



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:23 AM UTC

PDB ID : 1MA6 / pdb\_00001ma6  
Title : TPY4 Tachyplesin I tyrosine mutant in the presence of dodecylphosphocholine micelles (300 mM)  
Authors : Laederach, A.; Andreotti, A.H.; Fulton, D.B.  
Deposited on : 2002-07-31

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                                                             |

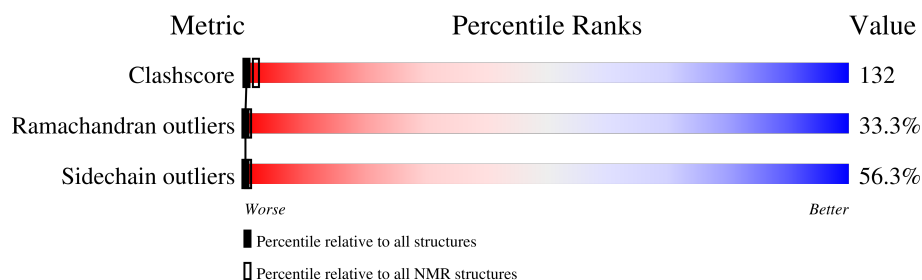
# 1 Overall quality at a glance

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     | 17     |                  |

## 2 Ensemble composition and analysis

This entry contains 31 models. Model 1 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:1-A:16 (16)         | 1.68              | 1            |

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 7 clusters and 1 single-model cluster was found.

| Cluster number        | Models                 |
|-----------------------|------------------------|
| 1                     | 1, 2, 5, 10, 14, 27    |
| 2                     | 12, 13, 17, 18, 20, 29 |
| 3                     | 3, 7, 9, 15, 24, 28    |
| 4                     | 11, 21, 22, 30         |
| 5                     | 6, 19, 26              |
| 6                     | 4, 23, 25              |
| 7                     | 16, 31                 |
| Single-model clusters | 8                      |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 357 atoms, of which 176 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tachyplesin I.

| Mol | Chain | Residues | Atoms |     |     |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|-------|
| 1   | A     | 17       | Total | C   | H   | N  | O  | 0     |
|     |       |          | 357   | 123 | 176 | 34 | 24 |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 3       | TYR      | CYS    | engineered mutation | UNP P14213 |
| A     | 7       | TYR      | CYS    | engineered mutation | UNP P14213 |
| A     | 12      | TYR      | CYS    | engineered mutation | UNP P14213 |
| A     | 16      | TYR      | CYS    | engineered mutation | UNP P14213 |

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

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

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

- Molecule 1: Tachyplesin I

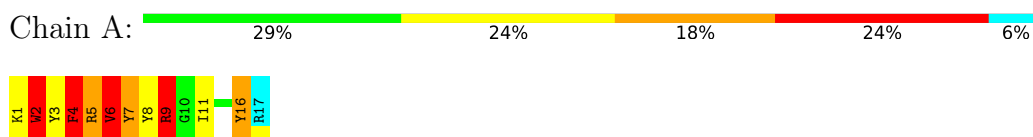


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

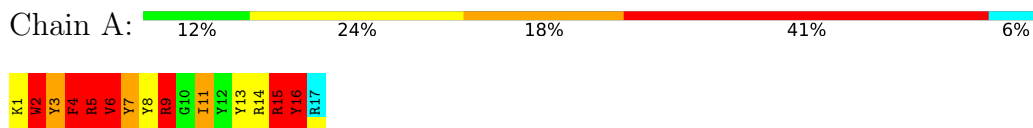
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Tachyplesin I



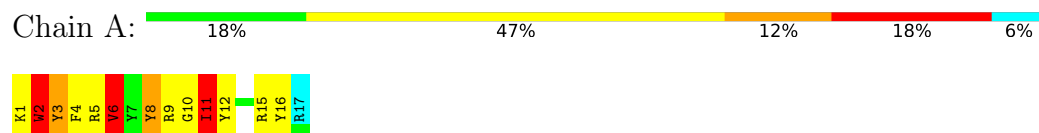
#### 4.2.2 Score per residue for model 2

- Molecule 1: Tachyplesin I



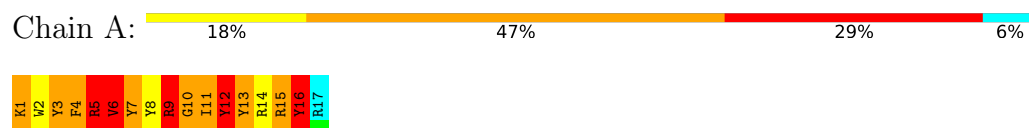
### 4.2.3 Score per residue for model 3

- Molecule 1: Tachyplesin I



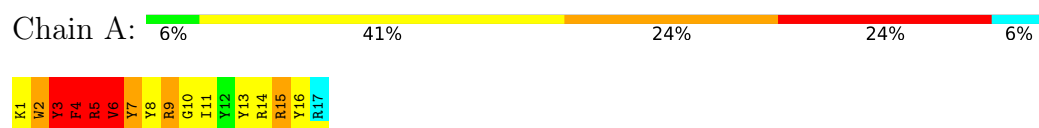
### 4.2.4 Score per residue for model 4

- Molecule 1: Tachyplesin I



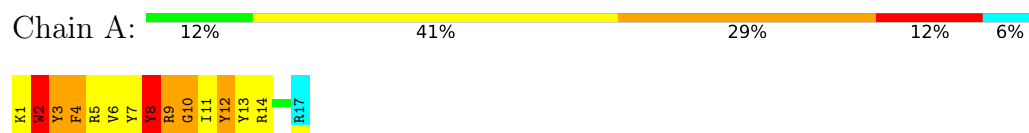
### 4.2.5 Score per residue for model 5

- Molecule 1: Tachyplesin I



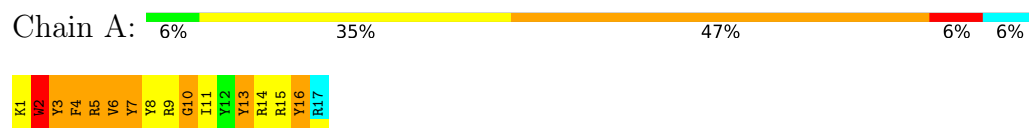
### 4.2.6 Score per residue for model 6

- Molecule 1: Tachyplesin I



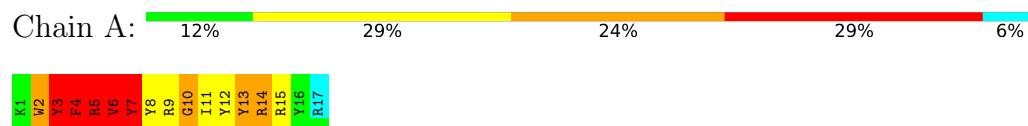
### 4.2.7 Score per residue for model 7

- Molecule 1: Tachyplesin I



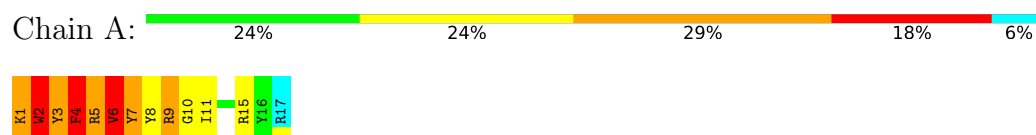
#### 4.2.8 Score per residue for model 8

- Molecule 1: Tachyplesin I



#### 4.2.9 Score per residue for model 9

- Molecule 1: Tachyplesin I



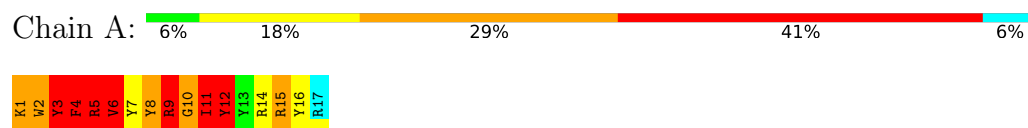
#### 4.2.10 Score per residue for model 10

- Molecule 1: Tachyplesin I



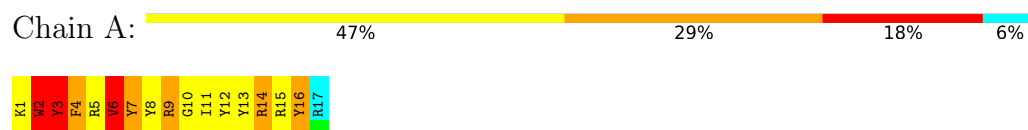
#### 4.2.11 Score per residue for model 11

- Molecule 1: Tachyplesin I



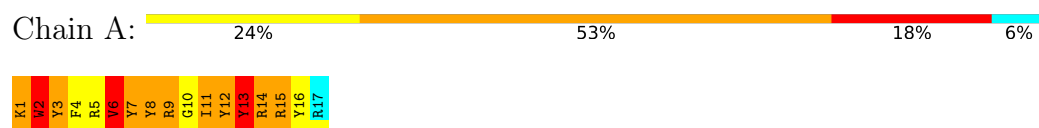
#### 4.2.12 Score per residue for model 12

- Molecule 1: Tachyplesin I



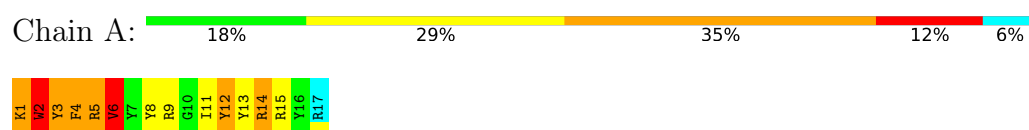
### 4.2.13 Score per residue for model 13

- Molecule 1: Tachyplesin I



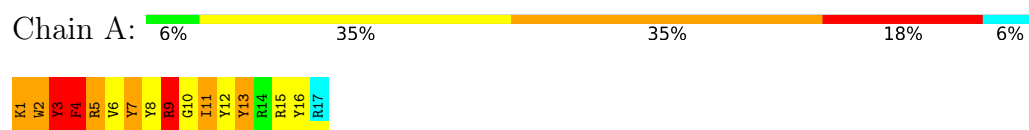
### 4.2.14 Score per residue for model 14

- Molecule 1: Tachyplesin I



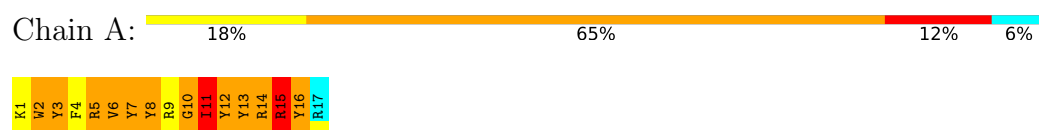
### 4.2.15 Score per residue for model 15

- Molecule 1: Tachyplesin I



### 4.2.16 Score per residue for model 16

- Molecule 1: Tachyplesin I



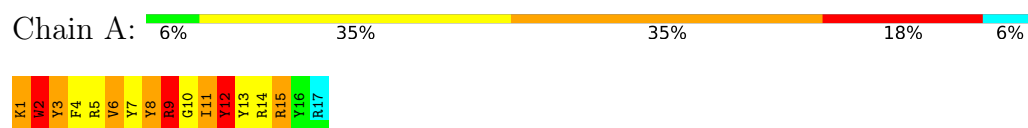
### 4.2.17 Score per residue for model 17

- Molecule 1: Tachyplesin I



#### 4.2.18 Score per residue for model 18

- Molecule 1: Tachyplesin I



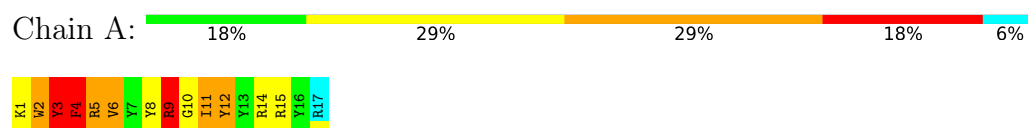
#### 4.2.19 Score per residue for model 19

- Molecule 1: Tachyplesin I



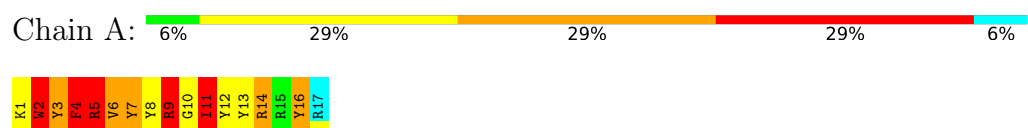
#### 4.2.20 Score per residue for model 20

- Molecule 1: Tachyplesin I



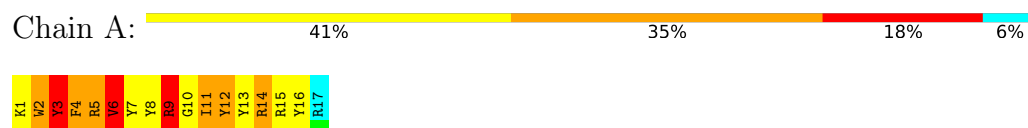
#### 4.2.21 Score per residue for model 21

- Molecule 1: Tachyplesin I



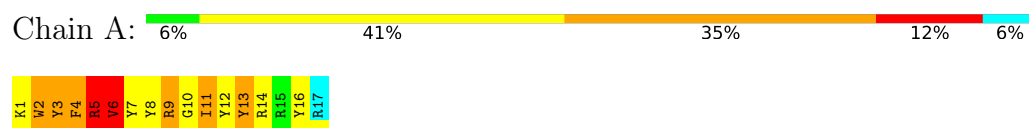
#### 4.2.22 Score per residue for model 22

- Molecule 1: Tachyplesin I



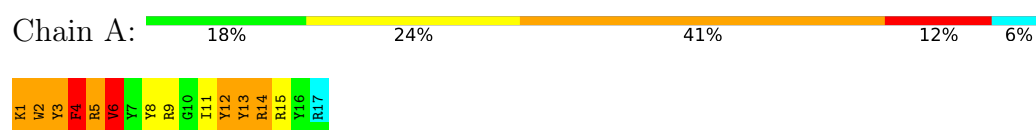
#### 4.2.23 Score per residue for model 23

- Molecule 1: Tachyplesin I



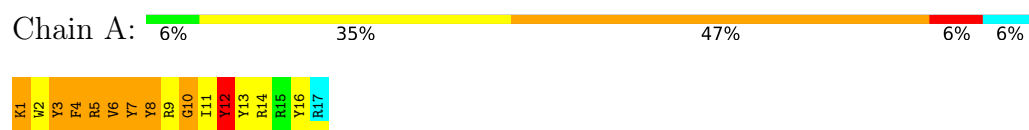
#### 4.2.24 Score per residue for model 24

- Molecule 1: Tachyplesin I



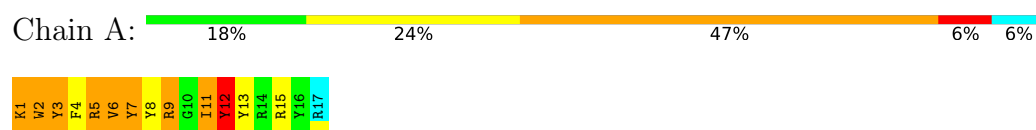
#### 4.2.25 Score per residue for model 25

- Molecule 1: Tachyplesin I



#### 4.2.26 Score per residue for model 26

- Molecule 1: Tachyplesin I



#### 4.2.27 Score per residue for model 27

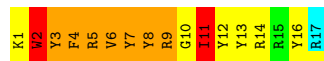
- Molecule 1: Tachyplesin I



#### 4.2.28 Score per residue for model 28

- Molecule 1: Tachyplesin I

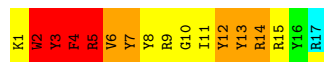
Chain A:  6% 35% 41% 12% 6%



#### 4.2.29 Score per residue for model 29

- Molecule 1: Tachyplesin I

Chain A:  6% 35% 29% 24% 6%



#### 4.2.30 Score per residue for model 30

- Molecule 1: Tachyplesin I

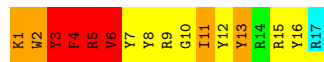
Chain A:  6% 29% 41% 18% 6%



#### 4.2.31 Score per residue for model 31

- Molecule 1: Tachyplesin I

Chain A:  6% 41% 24% 24% 6%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *Simulated annealing with complete cross validation.*

Of the 300 calculated structures, 31 were deposited, based on the following criterion: *structures with the lowest energy.*

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CNS           | structure solution | 1.0     |
| CNS           | refinement         | 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     | 0.43±0.06    | 0±0/178 ( 0.0± 0.0%) | 0.70±0.10   | 0±0/240 ( 0.0± 0.1%) |
| All | All   | 0.43         | 0/5518 ( 0.0%)       | 0.71        | 1/7440 ( 0.0%)       |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
|     |       |     |      |        |      |             |          | Worst  | Total |
| 1   | A     | 3   | TYR  | N-CA-C | 6.52 | 114.12      | 108.78   | 20     | 1     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 169   | 163      | 163      | 44±9    |
| All | All   | 5239  | 5053     | 5053     | 1361    |

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 132.

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

| Atom-1        | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|---------------|-----------------|----------|-------------|--------|-------|
|               |                 |          |             | Worst  | Total |
| 1:A:2:TRP:CD2 | 1:A:11:ILE:HD12 | 1.05     | 1.85        | 8      | 3     |

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| Atom-1        | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|---------------|-----------------|----------|-------------|--------|-------|
|               |                 |          |             | Worst  | Total |
| 1:A:2:TRP:CE2 | 1:A:11:ILE:HD13 | 1.03     | 1.88        | 13     | 12    |
| 1:A:2:TRP:C   | 1:A:3:TYR:HD1   | 1.02     | 1.63        | 26     | 2     |
| 1:A:2:TRP:CE3 | 1:A:3:TYR:CE1   | 1.02     | 2.48        | 26     | 3     |
| 1:A:5:ARG:NH2 | 1:A:8:TYR:HB3   | 0.99     | 1.71        | 27     | 2     |
| 1:A:2:TRP:CE3 | 1:A:3:TYR:N     | 0.97     | 2.32        | 7      | 3     |
| 1:A:2:TRP:CZ2 | 1:A:11:ILE:HG21 | 0.96     | 1.96        | 31     | 1     |
| 1:A:3:TYR:HD1 | 1:A:3:TYR:N     | 0.95     | 1.58        | 26     | 1     |
| 1:A:2:TRP:CD2 | 1:A:3:TYR:CE1   | 0.95     | 2.55        | 26     | 9     |
| 1:A:3:TYR:O   | 1:A:6:VAL:HG13  | 0.94     | 1.60        | 15     | 1     |
| 1:A:2:TRP:O   | 1:A:3:TYR:CG    | 0.93     | 2.21        | 10     | 3     |
| 1:A:2:TRP:CD2 | 1:A:11:ILE:HD13 | 0.93     | 1.97        | 22     | 10    |
| 1:A:1:LYS:CB  | 1:A:11:ILE:HD11 | 0.92     | 1.95        | 12     | 3     |
| 1:A:3:TYR:N   | 1:A:3:TYR:CD1   | 0.91     | 2.31        | 26     | 4     |
| 1:A:8:TYR:HD1 | 1:A:9:ARG:N     | 0.89     | 1.65        | 30     | 1     |
| 1:A:1:LYS:N   | 1:A:11:ILE:HD12 | 0.88     | 1.83        | 23     | 2     |
| 1:A:5:ARG:NH1 | 1:A:11:ILE:HD11 | 0.88     | 1.82        | 19     | 3     |
| 1:A:2:TRP:C   | 1:A:3:TYR:CD1   | 0.87     | 2.51        | 26     | 5     |
| 1:A:8:TYR:HD1 | 1:A:8:TYR:C     | 0.87     | 1.78        | 30     | 1     |
| 1:A:8:TYR:CD1 | 1:A:9:ARG:N     | 0.86     | 2.42        | 30     | 13    |
| 1:A:5:ARG:NE  | 1:A:7:TYR:CD1   | 0.84     | 2.46        | 26     | 1     |
| 1:A:2:TRP:CE3 | 1:A:4:PHE:CE1   | 0.83     | 2.65        | 26     | 1     |
| 1:A:8:TYR:C   | 1:A:8:TYR:CD1   | 0.83     | 2.55        | 30     | 1     |
| 1:A:2:TRP:CG  | 1:A:11:ILE:HD12 | 0.83     | 2.09        | 19     | 4     |
| 1:A:1:LYS:HA  | 1:A:11:ILE:HD11 | 0.82     | 1.49        | 20     | 1     |
| 1:A:2:TRP:O   | 1:A:3:TYR:CD1   | 0.81     | 2.33        | 10     | 4     |
| 1:A:6:VAL:C   | 1:A:7:TYR:CD1   | 0.81     | 2.59        | 7      | 2     |
| 1:A:9:ARG:O   | 1:A:11:ILE:N    | 0.80     | 2.13        | 25     | 4     |
| 1:A:2:TRP:CD1 | 1:A:3:TYR:CE1   | 0.79     | 2.70        | 1      | 9     |
| 1:A:2:TRP:CD1 | 1:A:11:ILE:HD13 | 0.79     | 2.12        | 21     | 9     |
| 1:A:6:VAL:O   | 1:A:6:VAL:HG22  | 0.78     | 1.76        | 6      | 26    |
| 1:A:2:TRP:CZ3 | 1:A:6:VAL:N     | 0.78     | 2.52        | 7      | 1     |
| 1:A:1:LYS:HB3 | 1:A:11:ILE:HD11 | 0.78     | 1.52        | 12     | 1     |
| 1:A:2:TRP:CZ3 | 1:A:4:PHE:CE1   | 0.77     | 2.72        | 31     | 3     |
| 1:A:1:LYS:CG  | 1:A:11:ILE:HD11 | 0.77     | 2.09        | 12     | 2     |
| 1:A:8:TYR:CD2 | 1:A:11:ILE:CG1  | 0.77     | 2.68        | 13     | 3     |
| 1:A:10:GLY:O  | 1:A:11:ILE:HD12 | 0.76     | 1.80        | 21     | 2     |
| 1:A:2:TRP:NE1 | 1:A:11:ILE:HG21 | 0.76     | 1.96        | 19     | 4     |
| 1:A:1:LYS:CB  | 1:A:6:VAL:HG23  | 0.76     | 2.11        | 19     | 1     |
| 1:A:1:LYS:HB3 | 1:A:6:VAL:HG23  | 0.76     | 1.58        | 19     | 3     |
| 1:A:5:ARG:O   | 1:A:6:VAL:HG13  | 0.76     | 1.80        | 7      | 4     |
| 1:A:1:LYS:O   | 1:A:2:TRP:CG    | 0.76     | 2.39        | 4      | 1     |

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| Atom-1        | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|---------------|-----------------|----------|-------------|--------|-------|
|               |                 |          |             | Worst  | Total |
| 1:A:1:LYS:O   | 1:A:3:TYR:CD1   | 0.75     | 2.39        | 4      | 1     |
| 1:A:8:TYR:CG  | 1:A:9:ARG:N     | 0.75     | 2.54        | 3      | 24    |
| 1:A:1:LYS:HB2 | 1:A:11:ILE:CD1  | 0.75     | 2.12        | 25     | 1     |
| 1:A:2:TRP:CZ3 | 1:A:5:ARG:CG    | 0.74     | 2.70        | 27     | 2     |
| 1:A:2:TRP:CZ3 | 1:A:5:ARG:HG2   | 0.74     | 2.18        | 27     | 3     |
| 1:A:1:LYS:HB3 | 1:A:2:TRP:CE3   | 0.74     | 2.17        | 12     | 1     |
| 1:A:5:ARG:CZ  | 1:A:11:ILE:HD11 | 0.73     | 2.13        | 22     | 2     |
| 1:A:2:TRP:CE2 | 1:A:3:TYR:CE1   | 0.73     | 2.77        | 16     | 13    |
| 1:A:3:TYR:CD1 | 1:A:3:TYR:N     | 0.73     | 2.56        | 15     | 15    |
| 1:A:8:TYR:CD2 | 1:A:11:ILE:HG12 | 0.72     | 2.18        | 13     | 2     |
| 1:A:8:TYR:CZ  | 1:A:11:ILE:HG12 | 0.72     | 2.18        | 30     | 1     |
| 1:A:2:TRP:NE1 | 1:A:11:ILE:HB   | 0.72     | 2.00        | 8      | 1     |
| 1:A:2:TRP:NE1 | 1:A:3:TYR:CE1   | 0.72     | 2.57        | 24     | 8     |
| 1:A:5:ARG:NH2 | 1:A:7:TYR:CE1   | 0.72     | 2.58        | 27     | 2     |
| 1:A:8:TYR:CE2 | 1:A:11:ILE:HG12 | 0.71     | 2.21        | 30     | 2     |
| 1:A:1:LYS:HB2 | 1:A:6:VAL:HG23  | 0.71     | 1.62        | 1      | 2     |
| 1:A:2:TRP:O   | 1:A:2:TRP:CG    | 0.71     | 2.44        | 10     | 1     |
| 1:A:2:TRP:CE2 | 1:A:11:ILE:HD12 | 0.70     | 2.19        | 8      | 2     |
| 1:A:8:TYR:CE1 | 1:A:10:GLY:N    | 0.70     | 2.59        | 19     | 2     |
| 1:A:2:TRP:CE3 | 1:A:4:PHE:CD1   | 0.70     | 2.79        | 26     | 1     |
| 1:A:5:ARG:CZ  | 1:A:7:TYR:CE1   | 0.70     | 2.75        | 31     | 3     |
| 1:A:2:TRP:CG  | 1:A:3:TYR:CE1   | 0.70     | 2.80        | 18     | 7     |
| 1:A:3:TYR:O   | 1:A:5:ARG:HG3   | 0.70     | 1.86        | 21     | 2     |
| 1:A:8:TYR:CZ  | 1:A:9:ARG:O     | 0.69     | 2.45        | 6      | 3     |
| 1:A:3:TYR:O   | 1:A:5:ARG:N     | 0.69     | 2.26        | 30     | 10    |
| 1:A:8:TYR:CD2 | 1:A:9:ARG:N     | 0.69     | 2.60        | 15     | 5     |
| 1:A:5:ARG:HB2 | 1:A:8:TYR:CE2   | 0.69     | 2.22        | 30     | 1     |
| 1:A:2:TRP:CH2 | 1:A:4:PHE:CD2   | 0.69     | 2.80        | 11     | 1     |
| 1:A:2:TRP:HA  | 1:A:2:TRP:CE3   | 0.69     | 2.22        | 29     | 1     |
| 1:A:8:TYR:CD1 | 1:A:8:TYR:C     | 0.69     | 2.70        | 6      | 11    |
| 1:A:1:LYS:HG3 | 1:A:7:TYR:CE1   | 0.69     | 2.23        | 25     | 2     |
| 1:A:3:TYR:CE1 | 1:A:4:PHE:CD1   | 0.68     | 2.81        | 6      | 10    |
| 1:A:6:VAL:O   | 1:A:6:VAL:CG2   | 0.68     | 2.41        | 16     | 21    |
| 1:A:2:TRP:CD2 | 1:A:11:ILE:CD1  | 0.68     | 2.76        | 24     | 14    |
| 1:A:5:ARG:NH2 | 1:A:6:VAL:H     | 0.68     | 1.87        | 23     | 1     |
| 1:A:2:TRP:CE3 | 1:A:5:ARG:CG    | 0.68     | 2.76        | 27     | 1     |
| 1:A:2:TRP:CE3 | 1:A:3:TYR:CZ    | 0.68     | 2.82        | 26     | 1     |
| 1:A:3:TYR:CD2 | 1:A:4:PHE:CD1   | 0.67     | 2.83        | 1      | 4     |
| 1:A:2:TRP:CE3 | 1:A:3:TYR:CD1   | 0.67     | 2.82        | 27     | 12    |
| 1:A:3:TYR:N   | 1:A:6:VAL:HG12  | 0.67     | 2.04        | 15     | 1     |
| 1:A:2:TRP:CE3 | 1:A:5:ARG:HG2   | 0.67     | 2.25        | 27     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:ARG:HG3   | 1:A:10:GLY:H    | 0.67     | 1.50        | 6      | 1     |
| 1:A:10:GLY:O    | 1:A:12:TYR:N    | 0.67     | 2.28        | 20     | 2     |
| 1:A:3:TYR:N     | 1:A:3:TYR:HD1   | 0.66     | 1.87        | 15     | 3     |
| 1:A:4:PHE:C     | 1:A:5:ARG:HG3   | 0.66     | 2.16        | 31     | 4     |
| 1:A:2:TRP:CZ3   | 1:A:4:PHE:CD1   | 0.66     | 2.83        | 31     | 2     |
| 1:A:11:ILE:HG22 | 1:A:13:TYR:HB3  | 0.66     | 1.65        | 7      | 3     |
| 1:A:5:ARG:CZ    | 1:A:6:VAL:HA    | 0.66     | 2.21        | 5      | 3     |
| 1:A:2:TRP:CE2   | 1:A:11:ILE:CD1  | 0.66     | 2.79        | 14     | 8     |
| 1:A:2:TRP:CE3   | 1:A:2:TRP:C     | 0.66     | 2.73        | 28     | 5     |
| 1:A:1:LYS:HB3   | 1:A:2:TRP:CZ3   | 0.65     | 2.25        | 12     | 1     |
| 1:A:3:TYR:CE1   | 1:A:4:PHE:CE2   | 0.65     | 2.84        | 14     | 2     |
| 1:A:12:TYR:CG   | 1:A:15:ARG:HG2  | 0.65     | 2.26        | 16     | 1     |
| 1:A:8:TYR:O     | 1:A:9:ARG:CB    | 0.65     | 2.43        | 6      | 9     |
| 1:A:11:ILE:HG22 | 1:A:12:TYR:H    | 0.65     | 1.50        | 31     | 1     |
| 1:A:5:ARG:C     | 1:A:6:VAL:CG1   | 0.65     | 2.70        | 30     | 17    |
| 1:A:1:LYS:HB2   | 1:A:11:ILE:HD11 | 0.65     | 1.68        | 4      | 2     |
| 1:A:2:TRP:O     | 1:A:3:TYR:CB    | 0.65     | 2.45        | 5      | 3     |
| 1:A:11:ILE:HG22 | 1:A:12:TYR:N    | 0.64     | 2.06        | 6      | 6     |
| 1:A:5:ARG:NH2   | 1:A:7:TYR:CD1   | 0.64     | 2.65        | 27     | 2     |
| 1:A:2:TRP:CE2   | 1:A:3:TYR:HE1   | 0.64     | 2.11        | 11     | 5     |
| 1:A:2:TRP:CZ2   | 1:A:3:TYR:HE1   | 0.64     | 2.11        | 22     | 1     |
| 1:A:3:TYR:CE1   | 1:A:4:PHE:CE1   | 0.64     | 2.85        | 31     | 14    |
| 1:A:2:TRP:CD1   | 1:A:11:ILE:HB   | 0.64     | 2.27        | 29     | 3     |
| 1:A:3:TYR:CE2   | 1:A:4:PHE:CE1   | 0.64     | 2.85        | 1      | 3     |
| 1:A:2:TRP:HB3   | 1:A:11:ILE:CG1  | 0.64     | 2.23        | 30     | 3     |
| 1:A:2:TRP:CG    | 1:A:11:ILE:CD1  | 0.64     | 2.81        | 11     | 3     |
| 1:A:8:TYR:CE1   | 1:A:9:ARG:CD    | 0.64     | 2.81        | 10     | 1     |
| 1:A:2:TRP:HE3   | 1:A:3:TYR:N     | 0.63     | 1.91        | 7      | 2     |
| 1:A:4:PHE:CE1   | 1:A:5:ARG:HG2   | 0.63     | 2.29        | 1      | 5     |
| 1:A:5:ARG:C     | 1:A:6:VAL:HG13  | 0.63     | 2.18        | 28     | 3     |
| 1:A:15:ARG:HD2  | 1:A:16:TYR:N    | 0.63     | 2.09        | 16     | 1     |
| 1:A:4:PHE:O     | 1:A:5:ARG:NE    | 0.63     | 2.30        | 30     | 1     |
| 1:A:8:TYR:CE1   | 1:A:9:ARG:O     | 0.63     | 2.52        | 6      | 4     |
| 1:A:12:TYR:C    | 1:A:12:TYR:CD1  | 0.63     | 2.74        | 18     | 1     |
| 1:A:2:TRP:CG    | 1:A:11:ILE:HD13 | 0.63     | 2.28        | 11     | 6     |
| 1:A:8:TYR:CZ    | 1:A:10:GLY:CA   | 0.62     | 2.82        | 23     | 6     |
| 1:A:8:TYR:CD1   | 1:A:11:ILE:CG1  | 0.62     | 2.82        | 9      | 1     |
| 1:A:1:LYS:HB3   | 1:A:9:ARG:HA    | 0.62     | 1.70        | 23     | 1     |
| 1:A:2:TRP:CD2   | 1:A:3:TYR:CD1   | 0.62     | 2.88        | 4      | 9     |
| 1:A:1:LYS:C     | 1:A:5:ARG:NH2   | 0.62     | 2.58        | 23     | 1     |
| 1:A:3:TYR:CD2   | 1:A:4:PHE:CE2   | 0.62     | 2.87        | 10     | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:8:TYR:CE2  | 1:A:11:ILE:HA   | 0.62     | 2.29        | 28     | 1     |
| 1:A:5:ARG:HD2  | 1:A:7:TYR:CE1   | 0.62     | 2.30        | 23     | 2     |
| 1:A:3:TYR:N    | 1:A:5:ARG:HH22  | 0.62     | 1.93        | 23     | 1     |
| 1:A:3:TYR:H    | 1:A:3:TYR:HD1   | 0.61     | 1.36        | 20     | 2     |
| 1:A:2:TRP:N    | 1:A:2:TRP:CE3   | 0.61     | 2.68        | 15     | 5     |
| 1:A:5:ARG:HB2  | 1:A:7:TYR:CE1   | 0.61     | 2.30        | 27     | 2     |
| 1:A:8:TYR:CD1  | 1:A:9:ARG:HB2   | 0.61     | 2.30        | 11     | 1     |
| 1:A:2:TRP:NE1  | 1:A:11:ILE:HD13 | 0.61     | 2.10        | 17     | 5     |
| 1:A:5:ARG:HD3  | 1:A:6:VAL:H     | 0.61     | 1.55        | 31     | 1     |
| 1:A:1:LYS:N    | 1:A:8:TYR:O     | 0.61     | 2.28        | 31     | 3     |
| 1:A:7:TYR:C    | 1:A:7:TYR:CD1   | 0.61     | 2.78        | 8      | 5     |
| 1:A:3:TYR:CD1  | 1:A:3:TYR:C     | 0.61     | 2.78        | 10     | 2     |
| 1:A:2:TRP:CE3  | 1:A:5:ARG:HD2   | 0.61     | 2.31        | 31     | 1     |
| 1:A:2:TRP:CZ3  | 1:A:3:TYR:CG    | 0.60     | 2.89        | 25     | 2     |
| 1:A:2:TRP:CH2  | 1:A:4:PHE:CE1   | 0.60     | 2.88        | 22     | 5     |
| 1:A:2:TRP:CE2  | 1:A:3:TYR:CD2   | 0.60     | 2.89        | 3      | 3     |
| 1:A:8:TYR:CE2  | 1:A:9:ARG:O     | 0.60     | 2.54        | 20     | 4     |
| 1:A:11:ILE:O   | 1:A:12:TYR:CB   | 0.60     | 2.49        | 20     | 4     |
| 1:A:12:TYR:O   | 1:A:14:ARG:N    | 0.60     | 2.33        | 24     | 2     |
| 1:A:8:TYR:CD2  | 1:A:11:ILE:HA   | 0.60     | 2.31        | 30     | 2     |
| 1:A:2:TRP:CD1  | 1:A:13:TYR:HB3  | 0.60     | 2.31        | 6      | 6     |
| 1:A:2:TRP:CZ2  | 1:A:3:TYR:CE1   | 0.60     | 2.90        | 25     | 3     |
| 1:A:12:TYR:CD1 | 1:A:12:TYR:O    | 0.60     | 2.54        | 18     | 2     |
| 1:A:1:LYS:HB3  | 1:A:11:ILE:HD12 | 0.60     | 1.72        | 10     | 1     |
| 1:A:1:LYS:HG3  | 1:A:6:VAL:HG23  | 0.60     | 1.72        | 17     | 1     |
| 1:A:4:PHE:CE1  | 1:A:5:ARG:HB3   | 0.60     | 2.32        | 26     | 1     |
| 1:A:5:ARG:HD2  | 1:A:7:TYR:CD1   | 0.60     | 2.32        | 4      | 3     |
| 1:A:1:LYS:O    | 1:A:3:TYR:HD1   | 0.59     | 1.76        | 4      | 1     |
| 1:A:1:LYS:O    | 1:A:2:TRP:CB    | 0.59     | 2.50        | 18     | 1     |
| 1:A:8:TYR:CD1  | 1:A:9:ARG:HD3   | 0.59     | 2.32        | 10     | 1     |
| 1:A:1:LYS:H2   | 1:A:11:ILE:HD12 | 0.59     | 1.56        | 23     | 1     |
| 1:A:8:TYR:CE1  | 1:A:9:ARG:HB2   | 0.59     | 2.32        | 3      | 3     |
| 1:A:8:TYR:CD2  | 1:A:11:ILE:HG13 | 0.59     | 2.30        | 13     | 4     |
| 1:A:2:TRP:CD2  | 1:A:3:TYR:HE1   | 0.59     | 2.11        | 26     | 3     |
| 1:A:1:LYS:CA   | 1:A:11:ILE:HD11 | 0.59     | 2.27        | 20     | 1     |
| 1:A:5:ARG:O    | 1:A:7:TYR:N     | 0.59     | 2.36        | 27     | 5     |
| 1:A:8:TYR:CD1  | 1:A:11:ILE:HG13 | 0.59     | 2.33        | 9      | 1     |
| 1:A:6:VAL:C    | 1:A:7:TYR:CG    | 0.59     | 2.81        | 28     | 2     |
| 1:A:4:PHE:CD1  | 1:A:5:ARG:HG2   | 0.59     | 2.32        | 1      | 7     |
| 1:A:1:LYS:HB2  | 1:A:7:TYR:CD1   | 0.58     | 2.33        | 18     | 1     |
| 1:A:5:ARG:HH11 | 1:A:11:ILE:HD11 | 0.58     | 1.56        | 27     | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:2:TRP:CZ2  | 1:A:5:ARG:CZ    | 0.58     | 2.87        | 15     | 1     |
| 1:A:1:LYS:H1   | 1:A:1:LYS:HD3   | 0.58     | 1.58        | 25     | 1     |
| 1:A:2:TRP:CE3  | 1:A:3:TYR:CG    | 0.58     | 2.92        | 18     | 2     |
| 1:A:2:TRP:NE1  | 1:A:3:TYR:CD2   | 0.58     | 2.71        | 28     | 1     |
| 1:A:8:TYR:OH   | 1:A:10:GLY:HA3  | 0.58     | 1.98        | 8      | 4     |
| 1:A:8:TYR:OH   | 1:A:10:GLY:C    | 0.58     | 2.47        | 31     | 5     |
| 1:A:2:TRP:CD1  | 1:A:11:ILE:HD12 | 0.58     | 2.34        | 19     | 4     |
| 1:A:2:TRP:HZ3  | 1:A:5:ARG:CG    | 0.58     | 2.11        | 31     | 2     |
| 1:A:2:TRP:CE2  | 1:A:3:TYR:CZ    | 0.58     | 2.92        | 7      | 2     |
| 1:A:5:ARG:NH1  | 1:A:11:ILE:CD1  | 0.58     | 2.67        | 31     | 2     |
| 1:A:3:TYR:C    | 1:A:3:TYR:HD1   | 0.58     | 2.07        | 10     | 1     |
| 1:A:1:LYS:HB2  | 1:A:7:TYR:CE1   | 0.58     | 2.34        | 18     | 1     |
| 1:A:2:TRP:CZ3  | 1:A:5:ARG:NH1   | 0.58     | 2.71        | 23     | 1     |
| 1:A:2:TRP:HB2  | 1:A:3:TYR:CD1   | 0.57     | 2.34        | 31     | 1     |
| 1:A:5:ARG:HA   | 1:A:5:ARG:NE    | 0.57     | 2.14        | 3      | 2     |
| 1:A:2:TRP:CD1  | 1:A:3:TYR:HE1   | 0.57     | 2.13        | 1      | 1     |
| 1:A:11:ILE:CG2 | 1:A:12:TYR:N    | 0.57     | 2.67        | 6      | 2     |
| 1:A:2:TRP:HB3  | 1:A:3:TYR:CD1   | 0.57     | 2.34        | 18     | 1     |
| 1:A:2:TRP:HE1  | 1:A:11:ILE:HG21 | 0.57     | 1.59        | 14     | 1     |
| 1:A:2:TRP:CE2  | 1:A:13:TYR:CD2  | 0.57     | 2.93        | 2      | 1     |
| 1:A:2:TRP:CD1  | 1:A:13:TYR:CG   | 0.57     | 2.93        | 10     | 2     |
| 1:A:1:LYS:O    | 1:A:2:TRP:CD1   | 0.57     | 2.57        | 4      | 1     |
| 1:A:8:TYR:CZ   | 1:A:10:GLY:HA3  | 0.57     | 2.34        | 8      | 4     |
| 1:A:8:TYR:CZ   | 1:A:10:GLY:C    | 0.57     | 2.82        | 28     | 4     |
| 1:A:4:PHE:CE2  | 1:A:5:ARG:HG2   | 0.57     | 2.35        | 17     | 3     |
| 1:A:2:TRP:CD1  | 1:A:13:TYR:CD1  | 0.57     | 2.92        | 21     | 2     |
| 1:A:2:TRP:HA   | 1:A:5:ARG:CZ    | 0.57     | 2.29        | 4      | 1     |
| 1:A:2:TRP:HB3  | 1:A:13:TYR:CD1  | 0.57     | 2.35        | 5      | 1     |
| 1:A:1:LYS:HA   | 1:A:9:ARG:O     | 0.57     | 2.00        | 30     | 1     |
| 1:A:10:GLY:O   | 1:A:11:ILE:CD1  | 0.57     | 2.53        | 21     | 1     |
| 1:A:3:TYR:CD2  | 1:A:4:PHE:CE1   | 0.56     | 2.93        | 28     | 3     |
| 1:A:8:TYR:CE2  | 1:A:10:GLY:C    | 0.56     | 2.83        | 28     | 2     |
| 1:A:2:TRP:CH2  | 1:A:4:PHE:CZ    | 0.56     | 2.93        | 12     | 2     |
| 1:A:4:PHE:CE2  | 1:A:5:ARG:CG    | 0.56     | 2.88        | 16     | 2     |
| 1:A:11:ILE:O   | 1:A:12:TYR:HD1  | 0.56     | 1.82        | 18     | 1     |
| 1:A:1:LYS:H3   | 1:A:11:ILE:HD12 | 0.56     | 1.57        | 23     | 1     |
| 1:A:13:TYR:CG  | 1:A:14:ARG:N    | 0.56     | 2.73        | 6      | 14    |
| 1:A:2:TRP:CG   | 1:A:3:TYR:N     | 0.56     | 2.73        | 28     | 2     |
| 1:A:10:GLY:O   | 1:A:11:ILE:C    | 0.56     | 2.47        | 30     | 9     |
| 1:A:2:TRP:CD1  | 1:A:11:ILE:CG2  | 0.56     | 2.88        | 6      | 2     |
| 1:A:8:TYR:CE2  | 1:A:11:ILE:CG1  | 0.56     | 2.88        | 13     | 2     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:1:LYS:HB2  | 1:A:8:TYR:O     | 0.56     | 2.00        | 16     | 1     |
| 1:A:5:ARG:CZ   | 1:A:6:VAL:H     | 0.56     | 2.12        | 23     | 1     |
| 1:A:2:TRP:CH2  | 1:A:4:PHE:CD1   | 0.56     | 2.94        | 27     | 2     |
| 1:A:1:LYS:CE   | 1:A:6:VAL:HG23  | 0.56     | 2.31        | 23     | 1     |
| 1:A:5:ARG:CB   | 1:A:8:TYR:CE2   | 0.56     | 2.89        | 30     | 1     |
| 1:A:14:ARG:O   | 1:A:16:TYR:N    | 0.56     | 2.39        | 27     | 3     |
| 1:A:5:ARG:NE   | 1:A:6:VAL:H     | 0.56     | 1.98        | 8      | 3     |
| 1:A:3:TYR:N    | 1:A:6:VAL:CG1   | 0.56     | 2.69        | 15     | 1     |
| 1:A:8:TYR:CE2  | 1:A:11:ILE:N    | 0.56     | 2.73        | 31     | 10    |
| 1:A:1:LYS:CA   | 1:A:6:VAL:HB    | 0.56     | 2.31        | 15     | 1     |
| 1:A:8:TYR:CE1  | 1:A:9:ARG:HB3   | 0.56     | 2.36        | 18     | 1     |
| 1:A:3:TYR:CZ   | 1:A:4:PHE:CE1   | 0.56     | 2.93        | 2      | 4     |
| 1:A:11:ILE:H   | 1:A:11:ILE:HD12 | 0.56     | 1.60        | 20     | 2     |
| 1:A:1:LYS:O    | 1:A:3:TYR:N     | 0.55     | 2.38        | 20     | 4     |
| 1:A:4:PHE:CE1  | 1:A:5:ARG:NE    | 0.55     | 2.75        | 15     | 1     |
| 1:A:2:TRP:O    | 1:A:5:ARG:HG3   | 0.55     | 2.01        | 29     | 1     |
| 1:A:2:TRP:CD1  | 1:A:11:ILE:CD1  | 0.55     | 2.89        | 9      | 3     |
| 1:A:5:ARG:O    | 1:A:6:VAL:CG1   | 0.55     | 2.53        | 7      | 1     |
| 1:A:8:TYR:CE1  | 1:A:9:ARG:HD3   | 0.55     | 2.37        | 10     | 1     |
| 1:A:2:TRP:CE3  | 1:A:5:ARG:NH1   | 0.55     | 2.75        | 23     | 1     |
| 1:A:9:ARG:O    | 1:A:9:ARG:HG3   | 0.55     | 2.00        | 28     | 1     |
| 1:A:2:TRP:HB2  | 1:A:13:TYR:CE1  | 0.55     | 2.37        | 10     | 1     |
| 1:A:8:TYR:O    | 1:A:9:ARG:CG    | 0.55     | 2.54        | 23     | 6     |
| 1:A:4:PHE:CE1  | 1:A:11:ILE:HD13 | 0.55     | 2.37        | 8      | 1     |
| 1:A:1:LYS:O    | 1:A:6:VAL:N     | 0.55     | 2.40        | 20     | 1     |
| 1:A:12:TYR:CZ  | 1:A:15:ARG:HD2  | 0.55     | 2.37        | 19     | 1     |
| 1:A:4:PHE:CZ   | 1:A:13:TYR:CZ   | 0.55     | 2.95        | 8      | 1     |
| 1:A:5:ARG:HD2  | 1:A:7:TYR:CZ    | 0.54     | 2.37        | 19     | 1     |
| 1:A:2:TRP:CD1  | 1:A:13:TYR:CE1  | 0.54     | 2.95        | 30     | 1     |
| 1:A:13:TYR:CD1 | 1:A:14:ARG:N    | 0.54     | 2.76        | 4      | 3     |
| 1:A:2:TRP:CE3  | 1:A:3:TYR:HD1   | 0.54     | 2.19        | 5      | 3     |
| 1:A:1:LYS:HB2  | 1:A:9:ARG:HA    | 0.54     | 1.79        | 27     | 3     |
| 1:A:9:ARG:O    | 1:A:9:ARG:HG2   | 0.54     | 2.02        | 20     | 2     |
| 1:A:9:ARG:O    | 1:A:10:GLY:C    | 0.54     | 2.50        | 25     | 1     |
| 1:A:2:TRP:CE2  | 1:A:11:ILE:HG21 | 0.54     | 2.38        | 31     | 1     |
| 1:A:5:ARG:O    | 1:A:6:VAL:C     | 0.54     | 2.50        | 3      | 15    |
| 1:A:8:TYR:CE1  | 1:A:9:ARG:C     | 0.54     | 2.86        | 6      | 4     |
| 1:A:2:TRP:CH2  | 1:A:5:ARG:NE    | 0.54     | 2.76        | 15     | 2     |
| 1:A:12:TYR:O   | 1:A:13:TYR:CD1  | 0.54     | 2.61        | 24     | 1     |
| 1:A:1:LYS:O    | 1:A:3:TYR:CE1   | 0.54     | 2.60        | 4      | 1     |
| 1:A:2:TRP:CZ2  | 1:A:3:TYR:CZ    | 0.54     | 2.96        | 20     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:2:TRP:HB2   | 1:A:11:ILE:HG13 | 0.54     | 1.78        | 18     | 1     |
| 1:A:11:ILE:HG22 | 1:A:13:TYR:N    | 0.54     | 2.18        | 23     | 2     |
| 1:A:13:TYR:C    | 1:A:13:TYR:CD1  | 0.54     | 2.86        | 8      | 1     |
| 1:A:1:LYS:CB    | 1:A:9:ARG:HA    | 0.54     | 2.33        | 23     | 1     |
| 1:A:2:TRP:CD1   | 1:A:11:ILE:HG21 | 0.54     | 2.38        | 6      | 4     |
| 1:A:2:TRP:O     | 1:A:5:ARG:NE    | 0.54     | 2.41        | 11     | 1     |
| 1:A:8:TYR:CE2   | 1:A:11:ILE:HG13 | 0.54     | 2.37        | 13     | 1     |
| 1:A:2:TRP:CZ3   | 1:A:5:ARG:NE    | 0.54     | 2.75        | 22     | 1     |
| 1:A:2:TRP:CG    | 1:A:13:TYR:CD1  | 0.54     | 2.96        | 2      | 2     |
| 1:A:4:PHE:O     | 1:A:4:PHE:CG    | 0.53     | 2.61        | 5      | 4     |
| 1:A:2:TRP:CZ3   | 1:A:7:TYR:CZ    | 0.53     | 2.96        | 9      | 1     |
| 1:A:2:TRP:CH2   | 1:A:4:PHE:HD2   | 0.53     | 2.22        | 11     | 1     |
| 1:A:5:ARG:HB2   | 1:A:7:TYR:CD1   | 0.53     | 2.39        | 27     | 4     |
| 1:A:2:TRP:CA    | 1:A:3:TYR:HD1   | 0.53     | 2.16        | 26     | 1     |
| 1:A:1:LYS:CA    | 1:A:6:VAL:HG21  | 0.53     | 2.34        | 28     | 1     |
| 1:A:2:TRP:N     | 1:A:2:TRP:HE3   | 0.53     | 2.01        | 1      | 4     |
| 1:A:2:TRP:NE1   | 1:A:3:TYR:CZ    | 0.53     | 2.77        | 7      | 2     |
| 1:A:2:TRP:CE3   | 1:A:2:TRP:N     | 0.53     | 2.75        | 23     | 2     |
| 1:A:2:TRP:CE3   | 1:A:6:VAL:HB    | 0.53     | 2.38        | 7      | 1     |
| 1:A:1:LYS:N     | 1:A:6:VAL:HG23  | 0.53     | 2.18        | 6      | 1     |
| 1:A:2:TRP:CD2   | 1:A:3:TYR:CZ    | 0.53     | 2.96        | 18     | 1     |
| 1:A:2:TRP:CZ3   | 1:A:3:TYR:CD2   | 0.53     | 2.97        | 18     | 1     |
| 1:A:2:TRP:CE2   | 1:A:3:TYR:CD1   | 0.53     | 2.97        | 24     | 3     |
| 1:A:4:PHE:C     | 1:A:5:ARG:HG2   | 0.53     | 2.28        | 13     | 3     |
| 1:A:3:TYR:CZ    | 1:A:4:PHE:CE2   | 0.53     | 2.97        | 14     | 1     |
| 1:A:15:ARG:CD   | 1:A:15:ARG:C    | 0.53     | 2.81        | 19     | 1     |
| 1:A:2:TRP:NE1   | 1:A:13:TYR:CD1  | 0.53     | 2.77        | 21     | 1     |
| 1:A:2:TRP:HB2   | 1:A:13:TYR:CD1  | 0.53     | 2.39        | 4      | 1     |
| 1:A:6:VAL:O     | 1:A:7:TYR:CD2   | 0.53     | 2.62        | 28     | 1     |
| 1:A:8:TYR:CE1   | 1:A:9:ARG:CB    | 0.53     | 2.92        | 18     | 2     |
| 1:A:3:TYR:CD1   | 1:A:4:PHE:CD2   | 0.53     | 2.96        | 10     | 2     |
| 1:A:3:TYR:CE1   | 1:A:4:PHE:CZ    | 0.53     | 2.97        | 11     | 3     |
| 1:A:8:TYR:CE2   | 1:A:11:ILE:CA   | 0.53     | 2.92        | 28     | 1     |
| 1:A:2:TRP:O     | 1:A:3:TYR:O     | 0.53     | 2.27        | 30     | 1     |
| 1:A:5:ARG:C     | 1:A:7:TYR:H     | 0.53     | 2.12        | 27     | 1     |
| 1:A:2:TRP:HD1   | 1:A:11:ILE:HD12 | 0.53     | 1.64        | 29     | 1     |
| 1:A:2:TRP:CH2   | 1:A:9:ARG:HA    | 0.52     | 2.39        | 8      | 1     |
| 1:A:4:PHE:O     | 1:A:5:ARG:CB    | 0.52     | 2.57        | 11     | 6     |
| 1:A:2:TRP:CZ2   | 1:A:5:ARG:NE    | 0.52     | 2.77        | 15     | 1     |
| 1:A:5:ARG:NE    | 1:A:6:VAL:N     | 0.52     | 2.56        | 8      | 2     |
| 1:A:2:TRP:CB    | 1:A:11:ILE:HG13 | 0.52     | 2.34        | 30     | 3     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:2:TRP:HB2  | 1:A:11:ILE:HD13 | 0.52     | 1.80        | 26     | 1     |
| 1:A:1:LYS:HA   | 1:A:8:TYR:CD2   | 0.52     | 2.39        | 18     | 1     |
| 1:A:7:TYR:CD1  | 1:A:7:TYR:N     | 0.52     | 2.78        | 7      | 1     |
| 1:A:3:TYR:HD1  | 1:A:3:TYR:H     | 0.52     | 1.45        | 15     | 1     |
| 1:A:1:LYS:O    | 1:A:2:TRP:HB2   | 0.52     | 2.04        | 18     | 1     |
| 1:A:12:TYR:HB2 | 1:A:15:ARG:CG   | 0.52     | 2.35        | 18     | 1     |
| 1:A:2:TRP:HA   | 1:A:2:TRP:HE3   | 0.52     | 1.59        | 29     | 1     |
| 1:A:1:LYS:CA   | 1:A:8:TYR:HB3   | 0.52     | 2.34        | 18     | 1     |
| 1:A:5:ARG:CZ   | 1:A:7:TYR:CD1   | 0.52     | 2.93        | 27     | 3     |
| 1:A:8:TYR:O    | 1:A:9:ARG:CD    | 0.52     | 2.58        | 23     | 3     |
| 1:A:1:LYS:N    | 1:A:5:ARG:HB2   | 0.52     | 2.20        | 20     | 1     |
| 1:A:2:TRP:CZ2  | 1:A:3:TYR:CD2   | 0.51     | 2.98        | 3      | 1     |
| 1:A:2:TRP:HB2  | 1:A:11:ILE:CD1  | 0.51     | 2.35        | 18     | 1     |
| 1:A:8:TYR:O    | 1:A:9:ARG:HD3   | 0.51     | 2.04        | 23     | 1     |
| 1:A:2:TRP:CH2  | 1:A:3:TYR:CD2   | 0.51     | 2.98        | 20     | 1     |
| 1:A:2:TRP:CB   | 1:A:11:ILE:CG1  | 0.51     | 2.89        | 3      | 3     |
| 1:A:4:PHE:CZ   | 1:A:13:TYR:CE1  | 0.51     | 2.98        | 8      | 1     |
| 1:A:2:TRP:CD2  | 1:A:13:TYR:CD2  | 0.51     | 2.99        | 10     | 1     |
| 1:A:1:LYS:CG   | 1:A:6:VAL:HG23  | 0.51     | 2.36        | 16     | 1     |
| 1:A:5:ARG:CD   | 1:A:7:TYR:CD1   | 0.51     | 2.93        | 26     | 1     |
| 1:A:2:TRP:O    | 1:A:3:TYR:HB3   | 0.51     | 2.03        | 5      | 3     |
| 1:A:2:TRP:CE2  | 1:A:13:TYR:HB3  | 0.51     | 2.40        | 6      | 1     |
| 1:A:1:LYS:O    | 1:A:2:TRP:C     | 0.51     | 2.53        | 20     | 5     |
| 1:A:2:TRP:CE3  | 1:A:3:TYR:CD2   | 0.51     | 2.98        | 18     | 1     |
| 1:A:3:TYR:HD2  | 1:A:4:PHE:CD1   | 0.51     | 2.21        | 9      | 2     |
| 1:A:12:TYR:CD1 | 1:A:15:ARG:HG2  | 0.51     | 2.41        | 19     | 1     |
| 1:A:5:ARG:NE   | 1:A:5:ARG:HA    | 0.51     | 2.21        | 30     | 2     |
| 1:A:12:TYR:O   | 1:A:15:ARG:HG3  | 0.51     | 2.06        | 16     | 1     |
| 1:A:2:TRP:CA   | 1:A:5:ARG:CZ    | 0.51     | 2.89        | 4      | 1     |
| 1:A:6:VAL:O    | 1:A:8:TYR:N     | 0.51     | 2.44        | 7      | 2     |
| 1:A:2:TRP:CG   | 1:A:13:TYR:CG   | 0.51     | 2.99        | 10     | 2     |
| 1:A:8:TYR:CD1  | 1:A:10:GLY:N    | 0.51     | 2.79        | 30     | 1     |
| 1:A:2:TRP:CE2  | 1:A:11:ILE:HB   | 0.51     | 2.40        | 8      | 1     |
| 1:A:11:ILE:CG2 | 1:A:13:TYR:HD1  | 0.51     | 2.18        | 16     | 1     |
| 1:A:2:TRP:CZ3  | 1:A:7:TYR:CE1   | 0.51     | 2.99        | 9      | 1     |
| 1:A:2:TRP:CD1  | 1:A:13:TYR:CB   | 0.51     | 2.94        | 10     | 1     |
| 1:A:5:ARG:HB3  | 1:A:7:TYR:CD1   | 0.50     | 2.41        | 18     | 1     |
| 1:A:3:TYR:CZ   | 1:A:4:PHE:CZ    | 0.50     | 2.99        | 11     | 1     |
| 1:A:5:ARG:CZ   | 1:A:7:TYR:OH    | 0.50     | 2.59        | 16     | 1     |
| 1:A:3:TYR:O    | 1:A:6:VAL:N     | 0.50     | 2.45        | 14     | 1     |
| 1:A:4:PHE:CE1  | 1:A:5:ARG:CZ    | 0.50     | 2.94        | 15     | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:2:TRP:N    | 1:A:6:VAL:HB    | 0.50     | 2.22        | 16     | 1     |
| 1:A:1:LYS:HE3  | 1:A:6:VAL:HG23  | 0.50     | 1.82        | 23     | 1     |
| 1:A:6:VAL:O    | 1:A:6:VAL:HG13  | 0.50     | 2.07        | 26     | 1     |
| 1:A:3:TYR:CD1  | 1:A:4:PHE:CD1   | 0.50     | 2.99        | 8      | 6     |
| 1:A:2:TRP:CZ3  | 1:A:4:PHE:CD2   | 0.50     | 2.99        | 11     | 1     |
| 1:A:12:TYR:C   | 1:A:13:TYR:CD1  | 0.50     | 2.89        | 16     | 2     |
| 1:A:3:TYR:CD1  | 1:A:4:PHE:CE1   | 0.50     | 2.98        | 19     | 1     |
| 1:A:2:TRP:C    | 1:A:2:TRP:HE3   | 0.50     | 2.14        | 2      | 1     |
| 1:A:3:TYR:CG   | 1:A:4:PHE:CD2   | 0.50     | 2.99        | 10     | 1     |
| 1:A:2:TRP:HE3  | 1:A:2:TRP:C     | 0.50     | 2.14        | 21     | 2     |
| 1:A:2:TRP:CH2  | 1:A:5:ARG:CD    | 0.50     | 2.94        | 22     | 1     |
| 1:A:2:TRP:CE3  | 1:A:4:PHE:HE1   | 0.50     | 2.20        | 26     | 1     |
| 1:A:2:TRP:HB3  | 1:A:11:ILE:HG13 | 0.50     | 1.84        | 28     | 2     |
| 1:A:9:ARG:CG   | 1:A:10:GLY:H    | 0.50     | 2.18        | 6      | 1     |
| 1:A:4:PHE:CD1  | 1:A:4:PHE:N     | 0.50     | 2.80        | 8      | 3     |
| 1:A:1:LYS:HA   | 1:A:6:VAL:HB    | 0.50     | 1.83        | 15     | 1     |
| 1:A:2:TRP:CZ3  | 1:A:5:ARG:HD2   | 0.50     | 2.42        | 31     | 1     |
| 1:A:2:TRP:CZ3  | 1:A:3:TYR:CZ    | 0.50     | 3.00        | 26     | 1     |
| 1:A:5:ARG:CB   | 1:A:7:TYR:CE1   | 0.50     | 2.94        | 12     | 2     |
| 1:A:2:TRP:HB2  | 1:A:5:ARG:CG    | 0.50     | 2.37        | 26     | 1     |
| 1:A:5:ARG:C    | 1:A:7:TYR:N     | 0.50     | 2.70        | 27     | 1     |
| 1:A:4:PHE:CZ   | 1:A:5:ARG:HG2   | 0.50     | 2.42        | 17     | 2     |
| 1:A:2:TRP:CB   | 1:A:11:ILE:HG12 | 0.49     | 2.37        | 3      | 1     |
| 1:A:4:PHE:CD2  | 1:A:5:ARG:CG    | 0.49     | 2.95        | 16     | 2     |
| 1:A:12:TYR:CE2 | 1:A:15:ARG:CB   | 0.49     | 2.95        | 31     | 1     |
| 1:A:7:TYR:CD1  | 1:A:7:TYR:C     | 0.49     | 2.90        | 4      | 4     |
| 1:A:4:PHE:CD2  | 1:A:5:ARG:NE    | 0.49     | 2.80        | 24     | 3     |
| 1:A:3:TYR:CZ   | 1:A:4:PHE:CD1   | 0.49     | 3.00        | 4      | 2     |
| 1:A:1:LYS:CG   | 1:A:7:TYR:CE1   | 0.49     | 2.96        | 25     | 2     |
| 1:A:2:TRP:CE2  | 1:A:11:ILE:HD11 | 0.49     | 2.42        | 16     | 1     |
| 1:A:13:TYR:CG  | 1:A:13:TYR:O    | 0.49     | 2.65        | 8      | 1     |
| 1:A:2:TRP:CZ3  | 1:A:5:ARG:HG3   | 0.49     | 2.42        | 22     | 1     |
| 1:A:8:TYR:CZ   | 1:A:9:ARG:HG2   | 0.49     | 2.42        | 22     | 1     |
| 1:A:2:TRP:C    | 1:A:3:TYR:CG    | 0.49     | 2.89        | 19     | 2     |
| 1:A:2:TRP:CZ3  | 1:A:3:TYR:CE2   | 0.49     | 3.01        | 18     | 1     |
| 1:A:8:TYR:CE1  | 1:A:9:ARG:CG    | 0.49     | 2.95        | 22     | 2     |
| 1:A:9:ARG:O    | 1:A:9:ARG:CG    | 0.49     | 2.59        | 28     | 1     |
| 1:A:2:TRP:CZ3  | 1:A:5:ARG:HB2   | 0.49     | 2.43        | 1      | 1     |
| 1:A:8:TYR:C    | 1:A:9:ARG:CG    | 0.49     | 2.85        | 25     | 1     |
| 1:A:5:ARG:HG3  | 1:A:6:VAL:N     | 0.49     | 2.22        | 26     | 1     |
| 1:A:2:TRP:CE3  | 1:A:5:ARG:HG3   | 0.49     | 2.41        | 27     | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:2:TRP:CE3  | 1:A:11:ILE:CD1  | 0.49     | 2.96        | 5      | 2     |
| 1:A:2:TRP:CE2  | 1:A:13:TYR:CB   | 0.49     | 2.96        | 6      | 1     |
| 1:A:1:LYS:O    | 1:A:11:ILE:HD11 | 0.49     | 2.08        | 18     | 1     |
| 1:A:1:LYS:HA   | 1:A:5:ARG:HD3   | 0.49     | 1.84        | 27     | 1     |
| 1:A:5:ARG:HA   | 1:A:5:ARG:HE    | 0.49     | 1.68        | 3      | 3     |
| 1:A:2:TRP:CH2  | 1:A:5:ARG:HD3   | 0.49     | 2.43        | 22     | 1     |
| 1:A:4:PHE:CZ   | 1:A:5:ARG:CZ    | 0.49     | 2.95        | 15     | 1     |
| 1:A:13:TYR:CD2 | 1:A:14:ARG:CG   | 0.49     | 2.96        | 16     | 1     |
| 1:A:8:TYR:CE2  | 1:A:10:GLY:N    | 0.49     | 2.81        | 4      | 4     |
| 1:A:2:TRP:CD1  | 1:A:3:TYR:CD1   | 0.49     | 3.01        | 3      | 1     |
| 1:A:12:TYR:HB3 | 1:A:15:ARG:NE   | 0.49     | 2.23        | 16     | 1     |
| 1:A:2:TRP:CZ2  | 1:A:3:TYR:CE2   | 0.49     | 3.00        | 20     | 1     |
| 1:A:8:TYR:CD1  | 1:A:9:ARG:C     | 0.49     | 2.91        | 30     | 1     |
| 1:A:2:TRP:CE2  | 1:A:3:TYR:CG    | 0.48     | 3.01        | 3      | 2     |
| 1:A:5:ARG:HE   | 1:A:5:ARG:CA    | 0.48     | 2.21        | 25     | 4     |
| 1:A:12:TYR:CG  | 1:A:12:TYR:O    | 0.48     | 2.66        | 22     | 2     |
| 1:A:1:LYS:HD3  | 1:A:1:LYS:N     | 0.48     | 2.23        | 25     | 1     |
| 1:A:9:ARG:CD   | 1:A:9:ARG:C     | 0.48     | 2.86        | 10     | 2     |
| 1:A:2:TRP:HD1  | 1:A:11:ILE:HD13 | 0.48     | 1.64        | 4      | 1     |
| 1:A:3:TYR:CE1  | 1:A:4:PHE:CD2   | 0.48     | 3.01        | 14     | 1     |
| 1:A:2:TRP:NE1  | 1:A:13:TYR:HB3  | 0.48     | 2.24        | 6      | 2     |
| 1:A:4:PHE:CZ   | 1:A:11:ILE:HD13 | 0.48     | 2.43        | 8      | 1     |
| 1:A:5:ARG:NH2  | 1:A:7:TYR:CZ    | 0.48     | 2.81        | 27     | 1     |
| 1:A:2:TRP:NE1  | 1:A:3:TYR:CE2   | 0.48     | 2.81        | 3      | 1     |
| 1:A:8:TYR:O    | 1:A:9:ARG:HB3   | 0.48     | 2.08        | 10     | 4     |
| 1:A:1:LYS:HG2  | 1:A:2:TRP:H     | 0.48     | 1.68        | 10     | 1     |
| 1:A:2:TRP:CE3  | 1:A:5:ARG:HD3   | 0.48     | 2.44        | 19     | 1     |
| 1:A:4:PHE:CD2  | 1:A:5:ARG:CZ    | 0.48     | 2.96        | 6      | 2     |
| 1:A:5:ARG:HE   | 1:A:5:ARG:HA    | 0.48     | 1.68        | 25     | 1     |
| 1:A:3:TYR:O    | 1:A:6:VAL:HG12  | 0.48     | 2.09        | 3      | 2     |
| 1:A:1:LYS:H3   | 1:A:6:VAL:HG23  | 0.48     | 1.67        | 6      | 1     |
| 1:A:14:ARG:O   | 1:A:15:ARG:C    | 0.48     | 2.56        | 2      | 3     |
| 1:A:15:ARG:O   | 1:A:16:TYR:C    | 0.47     | 2.57        | 19     | 1     |
| 1:A:9:ARG:O    | 1:A:11:ILE:HG13 | 0.47     | 2.09        | 25     | 2     |
| 1:A:1:LYS:HB3  | 1:A:5:ARG:HB2   | 0.47     | 1.85        | 18     | 1     |
| 1:A:5:ARG:O    | 1:A:7:TYR:CD1   | 0.47     | 2.67        | 2      | 1     |
| 1:A:1:LYS:CG   | 1:A:8:TYR:HB3   | 0.47     | 2.38        | 12     | 1     |
| 1:A:1:LYS:HD3  | 1:A:11:ILE:HD11 | 0.47     | 1.86        | 25     | 1     |
| 1:A:2:TRP:CD2  | 1:A:3:TYR:N     | 0.47     | 2.82        | 28     | 1     |
| 1:A:5:ARG:O    | 1:A:7:TYR:CD2   | 0.47     | 2.67        | 15     | 1     |
| 1:A:1:LYS:HA   | 1:A:5:ARG:NH2   | 0.47     | 2.24        | 5      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:14:ARG:O    | 1:A:15:ARG:HD2  | 0.47     | 2.10        | 16     | 1     |
| 1:A:5:ARG:HD2   | 1:A:11:ILE:HD11 | 0.47     | 1.86        | 2      | 1     |
| 1:A:4:PHE:CE1   | 1:A:11:ILE:CD1  | 0.47     | 2.97        | 8      | 1     |
| 1:A:2:TRP:CZ3   | 1:A:5:ARG:CB    | 0.47     | 2.98        | 27     | 1     |
| 1:A:4:PHE:C     | 1:A:5:ARG:CG    | 0.47     | 2.88        | 29     | 1     |
| 1:A:2:TRP:C     | 1:A:8:TYR:OH    | 0.47     | 2.57        | 30     | 1     |
| 1:A:4:PHE:CE2   | 1:A:5:ARG:NE    | 0.47     | 2.83        | 3      | 1     |
| 1:A:6:VAL:C     | 1:A:8:TYR:N     | 0.47     | 2.72        | 7      | 2     |
| 1:A:15:ARG:O    | 1:A:16:TYR:CD1  | 0.47     | 2.68        | 13     | 2     |
| 1:A:11:ILE:HG23 | 1:A:13:TYR:N    | 0.47     | 2.24        | 16     | 1     |
| 1:A:12:TYR:CD2  | 1:A:15:ARG:HD3  | 0.47     | 2.44        | 16     | 1     |
| 1:A:2:TRP:CH2   | 1:A:5:ARG:HB2   | 0.47     | 2.44        | 1      | 2     |
| 1:A:2:TRP:CZ3   | 1:A:3:TYR:CD1   | 0.47     | 3.02        | 4      | 1     |
| 1:A:8:TYR:CZ    | 1:A:11:ILE:N    | 0.47     | 2.83        | 19     | 2     |
| 1:A:2:TRP:HE3   | 1:A:4:PHE:CD1   | 0.47     | 2.24        | 26     | 1     |
| 1:A:8:TYR:CD1   | 1:A:9:ARG:O     | 0.47     | 2.68        | 6      | 2     |
| 1:A:1:LYS:CB    | 1:A:7:TYR:CE1   | 0.46     | 2.98        | 18     | 1     |
| 1:A:11:ILE:HG22 | 1:A:13:TYR:H    | 0.46     | 1.69        | 23     | 1     |
| 1:A:6:VAL:O     | 1:A:7:TYR:CG    | 0.46     | 2.69        | 28     | 1     |
| 1:A:1:LYS:N     | 1:A:9:ARG:HA    | 0.46     | 2.25        | 13     | 1     |
| 1:A:5:ARG:NH2   | 1:A:11:ILE:HG13 | 0.46     | 2.25        | 16     | 1     |
| 1:A:2:TRP:HB2   | 1:A:11:ILE:CG1  | 0.46     | 2.39        | 18     | 1     |
| 1:A:13:TYR:CD1  | 1:A:13:TYR:N    | 0.46     | 2.83        | 13     | 1     |
| 1:A:11:ILE:O    | 1:A:13:TYR:N    | 0.46     | 2.49        | 18     | 1     |
| 1:A:13:TYR:CD2  | 1:A:14:ARG:N    | 0.46     | 2.83        | 24     | 1     |
| 1:A:7:TYR:CE1   | 1:A:8:TYR:CD2   | 0.46     | 3.03        | 30     | 1     |
| 1:A:3:TYR:O     | 1:A:4:PHE:C     | 0.46     | 2.57        | 14     | 5     |
| 1:A:2:TRP:CZ2   | 1:A:11:ILE:HD13 | 0.46     | 2.45        | 31     | 2     |
| 1:A:5:ARG:HB3   | 1:A:7:TYR:CE1   | 0.46     | 2.45        | 12     | 1     |
| 1:A:2:TRP:CD1   | 1:A:3:TYR:CZ    | 0.46     | 3.03        | 13     | 2     |
| 1:A:12:TYR:CD2  | 1:A:15:ARG:CB   | 0.46     | 2.98        | 13     | 1     |
| 1:A:7:TYR:N     | 1:A:7:TYR:CD1   | 0.46     | 2.83        | 16     | 1     |
| 1:A:1:LYS:HA    | 1:A:7:TYR:CE1   | 0.46     | 2.45        | 25     | 1     |
| 1:A:1:LYS:HA    | 1:A:6:VAL:HA    | 0.46     | 1.87        | 17     | 2     |
| 1:A:2:TRP:CH2   | 1:A:4:PHE:CE2   | 0.46     | 3.03        | 11     | 1     |
| 1:A:13:TYR:CD1  | 1:A:13:TYR:C    | 0.46     | 2.93        | 7      | 3     |
| 1:A:2:TRP:HB2   | 1:A:13:TYR:CG   | 0.46     | 2.46        | 4      | 1     |
| 1:A:8:TYR:CD2   | 1:A:9:ARG:O     | 0.46     | 2.69        | 6      | 1     |
| 1:A:2:TRP:CG    | 1:A:3:TYR:HE1   | 0.46     | 2.27        | 26     | 1     |
| 1:A:4:PHE:CE1   | 1:A:5:ARG:CG    | 0.46     | 2.98        | 1      | 2     |
| 1:A:13:TYR:CE2  | 1:A:14:ARG:CG   | 0.46     | 2.98        | 24     | 3     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:2:TRP:CZ2  | 1:A:11:ILE:HG13 | 0.46     | 2.45        | 8      | 1     |
| 1:A:5:ARG:NH1  | 1:A:10:GLY:O    | 0.46     | 2.48        | 21     | 1     |
| 1:A:1:LYS:HA   | 1:A:6:VAL:HG21  | 0.46     | 1.88        | 28     | 1     |
| 1:A:2:TRP:C    | 1:A:2:TRP:CD2   | 0.46     | 2.93        | 28     | 1     |
| 1:A:13:TYR:CE2 | 1:A:14:ARG:HG3  | 0.46     | 2.45        | 24     | 1     |
| 1:A:5:ARG:CZ   | 1:A:5:ARG:HB2   | 0.46     | 2.41        | 26     | 1     |
| 1:A:2:TRP:CZ3  | 1:A:5:ARG:CD    | 0.46     | 2.99        | 31     | 1     |
| 1:A:2:TRP:NE1  | 1:A:13:TYR:CB   | 0.46     | 2.79        | 2      | 1     |
| 1:A:15:ARG:HD2 | 1:A:15:ARG:C    | 0.46     | 2.36        | 16     | 1     |
| 1:A:5:ARG:CD   | 1:A:6:VAL:N     | 0.45     | 2.79        | 27     | 3     |
| 1:A:4:PHE:CD1  | 1:A:4:PHE:O     | 0.45     | 2.69        | 5      | 2     |
| 1:A:1:LYS:N    | 1:A:9:ARG:O     | 0.45     | 2.48        | 22     | 1     |
| 1:A:4:PHE:CE2  | 1:A:5:ARG:CZ    | 0.45     | 2.99        | 6      | 1     |
| 1:A:2:TRP:HD1  | 1:A:11:ILE:HG21 | 0.45     | 1.71        | 10     | 1     |
| 1:A:16:TYR:C   | 1:A:16:TYR:CD1  | 0.45     | 2.94        | 12     | 1     |
| 1:A:2:TRP:NE1  | 1:A:13:TYR:CE1  | 0.45     | 2.84        | 21     | 1     |
| 1:A:2:TRP:CZ3  | 1:A:5:ARG:HB3   | 0.45     | 2.47        | 27     | 1     |
| 1:A:8:TYR:CE2  | 1:A:11:ILE:CD1  | 0.45     | 2.99        | 30     | 1     |
| 1:A:5:ARG:NE   | 1:A:5:ARG:C     | 0.45     | 2.75        | 26     | 2     |
| 1:A:1:LYS:CG   | 1:A:8:TYR:O     | 0.45     | 2.64        | 27     | 1     |
| 1:A:1:LYS:N    | 1:A:7:TYR:H     | 0.45     | 2.09        | 12     | 1     |
| 1:A:2:TRP:CE3  | 1:A:5:ARG:CZ    | 0.45     | 3.00        | 23     | 1     |
| 1:A:2:TRP:CA   | 1:A:3:TYR:CD1   | 0.45     | 2.99        | 26     | 1     |
| 1:A:1:LYS:HA   | 1:A:6:VAL:HG23  | 0.45     | 1.88        | 16     | 1     |
| 1:A:2:TRP:NE1  | 1:A:11:ILE:CG2  | 0.45     | 2.80        | 26     | 1     |
| 1:A:14:ARG:O   | 1:A:16:TYR:CD1  | 0.45     | 2.70        | 28     | 1     |
| 1:A:4:PHE:CZ   | 1:A:5:ARG:HD2   | 0.45     | 2.47        | 1      | 1     |
| 1:A:1:LYS:CB   | 1:A:5:ARG:HD3   | 0.45     | 2.42        | 4      | 1     |
| 1:A:6:VAL:O    | 1:A:7:TYR:CD1   | 0.45     | 2.69        | 7      | 1     |
| 1:A:2:TRP:HB3  | 1:A:13:TYR:HB3  | 0.45     | 1.88        | 23     | 1     |
| 1:A:5:ARG:CD   | 1:A:11:ILE:HD11 | 0.45     | 2.40        | 2      | 2     |
| 1:A:16:TYR:O   | 1:A:16:TYR:CD2  | 0.45     | 2.69        | 13     | 4     |
| 1:A:2:TRP:CZ2  | 1:A:5:ARG:NH2   | 0.45     | 2.84        | 15     | 1     |
| 1:A:1:LYS:HA   | 1:A:7:TYR:CD1   | 0.45     | 2.46        | 25     | 1     |
| 1:A:8:TYR:CE2  | 1:A:10:GLY:HA3  | 0.45     | 2.46        | 16     | 1     |
| 1:A:4:PHE:CD2  | 1:A:5:ARG:NH1   | 0.45     | 2.84        | 25     | 1     |
| 1:A:2:TRP:NE1  | 1:A:13:TYR:CG   | 0.45     | 2.85        | 2      | 1     |
| 1:A:4:PHE:CD2  | 1:A:5:ARG:HG2   | 0.45     | 2.46        | 16     | 3     |
| 1:A:12:TYR:CD2 | 1:A:15:ARG:HG2  | 0.45     | 2.47        | 16     | 1     |
| 1:A:4:PHE:CD2  | 1:A:5:ARG:HG3   | 0.45     | 2.47        | 23     | 1     |
| 1:A:5:ARG:CG   | 1:A:6:VAL:H     | 0.45     | 2.24        | 27     | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:2:TRP:CH2  | 1:A:15:ARG:NH1  | 0.45     | 2.85        | 29     | 1     |
| 1:A:2:TRP:CG   | 1:A:3:TYR:CD1   | 0.45     | 3.05        | 7      | 3     |
| 1:A:2:TRP:HD1  | 1:A:11:ILE:CB   | 0.44     | 2.24        | 6      | 1     |
| 1:A:15:ARG:C   | 1:A:16:TYR:CD1  | 0.44     | 2.95        | 10     | 1     |
| 1:A:1:LYS:CB   | 1:A:2:TRP:CZ3   | 0.44     | 2.99        | 12     | 1     |
| 1:A:2:TRP:HB3  | 1:A:13:TYR:CE1  | 0.44     | 2.47        | 25     | 1     |
| 1:A:4:PHE:O    | 1:A:5:ARG:CD    | 0.44     | 2.65        | 30     | 1     |
| 1:A:4:PHE:N    | 1:A:4:PHE:HD1   | 0.44     | 2.10        | 9      | 1     |
| 1:A:15:ARG:NH1 | 1:A:16:TYR:CD2  | 0.44     | 2.86        | 16     | 1     |
| 1:A:8:TYR:C    | 1:A:9:ARG:HG2   | 0.44     | 2.36        | 25     | 1     |
| 1:A:2:TRP:CH2  | 1:A:8:TYR:CD2   | 0.44     | 3.06        | 8      | 1     |
| 1:A:1:LYS:CB   | 1:A:6:VAL:HG21  | 0.44     | 2.43        | 7      | 2     |
| 1:A:13:TYR:CD2 | 1:A:14:ARG:HG2  | 0.44     | 2.48        | 16     | 1     |
| 1:A:2:TRP:CH2  | 1:A:11:ILE:HD11 | 0.44     | 2.48        | 23     | 1     |
| 1:A:1:LYS:H1   | 1:A:1:LYS:CD    | 0.44     | 2.25        | 25     | 1     |
| 1:A:5:ARG:NE   | 1:A:7:TYR:CZ    | 0.44     | 2.85        | 16     | 1     |
| 1:A:9:ARG:C    | 1:A:11:ILE:N    | 0.44     | 2.75        | 16     | 4     |
| 1:A:1:LYS:HD3  | 1:A:2:TRP:HB3   | 0.44     | 1.88        | 10     | 1     |
| 1:A:1:LYS:N    | 1:A:9:ARG:N     | 0.44     | 2.65        | 1      | 1     |
| 1:A:4:PHE:CD1  | 1:A:4:PHE:C     | 0.44     | 2.95        | 21     | 2     |
| 1:A:1:LYS:HB3  | 1:A:5:ARG:HG2   | 0.44     | 1.89        | 4      | 1     |
| 1:A:12:TYR:CD1 | 1:A:15:ARG:CG   | 0.44     | 3.01        | 19     | 1     |
| 1:A:4:PHE:CG   | 1:A:5:ARG:N     | 0.44     | 2.86        | 22     | 1     |
| 1:A:3:TYR:CG   | 1:A:4:PHE:N     | 0.44     | 2.83        | 21     | 2     |
| 1:A:11:ILE:CG2 | 1:A:12:TYR:H    | 0.44     | 2.26        | 6      | 2     |
| 1:A:1:LYS:HG3  | 1:A:9:ARG:HA    | 0.44     | 1.89        | 10     | 1     |
| 1:A:13:TYR:CZ  | 1:A:14:ARG:HG2  | 0.44     | 2.48        | 14     | 1     |
| 1:A:2:TRP:HZ3  | 1:A:4:PHE:C     | 0.44     | 2.21        | 27     | 1     |
| 1:A:2:TRP:CE3  | 1:A:2:TRP:HA    | 0.44     | 2.48        | 30     | 1     |
| 1:A:1:LYS:N    | 1:A:9:ARG:CA    | 0.44     | 2.80        | 1      | 1     |
| 1:A:1:LYS:N    | 1:A:9:ARG:C     | 0.44     | 2.76        | 3      | 2     |
| 1:A:3:TYR:CZ   | 1:A:4:PHE:HE1   | 0.44     | 2.31        | 3      | 1     |
| 1:A:8:TYR:HE2  | 1:A:11:ILE:N    | 0.44     | 2.10        | 20     | 1     |
| 1:A:5:ARG:HB2  | 1:A:7:TYR:CD2   | 0.43     | 2.48        | 11     | 1     |
| 1:A:2:TRP:CZ2  | 1:A:11:ILE:HD11 | 0.43     | 2.48        | 16     | 1     |
| 1:A:5:ARG:CG   | 1:A:6:VAL:N     | 0.43     | 2.81        | 27     | 1     |
| 1:A:5:ARG:CA   | 1:A:5:ARG:NE    | 0.43     | 2.81        | 6      | 1     |
| 1:A:2:TRP:HB3  | 1:A:6:VAL:HA    | 0.43     | 1.90        | 9      | 1     |
| 1:A:16:TYR:O   | 1:A:16:TYR:CG   | 0.43     | 2.71        | 12     | 3     |
| 1:A:9:ARG:N    | 1:A:9:ARG:HD3   | 0.43     | 2.28        | 10     | 1     |
| 1:A:2:TRP:CD1  | 1:A:2:TRP:N     | 0.43     | 2.87        | 20     | 1     |

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:12:TYR:O   | 1:A:13:TYR:O    | 0.43     | 2.36        | 23     | 1     |
| 1:A:12:TYR:CZ  | 1:A:15:ARG:HB2  | 0.43     | 2.49        | 31     | 1     |
| 1:A:3:TYR:O    | 1:A:6:VAL:CG1   | 0.43     | 2.67        | 16     | 1     |
| 1:A:2:TRP:CB   | 1:A:13:TYR:CD1  | 0.43     | 3.01        | 4      | 1     |
| 1:A:14:ARG:O   | 1:A:15:ARG:CD   | 0.43     | 2.67        | 16     | 1     |
| 1:A:4:PHE:CE2  | 1:A:5:ARG:HD2   | 0.43     | 2.48        | 20     | 1     |
| 1:A:8:TYR:CD1  | 1:A:11:ILE:N    | 0.43     | 2.87        | 30     | 1     |
| 1:A:1:LYS:C    | 1:A:11:ILE:CD1  | 0.43     | 2.91        | 4      | 1     |
| 1:A:1:LYS:HB3  | 1:A:6:VAL:HG21  | 0.43     | 1.89        | 7      | 1     |
| 1:A:8:TYR:CE1  | 1:A:9:ARG:HG3   | 0.43     | 2.48        | 21     | 2     |
| 1:A:2:TRP:CE2  | 1:A:13:TYR:CG   | 0.43     | 3.07        | 2      | 1     |
| 1:A:2:TRP:HB2  | 1:A:11:ILE:HG12 | 0.43     | 1.89        | 3      | 1     |
| 1:A:8:TYR:HE1  | 1:A:10:GLY:C    | 0.43     | 2.22        | 7      | 1     |
| 1:A:11:ILE:O   | 1:A:12:TYR:C    | 0.43     | 2.62        | 18     | 1     |
| 1:A:1:LYS:HG2  | 1:A:1:LYS:O     | 0.43     | 2.13        | 22     | 1     |
| 1:A:8:TYR:C    | 1:A:9:ARG:HG3   | 0.43     | 2.39        | 24     | 1     |
| 1:A:5:ARG:C    | 1:A:6:VAL:HG12  | 0.43     | 2.39        | 19     | 4     |
| 1:A:12:TYR:HA  | 1:A:15:ARG:HG3  | 0.43     | 1.89        | 24     | 1     |
| 1:A:13:TYR:CE1 | 1:A:14:ARG:HG2  | 0.43     | 2.49        | 5      | 1     |
| 1:A:12:TYR:CE2 | 1:A:15:ARG:O    | 0.43     | 2.72        | 18     | 3     |
| 1:A:8:TYR:CE1  | 1:A:11:ILE:HA   | 0.43     | 2.49        | 22     | 1     |
| 1:A:2:TRP:HZ3  | 1:A:5:ARG:HD3   | 0.43     | 1.72        | 23     | 1     |
| 1:A:1:LYS:CB   | 1:A:8:TYR:O     | 0.43     | 2.67        | 26     | 1     |
| 1:A:5:ARG:CD   | 1:A:7:TYR:HD1   | 0.43     | 2.27        | 26     | 1     |
| 1:A:2:TRP:HB3  | 1:A:5:ARG:CZ    | 0.42     | 2.43        | 11     | 2     |
| 1:A:7:TYR:O    | 1:A:7:TYR:CG    | 0.42     | 2.72        | 6      | 1     |
| 1:A:5:ARG:N    | 1:A:5:ARG:HE    | 0.42     | 2.11        | 7      | 1     |
| 1:A:8:TYR:CE1  | 1:A:10:GLY:C    | 0.42     | 2.97        | 25     | 1     |
| 1:A:5:ARG:CZ   | 1:A:8:TYR:HB3   | 0.42     | 2.42        | 27     | 1     |
| 1:A:1:LYS:O    | 1:A:2:TRP:CD2   | 0.42     | 2.71        | 4      | 1     |
| 1:A:1:LYS:HG3  | 1:A:8:TYR:HB3   | 0.42     | 1.91        | 12     | 1     |
| 1:A:6:VAL:C    | 1:A:8:TYR:H     | 0.42     | 2.22        | 28     | 1     |
| 1:A:5:ARG:HD3  | 1:A:11:ILE:CD1  | 0.42     | 2.44        | 2      | 1     |
| 1:A:8:TYR:CD1  | 1:A:9:ARG:CB    | 0.42     | 3.02        | 18     | 1     |
| 1:A:4:PHE:O    | 1:A:5:ARG:HB2   | 0.42     | 2.15        | 24     | 1     |
| 1:A:1:LYS:CA   | 1:A:5:ARG:NH2   | 0.42     | 2.82        | 29     | 1     |
| 1:A:5:ARG:HD3  | 1:A:11:ILE:HD11 | 0.42     | 1.92        | 29     | 1     |
| 1:A:9:ARG:C    | 1:A:11:ILE:H    | 0.42     | 2.21        | 6      | 3     |
| 1:A:12:TYR:CD2 | 1:A:15:ARG:O    | 0.42     | 2.72        | 29     | 3     |
| 1:A:8:TYR:CE1  | 1:A:9:ARG:HG2   | 0.42     | 2.50        | 22     | 1     |
| 1:A:13:TYR:CE1 | 1:A:14:ARG:CG   | 0.42     | 3.02        | 5      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:2:TRP:CH2   | 1:A:4:PHE:HE1   | 0.42     | 2.33        | 9      | 1     |
| 1:A:11:ILE:HD12 | 1:A:11:ILE:N    | 0.42     | 2.27        | 20     | 1     |
| 1:A:1:LYS:O     | 1:A:13:TYR:CE1  | 0.42     | 2.73        | 26     | 1     |
| 1:A:5:ARG:CD    | 1:A:6:VAL:H     | 0.42     | 2.26        | 31     | 1     |
| 1:A:5:ARG:CD    | 1:A:7:TYR:CE1   | 0.42     | 3.03        | 4      | 1     |
| 1:A:12:TYR:O    | 1:A:12:TYR:CG   | 0.42     | 2.72        | 18     | 2     |
| 1:A:10:GLY:O    | 1:A:11:ILE:O    | 0.42     | 2.38        | 19     | 1     |
| 1:A:8:TYR:CZ    | 1:A:10:GLY:N    | 0.42     | 2.88        | 5      | 1     |
| 1:A:1:LYS:CG    | 1:A:2:TRP:N     | 0.42     | 2.83        | 10     | 1     |
| 1:A:6:VAL:O     | 1:A:6:VAL:HG23  | 0.42     | 2.14        | 15     | 1     |
| 1:A:2:TRP:CH2   | 1:A:5:ARG:CG    | 0.42     | 3.03        | 22     | 1     |
| 1:A:2:TRP:CZ3   | 1:A:5:ARG:HD3   | 0.42     | 2.50        | 8      | 1     |
| 1:A:5:ARG:HB2   | 1:A:7:TYR:CE2   | 0.42     | 2.50        | 21     | 1     |
| 1:A:2:TRP:CE3   | 1:A:3:TYR:HB3   | 0.42     | 2.50        | 25     | 1     |
| 1:A:5:ARG:NE    | 1:A:5:ARG:CA    | 0.42     | 2.83        | 30     | 2     |
| 1:A:8:TYR:O     | 1:A:9:ARG:C     | 0.42     | 2.62        | 21     | 1     |
| 1:A:1:LYS:HB3   | 1:A:9:ARG:C     | 0.42     | 2.40        | 24     | 1     |
| 1:A:8:TYR:CE1   | 1:A:10:GLY:CA   | 0.42     | 3.03        | 19     | 1     |
| 1:A:4:PHE:CD1   | 1:A:5:ARG:N     | 0.42     | 2.88        | 26     | 1     |
| 1:A:2:TRP:HB3   | 1:A:11:ILE:CD1  | 0.42     | 2.45        | 30     | 1     |
| 1:A:9:ARG:CD    | 1:A:9:ARG:O     | 0.41     | 2.68        | 1      | 1     |
| 1:A:4:PHE:O     | 1:A:5:ARG:CG    | 0.41     | 2.68        | 11     | 2     |
| 1:A:2:TRP:CZ3   | 1:A:11:ILE:CD1  | 0.41     | 3.03        | 23     | 1     |
| 1:A:12:TYR:CD2  | 1:A:12:TYR:O    | 0.41     | 2.73        | 28     | 1     |
| 1:A:13:TYR:O    | 1:A:16:TYR:CD1  | 0.41     | 2.73        | 4      | 1     |
| 1:A:1:LYS:HG3   | 1:A:8:TYR:C     | 0.41     | 2.40        | 24     | 1     |
| 1:A:1:LYS:HA    | 1:A:8:TYR:O     | 0.41     | 2.14        | 26     | 1     |
| 1:A:2:TRP:CB    | 1:A:11:ILE:HD13 | 0.41     | 2.45        | 26     | 1     |
| 1:A:12:TYR:CD1  | 1:A:12:TYR:C    | 0.41     | 2.98        | 4      | 1     |
| 1:A:8:TYR:OH    | 1:A:10:GLY:CA   | 0.41     | 2.68        | 5      | 1     |
| 1:A:12:TYR:CD1  | 1:A:15:ARG:HG3  | 0.41     | 2.49        | 14     | 1     |
| 1:A:5:ARG:HD2   | 1:A:7:TYR:OH    | 0.41     | 2.15        | 16     | 1     |
| 1:A:12:TYR:CE1  | 1:A:15:ARG:HB2  | 0.41     | 2.51        | 31     | 1     |
| 1:A:5:ARG:HE    | 1:A:5:ARG:N     | 0.41     | 2.12        | 6      | 1     |
| 1:A:1:LYS:HB3   | 1:A:11:ILE:CD1  | 0.41     | 2.37        | 12     | 1     |
| 1:A:1:LYS:CD    | 1:A:11:ILE:HD11 | 0.41     | 2.45        | 25     | 1     |
| 1:A:13:TYR:O    | 1:A:16:TYR:CG   | 0.41     | 2.74        | 4      | 1     |
| 1:A:2:TRP:HE3   | 1:A:5:ARG:CZ    | 0.41     | 2.28        | 8      | 1     |
| 1:A:1:LYS:HG2   | 1:A:11:ILE:HD11 | 0.41     | 1.87        | 12     | 1     |
| 1:A:2:TRP:N     | 1:A:8:TYR:OH    | 0.41     | 2.53        | 30     | 1     |
| 1:A:12:TYR:CE2  | 1:A:15:ARG:HB2  | 0.41     | 2.49        | 31     | 1     |

*Continued on next page...*

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| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:9:ARG:CG   | 1:A:9:ARG:O     | 0.41     | 2.68        | 1      | 1     |
| 1:A:4:PHE:O    | 1:A:5:ARG:HB3   | 0.41     | 2.15        | 8      | 1     |
| 1:A:2:TRP:CE2  | 1:A:5:ARG:NH2   | 0.41     | 2.88        | 15     | 1     |
| 1:A:3:TYR:CD1  | 1:A:4:PHE:HD1   | 0.41     | 2.32        | 18     | 1     |
| 1:A:8:TYR:OH   | 1:A:11:ILE:N    | 0.41     | 2.53        | 16     | 1     |
| 1:A:10:GLY:O   | 1:A:11:ILE:CG1  | 0.41     | 2.69        | 21     | 1     |
| 1:A:2:TRP:NE1  | 1:A:3:TYR:CD1   | 0.41     | 2.88        | 24     | 1     |
| 1:A:2:TRP:CH2  | 1:A:14:ARG:NH1  | 0.41     | 2.89        | 28     | 1     |
| 1:A:16:TYR:CD1 | 1:A:16:TYR:C    | 0.41     | 2.99        | 4      | 1     |
| 1:A:8:TYR:CE1  | 1:A:11:ILE:CG1  | 0.41     | 3.04        | 9      | 1     |
| 1:A:3:TYR:CD1  | 1:A:4:PHE:N     | 0.41     | 2.89        | 10     | 1     |
| 1:A:5:ARG:NH2  | 1:A:11:ILE:CG1  | 0.41     | 2.83        | 16     | 1     |
| 1:A:12:TYR:HB2 | 1:A:15:ARG:HG3  | 0.41     | 1.93        | 18     | 1     |
| 1:A:1:LYS:CB   | 1:A:9:ARG:N     | 0.41     | 2.84        | 23     | 1     |
| 1:A:2:TRP:O    | 1:A:3:TYR:C     | 0.41     | 2.63        | 29     | 1     |
| 1:A:4:PHE:CD2  | 1:A:5:ARG:NH2   | 0.41     | 2.89        | 6      | 1     |
| 1:A:8:TYR:CZ   | 1:A:9:ARG:CG    | 0.41     | 3.03        | 22     | 1     |
| 1:A:8:TYR:CG   | 1:A:11:ILE:HA   | 0.41     | 2.51        | 30     | 1     |
| 1:A:5:ARG:NH1  | 1:A:8:TYR:O     | 0.40     | 2.54        | 5      | 1     |
| 1:A:3:TYR:C    | 1:A:6:VAL:HG13  | 0.40     | 2.37        | 15     | 1     |
| 1:A:8:TYR:CE2  | 1:A:10:GLY:CA   | 0.40     | 3.04        | 16     | 1     |
| 1:A:2:TRP:HB2  | 1:A:5:ARG:HG3   | 0.40     | 1.92        | 26     | 1     |
| 1:A:2:TRP:O    | 1:A:2:TRP:CD1   | 0.40     | 2.72        | 10     | 1     |
| 1:A:4:PHE:CB   | 1:A:5:ARG:NH2   | 0.40     | 2.85        | 10     | 1     |
| 1:A:2:TRP:CZ3  | 1:A:6:VAL:HA    | 0.40     | 2.52        | 15     | 1     |
| 1:A:8:TYR:O    | 1:A:10:GLY:N    | 0.40     | 2.54        | 21     | 1     |
| 1:A:2:TRP:HB3  | 1:A:11:ILE:HD11 | 0.40     | 1.92        | 30     | 1     |
| 1:A:12:TYR:O   | 1:A:13:TYR:C    | 0.40     | 2.65        | 25     | 2     |
| 1:A:11:ILE:O   | 1:A:13:TYR:CE1  | 0.40     | 2.74        | 31     | 1     |
| 1:A:5:ARG:CD   | 1:A:11:ILE:CD1  | 0.40     | 3.00        | 2      | 1     |
| 1:A:8:TYR:CD1  | 1:A:9:ARG:HG2   | 0.40     | 2.51        | 3      | 1     |
| 1:A:12:TYR:O   | 1:A:15:ARG:N    | 0.40     | 2.54        | 4      | 1     |
| 1:A:2:TRP:CD1  | 1:A:11:ILE:CB   | 0.40     | 3.04        | 6      | 1     |
| 1:A:3:TYR:CE2  | 1:A:4:PHE:CE2   | 0.40     | 3.10        | 10     | 1     |
| 1:A:12:TYR:O   | 1:A:13:TYR:CG   | 0.40     | 2.74        | 16     | 1     |
| 1:A:4:PHE:O    | 1:A:5:ARG:HG2   | 0.40     | 2.16        | 24     | 1     |
| 1:A:5:ARG:HB2  | 1:A:8:TYR:CZ    | 0.40     | 2.52        | 30     | 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     | 15/17 (88%)   | 5±2 (35±12%) | 5±2 (31±13%) | 5±2 (33±11%) | 0           | 0 |
| All | All   | 465/527 (88%) | 164 (35%)    | 146 (31%)    | 155 (33%)    | 0           | 0 |

All 15 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     | 4   | PHE  | 21             |
| 1   | A     | 6   | VAL  | 21             |
| 1   | A     | 2   | TRP  | 19             |
| 1   | A     | 9   | ARG  | 15             |
| 1   | A     | 10  | GLY  | 13             |
| 1   | A     | 11  | ILE  | 12             |
| 1   | A     | 3   | TYR  | 11             |
| 1   | A     | 5   | ARG  | 10             |
| 1   | A     | 12  | TYR  | 9              |
| 1   | A     | 16  | TYR  | 8              |
| 1   | A     | 15  | ARG  | 5              |
| 1   | A     | 7   | TYR  | 4              |
| 1   | A     | 13  | TYR  | 4              |
| 1   | A     | 8   | TYR  | 2              |
| 1   | A     | 14  | ARG  | 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     | 15/16 (94%)   | 7±2 (44±12%) | 8±2 (56±12%) | 0           | 0 |
| All | All   | 465/496 (94%) | 203 (44%)    | 262 (56%)    | 0           | 0 |

All 15 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     | 3   | TYR  | 29             |
| 1   | A     | 2   | TRP  | 26             |
| 1   | A     | 6   | VAL  | 26             |
| 1   | A     | 5   | ARG  | 23             |
| 1   | A     | 4   | PHE  | 19             |
| 1   | A     | 9   | ARG  | 19             |
| 1   | A     | 7   | TYR  | 17             |
| 1   | A     | 1   | LYS  | 17             |
| 1   | A     | 15  | ARG  | 17             |
| 1   | A     | 12  | TYR  | 15             |
| 1   | A     | 14  | ARG  | 14             |
| 1   | A     | 16  | TYR  | 12             |
| 1   | A     | 11  | ILE  | 12             |
| 1   | A     | 8   | TYR  | 9              |
| 1   | A     | 13  | TYR  | 7              |

### 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 ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided