



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 04:44 PM UTC

PDB ID : 1RLF / pdb\_00001rlf  
Title : STRUCTURE DETERMINATION OF THE RAS-BINDING DOMAIN OF  
THE RAL-SPECIFIC GUANINE NUCLEOTIDE EXCHANGE FACTOR  
RLF, NMR, 10 STRUCTURES  
Authors : Esser, D.; Bauer, B.; Wolthuis, R.M.F.; Wittinghofer, A.; Cool, R.H.; Bay, P.  
Deposited on : 1998-07-09

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                                                             |

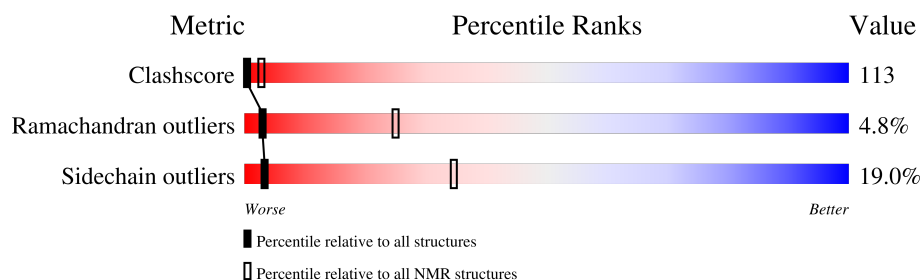
# 1 Overall quality at a glance

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     | 90     | <div> <div>17%</div> <div>58%</div> <div>22%</div> <div>.</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:649-A:735 (87)      | 0.58              | 7            |

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

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

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

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

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

There is only 1 type of molecule in this entry. The entry contains 1413 atoms, of which 709 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RLF.

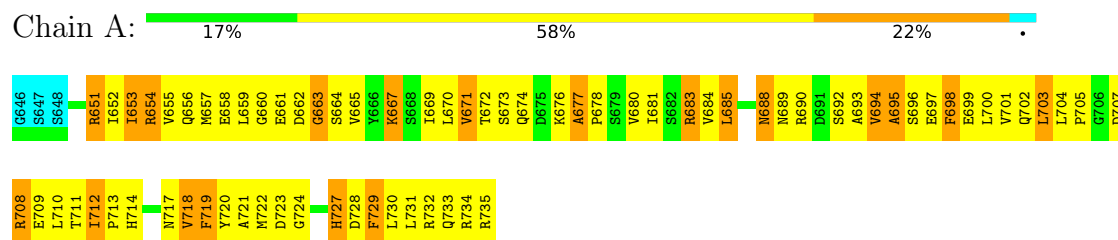
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 90       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1413  | 435 | 709 | 129 | 137 | 3 |       |

## 4 Residue-property plots

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

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

- Molecule 1: RLF

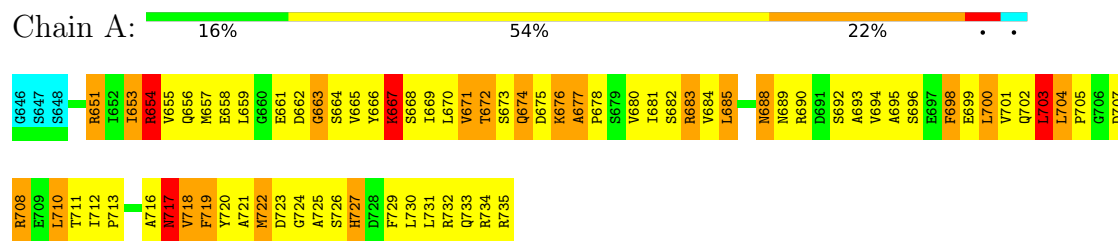


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

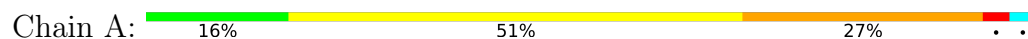
#### 4.2.1 Score per residue for model 1

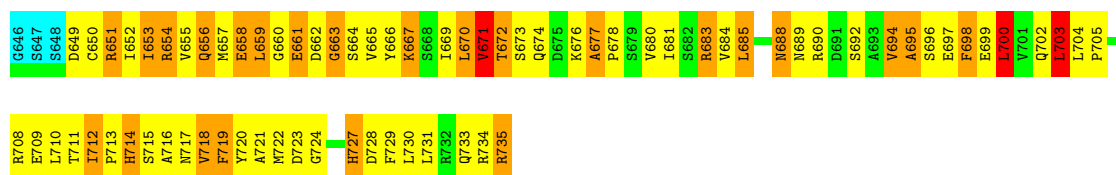
- Molecule 1: RLF



#### 4.2.2 Score per residue for model 2

- Molecule 1: RLF

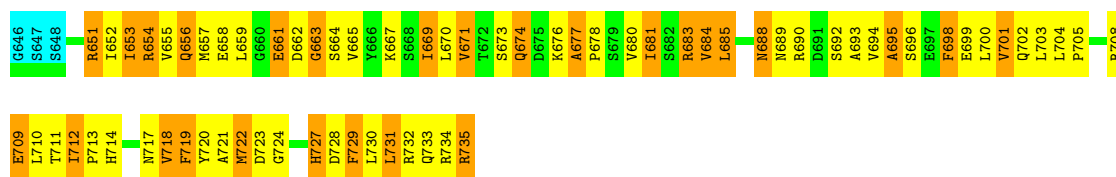




### 4.2.3 Score per residue for model 3

- Molecule 1: RLF

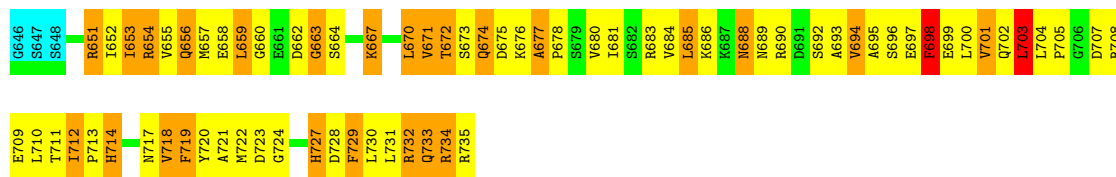
Chain A: 21% 46% 30% .



### 4.2.4 Score per residue for model 4

- Molecule 1: RLF

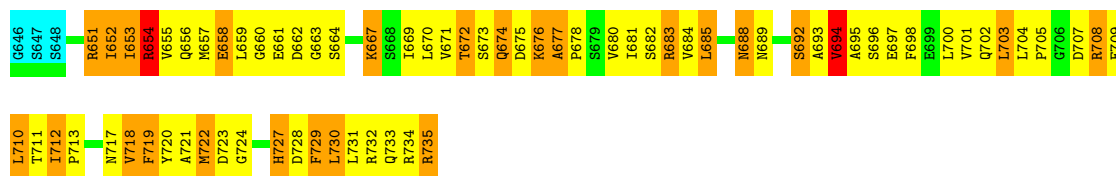
Chain A: 18% 49% 28% . .



### 4.2.5 Score per residue for model 5

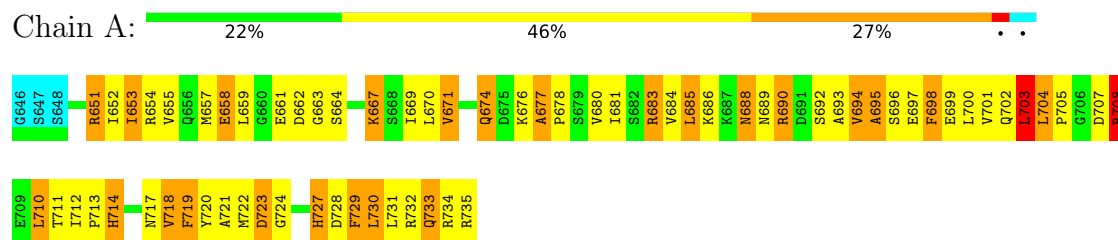
- Molecule 1: RLF

Chain A: 19% 49% 27% . .



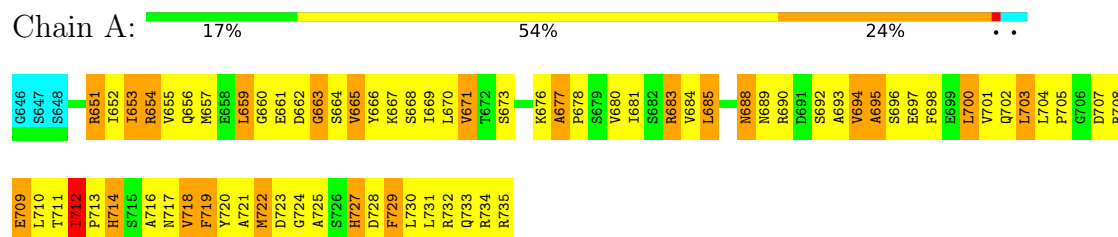
### 4.2.6 Score per residue for model 6

- Molecule 1: RLF



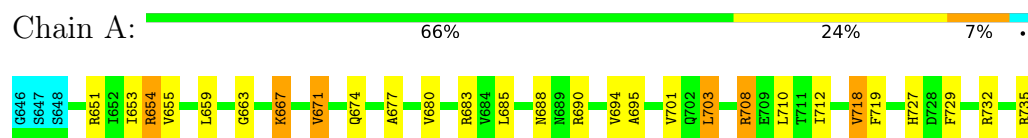
#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: RLF



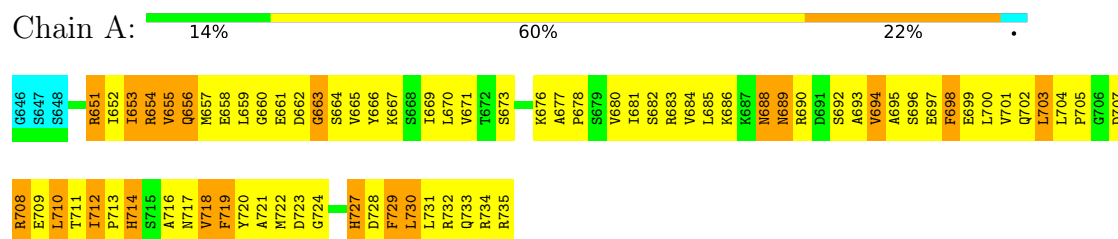
#### 4.2.8 Score per residue for model 8

- Molecule 1: RLF



#### 4.2.9 Score per residue for model 9

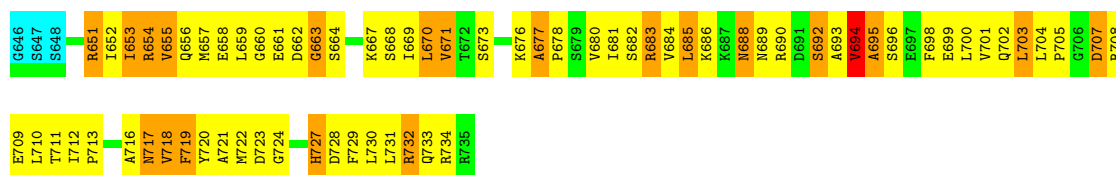
- Molecule 1: RLF



#### 4.2.10 Score per residue for model 10

- Molecule 1: RLF





## 5 Refinement protocol and experimental data overview

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

Of the 30 calculated structures, 10 were deposited, based on the following criterion: *ENERGY*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR        | refinement         | 3.851   |
| NDEE          | structure solution |         |
| X-PLOR        | structure solution | 3.851   |

No chemical shift data was provided.

## 6 Model quality

### 6.1 Standard geometry

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     | 1.51±0.02    | 0±0/697 ( 0.0± 0.1%) | 1.74±0.02   | 5±2/937 ( 0.6± 0.2%) |
| All | All   | 1.51         | 3/6970 ( 0.0%)       | 1.74        | 54/9370 ( 0.6%)      |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 7.1±0.5   |
| All | All   | 0         | 71        |

All unique bond 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(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 692 | SER  | N-CA  | 6.75 | 1.50        | 1.46     | 5      | 2     |
| 1   | A     | 725 | ALA  | N-CA  | 6.74 | 1.50        | 1.46     | 7      | 1     |

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     | 712 | ILE  | N-CA-CB  | -8.93 | 104.87      | 110.50   | 7      | 2     |
| 1   | A     | 719 | PHE  | CA-CB-CG | -7.09 | 106.71      | 113.80   | 7      | 10    |
| 1   | A     | 714 | HIS  | CA-CB-CG | -6.78 | 107.02      | 113.80   | 4      | 5     |
| 1   | A     | 694 | VAL  | N-CA-CB  | -6.12 | 103.95      | 112.52   | 4      | 7     |
| 1   | A     | 698 | PHE  | N-CA-CB  | -5.90 | 102.23      | 111.56   | 2      | 2     |
| 1   | A     | 671 | VAL  | N-CA-CB  | -5.89 | 105.00      | 112.60   | 8      | 2     |
| 1   | A     | 718 | VAL  | N-CA-CB  | -5.76 | 102.56      | 110.68   | 8      | 2     |
| 1   | A     | 674 | GLN  | N-CA-CB  | -5.59 | 101.98      | 111.20   | 3      | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 692 | SER  | CA-C-O  | 5.54  | 121.16      | 117.94   | 5      | 2     |
| 1   | A     | 655 | VAL  | N-CA-CB | -5.52 | 105.48      | 112.60   | 9      | 3     |
| 1   | A     | 659 | LEU  | N-CA-CB | -5.33 | 103.13      | 111.56   | 8      | 2     |
| 1   | A     | 701 | VAL  | N-CA-CB | -5.25 | 104.68      | 111.82   | 10     | 5     |
| 1   | A     | 654 | ARG  | N-CA-CB | -5.24 | 102.24      | 110.77   | 1      | 1     |
| 1   | A     | 658 | GLU  | N-CA-CB | -5.18 | 103.05      | 110.57   | 5      | 3     |
| 1   | A     | 710 | LEU  | N-CA-CB | -5.18 | 103.76      | 111.43   | 8      | 1     |
| 1   | A     | 714 | HIS  | N-CA-CB | -5.16 | 103.32      | 111.05   | 4      | 1     |
| 1   | A     | 665 | VAL  | N-CA-CB | -5.14 | 102.75      | 111.23   | 7      | 2     |
| 1   | A     | 666 | TYR  | N-CA-CB | -5.08 | 103.63      | 111.46   | 2      | 1     |
| 1   | A     | 700 | LEU  | N-CA-CB | -5.03 | 102.67      | 110.57   | 7      | 2     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 651 | ARG  | Sidechain | 10             |
| 1   | A     | 654 | ARG  | Sidechain | 9              |
| 1   | A     | 690 | ARG  | Sidechain | 9              |
| 1   | A     | 708 | ARG  | Sidechain | 9              |
| 1   | A     | 732 | ARG  | Sidechain | 9              |
| 1   | A     | 734 | ARG  | Sidechain | 9              |
| 1   | A     | 683 | ARG  | Sidechain | 8              |
| 1   | A     | 735 | ARG  | Sidechain | 8              |

## 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     | 688   | 694      | 694      | 148±50  |
| All | All   | 6880  | 6940     | 6246     | 1482    |

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 113.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:657:MET:HE3  | 1:A:693:ALA:HB3  | 1.12     | 1.19        | 6      | 1     |
| 1:A:698:PHE:CD2  | 1:A:700:LEU:HD11 | 1.09     | 1.81        | 2      | 1     |
| 1:A:698:PHE:CD1  | 1:A:700:LEU:HD21 | 1.08     | 1.83        | 9      | 3     |
| 1:A:700:LEU:HD22 | 1:A:731:LEU:HD22 | 1.06     | 1.16        | 4      | 4     |
| 1:A:669:ILE:HD13 | 1:A:680:VAL:HG21 | 0.99     | 1.33        | 6      | 2     |
| 1:A:698:PHE:CD1  | 1:A:700:LEU:HD11 | 0.98     | 1.93        | 3      | 2     |
| 1:A:681:ILE:O    | 1:A:685:LEU:HD23 | 0.96     | 1.60        | 9      | 5     |
| 1:A:669:ILE:HD13 | 1:A:680:VAL:HG11 | 0.94     | 1.37        | 5      | 2     |
| 1:A:669:ILE:HD13 | 1:A:670:LEU:N    | 0.94     | 1.76        | 3      | 1     |
| 1:A:700:LEU:HD22 | 1:A:731:LEU:CD2  | 0.93     | 1.92        | 6      | 4     |
| 1:A:659:LEU:HD23 | 1:A:733:GLN:CB   | 0.93     | 1.93        | 10     | 4     |
| 1:A:659:LEU:HD23 | 1:A:733:GLN:HB2  | 0.93     | 1.40        | 9      | 6     |
| 1:A:718:VAL:HG22 | 1:A:722:MET:HE2  | 0.93     | 1.41        | 7      | 1     |
| 1:A:730:LEU:C    | 1:A:731:LEU:HD23 | 0.92     | 1.89        | 3      | 9     |
| 1:A:652:ILE:HG22 | 1:A:670:LEU:HD13 | 0.92     | 1.42        | 2      | 1     |
| 1:A:700:LEU:HG   | 1:A:731:LEU:HD22 | 0.92     | 1.36        | 3      | 5     |
| 1:A:678:PRO:CB   | 1:A:710:LEU:HD21 | 0.92     | 1.95        | 10     | 1     |
| 1:A:698:PHE:CD2  | 1:A:700:LEU:HD21 | 0.90     | 2.02        | 4      | 1     |
| 1:A:700:LEU:CD2  | 1:A:731:LEU:HD22 | 0.90     | 1.95        | 6      | 6     |
| 1:A:655:VAL:HG11 | 1:A:731:LEU:HD11 | 0.89     | 1.41        | 9      | 4     |
| 1:A:700:LEU:CD1  | 1:A:731:LEU:HD22 | 0.89     | 1.97        | 2      | 1     |
| 1:A:657:MET:CG   | 1:A:731:LEU:HD12 | 0.89     | 1.97        | 3      | 1     |
| 1:A:659:LEU:HD12 | 1:A:733:GLN:CD   | 0.88     | 1.93        | 4      | 1     |
| 1:A:698:PHE:CE2  | 1:A:731:LEU:HD13 | 0.87     | 2.03        | 10     | 3     |
| 1:A:669:ILE:HD12 | 1:A:680:VAL:HG21 | 0.86     | 1.46        | 10     | 2     |
| 1:A:699:GLU:C    | 1:A:700:LEU:HD23 | 0.86     | 1.96        | 4      | 4     |
| 1:A:730:LEU:HD13 | 1:A:731:LEU:N    | 0.86     | 1.85        | 9      | 1     |
| 1:A:698:PHE:CE2  | 1:A:700:LEU:HD11 | 0.85     | 2.05        | 2      | 1     |
| 1:A:700:LEU:HD12 | 1:A:731:LEU:HD22 | 0.85     | 1.48        | 2      | 1     |
| 1:A:678:PRO:HB3  | 1:A:710:LEU:HD21 | 0.85     | 1.47        | 6      | 4     |
| 1:A:661:GLU:HG2  | 1:A:694:VAL:HG21 | 0.85     | 1.49        | 1      | 6     |
| 1:A:652:ILE:HG22 | 1:A:670:LEU:CD2  | 0.83     | 2.03        | 5      | 6     |
| 1:A:677:ALA:O    | 1:A:680:VAL:HG22 | 0.83     | 1.74        | 9      | 1     |
| 1:A:661:GLU:CG   | 1:A:694:VAL:HG21 | 0.83     | 2.04        | 1      | 6     |
| 1:A:689:ASN:HB2  | 1:A:694:VAL:HG22 | 0.82     | 1.52        | 9      | 5     |
| 1:A:672:THR:HG22 | 1:A:675:ASP:HB2  | 0.82     | 1.52        | 5      | 3     |
| 1:A:659:LEU:HD13 | 1:A:660:GLY:N    | 0.82     | 1.89        | 4      | 2     |
| 1:A:669:ILE:HD13 | 1:A:680:VAL:CG2  | 0.82     | 2.05        | 6      | 1     |
| 1:A:698:PHE:O    | 1:A:712:ILE:HD11 | 0.81     | 1.74        | 7      | 1     |
| 1:A:700:LEU:HD12 | 1:A:700:LEU:N    | 0.81     | 1.91        | 10     | 2     |
| 1:A:659:LEU:HD23 | 1:A:733:GLN:HB3  | 0.81     | 1.51        | 10     | 3     |
| 1:A:680:VAL:HG23 | 1:A:683:ARG:NE   | 0.80     | 1.91        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:678:PRO:HB2  | 1:A:710:LEU:HD21 | 0.80     | 1.50        | 10     | 1     |
| 1:A:657:MET:CE   | 1:A:693:ALA:HB3  | 0.80     | 2.06        | 6      | 2     |
| 1:A:678:PRO:HB3  | 1:A:710:LEU:HD11 | 0.79     | 1.52        | 1      | 1     |
| 1:A:657:MET:HB2  | 1:A:731:LEU:HD12 | 0.79     | 1.52        | 6      | 3     |
| 1:A:653:ILE:CG2  | 1:A:671:VAL:HG23 | 0.78     | 2.07        | 4      | 6     |
| 1:A:659:LEU:HD13 | 1:A:660:GLY:H    | 0.78     | 1.39        | 4      | 2     |
| 1:A:710:LEU:HD21 | 1:A:718:VAL:HG21 | 0.78     | 1.54        | 5      | 2     |
| 1:A:677:ALA:N    | 1:A:678:PRO:CD   | 0.78     | 2.47        | 9      | 9     |
| 1:A:718:VAL:HG22 | 1:A:722:MET:CE   | 0.78     | 2.09        | 7      | 1     |
| 1:A:669:ILE:CD1  | 1:A:680:VAL:HG21 | 0.77     | 2.10        | 10     | 5     |
| 1:A:670:LEU:HD13 | 1:A:671:VAL:N    | 0.77     | 1.95        | 3      | 7     |
| 1:A:653:ILE:C    | 1:A:653:ILE:HD13 | 0.77     | 2.05        | 9      | 1     |
| 1:A:655:VAL:HG13 | 1:A:729:PHE:HB2  | 0.76     | 1.57        | 10     | 2     |
| 1:A:655:VAL:CG1  | 1:A:731:LEU:HD21 | 0.76     | 2.10        | 3      | 9     |
| 1:A:659:LEU:HD23 | 1:A:660:GLY:N    | 0.76     | 1.94        | 7      | 1     |
| 1:A:670:LEU:C    | 1:A:670:LEU:HD13 | 0.76     | 2.05        | 7      | 3     |
| 1:A:700:LEU:H    | 1:A:711:THR:HG22 | 0.76     | 1.41        | 1      | 5     |
| 1:A:699:GLU:C    | 1:A:700:LEU:HD13 | 0.75     | 2.06        | 2      | 1     |
| 1:A:659:LEU:HD12 | 1:A:733:GLN:NE2  | 0.75     | 1.97        | 4      | 1     |
| 1:A:704:LEU:N    | 1:A:704:LEU:HD13 | 0.75     | 1.97        | 1      | 2     |
| 1:A:677:ALA:O    | 1:A:680:VAL:HG12 | 0.75     | 1.82        | 1      | 7     |
| 1:A:700:LEU:HD12 | 1:A:731:LEU:CD2  | 0.74     | 2.12        | 2      | 1     |
| 1:A:655:VAL:HG22 | 1:A:729:PHE:CD1  | 0.74     | 2.17        | 1      | 4     |
| 1:A:730:LEU:O    | 1:A:731:LEU:HD23 | 0.74     | 1.83        | 4      | 5     |
| 1:A:727:HIS:N    | 1:A:727:HIS:CD2  | 0.73     | 2.57        | 4      | 3     |
| 1:A:718:VAL:HG22 | 1:A:722:MET:SD   | 0.73     | 2.23        | 1      | 4     |
| 1:A:655:VAL:CG1  | 1:A:731:LEU:HD11 | 0.72     | 2.14        | 9      | 4     |
| 1:A:670:LEU:HD13 | 1:A:670:LEU:C    | 0.72     | 2.08        | 3      | 3     |
| 1:A:678:PRO:CG   | 1:A:718:VAL:HG11 | 0.72     | 2.15        | 10     | 4     |
| 1:A:712:ILE:C    | 1:A:712:ILE:HD12 | 0.71     | 2.09        | 1      | 1     |
| 1:A:700:LEU:HD23 | 1:A:731:LEU:CD2  | 0.71     | 2.15        | 7      | 2     |
| 1:A:710:LEU:HD13 | 1:A:722:MET:HE1  | 0.71     | 1.60        | 10     | 1     |
| 1:A:698:PHE:CD1  | 1:A:698:PHE:N    | 0.71     | 2.59        | 2      | 5     |
| 1:A:731:LEU:HD23 | 1:A:731:LEU:N    | 0.71     | 2.01        | 3      | 2     |
| 1:A:698:PHE:CD2  | 1:A:700:LEU:CD2  | 0.71     | 2.72        | 4      | 1     |
| 1:A:698:PHE:CE1  | 1:A:700:LEU:HD11 | 0.70     | 2.21        | 3      | 5     |
| 1:A:711:THR:C    | 1:A:713:PRO:HD2  | 0.70     | 2.11        | 1      | 8     |
| 1:A:698:PHE:HB3  | 1:A:733:GLN:HA   | 0.70     | 1.62        | 2      | 9     |
| 1:A:700:LEU:HD23 | 1:A:700:LEU:N    | 0.70     | 2.02        | 1      | 3     |
| 1:A:703:LEU:HD13 | 1:A:707:ASP:HB3  | 0.70     | 1.61        | 6      | 1     |
| 1:A:719:PHE:CE2  | 1:A:727:HIS:CD2  | 0.69     | 2.80        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:669:ILE:CD1  | 1:A:680:VAL:HG11 | 0.69     | 2.16        | 5      | 2     |
| 1:A:653:ILE:HD12 | 1:A:719:PHE:CZ   | 0.69     | 2.23        | 3      | 7     |
| 1:A:719:PHE:O    | 1:A:723:ASP:CG   | 0.68     | 2.37        | 1      | 9     |
| 1:A:685:LEU:HD11 | 1:A:693:ALA:HB3  | 0.68     | 1.64        | 9      | 2     |
| 1:A:712:ILE:N    | 1:A:713:PRO:CD   | 0.68     | 2.56        | 1      | 9     |
| 1:A:651:ARG:HB3  | 1:A:727:HIS:CE1  | 0.68     | 2.24        | 5      | 6     |
| 1:A:700:LEU:N    | 1:A:711:THR:HG22 | 0.67     | 2.03        | 2      | 4     |
| 1:A:653:ILE:HG23 | 1:A:669:ILE:HG23 | 0.67     | 1.66        | 6      | 5     |
| 1:A:729:PHE:CD1  | 1:A:729:PHE:N    | 0.67     | 2.62        | 2      | 5     |
| 1:A:698:PHE:CE1  | 1:A:700:LEU:HD21 | 0.67     | 2.23        | 5      | 5     |
| 1:A:680:VAL:HG23 | 1:A:683:ARG:CZ   | 0.67     | 2.19        | 2      | 1     |
| 1:A:657:MET:HE3  | 1:A:693:ALA:CB   | 0.67     | 2.10        | 6      | 1     |
| 1:A:667:LYS:HG2  | 1:A:681:ILE:HD13 | 0.67     | 1.64        | 9      | 1     |
| 1:A:704:LEU:N    | 1:A:705:PRO:CD   | 0.66     | 2.57        | 2      | 9     |
| 1:A:698:PHE:CD2  | 1:A:700:LEU:CD1  | 0.66     | 2.72        | 2      | 1     |
| 1:A:657:MET:HG3  | 1:A:731:LEU:HD12 | 0.66     | 1.66        | 3      | 1     |
| 1:A:710:LEU:HD22 | 1:A:729:PHE:CE2  | 0.66     | 2.25        | 2      | 2     |
| 1:A:652:ILE:HG22 | 1:A:670:LEU:HD22 | 0.66     | 1.68        | 5      | 4     |
| 1:A:698:PHE:HE2  | 1:A:731:LEU:HD13 | 0.66     | 1.49        | 2      | 2     |
| 1:A:702:GLN:O    | 1:A:703:LEU:HB2  | 0.65     | 1.92        | 3      | 7     |
| 1:A:677:ALA:N    | 1:A:678:PRO:HD3  | 0.65     | 2.07        | 3      | 9     |
| 1:A:655:VAL:HG13 | 1:A:731:LEU:HD21 | 0.65     | 1.67        | 3      | 3     |
| 1:A:723:ASP:HB2  | 1:A:727:HIS:CE1  | 0.65     | 2.27        | 10     | 7     |
| 1:A:652:ILE:HG22 | 1:A:670:LEU:CD1  | 0.65     | 2.21        | 2      | 1     |
| 1:A:653:ILE:HD11 | 1:A:655:VAL:HG23 | 0.65     | 1.67        | 9      | 1     |
| 1:A:659:LEU:HD22 | 1:A:733:GLN:NE2  | 0.64     | 2.07        | 7      | 1     |
| 1:A:656:GLN:HB2  | 1:A:730:LEU:HD12 | 0.64     | 1.69        | 3      | 1     |
| 1:A:717:ASN:ND2  | 1:A:720:TYR:HB3  | 0.64     | 2.08        | 10     | 2     |
| 1:A:659:LEU:O    | 1:A:693:ALA:HB1  | 0.64     | 1.93        | 4      | 3     |
| 1:A:680:VAL:HG23 | 1:A:683:ARG:HE   | 0.64     | 1.50        | 2      | 1     |
| 1:A:681:ILE:HA   | 1:A:684:VAL:CG2  | 0.64     | 2.23        | 6      | 2     |
| 1:A:657:MET:HE2  | 1:A:693:ALA:HB3  | 0.64     | 1.70        | 3      | 1     |
| 1:A:704:LEU:CD1  | 1:A:704:LEU:N    | 0.64     | 2.61        | 3      | 1     |
| 1:A:729:PHE:N    | 1:A:729:PHE:CD1  | 0.63     | 2.66        | 6      | 4     |
| 1:A:667:LYS:CE   | 1:A:681:ILE:CD1  | 0.63     | 2.75        | 9      | 1     |
| 1:A:704:LEU:N    | 1:A:704:LEU:HD12 | 0.63     | 2.08        | 2      | 3     |
| 1:A:658:GLU:HA   | 1:A:664:SER:O    | 0.63     | 1.94        | 9      | 8     |
| 1:A:685:LEU:HD12 | 1:A:694:VAL:HA   | 0.63     | 1.69        | 7      | 2     |
| 1:A:667:LYS:HE3  | 1:A:681:ILE:HD12 | 0.63     | 1.69        | 9      | 1     |
| 1:A:681:ILE:O    | 1:A:685:LEU:CD2  | 0.63     | 2.44        | 9      | 5     |
| 1:A:685:LEU:O    | 1:A:689:ASN:N    | 0.62     | 2.32        | 5      | 9     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:655:VAL:HG22 | 1:A:729:PHE:CD2  | 0.62     | 2.29        | 3      | 2     |
| 1:A:727:HIS:N    | 1:A:727:HIS:ND1  | 0.62     | 2.47        | 7      | 4     |
| 1:A:678:PRO:HG2  | 1:A:718:VAL:HG11 | 0.62     | 1.70        | 10     | 3     |
| 1:A:700:LEU:N    | 1:A:700:LEU:CD1  | 0.62     | 2.62        | 3      | 2     |
| 1:A:700:LEU:HD23 | 1:A:731:LEU:HD22 | 0.62     | 1.70        | 5      | 2     |
| 1:A:710:LEU:HD11 | 1:A:718:VAL:CG1  | 0.62     | 2.24        | 9      | 3     |
| 1:A:684:VAL:O    | 1:A:688:ASN:ND2  | 0.62     | 2.32        | 10     | 9     |
| 1:A:728:ASP:C    | 1:A:729:PHE:CD1  | 0.62     | 2.78        | 7      | 5     |
| 1:A:704:LEU:HD11 | 1:A:728:ASP:HB3  | 0.62     | 1.70        | 6      | 1     |
| 1:A:700:LEU:HD13 | 1:A:700:LEU:N    | 0.62     | 2.10        | 2      | 1     |
| 1:A:698:PHE:HD1  | 1:A:700:LEU:HD11 | 0.62     | 1.51        | 3      | 1     |
| 1:A:712:ILE:N    | 1:A:713:PRO:HD2  | 0.62     | 2.09        | 3      | 9     |
| 1:A:727:HIS:C    | 1:A:729:PHE:CE1  | 0.62     | 2.78        | 4      | 5     |
| 1:A:704:LEU:HB2  | 1:A:705:PRO:HD3  | 0.61     | 1.72        | 5      | 9     |
| 1:A:704:LEU:HD12 | 1:A:704:LEU:H    | 0.61     | 1.54        | 7      | 1     |
| 1:A:678:PRO:CB   | 1:A:710:LEU:HD11 | 0.61     | 2.25        | 1      | 1     |
| 1:A:652:ILE:HG22 | 1:A:670:LEU:HD23 | 0.61     | 1.72        | 4      | 2     |
| 1:A:655:VAL:HG13 | 1:A:729:PHE:O    | 0.61     | 1.95        | 7      | 2     |
| 1:A:685:LEU:O    | 1:A:689:ASN:HB3  | 0.61     | 1.96        | 10     | 9     |
| 1:A:723:ASP:HB2  | 1:A:727:HIS:NE2  | 0.61     | 2.10        | 4      | 4     |
| 1:A:700:LEU:CG   | 1:A:731:LEU:HD22 | 0.61     | 2.18        | 3      | 5     |
| 1:A:659:LEU:CB   | 1:A:733:GLN:HB2  | 0.61     | 2.26        | 4      | 2     |
| 1:A:723:ASP:CB   | 1:A:727:HIS:CD2  | 0.61     | 2.83        | 2      | 1     |
| 1:A:677:ALA:O    | 1:A:680:VAL:HG13 | 0.61     | 1.96        | 6      | 1     |
| 1:A:723:ASP:OD1  | 1:A:724:GLY:N    | 0.61     | 2.32        | 6      | 1     |
| 1:A:655:VAL:O    | 1:A:667:LYS:N    | 0.61     | 2.34        | 6      | 9     |
| 1:A:657:MET:SD   | 1:A:698:PHE:CD2  | 0.61     | 2.94        | 5      | 1     |
| 1:A:651:ARG:NH1  | 1:A:723:ASP:OD2  | 0.61     | 2.34        | 1      | 8     |
| 1:A:671:VAL:HG21 | 1:A:719:PHE:CD2  | 0.60     | 2.31        | 7      | 7     |
| 1:A:703:LEU:HD12 | 1:A:707:ASP:HB3  | 0.60     | 1.71        | 7      | 2     |
| 1:A:653:ILE:HD12 | 1:A:669:ILE:HG22 | 0.60     | 1.73        | 9      | 1     |
| 1:A:652:ILE:HD12 | 1:A:654:ARG:CZ   | 0.60     | 2.25        | 6      | 1     |
| 1:A:653:ILE:CG2  | 1:A:671:VAL:CG2  | 0.60     | 2.78        | 10     | 6     |
| 1:A:670:LEU:HD12 | 1:A:671:VAL:N    | 0.60     | 2.11        | 2      | 1     |
| 1:A:700:LEU:HB2  | 1:A:710:LEU:O    | 0.60     | 1.96        | 7      | 7     |
| 1:A:703:LEU:HD23 | 1:A:707:ASP:CB   | 0.60     | 2.27        | 10     | 1     |
| 1:A:653:ILE:HG21 | 1:A:671:VAL:HG23 | 0.60     | 1.72        | 5      | 6     |
| 1:A:704:LEU:N    | 1:A:705:PRO:HD2  | 0.60     | 2.11        | 4      | 9     |
| 1:A:718:VAL:O    | 1:A:722:MET:N    | 0.60     | 2.33        | 4      | 6     |
| 1:A:702:GLN:CD   | 1:A:729:PHE:CE1  | 0.60     | 2.79        | 5      | 2     |
| 1:A:685:LEU:HA   | 1:A:688:ASN:ND2  | 0.60     | 2.11        | 9      | 9     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:685:LEU:CD1  | 1:A:693:ALA:C    | 0.60     | 2.75        | 9      | 3     |
| 1:A:696:SER:HA   | 1:A:698:PHE:CE2  | 0.59     | 2.32        | 7      | 4     |
| 1:A:710:LEU:HD11 | 1:A:718:VAL:HG11 | 0.59     | 1.72        | 9      | 3     |
| 1:A:698:PHE:HE1  | 1:A:700:LEU:HD11 | 0.59     | 1.55        | 7      | 1     |
| 1:A:678:PRO:CG   | 1:A:718:VAL:CG1  | 0.59     | 2.79        | 1      | 6     |
| 1:A:678:PRO:HB3  | 1:A:710:LEU:CD2  | 0.59     | 2.27        | 10     | 1     |
| 1:A:657:MET:CE   | 1:A:695:ALA:O    | 0.59     | 2.50        | 9      | 1     |
| 1:A:710:LEU:HD13 | 1:A:722:MET:CE   | 0.59     | 2.28        | 10     | 1     |
| 1:A:655:VAL:HG11 | 1:A:731:LEU:HD21 | 0.59     | 1.73        | 2      | 4     |
| 1:A:651:ARG:HB3  | 1:A:727:HIS:NE2  | 0.59     | 2.12        | 4      | 4     |
| 1:A:710:LEU:HD23 | 1:A:729:PHE:CE2  | 0.59     | 2.32        | 4      | 2     |
| 1:A:698:PHE:CE1  | 1:A:712:ILE:HD11 | 0.59     | 2.33        | 9      | 1     |
| 1:A:661:GLU:HG2  | 1:A:694:VAL:CG2  | 0.59     | 2.24        | 1      | 6     |
| 1:A:704:LEU:N    | 1:A:704:LEU:CD1  | 0.59     | 2.66        | 1      | 4     |
| 1:A:702:GLN:NE2  | 1:A:722:MET:O    | 0.58     | 2.36        | 3      | 6     |
| 1:A:702:GLN:HG2  | 1:A:703:LEU:HD22 | 0.58     | 1.73        | 3      | 1     |
| 1:A:667:LYS:HE2  | 1:A:681:ILE:HD12 | 0.58     | 1.73        | 10     | 1     |
| 1:A:712:ILE:HG12 | 1:A:713:PRO:HD3  | 0.58     | 1.75        | 2      | 2     |
| 1:A:704:LEU:HD11 | 1:A:728:ASP:CB   | 0.58     | 2.29        | 6      | 3     |
| 1:A:654:ARG:NH1  | 1:A:668:SER:CB   | 0.58     | 2.66        | 10     | 1     |
| 1:A:702:GLN:O    | 1:A:703:LEU:CB   | 0.58     | 2.52        | 10     | 8     |
| 1:A:666:TYR:C    | 1:A:666:TYR:CD1  | 0.58     | 2.81        | 7      | 1     |
| 1:A:696:SER:CA   | 1:A:698:PHE:CE2  | 0.58     | 2.86        | 7      | 2     |
| 1:A:671:VAL:HG21 | 1:A:719:PHE:CE2  | 0.58     | 2.34        | 4      | 5     |
| 1:A:714:HIS:HB3  | 1:A:718:VAL:HG21 | 0.58     | 1.75        | 2      | 3     |
| 1:A:696:SER:HB2  | 1:A:698:PHE:CZ   | 0.58     | 2.34        | 3      | 1     |
| 1:A:699:GLU:C    | 1:A:700:LEU:HD12 | 0.58     | 2.23        | 3      | 1     |
| 1:A:698:PHE:CE2  | 1:A:700:LEU:HD21 | 0.58     | 2.33        | 10     | 2     |
| 1:A:680:VAL:HG23 | 1:A:683:ARG:HD2  | 0.58     | 1.75        | 1      | 1     |
| 1:A:711:THR:O    | 1:A:714:HIS:CD2  | 0.58     | 2.57        | 4      | 1     |
| 1:A:717:ASN:O    | 1:A:717:ASN:ND2  | 0.58     | 2.36        | 2      | 3     |
| 1:A:699:GLU:O    | 1:A:700:LEU:HD23 | 0.58     | 1.98        | 6      | 2     |
| 1:A:651:ARG:NH1  | 1:A:673:SER:HA   | 0.57     | 2.14        | 9      | 7     |
| 1:A:659:LEU:HD13 | 1:A:733:GLN:HB3  | 0.57     | 1.76        | 7      | 1     |
| 1:A:667:LYS:CE   | 1:A:681:ILE:HD12 | 0.57     | 2.29        | 9      | 1     |
| 1:A:718:VAL:HG13 | 1:A:719:PHE:N    | 0.57     | 2.14        | 10     | 1     |
| 1:A:670:LEU:C    | 1:A:670:LEU:CD1  | 0.57     | 2.76        | 7      | 6     |
| 1:A:655:VAL:CG1  | 1:A:731:LEU:CD2  | 0.57     | 2.83        | 3      | 4     |
| 1:A:704:LEU:H    | 1:A:704:LEU:HD22 | 0.57     | 1.60        | 6      | 1     |
| 1:A:698:PHE:CE2  | 1:A:700:LEU:HG   | 0.57     | 2.35        | 10     | 1     |
| 1:A:653:ILE:HG23 | 1:A:669:ILE:CG2  | 0.57     | 2.29        | 2      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:702:GLN:CD   | 1:A:729:PHE:CE2  | 0.57     | 2.83        | 10     | 3     |
| 1:A:730:LEU:C    | 1:A:730:LEU:CD1  | 0.57     | 2.78        | 9      | 1     |
| 1:A:659:LEU:HD12 | 1:A:733:GLN:HB2  | 0.57     | 1.76        | 2      | 1     |
| 1:A:699:GLU:HG3  | 1:A:711:THR:HG21 | 0.57     | 1.77        | 4      | 1     |
| 1:A:659:LEU:HD23 | 1:A:660:GLY:H    | 0.57     | 1.57        | 7      | 1     |
| 1:A:730:LEU:HD13 | 1:A:730:LEU:C    | 0.57     | 2.25        | 9      | 1     |
| 1:A:676:LYS:HG2  | 1:A:716:ALA:O    | 0.57     | 1.99        | 1      | 2     |
| 1:A:710:LEU:CD2  | 1:A:729:PHE:CE2  | 0.57     | 2.88        | 4      | 2     |
| 1:A:651:ARG:CD   | 1:A:723:ASP:O    | 0.57     | 2.53        | 1      | 5     |
| 1:A:684:VAL:O    | 1:A:688:ASN:N    | 0.57     | 2.37        | 1      | 6     |
| 1:A:677:ALA:N    | 1:A:678:PRO:HD2  | 0.57     | 2.15        | 9      | 3     |
| 1:A:667:LYS:HE2  | 1:A:681:ILE:CD1  | 0.57     | 2.30        | 9      | 2     |
| 1:A:672:THR:HG22 | 1:A:675:ASP:CB   | 0.56     | 2.27        | 5      | 3     |
| 1:A:685:LEU:HD12 | 1:A:694:VAL:CA   | 0.56     | 2.29        | 5      | 2     |
| 1:A:657:MET:O    | 1:A:664:SER:O    | 0.56     | 2.23        | 7      | 9     |
| 1:A:678:PRO:HG3  | 1:A:718:VAL:CG1  | 0.56     | 2.30        | 5      | 6     |
| 1:A:719:PHE:O    | 1:A:720:TYR:C    | 0.56     | 2.48        | 3      | 9     |
| 1:A:652:ILE:O    | 1:A:727:HIS:ND1  | 0.56     | 2.36        | 2      | 1     |
| 1:A:709:GLU:O    | 1:A:714:HIS:CE1  | 0.56     | 2.58        | 9      | 4     |
| 1:A:670:LEU:HD22 | 1:A:671:VAL:N    | 0.56     | 2.15        | 4      | 1     |
| 1:A:674:GLN:O    | 1:A:676:LYS:NZ   | 0.56     | 2.39        | 6      | 2     |
| 1:A:678:PRO:HG3  | 1:A:719:PHE:CE1  | 0.56     | 2.34        | 5      | 4     |
| 1:A:702:GLN:O    | 1:A:703:LEU:HB3  | 0.56     | 2.00        | 10     | 1     |
| 1:A:653:ILE:HG21 | 1:A:671:VAL:CG2  | 0.56     | 2.31        | 10     | 6     |
| 1:A:651:ARG:NH2  | 1:A:723:ASP:OD2  | 0.56     | 2.39        | 5      | 1     |
| 1:A:681:ILE:HD13 | 1:A:731:LEU:HD11 | 0.56     | 1.78        | 1      | 1     |
| 1:A:654:ARG:O    | 1:A:728:ASP:HA   | 0.56     | 2.01        | 7      | 7     |
| 1:A:676:LYS:CD   | 1:A:717:ASN:HA   | 0.56     | 2.31        | 6      | 5     |
| 1:A:711:THR:N    | 1:A:714:HIS:CD2  | 0.56     | 2.74        | 7      | 3     |
| 1:A:710:LEU:O    | 1:A:710:LEU:HG   | 0.56     | 2.01        | 10     | 3     |
| 1:A:709:GLU:HG3  | 1:A:714:HIS:CE1  | 0.55     | 2.36        | 4      | 1     |
| 1:A:652:ILE:HD12 | 1:A:654:ARG:NH2  | 0.55     | 2.16        | 6      | 1     |
| 1:A:676:LYS:CD   | 1:A:716:ALA:O    | 0.55     | 2.53        | 10     | 1     |
| 1:A:654:ARG:HA   | 1:A:667:LYS:O    | 0.55     | 2.01        | 1      | 5     |
| 1:A:695:ALA:O    | 1:A:733:GLN:NE2  | 0.55     | 2.39        | 5      | 2     |
| 1:A:657:MET:SD   | 1:A:693:ALA:CB   | 0.55     | 2.94        | 1      | 1     |
| 1:A:688:ASN:OD1  | 1:A:692:SER:CB   | 0.55     | 2.55        | 4      | 6     |
| 1:A:703:LEU:CD2  | 1:A:707:ASP:HB3  | 0.55     | 2.31        | 5      | 2     |
| 1:A:710:LEU:O    | 1:A:710:LEU:CD2  | 0.55     | 2.54        | 7      | 1     |
| 1:A:657:MET:HG3  | 1:A:731:LEU:CD1  | 0.55     | 2.30        | 3      | 1     |
| 1:A:723:ASP:O    | 1:A:724:GLY:C    | 0.55     | 2.50        | 9      | 8     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:676:LYS:C    | 1:A:678:PRO:CD   | 0.55     | 2.80        | 1      | 5     |
| 1:A:723:ASP:C    | 1:A:723:ASP:OD1  | 0.55     | 2.50        | 10     | 7     |
| 1:A:689:ASN:CB   | 1:A:694:VAL:HG22 | 0.55     | 2.31        | 3      | 3     |
| 1:A:657:MET:HA   | 1:A:731:LEU:HB2  | 0.55     | 1.78        | 10     | 2     |
| 1:A:698:PHE:CE2  | 1:A:700:LEU:CD2  | 0.55     | 2.89        | 10     | 2     |
| 1:A:712:ILE:CG2  | 1:A:713:PRO:HD3  | 0.55     | 2.31        | 5      | 1     |
| 1:A:719:PHE:CD2  | 1:A:727:HIS:CD2  | 0.55     | 2.95        | 2      | 1     |
| 1:A:681:ILE:O    | 1:A:684:VAL:CG2  | 0.55     | 2.55        | 5      | 1     |
| 1:A:664:SER:C    | 1:A:665:VAL:HG13 | 0.54     | 2.25        | 7      | 4     |
| 1:A:676:LYS:C    | 1:A:678:PRO:HD2  | 0.54     | 2.27        | 2      | 9     |
| 1:A:711:THR:OG1  | 1:A:713:PRO:HD2  | 0.54     | 2.02        | 2      | 7     |
| 1:A:657:MET:HE2  | 1:A:698:PHE:CE2  | 0.54     | 2.37        | 2      | 1     |
| 1:A:722:MET:N    | 1:A:722:MET:SD   | 0.54     | 2.81        | 4      | 1     |
| 1:A:672:THR:HG23 | 1:A:674:GLN:H    | 0.54     | 1.61        | 1      | 2     |
| 1:A:712:ILE:HD12 | 1:A:713:PRO:N    | 0.54     | 2.16        | 1      | 1     |
| 1:A:703:LEU:CD2  | 1:A:707:ASP:CB   | 0.54     | 2.85        | 10     | 1     |
| 1:A:667:LYS:CD   | 1:A:667:LYS:C    | 0.54     | 2.80        | 1      | 2     |
| 1:A:680:VAL:O    | 1:A:683:ARG:CG   | 0.54     | 2.55        | 1      | 1     |
| 1:A:716:ALA:O    | 1:A:718:VAL:N    | 0.54     | 2.41        | 2      | 3     |
| 1:A:685:LEU:O    | 1:A:689:ASN:CB   | 0.54     | 2.56        | 2      | 4     |
| 1:A:653:ILE:C    | 1:A:653:ILE:CD1  | 0.54     | 2.76        | 9      | 1     |
| 1:A:677:ALA:O    | 1:A:680:VAL:CG1  | 0.54     | 2.56        | 7      | 5     |
| 1:A:698:PHE:CD2  | 1:A:731:LEU:HB3  | 0.54     | 2.37        | 10     | 2     |
| 1:A:686:LYS:O    | 1:A:689:ASN:CG   | 0.54     | 2.50        | 10     | 3     |
| 1:A:661:GLU:CG   | 1:A:694:VAL:CG2  | 0.54     | 2.85        | 2      | 1     |
| 1:A:651:ARG:CZ   | 1:A:673:SER:HA   | 0.54     | 2.32        | 1      | 2     |
| 1:A:678:PRO:HD3  | 1:A:719:PHE:CD2  | 0.54     | 2.38        | 3      | 2     |
| 1:A:654:ARG:NH2  | 1:A:668:SER:OG   | 0.54     | 2.41        | 7      | 2     |
| 1:A:695:ALA:HB3  | 1:A:733:GLN:NE2  | 0.54     | 2.18        | 1      | 1     |
| 1:A:696:SER:O    | 1:A:698:PHE:CD1  | 0.54     | 2.61        | 1      | 4     |
| 1:A:698:PHE:HB3  | 1:A:733:GLN:CA   | 0.54     | 2.33        | 9      | 5     |
| 1:A:651:ARG:NH2  | 1:A:673:SER:O    | 0.54     | 2.40        | 5      | 2     |
| 1:A:688:ASN:ND2  | 1:A:688:ASN:C    | 0.54     | 2.66        | 2      | 8     |
| 1:A:651:ARG:HB3  | 1:A:727:HIS:HE2  | 0.53     | 1.63        | 1      | 1     |
| 1:A:655:VAL:O    | 1:A:667:LYS:HB3  | 0.53     | 2.03        | 7      | 6     |
| 1:A:702:GLN:HB2  | 1:A:729:PHE:CD2  | 0.53     | 2.38        | 6      | 3     |
| 1:A:702:GLN:CG   | 1:A:729:PHE:CE2  | 0.53     | 2.91        | 2      | 2     |
| 1:A:697:GLU:O    | 1:A:733:GLN:HA   | 0.53     | 2.03        | 9      | 1     |
| 1:A:717:ASN:ND2  | 1:A:720:TYR:CB   | 0.53     | 2.71        | 10     | 2     |
| 1:A:712:ILE:HD13 | 1:A:712:ILE:H    | 0.53     | 1.64        | 3      | 2     |
| 1:A:702:GLN:HG3  | 1:A:729:PHE:CD1  | 0.53     | 2.38        | 7      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:712:ILE:HG22 | 1:A:713:PRO:HD3  | 0.53     | 1.81        | 5      | 1     |
| 1:A:696:SER:CB   | 1:A:698:PHE:CE2  | 0.53     | 2.92        | 7      | 1     |
| 1:A:698:PHE:CE2  | 1:A:700:LEU:CG   | 0.53     | 2.91        | 10     | 1     |
| 1:A:669:ILE:HD13 | 1:A:669:ILE:C    | 0.53     | 2.29        | 3      | 1     |
| 1:A:680:VAL:HG23 | 1:A:683:ARG:HH11 | 0.53     | 1.63        | 7      | 1     |
| 1:A:680:VAL:O    | 1:A:683:ARG:HG2  | 0.53     | 2.04        | 1      | 7     |
| 1:A:709:GLU:N    | 1:A:709:GLU:OE1  | 0.53     | 2.42        | 2      | 1     |
| 1:A:670:LEU:HD22 | 1:A:670:LEU:C    | 0.53     | 2.28        | 4      | 1     |
| 1:A:711:THR:OG1  | 1:A:714:HIS:NE2  | 0.53     | 2.40        | 4      | 1     |
| 1:A:670:LEU:C    | 1:A:670:LEU:CD2  | 0.53     | 2.82        | 4      | 1     |
| 1:A:651:ARG:NH2  | 1:A:723:ASP:CG   | 0.53     | 2.67        | 5      | 1     |
| 1:A:651:ARG:CZ   | 1:A:723:ASP:OD1  | 0.53     | 2.57        | 5      | 2     |
| 1:A:700:LEU:CD2  | 1:A:700:LEU:N    | 0.53     | 2.67        | 1      | 2     |
| 1:A:703:LEU:HD22 | 1:A:707:ASP:HB3  | 0.53     | 1.78        | 5      | 3     |
| 1:A:680:VAL:HG23 | 1:A:683:ARG:NH1  | 0.53     | 2.19        | 7      | 1     |
| 1:A:655:VAL:CG1  | 1:A:731:LEU:CD1  | 0.53     | 2.86        | 9      | 1     |
| 1:A:714:HIS:CD2  | 1:A:714:HIS:N    | 0.53     | 2.77        | 4      | 1     |
| 1:A:674:GLN:N    | 1:A:674:GLN:CD   | 0.53     | 2.66        | 2      | 1     |
| 1:A:657:MET:SD   | 1:A:693:ALA:HB1  | 0.53     | 2.43        | 1      | 1     |
| 1:A:671:VAL:CG1  | 1:A:672:THR:N    | 0.53     | 2.71        | 2      | 1     |
| 1:A:677:ALA:CA   | 1:A:680:VAL:HG13 | 0.53     | 2.34        | 6      | 1     |
| 1:A:653:ILE:HD12 | 1:A:719:PHE:CE2  | 0.52     | 2.39        | 1      | 4     |
| 1:A:651:ARG:O    | 1:A:671:VAL:N    | 0.52     | 2.41        | 2      | 5     |
| 1:A:694:VAL:HG12 | 1:A:695:ALA:N    | 0.52     | 2.19        | 2      | 5     |
| 1:A:651:ARG:NH1  | 1:A:723:ASP:CG   | 0.52     | 2.68        | 3      | 3     |
| 1:A:712:ILE:CG1  | 1:A:713:PRO:HD3  | 0.52     | 2.34        | 2      | 3     |
| 1:A:722:MET:SD   | 1:A:722:MET:N    | 0.52     | 2.82        | 3      | 3     |
| 1:A:674:GLN:C    | 1:A:676:LYS:NZ   | 0.52     | 2.68        | 4      | 1     |
| 1:A:664:SER:OG   | 1:A:693:ALA:HB2  | 0.52     | 2.05        | 7      | 1     |
| 1:A:719:PHE:C    | 1:A:721:ALA:N    | 0.52     | 2.65        | 4      | 9     |
| 1:A:698:PHE:CB   | 1:A:733:GLN:HA   | 0.52     | 2.34        | 2      | 2     |
| 1:A:651:ARG:HB2  | 1:A:671:VAL:HG12 | 0.52     | 1.81        | 7      | 3     |
| 1:A:657:MET:HE3  | 1:A:657:MET:HA   | 0.52     | 1.80        | 4      | 2     |
| 1:A:654:ARG:HB2  | 1:A:654:ARG:CZ   | 0.52     | 2.34        | 7      | 1     |
| 1:A:685:LEU:CD1  | 1:A:693:ALA:O    | 0.52     | 2.58        | 10     | 1     |
| 1:A:681:ILE:HG22 | 1:A:685:LEU:HD23 | 0.52     | 1.81        | 2      | 3     |
| 1:A:710:LEU:HD23 | 1:A:729:PHE:CD2  | 0.52     | 2.40        | 4      | 2     |
| 1:A:727:HIS:CB   | 1:A:729:PHE:CZ   | 0.52     | 2.93        | 9      | 5     |
| 1:A:661:GLU:HG3  | 1:A:662:ASP:N    | 0.52     | 2.19        | 2      | 6     |
| 1:A:656:GLN:NE2  | 1:A:729:PHE:O    | 0.52     | 2.43        | 2      | 1     |
| 1:A:685:LEU:HD12 | 1:A:694:VAL:N    | 0.52     | 2.20        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:662:ASP:HB2  | 1:A:692:SER:O    | 0.52     | 2.05        | 10     | 5     |
| 1:A:673:SER:CB   | 1:A:674:GLN:OE1  | 0.52     | 2.57        | 2      | 1     |
| 1:A:653:ILE:HD12 | 1:A:719:PHE:HZ   | 0.52     | 1.64        | 4      | 2     |
| 1:A:696:SER:HB2  | 1:A:698:PHE:CE2  | 0.52     | 2.40        | 7      | 1     |
| 1:A:710:LEU:CD1  | 1:A:722:MET:HE1  | 0.52     | 2.33        | 10     | 1     |
| 1:A:704:LEU:HD11 | 1:A:728:ASP:OD2  | 0.51     | 2.04        | 10     | 1     |
| 1:A:659:LEU:O    | 1:A:733:GLN:OE1  | 0.51     | 2.27        | 1      | 1     |
| 1:A:676:LYS:HG2  | 1:A:717:ASN:HA   | 0.51     | 1.81        | 1      | 3     |
| 1:A:698:PHE:HE1  | 1:A:700:LEU:HD21 | 0.51     | 1.62        | 5      | 1     |
| 1:A:696:SER:O    | 1:A:698:PHE:N    | 0.51     | 2.44        | 6      | 4     |
| 1:A:712:ILE:C    | 1:A:712:ILE:CD1  | 0.51     | 2.84        | 1      | 1     |
| 1:A:653:ILE:HD12 | 1:A:669:ILE:CG2  | 0.51     | 2.36        | 9      | 1     |
| 1:A:710:LEU:C    | 1:A:710:LEU:HD22 | 0.51     | 2.31        | 1      | 1     |
| 1:A:653:ILE:HG22 | 1:A:671:VAL:CG2  | 0.51     | 2.35        | 4      | 2     |
| 1:A:698:PHE:HB2  | 1:A:732:ARG:O    | 0.51     | 2.06        | 4      | 1     |
| 1:A:673:SER:HB3  | 1:A:674:GLN:OE1  | 0.51     | 2.06        | 2      | 1     |
| 1:A:709:GLU:O    | 1:A:714:HIS:NE2  | 0.51     | 2.44        | 2      | 1     |
| 1:A:685:LEU:CD1  | 1:A:694:VAL:HA   | 0.51     | 2.35        | 7      | 2     |
| 1:A:712:ILE:CD1  | 1:A:713:PRO:HD3  | 0.51     | 2.36        | 2      | 2     |
| 1:A:704:LEU:CD1  | 1:A:728:ASP:HB2  | 0.51     | 2.36        | 5      | 1     |
| 1:A:652:ILE:O    | 1:A:727:HIS:CD2  | 0.51     | 2.64        | 10     | 1     |
| 1:A:651:ARG:CB   | 1:A:727:HIS:CE1  | 0.51     | 2.94        | 2      | 2     |
| 1:A:659:LEU:CG   | 1:A:733:GLN:HB2  | 0.51     | 2.36        | 2      | 1     |
| 1:A:676:LYS:CE   | 1:A:717:ASN:HA   | 0.50     | 2.36        | 3      | 3     |
| 1:A:710:LEU:C    | 1:A:710:LEU:HD23 | 0.50     | 2.31        | 7      | 1     |
| 1:A:670:LEU:CD1  | 1:A:670:LEU:C    | 0.50     | 2.84        | 10     | 1     |
| 1:A:671:VAL:HG13 | 1:A:672:THR:N    | 0.50     | 2.21        | 2      | 1     |
| 1:A:715:SER:O    | 1:A:718:VAL:HG23 | 0.50     | 2.06        | 2      | 1     |
| 1:A:653:ILE:HG22 | 1:A:671:VAL:HG23 | 0.50     | 1.80        | 4      | 1     |
| 1:A:678:PRO:HG3  | 1:A:719:PHE:CD1  | 0.50     | 2.42        | 5      | 2     |
| 1:A:719:PHE:O    | 1:A:723:ASP:OD2  | 0.50     | 2.29        | 9      | 2     |
| 1:A:659:LEU:HB3  | 1:A:733:GLN:HB2  | 0.50     | 1.83        | 2      | 4     |
| 1:A:659:LEU:HB3  | 1:A:733:GLN:CB   | 0.50     | 2.36        | 7      | 2     |
| 1:A:681:ILE:C    | 1:A:684:VAL:HG22 | 0.50     | 2.31        | 5      | 1     |
| 1:A:659:LEU:C    | 1:A:663:GLY:HA2  | 0.50     | 2.30        | 10     | 2     |
| 1:A:717:ASN:O    | 1:A:717:ASN:CG   | 0.50     | 2.55        | 7      | 2     |
| 1:A:670:LEU:CD2  | 1:A:671:VAL:N    | 0.50     | 2.75        | 4      | 1     |
| 1:A:669:ILE:CD1  | 1:A:670:LEU:O    | 0.50     | 2.59        | 3      | 1     |
| 1:A:703:LEU:HD23 | 1:A:707:ASP:HB2  | 0.50     | 1.82        | 10     | 1     |
| 1:A:655:VAL:O    | 1:A:667:LYS:CB   | 0.50     | 2.60        | 2      | 6     |
| 1:A:655:VAL:CG1  | 1:A:731:LEU:CG   | 0.50     | 2.89        | 1      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:723:ASP:HA   | 1:A:727:HIS:ND1  | 0.50     | 2.22        | 5      | 3     |
| 1:A:696:SER:HB3  | 1:A:698:PHE:CZ   | 0.50     | 2.42        | 9      | 2     |
| 1:A:702:GLN:N    | 1:A:708:ARG:O    | 0.50     | 2.43        | 5      | 4     |
| 1:A:696:SER:HA   | 1:A:698:PHE:CD2  | 0.50     | 2.40        | 7      | 1     |
| 1:A:659:LEU:C    | 1:A:733:GLN:OE1  | 0.50     | 2.54        | 9      | 1     |
| 1:A:718:VAL:CG2  | 1:A:722:MET:SD   | 0.50     | 3.00        | 10     | 1     |
| 1:A:659:LEU:CD2  | 1:A:733:GLN:HB2  | 0.50     | 2.34        | 1      | 3     |
| 1:A:694:VAL:O    | 1:A:695:ALA:O    | 0.50     | 2.30        | 2      | 4     |
| 1:A:680:VAL:O    | 1:A:684:VAL:HG22 | 0.50     | 2.06        | 6      | 1     |
| 1:A:664:SER:C    | 1:A:665:VAL:CG1  | 0.50     | 2.84        | 7      | 1     |
| 1:A:712:ILE:HB   | 1:A:713:PRO:HD3  | 0.50     | 1.83        | 10     | 1     |
| 1:A:712:ILE:HG13 | 1:A:713:PRO:CD   | 0.49     | 2.37        | 4      | 1     |
| 1:A:655:VAL:HA   | 1:A:729:PHE:O    | 0.49     | 2.07        | 10     | 6     |
| 1:A:700:LEU:CD1  | 1:A:711:THR:HA   | 0.49     | 2.37        | 5      | 1     |
| 1:A:708:ARG:HA   | 1:A:708:ARG:NE   | 0.49     | 2.22        | 9      | 2     |
| 1:A:678:PRO:CG   | 1:A:719:PHE:CE1  | 0.49     | 2.95        | 10     | 1     |
| 1:A:718:VAL:CG1  | 1:A:719:PHE:N    | 0.49     | 2.74        | 3      | 4     |
| 1:A:700:LEU:CD1  | 1:A:700:LEU:N    | 0.49     | 2.75        | 2      | 1     |
| 1:A:702:GLN:HG2  | 1:A:703:LEU:CD2  | 0.49     | 2.37        | 3      | 1     |
| 1:A:655:VAL:HG22 | 1:A:729:PHE:HD1  | 0.49     | 1.60        | 10     | 2     |
| 1:A:698:PHE:CD2  | 1:A:700:LEU:HG   | 0.49     | 2.42        | 10     | 1     |
| 1:A:718:VAL:O    | 1:A:722:MET:SD   | 0.49     | 2.70        | 9      | 4     |
| 1:A:676:LYS:CG   | 1:A:716:ALA:O    | 0.49     | 2.60        | 7      | 3     |
| 1:A:694:VAL:CG1  | 1:A:695:ALA:N    | 0.49     | 2.74        | 6      | 3     |
| 1:A:702:GLN:NE2  | 1:A:722:MET:HB3  | 0.49     | 2.23        | 9      | 1     |
| 1:A:651:ARG:O    | 1:A:671:VAL:O    | 0.49     | 2.30        | 7      | 2     |
| 1:A:710:LEU:HD11 | 1:A:722:MET:HG2  | 0.49     | 1.84        | 4      | 1     |
| 1:A:709:GLU:O    | 1:A:709:GLU:CG   | 0.49     | 2.61        | 5      | 2     |
| 1:A:677:ALA:HA   | 1:A:680:VAL:HG13 | 0.49     | 1.83        | 6      | 1     |
| 1:A:717:ASN:CG   | 1:A:717:ASN:O    | 0.49     | 2.53        | 6      | 1     |
| 1:A:697:GLU:OE1  | 1:A:735:ARG:HD2  | 0.49     | 2.07        | 2      | 1     |
| 1:A:723:ASP:OD1  | 1:A:723:ASP:C    | 0.49     | 2.54        | 5      | 1     |
| 1:A:677:ALA:HA   | 1:A:680:VAL:CG1  | 0.49     | 2.37        | 6      | 1     |
| 1:A:698:PHE:CA   | 1:A:733:GLN:HA   | 0.49     | 2.37        | 9      | 1     |
| 1:A:657:MET:O    | 1:A:664:SER:C    | 0.49     | 2.56        | 2      | 6     |
| 1:A:697:GLU:OE1  | 1:A:735:ARG:CD   | 0.49     | 2.61        | 2      | 1     |
| 1:A:702:GLN:HG3  | 1:A:729:PHE:CE1  | 0.49     | 2.43        | 7      | 2     |
| 1:A:727:HIS:CB   | 1:A:729:PHE:CE1  | 0.49     | 2.96        | 3      | 3     |
| 1:A:655:VAL:HG12 | 1:A:731:LEU:HG   | 0.48     | 1.85        | 10     | 7     |
| 1:A:681:ILE:CD1  | 1:A:731:LEU:HD11 | 0.48     | 2.38        | 1      | 1     |
| 1:A:701:VAL:O    | 1:A:729:PHE:HA   | 0.48     | 2.08        | 7      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:695:ALA:O    | 1:A:733:GLN:CD   | 0.48     | 2.56        | 9      | 3     |
| 1:A:657:MET:SD   | 1:A:733:GLN:OE1  | 0.48     | 2.71        | 2      | 1     |
| 1:A:676:LYS:HE2  | 1:A:717:ASN:HA   | 0.48     | 1.85        | 6      | 1     |
| 1:A:651:ARG:O    | 1:A:671:VAL:CB   | 0.48     | 2.61        | 10     | 1     |
| 1:A:653:ILE:HD13 | 1:A:669:ILE:CG2  | 0.48     | 2.38        | 1      | 2     |
| 1:A:697:GLU:HB3  | 1:A:735:ARG:CG   | 0.48     | 2.37        | 5      | 1     |
| 1:A:730:LEU:CD1  | 1:A:731:LEU:N    | 0.48     | 2.69        | 9      | 1     |
| 1:A:678:PRO:HG2  | 1:A:718:VAL:CG1  | 0.48     | 2.38        | 1      | 2     |
| 1:A:723:ASP:HA   | 1:A:727:HIS:CD2  | 0.48     | 2.43        | 1      | 3     |
| 1:A:726:SER:C    | 1:A:727:HIS:CD2  | 0.48     | 2.92        | 1      | 1     |
| 1:A:698:PHE:HB3  | 1:A:733:GLN:HG2  | 0.48     | 1.85        | 2      | 1     |
| 1:A:662:ASP:CB   | 1:A:692:SER:O    | 0.48     | 2.60        | 5      | 1     |
| 1:A:681:ILE:O    | 1:A:684:VAL:HG22 | 0.48     | 2.07        | 5      | 1     |
| 1:A:664:SER:CB   | 1:A:693:ALA:HB2  | 0.48     | 2.38        | 7      | 1     |
| 1:A:712:ILE:HG12 | 1:A:713:PRO:CD   | 0.48     | 2.38        | 2      | 1     |
| 1:A:655:VAL:CG1  | 1:A:729:PHE:O    | 0.48     | 2.62        | 7      | 1     |
| 1:A:712:ILE:HG13 | 1:A:713:PRO:HD3  | 0.48     | 1.85        | 4      | 2     |
| 1:A:702:GLN:HG2  | 1:A:703:LEU:N    | 0.48     | 2.24        | 2      | 1     |
| 1:A:651:ARG:CB   | 1:A:727:HIS:NE2  | 0.48     | 2.77        | 3      | 4     |
| 1:A:659:LEU:CD1  | 1:A:660:GLY:N    | 0.48     | 2.73        | 4      | 1     |
| 1:A:683:ARG:HG3  | 1:A:684:VAL:N    | 0.48     | 2.23        | 6      | 4     |
| 1:A:654:ARG:N    | 1:A:727:HIS:O    | 0.48     | 2.45        | 1      | 2     |
| 1:A:667:LYS:C    | 1:A:667:LYS:HD2  | 0.48     | 2.34        | 1      | 1     |
| 1:A:700:LEU:CB   | 1:A:731:LEU:HD22 | 0.48     | 2.39        | 1      | 1     |
| 1:A:677:ALA:C    | 1:A:680:VAL:HG13 | 0.48     | 2.33        | 6      | 1     |
| 1:A:662:ASP:O    | 1:A:663:GLY:O    | 0.47     | 2.32        | 7      | 6     |
| 1:A:697:GLU:N    | 1:A:733:GLN:OE1  | 0.47     | 2.47        | 6      | 1     |
| 1:A:702:GLN:CB   | 1:A:729:PHE:CD2  | 0.47     | 2.96        | 6      | 2     |
| 1:A:672:THR:CG2  | 1:A:675:ASP:HB2  | 0.47     | 2.34        | 5      | 2     |
| 1:A:657:MET:HE2  | 1:A:693:ALA:CB   | 0.47     | 2.39        | 3      | 1     |
| 1:A:719:PHE:O    | 1:A:721:ALA:N    | 0.47     | 2.47        | 9      | 5     |
| 1:A:655:VAL:HG12 | 1:A:731:LEU:CG   | 0.47     | 2.40        | 4      | 3     |
| 1:A:681:ILE:O    | 1:A:685:LEU:N    | 0.47     | 2.47        | 10     | 3     |
| 1:A:697:GLU:C    | 1:A:733:GLN:OE1  | 0.47     | 2.57        | 6      | 1     |
| 1:A:700:LEU:HD12 | 1:A:700:LEU:H    | 0.47     | 1.64        | 10     | 1     |
| 1:A:685:LEU:HD11 | 1:A:693:ALA:C    | 0.47     | 2.34        | 10     | 1     |
| 1:A:655:VAL:C    | 1:A:656:GLN:HG3  | 0.47     | 2.35        | 1      | 1     |
| 1:A:651:ARG:N    | 1:A:671:VAL:O    | 0.47     | 2.48        | 7      | 2     |
| 1:A:653:ILE:HG12 | 1:A:669:ILE:HG22 | 0.47     | 1.85        | 6      | 1     |
| 1:A:703:LEU:CD1  | 1:A:707:ASP:HB3  | 0.47     | 2.39        | 7      | 2     |
| 1:A:661:GLU:OE2  | 1:A:694:VAL:HG21 | 0.47     | 2.09        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:661:GLU:HG2  | 1:A:694:VAL:CB   | 0.47     | 2.40        | 2      | 1     |
| 1:A:686:LYS:O    | 1:A:689:ASN:ND2  | 0.47     | 2.47        | 9      | 1     |
| 1:A:727:HIS:ND1  | 1:A:727:HIS:N    | 0.47     | 2.60        | 6      | 2     |
| 1:A:659:LEU:CD1  | 1:A:733:GLN:CD   | 0.47     | 2.81        | 4      | 1     |
| 1:A:688:ASN:OD1  | 1:A:692:SER:HB2  | 0.46     | 2.10        | 1      | 8     |
| 1:A:700:LEU:HD23 | 1:A:731:LEU:HD21 | 0.46     | 1.85        | 7      | 2     |
| 1:A:715:SER:O    | 1:A:718:VAL:CG2  | 0.46     | 2.63        | 2      | 1     |
| 1:A:678:PRO:HD3  | 1:A:719:PHE:CE2  | 0.46     | 2.45        | 3      | 1     |
| 1:A:701:VAL:O    | 1:A:729:PHE:HB3  | 0.46     | 2.11        | 6      | 3     |
| 1:A:659:LEU:CD1  | 1:A:733:GLN:HB2  | 0.46     | 2.39        | 2      | 1     |
| 1:A:667:LYS:NZ   | 1:A:681:ILE:HB   | 0.46     | 2.26        | 5      | 1     |
| 1:A:708:ARG:HD3  | 1:A:722:MET:HE2  | 0.46     | 1.87        | 5      | 1     |
| 1:A:653:ILE:HB   | 1:A:727:HIS:ND1  | 0.46     | 2.26        | 9      | 1     |
| 1:A:697:GLU:OE1  | 1:A:735:ARG:HB2  | 0.46     | 2.11        | 2      | 2     |
| 1:A:712:ILE:HG13 | 1:A:713:PRO:N    | 0.46     | 2.25        | 4      | 1     |
| 1:A:654:ARG:HB3  | 1:A:728:ASP:OD1  | 0.46     | 2.11        | 5      | 2     |
| 1:A:667:LYS:CE   | 1:A:681:ILE:HB   | 0.46     | 2.39        | 6      | 1     |
| 1:A:655:VAL:N    | 1:A:667:LYS:O    | 0.46     | 2.46        | 1      | 1     |
| 1:A:700:LEU:HB2  | 1:A:710:LEU:C    | 0.46     | 2.36        | 9      | 2     |
| 1:A:653:ILE:HD13 | 1:A:653:ILE:O    | 0.46     | 2.10        | 9      | 1     |
| 1:A:657:MET:O    | 1:A:664:SER:OG   | 0.46     | 2.33        | 5      | 2     |
| 1:A:702:GLN:CD   | 1:A:722:MET:HB3  | 0.46     | 2.35        | 9      | 1     |
| 1:A:703:LEU:HG   | 1:A:705:PRO:HD2  | 0.46     | 1.86        | 10     | 1     |
| 1:A:694:VAL:O    | 1:A:695:ALA:HB3  | 0.46     | 2.11        | 4      | 1     |
| 1:A:698:PHE:CD1  | 1:A:698:PHE:C    | 0.46     | 2.94        | 7      | 1     |
| 1:A:704:LEU:CD1  | 1:A:704:LEU:H    | 0.46     | 2.22        | 2      | 1     |
| 1:A:659:LEU:O    | 1:A:693:ALA:CB   | 0.46     | 2.62        | 4      | 1     |
| 1:A:676:LYS:HD2  | 1:A:718:VAL:N    | 0.46     | 2.26        | 6      | 1     |
| 1:A:659:LEU:HD23 | 1:A:733:GLN:O    | 0.45     | 2.10        | 1      | 1     |
| 1:A:719:PHE:C    | 1:A:723:ASP:OD2  | 0.45     | 2.59        | 3      | 3     |
| 1:A:702:GLN:CG   | 1:A:729:PHE:CE1  | 0.45     | 2.99        | 5      | 1     |
| 1:A:660:GLY:O    | 1:A:661:GLU:C    | 0.45     | 2.58        | 10     | 3     |
| 1:A:677:ALA:O    | 1:A:680:VAL:CG2  | 0.45     | 2.58        | 9      | 1     |
| 1:A:681:ILE:CG2  | 1:A:682:SER:N    | 0.45     | 2.79        | 10     | 2     |
| 1:A:651:ARG:HD2  | 1:A:723:ASP:O    | 0.45     | 2.11        | 1      | 2     |
| 1:A:667:LYS:HE2  | 1:A:681:ILE:CG1  | 0.45     | 2.41        | 7      | 2     |
| 1:A:657:MET:HE1  | 1:A:685:LEU:HD21 | 0.45     | 1.88        | 6      | 1     |
| 1:A:723:ASP:CB   | 1:A:727:HIS:CE1  | 0.45     | 3.00        | 10     | 3     |
| 1:A:652:ILE:O    | 1:A:652:ILE:HG13 | 0.45     | 2.11        | 2      | 1     |
| 1:A:654:ARG:HD3  | 1:A:728:ASP:OD1  | 0.45     | 2.11        | 6      | 1     |
| 1:A:671:VAL:CG2  | 1:A:677:ALA:HB3  | 0.45     | 2.41        | 9      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:651:ARG:NH1  | 1:A:673:SER:O    | 0.45     | 2.47        | 9      | 3     |
| 1:A:704:LEU:HB2  | 1:A:705:PRO:CD   | 0.45     | 2.40        | 10     | 1     |
| 1:A:669:ILE:HD13 | 1:A:670:LEU:O    | 0.45     | 2.12        | 3      | 1     |
| 1:A:686:LYS:O    | 1:A:689:ASN:OD1  | 0.45     | 2.34        | 4      | 1     |
| 1:A:685:LEU:HD12 | 1:A:694:VAL:C    | 0.45     | 2.37        | 1      | 1     |
| 1:A:731:LEU:N    | 1:A:731:LEU:CD2  | 0.45     | 2.69        | 3      | 1     |
| 1:A:651:ARG:O    | 1:A:671:VAL:HB   | 0.45     | 2.11        | 9      | 3     |
| 1:A:656:GLN:HB2  | 1:A:730:LEU:HD22 | 0.45     | 1.89        | 9      | 1     |
| 1:A:651:ARG:NH2  | 1:A:723:ASP:OD1  | 0.45     | 2.50        | 5      | 1     |
| 1:A:657:MET:HE3  | 1:A:696:SER:HA   | 0.45     | 1.89        | 9      | 1     |
| 1:A:654:ARG:NH1  | 1:A:668:SER:OG   | 0.45     | 2.50        | 10     | 1     |
| 1:A:659:LEU:HG   | 1:A:733:GLN:CB   | 0.45     | 2.41        | 4      | 1     |
| 1:A:653:ILE:CD1  | 1:A:669:ILE:HG22 | 0.45     | 2.42        | 9      | 1     |
| 1:A:702:GLN:HG3  | 1:A:703:LEU:N    | 0.45     | 2.26        | 9      | 1     |
| 1:A:698:PHE:CD1  | 1:A:700:LEU:CD1  | 0.44     | 2.85        | 3      | 1     |
| 1:A:678:PRO:HG3  | 1:A:718:VAL:HG12 | 0.44     | 1.88        | 6      | 2     |
| 1:A:651:ARG:HD3  | 1:A:723:ASP:O    | 0.44     | 2.12        | 1      | 6     |
| 1:A:702:GLN:HG3  | 1:A:729:PHE:CE2  | 0.44     | 2.47        | 2      | 1     |
| 1:A:653:ILE:HB   | 1:A:727:HIS:HB2  | 0.44     | 1.88        | 3      | 2     |
| 1:A:699:GLU:HG3  | 1:A:711:THR:HG22 | 0.44     | 1.89        | 10     | 1     |
| 1:A:676:LYS:HD3  | 1:A:716:ALA:C    | 0.44     | 2.38        | 2      | 1     |
| 1:A:710:LEU:CD1  | 1:A:718:VAL:HG11 | 0.44     | 2.43        | 2      | 1     |
| 1:A:710:LEU:HD22 | 1:A:722:MET:SD   | 0.44     | 2.52        | 10     | 1     |
| 1:A:702:GLN:CA   | 1:A:729:PHE:CD2  | 0.44     | 3.01        | 6      | 1     |
| 1:A:703:LEU:C    | 1:A:705:PRO:HD2  | 0.44     | 2.37        | 9      | 1     |
| 1:A:702:GLN:OE1  | 1:A:722:MET:CG   | 0.44     | 2.66        | 10     | 1     |
| 1:A:718:VAL:O    | 1:A:722:MET:HB2  | 0.44     | 2.13        | 10     | 1     |
| 1:A:727:HIS:HB3  | 1:A:729:PHE:CZ   | 0.44     | 2.48        | 2      | 3     |
| 1:A:688:ASN:O    | 1:A:692:SER:HB2  | 0.44     | 2.13        | 3      | 1     |
| 1:A:710:LEU:CD1  | 1:A:718:VAL:HG21 | 0.44     | 2.42        | 3      | 1     |
| 1:A:710:LEU:O    | 1:A:710:LEU:HD23 | 0.44     | 2.13        | 7      | 1     |
| 1:A:655:VAL:HG12 | 1:A:656:GLN:N    | 0.44     | 2.28        | 10     | 1     |
| 1:A:667:LYS:HD2  | 1:A:667:LYS:C    | 0.44     | 2.38        | 4      | 1     |
| 1:A:710:LEU:C    | 1:A:710:LEU:CD2  | 0.44     | 2.90        | 5      | 1     |
| 1:A:676:LYS:HD2  | 1:A:716:ALA:O    | 0.44     | 2.13        | 10     | 1     |
| 1:A:698:PHE:HB2  | 1:A:732:ARG:C    | 0.44     | 2.38        | 10     | 1     |
| 1:A:710:LEU:HD13 | 1:A:710:LEU:O    | 0.44     | 2.13        | 1      | 1     |
| 1:A:689:ASN:OD1  | 1:A:690:ARG:N    | 0.44     | 2.51        | 6      | 1     |
| 1:A:710:LEU:O    | 1:A:710:LEU:CG   | 0.44     | 2.66        | 6      | 1     |
| 1:A:700:LEU:HD22 | 1:A:731:LEU:CB   | 0.43     | 2.43        | 1      | 1     |
| 1:A:710:LEU:HD13 | 1:A:722:MET:HG2  | 0.43     | 1.90        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:689:ASN:N    | 1:A:689:ASN:OD1  | 0.43     | 2.52        | 2      | 1     |
| 1:A:710:LEU:CD2  | 1:A:718:VAL:HG21 | 0.43     | 2.34        | 5      | 1     |
| 1:A:703:LEU:N    | 1:A:728:ASP:O    | 0.43     | 2.51        | 6      | 1     |
| 1:A:689:ASN:HA   | 1:A:693:ALA:O    | 0.43     | 2.12        | 1      | 3     |
| 1:A:657:MET:CE   | 1:A:733:GLN:HG3  | 0.43     | 2.44        | 5      | 1     |
| 1:A:704:LEU:CD1  | 1:A:728:ASP:CB   | 0.43     | 2.97        | 5      | 1     |
| 1:A:655:VAL:HG11 | 1:A:731:LEU:CD1  | 0.43     | 2.27        | 9      | 1     |
| 1:A:710:LEU:CD2  | 1:A:729:PHE:CZ   | 0.43     | 3.01        | 4      | 1     |
| 1:A:666:TYR:CD1  | 1:A:666:TYR:C    | 0.43     | 2.95        | 9      | 1     |
| 1:A:688:ASN:CG   | 1:A:692:SER:HB2  | 0.43     | 2.38        | 3      | 2     |
| 1:A:676:LYS:HB3  | 1:A:716:ALA:O    | 0.43     | 2.14        | 7      | 2     |
| 1:A:702:GLN:HA   | 1:A:729:PHE:CD2  | 0.43     | 2.49        | 6      | 1     |
| 1:A:671:VAL:HG21 | 1:A:719:PHE:HD2  | 0.43     | 1.71        | 7      | 1     |
| 1:A:697:GLU:OE1  | 1:A:735:ARG:CB   | 0.43     | 2.66        | 2      | 1     |
| 1:A:727:HIS:HB3  | 1:A:729:PHE:CE1  | 0.43     | 2.48        | 3      | 1     |
| 1:A:707:ASP:HB3  | 1:A:708:ARG:HD3  | 0.43     | 1.91        | 4      | 1     |
| 1:A:678:PRO:CG   | 1:A:718:VAL:HG12 | 0.43     | 2.44        | 9      | 1     |
| 1:A:702:GLN:OE1  | 1:A:722:MET:HG2  | 0.43     | 2.13        | 1      | 2     |
| 1:A:677:ALA:CA   | 1:A:680:VAL:CG1  | 0.43     | 2.97        | 6      | 1     |
| 1:A:651:ARG:CZ   | 1:A:723:ASP:CG   | 0.43     | 2.91        | 10     | 1     |
| 1:A:694:VAL:O    | 1:A:733:GLN:NE2  | 0.43     | 2.51        | 10     | 1     |
| 1:A:653:ILE:HB   | 1:A:719:PHE:CE2  | 0.43     | 2.49        | 2      | 1     |
| 1:A:671:VAL:CG1  | 1:A:672:THR:O    | 0.43     | 2.67        | 4      | 1     |
| 1:A:719:PHE:O    | 1:A:723:ASP:OD1  | 0.43     | 2.36        | 4      | 1     |
| 1:A:671:VAL:CG2  | 1:A:677:ALA:CB   | 0.42     | 2.97        | 9      | 1     |
| 1:A:659:LEU:O    | 1:A:663:GLY:HA2  | 0.42     | 2.15        | 1      | 1     |
| 1:A:685:LEU:O    | 1:A:689:ASN:CA   | 0.42     | 2.66        | 5      | 2     |
| 1:A:702:GLN:HB3  | 1:A:708:ARG:O    | 0.42     | 2.13        | 9      | 3     |
| 1:A:650:CYS:HA   | 1:A:672:THR:HA   | 0.42     | 1.90        | 2      | 1     |
| 1:A:693:ALA:C    | 1:A:694:VAL:HG23 | 0.42     | 2.40        | 5      | 2     |
| 1:A:655:VAL:C    | 1:A:667:LYS:HB3  | 0.42     | 2.39        | 10     | 1     |
| 1:A:714:HIS:HB3  | 1:A:718:VAL:CG2  | 0.42     | 2.44        | 2      | 1     |
| 1:A:725:ALA:O    | 1:A:727:HIS:CD2  | 0.42     | 2.72        | 1      | 1     |
| 1:A:657:MET:HG3  | 1:A:731:LEU:CG   | 0.42     | 2.44        | 3      | 1     |
| 1:A:698:PHE:CD1  | 1:A:712:ILE:HD11 | 0.42     | 2.50        | 9      | 1     |
| 1:A:698:PHE:CZ   | 1:A:731:LEU:HD13 | 0.42     | 2.46        | 10     | 1     |
| 1:A:700:LEU:O    | 1:A:710:LEU:N    | 0.42     | 2.50        | 3      | 1     |
| 1:A:657:MET:HE1  | 1:A:695:ALA:O    | 0.42     | 2.15        | 9      | 1     |
| 1:A:673:SER:OG   | 1:A:674:GLN:OE1  | 0.42     | 2.32        | 2      | 1     |
| 1:A:656:GLN:HB2  | 1:A:730:LEU:CD1  | 0.42     | 2.44        | 3      | 1     |
| 1:A:681:ILE:HG12 | 1:A:685:LEU:CD2  | 0.42     | 2.45        | 5      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:651:ARG:HB2  | 1:A:727:HIS:NE2  | 0.42     | 2.28        | 6      | 1     |
| 1:A:688:ASN:OD1  | 1:A:692:SER:OG   | 0.42     | 2.36        | 6      | 1     |
| 1:A:719:PHE:CZ   | 1:A:729:PHE:CZ   | 0.42     | 3.08        | 9      | 1     |
| 1:A:735:ARG:HB2  | 1:A:735:ARG:CZ   | 0.42     | 2.45        | 3      | 1     |
| 1:A:712:ILE:O    | 1:A:712:ILE:HD12 | 0.42     | 2.14        | 5      | 1     |
| 1:A:710:LEU:CD2  | 1:A:710:LEU:C    | 0.42     | 2.93        | 7      | 1     |
| 1:A:664:SER:HB3  | 1:A:693:ALA:N    | 0.42     | 2.29        | 9      | 1     |
| 1:A:709:GLU:O    | 1:A:709:GLU:HG3  | 0.42     | 2.13        | 10     | 1     |
| 1:A:655:VAL:HG12 | 1:A:731:LEU:HD11 | 0.42     | 1.91        | 4      | 1     |
| 1:A:655:VAL:CG2  | 1:A:729:PHE:CD2  | 0.42     | 3.03        | 4      | 1     |
| 1:A:653:ILE:HA   | 1:A:727:HIS:O    | 0.42     | 2.15        | 7      | 1     |
| 1:A:682:SER:O    | 1:A:685:LEU:HB2  | 0.41     | 2.14        | 1      | 2     |
| 1:A:700:LEU:HB3  | 1:A:731:LEU:CD2  | 0.41     | 2.45        | 1      | 1     |
| 1:A:651:ARG:HD2  | 1:A:723:ASP:HB2  | 0.41     | 1.91        | 6      | 2     |
| 1:A:657:MET:HE3  | 1:A:658:GLU:N    | 0.41     | 2.30        | 5      | 1     |
| 1:A:703:LEU:HG   | 1:A:705:PRO:CD   | 0.41     | 2.45        | 10     | 1     |
| 1:A:702:GLN:OE1  | 1:A:722:MET:HB3  | 0.41     | 2.15        | 4      | 2     |
| 1:A:696:SER:HB3  | 1:A:698:PHE:CE2  | 0.41     | 2.49        | 5      | 1     |
| 1:A:697:GLU:CB   | 1:A:735:ARG:HG3  | 0.41     | 2.44        | 5      | 1     |
| 1:A:702:GLN:OE1  | 1:A:710:LEU:HD12 | 0.41     | 2.15        | 9      | 1     |
| 1:A:658:GLU:HG2  | 1:A:658:GLU:O    | 0.41     | 2.15        | 1      | 2     |
| 1:A:676:LYS:N    | 1:A:676:LYS:HD3  | 0.41     | 2.30        | 1      | 1     |
| 1:A:656:GLN:O    | 1:A:731:LEU:HG   | 0.41     | 2.15        | 4      | 1     |
| 1:A:702:GLN:CG   | 1:A:729:PHE:CD1  | 0.41     | 3.03        | 5      | 1     |
| 1:A:657:MET:SD   | 1:A:731:LEU:HD12 | 0.41     | 2.55        | 3      | 1     |
| 1:A:653:ILE:C    | 1:A:654:ARG:HD2  | 0.41     | 2.40        | 6      | 1     |
| 1:A:681:ILE:O    | 1:A:685:LEU:HB2  | 0.41     | 2.15        | 6      | 1     |
| 1:A:655:VAL:CG2  | 1:A:729:PHE:CD1  | 0.41     | 2.98        | 1      | 1     |
| 1:A:661:GLU:CD   | 1:A:694:VAL:HG21 | 0.41     | 2.40        | 1      | 1     |
| 1:A:711:THR:CB   | 1:A:713:PRO:HD2  | 0.41     | 2.44        | 1      | 1     |
| 1:A:689:ASN:CA   | 1:A:694:VAL:HG22 | 0.41     | 2.46        | 3      | 2     |
| 1:A:683:ARG:CG   | 1:A:684:VAL:N    | 0.41     | 2.82        | 9      | 2     |
| 1:A:710:LEU:HD11 | 1:A:718:VAL:HG13 | 0.41     | 1.92        | 5      | 1     |
| 1:A:655:VAL:HG12 | 1:A:656:GLN:H    | 0.41     | 1.75        | 10     | 1     |
| 1:A:685:LEU:HG   | 1:A:696:SER:OG   | 0.41     | 2.14        | 10     | 1     |
| 1:A:649:ASP:O    | 1:A:673:SER:HB2  | 0.41     | 2.15        | 2      | 1     |
| 1:A:681:ILE:HD13 | 1:A:731:LEU:CD1  | 0.41     | 2.45        | 1      | 1     |
| 1:A:735:ARG:HB2  | 1:A:735:ARG:NH2  | 0.41     | 2.31        | 3      | 1     |
| 1:A:681:ILE:HG22 | 1:A:685:LEU:CD2  | 0.41     | 2.46        | 4      | 1     |
| 1:A:672:THR:HG23 | 1:A:673:SER:N    | 0.41     | 2.30        | 2      | 1     |
| 1:A:676:LYS:HG3  | 1:A:717:ASN:HA   | 0.41     | 1.92        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:697:GLU:O    | 1:A:734:ARG:HB3  | 0.41     | 2.16        | 4      | 1     |
| 1:A:698:PHE:N    | 1:A:698:PHE:HD1  | 0.41     | 2.12        | 4      | 1     |
| 1:A:685:LEU:CD2  | 1:A:696:SER:HB3  | 0.41     | 2.46        | 7      | 1     |
| 1:A:666:TYR:O    | 1:A:667:LYS:HB2  | 0.41     | 2.16        | 1      | 1     |
| 1:A:681:ILE:HD12 | 1:A:731:LEU:HD11 | 0.41     | 1.93        | 3      | 1     |
| 1:A:671:VAL:HG12 | 1:A:672:THR:O    | 0.41     | 2.16        | 4      | 1     |
| 1:A:727:HIS:CA   | 1:A:729:PHE:CE1  | 0.41     | 3.03        | 4      | 1     |
| 1:A:670:LEU:HD12 | 1:A:670:LEU:C    | 0.40     | 2.40        | 2      | 1     |
| 1:A:710:LEU:HD22 | 1:A:729:PHE:CD2  | 0.40     | 2.51        | 2      | 1     |
| 1:A:704:LEU:HD12 | 1:A:704:LEU:N    | 0.40     | 2.27        | 7      | 1     |
| 1:A:667:LYS:C    | 1:A:667:LYS:CD   | 0.40     | 2.94        | 3      | 1     |
| 1:A:655:VAL:HG12 | 1:A:731:LEU:CD1  | 0.40     | 2.46        | 4      | 1     |
| 1:A:696:SER:O    | 1:A:698:PHE:CE1  | 0.40     | 2.74        | 9      | 1     |
| 1:A:710:LEU:HD13 | 1:A:722:MET:SD   | 0.40     | 2.56        | 10     | 1     |
| 1:A:669:ILE:CD1  | 1:A:680:VAL:CG2  | 0.40     | 2.94        | 9      | 1     |
| 1:A:651:ARG:HB2  | 1:A:671:VAL:CG1  | 0.40     | 2.46        | 3      | 1     |
| 1:A:707:ASP:CB   | 1:A:708:ARG:HD3  | 0.40     | 2.47        | 4      | 1     |
| 1:A:685:LEU:HA   | 1:A:685:LEU:HD13 | 0.40     | 1.67        | 10     | 1     |
| 1:A:678:PRO:HD3  | 1:A:719:PHE:CD1  | 0.40     | 2.52        | 2      | 1     |
| 1:A:700:LEU:HD22 | 1:A:711:THR:HA   | 0.40     | 1.94        | 2      | 1     |
| 1:A:653:ILE:HB   | 1:A:727:HIS:CD2  | 0.40     | 2.52        | 7      | 1     |

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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     | 86/90 (96%)   | 71±2 (83±2%) | 11±2 (13±2%) | 4±1 (5±1%) | 3           | 25 |
| All | All   | 860/900 (96%) | 711 (83%)    | 108 (13%)    | 41 (5%)    | 3           | 25 |

All 9 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     | 663 | GLY  | 10             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 677 | ALA  | 9              |
| 1   | A     | 703 | LEU  | 9              |
| 1   | A     | 695 | ALA  | 6              |
| 1   | A     | 667 | LYS  | 2              |
| 1   | A     | 694 | VAL  | 2              |
| 1   | A     | 717 | ASN  | 1              |
| 1   | A     | 723 | ASP  | 1              |
| 1   | A     | 707 | ASP  | 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     | 77/79 (97%)   | 62±4 (81±5%) | 15±4 (19±5%) | 3           | 34 |
| All | All   | 770/790 (97%) | 624 (81%)    | 146 (19%)    | 3           | 34 |

All 38 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     | 653 | ILE  | 10             |
| 1   | A     | 688 | ASN  | 10             |
| 1   | A     | 727 | HIS  | 10             |
| 1   | A     | 685 | LEU  | 9              |
| 1   | A     | 718 | VAL  | 9              |
| 1   | A     | 671 | VAL  | 8              |
| 1   | A     | 729 | PHE  | 7              |
| 1   | A     | 667 | LYS  | 6              |
| 1   | A     | 674 | GLN  | 6              |
| 1   | A     | 656 | GLN  | 6              |
| 1   | A     | 712 | ILE  | 6              |
| 1   | A     | 698 | PHE  | 5              |
| 1   | A     | 703 | LEU  | 5              |
| 1   | A     | 672 | THR  | 4              |
| 1   | A     | 710 | LEU  | 4              |
| 1   | A     | 722 | MET  | 4              |
| 1   | A     | 670 | LEU  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 730 | LEU  | 3              |
| 1   | A     | 676 | LYS  | 2              |
| 1   | A     | 700 | LEU  | 2              |
| 1   | A     | 704 | LEU  | 2              |
| 1   | A     | 717 | ASN  | 2              |
| 1   | A     | 659 | LEU  | 2              |
| 1   | A     | 661 | GLU  | 2              |
| 1   | A     | 696 | SER  | 2              |
| 1   | A     | 709 | GLU  | 2              |
| 1   | A     | 733 | GLN  | 2              |
| 1   | A     | 654 | ARG  | 2              |
| 1   | A     | 708 | ARG  | 2              |
| 1   | A     | 669 | ILE  | 1              |
| 1   | A     | 681 | ILE  | 1              |
| 1   | A     | 683 | ARG  | 1              |
| 1   | A     | 684 | VAL  | 1              |
| 1   | A     | 731 | LEU  | 1              |
| 1   | A     | 652 | ILE  | 1              |
| 1   | A     | 680 | VAL  | 1              |
| 1   | A     | 689 | ASN  | 1              |
| 1   | A     | 694 | VAL  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided