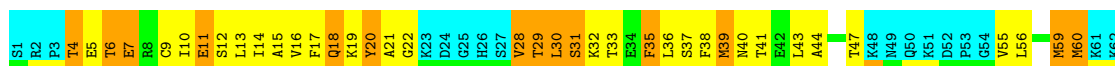


- Molecule 1: Calgizzarin

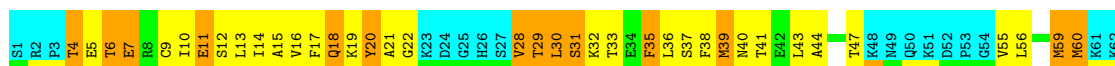


#### 4.2.18 Score per residue for model 18

- Molecule 1: Calgizzarin



- Molecule 1: Calgizzarin



### 4.2.19 Score per residue for model 19

#### • Molecule 1: Calgizzarin

Chain A:  16% 33% 18% • 33%



#### • Molecule 1: Calgizzarin

Chain B:  14% 34% 19% • 33%



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 19 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     |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

|  |                 |
|--|-----------------|
| Chemical shift file(s)                       | BMRB entry 5189 |
| Number of chemical shift lists               | 1               |
| Total number of shifts                       | 2458            |
| Number of shifts mapped to atoms             | 2458            |
| Number of unparsed shifts                    | 0               |
| Number of shifts with mapping errors         | 0               |
| Number of shifts with mapping warnings       | 0               |
| Assignment completeness (well-defined parts) | 90%             |

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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     | 536   | 531      | 532      | 83±11   |
| 1   | B     | 536   | 531      | 532      | 82±11   |
| All | All   | 20368 | 20178    | 20216    | 2693    |

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 66.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:59:MET:HE2  | 1:B:83:LEU:HD21 | 1.10     | 1.18        | 1      | 10    |
| 1:A:33:THR:HA   | 1:A:36:LEU:HD23 | 1.05     | 1.22        | 12     | 9     |
| 1:B:33:THR:HA   | 1:B:36:LEU:HD23 | 1.04     | 1.29        | 10     | 9     |
| 1:A:10:ILE:HG22 | 1:A:14:ILE:HD11 | 1.00     | 1.33        | 19     | 19    |
| 1:B:10:ILE:HG22 | 1:B:14:ILE:HD11 | 0.98     | 1.34        | 1      | 19    |
| 1:A:13:LEU:HD23 | 1:B:13:LEU:HD23 | 0.96     | 1.34        | 11     | 12    |
| 1:B:59:MET:HE3  | 1:B:83:LEU:HD21 | 0.96     | 1.36        | 8      | 9     |
| 1:A:59:MET:HE3  | 1:A:83:LEU:HD21 | 0.96     | 1.31        | 1      | 9     |
| 1:A:13:LEU:O    | 1:A:16:VAL:HG22 | 0.95     | 1.62        | 19     | 19    |
| 1:B:79:LEU:O    | 1:B:83:LEU:HG   | 0.95     | 1.60        | 5      | 15    |
| 1:A:79:LEU:O    | 1:A:83:LEU:HG   | 0.95     | 1.60        | 5      | 15    |
| 1:B:13:LEU:O    | 1:B:16:VAL:HG22 | 0.94     | 1.63        | 4      | 19    |
| 1:B:59:MET:HG3  | 1:B:83:LEU:HD21 | 0.92     | 1.39        | 13     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:59:MET:HG3  | 1:A:83:LEU:HD21 | 0.91     | 1.39        | 13     | 1     |
| 1:A:77:LEU:HD22 | 1:B:77:LEU:HD22 | 0.90     | 1.44        | 16     | 7     |
| 1:A:80:ILE:HD11 | 1:B:10:ILE:HG12 | 0.90     | 1.44        | 8      | 18    |
| 1:B:6:THR:O     | 1:B:10:ILE:HD12 | 0.89     | 1.67        | 2      | 19    |
| 1:A:6:THR:O     | 1:A:10:ILE:HD12 | 0.89     | 1.68        | 7      | 19    |
| 1:A:10:ILE:HG12 | 1:B:80:ILE:HD11 | 0.87     | 1.46        | 14     | 18    |
| 1:A:75:GLU:O    | 1:A:79:LEU:HD23 | 0.87     | 1.70        | 17     | 6     |
| 1:B:75:GLU:O    | 1:B:79:LEU:HD23 | 0.86     | 1.70        | 17     | 6     |
| 1:B:41:THR:HG23 | 1:B:42:GLU:HG2  | 0.86     | 1.46        | 9      | 9     |
| 1:A:41:THR:HG23 | 1:A:42:GLU:HG2  | 0.86     | 1.46        | 9      | 9     |
| 1:A:59:MET:CE   | 1:A:83:LEU:HD21 | 0.85     | 2.00        | 1      | 14    |
| 1:B:59:MET:CE   | 1:B:83:LEU:HD21 | 0.85     | 2.00        | 1      | 14    |
| 1:B:37:SER:O    | 1:B:41:THR:HG22 | 0.85     | 1.72        | 13     | 8     |
| 1:A:73:PHE:CD2  | 1:B:85:VAL:HG11 | 0.84     | 2.08        | 11     | 15    |
| 1:A:85:VAL:HG11 | 1:B:73:PHE:CD2  | 0.84     | 2.08        | 11     | 15    |
| 1:A:41:THR:HG23 | 1:A:42:GLU:CG   | 0.84     | 2.03        | 10     | 7     |
| 1:A:37:SER:O    | 1:A:41:THR:HG22 | 0.83     | 1.71        | 13     | 8     |
| 1:A:35:PHE:CD2  | 1:A:79:LEU:HD23 | 0.83     | 2.08        | 2      | 5     |
| 1:B:35:PHE:CD2  | 1:B:79:LEU:HD23 | 0.83     | 2.08        | 2      | 5     |
| 1:A:73:PHE:CG   | 1:B:85:VAL:HG11 | 0.83     | 2.09        | 17     | 17    |
| 1:B:71:LEU:HD13 | 1:B:75:GLU:HB3  | 0.83     | 1.51        | 10     | 9     |
| 1:B:41:THR:HG23 | 1:B:42:GLU:CG   | 0.82     | 2.04        | 1      | 7     |
| 1:A:85:VAL:HG11 | 1:B:73:PHE:CG   | 0.82     | 2.09        | 17     | 17    |
| 1:A:59:MET:HE2  | 1:A:83:LEU:HD21 | 0.82     | 1.48        | 2      | 11    |
| 1:A:71:LEU:HD13 | 1:A:75:GLU:HB3  | 0.82     | 1.51        | 10     | 9     |
| 1:A:11:GLU:HA   | 1:A:14:ILE:HD12 | 0.82     | 1.51        | 19     | 19    |
| 1:B:11:GLU:HA   | 1:B:14:ILE:HD12 | 0.80     | 1.52        | 5      | 19    |
| 1:A:38:PHE:O    | 1:A:41:THR:HG22 | 0.79     | 1.76        | 10     | 1     |
| 1:B:38:PHE:O    | 1:B:41:THR:HG22 | 0.78     | 1.76        | 10     | 1     |
| 1:A:85:VAL:HG11 | 1:B:73:PHE:CD1  | 0.78     | 2.13        | 10     | 2     |
| 1:B:59:MET:SD   | 1:B:79:LEU:HD13 | 0.78     | 2.18        | 1      | 1     |
| 1:B:14:ILE:O    | 1:B:18:GLN:HG2  | 0.78     | 1.78        | 3      | 15    |
| 1:A:59:MET:SD   | 1:A:79:LEU:HD13 | 0.78     | 2.19        | 1      | 1     |
| 1:A:14:ILE:HD13 | 1:B:88:HIS:CD2  | 0.78     | 2.13        | 4      | 2     |
| 1:A:10:ILE:HD11 | 1:B:43:LEU:HD21 | 0.78     | 1.55        | 8      | 13    |
| 1:A:14:ILE:O    | 1:A:18:GLN:HG2  | 0.77     | 1.78        | 3      | 15    |
| 1:A:73:PHE:CD1  | 1:B:85:VAL:HG11 | 0.77     | 2.13        | 10     | 2     |
| 1:B:33:THR:HA   | 1:B:36:LEU:CD2  | 0.77     | 2.09        | 8      | 3     |
| 1:B:56:LEU:HD23 | 1:B:57:ASP:N    | 0.76     | 1.95        | 4      | 6     |
| 1:A:56:LEU:HD23 | 1:A:57:ASP:N    | 0.76     | 1.95        | 4      | 6     |
| 1:A:33:THR:HA   | 1:A:36:LEU:CD2  | 0.76     | 2.09        | 8      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:88:HIS:CD2  | 1:B:14:ILE:HD13 | 0.76     | 2.13        | 4      | 2     |
| 1:B:18:GLN:HA   | 1:B:21:ALA:HB3  | 0.76     | 1.55        | 6      | 9     |
| 1:A:18:GLN:HA   | 1:A:21:ALA:HB3  | 0.76     | 1.55        | 6      | 9     |
| 1:B:71:LEU:HD13 | 1:B:75:GLU:HG2  | 0.76     | 1.58        | 16     | 1     |
| 1:A:43:LEU:HD21 | 1:B:10:ILE:HD11 | 0.76     | 1.55        | 8      | 13    |
| 1:B:59:MET:HE1  | 1:B:83:LEU:HD11 | 0.76     | 1.57        | 2      | 6     |
| 1:A:71:LEU:HD13 | 1:A:75:GLU:HG2  | 0.76     | 1.58        | 16     | 1     |
| 1:A:85:VAL:HG21 | 1:B:73:PHE:CD2  | 0.75     | 2.16        | 6      | 15    |
| 1:A:73:PHE:CD2  | 1:B:85:VAL:HG21 | 0.75     | 2.16        | 6      | 15    |
| 1:B:75:GLU:O    | 1:B:79:LEU:HD13 | 0.75     | 1.81        | 16     | 13    |
| 1:A:75:GLU:O    | 1:A:79:LEU:HD13 | 0.75     | 1.81        | 16     | 13    |
| 1:A:39:MET:HG2  | 1:A:47:THR:HG21 | 0.74     | 1.59        | 19     | 7     |
| 1:B:39:MET:HE2  | 1:B:43:LEU:HD12 | 0.74     | 1.57        | 19     | 1     |
| 1:B:39:MET:HG2  | 1:B:47:THR:HG21 | 0.74     | 1.58        | 19     | 7     |
| 1:A:59:MET:HG2  | 1:A:60:MET:N    | 0.73     | 1.98        | 4      | 1     |
| 1:B:59:MET:HE2  | 1:B:83:LEU:CD2  | 0.73     | 2.09        | 1      | 1     |
| 1:A:59:MET:HE3  | 1:A:83:LEU:HD11 | 0.72     | 1.60        | 19     | 5     |
| 1:A:10:ILE:CG1  | 1:B:80:ILE:HD11 | 0.72     | 2.15        | 1      | 16    |
| 1:B:59:MET:HE3  | 1:B:83:LEU:HD11 | 0.72     | 1.61        | 19     | 6     |
| 1:A:59:MET:CE   | 1:A:83:LEU:HD11 | 0.71     | 2.15        | 2      | 13    |
| 1:B:59:MET:CE   | 1:B:83:LEU:HD11 | 0.71     | 2.15        | 2      | 13    |
| 1:A:16:VAL:CG1  | 1:B:6:THR:HG23  | 0.71     | 2.15        | 4      | 1     |
| 1:A:80:ILE:HD11 | 1:B:10:ILE:CG1  | 0.71     | 2.15        | 1      | 16    |
| 1:B:59:MET:HG2  | 1:B:60:MET:N    | 0.71     | 1.98        | 4      | 1     |
| 1:A:77:LEU:HD12 | 1:B:77:LEU:HD12 | 0.71     | 1.62        | 11     | 1     |
| 1:A:73:PHE:CZ   | 1:B:84:ALA:HB1  | 0.71     | 2.21        | 19     | 1     |
| 1:B:20:TYR:HB3  | 1:B:30:LEU:HD21 | 0.71     | 1.63        | 14     | 5     |
| 1:A:40:ASN:O    | 1:A:44:ALA:HB2  | 0.70     | 1.86        | 18     | 5     |
| 1:A:71:LEU:HD11 | 1:A:79:LEU:CD2  | 0.70     | 2.16        | 10     | 3     |
| 1:A:14:ILE:HG22 | 1:A:18:GLN:NE2  | 0.70     | 2.01        | 3      | 5     |
| 1:A:59:MET:HE2  | 1:A:79:LEU:O    | 0.70     | 1.85        | 19     | 5     |
| 1:A:85:VAL:HG13 | 1:B:73:PHE:CB   | 0.70     | 2.16        | 19     | 1     |
| 1:A:84:ALA:HB1  | 1:B:73:PHE:CZ   | 0.70     | 2.21        | 19     | 1     |
| 1:A:90:SER:OG   | 1:B:14:ILE:HG23 | 0.70     | 1.85        | 3      | 1     |
| 1:A:20:TYR:HB3  | 1:A:30:LEU:HD21 | 0.70     | 1.62        | 13     | 5     |
| 1:A:14:ILE:HG23 | 1:B:90:SER:OG   | 0.70     | 1.85        | 3      | 1     |
| 1:A:6:THR:HG23  | 1:B:16:VAL:CG1  | 0.70     | 2.16        | 4      | 1     |
| 1:B:14:ILE:HG22 | 1:B:18:GLN:NE2  | 0.70     | 2.01        | 3      | 5     |
| 1:B:16:VAL:HG23 | 1:B:17:PHE:CD1  | 0.70     | 2.22        | 4      | 2     |
| 1:B:59:MET:CG   | 1:B:79:LEU:HD13 | 0.70     | 2.17        | 4      | 1     |
| 1:B:40:ASN:O    | 1:B:44:ALA:HB2  | 0.69     | 1.86        | 18     | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:16:VAL:HG23 | 1:A:17:PHE:CD1  | 0.69     | 2.22        | 4      | 2     |
| 1:B:12:SER:O    | 1:B:16:VAL:HG13 | 0.69     | 1.87        | 11     | 16    |
| 1:B:71:LEU:HD11 | 1:B:79:LEU:CD2  | 0.69     | 2.16        | 10     | 3     |
| 1:A:71:LEU:HD13 | 1:A:75:GLU:CG   | 0.69     | 2.17        | 16     | 1     |
| 1:B:59:MET:HB3  | 1:B:79:LEU:HG   | 0.69     | 1.65        | 13     | 1     |
| 1:A:73:PHE:CB   | 1:B:85:VAL:HG13 | 0.69     | 2.16        | 19     | 1     |
| 1:B:59:MET:HB2  | 1:B:79:LEU:HA   | 0.69     | 1.64        | 9      | 9     |
| 1:A:39:MET:HE2  | 1:A:43:LEU:HD12 | 0.69     | 1.65        | 19     | 1     |
| 1:B:71:LEU:HD13 | 1:B:75:GLU:CG   | 0.69     | 2.17        | 16     | 1     |
| 1:A:12:SER:O    | 1:A:16:VAL:HG13 | 0.69     | 1.87        | 11     | 16    |
| 1:A:59:MET:CG   | 1:A:79:LEU:HD13 | 0.68     | 2.17        | 4      | 1     |
| 1:A:59:MET:HB2  | 1:A:79:LEU:HA   | 0.68     | 1.66        | 10     | 10    |
| 1:A:39:MET:CE   | 1:A:43:LEU:HD12 | 0.68     | 2.18        | 19     | 3     |
| 1:A:30:LEU:HD12 | 1:A:35:PHE:CD2  | 0.68     | 2.24        | 3      | 1     |
| 1:A:4:THR:HG23  | 1:A:7:GLU:HB2   | 0.68     | 1.66        | 1      | 17    |
| 1:A:14:ILE:HG23 | 1:A:73:PHE:CE1  | 0.68     | 2.24        | 19     | 1     |
| 1:B:14:ILE:HG23 | 1:B:73:PHE:CE1  | 0.68     | 2.24        | 19     | 1     |
| 1:B:39:MET:CE   | 1:B:43:LEU:HD12 | 0.68     | 2.18        | 19     | 4     |
| 1:B:4:THR:HG23  | 1:B:7:GLU:HB2   | 0.67     | 1.66        | 1      | 17    |
| 1:B:55:VAL:HG22 | 1:B:86:ALA:O    | 0.67     | 1.89        | 12     | 7     |
| 1:A:59:MET:CE   | 1:A:83:LEU:HD23 | 0.67     | 2.20        | 6      | 3     |
| 1:B:30:LEU:HD12 | 1:B:35:PHE:CD2  | 0.67     | 2.24        | 3      | 1     |
| 1:A:59:MET:HB3  | 1:A:79:LEU:HG   | 0.67     | 1.65        | 13     | 1     |
| 1:B:14:ILE:O    | 1:B:18:GLN:HG3  | 0.66     | 1.90        | 9      | 4     |
| 1:B:21:ALA:HB1  | 1:B:29:THR:O    | 0.66     | 1.91        | 11     | 9     |
| 1:A:14:ILE:O    | 1:A:18:GLN:HG3  | 0.66     | 1.91        | 9      | 4     |
| 1:A:21:ALA:HB1  | 1:A:29:THR:O    | 0.66     | 1.91        | 11     | 9     |
| 1:A:28:VAL:HG12 | 1:B:90:SER:O    | 0.66     | 1.89        | 4      | 2     |
| 1:B:59:MET:HE2  | 1:B:79:LEU:O    | 0.66     | 1.91        | 19     | 6     |
| 1:A:43:LEU:HD22 | 1:A:46:PHE:CD2  | 0.66     | 2.25        | 12     | 2     |
| 1:A:90:SER:O    | 1:B:28:VAL:HG12 | 0.66     | 1.89        | 4      | 2     |
| 1:A:55:VAL:HG22 | 1:A:86:ALA:O    | 0.66     | 1.89        | 12     | 6     |
| 1:B:43:LEU:HD22 | 1:B:46:PHE:CD2  | 0.66     | 2.25        | 12     | 2     |
| 1:B:75:GLU:O    | 1:B:79:LEU:CD2  | 0.66     | 2.44        | 17     | 6     |
| 1:B:59:MET:CE   | 1:B:83:LEU:HD23 | 0.65     | 2.20        | 6      | 3     |
| 1:B:33:THR:O    | 1:B:36:LEU:HB2  | 0.65     | 1.91        | 9      | 16    |
| 1:A:33:THR:O    | 1:A:36:LEU:HB2  | 0.65     | 1.91        | 9      | 16    |
| 1:A:81:GLY:HA3  | 1:B:77:LEU:HD13 | 0.65     | 1.69        | 5      | 3     |
| 1:A:39:MET:SD   | 1:A:56:LEU:HD12 | 0.65     | 2.32        | 1      | 3     |
| 1:B:71:LEU:O    | 1:B:72:ASP:HB2  | 0.65     | 1.91        | 9      | 4     |
| 1:B:59:MET:HE1  | 1:B:79:LEU:O    | 0.65     | 1.92        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:75:GLU:O    | 1:A:79:LEU:CD2  | 0.65     | 2.44        | 17     | 6     |
| 1:A:30:LEU:HD12 | 1:A:35:PHE:CE2  | 0.65     | 2.27        | 3      | 1     |
| 1:B:59:MET:HE3  | 1:B:79:LEU:O    | 0.64     | 1.93        | 18     | 3     |
| 1:B:21:ALA:HB2  | 1:B:30:LEU:HB2  | 0.64     | 1.69        | 9      | 3     |
| 1:B:39:MET:SD   | 1:B:56:LEU:HD12 | 0.64     | 2.32        | 1      | 3     |
| 1:A:77:LEU:HD13 | 1:B:81:GLY:HA3  | 0.64     | 1.69        | 5      | 3     |
| 1:A:21:ALA:HB2  | 1:A:30:LEU:HB2  | 0.64     | 1.70        | 9      | 3     |
| 1:B:30:LEU:HD12 | 1:B:35:PHE:CE2  | 0.63     | 2.27        | 3      | 1     |
| 1:A:14:ILE:HG23 | 1:A:73:PHE:CZ   | 0.63     | 2.29        | 19     | 1     |
| 1:B:14:ILE:HG23 | 1:B:73:PHE:CZ   | 0.63     | 2.29        | 19     | 1     |
| 1:B:55:VAL:HG22 | 1:B:86:ALA:HB1  | 0.63     | 1.71        | 15     | 2     |
| 1:A:84:ALA:HB2  | 1:B:10:ILE:CG2  | 0.63     | 2.24        | 15     | 6     |
| 1:B:56:LEU:HD23 | 1:B:56:LEU:C    | 0.62     | 2.14        | 6      | 2     |
| 1:A:10:ILE:CG2  | 1:B:84:ALA:HB2  | 0.62     | 2.24        | 15     | 6     |
| 1:A:71:LEU:O    | 1:A:72:ASP:HB2  | 0.62     | 1.91        | 9      | 4     |
| 1:A:56:LEU:C    | 1:A:56:LEU:HD23 | 0.62     | 2.14        | 6      | 2     |
| 1:A:17:PHE:CD1  | 1:A:18:GLN:N    | 0.62     | 2.68        | 9      | 1     |
| 1:B:75:GLU:O    | 1:B:79:LEU:HD22 | 0.62     | 1.93        | 10     | 1     |
| 1:A:56:LEU:HD13 | 1:A:57:ASP:N    | 0.62     | 2.09        | 9      | 1     |
| 1:A:55:VAL:HG22 | 1:A:86:ALA:HB1  | 0.62     | 1.71        | 15     | 2     |
| 1:A:71:LEU:HD13 | 1:A:75:GLU:OE1  | 0.62     | 1.95        | 17     | 1     |
| 1:B:56:LEU:HD13 | 1:B:57:ASP:N    | 0.62     | 2.09        | 9      | 1     |
| 1:A:59:MET:HE1  | 1:A:79:LEU:O    | 0.61     | 1.95        | 5      | 1     |
| 1:A:4:THR:HG23  | 1:A:7:GLU:CB    | 0.61     | 2.25        | 1      | 11    |
| 1:A:75:GLU:O    | 1:A:79:LEU:HD22 | 0.61     | 1.93        | 10     | 1     |
| 1:B:59:MET:SD   | 1:B:79:LEU:HA   | 0.61     | 2.35        | 17     | 1     |
| 1:B:71:LEU:HD13 | 1:B:75:GLU:OE1  | 0.61     | 1.95        | 17     | 1     |
| 1:A:10:ILE:HG23 | 1:B:84:ALA:HB2  | 0.61     | 1.72        | 15     | 4     |
| 1:A:59:MET:SD   | 1:A:79:LEU:HA   | 0.61     | 2.36        | 17     | 1     |
| 1:B:85:VAL:HG12 | 1:B:91:PHE:HB2  | 0.61     | 1.72        | 17     | 8     |
| 1:B:4:THR:HG23  | 1:B:7:GLU:CB    | 0.61     | 2.25        | 1      | 10    |
| 1:A:75:GLU:N    | 1:A:75:GLU:OE1  | 0.61     | 2.33        | 16     | 1     |
| 1:B:17:PHE:CD1  | 1:B:18:GLN:N    | 0.61     | 2.68        | 9      | 1     |
| 1:B:75:GLU:OE1  | 1:B:75:GLU:N    | 0.61     | 2.33        | 16     | 1     |
| 1:A:85:VAL:HG12 | 1:A:91:PHE:HB2  | 0.60     | 1.74        | 3      | 8     |
| 1:A:84:ALA:HB2  | 1:B:10:ILE:HG23 | 0.60     | 1.72        | 15     | 4     |
| 1:B:75:GLU:O    | 1:B:79:LEU:HB2  | 0.60     | 1.97        | 5      | 3     |
| 1:A:74:GLN:O    | 1:A:78:ASN:N    | 0.60     | 2.30        | 11     | 5     |
| 1:A:30:LEU:HD22 | 1:A:31:SER:N    | 0.60     | 2.12        | 10     | 11    |
| 1:A:17:PHE:CD1  | 1:A:76:PHE:CB   | 0.60     | 2.84        | 4      | 2     |
| 1:B:17:PHE:CD1  | 1:B:76:PHE:CB   | 0.60     | 2.84        | 4      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:59:MET:CG   | 1:B:83:LEU:HD21 | 0.60     | 2.23        | 13     | 1     |
| 1:B:13:LEU:HD12 | 1:B:80:ILE:HG21 | 0.60     | 1.73        | 14     | 5     |
| 1:B:56:LEU:C    | 1:B:56:LEU:HD23 | 0.60     | 2.17        | 15     | 1     |
| 1:B:59:MET:CE   | 1:B:59:MET:HA   | 0.59     | 2.27        | 13     | 1     |
| 1:A:56:LEU:HD23 | 1:A:56:LEU:C    | 0.59     | 2.18        | 11     | 1     |
| 1:B:39:MET:HG2  | 1:B:56:LEU:HD12 | 0.59     | 1.75        | 4      | 2     |
| 1:B:30:LEU:HD22 | 1:B:31:SER:N    | 0.59     | 2.12        | 10     | 11    |
| 1:A:16:VAL:HG11 | 1:B:6:THR:HG23  | 0.59     | 1.73        | 4      | 1     |
| 1:A:89:GLU:HA   | 1:A:92:VAL:HG23 | 0.59     | 1.74        | 14     | 1     |
| 1:A:6:THR:HG22  | 1:A:10:ILE:HD11 | 0.59     | 1.75        | 16     | 3     |
| 1:A:13:LEU:HD12 | 1:A:80:ILE:HG21 | 0.59     | 1.73        | 14     | 5     |
| 1:B:30:LEU:C    | 1:B:71:LEU:HB2  | 0.59     | 2.18        | 14     | 4     |
| 1:A:59:MET:HE1  | 1:A:79:LEU:CA   | 0.59     | 2.28        | 17     | 1     |
| 1:B:17:PHE:CD1  | 1:B:76:PHE:HB2  | 0.59     | 2.33        | 4      | 1     |
| 1:A:75:GLU:O    | 1:A:79:LEU:HB2  | 0.59     | 1.97        | 5      | 3     |
| 1:A:59:MET:CG   | 1:A:83:LEU:HD21 | 0.59     | 2.23        | 13     | 1     |
| 1:A:73:PHE:CG   | 1:A:74:GLN:N    | 0.58     | 2.71        | 10     | 16    |
| 1:B:39:MET:CG   | 1:B:47:THR:HG21 | 0.58     | 2.27        | 19     | 4     |
| 1:A:39:MET:CG   | 1:A:47:THR:HG21 | 0.58     | 2.27        | 19     | 4     |
| 1:B:6:THR:HG22  | 1:B:10:ILE:HD11 | 0.58     | 1.75        | 16     | 3     |
| 1:A:17:PHE:CD1  | 1:A:76:PHE:HB2  | 0.58     | 2.32        | 4      | 1     |
| 1:A:59:MET:CE   | 1:A:59:MET:HA   | 0.58     | 2.27        | 13     | 1     |
| 1:B:74:GLN:O    | 1:B:78:ASN:N    | 0.58     | 2.30        | 11     | 8     |
| 1:A:13:LEU:HB3  | 1:A:77:LEU:HD21 | 0.58     | 1.74        | 8      | 2     |
| 1:B:73:PHE:CG   | 1:B:74:GLN:N    | 0.58     | 2.71        | 10     | 16    |
| 1:B:59:MET:HE1  | 1:B:79:LEU:CA   | 0.58     | 2.28        | 17     | 1     |
| 1:A:14:ILE:HD13 | 1:B:88:HIS:ND1  | 0.58     | 2.13        | 7      | 1     |
| 1:A:30:LEU:C    | 1:A:71:LEU:HB2  | 0.58     | 2.18        | 14     | 4     |
| 1:A:59:MET:HG2  | 1:A:60:MET:HE3  | 0.58     | 1.74        | 10     | 3     |
| 1:A:81:GLY:CA   | 1:B:77:LEU:HD13 | 0.58     | 2.28        | 5      | 2     |
| 1:B:13:LEU:HB3  | 1:B:77:LEU:HD21 | 0.58     | 1.74        | 8      | 2     |
| 1:A:59:MET:HE3  | 1:A:83:LEU:CD2  | 0.58     | 2.26        | 18     | 2     |
| 1:A:59:MET:HE1  | 1:A:83:LEU:HD11 | 0.58     | 1.76        | 2      | 5     |
| 1:A:6:THR:HG23  | 1:B:16:VAL:HG11 | 0.58     | 1.73        | 4      | 1     |
| 1:B:39:MET:HE3  | 1:B:43:LEU:HD13 | 0.58     | 1.74        | 11     | 1     |
| 1:B:89:GLU:HA   | 1:B:92:VAL:HG23 | 0.58     | 1.74        | 14     | 1     |
| 1:A:88:HIS:ND1  | 1:B:14:ILE:HD13 | 0.58     | 2.13        | 7      | 1     |
| 1:A:77:LEU:HD13 | 1:B:81:GLY:CA   | 0.58     | 2.28        | 5      | 2     |
| 1:B:59:MET:HG2  | 1:B:60:MET:HE3  | 0.57     | 1.75        | 10     | 3     |
| 1:A:39:MET:HG2  | 1:A:56:LEU:HD12 | 0.57     | 1.75        | 4      | 2     |
| 1:B:28:VAL:HG22 | 1:B:28:VAL:O    | 0.57     | 1.99        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:28:VAL:O    | 1:A:28:VAL:HG22 | 0.57     | 1.99        | 8      | 1     |
| 1:A:16:VAL:HG23 | 1:A:76:PHE:CE1  | 0.57     | 2.34        | 2      | 3     |
| 1:A:73:PHE:CE2  | 1:B:84:ALA:HB1  | 0.57     | 2.34        | 19     | 1     |
| 1:B:15:ALA:HA   | 1:B:18:GLN:NE2  | 0.57     | 2.14        | 9      | 4     |
| 1:B:16:VAL:HG23 | 1:B:76:PHE:CE1  | 0.57     | 2.34        | 2      | 3     |
| 1:A:16:VAL:CG2  | 1:A:17:PHE:CE1  | 0.57     | 2.87        | 4      | 2     |
| 1:B:59:MET:HE1  | 1:B:79:LEU:HA   | 0.57     | 1.77        | 17     | 1     |
| 1:B:16:VAL:CG2  | 1:B:17:PHE:CE1  | 0.57     | 2.87        | 4      | 2     |
| 1:B:55:VAL:HG12 | 1:B:83:LEU:HD22 | 0.57     | 1.77        | 19     | 2     |
| 1:A:59:MET:HE1  | 1:A:79:LEU:HA   | 0.56     | 1.77        | 17     | 1     |
| 1:A:15:ALA:HA   | 1:A:18:GLN:NE2  | 0.56     | 2.14        | 9      | 4     |
| 1:A:6:THR:HG21  | 1:B:43:LEU:HG   | 0.56     | 1.77        | 4      | 6     |
| 1:B:16:VAL:HG23 | 1:B:76:PHE:CD1  | 0.56     | 2.35        | 2      | 3     |
| 1:A:55:VAL:HG12 | 1:A:83:LEU:HD22 | 0.56     | 1.77        | 19     | 2     |
| 1:A:84:ALA:HB1  | 1:B:73:PHE:CE2  | 0.56     | 2.34        | 19     | 1     |
| 1:A:56:LEU:O    | 1:A:59:MET:HG3  | 0.56     | 2.01        | 19     | 1     |
| 1:B:56:LEU:O    | 1:B:59:MET:HG3  | 0.56     | 2.01        | 19     | 1     |
| 1:A:35:PHE:CZ   | 1:A:76:PHE:CE1  | 0.56     | 2.94        | 2      | 7     |
| 1:A:35:PHE:CE1  | 1:A:76:PHE:CZ   | 0.56     | 2.94        | 3      | 8     |
| 1:A:73:PHE:HB2  | 1:B:85:VAL:CG1  | 0.56     | 2.31        | 10     | 2     |
| 1:A:39:MET:HE3  | 1:A:43:LEU:HD13 | 0.56     | 1.77        | 11     | 1     |
| 1:B:80:ILE:HD13 | 1:B:80:ILE:O    | 0.56     | 2.01        | 8      | 4     |
| 1:B:35:PHE:CE1  | 1:B:76:PHE:CZ   | 0.56     | 2.94        | 3      | 8     |
| 1:A:20:TYR:CD1  | 1:A:38:PHE:CG   | 0.56     | 2.94        | 4      | 3     |
| 1:A:16:VAL:HG23 | 1:A:76:PHE:CD1  | 0.56     | 2.35        | 2      | 3     |
| 1:B:28:VAL:HG13 | 1:B:28:VAL:O    | 0.56     | 2.01        | 9      | 2     |
| 1:B:20:TYR:CD1  | 1:B:38:PHE:CG   | 0.56     | 2.94        | 4      | 3     |
| 1:B:35:PHE:CZ   | 1:B:76:PHE:CE1  | 0.55     | 2.94        | 15     | 7     |
| 1:A:43:LEU:HG   | 1:B:6:THR:HG21  | 0.55     | 1.78        | 4      | 5     |
| 1:A:20:TYR:OH   | 1:A:41:THR:HG21 | 0.55     | 2.02        | 5      | 1     |
| 1:A:13:LEU:CD1  | 1:A:80:ILE:HG21 | 0.55     | 2.31        | 10     | 18    |
| 1:B:20:TYR:OH   | 1:B:41:THR:HG21 | 0.55     | 2.01        | 5      | 1     |
| 1:B:59:MET:HG3  | 1:B:60:MET:N    | 0.55     | 2.16        | 14     | 9     |
| 1:A:71:LEU:O    | 1:A:72:ASP:HB3  | 0.55     | 2.01        | 19     | 2     |
| 1:B:71:LEU:O    | 1:B:72:ASP:HB3  | 0.55     | 2.02        | 19     | 2     |
| 1:A:20:TYR:CB   | 1:A:30:LEU:HD21 | 0.55     | 2.32        | 13     | 1     |
| 1:B:13:LEU:CD1  | 1:B:80:ILE:HG21 | 0.55     | 2.32        | 9      | 18    |
| 1:A:10:ILE:HG12 | 1:B:80:ILE:CD1  | 0.55     | 2.32        | 12     | 4     |
| 1:A:28:VAL:HG13 | 1:A:28:VAL:O    | 0.55     | 2.01        | 9      | 2     |
| 1:B:17:PHE:HB2  | 1:B:76:PHE:CG   | 0.55     | 2.36        | 9      | 2     |
| 1:A:17:PHE:HB2  | 1:A:76:PHE:CG   | 0.55     | 2.36        | 9      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:17:PHE:CG   | 1:A:76:PHE:CD2  | 0.55     | 2.95        | 9      | 1     |
| 1:B:59:MET:CG   | 1:B:60:MET:N    | 0.55     | 2.70        | 12     | 11    |
| 1:A:35:PHE:CD1  | 1:A:76:PHE:CE1  | 0.55     | 2.94        | 3      | 1     |
| 1:A:56:LEU:O    | 1:A:59:MET:HG2  | 0.55     | 2.02        | 18     | 1     |
| 1:A:39:MET:HB3  | 1:A:47:THR:HG21 | 0.55     | 1.78        | 11     | 2     |
| 1:A:17:PHE:CD1  | 1:A:76:PHE:CE2  | 0.55     | 2.95        | 9      | 1     |
| 1:B:17:PHE:CD1  | 1:B:76:PHE:CE2  | 0.55     | 2.95        | 9      | 1     |
| 1:B:10:ILE:O    | 1:B:14:ILE:HG13 | 0.55     | 2.02        | 2      | 18    |
| 1:A:80:ILE:CD1  | 1:B:10:ILE:HG12 | 0.55     | 2.32        | 12     | 7     |
| 1:B:35:PHE:CD1  | 1:B:76:PHE:CE1  | 0.55     | 2.94        | 3      | 1     |
| 1:A:14:ILE:HG22 | 1:A:18:GLN:CD   | 0.55     | 2.22        | 7      | 5     |
| 1:B:35:PHE:CE2  | 1:B:76:PHE:CD2  | 0.55     | 2.95        | 12     | 4     |
| 1:A:17:PHE:CD1  | 1:A:76:PHE:HB3  | 0.55     | 2.37        | 10     | 2     |
| 1:A:85:VAL:HG11 | 1:B:73:PHE:CB   | 0.55     | 2.31        | 15     | 13    |
| 1:B:39:MET:CG   | 1:B:56:LEU:HD12 | 0.55     | 2.32        | 6      | 1     |
| 1:A:59:MET:HG3  | 1:A:60:MET:N    | 0.55     | 2.16        | 14     | 9     |
| 1:A:10:ILE:O    | 1:A:14:ILE:HG13 | 0.55     | 2.02        | 2      | 18    |
| 1:B:14:ILE:HG22 | 1:B:18:GLN:CD   | 0.55     | 2.22        | 7      | 5     |
| 1:A:16:VAL:HG23 | 1:A:76:PHE:CD2  | 0.54     | 2.37        | 3      | 1     |
| 1:B:17:PHE:CD1  | 1:B:76:PHE:HB3  | 0.54     | 2.37        | 10     | 2     |
| 1:A:16:VAL:CG2  | 1:A:17:PHE:CD1  | 0.54     | 2.89        | 4      | 2     |
| 1:B:17:PHE:CG   | 1:B:76:PHE:CD2  | 0.54     | 2.95        | 9      | 1     |
| 1:A:85:VAL:CG1  | 1:B:73:PHE:HB2  | 0.54     | 2.31        | 10     | 2     |
| 1:B:16:VAL:CG2  | 1:B:17:PHE:CD1  | 0.54     | 2.90        | 10     | 2     |
| 1:B:38:PHE:HA   | 1:B:41:THR:HG22 | 0.54     | 1.80        | 1      | 2     |
| 1:B:55:VAL:HB   | 1:B:86:ALA:HB3  | 0.54     | 1.79        | 8      | 3     |
| 1:A:73:PHE:CB   | 1:B:85:VAL:HG11 | 0.54     | 2.32        | 15     | 13    |
| 1:A:21:ALA:HB2  | 1:A:30:LEU:HG   | 0.54     | 1.79        | 17     | 9     |
| 1:A:35:PHE:CE2  | 1:A:76:PHE:CD2  | 0.54     | 2.95        | 12     | 4     |
| 1:B:72:ASP:O    | 1:B:76:PHE:CE2  | 0.54     | 2.61        | 9      | 2     |
| 1:A:39:MET:CG   | 1:A:56:LEU:HD12 | 0.54     | 2.32        | 6      | 1     |
| 1:A:56:LEU:HD13 | 1:A:56:LEU:C    | 0.54     | 2.23        | 9      | 1     |
| 1:A:59:MET:CG   | 1:A:60:MET:N    | 0.54     | 2.70        | 12     | 11    |
| 1:A:72:ASP:O    | 1:A:76:PHE:CE2  | 0.54     | 2.61        | 9      | 2     |
| 1:A:55:VAL:HB   | 1:A:86:ALA:HB3  | 0.54     | 1.78        | 9      | 3     |
| 1:A:80:ILE:O    | 1:A:80:ILE:HD13 | 0.54     | 2.01        | 8      | 7     |
| 1:B:16:VAL:HG23 | 1:B:76:PHE:CD2  | 0.54     | 2.37        | 3      | 1     |
| 1:A:70:GLN:O    | 1:A:71:LEU:O    | 0.54     | 2.26        | 8      | 2     |
| 1:A:59:MET:HB2  | 1:A:79:LEU:CA   | 0.54     | 2.33        | 9      | 2     |
| 1:B:56:LEU:HD13 | 1:B:56:LEU:C    | 0.54     | 2.23        | 9      | 1     |
| 1:B:20:TYR:CB   | 1:B:30:LEU:HD21 | 0.54     | 2.32        | 13     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:59:MET:HB2  | 1:B:79:LEU:CA   | 0.53     | 2.33        | 9      | 2     |
| 1:B:56:LEU:HD12 | 1:B:59:MET:SD   | 0.53     | 2.43        | 19     | 1     |
| 1:A:35:PHE:CZ   | 1:A:76:PHE:CZ   | 0.53     | 2.96        | 18     | 3     |
| 1:B:56:LEU:O    | 1:B:59:MET:HG2  | 0.53     | 2.02        | 18     | 1     |
| 1:B:40:ASN:HA   | 1:B:44:ALA:HB2  | 0.53     | 1.80        | 10     | 2     |
| 1:B:35:PHE:CZ   | 1:B:76:PHE:CZ   | 0.53     | 2.96        | 18     | 3     |
| 1:B:21:ALA:HB2  | 1:B:30:LEU:CB   | 0.53     | 2.33        | 9      | 1     |
| 1:A:89:GLU:HG2  | 1:B:14:ILE:HG23 | 0.53     | 1.80        | 5      | 1     |
| 1:A:43:LEU:HD22 | 1:A:46:PHE:HD2  | 0.53     | 1.63        | 12     | 2     |
| 1:A:40:ASN:HA   | 1:A:44:ALA:HB2  | 0.53     | 1.80        | 10     | 2     |
| 1:A:14:ILE:HG23 | 1:B:89:GLU:HG2  | 0.53     | 1.80        | 5      | 1     |
| 1:A:43:LEU:HD11 | 1:A:80:ILE:HG13 | 0.53     | 1.81        | 17     | 2     |
| 1:B:21:ALA:HB2  | 1:B:30:LEU:HG   | 0.53     | 1.79        | 17     | 10    |
| 1:A:21:ALA:HB2  | 1:A:30:LEU:CB   | 0.53     | 2.33        | 9      | 1     |
| 1:A:85:VAL:HG12 | 1:A:91:PHE:CB   | 0.53     | 2.34        | 19     | 2     |
| 1:B:39:MET:HE2  | 1:B:43:LEU:HD13 | 0.53     | 1.80        | 4      | 1     |
| 1:B:70:GLN:O    | 1:B:71:LEU:O    | 0.53     | 2.26        | 8      | 2     |
| 1:A:38:PHE:HA   | 1:A:41:THR:HG22 | 0.53     | 1.79        | 1      | 2     |
| 1:B:85:VAL:HG13 | 1:B:90:SER:HB3  | 0.53     | 1.81        | 3      | 1     |
| 1:B:39:MET:HB3  | 1:B:47:THR:HG21 | 0.53     | 1.78        | 11     | 2     |
| 1:B:59:MET:HG2  | 1:B:79:LEU:HA   | 0.53     | 1.80        | 11     | 2     |
| 1:A:59:MET:HE3  | 1:A:79:LEU:O    | 0.53     | 2.03        | 18     | 3     |
| 1:B:85:VAL:HG12 | 1:B:91:PHE:CB   | 0.53     | 2.34        | 19     | 2     |
| 1:A:71:LEU:HD11 | 1:A:79:LEU:HD22 | 0.53     | 1.82        | 8      | 2     |
| 1:A:60:MET:HA   | 1:A:60:MET:HE3  | 0.53     | 1.79        | 13     | 1     |
| 1:A:59:MET:HG2  | 1:A:79:LEU:HA   | 0.52     | 1.80        | 11     | 2     |
| 1:A:56:LEU:HD12 | 1:A:59:MET:SD   | 0.52     | 2.43        | 19     | 1     |
| 1:A:30:LEU:HD12 | 1:A:35:PHE:CG   | 0.52     | 2.40        | 3      | 1     |
| 1:B:43:LEU:HD11 | 1:B:80:ILE:HG13 | 0.52     | 1.81        | 17     | 2     |
| 1:A:85:VAL:HG13 | 1:A:90:SER:HB3  | 0.52     | 1.81        | 3      | 1     |
| 1:A:71:LEU:HD12 | 1:A:76:PHE:HD1  | 0.52     | 1.65        | 4      | 2     |
| 1:B:35:PHE:CE2  | 1:B:76:PHE:CE1  | 0.52     | 2.98        | 16     | 1     |
| 1:A:91:PHE:O    | 1:A:92:VAL:HG22 | 0.52     | 2.05        | 3      | 1     |
| 1:B:91:PHE:O    | 1:B:92:VAL:HG22 | 0.52     | 2.04        | 3      | 1     |
| 1:B:20:TYR:CD1  | 1:B:20:TYR:N    | 0.52     | 2.77        | 4      | 2     |
| 1:A:39:MET:HE2  | 1:A:43:LEU:HD13 | 0.52     | 1.80        | 4      | 2     |
| 1:A:35:PHE:CE2  | 1:A:76:PHE:CE1  | 0.52     | 2.98        | 16     | 1     |
| 1:B:71:LEU:HD12 | 1:B:76:PHE:CD1  | 0.52     | 2.40        | 4      | 2     |
| 1:A:59:MET:HE3  | 1:A:79:LEU:HD13 | 0.52     | 1.80        | 17     | 1     |
| 1:B:71:LEU:HD11 | 1:B:79:LEU:HD22 | 0.52     | 1.82        | 8      | 2     |
| 1:A:6:THR:HG21  | 1:B:38:PHE:CE1  | 0.52     | 2.40        | 11     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:20:TYR:CG   | 1:B:38:PHE:CD2  | 0.52     | 2.98        | 18     | 3     |
| 1:B:20:TYR:HB2  | 1:B:30:LEU:HD11 | 0.52     | 1.81        | 10     | 2     |
| 1:A:35:PHE:CE2  | 1:A:76:PHE:CZ   | 0.52     | 2.98        | 16     | 1     |
| 1:A:59:MET:CE   | 1:A:83:LEU:CD2  | 0.52     | 2.88        | 5      | 3     |
| 1:B:30:LEU:HD12 | 1:B:35:PHE:CG   | 0.52     | 2.40        | 3      | 1     |
| 1:B:71:LEU:HD12 | 1:B:76:PHE:HD1  | 0.52     | 1.65        | 4      | 2     |
| 1:B:79:LEU:O    | 1:B:83:LEU:CG   | 0.52     | 2.57        | 6      | 3     |
| 1:A:38:PHE:CE1  | 1:B:6:THR:HG21  | 0.51     | 2.40        | 11     | 1     |
| 1:B:35:PHE:CE2  | 1:B:76:PHE:CZ   | 0.51     | 2.98        | 16     | 2     |
| 1:A:20:TYR:CE1  | 1:A:38:PHE:CD2  | 0.51     | 2.98        | 5      | 1     |
| 1:B:21:ALA:CA   | 1:B:30:LEU:HG   | 0.51     | 2.36        | 4      | 3     |
| 1:A:20:TYR:HB2  | 1:A:30:LEU:HD11 | 0.51     | 1.81        | 10     | 2     |
| 1:A:73:PHE:HB3  | 1:B:85:VAL:HG13 | 0.51     | 1.82        | 19     | 1     |
| 1:B:35:PHE:CE1  | 1:B:76:PHE:CE1  | 0.51     | 2.98        | 3      | 1     |
| 1:A:20:TYR:CD1  | 1:A:20:TYR:N    | 0.51     | 2.77        | 4      | 2     |
| 1:A:71:LEU:HD12 | 1:A:76:PHE:CD1  | 0.51     | 2.40        | 4      | 2     |
| 1:A:20:TYR:HB3  | 1:A:38:PHE:CE2  | 0.51     | 2.41        | 15     | 1     |
| 1:A:59:MET:HG3  | 1:A:79:LEU:HD13 | 0.51     | 1.81        | 4      | 1     |
| 1:B:59:MET:HG3  | 1:B:79:LEU:HD13 | 0.51     | 1.81        | 4      | 1     |
| 1:B:75:GLU:O    | 1:B:79:LEU:CG   | 0.51     | 2.59        | 11     | 6     |
| 1:B:20:TYR:HB3  | 1:B:38:PHE:CE2  | 0.51     | 2.41        | 15     | 1     |
| 1:A:72:ASP:C    | 1:A:75:GLU:OE1  | 0.51     | 2.49        | 16     | 1     |
| 1:B:59:MET:CE   | 1:B:83:LEU:CD2  | 0.51     | 2.88        | 5      | 3     |
| 1:A:20:TYR:CG   | 1:A:38:PHE:CD2  | 0.51     | 2.98        | 18     | 3     |
| 1:A:21:ALA:CA   | 1:A:30:LEU:HG   | 0.51     | 2.36        | 4      | 3     |
| 1:A:35:PHE:CD2  | 1:A:76:PHE:CE2  | 0.51     | 2.99        | 7      | 1     |
| 1:A:20:TYR:CE1  | 1:A:38:PHE:CD1  | 0.51     | 2.98        | 2      | 3     |
| 1:A:35:PHE:CD1  | 1:A:76:PHE:CZ   | 0.51     | 2.99        | 17     | 1     |
| 1:A:79:LEU:O    | 1:A:83:LEU:CG   | 0.51     | 2.52        | 11     | 3     |
| 1:A:14:ILE:O    | 1:A:17:PHE:CD2  | 0.51     | 2.64        | 9      | 1     |
| 1:A:4:THR:HG21  | 1:B:42:GLU:O    | 0.51     | 2.06        | 8      | 1     |
| 1:A:73:PHE:CD2  | 1:A:74:GLN:N    | 0.51     | 2.79        | 11     | 13    |
| 1:A:72:ASP:O    | 1:A:76:PHE:CZ   | 0.51     | 2.64        | 4      | 2     |
| 1:B:73:PHE:CD2  | 1:B:74:GLN:N    | 0.51     | 2.79        | 11     | 13    |
| 1:B:39:MET:HE2  | 1:B:43:LEU:CD1  | 0.51     | 2.33        | 19     | 1     |
| 1:A:42:GLU:O    | 1:B:4:THR:HG21  | 0.51     | 2.06        | 8      | 1     |
| 1:B:80:ILE:O    | 1:B:80:ILE:HD13 | 0.51     | 2.05        | 11     | 4     |
| 1:A:43:LEU:HD22 | 1:A:46:PHE:CD1  | 0.50     | 2.40        | 5      | 1     |
| 1:B:43:LEU:HD22 | 1:B:46:PHE:CD1  | 0.50     | 2.40        | 5      | 1     |
| 1:B:20:TYR:CE1  | 1:B:38:PHE:CD1  | 0.50     | 3.00        | 18     | 3     |
| 1:B:72:ASP:O    | 1:B:76:PHE:CZ   | 0.50     | 2.64        | 4      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:39:MET:CE   | 1:A:43:LEU:HD13 | 0.50     | 2.36        | 11     | 3     |
| 1:B:72:ASP:C    | 1:B:75:GLU:OE1  | 0.50     | 2.49        | 16     | 1     |
| 1:B:17:PHE:CD1  | 1:B:76:PHE:CD2  | 0.50     | 2.99        | 9      | 1     |
| 1:B:20:TYR:CE1  | 1:B:38:PHE:CD2  | 0.50     | 2.98        | 5      | 1     |
| 1:B:35:PHE:CD1  | 1:B:76:PHE:CZ   | 0.50     | 2.99        | 17     | 1     |
| 1:B:35:PHE:CD2  | 1:B:76:PHE:CE2  | 0.50     | 2.99        | 7      | 1     |
| 1:B:59:MET:CE   | 1:B:79:LEU:HA   | 0.50     | 2.36        | 17     | 2     |
| 1:A:75:GLU:O    | 1:A:79:LEU:CG   | 0.50     | 2.59        | 11     | 5     |
| 1:B:14:ILE:O    | 1:B:17:PHE:CD2  | 0.50     | 2.64        | 9      | 1     |
| 1:B:59:MET:HE2  | 1:B:83:LEU:HD23 | 0.50     | 1.84        | 5      | 1     |
| 1:A:35:PHE:CE1  | 1:A:76:PHE:CE1  | 0.50     | 2.98        | 3      | 2     |
| 1:B:41:THR:HG23 | 1:B:42:GLU:HG3  | 0.50     | 1.80        | 10     | 3     |
| 1:B:59:MET:CE   | 1:B:79:LEU:HD13 | 0.50     | 2.36        | 17     | 1     |
| 1:A:85:VAL:HA   | 1:A:89:GLU:HB2  | 0.50     | 1.83        | 2      | 2     |
| 1:A:17:PHE:CD1  | 1:A:76:PHE:CD2  | 0.50     | 2.99        | 9      | 1     |
| 1:B:85:VAL:HA   | 1:B:89:GLU:HB2  | 0.50     | 1.83        | 2      | 2     |
| 1:B:20:TYR:CD1  | 1:B:38:PHE:CD2  | 0.50     | 2.99        | 8      | 4     |
| 1:B:21:ALA:HA   | 1:B:30:LEU:HD23 | 0.50     | 1.83        | 2      | 2     |
| 1:B:76:PHE:O    | 1:B:80:ILE:N    | 0.50     | 2.40        | 5      | 4     |
| 1:B:84:ALA:O    | 1:B:88:HIS:N    | 0.50     | 2.45        | 5      | 1     |
| 1:A:35:PHE:CE2  | 1:A:76:PHE:CE2  | 0.50     | 3.00        | 2      | 2     |
| 1:A:59:MET:CE   | 1:A:79:LEU:O    | 0.49     | 2.60        | 5      | 1     |
| 1:B:59:MET:HE1  | 1:B:83:LEU:HD21 | 0.49     | 1.84        | 4      | 1     |
| 1:B:35:PHE:CE2  | 1:B:76:PHE:CE2  | 0.49     | 3.00        | 2      | 2     |
| 1:A:35:PHE:CZ   | 1:A:76:PHE:CD1  | 0.49     | 3.00        | 1      | 1     |
| 1:B:83:LEU:O    | 1:B:87:CYS:N    | 0.49     | 2.45        | 18     | 8     |
| 1:A:6:THR:O     | 1:A:9:CYS:SG    | 0.49     | 2.70        | 5      | 7     |
| 1:B:6:THR:O     | 1:B:9:CYS:SG    | 0.49     | 2.70        | 2      | 7     |
| 1:B:39:MET:CE   | 1:B:43:LEU:HD13 | 0.49     | 2.36        | 11     | 3     |
| 1:B:6:THR:O     | 1:B:10:ILE:CD1  | 0.49     | 2.58        | 14     | 6     |
| 1:A:59:MET:HE2  | 1:A:83:LEU:HD23 | 0.49     | 1.84        | 5      | 1     |
| 1:A:76:PHE:O    | 1:A:80:ILE:N    | 0.49     | 2.40        | 5      | 2     |
| 1:A:83:LEU:O    | 1:A:87:CYS:N    | 0.49     | 2.46        | 7      | 8     |
| 1:A:74:GLN:NE2  | 1:A:78:ASN:N    | 0.49     | 2.61        | 3      | 8     |
| 1:B:59:MET:CE   | 1:B:79:LEU:O    | 0.49     | 2.60        | 5      | 1     |
| 1:A:85:VAL:HG13 | 1:B:73:PHE:HB3  | 0.49     | 1.82        | 19     | 1     |
| 1:B:59:MET:CG   | 1:B:60:MET:CE   | 0.49     | 2.91        | 14     | 3     |
| 1:A:20:TYR:CD1  | 1:A:38:PHE:CD2  | 0.49     | 3.00        | 8      | 4     |
| 1:A:59:MET:CE   | 1:A:79:LEU:HA   | 0.49     | 2.37        | 17     | 2     |
| 1:A:16:VAL:HG23 | 1:A:76:PHE:CE2  | 0.49     | 2.43        | 3      | 1     |
| 1:B:16:VAL:HG23 | 1:B:76:PHE:CE2  | 0.49     | 2.43        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:43:LEU:HD22 | 1:B:46:PHE:HD2  | 0.49     | 1.63        | 12     | 1     |
| 1:B:30:LEU:HB2  | 1:B:76:PHE:CE1  | 0.49     | 2.43        | 4      | 1     |
| 1:A:21:ALA:HA   | 1:A:30:LEU:HD23 | 0.49     | 1.83        | 2      | 2     |
| 1:A:59:MET:CG   | 1:A:60:MET:CE   | 0.49     | 2.91        | 14     | 3     |
| 1:A:85:VAL:HG21 | 1:B:73:PHE:CE2  | 0.49     | 2.43        | 5      | 9     |
| 1:A:16:VAL:CG2  | 1:A:76:PHE:CE1  | 0.49     | 2.96        | 12     | 5     |
| 1:B:16:VAL:CG2  | 1:B:76:PHE:CE1  | 0.49     | 2.96        | 12     | 5     |
| 1:B:75:GLU:O    | 1:B:79:LEU:CD1  | 0.49     | 2.60        | 16     | 2     |
| 1:B:74:GLN:NE2  | 1:B:78:ASN:N    | 0.49     | 2.61        | 3      | 9     |
| 1:B:16:VAL:HG23 | 1:B:17:PHE:N    | 0.49     | 2.23        | 9      | 8     |
| 1:A:73:PHE:HB2  | 1:B:85:VAL:HG11 | 0.49     | 1.85        | 10     | 3     |
| 1:A:30:LEU:HB2  | 1:A:76:PHE:CE1  | 0.49     | 2.43        | 4      | 1     |
| 1:A:59:MET:CE   | 1:A:79:LEU:HD13 | 0.49     | 2.36        | 17     | 1     |
| 1:B:20:TYR:HB3  | 1:B:30:LEU:HD11 | 0.49     | 1.84        | 3      | 1     |
| 1:A:41:THR:HG23 | 1:A:42:GLU:HG3  | 0.49     | 1.80        | 10     | 2     |
| 1:B:86:ALA:HA   | 1:B:92:VAL:HG13 | 0.48     | 1.85        | 14     | 1     |
| 1:B:35:PHE:CZ   | 1:B:76:PHE:CD1  | 0.48     | 3.00        | 1      | 1     |
| 1:A:82:GLY:O    | 1:A:85:VAL:HG23 | 0.48     | 2.08        | 3      | 7     |
| 1:A:13:LEU:HD22 | 1:B:9:CYS:SG    | 0.48     | 2.48        | 1      | 2     |
| 1:A:80:ILE:CD1  | 1:B:10:ILE:CG1  | 0.48     | 2.92        | 5      | 2     |
| 1:A:30:LEU:HD12 | 1:A:76:PHE:CD2  | 0.48     | 2.44        | 14     | 2     |
| 1:A:86:ALA:HA   | 1:A:92:VAL:HG13 | 0.48     | 1.85        | 14     | 1     |
| 1:A:43:LEU:HD11 | 1:A:80:ILE:CG1  | 0.48     | 2.38        | 5      | 1     |
| 1:A:35:PHE:HD2  | 1:A:79:LEU:HD23 | 0.48     | 1.68        | 15     | 1     |
| 1:B:43:LEU:HD11 | 1:B:80:ILE:CG1  | 0.48     | 2.38        | 5      | 1     |
| 1:A:73:PHE:CE2  | 1:B:85:VAL:HG21 | 0.48     | 2.43        | 5      | 10    |
| 1:A:77:LEU:HD22 | 1:B:77:LEU:CD2  | 0.48     | 2.29        | 16     | 4     |
| 1:A:16:VAL:HG23 | 1:A:17:PHE:N    | 0.48     | 2.23        | 9      | 10    |
| 1:A:13:LEU:CD2  | 1:B:13:LEU:HD23 | 0.48     | 2.39        | 5      | 3     |
| 1:A:13:LEU:HD22 | 1:B:9:CYS:HB2   | 0.48     | 1.86        | 12     | 8     |
| 1:B:82:GLY:O    | 1:B:85:VAL:HG23 | 0.48     | 2.08        | 3      | 6     |
| 1:A:85:VAL:O    | 1:A:92:VAL:HG22 | 0.48     | 2.08        | 18     | 1     |
| 1:A:13:LEU:O    | 1:A:17:PHE:CE2  | 0.48     | 2.67        | 10     | 2     |
| 1:A:43:LEU:O    | 1:A:47:THR:HG22 | 0.48     | 2.09        | 4      | 1     |
| 1:B:43:LEU:O    | 1:B:47:THR:HG22 | 0.48     | 2.09        | 4      | 1     |
| 1:A:9:CYS:SG    | 1:B:13:LEU:HD22 | 0.48     | 2.48        | 1      | 2     |
| 1:A:90:SER:CB   | 1:B:73:PHE:CE2  | 0.48     | 2.97        | 19     | 1     |
| 1:A:10:ILE:CG1  | 1:B:80:ILE:CD1  | 0.48     | 2.92        | 5      | 2     |
| 1:A:20:TYR:HB3  | 1:A:30:LEU:HD11 | 0.48     | 1.84        | 3      | 1     |
| 1:A:60:MET:HE3  | 1:A:60:MET:HA   | 0.48     | 1.85        | 12     | 1     |
| 1:A:9:CYS:SG    | 1:B:16:VAL:HG11 | 0.48     | 2.49        | 11     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:33:THR:HA   | 1:B:36:LEU:CD1  | 0.48     | 2.39        | 7      | 1     |
| 1:A:13:LEU:HD23 | 1:B:13:LEU:CD2  | 0.47     | 2.39        | 5      | 2     |
| 1:B:55:VAL:HG13 | 1:B:86:ALA:HB3  | 0.47     | 1.86        | 5      | 3     |
| 1:B:75:GLU:O    | 1:B:79:LEU:N    | 0.47     | 2.47        | 6      | 3     |
| 1:A:33:THR:HA   | 1:A:36:LEU:CD1  | 0.47     | 2.39        | 7      | 1     |
| 1:A:85:VAL:HG13 | 1:B:73:PHE:HB2  | 0.47     | 1.85        | 19     | 1     |
| 1:A:6:THR:O     | 1:A:10:ILE:CD1  | 0.47     | 2.58        | 14     | 6     |
| 1:A:14:ILE:O    | 1:A:18:GLN:CG   | 0.47     | 2.61        | 9      | 7     |
| 1:A:77:LEU:CD2  | 1:B:77:LEU:HD22 | 0.47     | 2.29        | 16     | 5     |
| 1:A:17:PHE:CG   | 1:A:76:PHE:CB   | 0.47     | 2.97        | 10     | 1     |
| 1:B:13:LEU:O    | 1:B:17:PHE:CE2  | 0.47     | 2.67        | 10     | 2     |
| 1:A:13:LEU:HD12 | 1:A:80:ILE:CG2  | 0.47     | 2.39        | 11     | 1     |
| 1:B:13:LEU:HD12 | 1:B:80:ILE:CG2  | 0.47     | 2.39        | 11     | 1     |
| 1:A:9:CYS:HB2   | 1:B:13:LEU:HD22 | 0.47     | 1.86        | 12     | 8     |
| 1:A:85:VAL:HG11 | 1:B:73:PHE:HB2  | 0.47     | 1.85        | 10     | 3     |
| 1:A:84:ALA:O    | 1:A:89:GLU:N    | 0.47     | 2.47        | 2      | 1     |
| 1:A:73:PHE:CE2  | 1:B:90:SER:CB   | 0.47     | 2.97        | 19     | 1     |
| 1:B:59:MET:SD   | 1:B:83:LEU:HD21 | 0.47     | 2.50        | 18     | 1     |
| 1:A:33:THR:HA   | 1:A:36:LEU:HD13 | 0.47     | 1.86        | 7      | 1     |
| 1:A:73:PHE:HB2  | 1:B:85:VAL:HG13 | 0.47     | 1.84        | 19     | 1     |
| 1:B:55:VAL:CG2  | 1:B:56:LEU:N    | 0.47     | 2.77        | 16     | 3     |
| 1:A:73:PHE:CB   | 1:B:85:VAL:CG1  | 0.47     | 2.93        | 13     | 2     |
| 1:B:60:MET:HE3  | 1:B:60:MET:HA   | 0.47     | 1.85        | 5      | 2     |
| 1:B:17:PHE:CE1  | 1:B:21:ALA:CB   | 0.47     | 2.97        | 16     | 4     |
| 1:B:84:ALA:O    | 1:B:89:GLU:N    | 0.47     | 2.47        | 2      | 1     |
| 1:B:60:MET:HA   | 1:B:60:MET:HE3  | 0.47     | 1.86        | 13     | 1     |
| 1:B:30:LEU:HD12 | 1:B:76:PHE:CD2  | 0.47     | 2.44        | 14     | 2     |
| 1:B:13:LEU:O    | 1:B:16:VAL:CG2  | 0.47     | 2.56        | 12     | 7     |
| 1:A:46:PHE:CE2  | 1:A:88:HIS:NE2  | 0.47     | 2.83        | 10     | 2     |
| 1:A:77:LEU:O    | 1:A:81:GLY:N    | 0.47     | 2.46        | 8      | 9     |
| 1:A:75:GLU:O    | 1:A:79:LEU:CD1  | 0.47     | 2.60        | 16     | 2     |
| 1:B:85:VAL:O    | 1:B:92:VAL:HG22 | 0.47     | 2.09        | 18     | 1     |
| 1:B:17:PHE:CG   | 1:B:76:PHE:CB   | 0.47     | 2.97        | 10     | 1     |
| 1:B:9:CYS:SG    | 1:B:10:ILE:N    | 0.47     | 2.88        | 11     | 3     |
| 1:B:21:ALA:N    | 1:B:30:LEU:HG   | 0.47     | 2.24        | 4      | 2     |
| 1:A:21:ALA:N    | 1:A:30:LEU:HG   | 0.47     | 2.24        | 4      | 1     |
| 1:A:12:SER:CB   | 1:B:9:CYS:HB2   | 0.47     | 2.40        | 11     | 4     |
| 1:A:16:VAL:HG11 | 1:B:9:CYS:SG    | 0.47     | 2.49        | 11     | 1     |
| 1:A:55:VAL:CG2  | 1:A:56:LEU:N    | 0.47     | 2.77        | 16     | 3     |
| 1:A:85:VAL:CG1  | 1:B:73:PHE:CB   | 0.47     | 2.93        | 13     | 2     |
| 1:A:59:MET:SD   | 1:A:83:LEU:HD21 | 0.47     | 2.50        | 18     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:17:PHE:CD2  | 1:B:30:LEU:HD12 | 0.47     | 2.45        | 13     | 1     |
| 1:B:59:MET:CG   | 1:B:60:MET:HE3  | 0.47     | 2.39        | 14     | 2     |
| 1:A:13:LEU:O    | 1:A:16:VAL:CG2  | 0.47     | 2.51        | 19     | 9     |
| 1:A:55:VAL:HG13 | 1:A:86:ALA:HB3  | 0.47     | 1.87        | 2      | 3     |
| 1:A:4:THR:CG2   | 1:A:7:GLU:CG    | 0.47     | 2.93        | 1      | 4     |
| 1:B:59:MET:HE2  | 1:B:79:LEU:HB3  | 0.47     | 1.87        | 18     | 1     |
| 1:B:71:LEU:O    | 1:B:72:ASP:CB   | 0.47     | 2.63        | 9      | 4     |
| 1:A:72:ASP:HB3  | 1:A:75:GLU:HB2  | 0.47     | 1.86        | 11     | 2     |
| 1:B:4:THR:CG2   | 1:B:7:GLU:CG    | 0.47     | 2.93        | 1      | 3     |
| 1:A:28:VAL:HG23 | 1:A:28:VAL:O    | 0.47     | 2.10        | 12     | 1     |
| 1:B:55:VAL:HG22 | 1:B:56:LEU:N    | 0.47     | 2.25        | 9      | 3     |
| 1:B:59:MET:HE2  | 1:B:79:LEU:HA   | 0.47     | 1.85        | 13     | 1     |
| 1:B:4:THR:HG23  | 1:B:7:GLU:CG    | 0.46     | 2.40        | 1      | 5     |
| 1:A:17:PHE:CE1  | 1:A:21:ALA:CB   | 0.46     | 2.98        | 16     | 4     |
| 1:B:14:ILE:O    | 1:B:18:GLN:CG   | 0.46     | 2.61        | 9      | 6     |
| 1:A:30:LEU:HD12 | 1:A:35:PHE:CZ   | 0.46     | 2.46        | 3      | 1     |
| 1:B:17:PHE:CG   | 1:B:18:GLN:N    | 0.46     | 2.83        | 9      | 2     |
| 1:A:17:PHE:CG   | 1:A:18:GLN:N    | 0.46     | 2.83        | 9      | 2     |
| 1:A:59:MET:HG3  | 1:A:79:LEU:CB   | 0.46     | 2.41        | 4      | 1     |
| 1:B:59:MET:HE3  | 1:B:79:LEU:HD13 | 0.46     | 1.87        | 17     | 1     |
| 1:A:17:PHE:CE1  | 1:A:72:ASP:O    | 0.46     | 2.69        | 8      | 12    |
| 1:A:74:GLN:NE2  | 1:A:78:ASN:HB2  | 0.46     | 2.25        | 10     | 2     |
| 1:A:4:THR:HG23  | 1:A:7:GLU:CG    | 0.46     | 2.41        | 1      | 5     |
| 1:A:9:CYS:SG    | 1:A:10:ILE:N    | 0.46     | 2.88        | 11     | 3     |
| 1:A:34:GLU:O    | 1:A:38:PHE:CD2  | 0.46     | 2.69        | 15     | 1     |
| 1:B:17:PHE:CE1  | 1:B:72:ASP:O    | 0.46     | 2.69        | 8      | 12    |
| 1:B:74:GLN:NE2  | 1:B:78:ASN:HB2  | 0.46     | 2.25        | 10     | 2     |
| 1:B:72:ASP:HB3  | 1:B:75:GLU:HB2  | 0.46     | 1.86        | 11     | 2     |
| 1:A:38:PHE:CE1  | 1:A:42:GLU:CB   | 0.46     | 2.99        | 6      | 1     |
| 1:B:34:GLU:O    | 1:B:38:PHE:CD2  | 0.46     | 2.69        | 15     | 1     |
| 1:A:59:MET:HG3  | 1:A:60:MET:H    | 0.46     | 1.71        | 19     | 1     |
| 1:A:71:LEU:HG   | 1:A:75:GLU:HB3  | 0.46     | 1.88        | 8      | 1     |
| 1:B:46:PHE:CE2  | 1:B:88:HIS:NE2  | 0.46     | 2.83        | 10     | 2     |
| 1:A:20:TYR:CB   | 1:A:38:PHE:CE2  | 0.46     | 2.99        | 15     | 1     |
| 1:B:33:THR:HA   | 1:B:36:LEU:HD13 | 0.46     | 1.86        | 7      | 1     |
| 1:B:35:PHE:HD2  | 1:B:79:LEU:HD23 | 0.46     | 1.69        | 15     | 1     |
| 1:A:17:PHE:CD2  | 1:A:30:LEU:HD12 | 0.46     | 2.45        | 13     | 1     |
| 1:A:84:ALA:O    | 1:A:88:HIS:N    | 0.46     | 2.45        | 5      | 1     |
| 1:B:59:MET:HG3  | 1:B:79:LEU:CB   | 0.46     | 2.41        | 4      | 1     |
| 1:A:9:CYS:HB2   | 1:B:12:SER:CB   | 0.46     | 2.40        | 11     | 4     |
| 1:B:39:MET:HA   | 1:B:43:LEU:CB   | 0.46     | 2.41        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:20:TYR:CE2  | 1:B:34:GLU:O    | 0.46     | 2.69        | 16     | 5     |
| 1:B:80:ILE:CG2  | 1:B:81:GLY:N    | 0.46     | 2.79        | 13     | 7     |
| 1:A:73:PHE:CD1  | 1:A:74:GLN:N    | 0.46     | 2.84        | 10     | 1     |
| 1:B:39:MET:HE1  | 1:B:43:LEU:HD13 | 0.46     | 1.88        | 2      | 2     |
| 1:B:35:PHE:CE2  | 1:B:79:LEU:CB   | 0.46     | 2.99        | 19     | 2     |
| 1:A:55:VAL:HG22 | 1:A:56:LEU:N    | 0.46     | 2.25        | 9      | 3     |
| 1:A:38:PHE:CZ   | 1:A:42:GLU:CB   | 0.46     | 2.99        | 12     | 1     |
| 1:B:6:THR:C     | 1:B:10:ILE:HD12 | 0.46     | 2.28        | 12     | 3     |
| 1:A:6:THR:C     | 1:A:10:ILE:HD12 | 0.46     | 2.30        | 19     | 3     |
| 1:B:38:PHE:CZ   | 1:B:42:GLU:CB   | 0.45     | 2.98        | 12     | 1     |
| 1:A:20:TYR:CD2  | 1:A:38:PHE:CD2  | 0.45     | 3.04        | 15     | 1     |
| 1:B:20:TYR:CB   | 1:B:38:PHE:CE2  | 0.45     | 2.99        | 15     | 1     |
| 1:B:20:TYR:CD2  | 1:B:38:PHE:CD2  | 0.45     | 3.04        | 15     | 1     |
| 1:A:74:GLN:NE2  | 1:B:74:GLN:NE2  | 0.45     | 2.65        | 17     | 4     |
| 1:B:30:LEU:HD12 | 1:B:35:PHE:CZ   | 0.45     | 2.46        | 3      | 1     |
| 1:A:6:THR:HG21  | 1:B:43:LEU:CG   | 0.45     | 2.41        | 4      | 1     |
| 1:A:30:LEU:HD11 | 1:A:38:PHE:CE2  | 0.45     | 2.47        | 15     | 1     |
| 1:A:34:GLU:O    | 1:A:38:PHE:CE2  | 0.45     | 2.70        | 15     | 1     |
| 1:A:6:THR:HG21  | 1:B:38:PHE:HE1  | 0.45     | 1.71        | 11     | 1     |
| 1:A:75:GLU:CD   | 1:A:76:PHE:N    | 0.45     | 2.70        | 16     | 1     |
| 1:A:39:MET:HA   | 1:A:43:LEU:CB   | 0.45     | 2.41        | 8      | 1     |
| 1:A:59:MET:CG   | 1:A:60:MET:HE3  | 0.45     | 2.40        | 14     | 2     |
| 1:A:80:ILE:CG2  | 1:A:81:GLY:N    | 0.45     | 2.79        | 19     | 7     |
| 1:B:31:SER:OG   | 1:B:33:THR:HG22 | 0.45     | 2.12        | 7      | 1     |
| 1:B:75:GLU:CD   | 1:B:76:PHE:N    | 0.45     | 2.70        | 16     | 1     |
| 1:A:84:ALA:O    | 1:A:88:HIS:C    | 0.45     | 2.55        | 5      | 1     |
| 1:A:35:PHE:CE2  | 1:A:79:LEU:CB   | 0.45     | 2.99        | 19     | 2     |
| 1:A:38:PHE:HE1  | 1:B:6:THR:HG21  | 0.45     | 1.71        | 11     | 1     |
| 1:A:84:ALA:O    | 1:A:88:HIS:HB3  | 0.45     | 2.12        | 13     | 1     |
| 1:B:77:LEU:O    | 1:B:81:GLY:N    | 0.45     | 2.46        | 8      | 10    |
| 1:A:43:LEU:CG   | 1:B:6:THR:HG21  | 0.45     | 2.41        | 4      | 1     |
| 1:A:60:MET:HG2  | 1:A:79:LEU:CD1  | 0.45     | 2.41        | 1      | 1     |
| 1:B:20:TYR:N    | 1:B:20:TYR:CD1  | 0.45     | 2.82        | 18     | 1     |
| 1:B:73:PHE:CD1  | 1:B:74:GLN:N    | 0.45     | 2.84        | 10     | 1     |
| 1:B:56:LEU:C    | 1:B:56:LEU:CD2  | 0.45     | 2.85        | 6      | 3     |
| 1:A:35:PHE:CZ   | 1:A:76:PHE:CG   | 0.45     | 3.04        | 3      | 2     |
| 1:A:39:MET:CE   | 1:A:83:LEU:CD1  | 0.45     | 2.95        | 3      | 5     |
| 1:B:34:GLU:O    | 1:B:38:PHE:CE2  | 0.45     | 2.70        | 15     | 1     |
| 1:B:60:MET:HG2  | 1:B:79:LEU:CD1  | 0.45     | 2.40        | 1      | 1     |
| 1:B:39:MET:HE3  | 1:B:43:LEU:CD1  | 0.45     | 2.41        | 11     | 1     |
| 1:A:56:LEU:CD2  | 1:A:56:LEU:C    | 0.45     | 2.85        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:59:MET:HE2  | 1:A:79:LEU:HA   | 0.45     | 1.89        | 13     | 1     |
| 1:B:82:GLY:HA2  | 1:B:85:VAL:HG23 | 0.45     | 1.87        | 5      | 1     |
| 1:A:32:LYS:O    | 1:A:36:LEU:HD23 | 0.45     | 2.12        | 3      | 1     |
| 1:B:32:LYS:O    | 1:B:36:LEU:HD23 | 0.45     | 2.12        | 3      | 1     |
| 1:A:77:LEU:O    | 1:A:81:GLY:HA3  | 0.45     | 2.11        | 16     | 1     |
| 1:B:39:MET:O    | 1:B:44:ALA:N    | 0.45     | 2.50        | 9      | 4     |
| 1:A:80:ILE:HD13 | 1:A:80:ILE:O    | 0.45     | 2.11        | 10     | 1     |
| 1:B:38:PHE:CE1  | 1:B:42:GLU:CB   | 0.45     | 2.99        | 6      | 1     |
| 1:B:71:LEU:HG   | 1:B:75:GLU:HB3  | 0.45     | 1.88        | 8      | 1     |
| 1:B:84:ALA:O    | 1:B:88:HIS:HB3  | 0.45     | 2.11        | 13     | 1     |
| 1:B:28:VAL:O    | 1:B:28:VAL:HG23 | 0.45     | 2.10        | 12     | 1     |
| 1:A:75:GLU:O    | 1:A:79:LEU:N    | 0.45     | 2.47        | 6      | 2     |
| 1:A:31:SER:OG   | 1:A:33:THR:HG22 | 0.45     | 2.12        | 7      | 1     |
| 1:A:20:TYR:CE2  | 1:A:34:GLU:O    | 0.44     | 2.69        | 16     | 6     |
| 1:A:16:VAL:CG2  | 1:A:17:PHE:N    | 0.44     | 2.80        | 11     | 6     |
| 1:A:85:VAL:HG21 | 1:B:73:PHE:CD1  | 0.44     | 2.47        | 10     | 1     |
| 1:B:84:ALA:O    | 1:B:88:HIS:C    | 0.44     | 2.55        | 5      | 1     |
| 1:B:56:LEU:O    | 1:B:59:MET:CG   | 0.44     | 2.65        | 18     | 2     |
| 1:A:33:THR:O    | 1:A:37:SER:N    | 0.44     | 2.49        | 10     | 1     |
| 1:B:59:MET:HG3  | 1:B:60:MET:H    | 0.44     | 1.71        | 19     | 1     |
| 1:A:17:PHE:CB   | 1:A:76:PHE:HB3  | 0.44     | 2.42        | 9      | 1     |
| 1:B:59:MET:HG3  | 1:B:83:LEU:CD2  | 0.44     | 2.29        | 13     | 1     |
| 1:B:60:MET:HE3  | 1:B:79:LEU:HD21 | 0.44     | 1.89        | 13     | 1     |
| 1:A:39:MET:O    | 1:A:44:ALA:N    | 0.44     | 2.50        | 9      | 4     |
| 1:A:33:THR:HA   | 1:A:36:LEU:HD12 | 0.44     | 1.90        | 6      | 1     |
| 1:A:35:PHE:CE2  | 1:A:76:PHE:CG   | 0.44     | 3.06        | 12     | 1     |
| 1:B:30:LEU:HD11 | 1:B:38:PHE:CE2  | 0.44     | 2.47        | 15     | 1     |
| 1:B:30:LEU:HD11 | 1:B:38:PHE:HE2  | 0.44     | 1.73        | 15     | 1     |
| 1:A:30:LEU:HD12 | 1:A:76:PHE:HE2  | 0.44     | 1.73        | 16     | 1     |
| 1:B:71:LEU:HD21 | 1:B:76:PHE:N    | 0.44     | 2.28        | 8      | 1     |
| 1:B:35:PHE:CZ   | 1:B:76:PHE:CG   | 0.44     | 3.04        | 3      | 2     |
| 1:B:35:PHE:CE2  | 1:B:76:PHE:CG   | 0.44     | 3.06        | 12     | 1     |
| 1:A:30:LEU:HD11 | 1:A:38:PHE:HE2  | 0.44     | 1.73        | 15     | 1     |
| 1:A:13:LEU:CD2  | 1:B:9:CYS:O     | 0.44     | 2.66        | 11     | 2     |
| 1:A:72:ASP:O    | 1:A:75:GLU:OE2  | 0.44     | 2.36        | 16     | 1     |
| 1:B:17:PHE:CB   | 1:B:76:PHE:HB3  | 0.44     | 2.42        | 9      | 1     |
| 1:B:39:MET:CE   | 1:B:83:LEU:CD1  | 0.44     | 2.95        | 3      | 5     |
| 1:A:56:LEU:O    | 1:A:59:MET:CG   | 0.44     | 2.65        | 18     | 2     |
| 1:B:35:PHE:CE2  | 1:B:76:PHE:HA   | 0.44     | 2.47        | 12     | 1     |
| 1:A:59:MET:CG   | 1:A:79:LEU:HA   | 0.44     | 2.43        | 1      | 1     |
| 1:B:59:MET:CG   | 1:B:79:LEU:HA   | 0.44     | 2.43        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:38:PHE:CE1  | 1:A:42:GLU:CG   | 0.44     | 3.01        | 6      | 1     |
| 1:B:30:LEU:O    | 1:B:70:GLN:NE2  | 0.44     | 2.51        | 9      | 8     |
| 1:A:90:SER:O    | 1:A:91:PHE:CB   | 0.44     | 2.66        | 18     | 1     |
| 1:B:13:LEU:HD11 | 1:B:80:ILE:HD12 | 0.44     | 1.90        | 11     | 1     |
| 1:A:40:ASN:C    | 1:A:44:ALA:HB2  | 0.44     | 2.33        | 4      | 2     |
| 1:A:20:TYR:N    | 1:A:20:TYR:CD1  | 0.44     | 2.83        | 10     | 1     |
| 1:A:73:PHE:CD1  | 1:B:85:VAL:HG21 | 0.44     | 2.47        | 10     | 1     |
| 1:B:60:MET:HG2  | 1:B:79:LEU:HD13 | 0.44     | 1.89        | 1      | 2     |
| 1:B:35:PHE:CE1  | 1:B:39:MET:HE3  | 0.44     | 2.47        | 2      | 1     |
| 1:B:30:LEU:HD12 | 1:B:76:PHE:HE2  | 0.44     | 1.73        | 16     | 1     |
| 1:B:77:LEU:O    | 1:B:81:GLY:HA3  | 0.44     | 2.11        | 16     | 1     |
| 1:A:59:MET:CE   | 1:A:59:MET:CA   | 0.44     | 2.96        | 13     | 1     |
| 1:B:16:VAL:CG2  | 1:B:17:PHE:N    | 0.44     | 2.80        | 11     | 7     |
| 1:A:82:GLY:HA2  | 1:A:85:VAL:HG23 | 0.44     | 1.88        | 5      | 1     |
| 1:A:16:VAL:O    | 1:A:76:PHE:CZ   | 0.44     | 2.71        | 2      | 1     |
| 1:A:85:VAL:HG21 | 1:B:73:PHE:HD2  | 0.44     | 1.70        | 11     | 1     |
| 1:B:20:TYR:CD2  | 1:B:34:GLU:O    | 0.43     | 2.72        | 5      | 5     |
| 1:A:13:LEU:CB   | 1:A:77:LEU:HD21 | 0.43     | 2.43        | 13     | 2     |
| 1:B:80:ILE:HG23 | 1:B:81:GLY:N    | 0.43     | 2.28        | 6      | 2     |
| 1:A:9:CYS:O     | 1:B:13:LEU:CD2  | 0.43     | 2.66        | 11     | 2     |
| 1:A:59:MET:HE2  | 1:A:79:LEU:HB3  | 0.43     | 1.89        | 18     | 1     |
| 1:A:39:MET:O    | 1:A:43:LEU:N    | 0.43     | 2.51        | 19     | 5     |
| 1:A:28:VAL:O    | 1:A:29:THR:OG1  | 0.43     | 2.36        | 18     | 1     |
| 1:B:17:PHE:CZ   | 1:B:77:LEU:HG   | 0.43     | 2.48        | 10     | 1     |
| 1:A:71:LEU:HD21 | 1:A:76:PHE:N    | 0.43     | 2.28        | 8      | 1     |
| 1:B:84:ALA:O    | 1:B:88:HIS:HB2  | 0.43     | 2.13        | 14     | 1     |
| 1:A:20:TYR:CD2  | 1:A:34:GLU:O    | 0.43     | 2.72        | 5      | 5     |
| 1:B:40:ASN:C    | 1:B:44:ALA:HB2  | 0.43     | 2.33        | 4      | 2     |
| 1:B:74:GLN:NE2  | 1:B:78:ASN:CB   | 0.43     | 2.81        | 5      | 3     |
| 1:A:17:PHE:HA   | 1:A:76:PHE:CD2  | 0.43     | 2.48        | 12     | 2     |
| 1:A:35:PHE:CE2  | 1:A:76:PHE:HA   | 0.43     | 2.47        | 12     | 1     |
| 1:A:39:MET:HE1  | 1:A:43:LEU:HD13 | 0.43     | 1.91        | 10     | 1     |
| 1:A:60:MET:HG2  | 1:A:79:LEU:HD13 | 0.43     | 1.90        | 1      | 2     |
| 1:B:56:LEU:HD22 | 1:B:56:LEU:O    | 0.43     | 2.14        | 9      | 1     |
| 1:A:74:GLN:NE2  | 1:A:78:ASN:CB   | 0.43     | 2.81        | 17     | 3     |
| 1:B:17:PHE:HA   | 1:B:76:PHE:CD2  | 0.43     | 2.48        | 12     | 2     |
| 1:A:84:ALA:O    | 1:A:88:HIS:HB2  | 0.43     | 2.13        | 14     | 1     |
| 1:A:39:MET:CG   | 1:A:56:LEU:HD13 | 0.43     | 2.44        | 12     | 1     |
| 1:A:71:LEU:O    | 1:A:72:ASP:CB   | 0.43     | 2.67        | 10     | 4     |
| 1:B:16:VAL:O    | 1:B:76:PHE:CZ   | 0.43     | 2.71        | 2      | 1     |
| 1:B:11:GLU:CA   | 1:B:14:ILE:HD12 | 0.43     | 2.37        | 7      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:72:ASP:O    | 1:B:75:GLU:OE2  | 0.43     | 2.36        | 16     | 1     |
| 1:A:17:PHE:CE2  | 1:A:72:ASP:O    | 0.43     | 2.72        | 13     | 2     |
| 1:B:17:PHE:CE2  | 1:B:72:ASP:O    | 0.43     | 2.72        | 13     | 2     |
| 1:A:14:ILE:HA   | 1:A:17:PHE:CD2  | 0.43     | 2.49        | 10     | 1     |
| 1:B:39:MET:O    | 1:B:43:LEU:N    | 0.43     | 2.51        | 19     | 5     |
| 1:A:59:MET:HB3  | 1:A:79:LEU:HD13 | 0.43     | 1.89        | 11     | 1     |
| 1:B:35:PHE:CE2  | 1:B:79:LEU:HB3  | 0.43     | 2.49        | 8      | 1     |
| 1:A:30:LEU:O    | 1:A:70:GLN:NE2  | 0.43     | 2.51        | 9      | 7     |
| 1:A:73:PHE:HA   | 1:A:76:PHE:CE2  | 0.43     | 2.48        | 9      | 2     |
| 1:A:18:GLN:O    | 1:A:22:GLY:N    | 0.43     | 2.52        | 15     | 8     |
| 1:A:17:PHE:CZ   | 1:A:77:LEU:HG   | 0.43     | 2.48        | 10     | 1     |
| 1:B:73:PHE:HA   | 1:B:76:PHE:CE2  | 0.43     | 2.48        | 9      | 2     |
| 1:A:46:PHE:CZ   | 1:A:88:HIS:CE1  | 0.43     | 3.07        | 2      | 1     |
| 1:B:89:GLU:O    | 1:B:90:SER:CB   | 0.43     | 2.67        | 1      | 2     |
| 1:B:33:THR:HA   | 1:B:36:LEU:HD12 | 0.43     | 1.90        | 6      | 1     |
| 1:B:31:SER:N    | 1:B:71:LEU:HB2  | 0.43     | 2.29        | 13     | 1     |
| 1:A:38:PHE:CE2  | 1:A:42:GLU:CG   | 0.43     | 3.02        | 12     | 1     |
| 1:B:59:MET:HB3  | 1:B:79:LEU:HD13 | 0.43     | 1.90        | 11     | 1     |
| 1:B:38:PHE:CE1  | 1:B:42:GLU:CG   | 0.43     | 3.01        | 6      | 1     |
| 1:B:33:THR:HA   | 1:B:36:LEU:HB2  | 0.43     | 1.90        | 7      | 1     |
| 1:B:39:MET:CG   | 1:B:56:LEU:HD13 | 0.42     | 2.44        | 12     | 1     |
| 1:B:38:PHE:CE2  | 1:B:42:GLU:CG   | 0.42     | 3.02        | 12     | 1     |
| 1:A:59:MET:HE1  | 1:A:83:LEU:HD21 | 0.42     | 1.85        | 4      | 1     |
| 1:B:39:MET:HE1  | 1:B:83:LEU:CD1  | 0.42     | 2.43        | 15     | 1     |
| 1:A:13:LEU:HD11 | 1:A:80:ILE:HD12 | 0.42     | 1.90        | 11     | 1     |
| 1:A:56:LEU:O    | 1:A:56:LEU:HD22 | 0.42     | 2.14        | 9      | 1     |
| 1:B:30:LEU:CD1  | 1:B:35:PHE:CD2  | 0.42     | 3.01        | 3      | 1     |
| 1:B:90:SER:O    | 1:B:91:PHE:CB   | 0.42     | 2.66        | 18     | 1     |
| 1:A:14:ILE:CG2  | 1:A:18:GLN:NE2  | 0.42     | 2.81        | 17     | 3     |
| 1:A:80:ILE:HG23 | 1:A:81:GLY:N    | 0.42     | 2.28        | 6      | 1     |
| 1:A:30:LEU:CD1  | 1:A:35:PHE:CD2  | 0.42     | 3.01        | 3      | 1     |
| 1:B:13:LEU:CB   | 1:B:77:LEU:HD21 | 0.42     | 2.43        | 13     | 2     |
| 1:A:39:MET:HE1  | 1:A:83:LEU:CD1  | 0.42     | 2.45        | 15     | 1     |
| 1:B:46:PHE:CZ   | 1:B:88:HIS:CD2  | 0.42     | 3.07        | 15     | 1     |
| 1:A:13:LEU:CD1  | 1:A:80:ILE:CG2  | 0.42     | 2.98        | 11     | 1     |
| 1:B:74:GLN:O    | 1:B:78:ASN:HB2  | 0.42     | 2.14        | 11     | 1     |
| 1:A:33:THR:HA   | 1:A:36:LEU:HB2  | 0.42     | 1.90        | 7      | 1     |
| 1:A:85:VAL:HG13 | 1:A:90:SER:HB2  | 0.42     | 1.89        | 7      | 1     |
| 1:A:59:MET:HG3  | 1:A:83:LEU:CD2  | 0.42     | 2.29        | 13     | 1     |
| 1:B:18:GLN:O    | 1:B:22:GLY:N    | 0.42     | 2.52        | 15     | 7     |
| 1:A:4:THR:CG2   | 1:A:7:GLU:HB2   | 0.42     | 2.42        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:32:LYS:N    | 1:B:71:LEU:CD2  | 0.42     | 2.82        | 1      | 3     |
| 1:B:4:THR:CG2   | 1:B:7:GLU:HB2   | 0.42     | 2.42        | 1      | 1     |
| 1:A:13:LEU:HD22 | 1:B:9:CYS:HB3   | 0.42     | 1.91        | 6      | 1     |
| 1:A:28:VAL:HG21 | 1:B:90:SER:O    | 0.42     | 2.14        | 9      | 1     |
| 1:B:72:ASP:O    | 1:B:76:PHE:CD2  | 0.42     | 2.72        | 9      | 1     |
| 1:A:35:PHE:CE1  | 1:A:76:PHE:CE2  | 0.42     | 3.08        | 3      | 1     |
| 1:B:39:MET:O    | 1:B:43:LEU:C    | 0.42     | 2.58        | 12     | 2     |
| 1:B:46:PHE:CZ   | 1:B:88:HIS:CE1  | 0.42     | 3.07        | 2      | 1     |
| 1:A:89:GLU:O    | 1:A:90:SER:CB   | 0.42     | 2.67        | 1      | 2     |
| 1:A:73:PHE:HD2  | 1:B:85:VAL:HG21 | 0.42     | 1.70        | 11     | 1     |
| 1:A:9:CYS:HB3   | 1:B:13:LEU:HD22 | 0.42     | 1.91        | 6      | 1     |
| 1:B:85:VAL:HG13 | 1:B:90:SER:HB2  | 0.42     | 1.89        | 7      | 1     |
| 1:A:39:MET:CE   | 1:A:83:LEU:HD13 | 0.42     | 2.45        | 8      | 1     |
| 1:A:46:PHE:CZ   | 1:A:88:HIS:CD2  | 0.42     | 3.07        | 15     | 1     |
| 1:A:74:GLN:O    | 1:A:78:ASN:HB2  | 0.42     | 2.14        | 11     | 1     |
| 1:B:13:LEU:CD1  | 1:B:80:ILE:CG2  | 0.42     | 2.98        | 11     | 1     |
| 1:A:72:ASP:O    | 1:A:76:PHE:CD2  | 0.42     | 2.72        | 9      | 1     |
| 1:A:35:PHE:CE2  | 1:A:79:LEU:HB3  | 0.42     | 2.49        | 8      | 1     |
| 1:B:30:LEU:O    | 1:B:70:GLN:CD   | 0.42     | 2.58        | 8      | 1     |
| 1:A:32:LYS:N    | 1:A:71:LEU:CD2  | 0.42     | 2.82        | 1      | 3     |
| 1:A:90:SER:HB2  | 1:B:73:PHE:CD2  | 0.42     | 2.50        | 19     | 1     |
| 1:A:84:ALA:HA   | 1:A:88:HIS:HB2  | 0.42     | 1.92        | 13     | 1     |
| 1:B:14:ILE:CG2  | 1:B:18:GLN:NE2  | 0.42     | 2.80        | 3      | 3     |
| 1:A:39:MET:O    | 1:A:43:LEU:C    | 0.42     | 2.58        | 12     | 2     |
| 1:B:60:MET:CE   | 1:B:60:MET:HA   | 0.42     | 2.45        | 12     | 1     |
| 1:A:89:GLU:HA   | 1:B:14:ILE:CG2  | 0.42     | 2.45        | 2      | 1     |
| 1:A:43:LEU:HD21 | 1:B:10:ILE:CD1  | 0.42     | 2.45        | 5      | 1     |
| 1:A:9:CYS:CB    | 1:B:12:SER:OG   | 0.42     | 2.68        | 3      | 1     |
| 1:B:14:ILE:HA   | 1:B:17:PHE:CD2  | 0.42     | 2.49        | 10     | 1     |
| 1:B:72:ASP:OD1  | 1:B:73:PHE:CD1  | 0.42     | 2.73        | 4      | 2     |
| 1:A:10:ILE:CG2  | 1:B:84:ALA:CB   | 0.42     | 2.96        | 15     | 1     |
| 1:A:56:LEU:C    | 1:A:56:LEU:CD2  | 0.42     | 2.87        | 15     | 2     |
| 1:A:30:LEU:HD21 | 1:A:34:GLU:HB3  | 0.42     | 1.92        | 1      | 2     |
| 1:A:31:SER:N    | 1:A:71:LEU:HB2  | 0.42     | 2.29        | 13     | 1     |
| 1:A:10:ILE:CD1  | 1:B:43:LEU:HD21 | 0.42     | 2.45        | 5      | 1     |
| 1:B:35:PHE:CE1  | 1:B:76:PHE:CE2  | 0.42     | 3.08        | 3      | 1     |
| 1:A:39:MET:CE   | 1:A:43:LEU:CD1  | 0.42     | 2.98        | 9      | 4     |
| 1:A:17:PHE:HB2  | 1:A:76:PHE:CB   | 0.42     | 2.45        | 6      | 2     |
| 1:A:14:ILE:CG2  | 1:B:89:GLU:HA   | 0.42     | 2.45        | 2      | 1     |
| 1:B:35:PHE:CE2  | 1:B:79:LEU:HB2  | 0.42     | 2.50        | 1      | 1     |
| 1:A:41:THR:HG23 | 1:A:42:GLU:H    | 0.42     | 1.75        | 13     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:41:THR:HG23 | 1:B:42:GLU:H    | 0.42     | 1.75        | 13     | 1     |
| 1:B:16:VAL:O    | 1:B:20:TYR:CZ   | 0.41     | 2.73        | 4      | 1     |
| 1:B:17:PHE:HB2  | 1:B:76:PHE:CB   | 0.41     | 2.45        | 6      | 2     |
| 1:A:35:PHE:CE2  | 1:A:79:LEU:HB2  | 0.41     | 2.50        | 1      | 1     |
| 1:A:73:PHE:CE2  | 1:B:90:SER:HB2  | 0.41     | 2.50        | 19     | 1     |
| 1:A:90:SER:CB   | 1:B:73:PHE:CD2  | 0.41     | 3.03        | 19     | 1     |
| 1:A:90:SER:HB2  | 1:B:73:PHE:CE2  | 0.41     | 2.50        | 19     | 1     |
| 1:B:39:MET:CE   | 1:B:43:LEU:CD1  | 0.41     | 2.98        | 9      | 4     |
| 1:A:39:MET:HE2  | 1:A:43:LEU:CD1  | 0.41     | 2.43        | 19     | 1     |
| 1:A:73:PHE:CD2  | 1:B:90:SER:HB2  | 0.41     | 2.50        | 19     | 1     |
| 1:A:30:LEU:O    | 1:A:70:GLN:CD   | 0.41     | 2.58        | 8      | 1     |
| 1:B:39:MET:CE   | 1:B:83:LEU:HD13 | 0.41     | 2.45        | 8      | 1     |
| 1:A:70:GLN:HE21 | 1:A:70:GLN:HA   | 0.41     | 1.76        | 4      | 1     |
| 1:A:38:PHE:CA   | 1:A:41:THR:HG22 | 0.41     | 2.46        | 1      | 1     |
| 1:A:59:MET:SD   | 1:A:60:MET:N    | 0.41     | 2.94        | 1      | 1     |
| 1:A:59:MET:HB3  | 1:A:59:MET:HE2  | 0.41     | 1.71        | 15     | 2     |
| 1:A:70:GLN:HA   | 1:A:70:GLN:HE21 | 0.41     | 1.76        | 12     | 1     |
| 1:A:16:VAL:O    | 1:A:20:TYR:CE2  | 0.41     | 2.73        | 15     | 2     |
| 1:A:72:ASP:OD1  | 1:A:73:PHE:CD1  | 0.41     | 2.73        | 4      | 2     |
| 1:B:14:ILE:HA   | 1:B:17:PHE:CE2  | 0.41     | 2.51        | 4      | 1     |
| 1:A:86:ALA:C    | 1:A:92:VAL:HG11 | 0.41     | 2.36        | 17     | 1     |
| 1:A:17:PHE:CB   | 1:A:76:PHE:CG   | 0.41     | 3.04        | 9      | 1     |
| 1:A:60:MET:HA   | 1:A:60:MET:CE   | 0.41     | 2.45        | 12     | 1     |
| 1:A:84:ALA:CB   | 1:B:10:ILE:CG2  | 0.41     | 2.96        | 15     | 1     |
| 1:B:74:GLN:O    | 1:B:75:GLU:C    | 0.41     | 2.59        | 11     | 1     |
| 1:A:89:GLU:CG   | 1:B:14:ILE:HG23 | 0.41     | 2.44        | 5      | 1     |
| 1:B:70:GLN:HE21 | 1:B:70:GLN:HA   | 0.41     | 1.75        | 4      | 2     |
| 1:A:77:LEU:HD13 | 1:A:77:LEU:HA   | 0.41     | 1.80        | 11     | 1     |
| 1:B:17:PHE:CE1  | 1:B:76:PHE:CE2  | 0.41     | 3.09        | 9      | 1     |
| 1:A:72:ASP:OD1  | 1:A:73:PHE:N    | 0.41     | 2.54        | 8      | 1     |
| 1:A:30:LEU:CD2  | 1:A:34:GLU:CB   | 0.41     | 2.99        | 13     | 1     |
| 1:A:76:PHE:HA   | 1:A:79:LEU:HB2  | 0.41     | 1.92        | 3      | 1     |
| 1:B:76:PHE:HA   | 1:B:79:LEU:HB2  | 0.41     | 1.92        | 3      | 1     |
| 1:B:33:THR:O    | 1:B:37:SER:N    | 0.41     | 2.49        | 10     | 1     |
| 1:A:30:LEU:HD13 | 1:A:31:SER:H    | 0.41     | 1.76        | 15     | 1     |
| 1:A:59:MET:HE2  | 1:A:83:LEU:HD11 | 0.41     | 1.92        | 1      | 1     |
| 1:B:59:MET:HB2  | 1:B:79:LEU:HD13 | 0.41     | 1.93        | 19     | 1     |
| 1:B:80:ILE:C    | 1:B:80:ILE:HD13 | 0.41     | 2.36        | 8      | 1     |
| 1:A:12:SER:OG   | 1:B:9:CYS:CB    | 0.41     | 2.68        | 3      | 1     |
| 1:A:38:PHE:CE2  | 1:A:42:GLU:OE1  | 0.41     | 2.74        | 3      | 1     |
| 1:B:30:LEU:CD2  | 1:B:31:SER:N    | 0.41     | 2.84        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:80:ILE:C    | 1:A:80:ILE:HD13 | 0.41     | 2.36        | 8      | 2     |
| 1:B:16:VAL:O    | 1:B:20:TYR:CE2  | 0.41     | 2.73        | 15     | 1     |
| 1:B:5:GLU:CG    | 1:B:6:THR:N     | 0.41     | 2.84        | 11     | 1     |
| 1:A:59:MET:HB2  | 1:A:79:LEU:HD13 | 0.41     | 1.93        | 19     | 1     |
| 1:A:90:SER:O    | 1:B:28:VAL:HG21 | 0.41     | 2.15        | 9      | 1     |
| 1:A:59:MET:CG   | 1:A:79:LEU:HG   | 0.41     | 2.46        | 8      | 2     |
| 1:B:28:VAL:O    | 1:B:29:THR:OG1  | 0.41     | 2.37        | 18     | 1     |
| 1:A:13:LEU:HD21 | 1:B:10:ILE:HA   | 0.41     | 1.93        | 4      | 1     |
| 1:A:16:VAL:O    | 1:A:20:TYR:CZ   | 0.41     | 2.73        | 4      | 1     |
| 1:A:59:MET:HG3  | 1:A:79:LEU:HA   | 0.41     | 1.93        | 4      | 1     |
| 1:B:59:MET:HG3  | 1:B:79:LEU:HA   | 0.41     | 1.93        | 4      | 1     |
| 1:A:4:THR:O     | 1:A:7:GLU:HB2   | 0.41     | 2.16        | 17     | 1     |
| 1:B:59:MET:SD   | 1:B:60:MET:N    | 0.41     | 2.94        | 1      | 1     |
| 1:A:39:MET:HE3  | 1:A:43:LEU:CD1  | 0.41     | 2.45        | 11     | 1     |
| 1:A:32:LYS:O    | 1:A:36:LEU:N    | 0.41     | 2.54        | 7      | 1     |
| 1:A:73:PHE:CD2  | 1:B:90:SER:CB   | 0.41     | 3.03        | 19     | 1     |
| 1:B:17:PHE:CD1  | 1:B:17:PHE:C    | 0.41     | 2.94        | 9      | 1     |
| 1:A:59:MET:HG2  | 1:A:60:MET:CE   | 0.41     | 2.46        | 9      | 1     |
| 1:A:17:PHE:CE1  | 1:A:76:PHE:CE2  | 0.41     | 3.09        | 9      | 1     |
| 1:B:17:PHE:CB   | 1:B:76:PHE:CG   | 0.41     | 3.04        | 9      | 1     |
| 1:B:30:LEU:CD2  | 1:B:34:GLU:CB   | 0.41     | 2.99        | 13     | 1     |
| 1:B:84:ALA:HA   | 1:B:88:HIS:HB2  | 0.41     | 1.92        | 13     | 1     |
| 1:A:30:LEU:HD12 | 1:A:76:PHE:HD2  | 0.41     | 1.76        | 14     | 1     |
| 1:A:14:ILE:HG23 | 1:B:89:GLU:CG   | 0.41     | 2.44        | 5      | 1     |
| 1:A:15:ALA:O    | 1:A:19:LYS:CB   | 0.41     | 2.69        | 18     | 1     |
| 1:B:15:ALA:O    | 1:B:19:LYS:CB   | 0.41     | 2.69        | 18     | 1     |
| 1:B:60:MET:HE3  | 1:B:79:LEU:HG   | 0.41     | 1.92        | 18     | 1     |
| 1:B:30:LEU:HD21 | 1:B:34:GLU:HB3  | 0.41     | 1.92        | 1      | 1     |
| 1:A:28:VAL:O    | 1:A:29:THR:O    | 0.41     | 2.39        | 6      | 1     |
| 1:B:28:VAL:O    | 1:B:29:THR:O    | 0.41     | 2.39        | 6      | 1     |
| 1:A:14:ILE:CG2  | 1:A:73:PHE:CZ   | 0.41     | 3.03        | 19     | 1     |
| 1:A:56:LEU:HG   | 1:A:60:MET:CE   | 0.40     | 2.47        | 10     | 1     |
| 1:A:14:ILE:HA   | 1:A:17:PHE:CE2  | 0.40     | 2.51        | 4      | 1     |
| 1:B:80:ILE:HD13 | 1:B:80:ILE:C    | 0.40     | 2.37        | 4      | 1     |
| 1:B:86:ALA:C    | 1:B:92:VAL:HG11 | 0.40     | 2.36        | 17     | 1     |
| 1:A:17:PHE:CD1  | 1:A:17:PHE:C    | 0.40     | 2.94        | 9      | 1     |
| 1:A:59:MET:SD   | 1:A:79:LEU:HG   | 0.40     | 2.56        | 14     | 1     |
| 1:A:17:PHE:CE2  | 1:A:77:LEU:HG   | 0.40     | 2.51        | 10     | 1     |
| 1:A:30:LEU:CD2  | 1:A:31:SER:N    | 0.40     | 2.84        | 4      | 1     |
| 1:A:8:ARG:O     | 1:A:12:SER:OG   | 0.40     | 2.39        | 4      | 1     |
| 1:B:59:MET:HE3  | 1:B:83:LEU:CD2  | 0.40     | 2.40        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:38:PHE:N    | 1:B:38:PHE:CD1  | 0.40     | 2.88        | 15     | 1     |
| 1:A:5:GLU:CG    | 1:A:6:THR:N     | 0.40     | 2.84        | 11     | 1     |
| 1:B:32:LYS:O    | 1:B:36:LEU:N    | 0.40     | 2.54        | 7      | 1     |
| 1:A:17:PHE:CB   | 1:A:76:PHE:CB   | 0.40     | 3.00        | 9      | 1     |
| 1:A:39:MET:HE2  | 1:A:43:LEU:HB3  | 0.40     | 1.93        | 8      | 1     |
| 1:B:30:LEU:CD2  | 1:B:34:GLU:HB3  | 0.40     | 2.47        | 13     | 1     |
| 1:A:9:CYS:HB2   | 1:B:12:SER:HB3  | 0.40     | 1.94        | 5      | 1     |
| 1:A:73:PHE:CE1  | 1:B:85:VAL:HG21 | 0.40     | 2.51        | 10     | 1     |
| 1:B:8:ARG:O     | 1:B:12:SER:OG   | 0.40     | 2.39        | 4      | 1     |
| 1:A:38:PHE:CD1  | 1:A:38:PHE:N    | 0.40     | 2.88        | 15     | 1     |
| 1:A:41:THR:HG23 | 1:A:42:GLU:N    | 0.40     | 2.31        | 11     | 1     |
| 1:B:33:THR:HG23 | 1:B:34:GLU:N    | 0.40     | 2.32        | 7      | 1     |
| 1:B:17:PHE:CB   | 1:B:76:PHE:CB   | 0.40     | 3.00        | 9      | 1     |
| 1:B:59:MET:HB3  | 1:B:59:MET:HE2  | 0.40     | 1.78        | 10     | 1     |
| 1:A:72:ASP:O    | 1:A:76:PHE:CE1  | 0.40     | 2.75        | 4      | 1     |
| 1:A:12:SER:HB3  | 1:B:9:CYS:CB    | 0.40     | 2.47        | 15     | 1     |
| 1:A:33:THR:HG23 | 1:A:34:GLU:N    | 0.40     | 2.32        | 7      | 1     |
| 1:B:17:PHE:C    | 1:B:17:PHE:CD1  | 0.40     | 2.95        | 7      | 1     |
| 1:B:74:GLN:NE2  | 1:B:78:ASN:CA   | 0.40     | 2.85        | 5      | 1     |
| 1:A:76:PHE:O    | 1:A:79:LEU:N    | 0.40     | 2.55        | 3      | 1     |
| 1:B:59:MET:CG   | 1:B:79:LEU:HG   | 0.40     | 2.47        | 12     | 1     |
| 1:B:56:LEU:HG   | 1:B:60:MET:CE   | 0.40     | 2.47        | 10     | 1     |
| 1:A:79:LEU:HD23 | 1:A:79:LEU:N    | 0.40     | 2.32        | 1      | 1     |
| 1:A:38:PHE:O    | 1:A:41:THR:CG2  | 0.40     | 2.70        | 8      | 1     |
| 1:B:38:PHE:O    | 1:B:41:THR:CG2  | 0.40     | 2.70        | 8      | 1     |
| 1:A:38:PHE:CD1  | 1:A:38:PHE:O    | 0.40     | 2.75        | 13     | 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     | 68/101 (67%)    | 56±2 (83±2%) | 8±1 (12±2%) | 3±1 (5±2%) | 5           | 27 |
| 1   | B     | 68/101 (67%)    | 56±2 (83±2%) | 8±1 (12±2%) | 3±1 (5±2%) | 5           | 27 |
| All | All   | 2584/3838 (67%) | 2143 (83%)   | 315 (12%)   | 126 (5%)   | 5           | 27 |

All 26 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | B     | 71  | LEU  | 19             |
| 1   | A     | 71  | LEU  | 19             |
| 1   | A     | 72  | ASP  | 10             |
| 1   | B     | 72  | ASP  | 10             |
| 1   | B     | 90  | SER  | 8              |
| 1   | A     | 90  | SER  | 8              |
| 1   | A     | 89  | GLU  | 5              |
| 1   | B     | 89  | GLU  | 5              |
| 1   | A     | 47  | THR  | 4              |
| 1   | B     | 47  | THR  | 4              |
| 1   | A     | 87  | CYS  | 3              |
| 1   | A     | 28  | VAL  | 3              |
| 1   | B     | 87  | CYS  | 3              |
| 1   | B     | 28  | VAL  | 3              |
| 1   | A     | 22  | GLY  | 2              |
| 1   | A     | 29  | THR  | 2              |
| 1   | B     | 22  | GLY  | 2              |
| 1   | B     | 29  | THR  | 2              |
| 1   | A     | 92  | VAL  | 2              |
| 1   | B     | 31  | SER  | 2              |
| 1   | A     | 31  | SER  | 2              |
| 1   | A     | 91  | PHE  | 2              |
| 1   | B     | 91  | PHE  | 2              |
| 1   | B     | 92  | VAL  | 2              |
| 1   | B     | 70  | GLN  | 1              |
| 1   | A     | 70  | GLN  | 1              |

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |   |
|-----|-------|-----------------|--------------|--------------|-------------|---|
| 1   | A     | 59/87 (68%)     | 35±3 (59±5%) | 24±3 (41±5%) | 0           | 4 |
| 1   | B     | 59/87 (68%)     | 35±3 (59±5%) | 24±3 (41±5%) | 0           | 4 |
| All | All   | 2242/3306 (68%) | 1328 (59%)   | 914 (41%)    | 0           | 4 |

All 96 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   | B     | 71  | LEU  | 19             |
| 1   | B     | 80  | ILE  | 19             |
| 1   | A     | 71  | LEU  | 19             |
| 1   | A     | 80  | ILE  | 19             |
| 1   | A     | 85  | VAL  | 19             |
| 1   | B     | 85  | VAL  | 19             |
| 1   | A     | 30  | LEU  | 18             |
| 1   | B     | 4   | THR  | 18             |
| 1   | A     | 4   | THR  | 18             |
| 1   | B     | 30  | LEU  | 18             |
| 1   | A     | 78  | ASN  | 17             |
| 1   | B     | 78  | ASN  | 17             |
| 1   | B     | 11  | GLU  | 17             |
| 1   | A     | 11  | GLU  | 17             |
| 1   | A     | 91  | PHE  | 16             |
| 1   | B     | 91  | PHE  | 16             |
| 1   | A     | 7   | GLU  | 15             |
| 1   | B     | 7   | GLU  | 15             |
| 1   | A     | 35  | PHE  | 14             |
| 1   | A     | 75  | GLU  | 14             |
| 1   | B     | 75  | GLU  | 14             |
| 1   | B     | 60  | MET  | 14             |
| 1   | A     | 60  | MET  | 14             |
| 1   | B     | 35  | PHE  | 14             |
| 1   | B     | 32  | LYS  | 13             |
| 1   | A     | 32  | LYS  | 13             |
| 1   | B     | 39  | MET  | 12             |
| 1   | A     | 19  | LYS  | 12             |
| 1   | A     | 58  | ARG  | 12             |
| 1   | B     | 58  | ARG  | 12             |
| 1   | B     | 19  | LYS  | 12             |
| 1   | A     | 39  | MET  | 12             |
| 1   | A     | 5   | GLU  | 11             |
| 1   | B     | 5   | GLU  | 11             |
| 1   | A     | 31  | SER  | 10             |
| 1   | B     | 33  | THR  | 10             |
| 1   | A     | 8   | ARG  | 10             |
| 1   | A     | 12  | SER  | 10             |
| 1   | B     | 12  | SER  | 10             |
| 1   | B     | 31  | SER  | 10             |
| 1   | A     | 33  | THR  | 10             |
| 1   | B     | 8   | ARG  | 10             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 70  | GLN  | 9              |
| 1   | A     | 18  | GLN  | 9              |
| 1   | B     | 70  | GLN  | 9              |
| 1   | B     | 18  | GLN  | 9              |
| 1   | A     | 90  | SER  | 9              |
| 1   | A     | 59  | MET  | 9              |
| 1   | B     | 90  | SER  | 9              |
| 1   | B     | 6   | THR  | 9              |
| 1   | B     | 59  | MET  | 9              |
| 1   | A     | 6   | THR  | 9              |
| 1   | A     | 89  | GLU  | 8              |
| 1   | A     | 56  | LEU  | 8              |
| 1   | B     | 42  | GLU  | 8              |
| 1   | A     | 88  | HIS  | 8              |
| 1   | B     | 74  | GLN  | 8              |
| 1   | B     | 56  | LEU  | 8              |
| 1   | B     | 87  | CYS  | 8              |
| 1   | A     | 87  | CYS  | 8              |
| 1   | A     | 74  | GLN  | 8              |
| 1   | B     | 88  | HIS  | 8              |
| 1   | A     | 42  | GLU  | 8              |
| 1   | B     | 89  | GLU  | 8              |
| 1   | B     | 72  | ASP  | 7              |
| 1   | B     | 79  | LEU  | 7              |
| 1   | B     | 34  | GLU  | 7              |
| 1   | A     | 34  | GLU  | 7              |
| 1   | A     | 79  | LEU  | 7              |
| 1   | A     | 72  | ASP  | 7              |
| 1   | A     | 41  | THR  | 6              |
| 1   | B     | 36  | LEU  | 6              |
| 1   | B     | 41  | THR  | 6              |
| 1   | A     | 36  | LEU  | 6              |
| 1   | A     | 20  | TYR  | 5              |
| 1   | A     | 37  | SER  | 5              |
| 1   | B     | 20  | TYR  | 5              |
| 1   | B     | 9   | CYS  | 5              |
| 1   | B     | 37  | SER  | 5              |
| 1   | A     | 9   | CYS  | 5              |
| 1   | A     | 17  | PHE  | 4              |
| 1   | B     | 17  | PHE  | 4              |
| 1   | A     | 73  | PHE  | 3              |
| 1   | B     | 73  | PHE  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 76  | PHE  | 2              |
| 1   | B     | 92  | VAL  | 2              |
| 1   | A     | 92  | VAL  | 2              |
| 1   | B     | 76  | PHE  | 2              |
| 1   | B     | 57  | ASP  | 2              |
| 1   | A     | 57  | ASP  | 2              |
| 1   | B     | 77  | LEU  | 1              |
| 1   | A     | 77  | LEU  | 1              |
| 1   | A     | 40  | ASN  | 1              |
| 1   | B     | 38  | PHE  | 1              |
| 1   | A     | 38  | PHE  | 1              |
| 1   | B     | 40  | ASN  | 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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 89% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5189

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|   |      |
|---|------|
| Total number of shifts                  | 2458 |
| Number of shifts mapped to atoms        | 2458 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 2    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 200      | $-0.59 \pm 0.15$                | Should be applied          |
| $^{13}\text{C}_\beta$  | 186      | $0.07 \pm 0.09$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 184      | $-0.38 \pm 0.05$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 192      | $0.34 \pm 0.19$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1482 atoms were assigned a chemical shift out of a possible 1650. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 674/680 (99%) | 270/272 (99%) | 268/272 (99%)   | 136/136 (100%)  |
| Sidechain | 724/812 (89%) | 432/468 (92%) | 282/318 (89%)   | 10/26 (38%)     |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 84/158 (53%)    | 56/86 (65%)          | 28/68 (41%)           | 0/4 (0%)              |
| Overall  | 1482/1650 (90%) | 758/826 (92%)        | 578/658 (88%)         | 146/166 (88%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 2212 atoms were assigned a chemical shift out of a possible 2498. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 964/994 (97%)   | 388/396 (98%)        | 384/404 (95%)         | 192/194 (99%)         |
| Sidechain | 1142/1312 (87%) | 698/772 (90%)        | 426/480 (89%)         | 18/60 (30%)           |
| Aromatic  | 106/192 (55%)   | 66/104 (63%)         | 40/80 (50%)           | 0/8 (0%)              |
| Overall   | 2212/2498 (89%) | 1152/1272 (91%)      | 850/964 (88%)         | 210/262 (80%)         |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

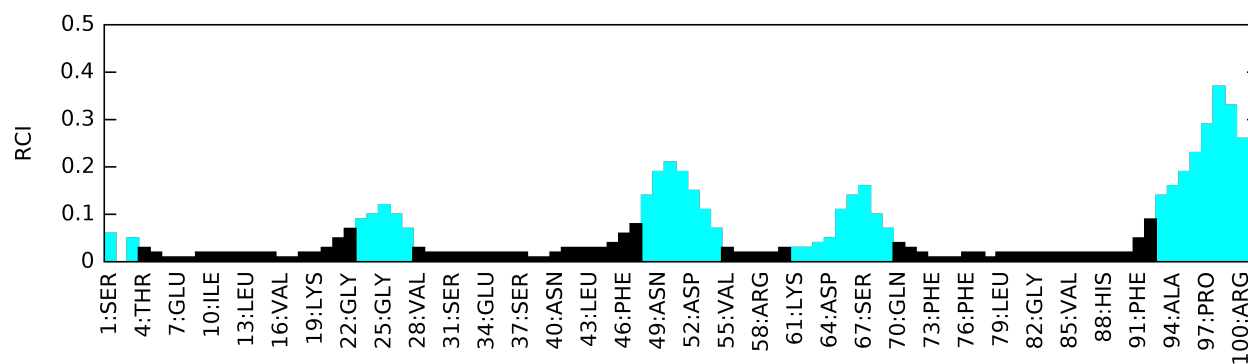
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| Mol | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|-----|-------|-----|------|------|------------|---------------------|---------|
| 1   | B     | 34  | GLU  | CG   | 27.08      | 42.24 – 29.94       | -7.3    |
| 1   | A     | 34  | GLU  | CG   | 27.08      | 42.24 – 29.94       | -7.3    |

#### 7.1.5 Random Coil Index (RCI) plots ⓘ

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

