



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 08:52 AM UTC

PDB ID : 1Q8G / pdb\_00001q8g  
Title : NMR structure of human Cofilin  
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Deposited on : 2003-08-21

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

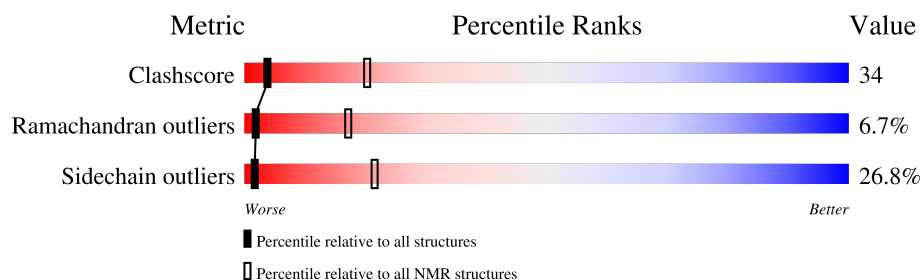
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 166    |  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:5-A:166 (162)       | 0.82              | 14           |

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

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

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 2642 atoms, of which 1346 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cofilin, non-muscle isoform.

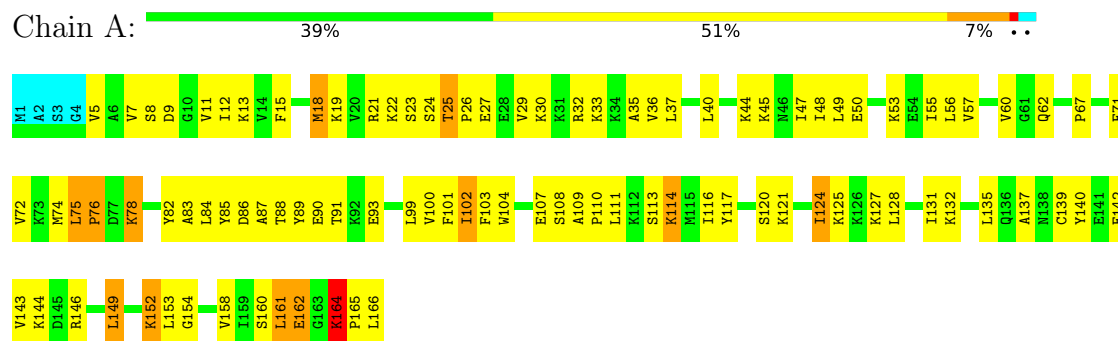
| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 166      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2642  | 826 | 1346 | 211 | 251 | 8 |       |

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

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

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

- Molecule 1: Cofilin, non-muscle isoform

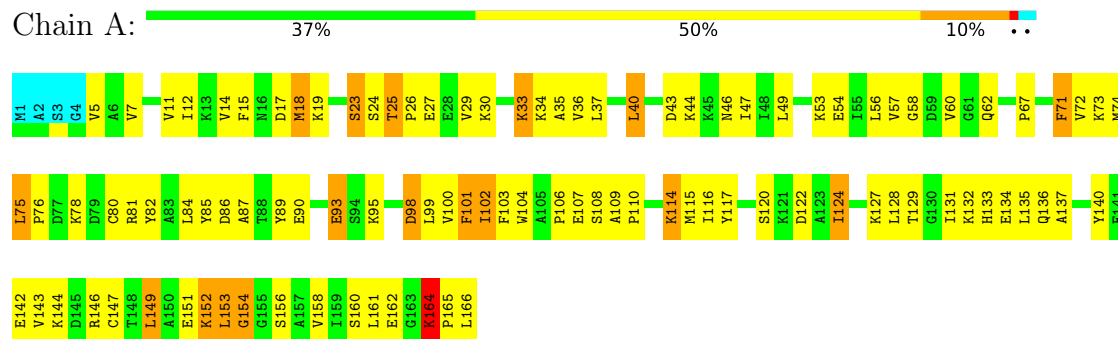


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

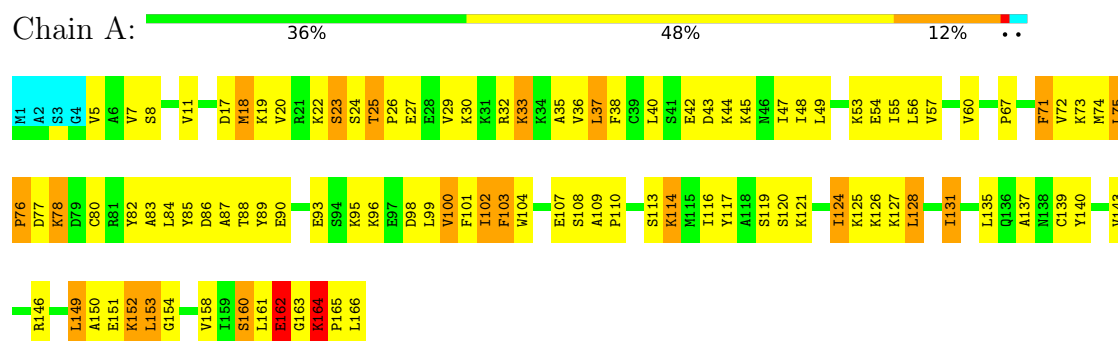
#### 4.2.1 Score per residue for model 1

- Molecule 1: Cofilin, non-muscle isoform



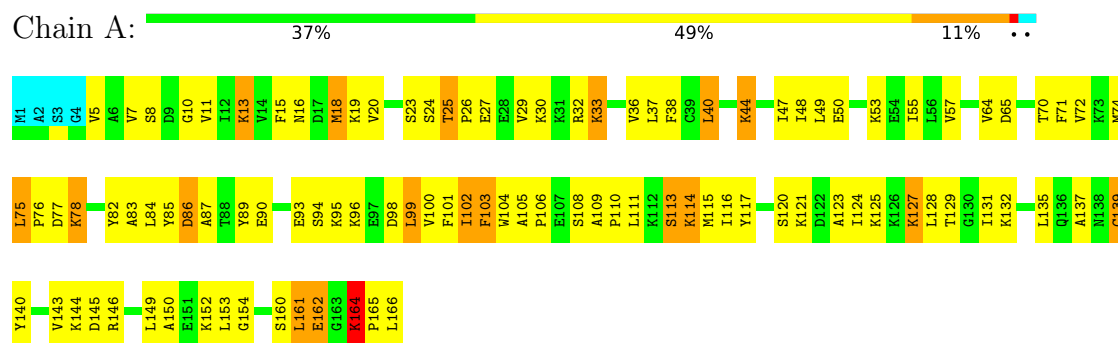
### 4.2.2 Score per residue for model 2

- Molecule 1: Cofilin, non-muscle isoform



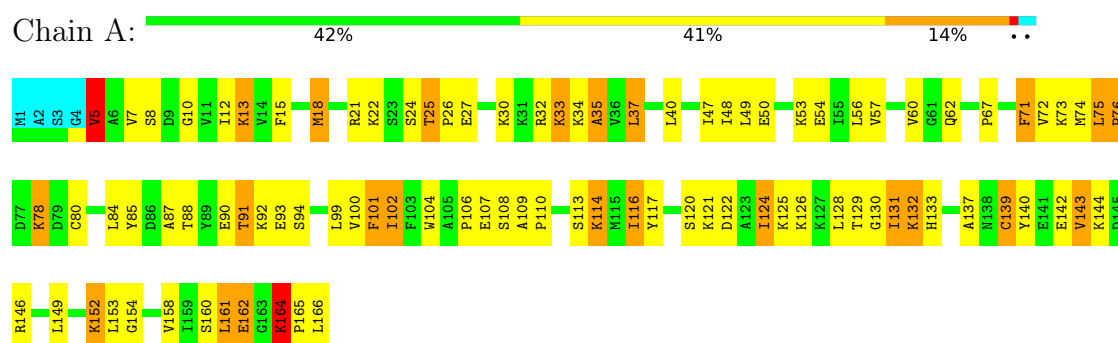
### 4.2.3 Score per residue for model 3

- Molecule 1: Cofilin, non-muscle isoform



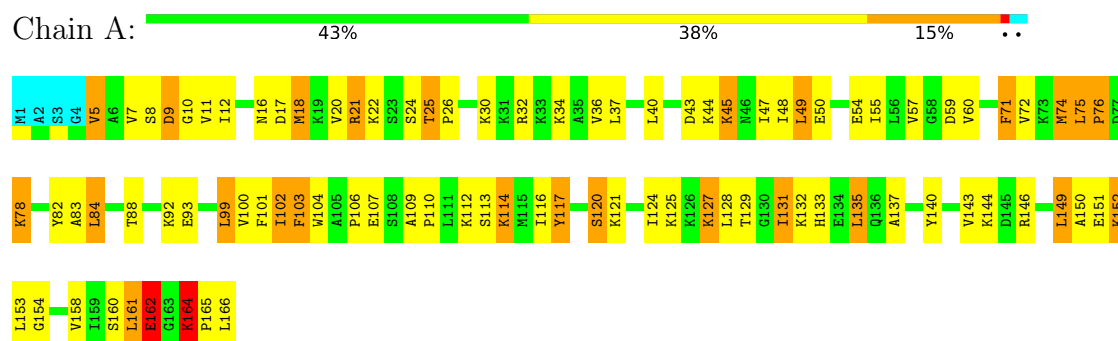
### 4.2.4 Score per residue for model 4

- Molecule 1: Cofilin, non-muscle isoform



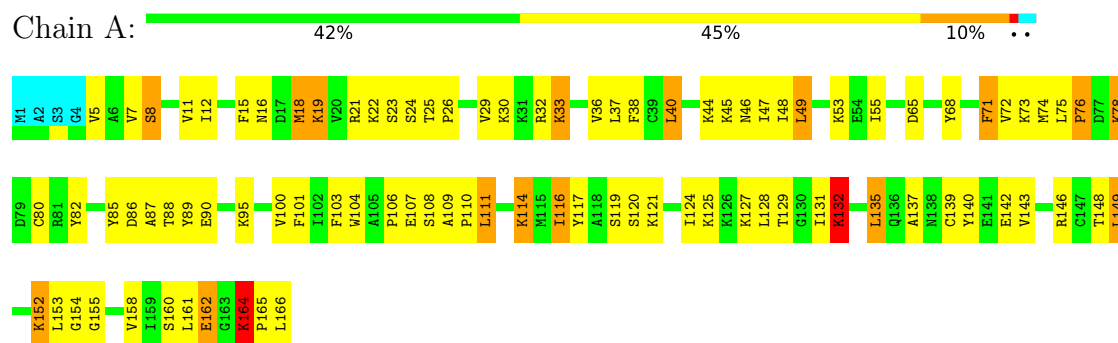
### 4.2.5 Score per residue for model 5

- Molecule 1: Cofilin, non-muscle isoform



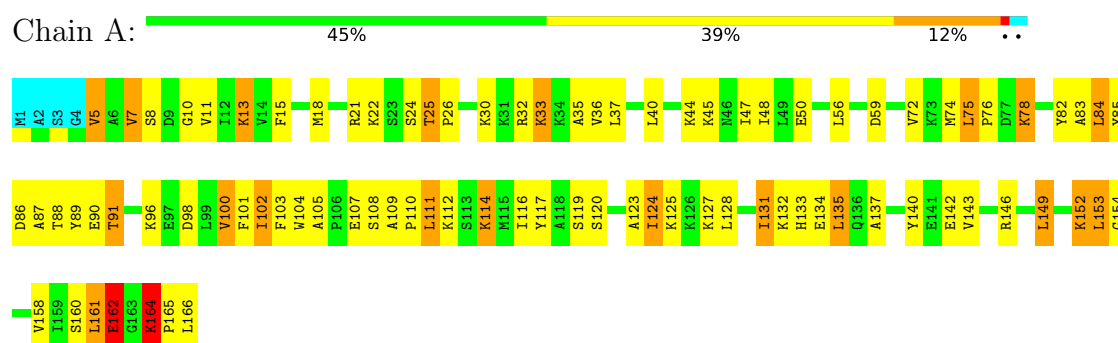
### 4.2.6 Score per residue for model 6

- Molecule 1: Cofilin, non-muscle isoform



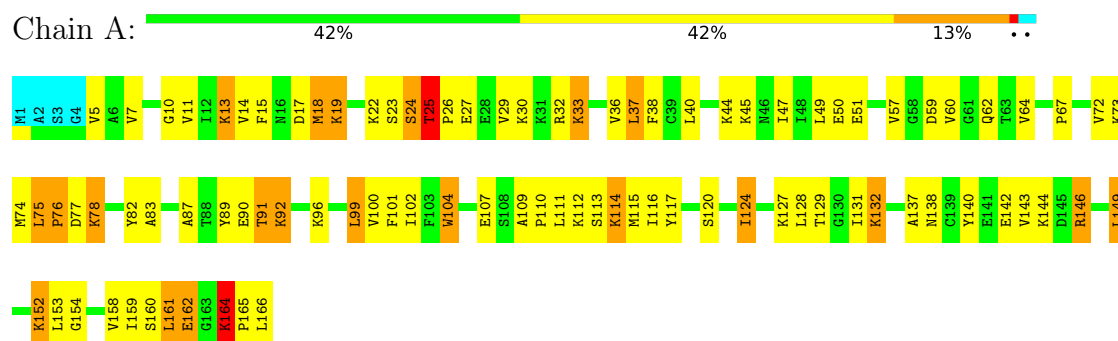
### 4.2.7 Score per residue for model 7

- Molecule 1: Cofilin, non-muscle isoform



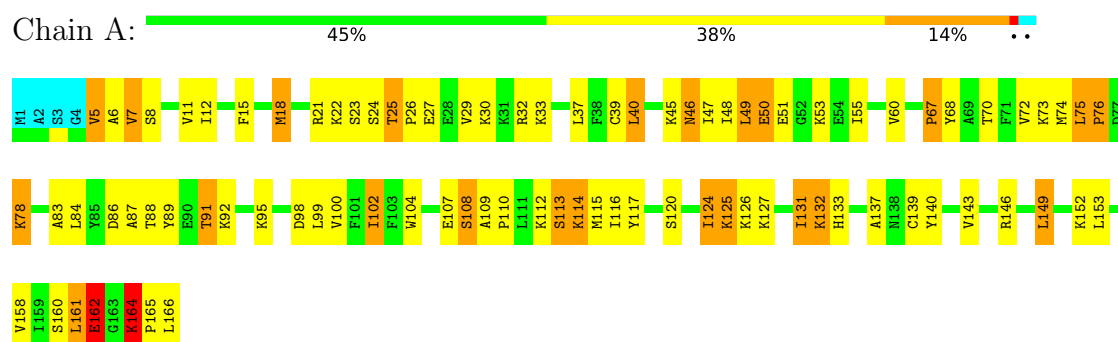
### 4.2.8 Score per residue for model 8

- Molecule 1: Cofilin, non-muscle isoform



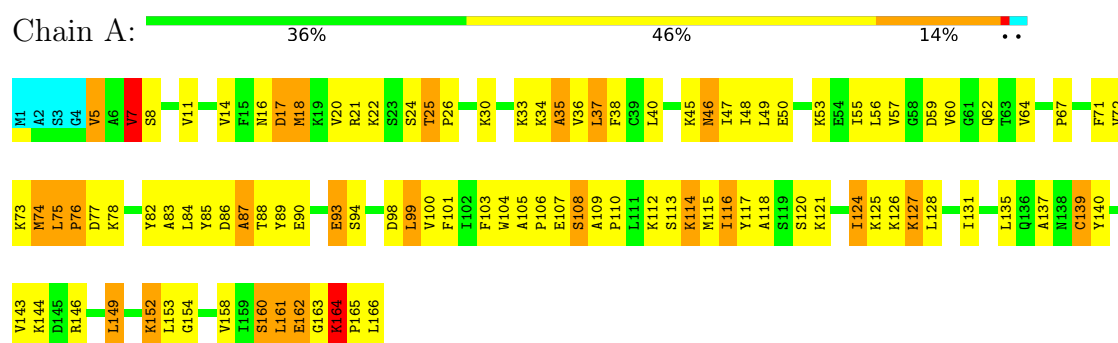
### 4.2.9 Score per residue for model 9

- Molecule 1: Cofilin, non-muscle isoform



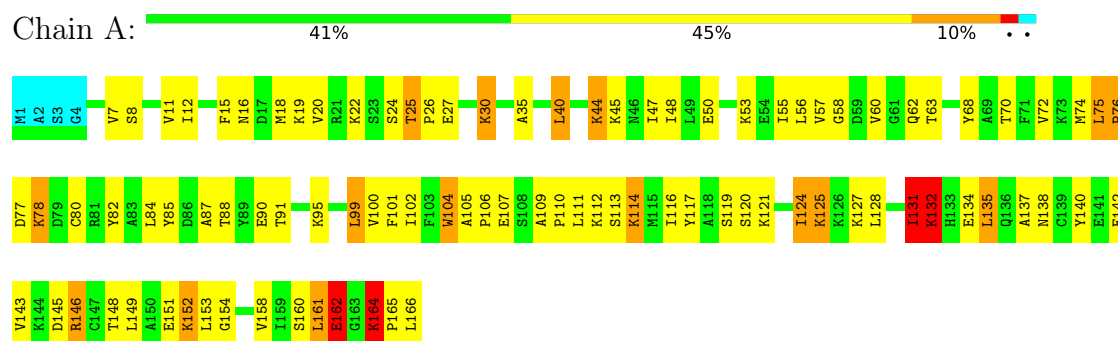
### 4.2.10 Score per residue for model 10

- Molecule 1: Cofilin, non-muscle isoform



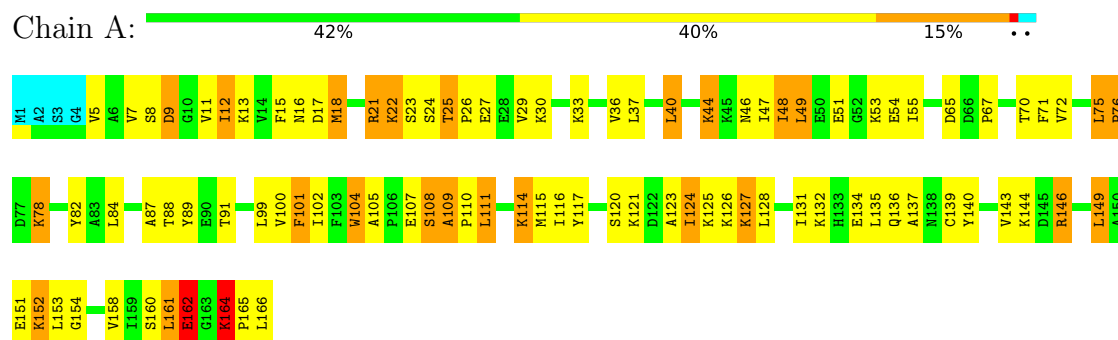
### 4.2.11 Score per residue for model 11

- Molecule 1: Cofilin, non-muscle isoform



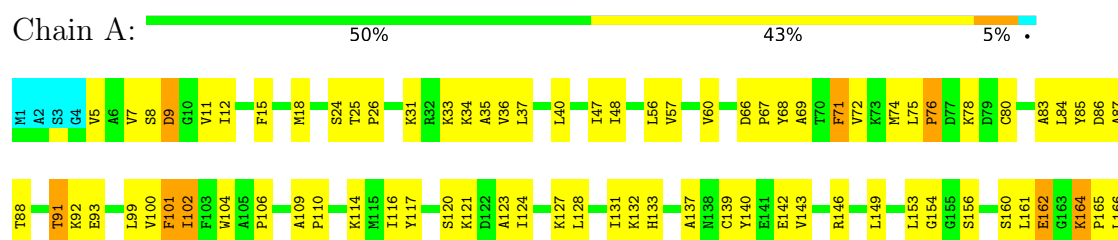
### 4.2.12 Score per residue for model 12

- Molecule 1: Cofilin, non-muscle isoform



### 4.2.13 Score per residue for model 13

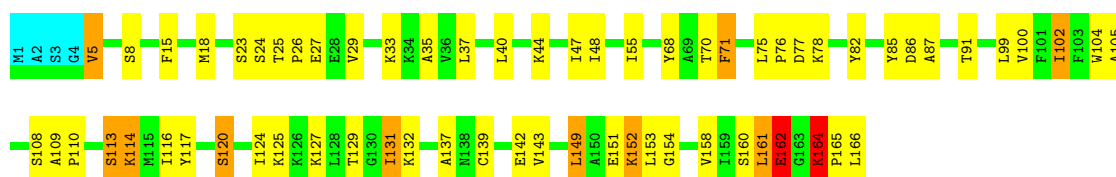
- Molecule 1: Cofilin, non-muscle isoform



### 4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Cofilin, non-muscle isoform

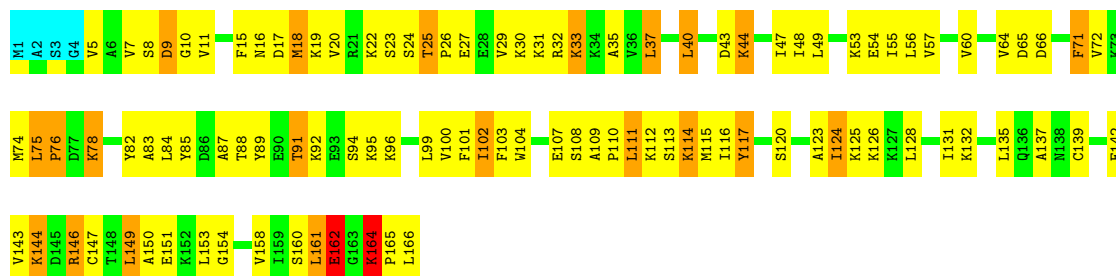




#### 4.2.15 Score per residue for model 15

- Molecule 1: Cofilin, non-muscle isoform

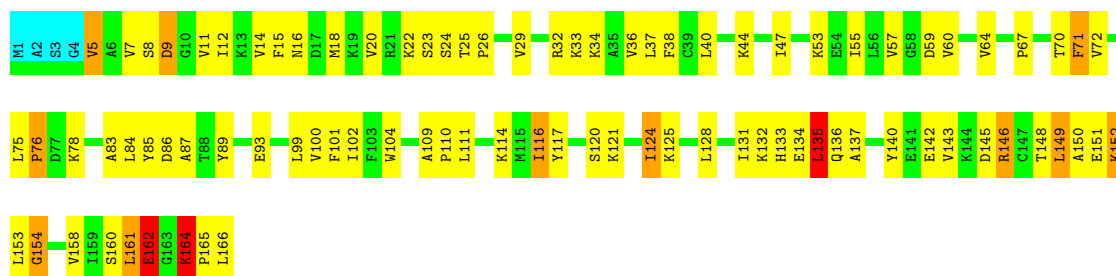
Chain A: 36% 48% 13% ..



#### 4.2.16 Score per residue for model 16

- Molecule 1: Cofilin, non-muscle isoform

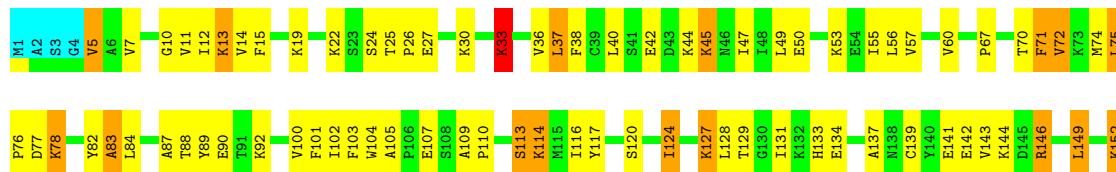
Chain A: 45% 45% 7% ..



#### 4.2.17 Score per residue for model 17

- Molecule 1: Cofilin, non-muscle isoform

Chain A: 45% 40% 11% ..

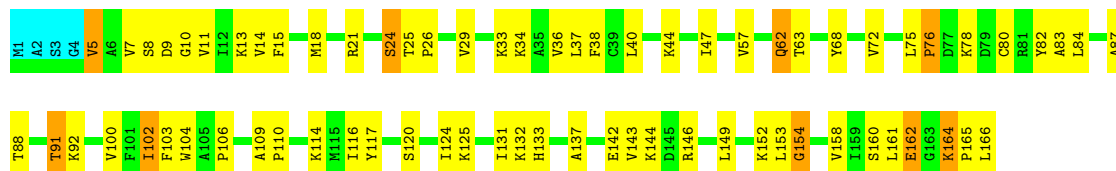




#### 4.2.18 Score per residue for model 18

- Molecule 1: Cofilin, non-muscle isoform

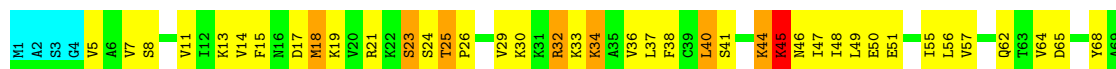
Chain A: 55% 37% 5% .



#### 4.2.19 Score per residue for model 19

- Molecule 1: Cofilin, non-muscle isoform

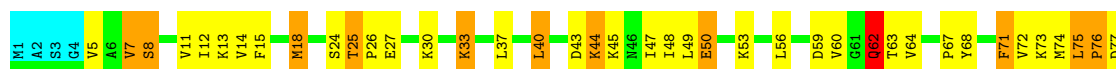
Chain A: 36% 46% 14% ..



#### 4.2.20 Score per residue for model 20

- Molecule 1: Cofilin, non-muscle isoform

Chain A: 42% 39% 16% ..



## 5 Refinement protocol and experimental data overview

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

Of the 140 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

No chemical shift data was provided.

## 6 Model quality ⓘ

### 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     | 1273  | 1322     | 1321     | 89±12   |
| All | All   | 25460 | 26440    | 26420    | 1778    |

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 34.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:100:VAL:HG21 | 1:A:149:LEU:HD21 | 1.09     | 1.20        | 1      | 1     |
| 1:A:100:VAL:HG11 | 1:A:149:LEU:HD21 | 1.05     | 1.18        | 12     | 2     |
| 1:A:55:ILE:HD13  | 1:A:70:THR:HG23  | 1.01     | 1.30        | 16     | 3     |
| 1:A:87:ALA:HB2   | 1:A:149:LEU:HD12 | 1.01     | 1.27        | 17     | 11    |
| 1:A:47:ILE:HG21  | 1:A:124:ILE:HD12 | 0.87     | 1.45        | 4      | 12    |
| 1:A:89:TYR:CD1   | 1:A:153:LEU:HD22 | 0.86     | 2.05        | 19     | 6     |
| 1:A:135:LEU:HD22 | 1:A:149:LEU:HD22 | 0.85     | 1.45        | 5      | 3     |
| 1:A:89:TYR:CD1   | 1:A:153:LEU:HD13 | 0.84     | 2.08        | 3      | 7     |
| 1:A:12:ILE:HD11  | 1:A:127:LYS:CD   | 0.84     | 2.02        | 20     | 2     |
| 1:A:153:LEU:HD12 | 1:A:158:VAL:HG21 | 0.83     | 1.49        | 20     | 1     |
| 1:A:12:ILE:HD12  | 1:A:127:LYS:CG   | 0.83     | 2.04        | 13     | 1     |
| 1:A:15:PHE:CE1   | 1:A:128:LEU:HD22 | 0.82     | 2.10        | 17     | 2     |
| 1:A:153:LEU:CD1  | 1:A:158:VAL:HG21 | 0.82     | 2.05        | 20     | 10    |
| 1:A:37:LEU:HD22  | 1:A:74:MET:HE3   | 0.81     | 1.52        | 5      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:109:ALA:HB1  | 1:A:110:PRO:HD2  | 0.81     | 1.53        | 6      | 20    |
| 1:A:87:ALA:HB2   | 1:A:149:LEU:CD1  | 0.81     | 2.06        | 17     | 9     |
| 1:A:37:LEU:HD23  | 1:A:74:MET:HE3   | 0.80     | 1.50        | 10     | 1     |
| 1:A:105:ALA:HB2  | 1:A:117:TYR:CE1  | 0.80     | 2.12        | 10     | 8     |
| 1:A:12:ILE:HD11  | 1:A:127:LYS:HD3  | 0.80     | 1.53        | 17     | 2     |
| 1:A:8:SER:OG     | 1:A:48:ILE:HG22  | 0.80     | 1.77        | 10     | 2     |
| 1:A:135:LEU:CD2  | 1:A:148:THR:HG22 | 0.80     | 2.07        | 16     | 2     |
| 1:A:15:PHE:CZ    | 1:A:131:ILE:HD12 | 0.79     | 2.11        | 14     | 9     |
| 1:A:109:ALA:HB3  | 1:A:114:LYS:HG3  | 0.79     | 1.52        | 7      | 19    |
| 1:A:120:SER:O    | 1:A:124:ILE:HG22 | 0.78     | 1.78        | 4      | 4     |
| 1:A:55:ILE:CD1   | 1:A:70:THR:HG23  | 0.78     | 2.08        | 16     | 2     |
| 1:A:44:LYS:O     | 1:A:116:ILE:HD13 | 0.77     | 1.77        | 19     | 5     |
| 1:A:146:ARG:CD   | 1:A:161:LEU:HD22 | 0.77     | 2.09        | 1      | 3     |
| 1:A:153:LEU:HD13 | 1:A:158:VAL:HG21 | 0.77     | 1.57        | 1      | 2     |
| 1:A:154:GLY:O    | 1:A:158:VAL:HG23 | 0.77     | 1.80        | 20     | 16    |
| 1:A:87:ALA:CB    | 1:A:149:LEU:HD12 | 0.76     | 2.10        | 17     | 10    |
| 1:A:137:ALA:HB3  | 1:A:143:VAL:HG22 | 0.76     | 1.58        | 17     | 17    |
| 1:A:161:LEU:HD13 | 1:A:161:LEU:O    | 0.76     | 1.81        | 6      | 10    |
| 1:A:146:ARG:HG3  | 1:A:161:LEU:HD22 | 0.76     | 1.55        | 2      | 4     |
| 1:A:84:LEU:HD22  | 1:A:99:LEU:HD11  | 0.76     | 1.56        | 2      | 2     |
| 1:A:67:PRO:O     | 1:A:70:THR:HG22  | 0.76     | 1.80        | 16     | 2     |
| 1:A:89:TYR:CE1   | 1:A:153:LEU:HD22 | 0.76     | 2.16        | 9      | 3     |
| 1:A:153:LEU:HD12 | 1:A:154:GLY:N    | 0.76     | 1.96        | 19     | 8     |
| 1:A:47:ILE:HD11  | 1:A:120:SER:OG   | 0.75     | 1.80        | 20     | 5     |
| 1:A:71:PHE:CE2   | 1:A:102:ILE:HG21 | 0.74     | 2.17        | 2      | 8     |
| 1:A:100:VAL:HG21 | 1:A:149:LEU:CD2  | 0.74     | 2.09        | 1      | 1     |
| 1:A:12:ILE:HD12  | 1:A:127:LYS:HG3  | 0.74     | 1.59        | 13     | 1     |
| 1:A:35:ALA:HB2   | 1:A:85:TYR:CD2   | 0.74     | 2.18        | 13     | 7     |
| 1:A:88:THR:HG23  | 1:A:162:GLU:HG2  | 0.73     | 1.58        | 11     | 6     |
| 1:A:109:ALA:HB3  | 1:A:114:LYS:CG   | 0.73     | 2.13        | 7      | 5     |
| 1:A:60:VAL:HG21  | 1:A:162:GLU:OE2  | 0.73     | 1.84        | 10     | 1     |
| 1:A:101:PHE:CE2  | 1:A:128:LEU:HD11 | 0.73     | 2.19        | 11     | 15    |
| 1:A:139:CYS:O    | 1:A:143:VAL:HG12 | 0.72     | 1.83        | 4      | 1     |
| 1:A:68:TYR:OH    | 1:A:149:LEU:HD23 | 0.72     | 1.84        | 19     | 5     |
| 1:A:60:VAL:HG22  | 1:A:67:PRO:HD3   | 0.72     | 1.60        | 1      | 1     |
| 1:A:149:LEU:HD13 | 1:A:149:LEU:O    | 0.71     | 1.85        | 3      | 7     |
| 1:A:84:LEU:HD21  | 1:A:131:ILE:HD11 | 0.71     | 1.60        | 18     | 6     |
| 1:A:72:VAL:HG11  | 1:A:144:LYS:HB2  | 0.71     | 1.62        | 18     | 4     |
| 1:A:5:VAL:HG11   | 1:A:120:SER:HB2  | 0.71     | 1.61        | 12     | 5     |
| 1:A:85:TYR:O     | 1:A:100:VAL:HG12 | 0.71     | 1.85        | 19     | 1     |
| 1:A:72:VAL:HG11  | 1:A:144:LYS:CD   | 0.71     | 2.15        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:40:LEU:CD2   | 1:A:47:ILE:HD13  | 0.71     | 2.16        | 20     | 7     |
| 1:A:109:ALA:HB3  | 1:A:114:LYS:HG2  | 0.71     | 1.61        | 3      | 1     |
| 1:A:47:ILE:CG2   | 1:A:124:ILE:HD12 | 0.70     | 2.15        | 19     | 3     |
| 1:A:37:LEU:CD2   | 1:A:74:MET:HE3   | 0.70     | 2.15        | 5      | 1     |
| 1:A:18:MET:SD    | 1:A:99:LEU:HD11  | 0.70     | 2.26        | 12     | 2     |
| 1:A:162:GLU:HB2  | 1:A:165:PRO:HG3  | 0.70     | 1.62        | 2      | 20    |
| 1:A:8:SER:HB2    | 1:A:48:ILE:HG22  | 0.70     | 1.63        | 3      | 8     |
| 1:A:59:ASP:HB3   | 1:A:64:VAL:HG21  | 0.70     | 1.63        | 10     | 3     |
| 1:A:8:SER:HB3    | 1:A:48:ILE:HG22  | 0.70     | 1.63        | 11     | 6     |
| 1:A:72:VAL:HG22  | 1:A:143:VAL:HG12 | 0.70     | 1.63        | 1      | 4     |
| 1:A:18:MET:HE1   | 1:A:84:LEU:O     | 0.70     | 1.86        | 20     | 2     |
| 1:A:104:TRP:CZ3  | 1:A:143:VAL:HG21 | 0.70     | 2.22        | 1      | 13    |
| 1:A:87:ALA:HB1   | 1:A:161:LEU:HD11 | 0.70     | 1.63        | 8      | 3     |
| 1:A:57:VAL:O     | 1:A:60:VAL:HG23  | 0.69     | 1.86        | 13     | 6     |
| 1:A:8:SER:CB     | 1:A:48:ILE:HG22  | 0.69     | 2.17        | 12     | 12    |
| 1:A:89:TYR:CE1   | 1:A:153:LEU:HD13 | 0.69     | 2.22        | 10     | 3     |
| 1:A:100:VAL:HG11 | 1:A:152:LYS:HG2  | 0.69     | 1.64        | 14     | 3     |
| 1:A:75:LEU:HD22  | 1:A:143:VAL:HG11 | 0.69     | 1.63        | 5      | 6     |
| 1:A:137:ALA:HB1  | 1:A:142:GLU:HB2  | 0.69     | 1.64        | 17     | 13    |
| 1:A:18:MET:HE3   | 1:A:33:LYS:CG    | 0.69     | 2.17        | 15     | 1     |
| 1:A:135:LEU:HD12 | 1:A:149:LEU:HD22 | 0.69     | 1.62        | 3      | 4     |
| 1:A:60:VAL:HG22  | 1:A:67:PRO:HG2   | 0.69     | 1.64        | 4      | 1     |
| 1:A:87:ALA:HB3   | 1:A:153:LEU:HD21 | 0.68     | 1.63        | 16     | 3     |
| 1:A:40:LEU:HD13  | 1:A:44:LYS:HG3   | 0.68     | 1.66        | 12     | 1     |
| 1:A:23:SER:CB    | 1:A:29:VAL:HG12  | 0.68     | 2.19        | 1      | 6     |
| 1:A:100:VAL:HG12 | 1:A:133:HIS:HB2  | 0.68     | 1.64        | 5      | 5     |
| 1:A:18:MET:HE3   | 1:A:84:LEU:O     | 0.67     | 1.89        | 10     | 5     |
| 1:A:18:MET:HE1   | 1:A:86:ASP:HB2   | 0.67     | 1.67        | 9      | 2     |
| 1:A:111:LEU:O    | 1:A:111:LEU:HD23 | 0.67     | 1.89        | 8      | 3     |
| 1:A:75:LEU:HD22  | 1:A:104:TRP:CD1  | 0.67     | 2.25        | 7      | 1     |
| 1:A:59:ASP:CB    | 1:A:64:VAL:HG21  | 0.67     | 2.20        | 10     | 1     |
| 1:A:5:VAL:CG1    | 1:A:47:ILE:HD11  | 0.66     | 2.21        | 4      | 1     |
| 1:A:111:LEU:HD11 | 1:A:115:MET:HE2  | 0.66     | 1.67        | 19     | 1     |
| 1:A:106:PRO:HG2  | 1:A:109:ALA:HB2  | 0.66     | 1.67        | 1      | 9     |
| 1:A:100:VAL:HG12 | 1:A:133:HIS:CB   | 0.66     | 2.20        | 5      | 4     |
| 1:A:16:ASN:O     | 1:A:20:VAL:HG22  | 0.66     | 1.89        | 3      | 3     |
| 1:A:47:ILE:HG21  | 1:A:124:ILE:CD1  | 0.66     | 2.21        | 15     | 4     |
| 1:A:87:ALA:HB1   | 1:A:153:LEU:HD11 | 0.65     | 1.68        | 6      | 4     |
| 1:A:72:VAL:HG21  | 1:A:144:LYS:HD3  | 0.65     | 1.66        | 15     | 2     |
| 1:A:62:GLN:OE1   | 1:A:63:THR:HG22  | 0.65     | 1.91        | 20     | 1     |
| 1:A:18:MET:O     | 1:A:99:LEU:HD21  | 0.65     | 1.91        | 13     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:87:ALA:HB2   | 1:A:149:LEU:HD11 | 0.65     | 1.68        | 3      | 2     |
| 1:A:139:CYS:O    | 1:A:143:VAL:HG23 | 0.65     | 1.91        | 12     | 9     |
| 1:A:149:LEU:HD22 | 1:A:152:LYS:HE2  | 0.65     | 1.67        | 1      | 1     |
| 1:A:102:ILE:HD11 | 1:A:149:LEU:HD21 | 0.64     | 1.68        | 7      | 2     |
| 1:A:87:ALA:HB3   | 1:A:149:LEU:CD1  | 0.64     | 2.21        | 2      | 1     |
| 1:A:5:VAL:HG13   | 1:A:47:ILE:HG12  | 0.64     | 1.69        | 10     | 1     |
| 1:A:134:GLU:O    | 1:A:135:LEU:HD12 | 0.64     | 1.92        | 16     | 1     |
| 1:A:146:ARG:CG   | 1:A:161:LEU:HD22 | 0.64     | 2.23        | 19     | 2     |
| 1:A:75:LEU:HD13  | 1:A:104:TRP:CE2  | 0.64     | 2.28        | 12     | 5     |
| 1:A:20:VAL:HG23  | 1:A:22:LYS:HG2   | 0.64     | 1.68        | 2      | 1     |
| 1:A:104:TRP:CH2  | 1:A:143:VAL:HG11 | 0.64     | 2.27        | 4      | 1     |
| 1:A:72:VAL:HG22  | 1:A:140:TYR:CE2  | 0.64     | 2.26        | 9      | 4     |
| 1:A:150:ALA:HB2  | 1:A:161:LEU:HD23 | 0.64     | 1.69        | 5      | 3     |
| 1:A:100:VAL:HG11 | 1:A:152:LYS:CG   | 0.64     | 2.23        | 14     | 3     |
| 1:A:18:MET:HE2   | 1:A:33:LYS:HG3   | 0.64     | 1.68        | 13     | 1     |
| 1:A:128:LEU:HD12 | 1:A:131:ILE:HG21 | 0.64     | 1.70        | 3      | 1     |
| 1:A:84:LEU:HD22  | 1:A:99:LEU:CD1   | 0.63     | 2.24        | 9      | 2     |
| 1:A:5:VAL:HG13   | 1:A:123:ALA:CB   | 0.63     | 2.24        | 3      | 5     |
| 1:A:5:VAL:CG1    | 1:A:40:LEU:HD11  | 0.63     | 2.23        | 6      | 2     |
| 1:A:49:LEU:N     | 1:A:49:LEU:HD13  | 0.63     | 2.09        | 6      | 2     |
| 1:A:84:LEU:HD22  | 1:A:99:LEU:HD22  | 0.63     | 1.71        | 11     | 1     |
| 1:A:5:VAL:HG11   | 1:A:40:LEU:HD21  | 0.63     | 1.71        | 6      | 1     |
| 1:A:36:VAL:HG23  | 1:A:38:PHE:CE1   | 0.63     | 2.29        | 18     | 3     |
| 1:A:75:LEU:HD13  | 1:A:104:TRP:CD1  | 0.63     | 2.28        | 18     | 3     |
| 1:A:57:VAL:O     | 1:A:60:VAL:HG12  | 0.63     | 1.94        | 15     | 4     |
| 1:A:7:VAL:HG13   | 1:A:11:VAL:HG21  | 0.62     | 1.69        | 16     | 14    |
| 1:A:161:LEU:N    | 1:A:166:LEU:HB2  | 0.62     | 2.09        | 14     | 13    |
| 1:A:100:VAL:HG21 | 1:A:149:LEU:HD11 | 0.62     | 1.72        | 16     | 1     |
| 1:A:100:VAL:HG11 | 1:A:149:LEU:CD2  | 0.62     | 2.10        | 12     | 1     |
| 1:A:7:VAL:HG21   | 1:A:127:LYS:HG3  | 0.62     | 1.70        | 8      | 6     |
| 1:A:75:LEU:HD12  | 1:A:143:VAL:HG11 | 0.62     | 1.71        | 9      | 4     |
| 1:A:60:VAL:HG22  | 1:A:67:PRO:HG3   | 0.62     | 1.71        | 13     | 1     |
| 1:A:12:ILE:HD12  | 1:A:127:LYS:HG2  | 0.62     | 1.72        | 13     | 1     |
| 1:A:15:PHE:CE1   | 1:A:131:ILE:HD12 | 0.62     | 2.29        | 11     | 3     |
| 1:A:75:LEU:CD2   | 1:A:143:VAL:HG11 | 0.61     | 2.24        | 19     | 6     |
| 1:A:18:MET:HE1   | 1:A:86:ASP:OD2   | 0.61     | 1.95        | 6      | 1     |
| 1:A:84:LEU:HD21  | 1:A:131:ILE:CD1  | 0.61     | 2.25        | 2      | 9     |
| 1:A:10:GLY:HA2   | 1:A:13:LYS:HB2   | 0.61     | 1.70        | 18     | 6     |
| 1:A:84:LEU:HD11  | 1:A:131:ILE:CD1  | 0.61     | 2.25        | 4      | 1     |
| 1:A:18:MET:HE1   | 1:A:86:ASP:OD1   | 0.61     | 1.96        | 1      | 4     |
| 1:A:100:VAL:CG2  | 1:A:149:LEU:HD21 | 0.61     | 2.13        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:7:VAL:HG13   | 1:A:11:VAL:CG2   | 0.61     | 2.26        | 16     | 5     |
| 1:A:153:LEU:HD11 | 1:A:158:VAL:HG21 | 0.61     | 1.72        | 15     | 2     |
| 1:A:84:LEU:HB3   | 1:A:99:LEU:HD11  | 0.61     | 1.72        | 15     | 1     |
| 1:A:72:VAL:HG12  | 1:A:140:TYR:CE2  | 0.61     | 2.30        | 16     | 11    |
| 1:A:40:LEU:CD1   | 1:A:47:ILE:HD13  | 0.61     | 2.26        | 10     | 1     |
| 1:A:37:LEU:HD21  | 1:A:75:LEU:CD1   | 0.61     | 2.25        | 15     | 1     |
| 1:A:32:ARG:NH1   | 1:A:57:VAL:HG11  | 0.61     | 2.10        | 19     | 2     |
| 1:A:5:VAL:HG21   | 1:A:47:ILE:CD1   | 0.61     | 2.26        | 17     | 2     |
| 1:A:71:PHE:CZ    | 1:A:75:LEU:HD11  | 0.61     | 2.31        | 10     | 12    |
| 1:A:135:LEU:CD1  | 1:A:149:LEU:HD22 | 0.61     | 2.26        | 3      | 3     |
| 1:A:5:VAL:HG11   | 1:A:120:SER:CB   | 0.61     | 2.25        | 3      | 4     |
| 1:A:25:THR:HG22  | 1:A:26:PRO:HD3   | 0.60     | 1.73        | 4      | 18    |
| 1:A:60:VAL:HG23  | 1:A:67:PRO:HG3   | 0.60     | 1.73        | 10     | 3     |
| 1:A:153:LEU:HD21 | 1:A:161:LEU:CD2  | 0.60     | 2.26        | 13     | 2     |
| 1:A:15:PHE:CD1   | 1:A:84:LEU:HD13  | 0.60     | 2.32        | 1      | 2     |
| 1:A:75:LEU:HD13  | 1:A:104:TRP:NE1  | 0.60     | 2.12        | 8      | 5     |
| 1:A:18:MET:CE    | 1:A:99:LEU:HD11  | 0.60     | 2.26        | 16     | 1     |
| 1:A:150:ALA:HB2  | 1:A:161:LEU:CD2  | 0.60     | 2.25        | 16     | 2     |
| 1:A:88:THR:HG23  | 1:A:162:GLU:CG   | 0.59     | 2.26        | 11     | 3     |
| 1:A:40:LEU:HD22  | 1:A:47:ILE:HD13  | 0.59     | 1.74        | 20     | 2     |
| 1:A:89:TYR:HE1   | 1:A:153:LEU:HD22 | 0.59     | 1.58        | 3      | 2     |
| 1:A:86:ASP:OD2   | 1:A:99:LEU:HD13  | 0.59     | 1.97        | 14     | 1     |
| 1:A:33:LYS:HA    | 1:A:56:LEU:HD23  | 0.59     | 1.74        | 17     | 9     |
| 1:A:146:ARG:HD2  | 1:A:161:LEU:HD22 | 0.59     | 1.72        | 3      | 3     |
| 1:A:57:VAL:HG22  | 1:A:57:VAL:O     | 0.59     | 1.97        | 3      | 2     |
| 1:A:18:MET:HE2   | 1:A:33:LYS:O     | 0.59     | 1.98        | 3      | 2     |
| 1:A:135:LEU:HD13 | 1:A:149:LEU:HD22 | 0.59     | 1.75        | 7      | 2     |
| 1:A:87:ALA:HB1   | 1:A:153:LEU:HD22 | 0.59     | 1.74        | 17     | 1     |
| 1:A:7:VAL:HG13   | 1:A:47:ILE:HB    | 0.59     | 1.73        | 10     | 1     |
| 1:A:5:VAL:HG22   | 1:A:47:ILE:HG12  | 0.58     | 1.74        | 16     | 8     |
| 1:A:11:VAL:HG21  | 1:A:47:ILE:HG22  | 0.58     | 1.75        | 8      | 6     |
| 1:A:72:VAL:HG11  | 1:A:144:LYS:HD3  | 0.58     | 1.75        | 8      | 1     |
| 1:A:34:LYS:HE3   | 1:A:88:THR:HG22  | 0.58     | 1.73        | 13     | 1     |
| 1:A:15:PHE:CD1   | 1:A:128:LEU:HD22 | 0.58     | 2.33        | 17     | 2     |
| 1:A:109:ALA:HB1  | 1:A:110:PRO:CD   | 0.58     | 2.29        | 14     | 13    |
| 1:A:104:TRP:CZ3  | 1:A:143:VAL:HG11 | 0.58     | 2.34        | 4      | 1     |
| 1:A:72:VAL:HG22  | 1:A:140:TYR:CD2  | 0.57     | 2.34        | 7      | 3     |
| 1:A:5:VAL:HG21   | 1:A:47:ILE:HD11  | 0.57     | 1.75        | 1      | 4     |
| 1:A:5:VAL:HG13   | 1:A:123:ALA:HB3  | 0.57     | 1.75        | 3      | 2     |
| 1:A:37:LEU:HD11  | 1:A:75:LEU:CD1   | 0.57     | 2.28        | 14     | 4     |
| 1:A:72:VAL:HG21  | 1:A:144:LYS:HB2  | 0.57     | 1.76        | 12     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:87:ALA:HB1   | 1:A:153:LEU:CD2  | 0.57     | 2.28        | 17     | 3     |
| 1:A:5:VAL:O      | 1:A:5:VAL:HG12   | 0.57     | 1.98        | 4      | 2     |
| 1:A:60:VAL:HG13  | 1:A:67:PRO:HG3   | 0.57     | 1.76        | 8      | 2     |
| 1:A:60:VAL:HG22  | 1:A:67:PRO:CG    | 0.57     | 2.29        | 13     | 1     |
| 1:A:99:LEU:C     | 1:A:99:LEU:HD13  | 0.57     | 2.24        | 2      | 1     |
| 1:A:7:VAL:HG22   | 1:A:47:ILE:HB    | 0.57     | 1.74        | 18     | 5     |
| 1:A:89:TYR:HB2   | 1:A:158:VAL:HG13 | 0.57     | 1.76        | 20     | 2     |
| 1:A:14:VAL:HB    | 1:A:49:LEU:HD13  | 0.57     | 1.77        | 19     | 6     |
| 1:A:14:VAL:CB    | 1:A:49:LEU:HD13  | 0.56     | 2.30        | 1      | 5     |
| 1:A:135:LEU:HD22 | 1:A:149:LEU:CD2  | 0.56     | 2.24        | 6      | 2     |
| 1:A:84:LEU:HD21  | 1:A:131:ILE:HD13 | 0.56     | 1.76        | 2      | 2     |
| 1:A:153:LEU:C    | 1:A:153:LEU:HD12 | 0.56     | 2.26        | 15     | 1     |
| 1:A:116:ILE:O    | 1:A:120:SER:N    | 0.56     | 2.37        | 7      | 17    |
| 1:A:18:MET:SD    | 1:A:99:LEU:HD21  | 0.56     | 2.40        | 3      | 1     |
| 1:A:88:THR:HG23  | 1:A:88:THR:O     | 0.56     | 2.00        | 10     | 11    |
| 1:A:60:VAL:HG21  | 1:A:162:GLU:OE1  | 0.56     | 2.01        | 5      | 1     |
| 1:A:25:THR:HG22  | 1:A:26:PRO:CD    | 0.56     | 2.30        | 12     | 5     |
| 1:A:18:MET:HE3   | 1:A:33:LYS:HG3   | 0.56     | 1.76        | 15     | 3     |
| 1:A:103:PHE:HB2  | 1:A:135:LEU:O    | 0.56     | 1.99        | 19     | 1     |
| 1:A:60:VAL:HG22  | 1:A:67:PRO:CD    | 0.56     | 2.30        | 1      | 1     |
| 1:A:40:LEU:HD23  | 1:A:117:TYR:CE1  | 0.56     | 2.35        | 15     | 2     |
| 1:A:12:ILE:N     | 1:A:12:ILE:HD12  | 0.56     | 2.15        | 4      | 2     |
| 1:A:5:VAL:HG12   | 1:A:45:LYS:C     | 0.56     | 2.24        | 6      | 1     |
| 1:A:49:LEU:HD12  | 1:A:49:LEU:O     | 0.56     | 2.01        | 12     | 1     |
| 1:A:128:LEU:N    | 1:A:128:LEU:HD23 | 0.56     | 2.15        | 19     | 1     |
| 1:A:75:LEU:N     | 1:A:76:PRO:HD3   | 0.56     | 2.15        | 18     | 18    |
| 1:A:161:LEU:H    | 1:A:166:LEU:HB2  | 0.56     | 1.61        | 14     | 15    |
| 1:A:18:MET:HE3   | 1:A:33:LYS:O     | 0.56     | 2.00        | 6      | 4     |
| 1:A:131:ILE:HG23 | 1:A:131:ILE:O    | 0.56     | 2.01        | 15     | 4     |
| 1:A:18:MET:SD    | 1:A:99:LEU:HD13  | 0.56     | 2.41        | 9      | 1     |
| 1:A:72:VAL:HG12  | 1:A:140:TYR:CD2  | 0.56     | 2.36        | 3      | 8     |
| 1:A:12:ILE:HD13  | 1:A:127:LYS:HB3  | 0.56     | 1.77        | 6      | 1     |
| 1:A:15:PHE:CD2   | 1:A:128:LEU:HD22 | 0.56     | 2.36        | 16     | 2     |
| 1:A:160:SER:HA   | 1:A:166:LEU:CB   | 0.55     | 2.32        | 10     | 20    |
| 1:A:37:LEU:HD12  | 1:A:83:ALA:HB2   | 0.55     | 1.77        | 16     | 4     |
| 1:A:5:VAL:HG11   | 1:A:40:LEU:HD11  | 0.55     | 1.78        | 6      | 1     |
| 1:A:100:VAL:HG21 | 1:A:135:LEU:HD12 | 0.55     | 1.77        | 10     | 3     |
| 1:A:59:ASP:HB2   | 1:A:64:VAL:HG21  | 0.55     | 1.77        | 20     | 1     |
| 1:A:36:VAL:O     | 1:A:83:ALA:HB1   | 0.54     | 2.03        | 13     | 2     |
| 1:A:84:LEU:HD22  | 1:A:99:LEU:CG    | 0.54     | 2.32        | 9      | 1     |
| 1:A:11:VAL:HA    | 1:A:49:LEU:HD12  | 0.54     | 1.78        | 9      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:62:GLN:HG3   | 1:A:63:THR:HG22  | 0.54     | 1.78        | 11     | 1     |
| 1:A:32:ARG:O     | 1:A:56:LEU:HD22  | 0.54     | 2.02        | 19     | 1     |
| 1:A:37:LEU:HD21  | 1:A:71:PHE:CE2   | 0.54     | 2.37        | 12     | 1     |
| 1:A:18:MET:HE1   | 1:A:99:LEU:HD11  | 0.54     | 1.79        | 16     | 1     |
| 1:A:87:ALA:HB1   | 1:A:153:LEU:HD23 | 0.54     | 1.80        | 19     | 1     |
| 1:A:111:LEU:O    | 1:A:111:LEU:HD13 | 0.54     | 2.03        | 16     | 3     |
| 1:A:87:ALA:CB    | 1:A:153:LEU:HD11 | 0.54     | 2.33        | 9      | 2     |
| 1:A:84:LEU:HD22  | 1:A:99:LEU:HD21  | 0.54     | 1.78        | 15     | 1     |
| 1:A:164:LYS:N    | 1:A:165:PRO:HD2  | 0.54     | 2.18        | 2      | 20    |
| 1:A:49:LEU:HD22  | 1:A:49:LEU:O     | 0.54     | 2.03        | 9      | 2     |
| 1:A:18:MET:O     | 1:A:99:LEU:HD22  | 0.54     | 2.02        | 16     | 1     |
| 1:A:160:SER:HA   | 1:A:166:LEU:HB2  | 0.53     | 1.79        | 13     | 18    |
| 1:A:82:TYR:CE1   | 1:A:117:TYR:CE2  | 0.53     | 2.96        | 11     | 9     |
| 1:A:55:ILE:HD11  | 1:A:74:MET:HE2   | 0.53     | 1.80        | 10     | 4     |
| 1:A:164:LYS:HG3  | 1:A:165:PRO:N    | 0.53     | 2.19        | 14     | 20    |
| 1:A:87:ALA:HB3   | 1:A:149:LEU:HD11 | 0.53     | 1.79        | 2      | 1     |
| 1:A:72:VAL:HG11  | 1:A:144:LYS:HD2  | 0.53     | 1.78        | 8      | 1     |
| 1:A:101:PHE:HB2  | 1:A:131:ILE:HD13 | 0.53     | 1.79        | 17     | 1     |
| 1:A:23:SER:HB3   | 1:A:29:VAL:HG12  | 0.53     | 1.80        | 2      | 4     |
| 1:A:82:TYR:O     | 1:A:83:ALA:HB2   | 0.53     | 2.04        | 20     | 5     |
| 1:A:12:ILE:HD12  | 1:A:127:LYS:HD3  | 0.53     | 1.79        | 12     | 1     |
| 1:A:40:LEU:HD23  | 1:A:117:TYR:CD1  | 0.53     | 2.38        | 15     | 2     |
| 1:A:137:ALA:CB   | 1:A:143:VAL:HG22 | 0.53     | 2.33        | 19     | 7     |
| 1:A:7:VAL:CG1    | 1:A:11:VAL:HG21  | 0.53     | 2.32        | 10     | 1     |
| 1:A:40:LEU:HD22  | 1:A:44:LYS:HA    | 0.53     | 1.80        | 12     | 1     |
| 1:A:18:MET:HE3   | 1:A:33:LYS:HG2   | 0.53     | 1.80        | 15     | 1     |
| 1:A:82:TYR:CD2   | 1:A:124:ILE:HD13 | 0.53     | 2.39        | 19     | 1     |
| 1:A:75:LEU:N     | 1:A:76:PRO:CD    | 0.53     | 2.72        | 18     | 16    |
| 1:A:5:VAL:HG13   | 1:A:47:ILE:HD11  | 0.53     | 1.79        | 4      | 1     |
| 1:A:12:ILE:HD11  | 1:A:127:LYS:HD2  | 0.53     | 1.75        | 20     | 1     |
| 1:A:60:VAL:HG12  | 1:A:60:VAL:O     | 0.53     | 2.04        | 8      | 1     |
| 1:A:100:VAL:O    | 1:A:100:VAL:HG13 | 0.53     | 2.04        | 12     | 6     |
| 1:A:36:VAL:HG23  | 1:A:36:VAL:O     | 0.52     | 2.05        | 5      | 2     |
| 1:A:37:LEU:HD21  | 1:A:75:LEU:HD11  | 0.52     | 1.81        | 15     | 1     |
| 1:A:135:LEU:HD11 | 1:A:152:LYS:NZ   | 0.52     | 2.19        | 1      | 1     |
| 1:A:31:LYS:O     | 1:A:56:LEU:HD22  | 0.52     | 2.04        | 13     | 2     |
| 1:A:114:LYS:NZ   | 1:A:118:ALA:HB2  | 0.52     | 2.19        | 10     | 1     |
| 1:A:37:LEU:HD12  | 1:A:74:MET:HE3   | 0.52     | 1.80        | 15     | 1     |
| 1:A:149:LEU:HD13 | 1:A:152:LYS:HD2  | 0.52     | 1.80        | 19     | 2     |
| 1:A:40:LEU:HD12  | 1:A:44:LYS:HA    | 0.52     | 1.81        | 6      | 3     |
| 1:A:89:TYR:CG    | 1:A:153:LEU:HD22 | 0.52     | 2.40        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:160:SER:C    | 1:A:166:LEU:HD12 | 0.52     | 2.29        | 11     | 4     |
| 1:A:116:ILE:HG22 | 1:A:116:ILE:O    | 0.52     | 2.05        | 15     | 2     |
| 1:A:131:ILE:HG23 | 1:A:132:LYS:H    | 0.52     | 1.64        | 11     | 1     |
| 1:A:88:THR:HG23  | 1:A:162:GLU:CD   | 0.52     | 2.29        | 13     | 1     |
| 1:A:71:PHE:CZ    | 1:A:102:ILE:HG21 | 0.52     | 2.39        | 1      | 5     |
| 1:A:153:LEU:HD12 | 1:A:154:GLY:H    | 0.52     | 1.64        | 1      | 1     |
| 1:A:87:ALA:CB    | 1:A:149:LEU:HD11 | 0.52     | 2.35        | 3      | 1     |
| 1:A:146:ARG:HG2  | 1:A:161:LEU:CB   | 0.52     | 2.35        | 20     | 4     |
| 1:A:60:VAL:HG21  | 1:A:162:GLU:CD   | 0.52     | 2.29        | 10     | 1     |
| 1:A:66:ASP:HB3   | 1:A:69:ALA:HB3   | 0.51     | 1.82        | 13     | 1     |
| 1:A:89:TYR:CD2   | 1:A:153:LEU:HD13 | 0.51     | 2.40        | 17     | 1     |
| 1:A:18:MET:HE1   | 1:A:86:ASP:CB    | 0.51     | 2.36        | 2      | 1     |
| 1:A:76:PRO:O     | 1:A:104:TRP:NE1  | 0.51     | 2.43        | 3      | 16    |
| 1:A:72:VAL:HG22  | 1:A:143:VAL:CG1  | 0.51     | 2.34        | 16     | 4     |
| 1:A:153:LEU:HD21 | 1:A:161:LEU:HD21 | 0.51     | 1.80        | 13     | 3     |
| 1:A:82:TYR:CZ    | 1:A:117:TYR:CD2  | 0.51     | 2.97        | 14     | 6     |
| 1:A:40:LEU:HD22  | 1:A:44:LYS:CA    | 0.51     | 2.34        | 12     | 1     |
| 1:A:105:ALA:HB2  | 1:A:117:TYR:HE1  | 0.51     | 1.58        | 3      | 3     |
| 1:A:48:ILE:HD12  | 1:A:48:ILE:C     | 0.51     | 2.30        | 9      | 4     |
| 1:A:149:LEU:HA   | 1:A:152:LYS:HE2  | 0.51     | 1.80        | 1      | 1     |
| 1:A:20:VAL:HG23  | 1:A:22:LYS:CG    | 0.51     | 2.36        | 2      | 1     |
| 1:A:85:TYR:O     | 1:A:100:VAL:HG22 | 0.51     | 2.05        | 6      | 1     |
| 1:A:82:TYR:CE1   | 1:A:103:PHE:CE2  | 0.51     | 2.99        | 5      | 1     |
| 1:A:60:VAL:HG13  | 1:A:67:PRO:HD3   | 0.51     | 1.83        | 9      | 1     |
| 1:A:59:ASP:CG    | 1:A:64:VAL:HG21  | 0.51     | 2.31        | 10     | 1     |
| 1:A:37:LEU:HD11  | 1:A:75:LEU:HD12  | 0.51     | 1.82        | 15     | 2     |
| 1:A:101:PHE:CE1  | 1:A:103:PHE:CE1  | 0.51     | 2.99        | 19     | 1     |
| 1:A:5:VAL:O      | 1:A:5:VAL:HG13   | 0.50     | 2.06        | 19     | 4     |
| 1:A:114:LYS:HZ1  | 1:A:118:ALA:HB2  | 0.50     | 1.66        | 10     | 1     |
| 1:A:149:LEU:HD22 | 1:A:152:LYS:CE   | 0.50     | 2.36        | 1      | 1     |
| 1:A:86:ASP:OD1   | 1:A:99:LEU:HD12  | 0.50     | 2.05        | 10     | 1     |
| 1:A:84:LEU:HD23  | 1:A:101:PHE:N    | 0.50     | 2.22        | 12     | 2     |
| 1:A:82:TYR:CD1   | 1:A:117:TYR:CE2  | 0.50     | 2.99        | 3      | 4     |
| 1:A:68:TYR:CD2   | 1:A:85:TYR:CZ    | 0.50     | 3.00        | 11     | 1     |
| 1:A:25:THR:O     | 1:A:29:VAL:HG22  | 0.50     | 2.05        | 18     | 2     |
| 1:A:8:SER:O      | 1:A:9:ASP:CB     | 0.50     | 2.59        | 16     | 4     |
| 1:A:146:ARG:HG3  | 1:A:161:LEU:HD13 | 0.50     | 1.83        | 1      | 1     |
| 1:A:135:LEU:HD21 | 1:A:148:THR:HG22 | 0.50     | 1.79        | 16     | 1     |
| 1:A:75:LEU:CD2   | 1:A:104:TRP:CD1  | 0.49     | 2.95        | 7      | 4     |
| 1:A:75:LEU:HD13  | 1:A:104:TRP:CG   | 0.49     | 2.43        | 7      | 3     |
| 1:A:100:VAL:HG11 | 1:A:152:LYS:CB   | 0.49     | 2.36        | 8      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:82:TYR:CE2   | 1:A:117:TYR:CZ   | 0.49     | 3.01        | 19     | 1     |
| 1:A:82:TYR:CE1   | 1:A:117:TYR:CD2  | 0.49     | 3.00        | 20     | 4     |
| 1:A:146:ARG:HG3  | 1:A:161:LEU:HG   | 0.49     | 1.83        | 8      | 8     |
| 1:A:14:VAL:CG2   | 1:A:36:VAL:HG11  | 0.49     | 2.37        | 18     | 2     |
| 1:A:23:SER:HB2   | 1:A:29:VAL:HG12  | 0.49     | 1.84        | 1      | 5     |
| 1:A:82:TYR:CE2   | 1:A:117:TYR:CE2  | 0.49     | 3.00        | 1      | 2     |
| 1:A:5:VAL:HG13   | 1:A:47:ILE:CD1   | 0.49     | 2.37        | 4      | 1     |
| 1:A:75:LEU:HD23  | 1:A:104:TRP:CD2  | 0.49     | 2.43        | 5      | 1     |
| 1:A:82:TYR:CZ    | 1:A:117:TYR:CE2  | 0.49     | 3.00        | 1      | 3     |
| 1:A:146:ARG:O    | 1:A:161:LEU:HD13 | 0.49     | 2.08        | 1      | 1     |
| 1:A:37:LEU:HD11  | 1:A:75:LEU:HD11  | 0.49     | 1.84        | 2      | 1     |
| 1:A:84:LEU:CD2   | 1:A:99:LEU:HD11  | 0.49     | 2.33        | 2      | 1     |
| 1:A:75:LEU:CD1   | 1:A:104:TRP:CG   | 0.49     | 2.96        | 7      | 3     |
| 1:A:104:TRP:CH2  | 1:A:143:VAL:HG21 | 0.49     | 2.43        | 12     | 1     |
| 1:A:82:TYR:CD2   | 1:A:117:TYR:CE2  | 0.49     | 3.01        | 19     | 1     |
| 1:A:25:THR:CB    | 1:A:26:PRO:CD    | 0.49     | 2.91        | 20     | 20    |
| 1:A:7:VAL:HG11   | 1:A:127:LYS:HG3  | 0.49     | 1.84        | 10     | 1     |
| 1:A:146:ARG:HG2  | 1:A:165:PRO:HB2  | 0.49     | 1.84        | 13     | 7     |
| 1:A:149:LEU:CD1  | 1:A:152:LYS:HZ2  | 0.49     | 2.20        | 8      | 1     |
| 1:A:154:GLY:C    | 1:A:158:VAL:HG23 | 0.49     | 2.32        | 16     | 1     |
| 1:A:5:VAL:HG13   | 1:A:40:LEU:HD11  | 0.49     | 1.85        | 9      | 1     |
| 1:A:15:PHE:HE2   | 1:A:131:ILE:HD12 | 0.49     | 1.67        | 13     | 1     |
| 1:A:159:ILE:HG23 | 1:A:160:SER:N    | 0.49     | 2.22        | 20     | 1     |
| 1:A:100:VAL:HG23 | 1:A:100:VAL:O    | 0.49     | 2.06        | 1      | 1     |
| 1:A:84:LEU:HD23  | 1:A:101:PHE:HA   | 0.48     | 1.83        | 16     | 2     |
| 1:A:11:VAL:CG2   | 1:A:47:ILE:HG22  | 0.48     | 2.36        | 8      | 3     |
| 1:A:135:LEU:HD23 | 1:A:148:THR:HG22 | 0.48     | 1.83        | 16     | 1     |
| 1:A:110:PRO:O    | 1:A:114:LYS:HB2  | 0.48     | 2.08        | 3      | 3     |
| 1:A:72:VAL:HG21  | 1:A:144:LYS:CB   | 0.48     | 2.38        | 12     | 2     |
| 1:A:8:SER:HG     | 1:A:48:ILE:HG22  | 0.48     | 1.66        | 10     | 1     |
| 1:A:15:PHE:CE1   | 1:A:84:LEU:HD13  | 0.48     | 2.43        | 1      | 1     |
| 1:A:55:ILE:HD13  | 1:A:70:THR:HB    | 0.48     | 1.85        | 14     | 2     |
| 1:A:27:GLU:O     | 1:A:27:GLU:CG    | 0.48     | 2.61        | 20     | 11    |
| 1:A:131:ILE:HG23 | 1:A:132:LYS:N    | 0.48     | 2.24        | 6      | 1     |
| 1:A:75:LEU:CD1   | 1:A:104:TRP:CE2  | 0.48     | 2.96        | 12     | 3     |
| 1:A:104:TRP:HA   | 1:A:104:TRP:CE3  | 0.48     | 2.43        | 12     | 3     |
| 1:A:140:TYR:HA   | 1:A:143:VAL:HG13 | 0.48     | 1.85        | 4      | 1     |
| 1:A:152:LYS:CE   | 1:A:153:LEU:HD23 | 0.48     | 2.38        | 16     | 1     |
| 1:A:25:THR:HB    | 1:A:26:PRO:CD    | 0.48     | 2.38        | 17     | 12    |
| 1:A:149:LEU:HD13 | 1:A:149:LEU:C    | 0.48     | 2.33        | 3      | 1     |
| 1:A:161:LEU:N    | 1:A:166:LEU:HD12 | 0.48     | 2.24        | 20     | 4     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:161:LEU:O    | 1:A:161:LEU:CD1 | 0.48     | 2.61        | 20     | 6     |
| 1:A:37:LEU:HD21  | 1:A:75:LEU:HD23 | 0.48     | 1.84        | 18     | 1     |
| 1:A:40:LEU:HD22  | 1:A:44:LYS:C    | 0.47     | 2.34        | 12     | 1     |
| 1:A:72:VAL:CG1   | 1:A:140:TYR:CD2 | 0.47     | 2.97        | 5      | 9     |
| 1:A:37:LEU:HD11  | 1:A:75:LEU:CD2  | 0.47     | 2.39        | 8      | 1     |
| 1:A:47:ILE:HD12  | 1:A:82:TYR:CE2  | 0.47     | 2.44        | 10     | 1     |
| 1:A:99:LEU:HD22  | 1:A:100:VAL:N   | 0.47     | 2.24        | 2      | 1     |
| 1:A:71:PHE:CE2   | 1:A:75:LEU:CD2  | 0.47     | 2.97        | 6      | 11    |
| 1:A:104:TRP:CZ3  | 1:A:143:VAL:CG2 | 0.47     | 2.97        | 7      | 12    |
| 1:A:103:PHE:CE2  | 1:A:121:LYS:CB  | 0.47     | 2.97        | 3      | 2     |
| 1:A:35:ALA:CB    | 1:A:85:TYR:CD2  | 0.47     | 2.98        | 15     | 4     |
| 1:A:71:PHE:CE1   | 1:A:75:LEU:CD1  | 0.47     | 2.97        | 5      | 3     |
| 1:A:47:ILE:O     | 1:A:48:ILE:HG23 | 0.47     | 2.10        | 6      | 2     |
| 1:A:68:TYR:CD1   | 1:A:146:ARG:NH2 | 0.47     | 2.83        | 11     | 2     |
| 1:A:72:VAL:HG21  | 1:A:144:LYS:CA  | 0.47     | 2.40        | 1      | 1     |
| 1:A:101:PHE:CE2  | 1:A:128:LEU:CD1 | 0.47     | 2.97        | 15     | 13    |
| 1:A:72:VAL:CG2   | 1:A:140:TYR:CD2 | 0.47     | 2.97        | 8      | 5     |
| 1:A:82:TYR:HB3   | 1:A:101:PHE:CE1 | 0.47     | 2.44        | 20     | 1     |
| 1:A:5:VAL:HG13   | 1:A:47:ILE:CG1  | 0.47     | 2.40        | 4      | 2     |
| 1:A:84:LEU:HD23  | 1:A:100:VAL:C   | 0.47     | 2.35        | 7      | 3     |
| 1:A:46:ASN:O     | 1:A:48:ILE:HG23 | 0.47     | 2.10        | 10     | 1     |
| 1:A:82:TYR:CE1   | 1:A:103:PHE:CE1 | 0.47     | 3.03        | 18     | 1     |
| 1:A:35:ALA:HB3   | 1:A:55:ILE:HB   | 0.47     | 1.85        | 10     | 2     |
| 1:A:149:LEU:HD11 | 1:A:152:LYS:NZ  | 0.46     | 2.25        | 18     | 1     |
| 1:A:160:SER:CA   | 1:A:166:LEU:HB2 | 0.46     | 2.40        | 17     | 7     |
| 1:A:37:LEU:HD13  | 1:A:74:MET:HE3  | 0.46     | 1.87        | 4      | 1     |
| 1:A:152:LYS:CD   | 1:A:152:LYS:C   | 0.46     | 2.88        | 6      | 5     |
| 1:A:7:VAL:HG22   | 1:A:47:ILE:CG1  | 0.46     | 2.40        | 17     | 1     |
| 1:A:92:LYS:HD2   | 1:A:157:ALA:HB1 | 0.46     | 1.85        | 17     | 1     |
| 1:A:110:PRO:O    | 1:A:113:SER:N   | 0.46     | 2.47        | 3      | 1     |
| 1:A:18:MET:HE2   | 1:A:36:VAL:HG13 | 0.46     | 1.86        | 5      | 2     |
| 1:A:62:GLN:OE1   | 1:A:63:THR:HG23 | 0.46     | 2.10        | 18     | 1     |
| 1:A:162:GLU:HB2  | 1:A:165:PRO:CG  | 0.46     | 2.39        | 9      | 14    |
| 1:A:77:ASP:O     | 1:A:77:ASP:CG   | 0.46     | 2.59        | 10     | 6     |
| 1:A:32:ARG:O     | 1:A:57:VAL:HG13 | 0.46     | 2.10        | 16     | 1     |
| 1:A:71:PHE:CZ    | 1:A:75:LEU:CD1  | 0.46     | 2.99        | 10     | 5     |
| 1:A:152:LYS:C    | 1:A:152:LYS:HD3 | 0.46     | 2.35        | 11     | 1     |
| 1:A:34:LYS:HB2   | 1:A:57:VAL:HG12 | 0.46     | 1.87        | 16     | 1     |
| 1:A:10:GLY:C     | 1:A:49:LEU:HD22 | 0.46     | 2.36        | 15     | 2     |
| 1:A:15:PHE:CE1   | 1:A:131:ILE:CD1 | 0.46     | 2.99        | 12     | 3     |
| 1:A:112:LYS:O    | 1:A:115:MET:HE2 | 0.46     | 2.11        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:100:VAL:HG13 | 1:A:152:LYS:NZ   | 0.46     | 2.26        | 16     | 1     |
| 1:A:104:TRP:CZ3  | 1:A:143:VAL:CG1  | 0.46     | 2.99        | 4      | 1     |
| 1:A:90:GLU:CB    | 1:A:159:ILE:HD11 | 0.46     | 2.40        | 8      | 1     |
| 1:A:153:LEU:HD12 | 1:A:153:LEU:C    | 0.46     | 2.36        | 5      | 2     |
| 1:A:40:LEU:HD23  | 1:A:46:ASN:O     | 0.46     | 2.11        | 12     | 1     |
| 1:A:35:ALA:HB2   | 1:A:85:TYR:CG    | 0.46     | 2.45        | 14     | 1     |
| 1:A:90:GLU:HB3   | 1:A:159:ILE:HD11 | 0.46     | 1.87        | 17     | 1     |
| 1:A:89:TYR:CE1   | 1:A:153:LEU:CB   | 0.45     | 2.99        | 1      | 1     |
| 1:A:71:PHE:HE2   | 1:A:102:ILE:HG21 | 0.45     | 1.71        | 5      | 1     |
| 1:A:15:PHE:CZ    | 1:A:131:ILE:CD1  | 0.45     | 2.99        | 20     | 4     |
| 1:A:83:ALA:HB3   | 1:A:102:ILE:HB   | 0.45     | 1.86        | 20     | 1     |
| 1:A:37:LEU:HD23  | 1:A:83:ALA:HB2   | 0.45     | 1.88        | 20     | 2     |
| 1:A:37:LEU:HG    | 1:A:83:ALA:HB2   | 0.45     | 1.88        | 5      | 1     |
| 1:A:11:VAL:HG21  | 1:A:47:ILE:CG2   | 0.45     | 2.40        | 8      | 2     |
| 1:A:44:LYS:NZ    | 1:A:116:ILE:HD13 | 0.45     | 2.25        | 11     | 1     |
| 1:A:55:ILE:HD12  | 1:A:70:THR:CG2   | 0.45     | 2.41        | 19     | 1     |
| 1:A:34:LYS:NZ    | 1:A:60:VAL:HG22  | 0.45     | 2.26        | 4      | 1     |
| 1:A:149:LEU:HD12 | 1:A:152:LYS:HZ2  | 0.45     | 1.72        | 8      | 1     |
| 1:A:160:SER:OG   | 1:A:166:LEU:HB2  | 0.45     | 2.10        | 8      | 2     |
| 1:A:5:VAL:HG13   | 1:A:5:VAL:O      | 0.45     | 2.11        | 3      | 3     |
| 1:A:71:PHE:CZ    | 1:A:75:LEU:CD2   | 0.45     | 3.00        | 6      | 1     |
| 1:A:37:LEU:CD2   | 1:A:71:PHE:CE2   | 0.45     | 3.00        | 12     | 1     |
| 1:A:12:ILE:HD11  | 1:A:127:LYS:HB2  | 0.45     | 1.89        | 1      | 1     |
| 1:A:84:LEU:CD2   | 1:A:131:ILE:HD11 | 0.45     | 2.36        | 3      | 2     |
| 1:A:117:TYR:O    | 1:A:121:LYS:N    | 0.45     | 2.49        | 4      | 9     |
| 1:A:152:LYS:HZ2  | 1:A:153:LEU:HD21 | 0.45     | 1.72        | 3      | 1     |
| 1:A:12:ILE:N     | 1:A:12:ILE:CD1   | 0.45     | 2.80        | 4      | 2     |
| 1:A:71:PHE:CE1   | 1:A:75:LEU:HD11  | 0.45     | 2.47        | 19     | 3     |
| 1:A:68:TYR:CD1   | 1:A:85:TYR:CE2   | 0.45     | 3.05        | 6      | 1     |
| 1:A:85:TYR:CD1   | 1:A:86:ASP:N     | 0.45     | 2.84        | 1      | 5     |
| 1:A:137:ALA:HB1  | 1:A:142:GLU:CB   | 0.45     | 2.41        | 1      | 2     |
| 1:A:12:ILE:CD1   | 1:A:128:LEU:HD23 | 0.45     | 2.42        | 6      | 1     |
| 1:A:36:VAL:HG23  | 1:A:38:PHE:CZ    | 0.45     | 2.47        | 16     | 2     |
| 1:A:36:VAL:CG2   | 1:A:38:PHE:CE2   | 0.45     | 2.99        | 10     | 1     |
| 1:A:103:PHE:N    | 1:A:135:LEU:O    | 0.45     | 2.50        | 15     | 2     |
| 1:A:84:LEU:HD21  | 1:A:101:PHE:CD2  | 0.45     | 2.46        | 17     | 1     |
| 1:A:40:LEU:HD21  | 1:A:47:ILE:CD1   | 0.44     | 2.41        | 11     | 2     |
| 1:A:15:PHE:CE1   | 1:A:19:LYS:CG    | 0.44     | 3.00        | 6      | 1     |
| 1:A:15:PHE:CZ    | 1:A:19:LYS:CG    | 0.44     | 3.00        | 8      | 2     |
| 1:A:49:LEU:N     | 1:A:49:LEU:CD1   | 0.44     | 2.80        | 9      | 1     |
| 1:A:71:PHE:CD2   | 1:A:75:LEU:HD13  | 0.44     | 2.48        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:72:VAL:HA    | 1:A:75:LEU:CB    | 0.44     | 2.43        | 2      | 10    |
| 1:A:11:VAL:N     | 1:A:49:LEU:HD22  | 0.44     | 2.28        | 15     | 1     |
| 1:A:5:VAL:HG21   | 1:A:120:SER:HB2  | 0.44     | 1.90        | 4      | 2     |
| 1:A:55:ILE:CD1   | 1:A:70:THR:HG22  | 0.44     | 2.42        | 11     | 2     |
| 1:A:40:LEU:HD12  | 1:A:44:LYS:C     | 0.44     | 2.38        | 14     | 1     |
| 1:A:113:SER:HA   | 1:A:116:ILE:HD12 | 0.44     | 1.90        | 17     | 2     |
| 1:A:80:CYS:HG    | 1:A:117:TYR:CB   | 0.44     | 2.26        | 4      | 2     |
| 1:A:44:LYS:O     | 1:A:116:ILE:HD12 | 0.44     | 2.12        | 12     | 1     |
| 1:A:37:LEU:HD21  | 1:A:75:LEU:HD12  | 0.44     | 1.88        | 10     | 1     |
| 1:A:75:LEU:CD2   | 1:A:143:VAL:HG21 | 0.44     | 2.43        | 4      | 1     |
| 1:A:101:PHE:HD2  | 1:A:131:ILE:HD13 | 0.44     | 1.72        | 5      | 1     |
| 1:A:55:ILE:HD11  | 1:A:74:MET:CE    | 0.44     | 2.42        | 6      | 1     |
| 1:A:99:LEU:HD23  | 1:A:100:VAL:H    | 0.44     | 1.73        | 8      | 1     |
| 1:A:47:ILE:HG21  | 1:A:124:ILE:HD13 | 0.44     | 1.90        | 15     | 1     |
| 1:A:60:VAL:HG22  | 1:A:67:PRO:HB3   | 0.44     | 1.88        | 17     | 1     |
| 1:A:78:LYS:N     | 1:A:78:LYS:CD    | 0.43     | 2.81        | 3      | 7     |
| 1:A:131:ILE:O    | 1:A:132:LYS:CB   | 0.43     | 2.66        | 6      | 1     |
| 1:A:117:TYR:C    | 1:A:117:TYR:CD1  | 0.43     | 2.96        | 7      | 1     |
| 1:A:83:ALA:O     | 1:A:102:ILE:N    | 0.43     | 2.51        | 9      | 3     |
| 1:A:68:TYR:CD2   | 1:A:146:ARG:CD   | 0.43     | 3.01        | 13     | 2     |
| 1:A:55:ILE:HD13  | 1:A:70:THR:CG2   | 0.43     | 2.21        | 16     | 1     |
| 1:A:100:VAL:HG21 | 1:A:135:LEU:CD1  | 0.43     | 2.43        | 19     | 1     |
| 1:A:84:LEU:HD11  | 1:A:101:PHE:CD2  | 0.43     | 2.48        | 10     | 1     |
| 1:A:135:LEU:HD22 | 1:A:148:THR:CG2  | 0.43     | 2.43        | 11     | 1     |
| 1:A:72:VAL:CG1   | 1:A:140:TYR:CG   | 0.43     | 3.01        | 13     | 1     |
| 1:A:34:LYS:N     | 1:A:55:ILE:O     | 0.43     | 2.51        | 16     | 2     |
| 1:A:15:PHE:CD1   | 1:A:128:LEU:CD2  | 0.43     | 3.01        | 17     | 1     |
| 1:A:37:LEU:CD2   | 1:A:71:PHE:CE1   | 0.43     | 3.01        | 1      | 1     |
| 1:A:124:ILE:O    | 1:A:127:LYS:CG   | 0.43     | 2.67        | 1      | 1     |
| 1:A:36:VAL:O     | 1:A:38:PHE:CE1   | 0.43     | 2.72        | 17     | 4     |
| 1:A:82:TYR:CD2   | 1:A:117:TYR:CZ   | 0.43     | 3.06        | 19     | 2     |
| 1:A:37:LEU:HD12  | 1:A:83:ALA:CB    | 0.43     | 2.43        | 2      | 1     |
| 1:A:160:SER:OG   | 1:A:161:LEU:N    | 0.43     | 2.52        | 20     | 4     |
| 1:A:78:LYS:CD    | 1:A:78:LYS:N     | 0.43     | 2.82        | 8      | 10    |
| 1:A:75:LEU:HD13  | 1:A:104:TRP:CD2  | 0.43     | 2.49        | 7      | 2     |
| 1:A:64:VAL:HG12  | 1:A:65:ASP:N     | 0.43     | 2.29        | 3      | 3     |
| 1:A:60:VAL:HG23  | 1:A:67:PRO:CD    | 0.43     | 2.44        | 16     | 1     |
| 1:A:20:VAL:HG12  | 1:A:21:ARG:N     | 0.43     | 2.29        | 5      | 2     |
| 1:A:12:ILE:O     | 1:A:16:ASN:N     | 0.43     | 2.51        | 6      | 1     |
| 1:A:25:THR:HB    | 1:A:26:PRO:HD2   | 0.43     | 1.91        | 6      | 1     |
| 1:A:48:ILE:HD12  | 1:A:49:LEU:O     | 0.43     | 2.13        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:15:PHE:CD1   | 1:A:84:LEU:CD1   | 0.43     | 3.01        | 1      | 2     |
| 1:A:9:ASP:CG     | 1:A:10:GLY:N     | 0.43     | 2.77        | 5      | 1     |
| 1:A:37:LEU:HD22  | 1:A:74:MET:CE    | 0.43     | 2.37        | 5      | 1     |
| 1:A:72:VAL:CG2   | 1:A:140:TYR:CE2  | 0.43     | 3.01        | 11     | 1     |
| 1:A:100:VAL:HG13 | 1:A:102:ILE:HG13 | 0.43     | 1.91        | 19     | 1     |
| 1:A:149:LEU:O    | 1:A:152:LYS:CD   | 0.43     | 2.67        | 1      | 3     |
| 1:A:131:ILE:O    | 1:A:133:HIS:N    | 0.43     | 2.52        | 4      | 1     |
| 1:A:89:TYR:CG    | 1:A:153:LEU:HD13 | 0.43     | 2.48        | 8      | 1     |
| 1:A:90:GLU:C     | 1:A:159:ILE:CG2  | 0.43     | 2.92        | 20     | 1     |
| 1:A:15:PHE:HZ    | 1:A:131:ILE:HD12 | 0.42     | 1.70        | 15     | 2     |
| 1:A:91:THR:O     | 1:A:93:GLU:N     | 0.42     | 2.51        | 13     | 1     |
| 1:A:149:LEU:O    | 1:A:153:LEU:HD23 | 0.42     | 2.13        | 17     | 1     |
| 1:A:40:LEU:N     | 1:A:117:TYR:CE1  | 0.42     | 2.87        | 19     | 1     |
| 1:A:82:TYR:CG    | 1:A:117:TYR:CE2  | 0.42     | 3.07        | 19     | 1     |
| 1:A:87:ALA:HB3   | 1:A:152:LYS:NZ   | 0.42     | 2.29        | 3      | 2     |
| 1:A:37:LEU:HD13  | 1:A:74:MET:CE    | 0.42     | 2.44        | 17     | 2     |
| 1:A:75:LEU:HG    | 1:A:104:TRP:CD1  | 0.42     | 2.50        | 6      | 1     |
| 1:A:82:TYR:CE1   | 1:A:103:PHE:CD1  | 0.42     | 3.08        | 18     | 2     |
| 1:A:40:LEU:HD12  | 1:A:45:LYS:N     | 0.42     | 2.29        | 10     | 1     |
| 1:A:111:LEU:HD13 | 1:A:111:LEU:O    | 0.42     | 2.14        | 12     | 1     |
| 1:A:89:TYR:CB    | 1:A:158:VAL:HG13 | 0.42     | 2.44        | 20     | 1     |
| 1:A:100:VAL:HG12 | 1:A:133:HIS:HB3  | 0.42     | 1.90        | 7      | 1     |
| 1:A:99:LEU:HD23  | 1:A:100:VAL:N    | 0.42     | 2.29        | 8      | 1     |
| 1:A:77:ASP:OD2   | 1:A:108:SER:CB   | 0.42     | 2.68        | 10     | 1     |
| 1:A:160:SER:OG   | 1:A:163:GLY:N    | 0.42     | 2.53        | 2      | 3     |
| 1:A:75:LEU:O     | 1:A:104:TRP:CZ2  | 0.42     | 2.73        | 3      | 1     |
| 1:A:87:ALA:CB    | 1:A:152:LYS:CE   | 0.42     | 2.98        | 3      | 1     |
| 1:A:8:SER:CB     | 1:A:48:ILE:CG2   | 0.42     | 2.96        | 9      | 3     |
| 1:A:68:TYR:CG    | 1:A:146:ARG:CZ   | 0.42     | 3.02        | 20     | 1     |
| 1:A:44:LYS:O     | 1:A:116:ILE:HG21 | 0.42     | 2.14        | 3      | 1     |
| 1:A:57:VAL:O     | 1:A:57:VAL:CG2   | 0.42     | 2.68        | 3      | 1     |
| 1:A:18:MET:O     | 1:A:99:LEU:HD11  | 0.42     | 2.14        | 5      | 1     |
| 1:A:75:LEU:HD23  | 1:A:104:TRP:CE2  | 0.42     | 2.50        | 5      | 1     |
| 1:A:38:PHE:CZ    | 1:A:84:LEU:HD12  | 0.42     | 2.50        | 17     | 1     |
| 1:A:14:VAL:CG1   | 1:A:49:LEU:HD22  | 0.42     | 2.45        | 20     | 1     |
| 1:A:135:LEU:HD11 | 1:A:152:LYS:HZ3  | 0.42     | 1.74        | 1      | 1     |
| 1:A:164:LYS:CB   | 1:A:165:PRO:CD   | 0.42     | 2.97        | 1      | 8     |
| 1:A:25:THR:HG22  | 1:A:26:PRO:HD2   | 0.42     | 1.91        | 2      | 2     |
| 1:A:72:VAL:CG2   | 1:A:140:TYR:CG   | 0.42     | 3.02        | 2      | 1     |
| 1:A:74:MET:C     | 1:A:76:PRO:HD3   | 0.42     | 2.40        | 5      | 4     |
| 1:A:100:VAL:CG1  | 1:A:152:LYS:CD   | 0.42     | 2.98        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:7:VAL:CG1    | 1:A:11:VAL:CG2   | 0.42     | 2.98        | 15     | 5     |
| 1:A:24:SER:O     | 1:A:29:VAL:HG13  | 0.42     | 2.15        | 18     | 2     |
| 1:A:127:LYS:O    | 1:A:129:THR:HG23 | 0.42     | 2.14        | 14     | 1     |
| 1:A:84:LEU:HD21  | 1:A:101:PHE:HD2  | 0.42     | 1.73        | 17     | 1     |
| 1:A:44:LYS:C     | 1:A:116:ILE:HG21 | 0.42     | 2.40        | 3      | 1     |
| 1:A:161:LEU:O    | 1:A:162:GLU:CB   | 0.42     | 2.67        | 8      | 1     |
| 1:A:19:LYS:HG3   | 1:A:20:VAL:HG13  | 0.42     | 1.91        | 15     | 1     |
| 1:A:40:LEU:HD21  | 1:A:47:ILE:HD13  | 0.41     | 1.91        | 3      | 1     |
| 1:A:89:TYR:CD2   | 1:A:158:VAL:HG22 | 0.41     | 2.49        | 9      | 1     |
| 1:A:57:VAL:HG23  | 1:A:58:GLY:N     | 0.41     | 2.30        | 1      | 1     |
| 1:A:18:MET:HE1   | 1:A:99:LEU:HD21  | 0.41     | 1.92        | 4      | 1     |
| 1:A:49:LEU:N     | 1:A:49:LEU:HD23  | 0.41     | 2.31        | 5      | 1     |
| 1:A:45:LYS:O     | 1:A:46:ASN:ND2   | 0.41     | 2.54        | 19     | 2     |
| 1:A:5:VAL:CG1    | 1:A:46:ASN:N     | 0.41     | 2.83        | 9      | 1     |
| 1:A:7:VAL:HG12   | 1:A:11:VAL:CG2   | 0.41     | 2.45        | 10     | 1     |
| 1:A:15:PHE:CE2   | 1:A:131:ILE:HD12 | 0.41     | 2.50        | 13     | 1     |
| 1:A:37:LEU:HD23  | 1:A:74:MET:CE    | 0.41     | 2.45        | 13     | 1     |
| 1:A:80:CYS:O     | 1:A:117:TYR:CE1  | 0.41     | 2.73        | 13     | 1     |
| 1:A:72:VAL:HA    | 1:A:75:LEU:HB2   | 0.41     | 1.92        | 2      | 3     |
| 1:A:124:ILE:HG23 | 1:A:125:LYS:N    | 0.41     | 2.30        | 9      | 5     |
| 1:A:146:ARG:NE   | 1:A:165:PRO:CB   | 0.41     | 2.84        | 9      | 1     |
| 1:A:89:TYR:CZ    | 1:A:96:LYS:CB    | 0.41     | 3.03        | 7      | 1     |
| 1:A:87:ALA:HB3   | 1:A:149:LEU:HD12 | 0.41     | 1.93        | 8      | 1     |
| 1:A:49:LEU:HD13  | 1:A:49:LEU:H     | 0.41     | 1.73        | 9      | 1     |
| 1:A:113:SER:O    | 1:A:117:TYR:CE1  | 0.41     | 2.73        | 9      | 1     |
| 1:A:104:TRP:O    | 1:A:117:TYR:CE2  | 0.41     | 2.74        | 11     | 1     |
| 1:A:10:GLY:CA    | 1:A:13:LYS:HB2   | 0.41     | 2.44        | 18     | 1     |
| 1:A:14:VAL:HG11  | 1:A:38:PHE:CE2   | 0.41     | 2.51        | 18     | 1     |
| 1:A:71:PHE:CZ    | 1:A:102:ILE:CG2  | 0.41     | 3.04        | 1      | 1     |
| 1:A:164:LYS:CG   | 1:A:165:PRO:HD3  | 0.41     | 2.46        | 17     | 3     |
| 1:A:104:TRP:CZ3  | 1:A:137:ALA:O    | 0.41     | 2.74        | 19     | 1     |
| 1:A:159:ILE:CG2  | 1:A:160:SER:N    | 0.41     | 2.83        | 20     | 1     |
| 1:A:135:LEU:HD12 | 1:A:149:LEU:CD2  | 0.41     | 2.46        | 1      | 1     |
| 1:A:130:GLY:O    | 1:A:132:LYS:N    | 0.41     | 2.54        | 4      | 1     |
| 1:A:135:LEU:CD1  | 1:A:152:LYS:CG   | 0.41     | 2.98        | 5      | 1     |
| 1:A:89:TYR:CE2   | 1:A:96:LYS:CD    | 0.41     | 3.03        | 7      | 1     |
| 1:A:7:VAL:HG12   | 1:A:8:SER:N      | 0.41     | 2.30        | 9      | 3     |
| 1:A:100:VAL:HG13 | 1:A:100:VAL:O    | 0.41     | 2.16        | 11     | 1     |
| 1:A:100:VAL:CG1  | 1:A:152:LYS:CE   | 0.41     | 2.98        | 17     | 1     |
| 1:A:90:GLU:C     | 1:A:159:ILE:HG22 | 0.41     | 2.41        | 20     | 1     |
| 1:A:150:ALA:HA   | 1:A:153:LEU:HD12 | 0.41     | 1.92        | 3      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:16:ASN:OD1  | 1:A:17:ASP:N     | 0.41     | 2.54        | 5      | 4     |
| 1:A:8:SER:HB2   | 1:A:48:ILE:HG23  | 0.41     | 1.92        | 6      | 1     |
| 1:A:30:LYS:O    | 1:A:58:GLY:N     | 0.41     | 2.54        | 11     | 1     |
| 1:A:7:VAL:HG11  | 1:A:11:VAL:HB    | 0.41     | 1.92        | 12     | 1     |
| 1:A:25:THR:CG2  | 1:A:26:PRO:CD    | 0.41     | 2.99        | 14     | 2     |
| 1:A:101:PHE:HE2 | 1:A:128:LEU:HD12 | 0.41     | 1.75        | 19     | 1     |
| 1:A:98:ASP:OD2  | 1:A:133:HIS:CD2  | 0.41     | 2.74        | 1      | 1     |
| 1:A:80:CYS:O    | 1:A:117:TYR:CZ   | 0.41     | 2.74        | 18     | 4     |
| 1:A:150:ALA:HA  | 1:A:153:LEU:HD21 | 0.41     | 1.93        | 2      | 1     |
| 1:A:5:VAL:CG1   | 1:A:123:ALA:HB3  | 0.41     | 2.46        | 3      | 1     |
| 1:A:25:THR:O    | 1:A:29:VAL:HG13  | 0.41     | 2.16        | 3      | 1     |
| 1:A:84:LEU:HD11 | 1:A:131:ILE:HD13 | 0.41     | 1.93        | 4      | 1     |
| 1:A:60:VAL:O    | 1:A:60:VAL:HG22  | 0.41     | 2.16        | 11     | 1     |
| 1:A:14:VAL:HG21 | 1:A:36:VAL:HG11  | 0.41     | 1.92        | 16     | 1     |
| 1:A:116:ILE:O   | 1:A:117:TYR:C    | 0.41     | 2.64        | 17     | 1     |
| 1:A:34:LYS:HE2  | 1:A:88:THR:HG22  | 0.41     | 1.92        | 18     | 1     |
| 1:A:91:THR:HG23 | 1:A:92:LYS:H     | 0.41     | 1.76        | 18     | 1     |
| 1:A:89:TYR:CE1  | 1:A:153:LEU:HB2  | 0.41     | 2.51        | 1      | 1     |
| 1:A:105:ALA:CB  | 1:A:117:TYR:CE1  | 0.41     | 3.00        | 7      | 1     |
| 1:A:5:VAL:CG2   | 1:A:47:ILE:CD1   | 0.41     | 2.99        | 8      | 1     |
| 1:A:6:ALA:O     | 1:A:7:VAL:O      | 0.41     | 2.39        | 9      | 1     |
| 1:A:132:LYS:O   | 1:A:133:HIS:CG   | 0.41     | 2.73        | 19     | 2     |
| 1:A:10:GLY:O    | 1:A:13:LYS:N     | 0.41     | 2.54        | 18     | 1     |
| 1:A:33:LYS:CD   | 1:A:36:VAL:CG1   | 0.40     | 3.00        | 1      | 1     |
| 1:A:89:TYR:CE2  | 1:A:96:LYS:HB2   | 0.40     | 2.51        | 7      | 1     |
| 1:A:60:VAL:HG11 | 1:A:162:GLU:CD   | 0.40     | 2.41        | 8      | 2     |
| 1:A:99:LEU:N    | 1:A:99:LEU:HD12  | 0.40     | 2.31        | 19     | 1     |
| 1:A:88:THR:CG2  | 1:A:162:GLU:CG   | 0.40     | 2.98        | 2      | 1     |
| 1:A:37:LEU:HD13 | 1:A:74:MET:HE1   | 0.40     | 1.92        | 5      | 1     |
| 1:A:75:LEU:CD1  | 1:A:104:TRP:CD1  | 0.40     | 3.05        | 6      | 1     |
| 1:A:40:LEU:HD13 | 1:A:44:LYS:HA    | 0.40     | 1.94        | 12     | 1     |
| 1:A:117:TYR:CD1 | 1:A:117:TYR:C    | 0.40     | 2.99        | 12     | 1     |
| 1:A:146:ARG:HG3 | 1:A:161:LEU:CG   | 0.40     | 2.46        | 18     | 1     |
| 1:A:101:PHE:CE1 | 1:A:103:PHE:CZ   | 0.40     | 3.10        | 19     | 1     |
| 1:A:149:LEU:CA  | 1:A:152:LYS:HE2  | 0.40     | 2.46        | 1      | 1     |
| 1:A:152:LYS:CD  | 1:A:153:LEU:N    | 0.40     | 2.84        | 12     | 3     |
| 1:A:131:ILE:CG1 | 1:A:132:LYS:N    | 0.40     | 2.83        | 11     | 1     |
| 1:A:68:TYR:CE2  | 1:A:143:VAL:O    | 0.40     | 2.74        | 13     | 1     |
| 1:A:25:THR:CB   | 1:A:26:PRO:HD2   | 0.40     | 2.47        | 14     | 1     |
| 1:A:80:CYS:SG   | 1:A:117:TYR:CG   | 0.40     | 3.14        | 1      | 1     |
| 1:A:149:LEU:CD1 | 1:A:152:LYS:HZ3  | 0.40     | 2.29        | 2      | 1     |

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| Atom-1         | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|----------------|------------------|----------|-------------|--------|-------|
|                |                  |          |             | Worst  | Total |
| 1:A:15:PHE:CZ  | 1:A:19:LYS:HG3   | 0.40     | 2.52        | 6      | 1     |
| 1:A:5:VAL:CG1  | 1:A:123:ALA:CB   | 0.40     | 3.00        | 7      | 1     |
| 1:A:161:LEU:O  | 1:A:161:LEU:HD13 | 0.40     | 2.15        | 12     | 1     |
| 1:A:152:LYS:CD | 1:A:153:LEU:CD2  | 0.40     | 2.99        | 16     | 1     |
| 1:A:146:ARG:CD | 1:A:165:PRO:HB2  | 0.40     | 2.46        | 1      | 1     |
| 1:A:25:THR:CG2 | 1:A:26:PRO:HD2   | 0.40     | 2.47        | 14     | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

| Mol | Chain | Analysed        | Favoured      | Allowed      | Outliers    | Percentiles |    |
|-----|-------|-----------------|---------------|--------------|-------------|-------------|----|
| 1   | A     | 161/166 (97%)   | 116±5 (72±3%) | 34±5 (21±3%) | 11±3 (7±2%) | 2           | 17 |
| All | All   | 3220/3320 (97%) | 2324 (72%)    | 681 (21%)    | 215 (7%)    | 2           | 17 |

All 38 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 24  | SER  | 20             |
| 1   | A     | 164 | LYS  | 20             |
| 1   | A     | 102 | ILE  | 18             |
| 1   | A     | 162 | GLU  | 16             |
| 1   | A     | 76  | PRO  | 14             |
| 1   | A     | 71  | PHE  | 12             |
| 1   | A     | 132 | LYS  | 12             |
| 1   | A     | 91  | THR  | 11             |
| 1   | A     | 5   | VAL  | 9              |
| 1   | A     | 7   | VAL  | 6              |
| 1   | A     | 21  | ARG  | 6              |
| 1   | A     | 22  | LYS  | 6              |
| 1   | A     | 93  | GLU  | 5              |
| 1   | A     | 101 | PHE  | 5              |
| 1   | A     | 154 | GLY  | 5              |
| 1   | A     | 9   | ASP  | 5              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 35  | ALA  | 4              |
| 1   | A     | 108 | SER  | 4              |
| 1   | A     | 62  | GLN  | 3              |
| 1   | A     | 131 | ILE  | 3              |
| 1   | A     | 129 | THR  | 3              |
| 1   | A     | 116 | ILE  | 3              |
| 1   | A     | 45  | LYS  | 3              |
| 1   | A     | 67  | PRO  | 2              |
| 1   | A     | 33  | LYS  | 2              |
| 1   | A     | 92  | LYS  | 2              |
| 1   | A     | 50  | GLU  | 2              |
| 1   | A     | 87  | ALA  | 2              |
| 1   | A     | 109 | ALA  | 2              |
| 1   | A     | 83  | ALA  | 2              |
| 1   | A     | 155 | GLY  | 1              |
| 1   | A     | 25  | THR  | 1              |
| 1   | A     | 156 | SER  | 1              |
| 1   | A     | 53  | LYS  | 1              |
| 1   | A     | 135 | LEU  | 1              |
| 1   | A     | 32  | ARG  | 1              |
| 1   | A     | 41  | SER  | 1              |
| 1   | A     | 130 | GLY  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric      | Outliers      | Percentiles |    |
|-----|-------|-----------------|----------------|---------------|-------------|----|
| 1   | A     | 142/144 (99%)   | 86±36 (61±26%) | 32±13 (22±9%) | 2           | 29 |
| All | All   | 2359/2880 (82%) | 1726 (73%)     | 633 (27%)     | 2           | 21 |

All 101 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 124 | ILE  | 18             |
| 1   | A     | 114 | LYS  | 17             |
| 1   | A     | 164 | LYS  | 17             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 30  | LYS  | 16             |
| 1   | A     | 78  | LYS  | 16             |
| 1   | A     | 149 | LEU  | 16             |
| 1   | A     | 152 | LYS  | 16             |
| 1   | A     | 75  | LEU  | 15             |
| 1   | A     | 18  | MET  | 14             |
| 1   | A     | 25  | THR  | 14             |
| 1   | A     | 40  | LEU  | 14             |
| 1   | A     | 107 | GLU  | 14             |
| 1   | A     | 161 | LEU  | 14             |
| 1   | A     | 125 | LYS  | 13             |
| 1   | A     | 162 | GLU  | 13             |
| 1   | A     | 33  | LYS  | 12             |
| 1   | A     | 53  | LYS  | 12             |
| 1   | A     | 108 | SER  | 12             |
| 1   | A     | 113 | SER  | 12             |
| 1   | A     | 50  | GLU  | 11             |
| 1   | A     | 90  | GLU  | 10             |
| 1   | A     | 44  | LYS  | 10             |
| 1   | A     | 73  | LYS  | 9              |
| 1   | A     | 37  | LEU  | 9              |
| 1   | A     | 45  | LYS  | 9              |
| 1   | A     | 127 | LYS  | 9              |
| 1   | A     | 19  | LYS  | 8              |
| 1   | A     | 74  | MET  | 8              |
| 1   | A     | 151 | GLU  | 8              |
| 1   | A     | 13  | LYS  | 8              |
| 1   | A     | 32  | ARG  | 8              |
| 1   | A     | 132 | LYS  | 8              |
| 1   | A     | 146 | ARG  | 8              |
| 1   | A     | 95  | LYS  | 7              |
| 1   | A     | 98  | ASP  | 7              |
| 1   | A     | 126 | LYS  | 7              |
| 1   | A     | 22  | LYS  | 7              |
| 1   | A     | 112 | LYS  | 7              |
| 1   | A     | 23  | SER  | 6              |
| 1   | A     | 54  | GLU  | 6              |
| 1   | A     | 103 | PHE  | 6              |
| 1   | A     | 115 | MET  | 6              |
| 1   | A     | 129 | THR  | 6              |
| 1   | A     | 134 | GLU  | 6              |
| 1   | A     | 49  | LEU  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 119 | SER  | 6              |
| 1   | A     | 139 | CYS  | 6              |
| 1   | A     | 91  | THR  | 6              |
| 1   | A     | 92  | LYS  | 6              |
| 1   | A     | 131 | ILE  | 6              |
| 1   | A     | 111 | LEU  | 6              |
| 1   | A     | 17  | ASP  | 5              |
| 1   | A     | 43  | ASP  | 5              |
| 1   | A     | 93  | GLU  | 5              |
| 1   | A     | 153 | LEU  | 5              |
| 1   | A     | 94  | SER  | 5              |
| 1   | A     | 99  | LEU  | 5              |
| 1   | A     | 62  | GLN  | 5              |
| 1   | A     | 135 | LEU  | 5              |
| 1   | A     | 34  | LYS  | 4              |
| 1   | A     | 96  | LYS  | 4              |
| 1   | A     | 12  | ILE  | 4              |
| 1   | A     | 51  | GLU  | 4              |
| 1   | A     | 46  | ASN  | 3              |
| 1   | A     | 136 | GLN  | 3              |
| 1   | A     | 100 | VAL  | 3              |
| 1   | A     | 160 | SER  | 3              |
| 1   | A     | 145 | ASP  | 3              |
| 1   | A     | 21  | ARG  | 3              |
| 1   | A     | 104 | TRP  | 3              |
| 1   | A     | 122 | ASP  | 2              |
| 1   | A     | 147 | CYS  | 2              |
| 1   | A     | 42  | GLU  | 2              |
| 1   | A     | 128 | LEU  | 2              |
| 1   | A     | 144 | LYS  | 2              |
| 1   | A     | 5   | VAL  | 2              |
| 1   | A     | 59  | ASP  | 2              |
| 1   | A     | 84  | LEU  | 2              |
| 1   | A     | 117 | TYR  | 2              |
| 1   | A     | 120 | SER  | 2              |
| 1   | A     | 8   | SER  | 2              |
| 1   | A     | 65  | ASP  | 2              |
| 1   | A     | 77  | ASP  | 2              |
| 1   | A     | 138 | ASN  | 2              |
| 1   | A     | 27  | GLU  | 1              |
| 1   | A     | 81  | ARG  | 1              |
| 1   | A     | 156 | SER  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 86  | ASP  | 1              |
| 1   | A     | 143 | VAL  | 1              |
| 1   | A     | 9   | ASP  | 1              |
| 1   | A     | 121 | LYS  | 1              |
| 1   | A     | 39  | CYS  | 1              |
| 1   | A     | 7   | VAL  | 1              |
| 1   | A     | 116 | ILE  | 1              |
| 1   | A     | 56  | LEU  | 1              |
| 1   | A     | 80  | CYS  | 1              |
| 1   | A     | 48  | ILE  | 1              |
| 1   | A     | 66  | ASP  | 1              |
| 1   | A     | 72  | VAL  | 1              |
| 1   | A     | 141 | GLU  | 1              |
| 1   | A     | 70  | THR  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided