



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 04:07 PM UTC

PDB ID : 1KKX / pdb\_00001kkx  
Title : Solution structure of the DNA-binding domain of ADR6  
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Deposited on : 2001-12-10

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                                                             |

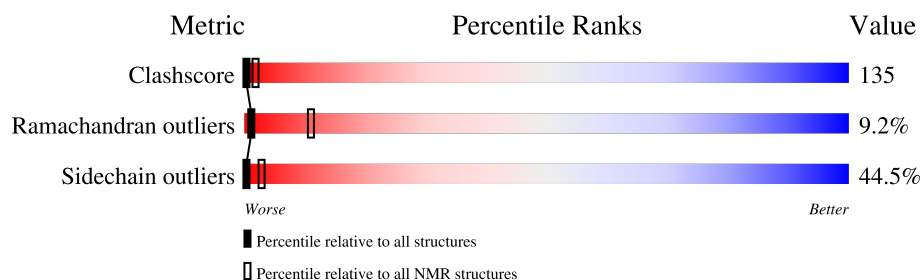
# 1 Overall quality at a glance

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     | 123    |                  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:7-A:89 (83)         | 0.89              | 3            |

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. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1741 atoms, of which 881 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription regulatory protein ADR6.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 102      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1741  | 549 | 881 | 152 | 153 | 6 |       |

There are 21 discrepancies between the modelled and reference sequences:

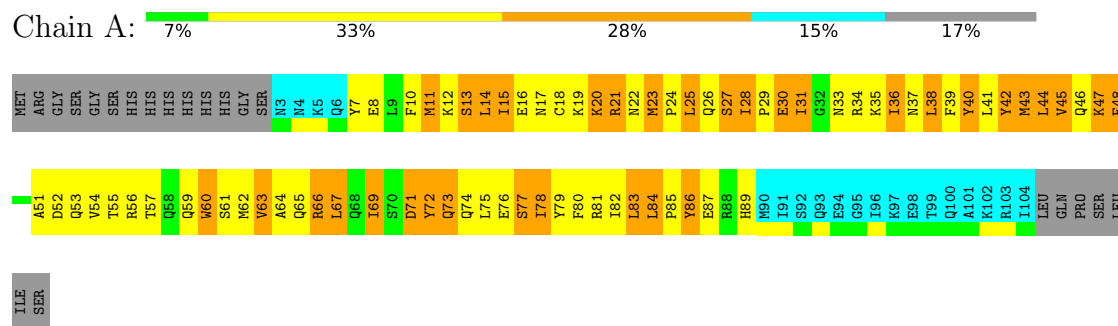
| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | -11     | MET      | -      | expression tag   | UNP P09547 |
| A     | -10     | ARG      | -      | expression tag   | UNP P09547 |
| A     | -9      | GLY      | -      | expression tag   | UNP P09547 |
| A     | -8      | SER      | -      | expression tag   | UNP P09547 |
| A     | -7      | GLY      | -      | expression tag   | UNP P09547 |
| A     | -6      | SER      | -      | expression tag   | UNP P09547 |
| A     | -5      | HIS      | -      | expression tag   | UNP P09547 |
| A     | -4      | HIS      | -      | expression tag   | UNP P09547 |
| A     | -3      | HIS      | -      | expression tag   | UNP P09547 |
| A     | -2      | HIS      | -      | expression tag   | UNP P09547 |
| A     | -1      | HIS      | -      | expression tag   | UNP P09547 |
| A     | 0       | HIS      | -      | expression tag   | UNP P09547 |
| A     | 1       | GLY      | -      | expression tag   | UNP P09547 |
| A     | 2       | SER      | -      | expression tag   | UNP P09547 |
| A     | 105     | LEU      | -      | cloning artifact | UNP P09547 |
| A     | 106     | GLN      | -      | cloning artifact | UNP P09547 |
| A     | 107     | PRO      | -      | cloning artifact | UNP P09547 |
| A     | 108     | SER      | -      | cloning artifact | UNP P09547 |
| A     | 109     | LEU      | -      | cloning artifact | UNP P09547 |
| A     | 110     | ILE      | -      | cloning artifact | UNP P09547 |
| A     | 111     | SER      | -      | cloning artifact | UNP P09547 |

## 4 Residue-property plots

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

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

- Molecule 1: Transcription regulatory protein ADR6

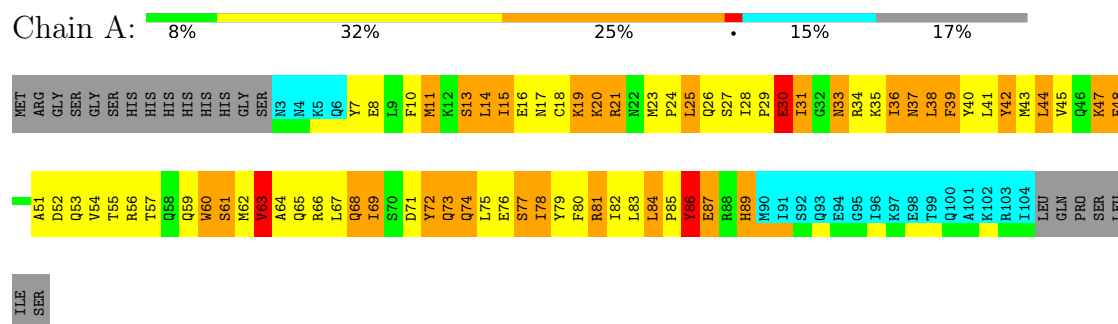


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Transcription regulatory protein ADR6

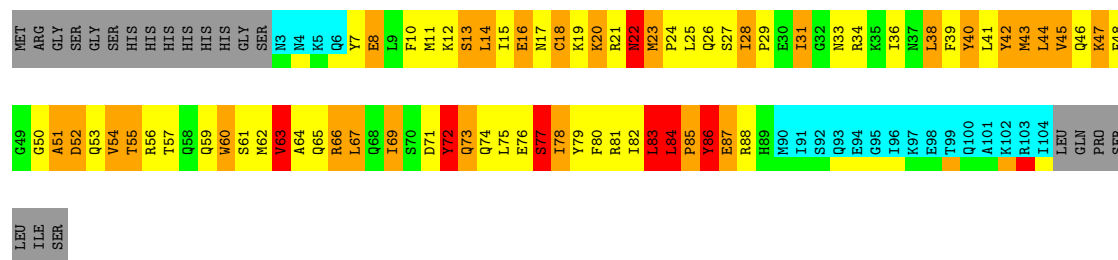






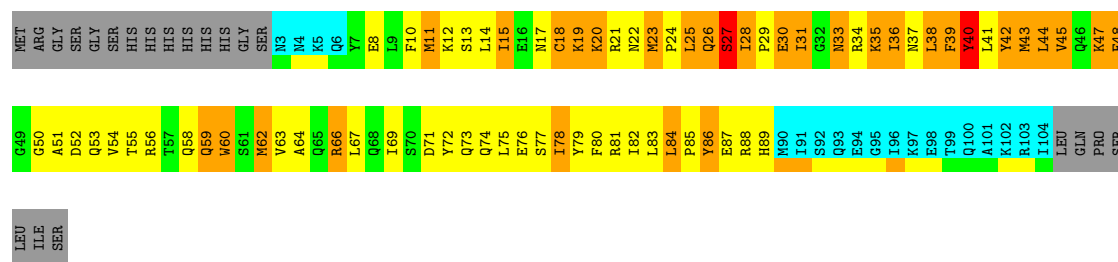
#### 4.2.6 Score per residue for model 6

- Molecule 1: Transcription regulatory protein ADR6



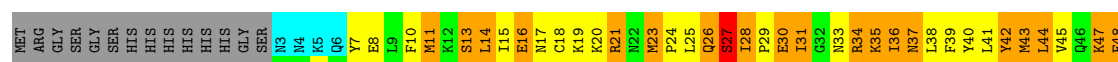
#### 4.2.7 Score per residue for model 7

- Molecule 1: Transcription regulatory protein ADR6



#### 4.2.8 Score per residue for model 8

- Molecule 1: Transcription regulatory protein ADR6





## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 10 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           | refinement     | v 1.0   |

No chemical shift data was provided.

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 0.46±0.01    | 0±0/723 ( 0.0± 0.0%) | 0.75±0.02   | 1±1/973 ( 0.1± 0.1%) |
| All | All   | 0.46         | 0/7230 ( 0.0%)       | 0.75        | 12/9730 ( 0.1%)      |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 77  | SER  | N-CA-C | -5.50 | 105.44      | 111.82   | 3      | 8     |
| 1   | A     | 84  | LEU  | CA-C-N | 5.27  | 126.42      | 119.84   | 4      | 2     |
| 1   | A     | 84  | LEU  | C-N-CA | 5.27  | 126.42      | 119.84   | 4      | 2     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 707   | 719      | 718      | 193±11  |
| All | All   | 7070  | 7190     | 7180     | 1928    |

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 135.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:75:LEU:O    | 1:A:78:ILE:HG12 | 1.18     | 1.36        | 5      | 10    |
| 1:A:42:TYR:O    | 1:A:45:VAL:HG12 | 1.16     | 1.37        | 9      | 9     |
| 1:A:63:VAL:HG12 | 1:A:75:LEU:HD12 | 1.13     | 1.13        | 3      | 7     |
| 1:A:78:ILE:HG13 | 1:A:79:TYR:N    | 1.08     | 1.59        | 9      | 9     |
| 1:A:31:ILE:HG21 | 1:A:69:ILE:HD12 | 1.06     | 1.26        | 7      | 1     |
| 1:A:45:VAL:HG23 | 1:A:54:VAL:HG11 | 1.05     | 1.22        | 1      | 9     |
| 1:A:55:THR:HA   | 1:A:60:TRP:CD1  | 1.05     | 1.86        | 7      | 10    |
| 1:A:41:LEU:HD11 | 1:A:78:ILE:HD13 | 1.05     | 1.28        | 10     | 9     |
| 1:A:14:LEU:HD21 | 1:A:82:ILE:HG22 | 1.04     | 1.18        | 2      | 8     |
| 1:A:41:LEU:HD12 | 1:A:63:VAL:HG13 | 1.03     | 1.22        | 6      | 3     |
| 1:A:23:MET:HA   | 1:A:23:MET:HE2  | 1.00     | 1.31        | 2      | 6     |
| 1:A:45:VAL:CG2  | 1:A:54:VAL:HG11 | 0.99     | 1.87        | 5      | 9     |
| 1:A:14:LEU:HD23 | 1:A:83:LEU:HB3  | 0.99     | 1.31        | 8      | 5     |
| 1:A:36:ILE:HD13 | 1:A:38:LEU:HD23 | 0.98     | 1.32        | 5      | 3     |
| 1:A:36:ILE:HD12 | 1:A:38:LEU:HD11 | 0.95     | 1.38        | 10     | 1     |
| 1:A:40:TYR:O    | 1:A:43:MET:HE1  | 0.95     | 1.61        | 9      | 1     |
| 1:A:84:LEU:C    | 1:A:84:LEU:HD12 | 0.94     | 1.87        | 4      | 9     |
| 1:A:41:LEU:CD1  | 1:A:78:ILE:HD13 | 0.92     | 1.94        | 9      | 9     |
| 1:A:63:VAL:CG1  | 1:A:75:LEU:HD12 | 0.92     | 1.94        | 2      | 10    |
| 1:A:14:LEU:HD13 | 1:A:15:ILE:N    | 0.91     | 1.80        | 6      | 9     |
| 1:A:41:LEU:O    | 1:A:63:VAL:HG22 | 0.91     | 1.63        | 10     | 7     |
| 1:A:63:VAL:HG12 | 1:A:75:LEU:CD1  | 0.90     | 1.96        | 2      | 10    |
| 1:A:83:LEU:O    | 1:A:87:GLU:HG3  | 0.90     | 1.66        | 10     | 10    |
| 1:A:44:LEU:HD11 | 1:A:66:ARG:CG   | 0.89     | 1.96        | 3      | 6     |
| 1:A:14:LEU:CD2  | 1:A:83:LEU:HD13 | 0.87     | 2.00        | 7      | 2     |
| 1:A:67:LEU:HD11 | 1:A:75:LEU:HD11 | 0.87     | 1.43        | 6      | 3     |
| 1:A:22:ASN:O    | 1:A:23:MET:HB3  | 0.87     | 1.70        | 10     | 1     |
| 1:A:41:LEU:HD21 | 1:A:78:ILE:CD1  | 0.87     | 2.00        | 6      | 5     |
| 1:A:51:ALA:O    | 1:A:55:THR:HG23 | 0.86     | 1.70        | 4      | 8     |
| 1:A:55:THR:HG22 | 1:A:60:TRP:CZ2  | 0.86     | 2.05        | 5      | 2     |
| 1:A:51:ALA:HB2  | 1:A:79:TYR:CG   | 0.85     | 2.05        | 9      | 9     |
| 1:A:72:TYR:CA   | 1:A:75:LEU:HD23 | 0.85     | 2.01        | 8      | 10    |
| 1:A:60:TRP:CZ3  | 1:A:63:VAL:HG21 | 0.84     | 2.06        | 1      | 10    |
| 1:A:41:LEU:HD13 | 1:A:67:LEU:HD22 | 0.84     | 1.47        | 7      | 4     |
| 1:A:55:THR:HA   | 1:A:60:TRP:NE1  | 0.84     | 1.87        | 3      | 10    |
| 1:A:42:TYR:O    | 1:A:45:VAL:CG1  | 0.83     | 2.26        | 9      | 9     |
| 1:A:41:LEU:CG   | 1:A:78:ILE:HD13 | 0.83     | 2.03        | 4      | 8     |
| 1:A:14:LEU:HD23 | 1:A:83:LEU:HD13 | 0.82     | 1.48        | 7      | 2     |
| 1:A:31:ILE:HG21 | 1:A:69:ILE:CD1  | 0.82     | 2.02        | 7      | 1     |
| 1:A:36:ILE:O    | 1:A:36:ILE:HD12 | 0.82     | 1.74        | 5      | 3     |
| 1:A:51:ALA:HB2  | 1:A:79:TYR:CD1  | 0.82     | 2.09        | 6      | 9     |
| 1:A:51:ALA:HB2  | 1:A:79:TYR:CD2  | 0.82     | 2.10        | 9      | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:14:LEU:CD2  | 1:A:82:ILE:HG22 | 0.82     | 2.05        | 2      | 7     |
| 1:A:72:TYR:HA   | 1:A:75:LEU:HD23 | 0.82     | 1.51        | 4      | 10    |
| 1:A:67:LEU:HD11 | 1:A:69:ILE:HB   | 0.82     | 1.50        | 1      | 2     |
| 1:A:55:THR:HG22 | 1:A:60:TRP:CE2  | 0.81     | 2.10        | 5      | 2     |
| 1:A:55:THR:HG21 | 1:A:76:GLU:CG   | 0.81     | 2.05        | 4      | 2     |
| 1:A:78:ILE:CG1  | 1:A:79:TYR:N    | 0.81     | 2.42        | 9      | 9     |
| 1:A:60:TRP:CE2  | 1:A:75:LEU:HB3  | 0.80     | 2.12        | 5      | 3     |
| 1:A:31:ILE:C    | 1:A:67:LEU:HD13 | 0.80     | 2.01        | 1      | 1     |
| 1:A:55:THR:HG22 | 1:A:76:GLU:HB2  | 0.80     | 1.53        | 9      | 5     |
| 1:A:28:ILE:HG22 | 1:A:29:PRO:HD2  | 0.79     | 1.50        | 8      | 3     |
| 1:A:60:TRP:HZ3  | 1:A:63:VAL:HG21 | 0.79     | 1.37        | 10     | 10    |
| 1:A:75:LEU:O    | 1:A:78:ILE:HG23 | 0.79     | 1.76        | 1      | 9     |
| 1:A:75:LEU:O    | 1:A:78:ILE:CG1  | 0.79     | 2.28        | 5      | 10    |
| 1:A:14:LEU:HD21 | 1:A:82:ILE:CG2  | 0.79     | 2.07        | 2      | 7     |
| 1:A:40:TYR:O    | 1:A:43:MET:HE3  | 0.79     | 1.76        | 6      | 1     |
| 1:A:36:ILE:HG23 | 1:A:38:LEU:HD21 | 0.79     | 1.51        | 4      | 1     |
| 1:A:80:PHE:CD1  | 1:A:84:LEU:HD23 | 0.79     | 2.12        | 6      | 7     |
| 1:A:41:LEU:HD12 | 1:A:63:VAL:CG1  | 0.79     | 2.07        | 8      | 8     |
| 1:A:42:TYR:O    | 1:A:45:VAL:HG22 | 0.79     | 1.77        | 6      | 1     |
| 1:A:38:LEU:HD22 | 1:A:82:ILE:HD13 | 0.79     | 1.55        | 4      | 1     |
| 1:A:45:VAL:HG23 | 1:A:54:VAL:CG1  | 0.78     | 2.04        | 5      | 8     |
| 1:A:55:THR:HG21 | 1:A:76:GLU:OE1  | 0.78     | 1.78        | 10     | 5     |
| 1:A:64:ALA:HB2  | 1:A:75:LEU:HD21 | 0.78     | 1.53        | 4      | 4     |
| 1:A:42:TYR:HA   | 1:A:45:VAL:HG12 | 0.78     | 1.55        | 7      | 8     |
| 1:A:38:LEU:HD13 | 1:A:82:ILE:CG2  | 0.78     | 2.08        | 4      | 1     |
| 1:A:41:LEU:HD21 | 1:A:78:ILE:CG2  | 0.78     | 2.09        | 5      | 1     |
| 1:A:55:THR:HG21 | 1:A:76:GLU:HG3  | 0.77     | 1.56        | 5      | 2     |
| 1:A:18:CYS:SG   | 1:A:25:LEU:HD21 | 0.77     | 2.19        | 7      | 1     |
| 1:A:14:LEU:CD2  | 1:A:38:LEU:HD12 | 0.77     | 2.10        | 3      | 1     |
| 1:A:23:MET:HA   | 1:A:23:MET:CE   | 0.77     | 2.10        | 2      | 9     |
| 1:A:40:TYR:O    | 1:A:43:MET:CE   | 0.77     | 2.31        | 9      | 2     |
| 1:A:38:LEU:HD13 | 1:A:82:ILE:HG21 | 0.76     | 1.55        | 4      | 1     |
| 1:A:42:TYR:C    | 1:A:42:TYR:CD1  | 0.76     | 2.61        | 6      | 9     |
| 1:A:41:LEU:HD21 | 1:A:78:ILE:HG21 | 0.76     | 1.55        | 5      | 1     |
| 1:A:84:LEU:HB3  | 1:A:85:PRO:CD   | 0.76     | 2.10        | 3      | 10    |
| 1:A:41:LEU:HD11 | 1:A:78:ILE:CD1  | 0.76     | 2.11        | 6      | 6     |
| 1:A:31:ILE:HB   | 1:A:67:LEU:HD12 | 0.76     | 1.58        | 10     | 2     |
| 1:A:44:LEU:HD11 | 1:A:66:ARG:HG3  | 0.75     | 1.58        | 2      | 3     |
| 1:A:41:LEU:HD12 | 1:A:75:LEU:CD1  | 0.75     | 2.11        | 3      | 9     |
| 1:A:28:ILE:HG21 | 1:A:36:ILE:CG1  | 0.75     | 2.12        | 8      | 1     |
| 1:A:31:ILE:CD1  | 1:A:67:LEU:HD12 | 0.75     | 2.11        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:44:LEU:HD12 | 1:A:62:MET:C    | 0.74     | 2.07        | 10     | 3     |
| 1:A:79:TYR:O    | 1:A:84:LEU:N    | 0.74     | 2.20        | 10     | 8     |
| 1:A:36:ILE:HD12 | 1:A:38:LEU:CD1  | 0.74     | 2.12        | 10     | 1     |
| 1:A:51:ALA:HA   | 1:A:54:VAL:HG12 | 0.74     | 1.60        | 5      | 8     |
| 1:A:51:ALA:HB1  | 1:A:76:GLU:HG3  | 0.73     | 1.60        | 6      | 10    |
| 1:A:59:GLN:HB2  | 1:A:62:MET:HE2  | 0.73     | 1.58        | 3      | 1     |
| 1:A:31:ILE:HG22 | 1:A:67:LEU:HD11 | 0.73     | 1.60        | 4      | 1     |
| 1:A:14:LEU:HD22 | 1:A:14:LEU:C    | 0.73     | 2.09        | 2      | 8     |
| 1:A:14:LEU:HD22 | 1:A:14:LEU:O    | 0.73     | 1.84        | 6      | 8     |
| 1:A:44:LEU:N    | 1:A:44:LEU:HD23 | 0.73     | 1.98        | 3      | 7     |
| 1:A:84:LEU:HB3  | 1:A:85:PRO:HD2  | 0.73     | 1.60        | 8      | 10    |
| 1:A:14:LEU:HD21 | 1:A:38:LEU:HD12 | 0.73     | 1.61        | 3      | 1     |
| 1:A:23:MET:N    | 1:A:23:MET:HE2  | 0.73     | 1.99        | 10     | 1     |
| 1:A:31:ILE:CG2  | 1:A:69:ILE:HD13 | 0.72     | 2.14        | 8      | 4     |
| 1:A:41:LEU:HD11 | 1:A:78:ILE:HG13 | 0.72     | 1.61        | 5      | 1     |
| 1:A:42:TYR:O    | 1:A:45:VAL:N    | 0.72     | 2.18        | 9      | 8     |
| 1:A:44:LEU:HD11 | 1:A:66:ARG:HG2  | 0.72     | 1.61        | 7      | 4     |
| 1:A:74:GLN:O    | 1:A:78:ILE:HG23 | 0.72     | 1.84        | 6      | 8     |
| 1:A:31:ILE:HG21 | 1:A:69:ILE:HB   | 0.72     | 1.61        | 8      | 1     |
| 1:A:38:LEU:HD12 | 1:A:83:LEU:HD21 | 0.72     | 1.60        | 9      | 2     |
| 1:A:83:LEU:HD23 | 1:A:87:GLU:OE2  | 0.72     | 1.85        | 3      | 1     |
| 1:A:47:LYS:HE2  | 1:A:62:MET:HE2  | 0.72     | 1.60        | 2      | 1     |
| 1:A:43:MET:N    | 1:A:43:MET:HE2  | 0.72     | 1.99        | 9      | 1     |
| 1:A:72:TYR:O    | 1:A:75:LEU:HB2  | 0.72     | 1.85        | 10     | 10    |
| 1:A:64:ALA:HA   | 1:A:75:LEU:HD11 | 0.71     | 1.59        | 7      | 8     |
| 1:A:60:TRP:HA   | 1:A:60:TRP:CE3  | 0.71     | 2.20        | 5      | 10    |
| 1:A:41:LEU:HD13 | 1:A:67:LEU:HD21 | 0.71     | 1.60        | 2      | 3     |
| 1:A:44:LEU:HD13 | 1:A:66:ARG:HG3  | 0.71     | 1.62        | 5      | 1     |
| 1:A:80:PHE:HA   | 1:A:84:LEU:HB2  | 0.71     | 1.60        | 7      | 9     |
| 1:A:25:LEU:HD23 | 1:A:82:ILE:HG12 | 0.71     | 1.61        | 7      | 1     |
| 1:A:41:LEU:HD12 | 1:A:75:LEU:HD12 | 0.71     | 1.61        | 6      | 8     |
| 1:A:45:VAL:HB   | 1:A:60:TRP:CZ3  | 0.71     | 2.20        | 10     | 8     |
| 1:A:41:LEU:O    | 1:A:44:LEU:HG   | 0.71     | 1.85        | 5      | 8     |
| 1:A:38:LEU:CD1  | 1:A:82:ILE:HG21 | 0.70     | 2.16        | 2      | 3     |
| 1:A:41:LEU:HG   | 1:A:78:ILE:HD13 | 0.70     | 1.62        | 4      | 2     |
| 1:A:42:TYR:C    | 1:A:45:VAL:HG12 | 0.70     | 2.11        | 9      | 6     |
| 1:A:18:CYS:SG   | 1:A:23:MET:HE1  | 0.70     | 2.27        | 9      | 3     |
| 1:A:44:LEU:HD12 | 1:A:63:VAL:HA   | 0.69     | 1.64        | 5      | 4     |
| 1:A:42:TYR:HA   | 1:A:45:VAL:HG13 | 0.69     | 1.64        | 6      | 1     |
| 1:A:23:MET:O    | 1:A:25:LEU:N    | 0.69     | 2.25        | 10     | 1     |
| 1:A:67:LEU:CD1  | 1:A:75:LEU:HD11 | 0.69     | 2.18        | 6      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:64:ALA:O    | 1:A:69:ILE:HG22 | 0.69     | 1.87        | 1      | 6     |
| 1:A:43:MET:HA   | 1:A:43:MET:HE2  | 0.69     | 1.63        | 1      | 4     |
| 1:A:11:MET:HE2  | 1:A:15:ILE:HD11 | 0.69     | 1.65        | 3      | 2     |
| 1:A:25:LEU:HD21 | 1:A:28:ILE:HA   | 0.69     | 1.65        | 3      | 1     |
| 1:A:42:TYR:CG   | 1:A:43:MET:N    | 0.69     | 2.59        | 9      | 2     |
| 1:A:42:TYR:CD2  | 1:A:43:MET:HE1  | 0.69     | 2.23        | 10     | 3     |
| 1:A:75:LEU:C    | 1:A:78:ILE:HG12 | 0.69     | 2.13        | 5      | 1     |
| 1:A:19:LYS:HA   | 1:A:23:MET:HE3  | 0.68     | 1.64        | 4      | 5     |
| 1:A:36:ILE:CD1  | 1:A:38:LEU:HD23 | 0.68     | 2.15        | 5      | 1     |
| 1:A:67:LEU:HD13 | 1:A:69:ILE:CG2  | 0.68     | 2.19        | 6      | 3     |
| 1:A:41:LEU:CD1  | 1:A:75:LEU:HD12 | 0.68     | 2.18        | 6      | 1     |
| 1:A:36:ILE:HD13 | 1:A:38:LEU:CD2  | 0.68     | 2.17        | 5      | 1     |
| 1:A:83:LEU:HD23 | 1:A:86:TYR:CB   | 0.67     | 2.19        | 10     | 1     |
| 1:A:55:THR:CG2  | 1:A:76:GLU:HB2  | 0.67     | 2.18        | 8      | 7     |
| 1:A:64:ALA:CB   | 1:A:75:LEU:HD21 | 0.67     | 2.20        | 5      | 5     |
| 1:A:84:LEU:C    | 1:A:84:LEU:CD1  | 0.67     | 2.67        | 1      | 10    |
| 1:A:42:TYR:CD1  | 1:A:42:TYR:C    | 0.67     | 2.72        | 8      | 1     |
| 1:A:55:THR:HG23 | 1:A:76:GLU:CB   | 0.67     | 2.19        | 6      | 2     |
| 1:A:80:PHE:CD2  | 1:A:84:LEU:HD22 | 0.67     | 2.25        | 4      | 2     |
| 1:A:83:LEU:HD23 | 1:A:86:TYR:HB2  | 0.67     | 1.65        | 10     | 1     |
| 1:A:45:VAL:HB   | 1:A:60:TRP:HZ3  | 0.66     | 1.50        | 10     | 8     |
| 1:A:14:LEU:HD23 | 1:A:83:LEU:HB2  | 0.66     | 1.64        | 6      | 2     |
| 1:A:48:PHE:CE1  | 1:A:57:THR:HG21 | 0.66     | 2.25        | 8      | 2     |
| 1:A:78:ILE:HG13 | 1:A:79:TYR:H    | 0.66     | 1.51        | 4      | 5     |
| 1:A:31:ILE:HG23 | 1:A:69:ILE:HD13 | 0.66     | 1.66        | 2      | 2     |
| 1:A:64:ALA:HB2  | 1:A:75:LEU:CD2  | 0.66     | 2.21        | 5      | 3     |
| 1:A:53:GLN:O    | 1:A:57:THR:HG22 | 0.66     | 1.91        | 4      | 2     |
| 1:A:43:MET:HE2  | 1:A:43:MET:CA   | 0.65     | 2.22        | 8      | 5     |
| 1:A:24:PRO:C    | 1:A:25:LEU:HD12 | 0.65     | 2.17        | 8      | 3     |
| 1:A:18:CYS:HB2  | 1:A:25:LEU:HD11 | 0.65     | 1.68        | 7      | 1     |
| 1:A:43:MET:HE2  | 1:A:43:MET:HA   | 0.65     | 1.69        | 8      | 1     |
| 1:A:43:MET:N    | 1:A:43:MET:HE3  | 0.65     | 2.06        | 10     | 3     |
| 1:A:45:VAL:HG21 | 1:A:79:TYR:CD2  | 0.64     | 2.27        | 5      | 4     |
| 1:A:77:SER:O    | 1:A:81:ARG:HB2  | 0.64     | 1.92        | 8      | 9     |
| 1:A:44:LEU:HD23 | 1:A:44:LEU:N    | 0.64     | 2.07        | 8      | 1     |
| 1:A:63:VAL:HG12 | 1:A:64:ALA:N    | 0.64     | 2.07        | 6      | 2     |
| 1:A:77:SER:HA   | 1:A:81:ARG:HG2  | 0.64     | 1.69        | 9      | 1     |
| 1:A:22:ASN:O    | 1:A:23:MET:CB   | 0.64     | 2.45        | 10     | 1     |
| 1:A:28:ILE:HD13 | 1:A:28:ILE:N    | 0.63     | 2.09        | 5      | 6     |
| 1:A:21:ARG:O    | 1:A:23:MET:HE1  | 0.63     | 1.93        | 10     | 1     |
| 1:A:42:TYR:HD1  | 1:A:45:VAL:CG1  | 0.63     | 2.07        | 4      | 8     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:51:ALA:O    | 1:A:54:VAL:HG12 | 0.63     | 1.92        | 7      | 2     |
| 1:A:14:LEU:C    | 1:A:14:LEU:HD13 | 0.63     | 2.19        | 7      | 2     |
| 1:A:41:LEU:CD2  | 1:A:78:ILE:HG21 | 0.63     | 2.23        | 5      | 1     |
| 1:A:29:PRO:O    | 1:A:30:GLU:C    | 0.62     | 2.42        | 10     | 5     |
| 1:A:45:VAL:HG12 | 1:A:63:VAL:HG21 | 0.62     | 1.71        | 6      | 1     |
| 1:A:14:LEU:HB2  | 1:A:83:LEU:HD11 | 0.62     | 1.70        | 10     | 1     |
| 1:A:25:LEU:HD23 | 1:A:81:ARG:O    | 0.62     | 1.93        | 5      | 1     |
| 1:A:38:LEU:HD13 | 1:A:78:ILE:HD12 | 0.62     | 1.71        | 7      | 1     |
| 1:A:31:ILE:HG13 | 1:A:67:LEU:HD12 | 0.62     | 1.71        | 8      | 1     |
| 1:A:45:VAL:HG21 | 1:A:79:TYR:CE2  | 0.62     | 2.30        | 6      | 2     |
| 1:A:14:LEU:HD11 | 1:A:82:ILE:CG2  | 0.62     | 2.25        | 3      | 1     |
| 1:A:42:TYR:CA   | 1:A:45:VAL:HG13 | 0.62     | 2.25        | 6      | 1     |
| 1:A:17:ASN:HA   | 1:A:20:LYS:HG3  | 0.62     | 1.70        | 8      | 1     |
| 1:A:38:LEU:HD12 | 1:A:83:LEU:CD2  | 0.62     | 2.25        | 9      | 2     |
| 1:A:41:LEU:HD11 | 1:A:78:ILE:CG1  | 0.62     | 2.25        | 5      | 1     |
| 1:A:23:MET:HA   | 1:A:23:MET:HE3  | 0.62     | 1.71        | 6      | 1     |
| 1:A:41:LEU:CD1  | 1:A:63:VAL:HG13 | 0.62     | 2.13        | 6      | 1     |
| 1:A:38:LEU:HA   | 1:A:41:LEU:HD21 | 0.61     | 1.72        | 1      | 6     |
| 1:A:76:GLU:HG2  | 1:A:80:PHE:HB2  | 0.61     | 1.71        | 4      | 3     |
| 1:A:47:LYS:HG2  | 1:A:62:MET:HE1  | 0.61     | 1.69        | 5      | 2     |
| 1:A:45:VAL:CG2  | 1:A:60:TRP:CZ3  | 0.61     | 2.83        | 9      | 1     |
| 1:A:14:LEU:CD2  | 1:A:82:ILE:O    | 0.61     | 2.48        | 5      | 9     |
| 1:A:28:ILE:HG21 | 1:A:36:ILE:HG12 | 0.61     | 1.71        | 6      | 4     |
| 1:A:31:ILE:CG1  | 1:A:67:LEU:HD12 | 0.61     | 2.26        | 8      | 1     |
| 1:A:41:LEU:HD23 | 1:A:42:TYR:H    | 0.61     | 1.53        | 6      | 3     |
| 1:A:60:TRP:HA   | 1:A:60:TRP:HE3  | 0.61     | 1.56        | 3      | 9     |
| 1:A:83:LEU:N    | 1:A:83:LEU:CD2  | 0.61     | 2.64        | 8      | 1     |
| 1:A:45:VAL:HG11 | 1:A:79:TYR:CD2  | 0.60     | 2.31        | 10     | 6     |
| 1:A:36:ILE:HD13 | 1:A:38:LEU:HG   | 0.60     | 1.72        | 2      | 1     |
| 1:A:78:ILE:HA   | 1:A:82:ILE:HD12 | 0.60     | 1.73        | 2      | 3     |
| 1:A:36:ILE:HG23 | 1:A:38:LEU:CD2  | 0.60     | 2.23        | 4      | 1     |
| 1:A:31:ILE:HG22 | 1:A:67:LEU:CD1  | 0.60     | 2.25        | 4      | 1     |
| 1:A:59:GLN:HB3  | 1:A:62:MET:HE2  | 0.60     | 1.72        | 7      | 2     |
| 1:A:42:TYR:CE2  | 1:A:43:MET:HE1  | 0.60     | 2.31        | 4      | 8     |
| 1:A:43:MET:HE3  | 1:A:43:MET:CA   | 0.60     | 2.27        | 7      | 3     |
| 1:A:41:LEU:O    | 1:A:44:LEU:HB3  | 0.60     | 1.96        | 6      | 1     |
| 1:A:41:LEU:HD11 | 1:A:78:ILE:HG21 | 0.60     | 1.74        | 4      | 3     |
| 1:A:42:TYR:HA   | 1:A:45:VAL:CG1  | 0.60     | 2.27        | 6      | 2     |
| 1:A:31:ILE:CG2  | 1:A:69:ILE:HD12 | 0.60     | 2.16        | 7      | 1     |
| 1:A:54:VAL:O    | 1:A:60:TRP:CG   | 0.60     | 2.55        | 6      | 9     |
| 1:A:41:LEU:HD12 | 1:A:63:VAL:HG12 | 0.59     | 1.71        | 4      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:23:MET:HE2  | 1:A:24:PRO:HD3  | 0.59     | 1.73        | 10     | 1     |
| 1:A:84:LEU:CB   | 1:A:85:PRO:CD   | 0.59     | 2.80        | 5      | 10    |
| 1:A:59:GLN:O    | 1:A:62:MET:HE2  | 0.59     | 1.97        | 6      | 1     |
| 1:A:10:PHE:CD1  | 1:A:39:PHE:CD2  | 0.59     | 2.91        | 10     | 1     |
| 1:A:67:LEU:HD12 | 1:A:67:LEU:H    | 0.59     | 1.57        | 6      | 3     |
| 1:A:14:LEU:HD13 | 1:A:14:LEU:C    | 0.59     | 2.21        | 9      | 8     |
| 1:A:41:LEU:HB2  | 1:A:63:VAL:HG13 | 0.59     | 1.75        | 8      | 4     |
| 1:A:28:ILE:HG21 | 1:A:36:ILE:HG13 | 0.59     | 1.75        | 8      | 1     |
| 1:A:74:GLN:O    | 1:A:78:ILE:HD13 | 0.59     | 1.98        | 5      | 1     |
| 1:A:18:CYS:O    | 1:A:23:MET:N    | 0.59     | 2.35        | 7      | 9     |
| 1:A:75:LEU:O    | 1:A:78:ILE:CG2  | 0.59     | 2.51        | 1      | 6     |
| 1:A:10:PHE:CZ   | 1:A:39:PHE:CE1  | 0.59     | 2.91        | 7      | 2     |
| 1:A:47:LYS:CE   | 1:A:62:MET:HE2  | 0.59     | 2.27        | 2      | 1     |
| 1:A:67:LEU:HD11 | 1:A:75:LEU:CD1  | 0.59     | 2.27        | 9      | 3     |
| 1:A:50:GLY:O    | 1:A:52:ASP:N    | 0.59     | 2.36        | 6      | 1     |
| 1:A:42:TYR:CA   | 1:A:45:VAL:HG12 | 0.58     | 2.26        | 7      | 8     |
| 1:A:60:TRP:CZ3  | 1:A:63:VAL:HG11 | 0.58     | 2.33        | 9      | 4     |
| 1:A:29:PRO:CD   | 1:A:82:ILE:HD11 | 0.58     | 2.28        | 6      | 2     |
| 1:A:55:THR:HG21 | 1:A:76:GLU:CD   | 0.58     | 2.23        | 9      | 2     |
| 1:A:39:PHE:CE1  | 1:A:83:LEU:HD21 | 0.58     | 2.33        | 3      | 2     |
| 1:A:42:TYR:O    | 1:A:45:VAL:HG13 | 0.58     | 1.98        | 6      | 1     |
| 1:A:14:LEU:HD23 | 1:A:83:LEU:CD1  | 0.58     | 2.27        | 7      | 1     |
| 1:A:17:ASN:HA   | 1:A:20:LYS:CG   | 0.58     | 2.28        | 4      | 6     |
| 1:A:75:LEU:O    | 1:A:78:ILE:N    | 0.58     | 2.36        | 2      | 10    |
| 1:A:14:LEU:HD23 | 1:A:83:LEU:HG   | 0.58     | 1.73        | 4      | 2     |
| 1:A:19:LYS:HG3  | 1:A:23:MET:HE3  | 0.58     | 1.74        | 2      | 1     |
| 1:A:83:LEU:N    | 1:A:83:LEU:HD23 | 0.58     | 2.13        | 8      | 2     |
| 1:A:18:CYS:CB   | 1:A:25:LEU:HD11 | 0.58     | 2.29        | 7      | 1     |
| 1:A:20:LYS:HG3  | 1:A:21:ARG:N    | 0.58     | 2.13        | 10     | 1     |
| 1:A:43:MET:HE2  | 1:A:43:MET:N    | 0.57     | 2.13        | 8      | 5     |
| 1:A:54:VAL:HG13 | 1:A:60:TRP:CD2  | 0.57     | 2.34        | 2      | 3     |
| 1:A:71:ASP:O    | 1:A:74:GLN:N    | 0.57     | 2.37        | 4      | 10    |
| 1:A:28:ILE:HG22 | 1:A:29:PRO:CD   | 0.57     | 2.29        | 3      | 1     |
| 1:A:67:LEU:HD13 | 1:A:69:ILE:HG22 | 0.57     | 1.74        | 6      | 1     |
| 1:A:75:LEU:HD22 | 1:A:75:LEU:N    | 0.57     | 2.14        | 2      | 8     |
| 1:A:47:LYS:CB   | 1:A:62:MET:HE1  | 0.57     | 2.30        | 6      | 2     |
| 1:A:82:ILE:HG22 | 1:A:82:ILE:O    | 0.57     | 2.00        | 10     | 1     |
| 1:A:12:LYS:HA   | 1:A:15:ILE:HD11 | 0.57     | 1.76        | 7      | 1     |
| 1:A:84:LEU:CB   | 1:A:85:PRO:HD2  | 0.57     | 2.29        | 5      | 8     |
| 1:A:10:PHE:CE1  | 1:A:39:PHE:CE1  | 0.57     | 2.92        | 7      | 2     |
| 1:A:54:VAL:HG23 | 1:A:59:GLN:HB2  | 0.57     | 1.75        | 4      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:7:TYR:CD1   | 1:A:8:GLU:N     | 0.57     | 2.73        | 6      | 2     |
| 1:A:63:VAL:CG1  | 1:A:75:LEU:CD1  | 0.57     | 2.83        | 5      | 3     |
| 1:A:47:LYS:HE2  | 1:A:62:MET:CE   | 0.56     | 2.30        | 2      | 1     |
| 1:A:23:MET:H    | 1:A:24:PRO:HD3  | 0.56     | 1.59        | 10     | 1     |
| 1:A:55:THR:HG23 | 1:A:76:GLU:HB2  | 0.56     | 1.75        | 6      | 2     |
| 1:A:14:LEU:HD23 | 1:A:83:LEU:CB   | 0.56     | 2.19        | 8      | 3     |
| 1:A:81:ARG:N    | 1:A:81:ARG:HD3  | 0.56     | 2.16        | 2      | 3     |
| 1:A:29:PRO:HD3  | 1:A:82:ILE:HD13 | 0.56     | 1.77        | 3      | 1     |
| 1:A:41:LEU:HD21 | 1:A:78:ILE:HD11 | 0.56     | 1.77        | 6      | 1     |
| 1:A:47:LYS:HB3  | 1:A:62:MET:HE1  | 0.56     | 1.77        | 6      | 2     |
| 1:A:14:LEU:HD11 | 1:A:82:ILE:HG22 | 0.56     | 1.77        | 3      | 1     |
| 1:A:67:LEU:H    | 1:A:67:LEU:HD23 | 0.56     | 1.60        | 10     | 3     |
| 1:A:45:VAL:HG21 | 1:A:79:TYR:HD2  | 0.56     | 1.60        | 5      | 1     |
| 1:A:45:VAL:HG23 | 1:A:60:TRP:CZ3  | 0.56     | 2.35        | 9      | 1     |
| 1:A:29:PRO:O    | 1:A:31:ILE:HD13 | 0.56     | 2.00        | 5      | 2     |
| 1:A:41:LEU:CG   | 1:A:63:VAL:HG13 | 0.56     | 2.30        | 10     | 3     |
| 1:A:59:GLN:CB   | 1:A:62:MET:HE2  | 0.56     | 2.28        | 3      | 2     |
| 1:A:74:GLN:O    | 1:A:78:ILE:CD1  | 0.56     | 2.54        | 5      | 1     |
| 1:A:44:LEU:HD13 | 1:A:66:ARG:CG   | 0.56     | 2.29        | 5      | 2     |
| 1:A:44:LEU:HD11 | 1:A:66:ARG:HD2  | 0.56     | 1.78        | 8      | 1     |
| 1:A:7:TYR:CG    | 1:A:8:GLU:N     | 0.55     | 2.74        | 9      | 4     |
| 1:A:28:ILE:HG22 | 1:A:28:ILE:O    | 0.55     | 1.99        | 9      | 1     |
| 1:A:67:LEU:HD12 | 1:A:67:LEU:C    | 0.55     | 2.26        | 1      | 1     |
| 1:A:84:LEU:HD12 | 1:A:84:LEU:O    | 0.55     | 1.99        | 4      | 2     |
| 1:A:38:LEU:O    | 1:A:41:LEU:HD23 | 0.55     | 2.01        | 5      | 1     |
| 1:A:71:ASP:C    | 1:A:75:LEU:HD23 | 0.55     | 2.27        | 5      | 8     |
| 1:A:76:GLU:HG2  | 1:A:80:PHE:CB   | 0.55     | 2.32        | 4      | 10    |
| 1:A:29:PRO:O    | 1:A:36:ILE:HG22 | 0.55     | 2.01        | 7      | 1     |
| 1:A:71:ASP:O    | 1:A:75:LEU:HD23 | 0.55     | 2.02        | 2      | 8     |
| 1:A:67:LEU:HD21 | 1:A:69:ILE:CG2  | 0.55     | 2.32        | 8      | 4     |
| 1:A:18:CYS:SG   | 1:A:25:LEU:HD22 | 0.55     | 2.41        | 2      | 1     |
| 1:A:55:THR:HG22 | 1:A:60:TRP:NE1  | 0.55     | 2.16        | 5      | 2     |
| 1:A:74:GLN:O    | 1:A:77:SER:CB   | 0.55     | 2.55        | 5      | 1     |
| 1:A:80:PHE:HA   | 1:A:84:LEU:CD2  | 0.54     | 2.31        | 7      | 3     |
| 1:A:25:LEU:HD22 | 1:A:28:ILE:HD12 | 0.54     | 1.77        | 10     | 1     |
| 1:A:37:ASN:O    | 1:A:41:LEU:HD23 | 0.54     | 2.02        | 8      | 2     |
| 1:A:28:ILE:O    | 1:A:30:GLU:N    | 0.54     | 2.41        | 7      | 3     |
| 1:A:43:MET:HA   | 1:A:43:MET:CE   | 0.54     | 2.33        | 5      | 7     |
| 1:A:48:PHE:CE1  | 1:A:53:GLN:CG   | 0.54     | 2.90        | 7      | 3     |
| 1:A:59:GLN:CA   | 1:A:62:MET:HE2  | 0.54     | 2.32        | 5      | 1     |
| 1:A:17:ASN:HA   | 1:A:20:LYS:HG2  | 0.54     | 1.80        | 4      | 7     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:41:LEU:C    | 1:A:44:LEU:HG   | 0.54     | 2.27        | 5      | 2     |
| 1:A:42:TYR:CZ   | 1:A:43:MET:HE1  | 0.54     | 2.37        | 5      | 2     |
| 1:A:76:GLU:O    | 1:A:80:PHE:N    | 0.54     | 2.39        | 7      | 9     |
| 1:A:81:ARG:CD   | 1:A:81:ARG:N    | 0.54     | 2.70        | 3      | 5     |
| 1:A:38:LEU:HA   | 1:A:41:LEU:CD2  | 0.54     | 2.32        | 4      | 1     |
| 1:A:18:CYS:C    | 1:A:24:PRO:HD2  | 0.54     | 2.27        | 10     | 1     |
| 1:A:25:LEU:HD23 | 1:A:82:ILE:HA   | 0.54     | 1.80        | 5      | 2     |
| 1:A:24:PRO:O    | 1:A:25:LEU:HD12 | 0.54     | 2.03        | 6      | 3     |
| 1:A:47:LYS:CG   | 1:A:62:MET:HE1  | 0.54     | 2.33        | 5      | 1     |
| 1:A:25:LEU:HD23 | 1:A:28:ILE:HG12 | 0.54     | 1.80        | 9      | 1     |
| 1:A:31:ILE:HD12 | 1:A:31:ILE:N    | 0.54     | 2.18        | 2      | 1     |
| 1:A:41:LEU:HG   | 1:A:63:VAL:HG13 | 0.54     | 1.80        | 10     | 2     |
| 1:A:28:ILE:HG13 | 1:A:36:ILE:HD11 | 0.54     | 1.80        | 3      | 1     |
| 1:A:14:LEU:CD2  | 1:A:83:LEU:HB3  | 0.54     | 2.21        | 8      | 1     |
| 1:A:23:MET:HE2  | 1:A:24:PRO:CD   | 0.54     | 2.32        | 10     | 1     |
| 1:A:17:ASN:O    | 1:A:20:LYS:HG2  | 0.53     | 2.03        | 5      | 1     |
| 1:A:76:GLU:HG2  | 1:A:80:PHE:HB3  | 0.53     | 1.78        | 1      | 3     |
| 1:A:14:LEU:HD12 | 1:A:15:ILE:HD13 | 0.53     | 1.80        | 3      | 1     |
| 1:A:41:LEU:CG   | 1:A:78:ILE:HG21 | 0.53     | 2.33        | 5      | 1     |
| 1:A:41:LEU:CD1  | 1:A:75:LEU:CD1  | 0.53     | 2.86        | 6      | 5     |
| 1:A:38:LEU:HD21 | 1:A:82:ILE:HD12 | 0.53     | 1.79        | 8      | 1     |
| 1:A:59:GLN:HA   | 1:A:62:MET:HE2  | 0.53     | 1.80        | 5      | 1     |
| 1:A:18:CYS:C    | 1:A:23:MET:CE   | 0.53     | 2.82        | 9      | 6     |
| 1:A:31:ILE:HD12 | 1:A:31:ILE:H    | 0.53     | 1.64        | 2      | 1     |
| 1:A:61:SER:O    | 1:A:65:GLN:HB2  | 0.53     | 2.04        | 9      | 3     |
| 1:A:14:LEU:HD13 | 1:A:15:ILE:CA   | 0.53     | 2.34        | 4      | 7     |
| 1:A:41:LEU:HD23 | 1:A:42:TYR:N    | 0.53     | 2.18        | 6      | 1     |
| 1:A:79:TYR:O    | 1:A:84:LEU:HA   | 0.53     | 2.04        | 5      | 7     |
| 1:A:10:PHE:CD1  | 1:A:10:PHE:C    | 0.53     | 2.87        | 10     | 5     |
| 1:A:14:LEU:HD22 | 1:A:82:ILE:O    | 0.53     | 2.04        | 3      | 1     |
| 1:A:26:GLN:O    | 1:A:27:SER:CB   | 0.53     | 2.56        | 10     | 3     |
| 1:A:41:LEU:HD21 | 1:A:78:ILE:HD13 | 0.52     | 1.82        | 10     | 3     |
| 1:A:14:LEU:HD22 | 1:A:83:LEU:HD13 | 0.52     | 1.81        | 7      | 1     |
| 1:A:64:ALA:CA   | 1:A:75:LEU:HD11 | 0.52     | 2.33        | 7      | 2     |
| 1:A:42:TYR:CD1  | 1:A:43:MET:N    | 0.52     | 2.77        | 9      | 1     |
| 1:A:54:VAL:HG13 | 1:A:60:TRP:CE2  | 0.52     | 2.38        | 8      | 3     |
| 1:A:71:ASP:O    | 1:A:75:LEU:CD2  | 0.52     | 2.57        | 2      | 9     |
| 1:A:38:LEU:O    | 1:A:42:TYR:HB3  | 0.52     | 2.03        | 8      | 2     |
| 1:A:10:PHE:CD1  | 1:A:39:PHE:CE1  | 0.52     | 2.96        | 8      | 1     |
| 1:A:10:PHE:CD1  | 1:A:39:PHE:CE2  | 0.52     | 2.97        | 10     | 1     |
| 1:A:80:PHE:CB   | 1:A:84:LEU:HD23 | 0.52     | 2.34        | 7      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:54:VAL:HG13 | 1:A:60:TRP:CH2  | 0.52     | 2.39        | 5      | 2     |
| 1:A:41:LEU:CD1  | 1:A:78:ILE:HG13 | 0.52     | 2.32        | 5      | 1     |
| 1:A:17:ASN:O    | 1:A:24:PRO:HD2  | 0.52     | 2.04        | 10     | 1     |
| 1:A:42:TYR:HD1  | 1:A:45:VAL:HG13 | 0.52     | 1.65        | 7      | 1     |
| 1:A:76:GLU:O    | 1:A:80:PHE:HB3  | 0.52     | 2.04        | 7      | 7     |
| 1:A:43:MET:HE3  | 1:A:43:MET:HA   | 0.52     | 1.81        | 7      | 3     |
| 1:A:18:CYS:O    | 1:A:24:PRO:HD2  | 0.52     | 2.05        | 10     | 3     |
| 1:A:25:LEU:HD11 | 1:A:27:SER:O    | 0.52     | 2.04        | 3      | 1     |
| 1:A:39:PHE:HE1  | 1:A:83:LEU:HD21 | 0.52     | 1.64        | 3      | 1     |
| 1:A:14:LEU:CD1  | 1:A:15:ILE:N    | 0.51     | 2.66        | 4      | 5     |
| 1:A:10:PHE:C    | 1:A:10:PHE:CD1  | 0.51     | 2.88        | 6      | 3     |
| 1:A:73:GLN:HG3  | 1:A:74:GLN:N    | 0.51     | 2.19        | 9      | 6     |
| 1:A:54:VAL:HG13 | 1:A:60:TRP:CE3  | 0.51     | 2.40        | 2      | 1     |
| 1:A:38:LEU:HD23 | 1:A:38:LEU:N    | 0.51     | 2.20        | 3      | 2     |
| 1:A:55:THR:CA   | 1:A:60:TRP:CD1  | 0.51     | 2.79        | 7      | 1     |
| 1:A:41:LEU:HG   | 1:A:78:ILE:CD1  | 0.51     | 2.35        | 4      | 1     |
| 1:A:85:PRO:O    | 1:A:89:HIS:HB2  | 0.51     | 2.05        | 7      | 1     |
| 1:A:54:VAL:HG23 | 1:A:59:GLN:CB   | 0.51     | 2.36        | 4      | 2     |
| 1:A:18:CYS:O    | 1:A:23:MET:HE2  | 0.51     | 2.06        | 9      | 3     |
| 1:A:44:LEU:HB2  | 1:A:63:VAL:HG22 | 0.51     | 1.81        | 4      | 1     |
| 1:A:59:GLN:O    | 1:A:62:MET:HG3  | 0.51     | 2.05        | 7      | 1     |
| 1:A:10:PHE:CE2  | 1:A:39:PHE:CZ   | 0.51     | 2.98        | 7      | 1     |
| 1:A:51:ALA:CB   | 1:A:79:TYR:CD1  | 0.50     | 2.94        | 1      | 2     |
| 1:A:74:GLN:O    | 1:A:78:ILE:CG2  | 0.50     | 2.58        | 6      | 4     |
| 1:A:80:PHE:CD2  | 1:A:81:ARG:NE   | 0.50     | 2.80        | 10     | 3     |
| 1:A:16:GLU:O    | 1:A:20:LYS:CG   | 0.50     | 2.59        | 8      | 1     |
| 1:A:41:LEU:HD13 | 1:A:67:LEU:HD23 | 0.50     | 1.84        | 1      | 1     |
| 1:A:48:PHE:CE1  | 1:A:53:GLN:HG2  | 0.50     | 2.41        | 10     | 3     |
| 1:A:51:ALA:HB1  | 1:A:76:GLU:CG   | 0.50     | 2.36        | 6      | 1     |
| 1:A:14:LEU:HD23 | 1:A:82:ILE:O    | 0.50     | 2.07        | 10     | 1     |
| 1:A:28:ILE:HG23 | 1:A:36:ILE:CG2  | 0.50     | 2.35        | 10     | 1     |
| 1:A:7:TYR:HA    | 1:A:10:PHE:CE2  | 0.50     | 2.41        | 9      | 3     |
| 1:A:50:GLY:O    | 1:A:51:ALA:C    | 0.50     | 2.54        | 6      | 2     |
| 1:A:54:VAL:O    | 1:A:57:THR:HG22 | 0.50     | 2.07        | 2      | 1     |
| 1:A:25:LEU:HD11 | 1:A:28:ILE:HA   | 0.50     | 1.83        | 1      | 1     |
| 1:A:83:LEU:CD2  | 1:A:86:TYR:HB2  | 0.50     | 2.36        | 4      | 1     |
| 1:A:21:ARG:CD   | 1:A:24:PRO:HB3  | 0.50     | 2.37        | 8      | 1     |
| 1:A:47:LYS:CG   | 1:A:59:GLN:HG3  | 0.50     | 2.37        | 8      | 2     |
| 1:A:21:ARG:CD   | 1:A:21:ARG:O    | 0.50     | 2.60        | 3      | 3     |
| 1:A:21:ARG:HB3  | 1:A:23:MET:HE1  | 0.50     | 1.83        | 10     | 1     |
| 1:A:29:PRO:HD2  | 1:A:82:ILE:HD11 | 0.50     | 1.83        | 5      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:72:TYR:N    | 1:A:75:LEU:HD23 | 0.50     | 2.22        | 8      | 2     |
| 1:A:83:LEU:O    | 1:A:87:GLU:CG   | 0.50     | 2.59        | 6      | 2     |
| 1:A:25:LEU:HD11 | 1:A:81:ARG:O    | 0.50     | 2.06        | 8      | 1     |
| 1:A:61:SER:O    | 1:A:65:GLN:HB3  | 0.49     | 2.07        | 6      | 4     |
| 1:A:61:SER:O    | 1:A:65:GLN:CB   | 0.49     | 2.60        | 2      | 4     |
| 1:A:48:PHE:CB   | 1:A:54:VAL:HB   | 0.49     | 2.37        | 8      | 2     |
| 1:A:41:LEU:HG   | 1:A:42:TYR:N    | 0.49     | 2.20        | 9      | 1     |
| 1:A:28:ILE:HG23 | 1:A:36:ILE:HG21 | 0.49     | 1.83        | 10     | 1     |
| 1:A:36:ILE:HG22 | 1:A:37:ASN:N    | 0.49     | 2.22        | 3      | 2     |
| 1:A:59:GLN:O    | 1:A:62:MET:CG   | 0.49     | 2.59        | 7      | 2     |
| 1:A:48:PHE:CZ   | 1:A:53:GLN:CB   | 0.49     | 2.95        | 4      | 2     |
| 1:A:48:PHE:HB2  | 1:A:54:VAL:HG23 | 0.49     | 1.84        | 6      | 1     |
| 1:A:18:CYS:CA   | 1:A:24:PRO:HD2  | 0.49     | 2.37        | 7      | 1     |
| 1:A:75:LEU:N    | 1:A:75:LEU:CD2  | 0.49     | 2.74        | 2      | 7     |
| 1:A:28:ILE:HG21 | 1:A:36:ILE:HD12 | 0.49     | 1.85        | 7      | 1     |
| 1:A:80:PHE:CD1  | 1:A:84:LEU:CD2  | 0.49     | 2.94        | 1      | 4     |
| 1:A:47:LYS:NZ   | 1:A:54:VAL:HG21 | 0.49     | 2.22        | 2      | 1     |
| 1:A:37:ASN:O    | 1:A:41:LEU:HD22 | 0.49     | 2.07        | 3      | 2     |
| 1:A:44:LEU:HD13 | 1:A:66:ARG:HG2  | 0.49     | 1.82        | 4      | 1     |
| 1:A:80:PHE:CD2  | 1:A:84:LEU:CD2  | 0.49     | 2.95        | 4      | 3     |
| 1:A:25:LEU:HD11 | 1:A:82:ILE:HG12 | 0.49     | 1.84        | 9      | 1     |
| 1:A:19:LYS:HA   | 1:A:23:MET:CE   | 0.49     | 2.37        | 7      | 2     |
| 1:A:40:TYR:C    | 1:A:43:MET:HE1  | 0.49     | 2.31        | 9      | 1     |
| 1:A:61:SER:O    | 1:A:65:GLN:CG   | 0.49     | 2.61        | 1      | 7     |
| 1:A:60:TRP:CD1  | 1:A:72:TYR:O    | 0.49     | 2.65        | 6      | 1     |
| 1:A:14:LEU:HD21 | 1:A:82:ILE:O    | 0.49     | 2.07        | 8      | 2     |
| 1:A:44:LEU:HD11 | 1:A:66:ARG:CD   | 0.49     | 2.38        | 8      | 1     |
| 1:A:82:ILE:O    | 1:A:82:ILE:CG2  | 0.49     | 2.61        | 10     | 1     |
| 1:A:47:LYS:HG3  | 1:A:59:GLN:HG3  | 0.49     | 1.84        | 9      | 5     |
| 1:A:11:MET:CE   | 1:A:14:LEU:HD12 | 0.49     | 2.37        | 2      | 1     |
| 1:A:64:ALA:HA   | 1:A:75:LEU:HD21 | 0.49     | 1.83        | 2      | 2     |
| 1:A:21:ARG:O    | 1:A:22:ASN:HB3  | 0.49     | 2.08        | 10     | 3     |
| 1:A:21:ARG:CB   | 1:A:24:PRO:HG3  | 0.49     | 2.38        | 10     | 1     |
| 1:A:44:LEU:N    | 1:A:44:LEU:CD2  | 0.49     | 2.70        | 3      | 6     |
| 1:A:63:VAL:CG1  | 1:A:64:ALA:N    | 0.49     | 2.76        | 1      | 2     |
| 1:A:80:PHE:CD2  | 1:A:81:ARG:CD   | 0.49     | 2.96        | 7      | 3     |
| 1:A:67:LEU:CD2  | 1:A:69:ILE:HG22 | 0.49     | 2.38        | 8      | 3     |
| 1:A:38:LEU:HD11 | 1:A:82:ILE:HG21 | 0.49     | 1.85        | 1      | 2     |
| 1:A:23:MET:H    | 1:A:24:PRO:CD   | 0.49     | 2.21        | 10     | 1     |
| 1:A:13:SER:CB   | 1:A:86:TYR:CZ   | 0.49     | 2.96        | 5      | 4     |
| 1:A:51:ALA:CB   | 1:A:79:TYR:CG   | 0.49     | 2.96        | 8      | 4     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:47:LYS:HG2  | 1:A:59:GLN:HB3  | 0.49     | 1.85        | 3      | 2     |
| 1:A:10:PHE:CE1  | 1:A:39:PHE:CZ   | 0.48     | 3.01        | 2      | 1     |
| 1:A:54:VAL:HG13 | 1:A:60:TRP:CZ3  | 0.48     | 2.42        | 5      | 2     |
| 1:A:39:PHE:CZ   | 1:A:86:TYR:CE2  | 0.48     | 3.00        | 9      | 1     |
| 1:A:42:TYR:CD2  | 1:A:43:MET:CE   | 0.48     | 2.96        | 3      | 7     |
| 1:A:41:LEU:CB   | 1:A:63:VAL:HG13 | 0.48     | 2.38        | 7      | 3     |
| 1:A:21:ARG:HD2  | 1:A:24:PRO:HB3  | 0.48     | 1.85        | 8      | 1     |
| 1:A:16:GLU:O    | 1:A:20:LYS:N    | 0.48     | 2.46        | 2      | 2     |
| 1:A:31:ILE:HG13 | 1:A:69:ILE:HD12 | 0.48     | 1.85        | 3      | 1     |
| 1:A:79:TYR:O    | 1:A:84:LEU:CA   | 0.48     | 2.61        | 9      | 7     |
| 1:A:51:ALA:O    | 1:A:55:THR:CG2  | 0.48     | 2.54        | 4      | 2     |
| 1:A:54:VAL:CG1  | 1:A:60:TRP:CH2  | 0.48     | 2.95        | 6      | 2     |
| 1:A:80:PHE:CE2  | 1:A:81:ARG:CZ   | 0.48     | 2.96        | 3      | 2     |
| 1:A:28:ILE:HG21 | 1:A:36:ILE:CD1  | 0.48     | 2.38        | 8      | 1     |
| 1:A:31:ILE:HD11 | 1:A:67:LEU:HD12 | 0.48     | 1.85        | 8      | 1     |
| 1:A:55:THR:HG21 | 1:A:76:GLU:CB   | 0.48     | 2.37        | 4      | 2     |
| 1:A:14:LEU:HB2  | 1:A:83:LEU:HD13 | 0.48     | 1.85        | 8      | 1     |
| 1:A:79:TYR:CG   | 1:A:87:GLU:OE2  | 0.48     | 2.67        | 6      | 1     |
| 1:A:72:TYR:HA   | 1:A:75:LEU:CD2  | 0.48     | 2.34        | 4      | 1     |
| 1:A:42:TYR:C    | 1:A:45:VAL:HG13 | 0.48     | 2.34        | 6      | 1     |
| 1:A:44:LEU:HD12 | 1:A:62:MET:O    | 0.48     | 2.08        | 3      | 2     |
| 1:A:55:THR:CA   | 1:A:60:TRP:NE1  | 0.48     | 2.76        | 4      | 2     |
| 1:A:48:PHE:CB   | 1:A:54:VAL:CG2  | 0.48     | 2.92        | 6      | 1     |
| 1:A:29:PRO:HD3  | 1:A:82:ILE:HD11 | 0.48     | 1.86        | 1      | 1     |
| 1:A:23:MET:N    | 1:A:24:PRO:HD3  | 0.48     | 2.24        | 2      | 3     |
| 1:A:45:VAL:HB   | 1:A:63:VAL:HG21 | 0.48     | 1.86        | 9      | 1     |
| 1:A:40:TYR:O    | 1:A:43:MET:N    | 0.47     | 2.47        | 10     | 4     |
| 1:A:48:PHE:CD2  | 1:A:57:THR:HG21 | 0.47     | 2.44        | 10     | 2     |
| 1:A:55:THR:HA   | 1:A:60:TRP:CG   | 0.47     | 2.43        | 5      | 2     |
| 1:A:60:TRP:CE2  | 1:A:75:LEU:CB   | 0.47     | 2.97        | 4      | 1     |
| 1:A:48:PHE:CZ   | 1:A:57:THR:CB   | 0.47     | 2.97        | 9      | 2     |
| 1:A:47:LYS:CD   | 1:A:47:LYS:C    | 0.47     | 2.87        | 5      | 6     |
| 1:A:78:ILE:HD13 | 1:A:78:ILE:N    | 0.47     | 2.23        | 5      | 1     |
| 1:A:42:TYR:O    | 1:A:45:VAL:CG2  | 0.47     | 2.57        | 6      | 1     |
| 1:A:25:LEU:HD23 | 1:A:82:ILE:CG1  | 0.47     | 2.35        | 7      | 1     |
| 1:A:39:PHE:O    | 1:A:42:TYR:N    | 0.47     | 2.47        | 9      | 1     |
| 1:A:39:PHE:CZ   | 1:A:83:LEU:HD21 | 0.47     | 2.44        | 10     | 1     |
| 1:A:60:TRP:CZ2  | 1:A:75:LEU:HB3  | 0.47     | 2.45        | 9      | 4     |
| 1:A:64:ALA:O    | 1:A:69:ILE:CG2  | 0.47     | 2.63        | 3      | 3     |
| 1:A:75:LEU:C    | 1:A:78:ILE:HG23 | 0.47     | 2.34        | 1      | 5     |
| 1:A:16:GLU:O    | 1:A:20:LYS:HG2  | 0.47     | 2.09        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:14:LEU:CD2  | 1:A:14:LEU:C    | 0.47     | 2.81        | 2      | 2     |
| 1:A:42:TYR:CD1  | 1:A:42:TYR:O    | 0.47     | 2.68        | 7      | 4     |
| 1:A:25:LEU:HD22 | 1:A:82:ILE:CG2  | 0.47     | 2.39        | 3      | 1     |
| 1:A:75:LEU:N    | 1:A:75:LEU:HD22 | 0.47     | 2.25        | 8      | 1     |
| 1:A:7:TYR:HA    | 1:A:10:PHE:CD2  | 0.47     | 2.44        | 6      | 2     |
| 1:A:42:TYR:CE2  | 1:A:43:MET:CE   | 0.47     | 2.98        | 1      | 5     |
| 1:A:10:PHE:CD1  | 1:A:11:MET:N    | 0.47     | 2.83        | 8      | 4     |
| 1:A:48:PHE:CB   | 1:A:54:VAL:HG23 | 0.47     | 2.38        | 6      | 1     |
| 1:A:62:MET:O    | 1:A:66:ARG:HB2  | 0.47     | 2.10        | 1      | 1     |
| 1:A:7:TYR:CD2   | 1:A:8:GLU:N     | 0.47     | 2.83        | 2      | 1     |
| 1:A:42:TYR:O    | 1:A:43:MET:C    | 0.47     | 2.58        | 4      | 9     |
| 1:A:47:LYS:CE   | 1:A:62:MET:CE   | 0.47     | 2.92        | 2      | 1     |
| 1:A:13:SER:CB   | 1:A:86:TYR:CE2  | 0.47     | 2.98        | 3      | 3     |
| 1:A:41:LEU:CD2  | 1:A:78:ILE:CD1  | 0.47     | 2.90        | 3      | 3     |
| 1:A:60:TRP:O    | 1:A:64:ALA:N    | 0.47     | 2.48        | 6      | 2     |
| 1:A:25:LEU:CD2  | 1:A:82:ILE:HD13 | 0.47     | 2.40        | 10     | 1     |
| 1:A:55:THR:CG2  | 1:A:76:GLU:CB   | 0.47     | 2.93        | 1      | 3     |
| 1:A:79:TYR:CD2  | 1:A:87:GLU:OE1  | 0.47     | 2.68        | 1      | 5     |
| 1:A:47:LYS:HG3  | 1:A:59:GLN:CG   | 0.47     | 2.40        | 5      | 2     |
| 1:A:79:TYR:O    | 1:A:83:LEU:C    | 0.46     | 2.58        | 4      | 4     |
| 1:A:80:PHE:CG   | 1:A:84:LEU:HD23 | 0.46     | 2.45        | 3      | 2     |
| 1:A:47:LYS:C    | 1:A:47:LYS:CD   | 0.46     | 2.88        | 8      | 2     |
| 1:A:45:VAL:HG11 | 1:A:79:TYR:HD2  | 0.46     | 1.68        | 2      | 2     |
| 1:A:14:LEU:HG   | 1:A:38:LEU:HD11 | 0.46     | 1.87        | 4      | 1     |
| 1:A:22:ASN:C    | 1:A:23:MET:SD   | 0.46     | 2.98        | 10     | 1     |
| 1:A:80:PHE:CD1  | 1:A:80:PHE:C    | 0.46     | 2.93        | 1      | 8     |
| 1:A:54:VAL:HG13 | 1:A:60:TRP:CZ2  | 0.46     | 2.45        | 6      | 1     |
| 1:A:46:GLN:O    | 1:A:47:LYS:C    | 0.46     | 2.59        | 5      | 4     |
| 1:A:38:LEU:HD21 | 1:A:82:ILE:HD13 | 0.46     | 1.87        | 9      | 1     |
| 1:A:14:LEU:HD23 | 1:A:83:LEU:CG   | 0.46     | 2.41        | 4      | 2     |
| 1:A:36:ILE:HD12 | 1:A:36:ILE:C    | 0.46     | 2.36        | 5      | 2     |
| 1:A:75:LEU:HA   | 1:A:78:ILE:CG1  | 0.46     | 2.41        | 5      | 1     |
| 1:A:75:LEU:HA   | 1:A:78:ILE:HG23 | 0.46     | 1.87        | 9      | 6     |
| 1:A:47:LYS:HD3  | 1:A:54:VAL:HG21 | 0.46     | 1.87        | 2      | 1     |
| 1:A:67:LEU:CD2  | 1:A:69:ILE:CG2  | 0.46     | 2.94        | 8      | 2     |
| 1:A:57:THR:HG21 | 1:A:59:GLN:CD   | 0.46     | 2.35        | 5      | 1     |
| 1:A:38:LEU:HD23 | 1:A:78:ILE:HB   | 0.46     | 1.88        | 10     | 1     |
| 1:A:41:LEU:CD2  | 1:A:78:ILE:HD13 | 0.46     | 2.39        | 1      | 5     |
| 1:A:10:PHE:CZ   | 1:A:39:PHE:HB2  | 0.46     | 2.46        | 9      | 1     |
| 1:A:47:LYS:CD   | 1:A:47:LYS:O    | 0.46     | 2.64        | 5      | 2     |
| 1:A:14:LEU:CD2  | 1:A:83:LEU:HG   | 0.46     | 2.41        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:83:LEU:CD1  | 1:A:86:TYR:HB2  | 0.46     | 2.41        | 4      | 1     |
| 1:A:48:PHE:CD1  | 1:A:53:GLN:HB3  | 0.46     | 2.46        | 5      | 1     |
| 1:A:14:LEU:CD2  | 1:A:83:LEU:HB2  | 0.46     | 2.41        | 3      | 2     |
| 1:A:48:PHE:CD2  | 1:A:53:GLN:HB3  | 0.46     | 2.46        | 4      | 1     |
| 1:A:83:LEU:CD1  | 1:A:86:TYR:CB   | 0.46     | 2.94        | 6      | 2     |
| 1:A:64:ALA:HA   | 1:A:75:LEU:CG   | 0.46     | 2.41        | 2      | 1     |
| 1:A:18:CYS:CB   | 1:A:25:LEU:HD22 | 0.45     | 2.41        | 2      | 1     |
| 1:A:29:PRO:O    | 1:A:31:ILE:N    | 0.45     | 2.48        | 7      | 2     |
| 1:A:80:PHE:CE2  | 1:A:81:ARG:NH1  | 0.45     | 2.85        | 8      | 1     |
| 1:A:48:PHE:CZ   | 1:A:53:GLN:HG2  | 0.45     | 2.47        | 1      | 2     |
| 1:A:11:MET:HE3  | 1:A:11:MET:HA   | 0.45     | 1.87        | 7      | 1     |
| 1:A:83:LEU:HD21 | 1:A:87:GLU:OE2  | 0.45     | 2.11        | 8      | 1     |
| 1:A:42:TYR:C    | 1:A:44:LEU:N    | 0.45     | 2.74        | 4      | 7     |
| 1:A:14:LEU:CD1  | 1:A:82:ILE:HG22 | 0.45     | 2.41        | 3      | 1     |
| 1:A:48:PHE:CE1  | 1:A:53:GLN:HG3  | 0.45     | 2.47        | 7      | 2     |
| 1:A:48:PHE:CG   | 1:A:53:GLN:HB3  | 0.45     | 2.46        | 4      | 1     |
| 1:A:54:VAL:HA   | 1:A:57:THR:CG2  | 0.45     | 2.42        | 6      | 2     |
| 1:A:14:LEU:O    | 1:A:17:ASN:N    | 0.45     | 2.50        | 8      | 1     |
| 1:A:44:LEU:O    | 1:A:47:LYS:HE3  | 0.45     | 2.11        | 2      | 1     |
| 1:A:54:VAL:HG23 | 1:A:59:GLN:HG3  | 0.45     | 1.87        | 3      | 1     |
| 1:A:31:ILE:HD13 | 1:A:31:ILE:N    | 0.45     | 2.27        | 6      | 1     |
| 1:A:14:LEU:C    | 1:A:14:LEU:CD1  | 0.45     | 2.89        | 7      | 3     |
| 1:A:13:SER:HB3  | 1:A:86:TYR:CE2  | 0.45     | 2.47        | 7      | 3     |
| 1:A:31:ILE:HG22 | 1:A:69:ILE:HD13 | 0.45     | 1.87        | 4      | 2     |
| 1:A:48:PHE:CE2  | 1:A:53:GLN:CB   | 0.45     | 3.00        | 4      | 1     |
| 1:A:57:THR:HG23 | 1:A:59:GLN:H    | 0.45     | 1.72        | 5      | 1     |
| 1:A:37:ASN:O    | 1:A:41:LEU:CD2  | 0.45     | 2.65        | 8      | 4     |
| 1:A:42:TYR:CZ   | 1:A:87:GLU:HB3  | 0.45     | 2.47        | 10     | 3     |
| 1:A:79:TYR:CG   | 1:A:87:GLU:OE1  | 0.45     | 2.69        | 8      | 5     |
| 1:A:71:ASP:O    | 1:A:72:TYR:C    | 0.45     | 2.60        | 8      | 3     |
| 1:A:43:MET:CE   | 1:A:43:MET:N    | 0.45     | 2.79        | 9      | 1     |
| 1:A:13:SER:OG   | 1:A:86:TYR:CZ   | 0.45     | 2.70        | 4      | 1     |
| 1:A:80:PHE:CE2  | 1:A:84:LEU:CD2  | 0.45     | 3.00        | 5      | 2     |
| 1:A:83:LEU:HD11 | 1:A:86:TYR:CB   | 0.45     | 2.42        | 6      | 1     |
| 1:A:10:PHE:HB2  | 1:A:39:PHE:CZ   | 0.44     | 2.47        | 1      | 2     |
| 1:A:75:LEU:CA   | 1:A:78:ILE:HG23 | 0.44     | 2.43        | 10     | 7     |
| 1:A:60:TRP:CZ3  | 1:A:63:VAL:CG2  | 0.44     | 2.95        | 9      | 6     |
| 1:A:14:LEU:HA   | 1:A:83:LEU:HD13 | 0.44     | 1.88        | 3      | 1     |
| 1:A:85:PRO:O    | 1:A:89:HIS:N    | 0.44     | 2.50        | 5      | 4     |
| 1:A:19:LYS:CG   | 1:A:23:MET:HE3  | 0.44     | 2.42        | 2      | 1     |
| 1:A:13:SER:HB2  | 1:A:86:TYR:CE2  | 0.44     | 2.47        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:17:ASN:O    | 1:A:21:ARG:N    | 0.44     | 2.47        | 1      | 2     |
| 1:A:31:ILE:HG21 | 1:A:69:ILE:CG1  | 0.44     | 2.42        | 6      | 2     |
| 1:A:64:ALA:CA   | 1:A:75:LEU:HD21 | 0.44     | 2.43        | 5      | 1     |
| 1:A:41:LEU:CD1  | 1:A:67:LEU:HD22 | 0.44     | 2.32        | 7      | 2     |
| 1:A:25:LEU:HD21 | 1:A:28:ILE:HG13 | 0.44     | 1.89        | 1      | 1     |
| 1:A:85:PRO:O    | 1:A:89:HIS:CB   | 0.44     | 2.66        | 3      | 1     |
| 1:A:41:LEU:HD23 | 1:A:41:LEU:N    | 0.44     | 2.28        | 1      | 2     |
| 1:A:43:MET:CA   | 1:A:43:MET:CE   | 0.44     | 2.94        | 8      | 7     |
| 1:A:71:ASP:C    | 1:A:75:LEU:CD2  | 0.44     | 2.90        | 8      | 2     |
| 1:A:79:TYR:CD1  | 1:A:79:TYR:C    | 0.44     | 2.96        | 2      | 4     |
| 1:A:59:GLN:C    | 1:A:62:MET:HE2  | 0.44     | 2.37        | 6      | 1     |
| 1:A:14:LEU:CG   | 1:A:83:LEU:HD13 | 0.44     | 2.43        | 8      | 1     |
| 1:A:27:SER:O    | 1:A:28:ILE:O    | 0.44     | 2.36        | 9      | 1     |
| 1:A:47:LYS:CG   | 1:A:59:GLN:HB3  | 0.44     | 2.42        | 6      | 3     |
| 1:A:47:LYS:HE2  | 1:A:59:GLN:CB   | 0.44     | 2.43        | 2      | 1     |
| 1:A:71:ASP:O    | 1:A:73:GLN:N    | 0.44     | 2.50        | 9      | 2     |
| 1:A:29:PRO:CG   | 1:A:82:ILE:CD1  | 0.44     | 2.95        | 3      | 2     |
| 1:A:44:LEU:CD1  | 1:A:66:ARG:CB   | 0.44     | 2.96        | 4      | 2     |
| 1:A:44:LEU:HD23 | 1:A:66:ARG:HG2  | 0.44     | 1.90        | 6      | 1     |
| 1:A:54:VAL:HG22 | 1:A:60:TRP:CE3  | 0.44     | 2.47        | 1      | 1     |
| 1:A:14:LEU:C    | 1:A:14:LEU:CD2  | 0.44     | 2.82        | 6      | 1     |
| 1:A:63:VAL:HG12 | 1:A:75:LEU:CG   | 0.44     | 2.43        | 6      | 1     |
| 1:A:13:SER:HB3  | 1:A:86:TYR:CZ   | 0.44     | 2.48        | 8      | 3     |
| 1:A:22:ASN:O    | 1:A:23:MET:C    | 0.44     | 2.61        | 6      | 1     |
| 1:A:29:PRO:O    | 1:A:31:ILE:CD1  | 0.44     | 2.65        | 6      | 1     |
| 1:A:69:ILE:CD1  | 1:A:71:ASP:CB   | 0.44     | 2.96        | 6      | 1     |
| 1:A:21:ARG:C    | 1:A:23:MET:HE1  | 0.44     | 2.38        | 10     | 1     |
| 1:A:38:LEU:O    | 1:A:42:TYR:CB   | 0.44     | 2.66        | 3      | 1     |
| 1:A:23:MET:HE2  | 1:A:23:MET:C    | 0.44     | 2.38        | 10     | 1     |
| 1:A:25:LEU:CG   | 1:A:82:ILE:HG23 | 0.44     | 2.43        | 10     | 1     |
| 1:A:63:VAL:HG12 | 1:A:75:LEU:HG   | 0.43     | 1.90        | 6      | 1     |
| 1:A:78:ILE:O    | 1:A:82:ILE:HB   | 0.43     | 2.11        | 6      | 2     |
| 1:A:23:MET:HE2  | 1:A:23:MET:CA   | 0.43     | 2.43        | 10     | 2     |
| 1:A:23:MET:CE   | 1:A:23:MET:CA   | 0.43     | 2.96        | 3      | 2     |
| 1:A:48:PHE:CZ   | 1:A:53:GLN:HB2  | 0.43     | 2.49        | 5      | 2     |
| 1:A:45:VAL:HG21 | 1:A:54:VAL:HG11 | 0.43     | 1.86        | 7      | 1     |
| 1:A:69:ILE:HG13 | 1:A:71:ASP:CB   | 0.43     | 2.43        | 8      | 1     |
| 1:A:28:ILE:HD12 | 1:A:28:ILE:N    | 0.43     | 2.28        | 10     | 1     |
| 1:A:25:LEU:HD21 | 1:A:82:ILE:HG23 | 0.43     | 1.90        | 2      | 1     |
| 1:A:47:LYS:O    | 1:A:47:LYS:CD   | 0.43     | 2.66        | 4      | 1     |
| 1:A:48:PHE:C    | 1:A:50:GLY:N    | 0.43     | 2.75        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:14:LEU:O    | 1:A:17:ASN:HB3  | 0.43     | 2.13        | 10     | 1     |
| 1:A:69:ILE:HD12 | 1:A:70:SER:N    | 0.43     | 2.28        | 10     | 1     |
| 1:A:41:LEU:CG   | 1:A:78:ILE:CD1  | 0.43     | 2.95        | 8      | 4     |
| 1:A:64:ALA:O    | 1:A:69:ILE:O    | 0.43     | 2.35        | 10     | 1     |
| 1:A:18:CYS:CB   | 1:A:24:PRO:HD2  | 0.43     | 2.44        | 7      | 1     |
| 1:A:39:PHE:O    | 1:A:43:MET:N    | 0.43     | 2.49        | 7      | 1     |
| 1:A:38:LEU:CD1  | 1:A:82:ILE:CG2  | 0.43     | 2.96        | 1      | 2     |
| 1:A:54:VAL:CG1  | 1:A:60:TRP:CZ3  | 0.43     | 3.01        | 2      | 2     |
| 1:A:78:ILE:CG1  | 1:A:79:TYR:H    | 0.43     | 2.22        | 3      | 2     |
| 1:A:64:ALA:HA   | 1:A:67:LEU:HD21 | 0.43     | 1.90        | 8      | 1     |
| 1:A:29:PRO:CD   | 1:A:82:ILE:HD13 | 0.43     | 2.44        | 3      | 1     |
| 1:A:41:LEU:CD1  | 1:A:75:LEU:HD13 | 0.43     | 2.44        | 4      | 1     |
| 1:A:48:PHE:CE1  | 1:A:53:GLN:CB   | 0.43     | 3.01        | 5      | 1     |
| 1:A:51:ALA:HB2  | 1:A:79:TYR:CB   | 0.43     | 2.43        | 5      | 1     |
| 1:A:43:MET:O    | 1:A:46:GLN:HB2  | 0.43     | 2.14        | 9      | 2     |
| 1:A:60:TRP:CE3  | 1:A:63:VAL:HB   | 0.43     | 2.49        | 9      | 2     |
| 1:A:21:ARG:O    | 1:A:23:MET:CE   | 0.43     | 2.66        | 10     | 1     |
| 1:A:39:PHE:CD1  | 1:A:83:LEU:HD21 | 0.43     | 2.49        | 7      | 1     |
| 1:A:35:LYS:HG3  | 1:A:35:LYS:O    | 0.43     | 2.13        | 8      | 1     |
| 1:A:47:LYS:CG   | 1:A:59:GLN:CG   | 0.43     | 2.97        | 9      | 2     |
| 1:A:54:VAL:HA   | 1:A:57:THR:HG22 | 0.43     | 1.90        | 5      | 1     |
| 1:A:11:MET:HA   | 1:A:11:MET:CE   | 0.43     | 2.43        | 7      | 1     |
| 1:A:48:PHE:CZ   | 1:A:57:THR:OG1  | 0.43     | 2.72        | 9      | 1     |
| 1:A:25:LEU:HG   | 1:A:82:ILE:HG23 | 0.43     | 1.91        | 10     | 1     |
| 1:A:13:SER:OG   | 1:A:86:TYR:CE1  | 0.42     | 2.71        | 1      | 1     |
| 1:A:19:LYS:CA   | 1:A:23:MET:HE3  | 0.42     | 2.39        | 4      | 2     |
| 1:A:28:ILE:HG21 | 1:A:36:ILE:HD11 | 0.42     | 1.90        | 8      | 1     |
| 1:A:28:ILE:CG2  | 1:A:38:LEU:HD21 | 0.42     | 2.44        | 1      | 1     |
| 1:A:55:THR:CG2  | 1:A:76:GLU:HB3  | 0.42     | 2.44        | 6      | 1     |
| 1:A:25:LEU:HD21 | 1:A:28:ILE:N    | 0.42     | 2.29        | 1      | 1     |
| 1:A:25:LEU:HD13 | 1:A:82:ILE:HG12 | 0.42     | 1.89        | 1      | 1     |
| 1:A:45:VAL:C    | 1:A:47:LYS:HD2  | 0.42     | 2.39        | 2      | 1     |
| 1:A:45:VAL:C    | 1:A:47:LYS:N    | 0.42     | 2.77        | 9      | 5     |
| 1:A:77:SER:CA   | 1:A:81:ARG:HB2  | 0.42     | 2.44        | 5      | 1     |
| 1:A:31:ILE:N    | 1:A:31:ILE:HD13 | 0.42     | 2.28        | 7      | 1     |
| 1:A:48:PHE:CD1  | 1:A:57:THR:HG21 | 0.42     | 2.48        | 8      | 1     |
| 1:A:67:LEU:HD21 | 1:A:69:ILE:HG21 | 0.42     | 1.90        | 8      | 1     |
| 1:A:17:ASN:O    | 1:A:24:PRO:HG2  | 0.42     | 2.14        | 10     | 1     |
| 1:A:11:MET:CE   | 1:A:11:MET:HA   | 0.42     | 2.45        | 1      | 1     |
| 1:A:83:LEU:CD1  | 1:A:87:GLU:HG2  | 0.42     | 2.45        | 1      | 1     |
| 1:A:83:LEU:HD12 | 1:A:87:GLU:HG2  | 0.42     | 1.91        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:77:SER:HA   | 1:A:81:ARG:HB2  | 0.42     | 1.92        | 4      | 2     |
| 1:A:22:ASN:OD1  | 1:A:22:ASN:N    | 0.42     | 2.52        | 6      | 1     |
| 1:A:42:TYR:CE2  | 1:A:87:GLU:HB3  | 0.42     | 2.49        | 8      | 1     |
| 1:A:18:CYS:O    | 1:A:23:MET:CA   | 0.42     | 2.68        | 10     | 1     |
| 1:A:27:SER:O    | 1:A:28:ILE:C    | 0.42     | 2.62        | 9      | 2     |
| 1:A:18:CYS:O    | 1:A:23:MET:HA   | 0.42     | 2.14        | 10     | 2     |
| 1:A:23:MET:HE3  | 1:A:23:MET:CA   | 0.42     | 2.45        | 5      | 1     |
| 1:A:63:VAL:O    | 1:A:66:ARG:HB2  | 0.42     | 2.14        | 7      | 1     |
| 1:A:17:ASN:O    | 1:A:20:LYS:HB2  | 0.42     | 2.15        | 8      | 1     |
| 1:A:43:MET:CE   | 1:A:43:MET:CA   | 0.42     | 2.96        | 9      | 1     |
| 1:A:11:MET:O    | 1:A:15:ILE:CG1  | 0.42     | 2.68        | 4      | 3     |
| 1:A:79:TYR:CE2  | 1:A:87:GLU:HB2  | 0.42     | 2.50        | 1      | 1     |
| 1:A:23:MET:N    | 1:A:24:PRO:CD   | 0.42     | 2.82        | 2      | 1     |
| 1:A:38:LEU:CD1  | 1:A:82:ILE:HD13 | 0.42     | 2.45        | 2      | 1     |
| 1:A:41:LEU:CB   | 1:A:67:LEU:HD22 | 0.42     | 2.45        | 4      | 1     |
| 1:A:63:VAL:HG12 | 1:A:75:LEU:HD11 | 0.42     | 1.92        | 5      | 1     |
| 1:A:21:ARG:O    | 1:A:21:ARG:CG   | 0.42     | 2.67        | 8      | 1     |
| 1:A:39:PHE:O    | 1:A:40:TYR:C    | 0.42     | 2.61        | 9      | 1     |
| 1:A:13:SER:O    | 1:A:86:TYR:CE2  | 0.42     | 2.73        | 10     | 3     |
| 1:A:42:TYR:CD1  | 1:A:45:VAL:CG1  | 0.42     | 2.97        | 4      | 1     |
| 1:A:31:ILE:HG13 | 1:A:67:LEU:CD1  | 0.42     | 2.45        | 5      | 1     |
| 1:A:41:LEU:CD1  | 1:A:78:ILE:CD1  | 0.42     | 2.93        | 6      | 1     |
| 1:A:47:LYS:O    | 1:A:47:LYS:CE   | 0.42     | 2.67        | 8      | 1     |
| 1:A:83:LEU:CD2  | 1:A:87:GLU:OE2  | 0.42     | 2.67        | 8      | 1     |
| 1:A:42:TYR:CE1  | 1:A:87:GLU:HB3  | 0.42     | 2.50        | 9      | 1     |
| 1:A:14:LEU:HD13 | 1:A:15:ILE:CG1  | 0.42     | 2.44        | 2      | 1     |
| 1:A:47:LYS:HG3  | 1:A:59:GLN:HB3  | 0.42     | 1.90        | 6      | 1     |
| 1:A:28:ILE:N    | 1:A:28:ILE:CD1  | 0.42     | 2.83        | 10     | 1     |
| 1:A:28:ILE:HG22 | 1:A:30:GLU:H    | 0.42     | 1.75        | 10     | 1     |
| 1:A:67:LEU:O    | 1:A:68:GLN:CB   | 0.42     | 2.68        | 1      | 1     |
| 1:A:80:PHE:CD1  | 1:A:80:PHE:O    | 0.42     | 2.73        | 2      | 4     |
| 1:A:25:LEU:O    | 1:A:26:GLN:HB2  | 0.42     | 2.15        | 4      | 1     |
| 1:A:48:PHE:CE2  | 1:A:53:GLN:HB2  | 0.42     | 2.49        | 4      | 1     |
| 1:A:25:LEU:HD21 | 1:A:82:ILE:HG12 | 0.42     | 1.92        | 8      | 1     |
| 1:A:18:CYS:C    | 1:A:23:MET:HE2  | 0.42     | 2.39        | 9      | 1     |
| 1:A:63:VAL:HG13 | 1:A:75:LEU:HD12 | 0.42     | 1.89        | 1      | 2     |
| 1:A:52:ASP:CA   | 1:A:76:GLU:OE2  | 0.42     | 2.68        | 3      | 2     |
| 1:A:14:LEU:HA   | 1:A:83:LEU:CD1  | 0.42     | 2.45        | 3      | 1     |
| 1:A:67:LEU:HG   | 1:A:69:ILE:HG22 | 0.42     | 1.92        | 10     | 2     |
| 1:A:39:PHE:CE1  | 1:A:86:TYR:CE2  | 0.42     | 3.08        | 9      | 1     |
| 1:A:40:TYR:O    | 1:A:41:LEU:C    | 0.42     | 2.63        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:16:GLU:O    | 1:A:20:LYS:HB3  | 0.41     | 2.15        | 9      | 2     |
| 1:A:47:LYS:HZ2  | 1:A:54:VAL:HG21 | 0.41     | 1.75        | 2      | 1     |
| 1:A:39:PHE:O    | 1:A:43:MET:HG2  | 0.41     | 2.15        | 5      | 1     |
| 1:A:55:THR:HG23 | 1:A:76:GLU:HB3  | 0.41     | 1.91        | 6      | 1     |
| 1:A:48:PHE:CE2  | 1:A:53:GLN:O    | 0.41     | 2.73        | 8      | 1     |
| 1:A:64:ALA:HA   | 1:A:75:LEU:CD1  | 0.41     | 2.45        | 9      | 2     |
| 1:A:11:MET:O    | 1:A:15:ILE:HG13 | 0.41     | 2.15        | 9      | 1     |
| 1:A:42:TYR:O    | 1:A:42:TYR:CD1  | 0.41     | 2.74        | 5      | 1     |
| 1:A:51:ALA:HB1  | 1:A:55:THR:CG2  | 0.41     | 2.45        | 5      | 1     |
| 1:A:29:PRO:CD   | 1:A:82:ILE:CD1  | 0.41     | 2.98        | 6      | 1     |
| 1:A:23:MET:HE2  | 1:A:24:PRO:N    | 0.41     | 2.31        | 10     | 1     |
| 1:A:67:LEU:H    | 1:A:67:LEU:CD2  | 0.41     | 2.28        | 10     | 1     |
| 1:A:18:CYS:HA   | 1:A:24:PRO:HD2  | 0.41     | 1.92        | 1      | 2     |
| 1:A:25:LEU:CD1  | 1:A:27:SER:O    | 0.41     | 2.69        | 3      | 1     |
| 1:A:14:LEU:CB   | 1:A:83:LEU:HD13 | 0.41     | 2.46        | 8      | 1     |
| 1:A:21:ARG:HB3  | 1:A:24:PRO:HG3  | 0.41     | 1.93        | 10     | 1     |
| 1:A:25:LEU:HD22 | 1:A:28:ILE:CD1  | 0.41     | 2.45        | 10     | 1     |
| 1:A:30:GLU:HA   | 1:A:36:ILE:CG2  | 0.41     | 2.46        | 10     | 1     |
| 1:A:79:TYR:CZ   | 1:A:87:GLU:HB2  | 0.41     | 2.50        | 1      | 1     |
| 1:A:36:ILE:CG2  | 1:A:37:ASN:N    | 0.41     | 2.84        | 1      | 1     |
| 1:A:11:MET:CE   | 1:A:15:ILE:HD11 | 0.41     | 2.43        | 3      | 2     |
| 1:A:45:VAL:O    | 1:A:46:GLN:C    | 0.41     | 2.63        | 3      | 2     |
| 1:A:80:PHE:C    | 1:A:80:PHE:CD1  | 0.41     | 2.99        | 4      | 1     |
| 1:A:37:ASN:O    | 1:A:39:PHE:N    | 0.41     | 2.54        | 9      | 1     |
| 1:A:38:LEU:HD11 | 1:A:82:ILE:HD13 | 0.41     | 1.93        | 2      | 1     |
| 1:A:55:THR:CB   | 1:A:60:TRP:NE1  | 0.41     | 2.83        | 5      | 1     |
| 1:A:38:LEU:O    | 1:A:41:LEU:CD2  | 0.41     | 2.69        | 7      | 1     |
| 1:A:81:ARG:N    | 1:A:81:ARG:CD   | 0.41     | 2.83        | 8      | 1     |
| 1:A:33:ASN:O    | 1:A:35:LYS:N    | 0.41     | 2.54        | 9      | 1     |
| 1:A:14:LEU:HD21 | 1:A:38:LEU:CD1  | 0.41     | 2.38        | 3      | 1     |
| 1:A:42:TYR:O    | 1:A:44:LEU:N    | 0.41     | 2.54        | 4      | 1     |
| 1:A:83:LEU:HD13 | 1:A:86:TYR:CB   | 0.41     | 2.46        | 4      | 1     |
| 1:A:18:CYS:O    | 1:A:24:PRO:CD   | 0.41     | 2.69        | 5      | 1     |
| 1:A:23:MET:C    | 1:A:25:LEU:H    | 0.41     | 2.24        | 5      | 1     |
| 1:A:52:ASP:O    | 1:A:56:ARG:CG   | 0.41     | 2.68        | 5      | 1     |
| 1:A:75:LEU:CD2  | 1:A:75:LEU:H    | 0.41     | 2.29        | 6      | 1     |
| 1:A:79:TYR:CD2  | 1:A:87:GLU:OE2  | 0.41     | 2.74        | 6      | 1     |
| 1:A:80:PHE:O    | 1:A:84:LEU:HB2  | 0.41     | 2.16        | 9      | 1     |
| 1:A:7:TYR:CZ    | 1:A:8:GLU:OE1   | 0.41     | 2.74        | 2      | 1     |
| 1:A:43:MET:CE   | 1:A:44:LEU:N    | 0.41     | 2.83        | 9      | 1     |
| 1:A:10:PHE:CB   | 1:A:39:PHE:CD2  | 0.40     | 3.04        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:75:LEU:O    | 1:A:78:ILE:CB   | 0.40     | 2.70        | 1      | 1     |
| 1:A:13:SER:HB3  | 1:A:86:TYR:CE1  | 0.40     | 2.52        | 1      | 1     |
| 1:A:41:LEU:HD11 | 1:A:78:ILE:CG2  | 0.40     | 2.46        | 5      | 1     |
| 1:A:41:LEU:O    | 1:A:44:LEU:CB   | 0.40     | 2.68        | 6      | 1     |
| 1:A:72:TYR:C    | 1:A:75:LEU:HD23 | 0.40     | 2.41        | 7      | 1     |
| 1:A:25:LEU:N    | 1:A:25:LEU:CD1  | 0.40     | 2.84        | 8      | 1     |
| 1:A:23:MET:O    | 1:A:23:MET:HG2  | 0.40     | 2.16        | 10     | 1     |
| 1:A:12:LYS:O    | 1:A:16:GLU:N    | 0.40     | 2.54        | 2      | 1     |
| 1:A:64:ALA:HA   | 1:A:69:ILE:CG2  | 0.40     | 2.47        | 4      | 1     |
| 1:A:40:TYR:O    | 1:A:43:MET:HB2  | 0.40     | 2.17        | 10     | 1     |
| 1:A:47:LYS:HD3  | 1:A:47:LYS:O    | 0.40     | 2.16        | 10     | 1     |
| 1:A:80:PHE:HA   | 1:A:84:LEU:HD23 | 0.40     | 1.93        | 10     | 1     |
| 1:A:48:PHE:CD2  | 1:A:53:GLN:C    | 0.40     | 2.99        | 2      | 1     |
| 1:A:57:THR:CG2  | 1:A:59:GLN:HG2  | 0.40     | 2.46        | 3      | 1     |
| 1:A:51:ALA:O    | 1:A:55:THR:OG1  | 0.40     | 2.38        | 6      | 1     |
| 1:A:37:ASN:O    | 1:A:38:LEU:C    | 0.40     | 2.64        | 7      | 1     |
| 1:A:45:VAL:O    | 1:A:48:PHE:N    | 0.40     | 2.52        | 8      | 1     |
| 1:A:24:PRO:O    | 1:A:25:LEU:CG   | 0.40     | 2.69        | 10     | 1     |
| 1:A:28:ILE:HG23 | 1:A:36:ILE:HD13 | 0.40     | 1.94        | 10     | 1     |
| 1:A:13:SER:CB   | 1:A:86:TYR:CE1  | 0.40     | 3.05        | 1      | 1     |
| 1:A:25:LEU:HD22 | 1:A:82:ILE:HG12 | 0.40     | 1.93        | 4      | 1     |
| 1:A:69:ILE:HG12 | 1:A:71:ASP:HB2  | 0.40     | 1.93        | 6      | 1     |
| 1:A:17:ASN:O    | 1:A:20:LYS:HG3  | 0.40     | 2.16        | 7      | 1     |
| 1:A:48:PHE:CD2  | 1:A:53:GLN:HG2  | 0.40     | 2.51        | 8      | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed       | Favoured     | Allowed      | Outliers   | Percentiles |    |
|-----|-------|----------------|--------------|--------------|------------|-------------|----|
| 1   | A     | 83/123 (67%)   | 52±3 (62±4%) | 24±4 (28±4%) | 8±2 (9±2%) | 1           | 11 |
| All | All   | 830/1230 (67%) | 518 (62%)    | 236 (28%)    | 76 (9%)    | 1           | 11 |

All 25 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     | 63  | VAL  | 8              |
| 1   | A     | 27  | SER  | 8              |
| 1   | A     | 72  | TYR  | 7              |
| 1   | A     | 30  | GLU  | 6              |
| 1   | A     | 40  | TYR  | 6              |
| 1   | A     | 33  | ASN  | 5              |
| 1   | A     | 36  | ILE  | 4              |
| 1   | A     | 38  | LEU  | 4              |
| 1   | A     | 37  | ASN  | 3              |
| 1   | A     | 34  | ARG  | 3              |
| 1   | A     | 86  | TYR  | 2              |
| 1   | A     | 22  | ASN  | 2              |
| 1   | A     | 35  | LYS  | 2              |
| 1   | A     | 85  | PRO  | 2              |
| 1   | A     | 29  | PRO  | 2              |
| 1   | A     | 84  | LEU  | 2              |
| 1   | A     | 83  | LEU  | 2              |
| 1   | A     | 68  | GLN  | 1              |
| 1   | A     | 51  | ALA  | 1              |
| 1   | A     | 28  | ILE  | 1              |
| 1   | A     | 31  | ILE  | 1              |
| 1   | A     | 42  | TYR  | 1              |
| 1   | A     | 23  | MET  | 1              |
| 1   | A     | 24  | PRO  | 1              |
| 1   | A     | 25  | LEU  | 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     | 78/113 (69%)   | 43±3 (56±4%) | 35±3 (44±4%) | 0 3         |
| All | All   | 780/1130 (69%) | 433 (56%)    | 347 (44%)    | 0 3         |

All 65 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     | 34  | ARG  | 10             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 42  | TYR  | 10             |
| 1   | A     | 47  | LYS  | 10             |
| 1   | A     | 60  | TRP  | 10             |
| 1   | A     | 73  | GLN  | 10             |
| 1   | A     | 78  | ILE  | 10             |
| 1   | A     | 84  | LEU  | 10             |
| 1   | A     | 8   | GLU  | 9              |
| 1   | A     | 16  | GLU  | 9              |
| 1   | A     | 20  | LYS  | 9              |
| 1   | A     | 26  | GLN  | 9              |
| 1   | A     | 31  | ILE  | 9              |
| 1   | A     | 44  | LEU  | 9              |
| 1   | A     | 11  | MET  | 8              |
| 1   | A     | 14  | LEU  | 8              |
| 1   | A     | 35  | LYS  | 8              |
| 1   | A     | 66  | ARG  | 8              |
| 1   | A     | 21  | ARG  | 7              |
| 1   | A     | 38  | LEU  | 7              |
| 1   | A     | 48  | PHE  | 7              |
| 1   | A     | 52  | ASP  | 7              |
| 1   | A     | 77  | SER  | 7              |
| 1   | A     | 23  | MET  | 7              |
| 1   | A     | 28  | ILE  | 7              |
| 1   | A     | 43  | MET  | 7              |
| 1   | A     | 13  | SER  | 6              |
| 1   | A     | 19  | LYS  | 6              |
| 1   | A     | 39  | PHE  | 6              |
| 1   | A     | 56  | ARG  | 6              |
| 1   | A     | 69  | ILE  | 6              |
| 1   | A     | 40  | TYR  | 6              |
| 1   | A     | 45  | VAL  | 6              |
| 1   | A     | 15  | ILE  | 5              |
| 1   | A     | 25  | LEU  | 5              |
| 1   | A     | 86  | TYR  | 5              |
| 1   | A     | 89  | HIS  | 5              |
| 1   | A     | 27  | SER  | 5              |
| 1   | A     | 67  | LEU  | 5              |
| 1   | A     | 71  | ASP  | 5              |
| 1   | A     | 33  | ASN  | 4              |
| 1   | A     | 81  | ARG  | 4              |
| 1   | A     | 12  | LYS  | 4              |
| 1   | A     | 83  | LEU  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 61  | SER  | 3              |
| 1   | A     | 74  | GLN  | 3              |
| 1   | A     | 46  | GLN  | 3              |
| 1   | A     | 54  | VAL  | 3              |
| 1   | A     | 88  | ARG  | 3              |
| 1   | A     | 59  | GLN  | 3              |
| 1   | A     | 58  | GLN  | 3              |
| 1   | A     | 30  | GLU  | 2              |
| 1   | A     | 63  | VAL  | 2              |
| 1   | A     | 87  | GLU  | 2              |
| 1   | A     | 37  | ASN  | 2              |
| 1   | A     | 17  | ASN  | 2              |
| 1   | A     | 18  | CYS  | 2              |
| 1   | A     | 41  | LEU  | 1              |
| 1   | A     | 53  | GLN  | 1              |
| 1   | A     | 22  | ASN  | 1              |
| 1   | A     | 55  | THR  | 1              |
| 1   | A     | 72  | TYR  | 1              |
| 1   | A     | 36  | ILE  | 1              |
| 1   | A     | 62  | MET  | 1              |
| 1   | A     | 65  | GLN  | 1              |
| 1   | A     | 68  | GLN  | 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