



# Full wwPDB NMR Structure Validation Report i

Apr 26, 2016 – 05:02 PM BST

PDB ID : 1FJE  
Title : SOLUTION STRUCTURE OF NUCLEOLIN RBD12 IN COMPLEX WITH SNRE RNA  
Authors : Allain, F.H.T.; Bouvet, P.; Dieckmann, T.; Feigon, J.  
Deposited on : 2000-08-08

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the i symbol.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

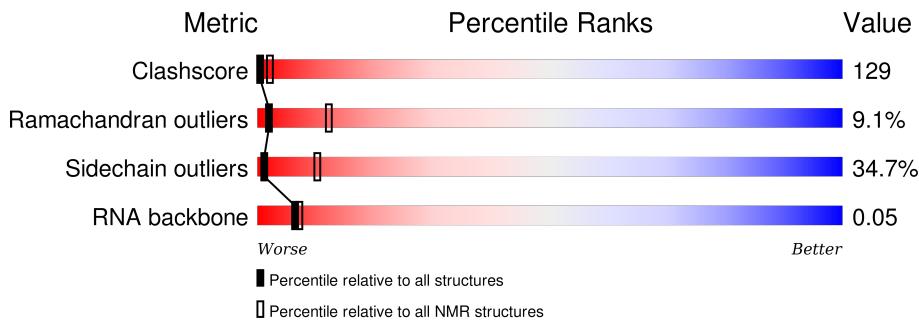
|                                |   |  |
|--------------------------------|---|--|
| Cyrange                        | : | Kirchner and Güntert (2011)  |
| NmrClust                       | : | Kelley et al. (1996)   |
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | unknown  |
| Percentile statistics          | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| RCI                            | : | v_1n_11_5_13_A (Berjanski et al., 2005)                            |
| PANAV                          | : | Wang et al. (2010)   |
| ShiftChecker                   | : | rb-20027457  |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | rb-20027457  |

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*SOLUTION NMR*

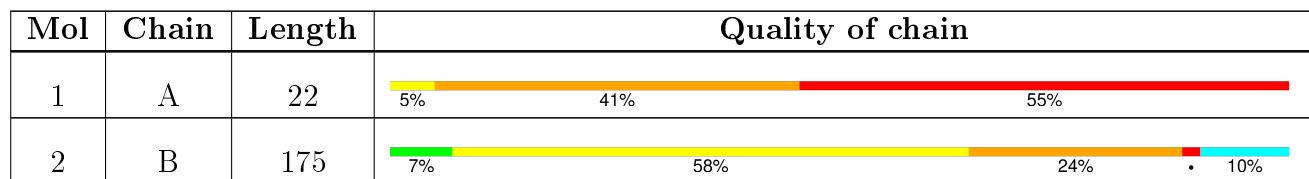
The overall completeness of chemical shifts assignment was not calculated.

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 (#Entries) | NMR archive (#Entries) |
|-----------------------|--------------------------|------------------------|
| Clashscore            | 114402                   | 11133                  |
| Ramachandran outliers | 111179                   | 9975                   |
| Sidechain outliers    | 111093                   | 9958                   |
| RNA backbone          | 3027                     | 600                    |

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  $\leq 5\%$ .



## 2 Ensemble composition and analysis

This entry contains 19 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                                  |                   |              |
|--------------------------------------|----------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)            | Backbone RMSD (Å) | Medoid model |
| 1                                    | B:10-B:130, B:136-B:172<br>(158) | 0.84              | 10           |

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 4 clusters and 3 single-model clusters were found.

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

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

There are 2 unique types of molecules in this entry. The entry contains 3444 atoms, of which 1611 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called SNRE RNA.

| Mol | Chain | Residues | Atoms |     |     |    |     |    | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|----|-------|
|     |       |          | Total | C   | H   | N  | O   | P  |       |
| 1   | A     | 22       | 712   | 211 | 242 | 90 | 148 | 21 | 0     |

- Molecule 2 is a protein called NUCLEOLIN RBD12.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
|     |       |          | Total | C   | H    | N   | O   | S |       |
| 2   | B     | 175      | 2732  | 856 | 1369 | 229 | 277 | 1 | 0     |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 1       | GLY      | LYS    | CONFLICT | UNP P08199 |
| B     | 2       | SER      | LYS    | CONFLICT | UNP P08199 |
| B     | 3       | HIS      | GLN    | CONFLICT | UNP P08199 |
| B     | 4       | MET      | LYS    | CONFLICT | UNP P08199 |
| B     | 37      | LEU      | PRO    | CONFLICT | UNP P08199 |

## 4 Residue-property plots

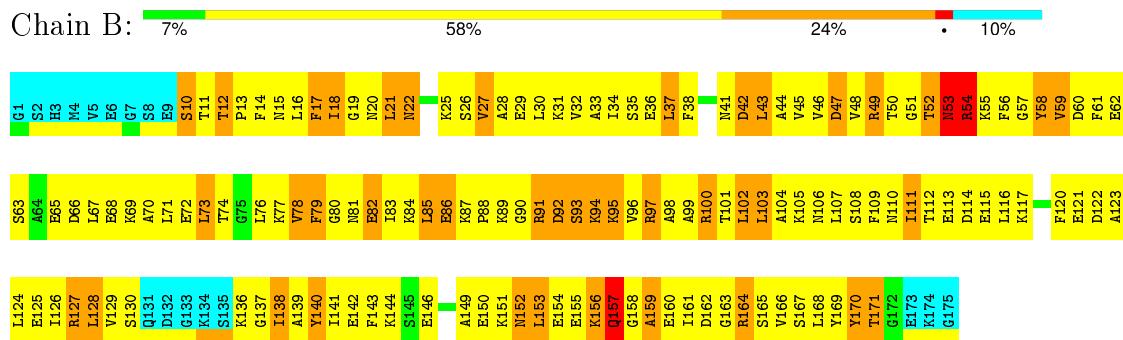
### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: SNRE RNA



- Molecule 2: NUCLEOLIN RBD12



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

Colouring as in section 4.1 above.

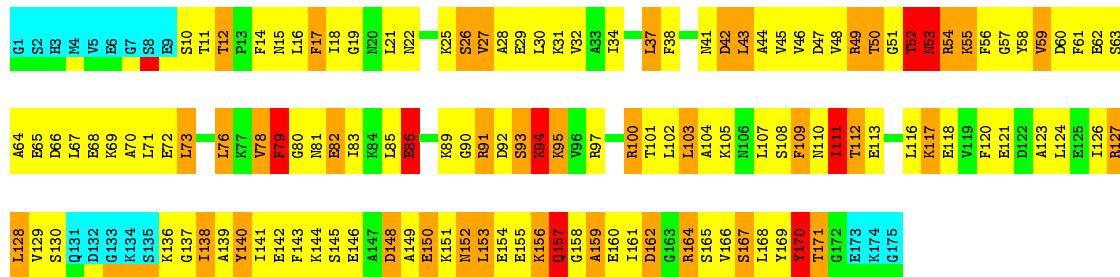
#### 4.2.1 Score per residue for model 1

- Molecule 1: SNRE RNA



- Molecule 2: NUCLEOLIN RBD12

A horizontal progress bar for Chain B. The bar is divided into five colored segments: green (15%), yellow (49%), orange (22%), red (5%), and blue (10%). The total length of the bar is 100%, indicating full completion.



#### 4.2.2 Score per residue for model 2

- Molecule 1: SNRE RNA

Chain A: 45% 55%

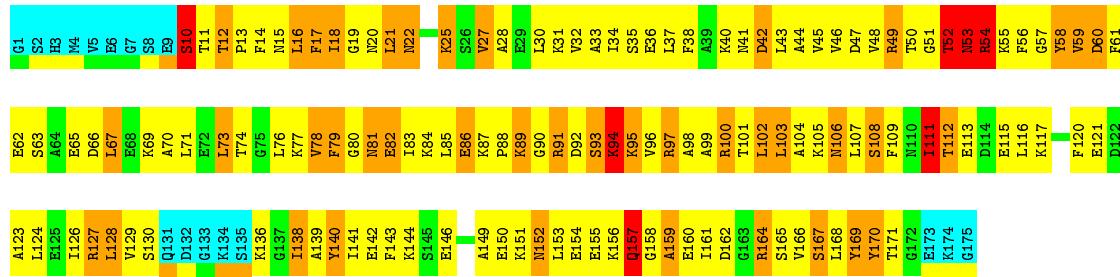
A horizontal progress bar for Chain A. The bar is divided into two segments: a yellow segment on the left representing 45% completion, and a red segment on the right representing 55% completion. The percentage values are displayed in white text inside each segment.



- Molecule 2: NUCLEOLIN RBD12

Chain B: 12% 51% 23% • 10%

A horizontal progress bar for 'Chain B' is shown, consisting of four colored segments: green (12%), yellow (51%), orange (23%), and red (10%). A black dot is positioned between the orange and red segments, indicating the current progress point.



#### 4.2.3 Score per residue for model 3

- Molecule 1: SNRE RNA

Chain A: 9% 55% 36%

A horizontal progress bar divided into three segments: yellow (9%), orange (55%), and red (36%).



- Molecule 2: NUCLEOLIN RBD12

Chain B:  14% 49% 25% • 10%



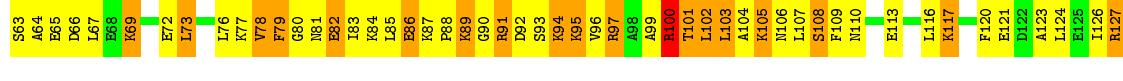
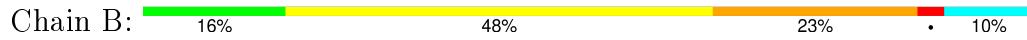


#### 4.2.4 Score per residue for model 4

- Molecule 1: SNRE RNA



- Molecule 2: NUCLEOLIN RBD12



#### 4.2.5 Score per residue for model 5

- Molecule 1: SNRE RNA

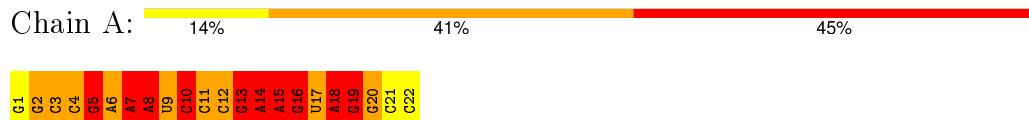


- Molecule 2: NUCLEOLIN RBD12

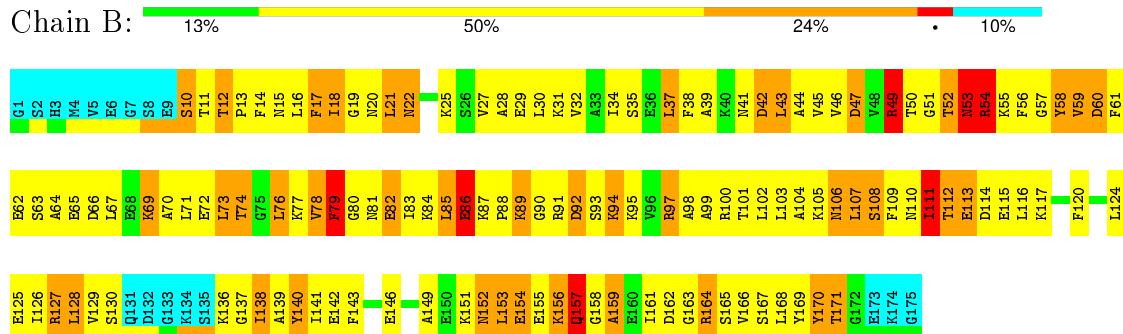


#### 4.2.6 Score per residue for model 6

- Molecule 1: SNRE RNA

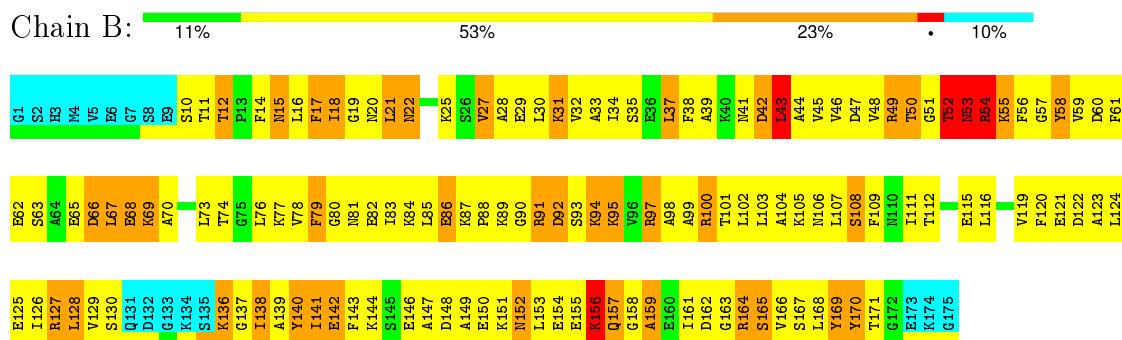


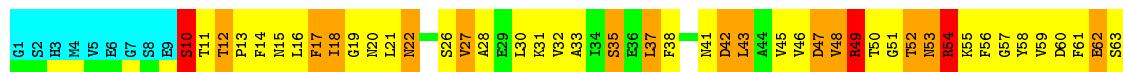
- Molecule 2: NUCLEOLIN RBD12





- Molecule 2: NUCLEOLIN RBD12



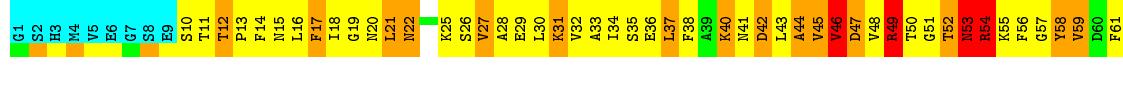


#### 4.2.11 Score per residue for model 11

- Molecule 1: SNRE RNA



- Molecule 2: NUCLEOLIN RBD12



#### 4.2.12 Score per residue for model 12

- Molecule 1: SNRE RNA



- Molecule 2: NUCLEOLIN RBD12





#### 4.2.13 Score per residue for model 13

- Molecule 1: SNRE RNA

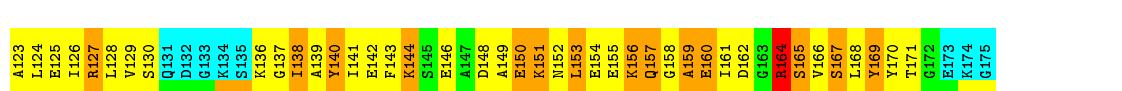


- Molecule 2: NUCLEOLIN RBD12



#### 4.2.14 Score per residue for model 14

- Molecule 1: SNRE RNA



#### 4.2.15 Score per residue for model 15

- Molecule 1: SNRE RNA



- Molecule 2: NUCLEOLIN RBD12



#### 4.2.16 Score per residue for model 16

- Molecule 1: SNRE RNA



- Molecule 2: NUCLEOLIN RBD12



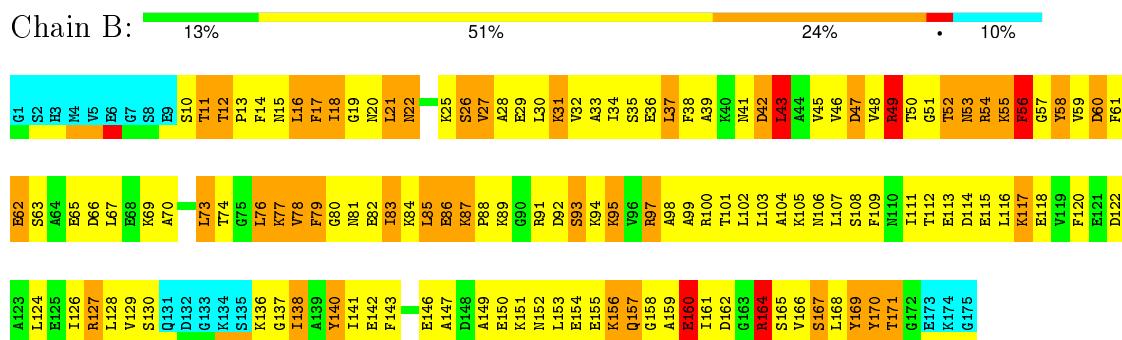
#### 4.2.17 Score per residue for model 17

- Molecule 1: SNRE RNA





- Molecule 2: NUCLEOLIN RBD12

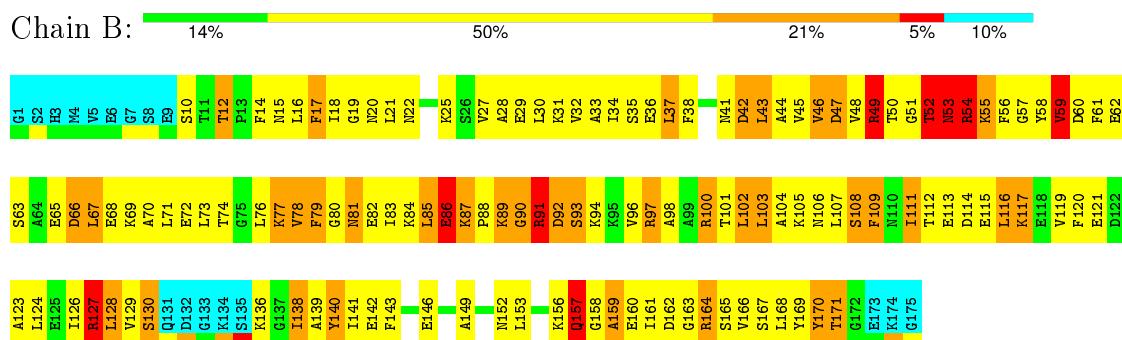


#### 4.2.18 Score per residue for model 18

- Molecule 1: SNRE RNA



- Molecule 2: NUCLEOLIN RBD12



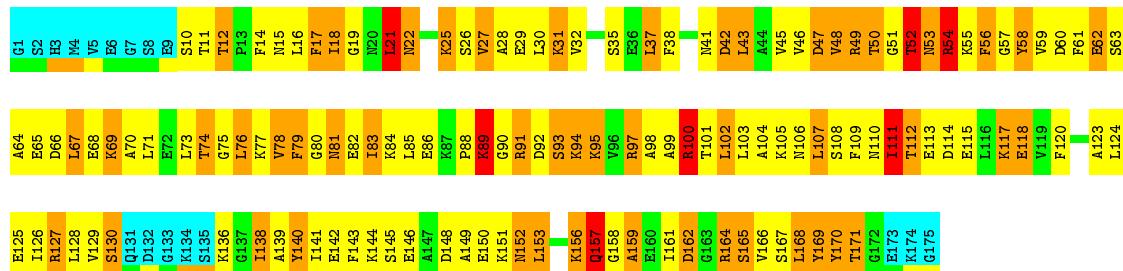
#### 4.2.19 Score per residue for model 19

- Molecule 1: SNRE RNA



- Molecule 2: NUCLEOLIN RBD12





## 5 Refinement protocol and experimental data overview i

The models were refined using the following method: *simulated annealing using XPLOR 3.841*.

Of the 40 calculated structures, 19 were deposited, based on the following criterion: *all calculated structures submitted*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR        | refinement         | 3.841   |
| X-PLOR        | structure solution | 3.841   |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 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     | 1.21±0.01    | 0±1/526 (0.1±0.1%)  | 2.10±0.01   | 32±2/819 (3.9±0.2%) |
| 2   | B     | 1.05±0.01    | 0±0/1257 (0.0±0.0%) | 1.25±0.01   | 0±0/1690 (0.0±0.0%) |
| All | All   | 1.10         | 9/33877 (0.0%)      | 1.58        | 614/47671 (1.3%)    |

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   | 0.1±0.2   |
| 2   | B     | 0.0±0.0   | 6.8±0.4   |
| All | All   | 0         | 131       |

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     | 11  | C    | N1-C6 | -5.76 | 1.33        | 1.37     | 14     | 1     |
| 1   | A     | 10  | C    | N1-C6 | -5.50 | 1.33        | 1.37     | 16     | 4     |
| 1   | A     | 12  | C    | N1-C6 | -5.41 | 1.33        | 1.37     | 18     | 1     |
| 1   | A     | 13  | G    | N9-C8 | -5.28 | 1.34        | 1.37     | 17     | 3     |

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     | 13  | G    | N7-C8-N9 | 10.33 | 118.26      | 113.10   | 14     | 19    |
| 1   | A     | 5   | G    | N7-C8-N9 | 9.73  | 117.96      | 113.10   | 11     | 19    |
| 1   | A     | 20  | G    | N7-C8-N9 | 9.51  | 117.86      | 113.10   | 4      | 19    |
| 1   | A     | 1   | G    | N7-C8-N9 | 9.39  | 117.80      | 113.10   | 12     | 19    |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 16  | G    | N7-C8-N9   | 9.36  | 117.78      | 113.10   | 15     | 19    |
| 1   | A     | 19  | G    | N7-C8-N9   | 9.32  | 117.76      | 113.10   | 8      | 19    |
| 1   | A     | 2   | G    | N7-C8-N9   | 9.28  | 117.74      | 113.10   | 6      | 19    |
| 1   | A     | 15  | A    | N7-C8-N9   | 8.44  | 118.02      | 113.80   | 7      | 19    |
| 1   | A     | 8   | A    | N7-C8-N9   | 8.15  | 117.87      | 113.80   | 11     | 19    |
| 1   | A     | 7   | A    | N7-C8-N9   | 7.97  | 117.79      | 113.80   | 7      | 19    |
| 1   | A     | 16  | G    | C8-N9-C4   | -7.96 | 103.21      | 106.40   | 9      | 19    |
| 1   | A     | 6   | A    | N7-C8-N9   | 7.63  | 117.61      | 113.80   | 18     | 19    |
| 1   | A     | 18  | A    | N7-C8-N9   | 7.59  | 117.59      | 113.80   | 2      | 19    |
| 1   | A     | 14  | A    | N7-C8-N9   | 7.55  | 117.58      | 113.80   | 13     | 19    |
| 1   | A     | 5   | G    | C8-N9-C4   | -7.55 | 103.38      | 106.40   | 8      | 19    |
| 1   | A     | 20  | G    | C8-N9-C4   | -7.26 | 103.50      | 106.40   | 4      | 19    |
| 1   | A     | 1   | G    | C8-N9-C4   | -7.26 | 103.50      | 106.40   | 12     | 19    |
| 1   | A     | 13  | G    | C8-N9-C4   | -7.22 | 103.51      | 106.40   | 5      | 19    |
| 1   | A     | 19  | G    | C8-N9-C4   | -7.02 | 103.59      | 106.40   | 17     | 19    |
| 1   | A     | 2   | G    | C8-N9-C4   | -6.75 | 103.70      | 106.40   | 2      | 19    |
| 2   | B     | 56  | PHE  | N-CA-CB    | -6.12 | 99.58       | 110.60   | 17     | 1     |
| 1   | A     | 13  | G    | O4'-C1'-N9 | 5.95  | 112.96      | 108.20   | 11     | 8     |
| 1   | A     | 20  | G    | O4'-C1'-N9 | 5.87  | 112.90      | 108.20   | 9      | 2     |
| 1   | A     | 8   | A    | C5-N7-C8   | -5.84 | 100.98      | 103.90   | 17     | 13    |
| 1   | A     | 8   | A    | C8-N9-C4   | -5.83 | 103.47      | 105.80   | 11     | 19    |
| 1   | A     | 18  | A    | C8-N9-C4   | -5.81 | 103.47      | 105.80   | 11     | 19    |
| 1   | A     | 21  | C    | O4'-C1'-N1 | 5.78  | 112.82      | 108.20   | 11     | 3     |
| 1   | A     | 7   | A    | C8-N9-C4   | -5.69 | 103.52      | 105.80   | 10     | 17    |
| 1   | A     | 15  | A    | C5-N7-C8   | -5.69 | 101.06      | 103.90   | 17     | 18    |
| 1   | A     | 6   | A    | C8-N9-C4   | -5.67 | 103.53      | 105.80   | 12     | 19    |
| 1   | A     | 16  | G    | O4'-C1'-N9 | 5.62  | 112.69      | 108.20   | 13     | 2     |
| 1   | A     | 10  | C    | C6-N1-C2   | 5.59  | 122.54      | 120.30   | 16     | 2     |
| 1   | A     | 19  | G    | C5-N7-C8   | -5.57 | 101.52      | 104.30   | 12     | 15    |
| 1   | A     | 13  | G    | C5-N7-C8   | -5.45 | 101.58      | 104.30   | 17     | 10    |
| 1   | A     | 15  | A    | O4'-C1'-N9 | 5.44  | 112.55      | 108.20   | 13     | 4     |
| 1   | A     | 14  | A    | C8-N9-C4   | -5.37 | 103.65      | 105.80   | 6      | 5     |
| 2   | B     | 10  | SER  | N-CA-CB    | -5.33 | 102.50      | 110.50   | 15     | 1     |
| 1   | A     | 9   | U    | O4'-C1'-N1 | 5.27  | 112.42      | 108.20   | 1      | 1     |
| 1   | A     | 20  | G    | C5-N7-C8   | -5.26 | 101.67      | 104.30   | 18     | 16    |
| 1   | A     | 2   | G    | C5-N7-C8   | -5.24 | 101.68      | 104.30   | 3      | 17    |
| 1   | A     | 5   | G    | C5-N7-C8   | -5.24 | 101.68      | 104.30   | 7      | 12    |
| 1   | A     | 15  | A    | C8-N9-C4   | -5.19 | 103.72      | 105.80   | 12     | 2     |
| 1   | A     | 14  | A    | C5-N7-C8   | -5.18 | 101.31      | 103.90   | 8      | 8     |
| 1   | A     | 1   | G    | C5-N7-C8   | -5.15 | 101.72      | 104.30   | 17     | 15    |
| 1   | A     | 7   | A    | O4'-C1'-N9 | 5.09  | 112.27      | 108.20   | 17     | 1     |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 14  | A    | O4'-C1'-N9 | 5.08  | 112.27      | 108.20   | 14     | 1     |
| 1   | A     | 7   | A    | C5-N7-C8   | -5.07 | 101.37      | 103.90   | 17     | 2     |
| 1   | A     | 16  | G    | C5-N7-C8   | -5.02 | 101.79      | 104.30   | 18     | 1     |

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) |
|-----|-------|-----|------|-----------|----------------|
| 2   | B     | 164 | ARG  | Sidechain | 19             |
| 2   | B     | 49  | ARG  | Sidechain | 19             |
| 2   | B     | 97  | ARG  | Sidechain | 19             |
| 2   | B     | 127 | ARG  | Sidechain | 19             |
| 2   | B     | 100 | ARG  | Sidechain | 19             |
| 2   | B     | 54  | ARG  | Sidechain | 18             |
| 2   | B     | 91  | ARG  | Sidechain | 17             |
| 1   | A     | 14  | A    | Sidechain | 1              |

## 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     | 470   | 242      | 242      | 172±15  |
| 2   | B     | 1241  | 1259     | 1259     | 297±19  |
| All | All   | 32509 | 28519    | 28519    | 7866    |

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 129.

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

| Atom-1           |  | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|--|-----------------|----------|-------------|--------|-------|
|                  |  |                 |          |             | Worst  | Total |
| 2:B:102:LEU:HD21 |  | 2:B:149:ALA:HB1 | 1.14     | 1.18        | 3      | 6     |
| 2:B:21:LEU:HD22  |  | 2:B:30:LEU:HD22 | 1.12     | 1.19        | 18     | 1     |
| 2:B:102:LEU:HD23 |  | 2:B:149:ALA:HB1 | 1.12     | 1.18        | 14     | 5     |
| 2:B:73:LEU:HD12  |  | 2:B:76:LEU:HD11 | 1.11     | 1.14        | 12     | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:3:C:O2'      | 1:A:4:C:H5'      | 1.08     | 1.48        | 8      | 11    |
| 2:B:104:ALA:HB3  | 2:B:139:ALA:HB3  | 1.07     | 1.25        | 19     | 15    |
| 2:B:102:LEU:HD11 | 2:B:149:ALA:HB1  | 1.06     | 1.20        | 12     | 7     |
| 1:A:10:C:O4'     | 2:B:129:VAL:HG13 | 1.05     | 1.51        | 4      | 19    |
| 2:B:48:VAL:HG22  | 2:B:59:VAL:HG13  | 1.04     | 1.25        | 5      | 2     |
| 2:B:73:LEU:HD13  | 2:B:76:LEU:HD12  | 1.04     | 1.29        | 7      | 4     |
| 1:A:5:G:O2'      | 1:A:6:A:H5"      | 1.03     | 1.52        | 9      | 11    |
| 2:B:12:THR:HG21  | 2:B:46:VAL:HG11  | 1.03     | 1.25        | 3      | 11    |
| 2:B:37:LEU:HD13  | 2:B:76:LEU:HD13  | 1.02     | 1.31        | 19     | 2     |
| 2:B:38:PHE:CD1   | 2:B:43:LEU:HD22  | 1.02     | 1.88        | 16     | 1     |
| 1:A:19:G:H2'     | 1:A:20:G:O4'     | 1.02     | 1.54        | 10     | 15    |
| 1:A:8:A:N1       | 1:A:14:A:H1'     | 1.02     | 1.70        | 16     | 18    |
| 2:B:102:LEU:HD21 | 2:B:143:PHE:CE1  | 1.01     | 1.91        | 8      | 8     |
| 2:B:107:LEU:HD21 | 2:B:139:ALA:HB2  | 1.00     | 1.31        | 10     | 2     |
| 2:B:38:PHE:CD2   | 2:B:45:VAL:HG11  | 0.99     | 1.92        | 11     | 4     |
| 1:A:15:A:C4      | 2:B:52:THR:HG23  | 0.99     | 1.92        | 13     | 19    |
| 2:B:85:LEU:HD13  | 2:B:86:GLU:N     | 0.99     | 1.73        | 5      | 1     |
| 1:A:13:G:H5'     | 2:B:90:GLY:O     | 0.99     | 1.58        | 7      | 2     |
| 1:A:13:G:O2'     | 1:A:15:A:H3'     | 0.99     | 1.57        | 18     | 1     |
| 2:B:73:LEU:HD12  | 2:B:76:LEU:CD1   | 0.99     | 1.87        | 12     | 4     |
| 2:B:22:ASN:CB    | 2:B:30:LEU:HD21  | 0.98     | 1.87        | 19     | 12    |
| 1:A:15:A:OP1     | 1:A:17:U:H1'     | 0.98     | 1.56        | 7      | 12    |
| 2:B:107:LEU:HD23 | 2:B:166:VAL:HG21 | 0.98     | 1.34        | 15     | 3     |
| 1:A:14:A:O2'     | 2:B:52:THR:HG21  | 0.97     | 1.58        | 14     | 11    |
| 1:A:11:C:O2'     | 1:A:12:C:H5'     | 0.97     | 1.56        | 15     | 10    |
| 2:B:102:LEU:HD21 | 2:B:168:LEU:HD12 | 0.97     | 1.34        | 18     | 1     |
| 1:A:13:G:H3'     | 1:A:13:G:N3      | 0.96     | 1.75        | 1      | 8     |
| 1:A:13:G:N3      | 1:A:13:G:H3'     | 0.96     | 1.75        | 7      | 11    |
| 2:B:38:PHE:CD2   | 2:B:43:LEU:HD23  | 0.96     | 1.95        | 2      | 1     |
| 2:B:103:LEU:HD11 | 2:B:171:THR:HG23 | 0.96     | 1.38        | 6      | 1     |
| 2:B:17:PHE:O     | 2:B:85:LEU:HD12  | 0.95     | 1.60        | 1      | 1     |
| 2:B:12:THR:CG2   | 2:B:46:VAL:HG11  | 0.95     | 1.92        | 3      | 16    |
| 2:B:48:VAL:HG22  | 2:B:59:VAL:HG22  | 0.95     | 1.38        | 17     | 4     |
| 1:A:15:A:H4'     | 1:A:17:U:OP1     | 0.94     | 1.60        | 9      | 6     |
| 2:B:101:THR:C    | 2:B:102:LEU:HD13 | 0.94     | 1.81        | 12     | 8     |
| 1:A:4:C:H4'      | 1:A:5:G:OP1      | 0.94     | 1.63        | 1      | 9     |
| 2:B:21:LEU:HD13  | 2:B:56:PHE:C     | 0.93     | 1.84        | 2      | 10    |
| 2:B:70:ALA:O     | 2:B:85:LEU:HD13  | 0.93     | 1.64        | 15     | 4     |
| 1:A:10:C:C2      | 1:A:11:C:C6      | 0.93     | 2.57        | 18     | 19    |
| 2:B:30:LEU:HD12  | 2:B:31:LYS:N     | 0.93     | 1.79        | 14     | 1     |
| 2:B:37:LEU:HD13  | 2:B:76:LEU:HD23  | 0.93     | 1.41        | 15     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:37:LEU:CD2   | 2:B:76:LEU:HD13  | 0.92     | 1.94        | 7      | 2     |
| 2:B:22:ASN:HB3   | 2:B:30:LEU:HD21  | 0.92     | 1.40        | 19     | 12    |
| 2:B:38:PHE:CD2   | 2:B:43:LEU:HD13  | 0.92     | 2.00        | 8      | 8     |
| 2:B:102:LEU:HD12 | 2:B:170:TYR:CD1  | 0.92     | 1.99        | 7      | 6     |
| 2:B:38:PHE:CZ    | 2:B:73:LEU:HD13  | 0.92     | 2.00        | 9      | 1     |
| 1:A:18:A:O2'     | 1:A:19:G:H5'     | 0.92     | 1.64        | 19     | 9     |
| 1:A:9:U:O2'      | 1:A:10:C:H6      | 0.91     | 1.48        | 2      | 19    |
| 2:B:30:LEU:O     | 2:B:34:ILE:HD12  | 0.91     | 1.64        | 18     | 5     |
| 2:B:107:LEU:CD2  | 2:B:166:VAL:HG21 | 0.91     | 1.94        | 15     | 2     |
| 2:B:21:LEU:HD22  | 2:B:56:PHE:O     | 0.91     | 1.64        | 5      | 11    |
| 2:B:73:LEU:CD1   | 2:B:76:LEU:HD11  | 0.91     | 1.95        | 12     | 2     |
| 1:A:13:G:C8      | 2:B:58:TYR:CD1   | 0.91     | 2.58        | 18     | 11    |
| 1:A:14:A:H4'     | 1:A:15:A:OP2     | 0.91     | 1.65        | 18     | 6     |
| 2:B:37:LEU:HD23  | 2:B:76:LEU:HD13  | 0.91     | 1.43        | 7      | 3     |
| 2:B:120:PHE:CZ   | 2:B:168:LEU:HD11 | 0.90     | 2.00        | 18     | 10    |
| 2:B:73:LEU:O     | 2:B:76:LEU:HD12  | 0.90     | 1.65        | 1      | 4     |
| 2:B:28:ALA:O     | 2:B:32:VAL:HG23  | 0.90     | 1.67        | 16     | 18    |
| 2:B:37:LEU:HD13  | 2:B:76:LEU:HD12  | 0.90     | 1.43        | 9      | 1     |
| 1:A:5:G:H3'      | 1:A:5:G:OP2      | 0.90     | 1.67        | 4      | 2     |
| 2:B:73:LEU:CD1   | 2:B:76:LEU:HD12  | 0.89     | 1.97        | 7      | 4     |
| 2:B:98:ALA:HB1   | 2:B:171:THR:CG2  | 0.89     | 1.96        | 15     | 1     |
| 2:B:73:LEU:HD22  | 2:B:76:LEU:HD11  | 0.89     | 1.44        | 13     | 2     |
| 2:B:102:LEU:HD12 | 2:B:103:LEU:N    | 0.89     | 1.82        | 18     | 1     |
| 1:A:8:A:H5"      | 1:A:9:U:OP2      | 0.89     | 1.68        | 3      | 4     |
| 1:A:6:A:OP1      | 1:A:6:A:H4'      | 0.89     | 1.68        | 15     | 3     |
| 2:B:11:THR:HG21  | 2:B:47:ASP:OD2   | 0.89     | 1.68        | 6      | 3     |
| 2:B:37:LEU:HD11  | 2:B:76:LEU:HD22  | 0.89     | 1.42        | 14     | 1     |
| 2:B:69:LYS:O     | 2:B:73:LEU:HD23  | 0.89     | 1.67        | 19     | 12    |
| 1:A:9:U:H3'      | 1:A:9:U:OP1      | 0.88     | 1.67        | 19     | 1     |
| 1:A:10:C:C1'     | 2:B:129:VAL:HG13 | 0.88     | 1.97        | 16     | 19    |
| 2:B:127:ARG:HB3  | 2:B:127:ARG:CZ   | 0.88     | 1.99        | 18     | 1     |
| 1:A:18:A:H2'     | 1:A:19:G:O4'     | 0.87     | 1.69        | 15     | 13    |
| 2:B:140:TYR:O    | 2:B:141:ILE:HD13 | 0.87     | 1.70        | 9      | 6     |
| 2:B:38:PHE:CE2   | 2:B:43:LEU:HD22  | 0.87     | 2.03        | 19     | 1     |
| 2:B:102:LEU:HD23 | 2:B:149:ALA:CB   | 0.87     | 1.98        | 14     | 2     |
| 2:B:61:PHE:CZ    | 2:B:70:ALA:HB1   | 0.87     | 2.04        | 9      | 9     |
| 2:B:107:LEU:HD12 | 2:B:137:GLY:O    | 0.87     | 1.69        | 6      | 6     |
| 1:A:14:A:H8      | 2:B:52:THR:HG1   | 0.87     | 1.12        | 1      | 1     |
| 1:A:10:C:O2      | 1:A:10:C:H2'     | 0.87     | 1.70        | 9      | 12    |
| 2:B:103:LEU:HD13 | 2:B:140:TYR:CE1  | 0.87     | 2.05        | 14     | 9     |
| 2:B:125:GLU:O    | 2:B:126:ILE:HD13 | 0.87     | 1.69        | 16     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:102:LEU:O    | 2:B:102:LEU:HD12 | 0.87     | 1.70        | 11     | 2     |
| 2:B:73:LEU:O     | 2:B:76:LEU:HD22  | 0.87     | 1.70        | 9      | 1     |
| 2:B:37:LEU:HD22  | 2:B:76:LEU:CD2   | 0.86     | 2.00        | 16     | 5     |
| 2:B:103:LEU:HD13 | 2:B:140:TYR:CD1  | 0.86     | 2.05        | 14     | 2     |
| 1:A:10:C:C2      | 2:B:127:ARG:NH2  | 0.86     | 2.43        | 18     | 2     |
| 2:B:107:LEU:CD2  | 2:B:139:ALA:HB2  | 0.86     | 1.99        | 10     | 2     |
| 2:B:102:LEU:HD21 | 2:B:149:ALA:CB   | 0.86     | 2.01        | 3      | 6     |
| 1:A:13:G:H4'     | 1:A:13:G:OP1     | 0.86     | 1.68        | 18     | 2     |
| 2:B:107:LEU:HD23 | 2:B:166:VAL:HG22 | 0.86     | 1.48        | 18     | 1     |
| 1:A:13:G:C8      | 2:B:58:TYR:CD2   | 0.86     | 2.63        | 8      | 5     |
| 1:A:14:A:OP2     | 1:A:14:A:H4'     | 0.86     | 1.68        | 1      | 1     |
| 2:B:102:LEU:HD13 | 2:B:102:LEU:N    | 0.86     | 1.86        | 10     | 6     |
| 2:B:160:GLU:O    | 2:B:161:ILE:HD13 | 0.85     | 1.69        | 10     | 3     |
| 2:B:103:LEU:HD21 | 2:B:140:TYR:CE1  | 0.85     | 2.06        | 10     | 7     |
| 2:B:56:PHE:CD1   | 2:B:57:GLY:N     | 0.85     | 2.44        | 17     | 3     |
| 1:A:21:C:HO2'    | 1:A:22:C:H6      | 0.85     | 0.88        | 11     | 1     |
| 1:A:13:G:N3      | 1:A:13:G:H5'     | 0.85     | 1.85        | 10     | 4     |
| 1:A:10:C:C5      | 2:B:140:TYR:CZ   | 0.85     | 2.64        | 14     | 18    |
| 2:B:102:LEU:CD1  | 2:B:168:LEU:HD22 | 0.85     | 2.01        | 4      | 4     |
| 2:B:16:LEU:HD12  | 2:B:17:PHE:N     | 0.85     | 1.87        | 9      | 9     |
| 1:A:14:A:N3      | 2:B:94:LYS:HG3   | 0.85     | 1.87        | 11     | 4     |
| 2:B:126:ILE:HG23 | 2:B:141:ILE:CD1  | 0.85     | 2.02        | 9      | 2     |
| 1:A:10:C:H2'     | 1:A:10:C:O2      | 0.84     | 1.71        | 18     | 7     |
| 2:B:67:LEU:HD22  | 2:B:67:LEU:O     | 0.84     | 1.72        | 8      | 1     |
| 2:B:120:PHE:CE2  | 2:B:141:ILE:HD13 | 0.84     | 2.08        | 11     | 4     |
| 2:B:102:LEU:CD2  | 2:B:149:ALA:HB1  | 0.84     | 2.02        | 3      | 9     |
| 2:B:16:LEU:HD22  | 2:B:17:PHE:N     | 0.84     | 1.87        | 2      | 4     |
| 2:B:21:LEU:HD13  | 2:B:30:LEU:HD13  | 0.84     | 1.48        | 18     | 3     |
| 2:B:38:PHE:CE2   | 2:B:43:LEU:HD13  | 0.83     | 2.07        | 19     | 7     |
| 2:B:103:LEU:HD11 | 2:B:138:ILE:CG2  | 0.83     | 2.02        | 12     | 5     |
| 2:B:37:LEU:HG    | 2:B:76:LEU:HD13  | 0.83     | 1.47        | 14     | 1     |
| 2:B:21:LEU:HD12  | 2:B:30:LEU:HD13  | 0.83     | 1.50        | 12     | 3     |
| 1:A:9:U:HO2'     | 1:A:10:C:H6      | 0.83     | 0.84        | 16     | 14    |
| 2:B:103:LEU:HD11 | 2:B:140:TYR:CE1  | 0.83     | 2.09        | 4      | 4     |
| 2:B:111:ILE:O    | 2:B:112:THR:HG23 | 0.83     | 1.74        | 10     | 16    |
| 2:B:103:LEU:HD12 | 2:B:171:THR:CG2  | 0.83     | 2.04        | 4      | 1     |
| 1:A:10:C:C5      | 2:B:140:TYR:CE1  | 0.82     | 2.67        | 4      | 18    |
| 2:B:50:THR:C     | 2:B:56:PHE:O     | 0.82     | 2.17        | 19     | 1     |
| 1:A:14:A:O2'     | 1:A:15:A:C8      | 0.82     | 2.32        | 17     | 18    |
| 1:A:13:G:H5'     | 1:A:13:G:N3      | 0.82     | 1.89        | 3      | 2     |
| 1:A:10:C:C2      | 2:B:127:ARG:CZ   | 0.82     | 2.61        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:153:LEU:HA   | 2:B:168:LEU:HD13 | 0.82     | 1.52        | 1      | 4     |
| 2:B:34:ILE:HD11  | 2:B:78:VAL:HG23  | 0.82     | 1.52        | 13     | 4     |
| 1:A:10:C:C2      | 1:A:11:C:C5      | 0.81     | 2.68        | 13     | 19    |
| 2:B:130:SER:HA   | 2:B:136:LYS:HA   | 0.81     | 1.49        | 15     | 1     |
| 2:B:143:PHE:HB2  | 2:B:149:ALA:HB2  | 0.81     | 1.49        | 16     | 18    |
| 2:B:101:THR:C    | 2:B:102:LEU:HD23 | 0.81     | 1.96        | 9      | 1     |
| 1:A:8:A:C6       | 1:A:14:A:C4      | 0.81     | 2.69        | 17     | 19    |
| 1:A:20:G:C5      | 1:A:21:C:C5      | 0.81     | 2.68        | 8      | 17    |
| 2:B:102:LEU:HD13 | 2:B:168:LEU:HD22 | 0.81     | 1.51        | 8      | 4     |
| 2:B:126:ILE:HG23 | 2:B:140:TYR:O    | 0.81     | 1.75        | 15     | 13    |
| 2:B:48:VAL:HG13  | 2:B:59:VAL:CG2   | 0.81     | 2.05        | 18     | 3     |
| 2:B:111:ILE:HD12 | 2:B:162:ASP:OD2  | 0.81     | 1.76        | 3      | 1     |
| 2:B:101:THR:O    | 2:B:102:LEU:HD13 | 0.81     | 1.76        | 13     | 5     |
| 2:B:103:LEU:HD23 | 2:B:129:VAL:HG21 | 0.81     | 1.53        | 9      | 4     |
| 2:B:102:LEU:CD1  | 2:B:149:ALA:HB1  | 0.80     | 2.05        | 12     | 4     |
| 2:B:102:LEU:N    | 2:B:102:LEU:HD22 | 0.80     | 1.92        | 16     | 2     |
| 1:A:14:A:H2'     | 2:B:52:THR:HG21  | 0.80     | 1.54        | 8      | 18    |
| 2:B:43:LEU:HD21  | 2:B:69:LYS:HB3   | 0.80     | 1.51        | 14     | 3     |
| 2:B:160:GLU:C    | 2:B:161:ILE:HD13 | 0.80     | 1.95        | 10     | 1     |
| 2:B:140:TYR:CE2  | 2:B:171:THR:HG21 | 0.80     | 2.12        | 7      | 7     |
| 2:B:102:LEU:HD23 | 2:B:153:LEU:HD12 | 0.80     | 1.49        | 2      | 1     |
| 2:B:153:LEU:HD23 | 2:B:154:GLU:N    | 0.80     | 1.92        | 1      | 5     |
| 2:B:58:TYR:O     | 2:B:59:VAL:HG23  | 0.80     | 1.77        | 9      | 8     |
| 1:A:7:A:O2'      | 1:A:8:A:P        | 0.79     | 2.40        | 14     | 4     |
| 1:A:14:A:H2'     | 2:B:52:THR:OG1   | 0.79     | 1.76        | 17     | 9     |
| 2:B:116:LEU:HB3  | 2:B:126:ILE:HD13 | 0.79     | 1.54        | 6      | 1     |
| 1:A:10:C:C6      | 2:B:140:TYR:CE1  | 0.79     | 2.71        | 11     | 18    |
| 1:A:13:G:C8      | 2:B:49:ARG:HD2   | 0.79     | 2.13        | 12     | 10    |
| 2:B:50:THR:O     | 2:B:56:PHE:O     | 0.79     | 2.01        | 19     | 1     |
| 2:B:128:LEU:C    | 2:B:128:LEU:HD22 | 0.79     | 1.96        | 16     | 1     |
| 1:A:11:C:O2'     | 1:A:12:C:P       | 0.79     | 2.40        | 8      | 9     |
| 1:A:13:G:H5"     | 1:A:13:G:N3      | 0.79     | 1.91        | 18     | 4     |
| 1:A:10:C:O2      | 2:B:127:ARG:CZ   | 0.79     | 2.31        | 16     | 2     |
| 2:B:69:LYS:O     | 2:B:73:LEU:HD13  | 0.79     | 1.78        | 8      | 4     |
| 2:B:27:VAL:HG23  | 2:B:54:ARG:NE    | 0.79     | 1.93        | 18     | 4     |
| 2:B:102:LEU:HD13 | 2:B:168:LEU:HD13 | 0.79     | 1.53        | 6      | 1     |
| 2:B:37:LEU:HD22  | 2:B:76:LEU:CD1   | 0.79     | 2.08        | 9      | 1     |
| 1:A:19:G:C4      | 1:A:20:G:C8      | 0.78     | 2.71        | 18     | 17    |
| 2:B:102:LEU:HD22 | 2:B:102:LEU:N    | 0.78     | 1.93        | 15     | 5     |
| 1:A:10:C:N3      | 2:B:127:ARG:NH1  | 0.78     | 2.31        | 16     | 1     |
| 1:A:10:C:N3      | 1:A:11:C:C5      | 0.78     | 2.51        | 16     | 15    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:21:C:O2'     | 1:A:22:C:H6      | 0.78     | 1.61        | 11     | 3     |
| 2:B:21:LEU:HD13  | 2:B:56:PHE:O     | 0.78     | 1.79        | 10     | 10    |
| 1:A:10:C:C4      | 2:B:140:TYR:CZ   | 0.78     | 2.71        | 13     | 19    |
| 2:B:67:LEU:HD13  | 2:B:68:GLU:N     | 0.78     | 1.93        | 8      | 1     |
| 2:B:120:PHE:CE1  | 2:B:168:LEU:HD11 | 0.78     | 2.13        | 9      | 8     |
| 2:B:98:ALA:HB1   | 2:B:171:THR:HG22 | 0.78     | 1.54        | 15     | 1     |
| 2:B:16:LEU:HD22  | 2:B:16:LEU:C     | 0.78     | 1.99        | 17     | 2     |
| 1:A:19:G:O2'     | 1:A:20:G:P       | 0.77     | 2.42        | 9      | 7     |
| 1:A:16:G:N7      | 2:B:27:VAL:HG21  | 0.77     | 1.93        | 9      | 9     |
| 2:B:70:ALA:O     | 2:B:85:LEU:HD22  | 0.77     | 1.79        | 10     | 1     |
| 2:B:120:PHE:CZ   | 2:B:168:LEU:HD21 | 0.77     | 2.14        | 4      | 8     |
| 2:B:103:LEU:CD1  | 2:B:171:THR:HG23 | 0.77     | 2.09        | 6      | 1     |
| 2:B:18:ILE:HD13  | 2:B:59:VAL:CG2   | 0.77     | 2.09        | 19     | 1     |
| 2:B:103:LEU:HD12 | 2:B:171:THR:HG22 | 0.77     | 1.55        | 4      | 1     |
| 1:A:16:G:OP1     | 1:A:16:G:H4'     | 0.77     | 1.80        | 18     | 2     |
| 1:A:18:A:O2'     | 1:A:19:G:P       | 0.77     | 2.43        | 17     | 2     |
| 2:B:98:ALA:HB1   | 2:B:171:THR:O    | 0.77     | 1.79        | 18     | 4     |
| 2:B:85:LEU:HD23  | 2:B:86:GLU:N     | 0.77     | 1.94        | 7      | 1     |
| 2:B:102:LEU:HD11 | 2:B:153:LEU:HD12 | 0.77     | 1.55        | 14     | 1     |
| 2:B:51:GLY:N     | 2:B:56:PHE:O     | 0.77     | 2.18        | 17     | 19    |
| 1:A:10:C:C4      | 1:A:11:C:C4      | 0.77     | 2.72        | 14     | 14    |
| 1:A:12:C:O2'     | 2:B:56:PHE:CE2   | 0.76     | 2.37        | 19     | 11    |
| 2:B:74:THR:HG23  | 2:B:84:LYS:HA    | 0.76     | 1.56        | 8      | 2     |
| 2:B:16:LEU:C     | 2:B:16:LEU:HD22  | 0.76     | 2.01        | 13     | 2     |
| 1:A:10:C:C5      | 2:B:140:TYR:CE2  | 0.76     | 2.72        | 15     | 1     |
| 1:A:2:G:C5       | 1:A:3:C:C5       | 0.76     | 2.74        | 1      | 7     |
| 2:B:30:LEU:HD11  | 2:B:31:LYS:HE2   | 0.76     | 1.57        | 14     | 1     |
| 1:A:8:A:C2       | 1:A:14:A:N3      | 0.76     | 2.53        | 11     | 19    |
| 2:B:30:LEU:HD11  | 2:B:54:ARG:HB3   | 0.76     | 1.55        | 3      | 7     |
| 2:B:102:LEU:O    | 2:B:102:LEU:HD22 | 0.76     | 1.81        | 10     | 1     |
| 1:A:13:G:N7      | 2:B:58:TYR:CD1   | 0.76     | 2.53        | 12     | 3     |
| 1:A:14:A:C2'     | 2:B:52:THR:HG21  | 0.76     | 2.11        | 11     | 15    |
| 1:A:12:C:C2      | 2:B:17:PHE:CZ    | 0.76     | 2.74        | 6      | 18    |
| 1:A:2:G:O2'      | 1:A:3:C:P        | 0.76     | 2.43        | 10     | 3     |
| 1:A:13:G:C8      | 2:B:49:ARG:CD    | 0.76     | 2.69        | 18     | 5     |
| 1:A:1:G:H2'      | 1:A:1:G:N3       | 0.75     | 1.95        | 12     | 2     |
| 1:A:20:G:O2'     | 1:A:21:C:P       | 0.75     | 2.43        | 13     | 3     |
| 2:B:107:LEU:HD11 | 2:B:139:ALA:HB2  | 0.75     | 1.59        | 4      | 1     |
| 1:A:12:C:C6      | 1:A:12:C:P       | 0.75     | 2.79        | 3      | 4     |
| 2:B:30:LEU:HD23  | 2:B:78:VAL:HG11  | 0.75     | 1.57        | 16     | 3     |
| 1:A:1:G:O2'      | 1:A:2:G:P        | 0.75     | 2.44        | 2      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:37:LEU:HD21  | 2:B:76:LEU:HB3   | 0.75     | 1.56        | 14     | 2     |
| 1:A:15:A:C5      | 2:B:52:THR:CG2   | 0.75     | 2.70        | 1      | 19    |
| 1:A:19:G:C6      | 1:A:20:G:N7      | 0.75     | 2.55        | 5      | 12    |
| 1:A:10:C:C4      | 2:B:140:TYR:CE2  | 0.75     | 2.75        | 15     | 5     |
| 2:B:18:ILE:CG1   | 2:B:85:LEU:HD12  | 0.75     | 2.12        | 6      | 1     |
| 1:A:9:U:O2'      | 1:A:10:C:P       | 0.75     | 2.44        | 6      | 4     |
| 2:B:38:PHE:HD2   | 2:B:45:VAL:HG11  | 0.75     | 1.42        | 11     | 1     |
| 2:B:21:LEU:HD23  | 2:B:30:LEU:HD13  | 0.75     | 1.58        | 15     | 8     |
| 2:B:17:PHE:CD1   | 2:B:56:PHE:CE2   | 0.75     | 2.75        | 17     | 2     |
| 1:A:20:G:C8      | 1:A:21:C:C5      | 0.75     | 2.75        | 11     | 6     |
| 2:B:70:ALA:HA    | 2:B:73:LEU:HD22  | 0.75     | 1.56        | 15     | 4     |
| 2:B:103:LEU:HD12 | 2:B:138:ILE:HG22 | 0.75     | 1.56        | 1      | 2     |
| 2:B:78:VAL:HB    | 2:B:83:ILE:HG23  | 0.74     | 1.58        | 14     | 9     |
| 1:A:13:G:N3      | 1:A:13:G:C5'     | 0.74     | 2.50        | 17     | 9     |
| 2:B:38:PHE:CE2   | 2:B:43:LEU:HD23  | 0.74     | 2.16        | 2      | 1     |
| 2:B:104:ALA:O    | 2:B:107:LEU:HD11 | 0.74     | 1.82        | 6      | 2     |
| 1:A:20:G:H2'     | 1:A:21:C:O4'     | 0.74     | 1.81        | 11     | 4     |
| 1:A:8:A:H5"      | 1:A:9:U:O5'      | 0.74     | 1.83        | 11     | 6     |
| 2:B:30:LEU:HD11  | 2:B:54:ARG:CG    | 0.74     | 2.11        | 16     | 2     |
| 2:B:21:LEU:CD2   | 2:B:30:LEU:HD22  | 0.74     | 2.08        | 18     | 1     |
| 2:B:17:PHE:C     | 2:B:18:ILE:HD12  | 0.74     | 2.03        | 12     | 1     |
| 2:B:153:LEU:HD13 | 2:B:153:LEU:C    | 0.74     | 2.01        | 15     | 1     |
| 1:A:2:G:C6       | 1:A:3:C:C4       | 0.74     | 2.76        | 3      | 11    |
| 1:A:13:G:N7      | 2:B:49:ARG:NE    | 0.74     | 2.35        | 19     | 19    |
| 2:B:103:LEU:HD21 | 2:B:140:TYR:HE1  | 0.74     | 1.42        | 8      | 4     |
| 1:A:21:C:O2'     | 1:A:22:C:H5"     | 0.74     | 1.83        | 17     | 2     |
| 1:A:19:G:H4'     | 1:A:20:G:OP1     | 0.74     | 1.83        | 10     | 5     |
| 2:B:126:ILE:HG23 | 2:B:141:ILE:HG13 | 0.74     | 1.59        | 10     | 1     |
| 1:A:4:C:O2'      | 1:A:5:G:P        | 0.74     | 2.46        | 19     | 10    |
| 2:B:116:LEU:HD12 | 2:B:141:ILE:HD11 | 0.74     | 1.60        | 17     | 1     |
| 2:B:140:TYR:C    | 2:B:141:ILE:HD13 | 0.74     | 2.03        | 7      | 4     |
| 1:A:15:A:C4      | 1:A:17:U:C5      | 0.73     | 2.76        | 15     | 16    |
| 1:A:4:C:H1'      | 1:A:5:G:O4'      | 0.73     | 1.83        | 13     | 7     |
| 1:A:13:G:C8      | 2:B:58:TYR:CG    | 0.73     | 2.75        | 7      | 6     |
| 1:A:13:G:N3      | 1:A:13:G:C3'     | 0.73     | 2.51        | 10     | 13    |
| 1:A:13:G:N7      | 2:B:58:TYR:CG    | 0.73     | 2.57        | 1      | 8     |
| 2:B:63:SER:N     | 2:B:66:ASP:OD2   | 0.73     | 2.20        | 8      | 3     |
| 1:A:7:A:C6       | 1:A:8:A:C2       | 0.73     | 2.76        | 18     | 14    |
| 2:B:74:THR:OG1   | 2:B:85:LEU:HD21  | 0.73     | 1.84        | 17     | 3     |
| 1:A:9:U:C5       | 2:B:103:LEU:HD21 | 0.73     | 2.17        | 16     | 4     |
| 1:A:19:G:O2'     | 1:A:20:G:H5'     | 0.73     | 1.83        | 6      | 3     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 2:B:37:LEU:CG    | 2:B:76:LEU:HD13 | 0.73     | 2.14        | 14     | 1     |
| 2:B:159:ALA:HB3  | 2:B:166:VAL:HB  | 0.73     | 1.61        | 18     | 1     |
| 1:A:15:A:H8      | 1:A:15:A:OP1    | 0.73     | 1.67        | 7      | 1     |
| 2:B:171:THR:HG22 | 2:B:171:THR:O   | 0.73     | 1.83        | 9      | 1     |
| 1:A:10:C:C2      | 2:B:127:ARG:NH1 | 0.73     | 2.56        | 16     | 1     |
| 1:A:20:G:C2      | 1:A:21:C:C6     | 0.73     | 2.77        | 9      | 5     |
| 1:A:21:C:C2      | 1:A:22:C:C5     | 0.73     | 2.77        | 14     | 14    |
| 2:B:44:ALA:HB1   | 2:B:62:GLU:CG   | 0.73     | 2.14        | 8      | 1     |
| 2:B:103:LEU:HD12 | 2:B:171:THR:OG1 | 0.73     | 1.83        | 9      | 1     |
| 2:B:48:VAL:HG13  | 2:B:59:VAL:HG23 | 0.73     | 1.59        | 18     | 3     |
| 2:B:67:LEU:C     | 2:B:67:LEU:HD13 | 0.73     | 2.04        | 1      | 1     |
| 1:A:13:G:C3'     | 1:A:13:G:N3     | 0.73     | 2.52        | 13     | 6     |
| 1:A:20:G:C4      | 1:A:21:C:C6     | 0.73     | 2.77        | 19     | 15    |
| 1:A:6:A:C5       | 1:A:18:A:C2     | 0.73     | 2.77        | 16     | 5     |
| 2:B:38:PHE:CG    | 2:B:43:LEU:HD22 | 0.73     | 2.18        | 16     | 1     |
| 2:B:124:LEU:HD11 | 2:B:144:LYS:CG  | 0.73     | 2.14        | 16     | 1     |
| 2:B:16:LEU:HD12  | 2:B:16:LEU:C    | 0.72     | 2.04        | 10     | 7     |
| 1:A:2:G:C2       | 1:A:22:C:C2     | 0.72     | 2.76        | 18     | 8     |
| 1:A:19:G:C2      | 1:A:20:G:C4     | 0.72     | 2.76        | 17     | 9     |
| 1:A:10:C:C2      | 2:B:140:TYR:CD2 | 0.72     | 2.77        | 15     | 1     |
| 2:B:51:GLY:HA3   | 2:B:56:PHE:CG   | 0.72     | 2.19        | 11     | 17    |
| 2:B:38:PHE:CD2   | 2:B:43:LEU:HD22 | 0.72     | 2.18        | 19     | 4     |
| 2:B:37:LEU:HD21  | 2:B:76:LEU:HD22 | 0.72     | 1.60        | 2      | 2     |
| 1:A:15:A:C5      | 1:A:17:U:C4     | 0.72     | 2.77        | 3      | 15    |
| 1:A:19:G:C5      | 1:A:20:G:C8     | 0.72     | 2.77        | 18     | 15    |
| 2:B:67:LEU:HD13  | 2:B:67:LEU:C    | 0.72     | 2.04        | 6      | 3     |
| 1:A:15:A:H1'     | 1:A:16:G:OP1    | 0.72     | 1.83        | 18     | 1     |
| 1:A:16:G:H4'     | 1:A:17:U:OP1    | 0.72     | 1.82        | 13     | 1     |
| 2:B:27:VAL:HG23  | 2:B:50:THR:HG21 | 0.72     | 1.59        | 19     | 1     |
| 1:A:11:C:O2'     | 1:A:12:C:C5'    | 0.72     | 2.38        | 5      | 13    |
| 1:A:10:C:O4'     | 2:B:129:VAL:CG1 | 0.72     | 2.38        | 16     | 13    |
| 1:A:6:A:C4       | 1:A:18:A:C2     | 0.72     | 2.78        | 17     | 11    |
| 1:A:8:A:H4'      | 1:A:9:U:OP2     | 0.72     | 1.84        | 8      | 7     |
| 1:A:13:G:N7      | 2:B:58:TYR:CD2  | 0.72     | 2.58        | 7      | 6     |
| 1:A:10:C:N3      | 1:A:11:C:C4     | 0.72     | 2.57        | 16     | 6     |
| 1:A:5:G:O2'      | 1:A:6:A:P       | 0.72     | 2.47        | 4      | 1     |
| 1:A:9:U:H1'      | 1:A:10:C:OP1    | 0.72     | 1.85        | 9      | 10    |
| 1:A:13:G:N3      | 1:A:13:G:H5"    | 0.72     | 1.98        | 15     | 5     |
| 1:A:16:G:O2'     | 1:A:17:U:P      | 0.72     | 2.47        | 11     | 2     |
| 1:A:8:A:N1       | 1:A:14:A:N3     | 0.72     | 2.38        | 11     | 18    |
| 2:B:18:ILE:HD13  | 2:B:59:VAL:HG21 | 0.72     | 1.60        | 19     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:10:C:O2      | 1:A:11:C:C6      | 0.72     | 2.42        | 16     | 14    |
| 2:B:38:PHE:CE1   | 2:B:73:LEU:HD13  | 0.72     | 2.20        | 9      | 2     |
| 1:A:14:A:C4      | 2:B:94:LYS:CG    | 0.72     | 2.73        | 1      | 6     |
| 1:A:3:C:O2'      | 1:A:4:C:P        | 0.72     | 2.48        | 1      | 10    |
| 1:A:8:A:N1       | 1:A:14:A:C1'     | 0.72     | 2.53        | 3      | 16    |
| 2:B:33:ALA:HB2   | 2:B:79:PHE:CD2   | 0.72     | 2.20        | 17     | 2     |
| 1:A:15:A:H4'     | 1:A:16:G:OP1     | 0.72     | 1.84        | 1      | 5     |
| 1:A:21:C:H4'     | 1:A:21:C:OP1     | 0.72     | 1.83        | 18     | 1     |
| 2:B:102:LEU:HD23 | 2:B:168:LEU:HD23 | 0.72     | 1.61        | 10     | 1     |
| 1:A:20:G:C5      | 1:A:21:C:C4      | 0.72     | 2.78        | 2      | 6     |
| 1:A:20:G:C6      | 1:A:21:C:C4      | 0.72     | 2.78        | 5      | 16    |
| 2:B:44:ALA:HB1   | 2:B:62:GLU:HG2   | 0.71     | 1.60        | 5      | 1     |
| 1:A:16:G:C8      | 2:B:27:VAL:HG21  | 0.71     | 2.20        | 17     | 11    |
| 1:A:12:C:O2'     | 2:B:56:PHE:CZ    | 0.71     | 2.42        | 14     | 3     |
| 1:A:11:C:O2'     | 1:A:12:C:OP1     | 0.71     | 2.08        | 5      | 6     |
| 1:A:15:A:C8      | 1:A:17:U:C2      | 0.71     | 2.78        | 3      | 13    |
| 1:A:14:A:N6      | 2:B:94:LYS:NZ    | 0.71     | 2.39        | 5      | 1     |
| 2:B:30:LEU:HD23  | 2:B:78:VAL:CG1   | 0.71     | 2.15        | 8      | 8     |
| 2:B:126:ILE:HG12 | 2:B:141:ILE:HG23 | 0.71     | 1.60        | 5      | 8     |
| 2:B:93:SER:O     | 2:B:95:LYS:N     | 0.71     | 2.23        | 10     | 14    |
| 2:B:92:ASP:CA    | 2:B:96:VAL:HG11  | 0.71     | 2.15        | 16     | 1     |
| 1:A:9:U:O2'      | 1:A:10:C:C6      | 0.71     | 2.43        | 5      | 18    |
| 2:B:16:LEU:C     | 2:B:16:LEU:HD12  | 0.71     | 2.06        | 19     | 3     |
| 2:B:37:LEU:HD13  | 2:B:76:LEU:CD2   | 0.71     | 2.15        | 15     | 1     |
| 2:B:21:LEU:HD22  | 2:B:30:LEU:CD2   | 0.71     | 2.10        | 18     | 1     |
| 1:A:4:C:O2'      | 1:A:5:G:O5'      | 0.71     | 2.08        | 5      | 19    |
| 2:B:103:LEU:HD23 | 2:B:169:TYR:O    | 0.71     | 1.86        | 5      | 3     |
| 1:A:20:G:N3      | 1:A:21:C:C6      | 0.71     | 2.59        | 9      | 5     |
| 2:B:103:LEU:HD12 | 2:B:138:ILE:CG2  | 0.70     | 2.16        | 1      | 3     |
| 2:B:37:LEU:HD22  | 2:B:76:LEU:HD21  | 0.70     | 1.61        | 11     | 2     |
| 1:A:3:C:C2       | 1:A:4:C:C5       | 0.70     | 2.78        | 19     | 2     |
| 1:A:13:G:C5'     | 1:A:13:G:N3      | 0.70     | 2.54        | 8      | 6     |
| 1:A:12:C:O2'     | 2:B:56:PHE:CE1   | 0.70     | 2.43        | 6      | 1     |
| 2:B:37:LEU:HD22  | 2:B:76:LEU:HD22  | 0.70     | 1.63        | 10     | 1     |
| 2:B:41:ASN:O     | 2:B:42:ASP:CB    | 0.70     | 2.40        | 4      | 19    |
| 1:A:15:A:C5      | 2:B:52:THR:HG23  | 0.70     | 2.20        | 3      | 3     |
| 2:B:43:LEU:HD12  | 2:B:66:ASP:OD1   | 0.70     | 1.85        | 17     | 2     |
| 2:B:38:PHE:CZ    | 2:B:43:LEU:HD13  | 0.70     | 2.22        | 19     | 1     |
| 1:A:12:C:P       | 1:A:12:C:C2      | 0.70     | 2.85        | 6      | 1     |
| 2:B:37:LEU:HD23  | 2:B:76:LEU:CD2   | 0.70     | 2.15        | 3      | 1     |
| 1:A:15:A:C4      | 2:B:52:THR:CG2   | 0.70     | 2.75        | 15     | 18    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:13:G:O2'     | 1:A:14:A:H5"     | 0.70     | 1.85        | 11     | 3     |
| 1:A:14:A:O2'     | 1:A:15:A:N7      | 0.70     | 2.25        | 16     | 15    |
| 1:A:19:G:C2'     | 1:A:20:G:O4'     | 0.70     | 2.39        | 10     | 8     |
| 2:B:103:LEU:HD12 | 2:B:129:VAL:HG21 | 0.70     | 1.62        | 15     | 2     |
| 2:B:77:LYS:O     | 2:B:78:VAL:O     | 0.70     | 2.10        | 10     | 8     |
| 1:A:13:G:O2'     | 2:B:56:PHE:CZ    | 0.70     | 2.43        | 16     | 3     |
| 1:A:13:G:C5      | 2:B:58:TYR:CE2   | 0.70     | 2.80        | 1      | 5     |
| 2:B:102:LEU:HD22 | 2:B:141:ILE:O    | 0.70     | 1.85        | 12     | 4     |
| 2:B:27:VAL:HA    | 2:B:30:LEU:HD12  | 0.70     | 1.61        | 16     | 5     |
| 1:A:15:A:OP1     | 1:A:15:A:C8      | 0.70     | 2.45        | 7      | 1     |
| 1:A:15:A:C6      | 1:A:17:U:C4      | 0.70     | 2.80        | 5      | 10    |
| 2:B:12:THR:HG21  | 2:B:46:VAL:HG21  | 0.70     | 1.64        | 17     | 5     |
| 2:B:12:THR:HG21  | 2:B:46:VAL:HB    | 0.70     | 1.63        | 19     | 1     |
| 2:B:12:THR:HG22  | 2:B:13:PRO:HD2   | 0.70     | 1.64        | 11     | 6     |
| 2:B:129:VAL:HB   | 2:B:138:ILE:HB   | 0.69     | 1.62        | 10     | 19    |
| 1:A:21:C:N3      | 1:A:22:C:C5      | 0.69     | 2.60        | 12     | 6     |
| 1:A:3:C:N4       | 1:A:4:C:N4       | 0.69     | 2.40        | 14     | 2     |
| 2:B:116:LEU:HD23 | 2:B:141:ILE:HD11 | 0.69     | 1.62        | 8      | 2     |
| 2:B:56:PHE:CD1   | 2:B:56:PHE:C     | 0.69     | 2.66        | 19     | 2     |
| 2:B:78:VAL:O     | 2:B:80:GLY:N     | 0.69     | 2.24        | 4      | 18    |
| 2:B:107:LEU:HD11 | 2:B:139:ALA:CB   | 0.69     | 2.17        | 4      | 3     |
| 1:A:4:C:H3'      | 1:A:4:C:OP2      | 0.69     | 1.87        | 8      | 1     |
| 1:A:9:U:C5       | 2:B:138:ILE:HD13 | 0.69     | 2.21        | 17     | 9     |
| 1:A:15:A:C4      | 1:A:17:U:C4      | 0.69     | 2.80        | 1      | 15    |
| 2:B:127:ARG:CZ   | 2:B:127:ARG:HB3  | 0.69     | 2.18        | 16     | 1     |
| 2:B:126:ILE:HG23 | 2:B:141:ILE:HD13 | 0.69     | 1.64        | 9      | 3     |
| 2:B:37:LEU:HD21  | 2:B:76:LEU:CB    | 0.69     | 2.16        | 14     | 1     |
| 2:B:34:ILE:HD11  | 2:B:83:ILE:HG21  | 0.69     | 1.63        | 14     | 1     |
| 1:A:10:C:OP2     | 1:A:11:C:H5      | 0.68     | 1.71        | 13     | 1     |
| 1:A:12:C:C6      | 1:A:12:C:OP1     | 0.68     | 2.46        | 13     | 1     |
| 1:A:8:A:N1       | 1:A:14:A:C4      | 0.68     | 2.61        | 5      | 16    |
| 1:A:10:C:H1'     | 2:B:129:VAL:HG22 | 0.68     | 1.65        | 4      | 19    |
| 1:A:19:G:C2      | 1:A:20:G:N9      | 0.68     | 2.61        | 10     | 5     |
| 2:B:103:LEU:CD2  | 2:B:140:TYR:CE1  | 0.68     | 2.76        | 10     | 6     |
| 2:B:12:THR:HG22  | 2:B:13:PRO:CD    | 0.68     | 2.18        | 17     | 4     |
| 1:A:14:A:N7      | 2:B:94:LYS:NZ    | 0.68     | 2.40        | 7      | 1     |
| 1:A:15:A:N3      | 1:A:17:U:C5      | 0.68     | 2.61        | 5      | 11    |
| 1:A:13:G:O2'     | 1:A:14:A:P       | 0.68     | 2.51        | 6      | 5     |
| 2:B:78:VAL:HG13  | 2:B:79:PHE:N     | 0.68     | 2.04        | 18     | 7     |
| 2:B:98:ALA:HB1   | 2:B:171:THR:HB   | 0.68     | 1.63        | 19     | 4     |
| 1:A:15:A:C5      | 2:B:52:THR:HG22  | 0.68     | 2.24        | 8      | 13    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:12:C:C5      | 2:B:17:PHE:CZ    | 0.68     | 2.81        | 3      | 4     |
| 1:A:10:C:N4      | 1:A:11:C:N4      | 0.68     | 2.40        | 13     | 3     |
| 2:B:16:LEU:CD2   | 2:B:85:LEU:HD21  | 0.68     | 2.18        | 6      | 2     |
| 2:B:111:ILE:HD12 | 2:B:161:ILE:HG21 | 0.68     | 1.66        | 17     | 1     |
| 1:A:14:A:N6      | 2:B:94:LYS:CE    | 0.68     | 2.57        | 2      | 4     |
| 2:B:37:LEU:HD23  | 2:B:76:LEU:HD23  | 0.68     | 1.66        | 3      | 1     |
| 2:B:74:THR:OG1   | 2:B:85:LEU:HD11  | 0.68     | 1.88        | 12     | 1     |
| 1:A:14:A:OP2     | 1:A:14:A:C8      | 0.68     | 2.47        | 4      | 3     |
| 2:B:157:GLN:HA   | 2:B:168:LEU:HD12 | 0.68     | 1.66        | 13     | 4     |
| 2:B:38:PHE:CD2   | 2:B:45:VAL:CG1   | 0.67     | 2.78        | 19     | 15    |
| 1:A:16:G:N7      | 2:B:27:VAL:CG2   | 0.67     | 2.57        | 9      | 11    |
| 2:B:78:VAL:CG2   | 2:B:83:ILE:HG21  | 0.67     | 2.18        | 8      | 10    |
| 1:A:13:G:O4'     | 2:B:56:PHE:CE1   | 0.67     | 2.46        | 17     | 2     |
| 2:B:153:LEU:HA   | 2:B:168:LEU:HD22 | 0.67     | 1.64        | 7      | 3     |
| 2:B:102:LEU:HA   | 2:B:171:THR:HG23 | 0.67     | 1.65        | 2      | 3     |
| 1:A:12:C:C5      | 1:A:12:C:OP2     | 0.67     | 2.47        | 18     | 5     |
| 2:B:103:LEU:CG   | 2:B:140:TYR:CE1  | 0.67     | 2.77        | 11     | 5     |
| 2:B:103:LEU:CD1  | 2:B:140:TYR:CE1  | 0.67     | 2.77        | 4      | 6     |
| 1:A:19:G:HO2'    | 1:A:20:G:P       | 0.67     | 2.12        | 7      | 3     |
| 2:B:111:ILE:HD11 | 2:B:161:ILE:CG2  | 0.67     | 2.19        | 2      | 1     |
| 2:B:31:LYS:HG2   | 2:B:48:VAL:HG13  | 0.67     | 1.66        | 12     | 3     |
| 2:B:102:LEU:CD2  | 2:B:168:LEU:HD12 | 0.67     | 2.18        | 18     | 1     |
| 2:B:130:SER:O    | 2:B:138:ILE:HD11 | 0.67     | 1.89        | 15     | 1     |
| 2:B:85:LEU:N     | 2:B:85:LEU:HD23  | 0.67     | 2.04        | 18     | 2     |
| 2:B:61:PHE:CE2   | 2:B:70:ALA:HB1   | 0.67     | 2.25        | 12     | 9     |
| 2:B:123:ALA:HB2  | 2:B:143:PHE:CZ   | 0.67     | 2.25        | 1      | 6     |
| 2:B:85:LEU:N     | 2:B:85:LEU:HD12  | 0.67     | 2.04        | 10     | 1     |
| 2:B:69:LYS:C     | 2:B:73:LEU:HD13  | 0.67     | 2.09        | 8      | 3     |
| 2:B:127:ARG:NH2  | 2:B:140:TYR:HB2  | 0.67     | 2.04        | 18     | 2     |
| 2:B:104:ALA:HB1  | 2:B:166:VAL:HG11 | 0.67     | 1.66        | 9      | 1     |
| 1:A:10:C:H4'     | 2:B:128:LEU:O    | 0.67     | 1.90        | 15     | 1     |
| 1:A:11:C:N3      | 2:B:94:LYS:HB2   | 0.67     | 2.05        | 18     | 2     |
| 2:B:107:LEU:HD23 | 2:B:166:VAL:CG2  | 0.67     | 2.17        | 4      | 3     |
| 2:B:94:LYS:HG2   | 2:B:95:LYS:N     | 0.67     | 2.03        | 11     | 1     |
| 2:B:161:ILE:HD12 | 2:B:166:VAL:HG21 | 0.67     | 1.66        | 17     | 1     |
| 2:B:46:VAL:HG22  | 2:B:62:GLU:HG3   | 0.67     | 1.64        | 17     | 6     |
| 1:A:13:G:O2'     | 1:A:14:A:C5'     | 0.67     | 2.43        | 8      | 6     |
| 1:A:9:U:C1'      | 1:A:10:C:OP1     | 0.67     | 2.43        | 8      | 11    |
| 2:B:102:LEU:HD23 | 2:B:143:PHE:CE1  | 0.67     | 2.24        | 15     | 4     |
| 2:B:127:ARG:NH2  | 2:B:140:TYR:CG   | 0.67     | 2.62        | 18     | 1     |
| 2:B:21:LEU:HD12  | 2:B:56:PHE:O     | 0.67     | 1.90        | 18     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:7:A:N1       | 1:A:8:A:C2       | 0.67     | 2.63        | 17     | 10    |
| 2:B:153:LEU:HD23 | 2:B:153:LEU:C    | 0.67     | 2.09        | 14     | 4     |
| 1:A:5:G:HO2'     | 1:A:6:A:H5'      | 0.67     | 1.47        | 9      | 2     |
| 2:B:26:SER:O     | 2:B:30:LEU:HD13  | 0.67     | 1.88        | 4      | 2     |
| 1:A:9:U:C4       | 2:B:138:ILE:HD13 | 0.67     | 2.24        | 4      | 5     |
| 1:A:8:A:N3       | 2:B:95:LYS:HD3   | 0.67     | 2.05        | 11     | 1     |
| 1:A:6:A:O2'      | 1:A:7:A:H5'      | 0.66     | 1.90        | 5      | 1     |
| 2:B:102:LEU:HD12 | 2:B:102:LEU:C    | 0.66     | 2.10        | 18     | 2     |
| 1:A:14:A:O3'     | 1:A:15:A:H8      | 0.66     | 1.71        | 14     | 3     |
| 2:B:61:PHE:CE2   | 2:B:70:ALA:CB    | 0.66     | 2.79        | 2      | 9     |
| 1:A:20:G:C4      | 1:A:21:C:C5      | 0.66     | 2.83        | 9      | 13    |
| 2:B:107:LEU:CD1  | 2:B:139:ALA:HB2  | 0.66     | 2.19        | 4      | 2     |
| 2:B:116:LEU:HD13 | 2:B:126:ILE:HG21 | 0.66     | 1.67        | 3      | 1     |
| 2:B:102:LEU:HD11 | 2:B:149:ALA:O    | 0.66     | 1.90        | 17     | 1     |
| 2:B:126:ILE:CG1  | 2:B:141:ILE:HG23 | 0.66     | 2.21        | 3      | 4     |
| 1:A:14:A:C6      | 2:B:94:LYS:CG    | 0.66     | 2.78        | 6      | 4     |
| 2:B:37:LEU:HD22  | 2:B:76:LEU:HD23  | 0.66     | 1.67        | 16     | 2     |
| 1:A:16:G:H1'     | 1:A:17:U:OP2     | 0.66     | 1.89        | 16     | 1     |
| 2:B:127:ARG:HB3  | 2:B:127:ARG:NH2  | 0.66     | 2.05        | 16     | 1     |
| 2:B:48:VAL:HG22  | 2:B:59:VAL:CG1   | 0.66     | 2.13        | 5      | 1     |
| 1:A:12:C:OP1     | 1:A:12:C:C5      | 0.66     | 2.48        | 10     | 5     |
| 1:A:12:C:C6      | 1:A:12:C:O5'     | 0.66     | 2.48        | 8      | 3     |
| 1:A:9:U:H1'      | 2:B:129:VAL:HG12 | 0.66     | 1.66        | 15     | 1     |
| 2:B:73:LEU:HD12  | 2:B:76:LEU:HD21  | 0.66     | 1.67        | 19     | 1     |
| 2:B:27:VAL:HG22  | 2:B:31:LYS:HE3   | 0.66     | 1.67        | 19     | 2     |
| 1:A:12:C:O3'     | 1:A:13:G:H4'     | 0.66     | 1.91        | 4      | 1     |
| 1:A:21:C:O2'     | 1:A:22:C:C5'     | 0.66     | 2.44        | 17     | 4     |
| 1:A:13:G:N7      | 2:B:49:ARG:CD    | 0.66     | 2.58        | 19     | 14    |
| 2:B:120:PHE:CE2  | 2:B:141:ILE:CD1  | 0.66     | 2.79        | 1      | 8     |
| 1:A:11:C:C2'     | 1:A:12:C:O5'     | 0.66     | 2.43        | 19     | 9     |
| 1:A:13:G:N7      | 2:B:49:ARG:HD3   | 0.66     | 2.06        | 11     | 6     |
| 1:A:3:C:O2'      | 1:A:4:C:C5'      | 0.66     | 2.43        | 10     | 16    |
| 2:B:69:LYS:C     | 2:B:73:LEU:HD23  | 0.66     | 2.10        | 4      | 7     |
| 1:A:10:C:O2'     | 2:B:128:LEU:N    | 0.66     | 2.29        | 15     | 1     |
| 1:A:20:G:H3'     | 1:A:21:C:O4'     | 0.66     | 1.91        | 18     | 3     |
| 1:A:13:G:O2'     | 1:A:14:A:O5'     | 0.66     | 2.14        | 6      | 4     |
| 2:B:102:LEU:HD13 | 2:B:168:LEU:CD1  | 0.66     | 2.20        | 6      | 1     |
| 1:A:7:A:N1       | 1:A:8:A:N3       | 0.66     | 2.44        | 4      | 15    |
| 2:B:128:LEU:HD21 | 2:B:136:LYS:CB   | 0.66     | 2.21        | 15     | 1     |
| 2:B:16:LEU:HD22  | 2:B:85:LEU:HD21  | 0.66     | 1.66        | 6      | 1     |
| 2:B:21:LEU:HG    | 2:B:30:LEU:HD22  | 0.65     | 1.68        | 2      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:116:LEU:CB   | 2:B:126:ILE:HD13 | 0.65     | 2.21        | 6      | 1     |
| 2:B:103:LEU:HD13 | 2:B:140:TYR:HE1  | 0.65     | 1.52        | 5      | 2     |
| 2:B:61:PHE:CZ    | 2:B:70:ALA:CB    | 0.65     | 2.79        | 1      | 7     |
| 1:A:4:C:O2'      | 1:A:5:G:C5'      | 0.65     | 2.44        | 18     | 9     |
| 2:B:104:ALA:HB2  | 2:B:141:ILE:CD1  | 0.65     | 2.22        | 10     | 1     |
| 2:B:44:ALA:HB3   | 2:B:66:ASP:OD2   | 0.65     | 1.90        | 11     | 3     |
| 1:A:13:G:OP1     | 1:A:13:G:H4'     | 0.65     | 1.91        | 5      | 2     |
| 1:A:14:A:C6      | 2:B:94:LYS:CE    | 0.65     | 2.79        | 16     | 4     |
| 1:A:20:G:N7      | 1:A:21:C:C5      | 0.65     | 2.65        | 11     | 7     |
| 1:A:9:U:C5       | 2:B:138:ILE:HG21 | 0.65     | 2.27        | 14     | 2     |
| 1:A:14:A:N1      | 2:B:94:LYS:HG3   | 0.65     | 2.06        | 6      | 3     |
| 2:B:102:LEU:HD11 | 2:B:143:PHE:CE1  | 0.65     | 2.26        | 9      | 1     |
| 2:B:101:THR:HG23 | 2:B:141:ILE:O    | 0.65     | 1.91        | 7      | 3     |
| 1:A:11:C:O2'     | 1:A:12:C:H5"     | 0.65     | 1.90        | 5      | 1     |
| 2:B:18:ILE:HD12  | 2:B:59:VAL:CG2   | 0.65     | 2.22        | 10     | 1     |
| 1:A:14:A:C5      | 2:B:94:LYS:HG2   | 0.65     | 2.27        | 15     | 8     |
| 1:A:19:G:N3      | 1:A:20:G:H1'     | 0.65     | 2.05        | 16     | 4     |
| 2:B:67:LEU:O     | 2:B:70:ALA:HB3   | 0.65     | 1.92        | 15     | 5     |
| 2:B:107:LEU:HD21 | 2:B:166:VAL:HG13 | 0.65     | 1.67        | 7      | 1     |
| 1:A:11:C:H4'     | 1:A:12:C:OP1     | 0.65     | 1.89        | 17     | 2     |
| 2:B:59:VAL:CG1   | 2:B:61:PHE:CZ    | 0.65     | 2.80        | 18     | 7     |
| 1:A:14:A:C4      | 2:B:94:LYS:HG3   | 0.65     | 2.27        | 15     | 4     |
| 1:A:12:C:H4'     | 1:A:13:G:OP2     | 0.65     | 1.89        | 8      | 1     |
| 2:B:21:LEU:HG    | 2:B:56:PHE:O     | 0.65     | 1.92        | 13     | 3     |
| 1:A:12:C:C4      | 1:A:12:C:OP2     | 0.65     | 2.50        | 7      | 6     |
| 2:B:38:PHE:CB    | 2:B:45:VAL:HG13  | 0.65     | 2.22        | 9      | 3     |
| 1:A:12:C:C2      | 2:B:17:PHE:CE1   | 0.65     | 2.84        | 14     | 8     |
| 2:B:105:LYS:CG   | 2:B:138:ILE:HG23 | 0.65     | 2.21        | 15     | 3     |
| 2:B:103:LEU:HD11 | 2:B:138:ILE:HG21 | 0.65     | 1.67        | 12     | 5     |
| 2:B:30:LEU:HD23  | 2:B:78:VAL:HG13  | 0.65     | 1.67        | 19     | 5     |
| 1:A:13:G:HO2'    | 1:A:14:A:C5'     | 0.65     | 2.04        | 3      | 2     |
| 2:B:102:LEU:HD12 | 2:B:170:TYR:HD1  | 0.65     | 1.51        | 7      | 1     |
| 2:B:27:VAL:CG2   | 2:B:50:THR:HG21  | 0.65     | 2.22        | 19     | 3     |
| 1:A:19:G:O2'     | 1:A:20:G:C5'     | 0.65     | 2.45        | 1      | 5     |
| 1:A:13:G:H4'     | 1:A:14:A:OP1     | 0.65     | 1.90        | 3      | 2     |
| 1:A:19:G:H8      | 1:A:19:G:OP2     | 0.65     | 1.75        | 11     | 1     |
| 1:A:21:C:O2'     | 1:A:22:C:P       | 0.65     | 2.54        | 14     | 2     |
| 1:A:7:A:N6       | 1:A:8:A:N1       | 0.65     | 2.44        | 4      | 10    |
| 2:B:140:TYR:OH   | 2:B:171:THR:CG2  | 0.65     | 2.45        | 15     | 4     |
| 2:B:128:LEU:HD21 | 2:B:136:LYS:HB2  | 0.65     | 1.69        | 15     | 1     |
| 1:A:14:A:P       | 1:A:14:A:C8      | 0.65     | 2.90        | 16     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:30:LEU:HD11  | 2:B:31:LYS:CE    | 0.65     | 2.21        | 14     | 1     |
| 2:B:102:LEU:HD21 | 2:B:153:LEU:HD12 | 0.65     | 1.69        | 17     | 1     |
| 1:A:13:G:N2      | 2:B:92:ASP:O     | 0.65     | 2.30        | 17     | 1     |
| 2:B:53:ASN:OD1   | 2:B:55:LYS:CB    | 0.64     | 2.45        | 13     | 19    |
| 1:A:8:A:N1       | 1:A:14:A:O2'     | 0.64     | 2.28        | 13     | 4     |
| 1:A:1:G:H4'      | 1:A:2:G:OP1      | 0.64     | 1.91        | 2      | 1     |
| 1:A:20:G:O2'     | 1:A:21:C:OP1     | 0.64     | 2.14        | 13     | 1     |
| 2:B:140:TYR:OH   | 2:B:171:THR:OG1  | 0.64     | 2.10        | 11     | 1     |
| 1:A:12:C:C2      | 1:A:12:C:OP1     | 0.64     | 2.50        | 14     | 1     |
| 1:A:14:A:C6      | 2:B:94:LYS:CD    | 0.64     | 2.80        | 13     | 3     |
| 1:A:13:G:O2'     | 2:B:52:THR:OG1   | 0.64     | 2.14        | 14     | 2     |
| 1:A:12:C:OP1     | 1:A:12:C:C6      | 0.64     | 2.50        | 6      | 5     |
| 1:A:20:G:O2'     | 1:A:21:C:C5'     | 0.64     | 2.44        | 9      | 4     |
| 1:A:14:A:P       | 1:A:14:A:O4'     | 0.64     | 2.56        | 2      | 1     |
| 1:A:12:C:O5'     | 1:A:12:C:C6      | 0.64     | 2.49        | 16     | 4     |
| 2:B:73:LEU:HD22  | 2:B:76:LEU:CD1   | 0.64     | 2.20        | 13     | 1     |
| 1:A:19:G:C5      | 1:A:20:G:N7      | 0.64     | 2.65        | 5      | 11    |
| 1:A:4:C:O2'      | 1:A:5:G:C8       | 0.64     | 2.51        | 8      | 17    |
| 2:B:116:LEU:CD1  | 2:B:139:ALA:HB1  | 0.64     | 2.22        | 10     | 3     |
| 2:B:104:ALA:HB1  | 2:B:166:VAL:CG1  | 0.64     | 2.22        | 9      | 4     |
| 2:B:129:VAL:CB   | 2:B:138:ILE:HB   | 0.64     | 2.23        | 15     | 19    |
| 1:A:2:G:N1       | 1:A:22:C:C4      | 0.64     | 2.65        | 10     | 6     |
| 2:B:102:LEU:HD21 | 2:B:143:PHE:HE1  | 0.64     | 1.51        | 19     | 1     |
| 1:A:7:A:H4'      | 1:A:7:A:OP1      | 0.64     | 1.91        | 14     | 1     |
| 1:A:12:C:C4      | 2:B:17:PHE:CZ    | 0.64     | 2.86        | 3      | 12    |
| 2:B:38:PHE:CE2   | 2:B:73:LEU:HD13  | 0.64     | 2.27        | 9      | 1     |
| 1:A:12:C:OP1     | 1:A:12:C:C4      | 0.64     | 2.51        | 6      | 2     |
| 2:B:103:LEU:CB   | 2:B:140:TYR:CD1  | 0.64     | 2.80        | 18     | 3     |
| 1:A:16:G:C6      | 2:B:54:ARG:NH1   | 0.64     | 2.65        | 13     | 2     |
| 1:A:12:C:C2      | 1:A:12:C:OP2     | 0.64     | 2.51        | 19     | 4     |
| 2:B:16:LEU:CD1   | 2:B:16:LEU:N     | 0.64     | 2.60        | 13     | 1     |
| 1:A:10:C:C6      | 2:B:140:TYR:CE2  | 0.64     | 2.86        | 15     | 1     |
| 1:A:9:U:N3       | 2:B:138:ILE:CD1  | 0.64     | 2.60        | 4      | 3     |
| 2:B:103:LEU:HD11 | 2:B:171:THR:CG2  | 0.64     | 2.20        | 6      | 1     |
| 1:A:7:A:O2'      | 1:A:8:A:O5'      | 0.64     | 2.16        | 14     | 3     |
| 2:B:16:LEU:N     | 2:B:16:LEU:CD1   | 0.64     | 2.60        | 2      | 3     |
| 1:A:14:A:C4'     | 1:A:14:A:OP2     | 0.64     | 2.45        | 3      | 2     |
| 2:B:33:ALA:CB    | 2:B:78:VAL:HG13  | 0.64     | 2.23        | 3      | 1     |
| 2:B:102:LEU:HD22 | 2:B:170:TYR:HB3  | 0.64     | 1.70        | 14     | 1     |
| 1:A:11:C:O2      | 2:B:94:LYS:NZ    | 0.64     | 2.31        | 14     | 1     |
| 1:A:20:G:C6      | 1:A:21:C:C5      | 0.64     | 2.86        | 3      | 8     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:52:THR:O     | 2:B:53:ASN:CB    | 0.63     | 2.46        | 19     | 19    |
| 2:B:17:PHE:CD1   | 2:B:18:ILE:N     | 0.63     | 2.66        | 14     | 16    |
| 2:B:120:PHE:HZ   | 2:B:168:LEU:HD11 | 0.63     | 1.53        | 18     | 6     |
| 2:B:102:LEU:HD12 | 2:B:170:TYR:CE1  | 0.63     | 2.28        | 12     | 1     |
| 1:A:18:A:O2'     | 1:A:19:G:C5'     | 0.63     | 2.46        | 3      | 6     |
| 2:B:123:ALA:CB   | 2:B:141:ILE:HG23 | 0.63     | 2.24        | 11     | 1     |
| 1:A:20:G:N1      | 1:A:21:C:C4      | 0.63     | 2.66        | 9      | 5     |
| 1:A:7:A:HO2'     | 1:A:8:A:P        | 0.63     | 2.15        | 10     | 1     |
| 2:B:30:LEU:HD12  | 2:B:54:ARG:HD2   | 0.63     | 1.69        | 3      | 6     |
| 1:A:11:C:N3      | 2:B:94:LYS:CD    | 0.63     | 2.61        | 2      | 2     |
| 1:A:14:A:N1      | 2:B:94:LYS:CG    | 0.63     | 2.61        | 12     | 3     |
| 1:A:16:G:C4'     | 1:A:16:G:OP1     | 0.63     | 2.46        | 18     | 1     |
| 1:A:13:G:C6      | 2:B:58:TYR:CE2   | 0.63     | 2.85        | 1      | 2     |
| 2:B:11:THR:HG21  | 2:B:47:ASP:CG    | 0.63     | 2.13        | 17     | 1     |
| 2:B:127:ARG:CZ   | 2:B:140:TYR:CD2  | 0.63     | 2.82        | 12     | 3     |
| 1:A:19:G:O2'     | 1:A:20:G:O4'     | 0.63     | 2.16        | 15     | 2     |
| 2:B:33:ALA:HB3   | 2:B:78:VAL:HG13  | 0.63     | 1.70        | 3      | 1     |
| 2:B:127:ARG:NH2  | 2:B:140:TYR:CD2  | 0.63     | 2.67        | 12     | 5     |
| 2:B:21:LEU:HD23  | 2:B:30:LEU:HD23  | 0.63     | 1.69        | 4      | 2     |
| 1:A:8:A:C4'      | 1:A:9:U:OP2      | 0.63     | 2.45        | 17     | 5     |
| 2:B:102:LEU:CA   | 2:B:171:THR:HG23 | 0.63     | 2.24        | 2      | 3     |
| 2:B:38:PHE:CD1   | 2:B:43:LEU:CD2   | 0.63     | 2.78        | 16     | 1     |
| 2:B:34:ILE:CG2   | 2:B:38:PHE:CE2   | 0.63     | 2.82        | 11     | 1     |
| 2:B:22:ASN:HB2   | 2:B:30:LEU:HD21  | 0.63     | 1.69        | 19     | 6     |
| 2:B:38:PHE:CE2   | 2:B:43:LEU:CD2   | 0.63     | 2.82        | 19     | 1     |
| 2:B:61:PHE:CE1   | 2:B:70:ALA:HB1   | 0.63     | 2.28        | 16     | 1     |
| 1:A:19:G:H8      | 1:A:19:G:O5'     | 0.63     | 1.76        | 13     | 1     |
| 1:A:17:U:C2'     | 1:A:18:A:OP1     | 0.63     | 2.46        | 11     | 1     |
| 1:A:15:A:HO2'    | 1:A:16:G:P       | 0.63     | 2.16        | 5      | 2     |
| 2:B:97:ARG:O     | 2:B:101:THR:OG1  | 0.63     | 2.17        | 7      | 11    |
| 1:A:2:G:N2       | 1:A:22:C:C6      | 0.63     | 2.66        | 18     | 3     |
| 1:A:9:U:C4'      | 1:A:10:C:OP1     | 0.63     | 2.47        | 16     | 5     |
| 1:A:11:C:HO2'    | 1:A:12:C:H5'     | 0.63     | 1.53        | 1      | 4     |
| 2:B:18:ILE:HD12  | 2:B:59:VAL:HG21  | 0.63     | 1.69        | 5      | 2     |
| 2:B:38:PHE:CD2   | 2:B:45:VAL:HG13  | 0.63     | 2.29        | 19     | 7     |
| 1:A:12:C:C6      | 1:A:12:C:OP2     | 0.63     | 2.52        | 19     | 2     |
| 2:B:17:PHE:C     | 2:B:17:PHE:CD1   | 0.63     | 2.72        | 19     | 1     |
| 1:A:12:C:OP1     | 1:A:12:C:N3      | 0.63     | 2.32        | 16     | 2     |
| 1:A:12:C:OP2     | 1:A:12:C:C2      | 0.63     | 2.52        | 6      | 1     |
| 1:A:7:A:O2'      | 1:A:8:A:OP1      | 0.63     | 2.16        | 14     | 4     |
| 1:A:13:G:N2      | 2:B:90:GLY:O     | 0.63     | 2.32        | 6      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:13:G:N7      | 2:B:49:ARG:HD2   | 0.63     | 2.08        | 13     | 4     |
| 2:B:101:THR:O    | 2:B:171:THR:OG1  | 0.62     | 2.17        | 10     | 13    |
| 1:A:7:A:N6       | 1:A:8:A:C2       | 0.62     | 2.67        | 18     | 8     |
| 2:B:17:PHE:CE1   | 2:B:18:ILE:O     | 0.62     | 2.53        | 6      | 12    |
| 1:A:19:G:O2'     | 1:A:20:G:O5'     | 0.62     | 2.17        | 9      | 6     |
| 2:B:67:LEU:HD22  | 2:B:67:LEU:C     | 0.62     | 2.10        | 8      | 1     |
| 1:A:13:G:HO2'    | 1:A:14:A:P       | 0.62     | 2.17        | 9      | 1     |
| 2:B:102:LEU:N    | 2:B:102:LEU:HD12 | 0.62     | 2.09        | 2      | 1     |
| 2:B:43:LEU:HD11  | 2:B:73:LEU:HD21  | 0.62     | 1.71        | 7      | 2     |
| 1:A:12:C:OP1     | 1:A:12:C:C2      | 0.62     | 2.52        | 6      | 3     |
| 2:B:120:PHE:CD2  | 2:B:141:ILE:HD13 | 0.62     | 2.30        | 5      | 7     |
| 1:A:14:A:C4      | 2:B:94:LYS:HG2   | 0.62     | 2.29        | 4      | 5     |
| 2:B:124:LEU:HD11 | 2:B:144:LYS:N    | 0.62     | 2.10        | 15     | 5     |
| 1:A:19:G:C2'     | 1:A:20:G:O5'     | 0.62     | 2.47        | 7      | 4     |
| 2:B:51:GLY:HA3   | 2:B:56:PHE:CD2   | 0.62     | 2.29        | 14     | 3     |
| 2:B:107:LEU:HD11 | 2:B:116:LEU:HD21 | 0.62     | 1.70        | 13     | 1     |
| 2:B:101:THR:OG1  | 2:B:142:GLU:CG   | 0.62     | 2.47        | 3      | 1     |
| 1:A:21:C:O2      | 1:A:22:C:C6      | 0.62     | 2.51        | 10     | 8     |
| 1:A:15:A:O2'     | 1:A:16:G:OP2     | 0.62     | 2.17        | 14     | 7     |
| 2:B:102:LEU:HD12 | 2:B:168:LEU:HD22 | 0.62     | 1.70        | 9      | 2     |
| 2:B:161:ILE:HD12 | 2:B:166:VAL:CG2  | 0.62     | 2.24        | 17     | 1     |
| 1:A:2:G:N2       | 1:A:22:C:N1      | 0.62     | 2.47        | 18     | 4     |
| 1:A:14:A:N3      | 2:B:95:LYS:HB3   | 0.62     | 2.09        | 8      | 4     |
| 1:A:9:U:H4'      | 1:A:10:C:OP2     | 0.62     | 1.92        | 19     | 4     |
| 1:A:4:C:O2'      | 1:A:5:G:O4'      | 0.62     | 2.17        | 1      | 18    |
| 2:B:51:GLY:HA3   | 2:B:56:PHE:CD1   | 0.62     | 2.30        | 3      | 13    |
| 1:A:15:A:H1'     | 1:A:17:U:OP1     | 0.62     | 1.95        | 8      | 1     |
| 1:A:12:C:OP2     | 1:A:12:C:C5      | 0.62     | 2.52        | 3      | 3     |
| 1:A:12:C:N3      | 2:B:17:PHE:CZ    | 0.62     | 2.68        | 19     | 9     |
| 1:A:12:C:C5      | 1:A:12:C:OP1     | 0.62     | 2.52        | 2      | 1     |
| 1:A:9:U:O2'      | 1:A:10:C:O5'     | 0.62     | 2.17        | 6      | 3     |
| 2:B:128:LEU:HD23 | 2:B:129:VAL:N    | 0.62     | 2.10        | 12     | 2     |
| 2:B:70:ALA:HA    | 2:B:73:LEU:HD12  | 0.62     | 1.71        | 13     | 1     |
| 2:B:30:LEU:C     | 2:B:30:LEU:HD12  | 0.62     | 2.13        | 14     | 1     |
| 1:A:8:A:C6       | 1:A:14:A:N3      | 0.62     | 2.68        | 14     | 12    |
| 1:A:20:G:C2      | 1:A:21:C:C5      | 0.62     | 2.88        | 9      | 3     |
| 2:B:14:PHE:CE2   | 2:B:63:SER:O     | 0.62     | 2.53        | 18     | 1     |
| 1:A:20:G:C6      | 1:A:21:C:N4      | 0.62     | 2.68        | 5      | 4     |
| 2:B:16:LEU:CD1   | 2:B:85:LEU:HD21  | 0.62     | 2.25        | 5      | 1     |
| 2:B:128:LEU:HD13 | 2:B:129:VAL:N    | 0.62     | 2.09        | 2      | 3     |
| 2:B:98:ALA:HB1   | 2:B:171:THR:CB   | 0.62     | 2.25        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:11:C:N3      | 2:B:94:LYS:HD2   | 0.62     | 2.10        | 2      | 2     |
| 1:A:17:U:C6      | 1:A:17:U:OP2     | 0.62     | 2.53        | 16     | 1     |
| 1:A:20:G:HO2'    | 1:A:21:C:C5'     | 0.62     | 2.08        | 6      | 1     |
| 2:B:124:LEU:N    | 2:B:124:LEU:HD23 | 0.62     | 2.08        | 14     | 1     |
| 1:A:15:A:C4      | 1:A:17:U:C6      | 0.62     | 2.88        | 18     | 6     |
| 2:B:16:LEU:O     | 2:B:58:TYR:CD2   | 0.62     | 2.53        | 12     | 5     |
| 1:A:11:C:O2'     | 1:A:12:C:O5'     | 0.62     | 2.17        | 17     | 3     |
| 1:A:14:A:C5      | 2:B:94:LYS:CG    | 0.62     | 2.83        | 15     | 3     |
| 1:A:10:C:C4      | 1:A:11:C:N4      | 0.62     | 2.68        | 13     | 4     |
| 2:B:12:THR:OG1   | 2:B:15:ASN:ND2   | 0.62     | 2.33        | 19     | 1     |
| 2:B:30:LEU:CD1   | 2:B:31:LYS:N     | 0.62     | 2.59        | 14     | 1     |
| 2:B:103:LEU:CD2  | 2:B:129:VAL:HG21 | 0.61     | 2.24        | 9      | 3     |
| 2:B:103:LEU:HB3  | 2:B:140:TYR:CD1  | 0.61     | 2.30        | 18     | 2     |
| 2:B:74:THR:CA    | 2:B:85:LEU:HD21  | 0.61     | 2.25        | 18     | 1     |
| 1:A:14:A:C8      | 1:A:14:A:OP1     | 0.61     | 2.52        | 9      | 3     |
| 2:B:51:GLY:HA3   | 2:B:56:PHE:O     | 0.61     | 1.96        | 19     | 2     |
| 1:A:7:A:C4'      | 1:A:7:A:OP1      | 0.61     | 2.48        | 14     | 1     |
| 2:B:34:ILE:O     | 2:B:38:PHE:CD1   | 0.61     | 2.53        | 15     | 6     |
| 1:A:13:G:O2'     | 1:A:14:A:OP1     | 0.61     | 2.18        | 9      | 3     |
| 2:B:17:PHE:CD1   | 2:B:17:PHE:C     | 0.61     | 2.73        | 17     | 4     |
| 2:B:30:LEU:HD12  | 2:B:54:ARG:HD3   | 0.61     | 1.72        | 7      | 1     |
| 1:A:8:A:N6       | 1:A:14:A:N9      | 0.61     | 2.48        | 17     | 10    |
| 2:B:98:ALA:O     | 2:B:171:THR:OG1  | 0.61     | 2.18        | 3      | 3     |
| 2:B:34:ILE:HD11  | 2:B:78:VAL:CG2   | 0.61     | 2.23        | 13     | 2     |
| 1:A:15:A:O2'     | 1:A:16:G:P       | 0.61     | 2.58        | 5      | 5     |
| 1:A:15:A:C5      | 1:A:17:U:N3      | 0.61     | 2.69        | 18     | 10    |
| 1:A:2:G:N2       | 1:A:22:C:C2      | 0.61     | 2.69        | 15     | 5     |
| 2:B:92:ASP:O     | 2:B:94:LYS:N     | 0.61     | 2.33        | 14     | 7     |
| 1:A:1:G:C6       | 1:A:2:G:C5       | 0.61     | 2.88        | 12     | 3     |
| 2:B:12:THR:HG21  | 2:B:46:VAL:CB    | 0.61     | 2.26        | 19     | 1     |
| 1:A:3:C:HO2'     | 1:A:4:C:P        | 0.61     | 2.19        | 4      | 3     |
| 1:A:12:C:OP2     | 1:A:12:C:C6      | 0.61     | 2.53        | 18     | 1     |
| 2:B:107:LEU:HD23 | 2:B:111:ILE:CG2  | 0.61     | 2.26        | 5      | 1     |
| 1:A:20:G:O2'     | 1:A:21:C:O5'     | 0.61     | 2.19        | 9      | 8     |
| 2:B:92:ASP:CB    | 2:B:96:VAL:HG11  | 0.61     | 2.24        | 16     | 1     |
| 2:B:63:SER:OG    | 2:B:66:ASP:CB    | 0.61     | 2.49        | 5      | 3     |
| 1:A:13:G:C2      | 2:B:92:ASP:O     | 0.61     | 2.54        | 17     | 1     |
| 2:B:156:LYS:O    | 2:B:157:GLN:C    | 0.61     | 2.39        | 5      | 18    |
| 2:B:16:LEU:HD21  | 2:B:61:PHE:HE2   | 0.61     | 1.56        | 5      | 2     |
| 1:A:18:A:O2'     | 1:A:19:G:O5'     | 0.61     | 2.18        | 17     | 3     |
| 1:A:14:A:C2      | 2:B:95:LYS:HB3   | 0.61     | 2.31        | 12     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:102:LEU:H    | 2:B:102:LEU:HD22 | 0.61     | 1.55        | 12     | 7     |
| 1:A:12:C:C2      | 2:B:17:PHE:CE2   | 0.61     | 2.88        | 12     | 1     |
| 2:B:14:PHE:CZ    | 2:B:64:ALA:HB2   | 0.61     | 2.31        | 19     | 2     |
| 2:B:107:LEU:HD12 | 2:B:111:ILE:CG2  | 0.61     | 2.26        | 11     | 2     |
| 1:A:12:C:O5'     | 1:A:12:C:N1      | 0.61     | 2.34        | 11     | 3     |
| 1:A:16:G:O2'     | 1:A:17:U:OP1     | 0.61     | 2.19        | 16     | 1     |
| 2:B:136:LYS:HD3  | 2:B:138:ILE:HD11 | 0.61     | 1.71        | 7      | 1     |
| 1:A:6:A:O2'      | 1:A:7:A:OP1      | 0.61     | 2.17        | 14     | 1     |
| 2:B:102:LEU:HD23 | 2:B:168:LEU:CD2  | 0.60     | 2.25        | 10     | 1     |
| 1:A:20:G:O2'     | 1:A:21:C:O4'     | 0.60     | 2.19        | 7      | 3     |
| 1:A:20:G:H4'     | 1:A:21:C:OP1     | 0.60     | 1.96        | 9      | 1     |
| 2:B:18:ILE:HD12  | 2:B:59:VAL:HB    | 0.60     | 1.72        | 9      | 1     |
| 2:B:158:GLY:O    | 2:B:159:ALA:C    | 0.60     | 2.39        | 18     | 12    |
| 1:A:19:G:O2'     | 1:A:20:G:OP1     | 0.60     | 2.19        | 7      | 7     |
| 1:A:1:G:C6       | 1:A:2:G:N7       | 0.60     | 2.69        | 12     | 2     |
| 1:A:2:G:C6       | 1:A:3:C:C5       | 0.60     | 2.89        | 3      | 6     |
| 1:A:12:C:O2'     | 2:B:56:PHE:CD2   | 0.60     | 2.50        | 7      | 2     |
| 1:A:1:G:N1       | 1:A:2:G:C5       | 0.60     | 2.70        | 12     | 2     |
| 1:A:12:C:O2'     | 1:A:13:G:P       | 0.60     | 2.60        | 15     | 2     |
| 2:B:159:ALA:HB3  | 2:B:161:ILE:HD11 | 0.60     | 1.71        | 9      | 1     |
| 2:B:71:LEU:O     | 2:B:71:LEU:HD13  | 0.60     | 1.96        | 6      | 1     |
| 2:B:22:ASN:CB    | 2:B:30:LEU:CD2   | 0.60     | 2.79        | 17     | 3     |
| 2:B:44:ALA:HB3   | 2:B:66:ASP:CG    | 0.60     | 2.16        | 14     | 2     |
| 1:A:14:A:C2      | 2:B:94:LYS:HG3   | 0.60     | 2.30        | 10     | 7     |
| 1:A:8:A:N6       | 1:A:14:A:O2'     | 0.60     | 2.34        | 14     | 7     |
| 2:B:128:LEU:CD2  | 2:B:136:LYS:CB   | 0.60     | 2.79        | 15     | 1     |
| 2:B:129:VAL:O    | 2:B:136:LYS:HA   | 0.60     | 1.95        | 15     | 1     |
| 1:A:14:A:O4'     | 1:A:14:A:P       | 0.60     | 2.60        | 14     | 2     |
| 1:A:9:U:O4       | 2:B:105:LYS:NZ   | 0.60     | 2.34        | 4      | 2     |
| 1:A:9:U:OP2      | 1:A:11:C:N4      | 0.60     | 2.34        | 14     | 2     |
| 2:B:92:ASP:HA    | 2:B:96:VAL:HG11  | 0.60     | 1.71        | 16     | 2     |
| 1:A:21:C:O2'     | 1:A:22:C:O5'     | 0.60     | 2.19        | 5      | 9     |
| 2:B:21:LEU:O     | 2:B:22:ASN:HB2   | 0.60     | 1.97        | 12     | 18    |
| 1:A:4:C:HO2'     | 1:A:5:G:C1'      | 0.60     | 2.08        | 9      | 15    |
| 1:A:10:C:O2'     | 2:B:128:LEU:O    | 0.60     | 2.19        | 12     | 13    |
| 2:B:78:VAL:HG21  | 2:B:83:ILE:HG21  | 0.60     | 1.73        | 16     | 7     |
| 1:A:14:A:OP2     | 2:B:94:LYS:CB    | 0.60     | 2.49        | 4      | 1     |
| 1:A:15:A:C1'     | 1:A:16:G:OP1     | 0.60     | 2.50        | 18     | 1     |
| 2:B:157:GLN:O    | 2:B:159:ALA:N    | 0.60     | 2.34        | 16     | 1     |
| 2:B:153:LEU:HD23 | 2:B:154:GLU:HG3  | 0.60     | 1.71        | 7      | 1     |
| 2:B:14:PHE:CE2   | 2:B:63:SER:CA    | 0.60     | 2.85        | 7      | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:171:THR:CG2  | 2:B:171:THR:O    | 0.60     | 2.49        | 9      | 1     |
| 2:B:102:LEU:C    | 2:B:102:LEU:HD12 | 0.60     | 2.17        | 11     | 1     |
| 2:B:61:PHE:CD1   | 2:B:66:ASP:OD1   | 0.60     | 2.55        | 5      | 1     |
| 2:B:18:ILE:HA    | 2:B:84:LYS:O     | 0.60     | 1.97        | 13     | 15    |
| 2:B:48:VAL:HG23  | 2:B:59:VAL:HG23  | 0.60     | 1.73        | 9      | 1     |
| 2:B:71:LEU:HD13  | 2:B:71:LEU:C     | 0.60     | 2.16        | 6      | 1     |
| 2:B:107:LEU:HD12 | 2:B:138:ILE:HA   | 0.60     | 1.73        | 1      | 2     |
| 1:A:15:A:C2      | 1:A:17:U:C4      | 0.60     | 2.90        | 8      | 5     |
| 2:B:156:LYS:O    | 2:B:158:GLY:N    | 0.60     | 2.34        | 9      | 4     |
| 1:A:10:C:C2'     | 1:A:10:C:O2      | 0.60     | 2.45        | 16     | 11    |
| 2:B:78:VAL:CG2   | 2:B:83:ILE:CG2   | 0.60     | 2.79        | 15     | 9     |
| 1:A:3:C:H4'      | 1:A:4:C:OP1      | 0.60     | 1.96        | 12     | 5     |
| 1:A:12:C:C6      | 2:B:17:PHE:CE2   | 0.60     | 2.89        | 15     | 1     |
| 2:B:123:ALA:CB   | 2:B:141:ILE:HG22 | 0.60     | 2.27        | 2      | 3     |
| 2:B:73:LEU:HD12  | 2:B:76:LEU:CD2   | 0.60     | 2.27        | 19     | 1     |
| 2:B:17:PHE:CE2   | 2:B:86:GLU:CG    | 0.60     | 2.84        | 4      | 3     |
| 1:A:16:G:HO2'    | 1:A:17:U:P       | 0.60     | 2.18        | 16     | 2     |
| 1:A:10:C:C4      | 1:A:11:C:C5      | 0.60     | 2.89        | 10     | 9     |
| 2:B:21:LEU:O     | 2:B:78:VAL:HG11  | 0.60     | 1.96        | 4      | 7     |
| 2:B:130:SER:O    | 2:B:136:LYS:NZ   | 0.60     | 2.35        | 1      | 2     |
| 2:B:128:LEU:C    | 2:B:128:LEU:HD13 | 0.60     | 2.16        | 4      | 1     |
| 2:B:27:VAL:HG23  | 2:B:54:ARG:HE    | 0.60     | 1.56        | 18     | 2     |
| 2:B:59:VAL:CG1   | 2:B:61:PHE:CE1   | 0.60     | 2.85        | 18     | 2     |
| 2:B:128:LEU:CD1  | 2:B:128:LEU:N    | 0.60     | 2.65        | 16     | 1     |
| 1:A:14:A:O3'     | 1:A:15:A:C8      | 0.60     | 2.53        | 14     | 2     |
| 2:B:126:ILE:HG13 | 2:B:141:ILE:HG23 | 0.60     | 1.73        | 3      | 1     |
| 2:B:140:TYR:HE2  | 2:B:171:THR:HG21 | 0.60     | 1.56        | 1      | 2     |
| 1:A:11:C:N3      | 2:B:94:LYS:CE    | 0.60     | 2.65        | 5      | 6     |
| 2:B:35:SER:HA    | 2:B:45:VAL:HG21  | 0.60     | 1.74        | 10     | 3     |
| 2:B:38:PHE:CB    | 2:B:45:VAL:CG2   | 0.60     | 2.79        | 14     | 3     |
| 2:B:158:GLY:O    | 2:B:159:ALA:HB3  | 0.60     | 1.96        | 16     | 2     |
| 1:A:18:A:C2'     | 1:A:19:G:O4'     | 0.59     | 2.50        | 17     | 6     |
| 1:A:1:G:O2'      | 1:A:2:G:O5'      | 0.59     | 2.19        | 4      | 5     |
| 1:A:12:C:O2'     | 1:A:13:G:OP1     | 0.59     | 2.18        | 8      | 2     |
| 1:A:14:A:N6      | 2:B:94:LYS:HE3   | 0.59     | 2.12        | 2      | 2     |
| 2:B:124:LEU:HD11 | 2:B:144:LYS:HG2  | 0.59     | 1.73        | 16     | 1     |
| 1:A:20:G:OP1     | 1:A:20:G:H4'     | 0.59     | 1.97        | 3      | 1     |
| 2:B:43:LEU:HD21  | 2:B:69:LYS:CB    | 0.59     | 2.27        | 17     | 3     |
| 2:B:85:LEU:O     | 2:B:86:GLU:CB    | 0.59     | 2.50        | 16     | 19    |
| 2:B:78:VAL:HG23  | 2:B:83:ILE:HG21  | 0.59     | 1.74        | 6      | 4     |
| 2:B:30:LEU:CD1   | 2:B:54:ARG:CG    | 0.59     | 2.80        | 16     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:116:LEU:HD13 | 2:B:139:ALA:HB1  | 0.59     | 1.74        | 13     | 4     |
| 2:B:107:LEU:CD2  | 2:B:166:VAL:HG13 | 0.59     | 2.26        | 7      | 1     |
| 1:A:19:G:C6      | 1:A:20:G:C5      | 0.59     | 2.89        | 19     | 9     |
| 1:A:19:G:N1      | 1:A:20:G:C5      | 0.59     | 2.70        | 19     | 12    |
| 2:B:107:LEU:HD21 | 2:B:139:ALA:CB   | 0.59     | 2.20        | 10     | 1     |
| 1:A:7:A:O2'      | 1:A:8:A:H5'      | 0.59     | 1.97        | 7      | 6     |
| 1:A:14:A:C5      | 2:B:94:LYS:HE2   | 0.59     | 2.33        | 9      | 1     |
| 2:B:158:GLY:O    | 2:B:166:VAL:HG12 | 0.59     | 1.97        | 13     | 2     |
| 2:B:116:LEU:CD1  | 2:B:139:ALA:CB   | 0.59     | 2.80        | 10     | 1     |
| 2:B:73:LEU:HD12  | 2:B:76:LEU:CG    | 0.59     | 2.27        | 10     | 3     |
| 1:A:13:G:H21     | 2:B:91:ARG:CB    | 0.59     | 2.11        | 9      | 1     |
| 1:A:9:U:H5       | 2:B:103:LEU:HD21 | 0.59     | 1.58        | 16     | 5     |
| 1:A:3:C:O2'      | 1:A:4:C:O5'      | 0.59     | 2.20        | 16     | 12    |
| 2:B:103:LEU:CD1  | 2:B:138:ILE:HG22 | 0.59     | 2.27        | 3      | 2     |
| 2:B:107:LEU:HD13 | 2:B:138:ILE:C    | 0.59     | 2.18        | 6      | 3     |
| 1:A:11:C:C2      | 2:B:94:LYS:HE2   | 0.59     | 2.32        | 6      | 1     |
| 1:A:14:A:C5      | 2:B:94:LYS:HD3   | 0.59     | 2.32        | 16     | 4     |
| 2:B:103:LEU:HG   | 2:B:140:TYR:CD1  | 0.59     | 2.33        | 4      | 4     |
| 2:B:73:LEU:CD1   | 2:B:76:LEU:HD21  | 0.59     | 2.28        | 19     | 1     |
| 2:B:102:LEU:HD12 | 2:B:141:ILE:O    | 0.59     | 1.96        | 2      | 1     |
| 1:A:18:A:O2'     | 1:A:19:G:OP1     | 0.59     | 2.20        | 5      | 2     |
| 2:B:48:VAL:CG2   | 2:B:59:VAL:HG13  | 0.59     | 2.16        | 5      | 1     |
| 1:A:15:A:H5"     | 1:A:16:G:OP1     | 0.59     | 1.97        | 10     | 3     |
| 2:B:14:PHE:CE2   | 2:B:63:SER:C     | 0.59     | 2.76        | 4      | 9     |
| 1:A:9:U:O2'      | 1:A:10:C:OP1     | 0.59     | 2.21        | 14     | 5     |
| 2:B:46:VAL:HG21  | 2:B:61:PHE:O     | 0.59     | 1.97        | 13     | 6     |
| 1:A:8:A:C5'      | 1:A:9:U:O5'      | 0.59     | 2.51        | 11     | 4     |
| 1:A:10:C:C4'     | 2:B:128:LEU:O    | 0.59     | 2.50        | 15     | 1     |
| 2:B:29:GLU:CD    | 2:B:79:PHE:CZ    | 0.59     | 2.76        | 11     | 6     |
| 2:B:37:LEU:CD2   | 2:B:73:LEU:HD22  | 0.59     | 2.28        | 16     | 1     |
| 2:B:21:LEU:HD22  | 2:B:30:LEU:HB3   | 0.59     | 1.73        | 17     | 2     |
| 2:B:108:SER:OG   | 2:B:164:ARG:NH1  | 0.59     | 2.36        | 10     | 1     |
| 2:B:29:GLU:OE1   | 2:B:79:PHE:CE1   | 0.59     | 2.55        | 17     | 2     |
| 1:A:15:A:C4'     | 1:A:16:G:OP1     | 0.59     | 2.51        | 6      | 8     |
| 1:A:5:G:O2'      | 1:A:6:A:O5'      | 0.59     | 2.20        | 18     | 3     |
| 1:A:10:C:C2'     | 1:A:11:C:OP1     | 0.59     | 2.51        | 2      | 1     |
| 1:A:9:U:C2       | 2:B:138:ILE:CD1  | 0.59     | 2.85        | 6      | 3     |
| 2:B:14:PHE:CZ    | 2:B:63:SER:C     | 0.59     | 2.75        | 13     | 2     |
| 2:B:107:LEU:HD13 | 2:B:139:ALA:HB2  | 0.59     | 1.75        | 11     | 2     |
| 2:B:45:VAL:O     | 2:B:45:VAL:HG23  | 0.59     | 1.97        | 3      | 8     |
| 2:B:103:LEU:CD1  | 2:B:140:TYR:CE2  | 0.59     | 2.86        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:12:THR:CB    | 2:B:13:PRO:CD    | 0.59     | 2.81        | 13     | 4     |
| 1:A:11:C:N3      | 2:B:94:LYS:HE3   | 0.59     | 2.13        | 6      | 5     |
| 2:B:65:GLU:OE2   | 2:B:69:LYS:NZ    | 0.59     | 2.35        | 16     | 1     |
| 2:B:129:VAL:N    | 2:B:138:ILE:O    | 0.58     | 2.36        | 16     | 13    |
| 1:A:4:C:O2'      | 1:A:5:G:H8       | 0.58     | 1.79        | 8      | 10    |
| 1:A:10:C:C5      | 1:A:11:C:N4      | 0.58     | 2.71        | 15     | 1     |
| 2:B:103:LEU:HG   | 2:B:140:TYR:CE1  | 0.58     | 2.33        | 11     | 4     |
| 1:A:9:U:N3       | 2:B:138:ILE:HD13 | 0.58     | 2.13        | 11     | 3     |
| 2:B:127:ARG:NH2  | 2:B:140:TYR:CD1  | 0.58     | 2.70        | 18     | 1     |
| 2:B:63:SER:OG    | 2:B:66:ASP:OD2   | 0.58     | 2.21        | 11     | 12    |
| 1:A:14:A:OP1     | 2:B:52:THR:OG1   | 0.58     | 2.22        | 16     | 3     |
| 1:A:10:C:O2      | 1:A:11:C:O4'     | 0.58     | 2.21        | 18     | 1     |
| 2:B:116:LEU:CD2  | 2:B:141:ILE:HD11 | 0.58     | 2.28        | 18     | 2     |
| 2:B:50:THR:C     | 2:B:57:GLY:HA2   | 0.58     | 2.18        | 9      | 16    |
| 1:A:15:A:OP1     | 1:A:17:U:C1'     | 0.58     | 2.50        | 10     | 7     |
| 1:A:19:G:C2      | 1:A:20:G:C8      | 0.58     | 2.92        | 11     | 5     |
| 1:A:14:A:C6      | 2:B:94:LYS:HG2   | 0.58     | 2.33        | 8      | 5     |
| 1:A:14:A:N9      | 1:A:14:A:OP2     | 0.58     | 2.36        | 4      | 1     |
| 1:A:5:G:H4'      | 1:A:6:A:OP1      | 0.58     | 1.97        | 4      | 1     |
| 2:B:127:ARG:NH2  | 2:B:140:TYR:CB   | 0.58     | 2.66        | 18     | 1     |
| 2:B:102:LEU:C    | 2:B:171:THR:HG23 | 0.58     | 2.18        | 13     | 2     |
| 2:B:158:GLY:N    | 2:B:166:VAL:O    | 0.58     | 2.36        | 9      | 13    |
| 1:A:15:A:C2      | 1:A:16:G:N3      | 0.58     | 2.71        | 15     | 3     |
| 1:A:13:G:N2      | 2:B:90:GLY:CA    | 0.58     | 2.66        | 3      | 2     |
| 2:B:34:ILE:CD1   | 2:B:34:ILE:N     | 0.58     | 2.66        | 9      | 1     |
| 1:A:14:A:OP2     | 2:B:94:LYS:N     | 0.58     | 2.36        | 19     | 1     |
| 1:A:9:U:C5       | 2:B:103:LEU:HD11 | 0.58     | 2.33        | 5      | 3     |
| 2:B:58:TYR:C     | 2:B:59:VAL:CG2   | 0.58     | 2.72        | 19     | 4     |
| 2:B:141:ILE:HG22 | 2:B:143:PHE:CE1  | 0.58     | 2.34        | 10     | 4     |
| 2:B:61:PHE:CB    | 2:B:66:ASP:CG    | 0.58     | 2.72        | 18     | 3     |
| 1:A:2:G:C5       | 1:A:3:C:C6       | 0.58     | 2.92        | 9      | 2     |
| 2:B:145:SER:N    | 2:B:148:ASP:OD1  | 0.58     | 2.36        | 19     | 1     |
| 1:A:12:C:H1'     | 2:B:56:PHE:CE2   | 0.58     | 2.34        | 19     | 2     |
| 1:A:14:A:C6      | 2:B:94:LYS:HE2   | 0.58     | 2.34        | 2      | 4     |
| 2:B:102:LEU:CD1  | 2:B:170:TYR:CD1  | 0.58     | 2.85        | 13     | 4     |
| 2:B:169:TYR:O    | 2:B:170:TYR:O    | 0.58     | 2.21        | 8      | 17    |
| 1:A:10:C:O2      | 1:A:10:C:C2'     | 0.58     | 2.47        | 9      | 8     |
| 2:B:54:ARG:CD    | 2:B:54:ARG:N     | 0.58     | 2.66        | 15     | 4     |
| 2:B:104:ALA:O    | 2:B:107:LEU:HD13 | 0.58     | 1.99        | 10     | 2     |
| 2:B:46:VAL:HG22  | 2:B:62:GLU:CG    | 0.58     | 2.28        | 17     | 4     |
| 2:B:12:THR:HG21  | 2:B:46:VAL:CG1   | 0.58     | 2.15        | 3      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:146:GLU:CG   | 2:B:170:TYR:OH   | 0.58     | 2.52        | 7      | 4     |
| 1:A:5:G:HO2'     | 1:A:6:A:C5'      | 0.58     | 2.10        | 15     | 1     |
| 2:B:130:SER:CB   | 2:B:136:LYS:HD2  | 0.58     | 2.29        | 15     | 1     |
| 2:B:26:SER:O     | 2:B:30:LEU:CD1   | 0.58     | 2.51        | 4      | 2     |
| 1:A:15:A:OP1     | 1:A:15:A:O4'     | 0.58     | 2.21        | 7      | 5     |
| 1:A:8:A:C5'      | 1:A:9:U:OP2      | 0.58     | 2.52        | 17     | 4     |
| 2:B:11:THR:HG22  | 2:B:11:THR:O     | 0.58     | 1.98        | 3      | 4     |
| 2:B:73:LEU:O     | 2:B:75:GLY:N     | 0.58     | 2.37        | 9      | 4     |
| 1:A:13:G:N2      | 2:B:91:ARG:CB    | 0.58     | 2.66        | 9      | 1     |
| 1:A:8:A:N6       | 1:A:14:A:C8      | 0.58     | 2.71        | 17     | 6     |
| 2:B:21:LEU:CB    | 2:B:30:LEU:HD22  | 0.58     | 2.29        | 16     | 1     |
| 2:B:140:TYR:CZ   | 2:B:171:THR:CG2  | 0.58     | 2.87        | 13     | 2     |
| 2:B:105:LYS:N    | 2:B:167:SER:O    | 0.58     | 2.35        | 9      | 11    |
| 2:B:156:LYS:O    | 2:B:157:GLN:O    | 0.58     | 2.20        | 8      | 12    |
| 2:B:103:LEU:HD13 | 2:B:140:TYR:CE2  | 0.58     | 2.34        | 15     | 1     |
| 1:A:14:A:OP1     | 2:B:94:LYS:N     | 0.58     | 2.37        | 1      | 2     |
| 2:B:14:PHE:CD1   | 2:B:67:LEU:HD13  | 0.58     | 2.33        | 9      | 1     |
| 2:B:107:LEU:HD13 | 2:B:166:VAL:CG2  | 0.58     | 2.29        | 7      | 1     |
| 2:B:116:LEU:HD22 | 2:B:141:ILE:HD11 | 0.58     | 1.75        | 1      | 1     |
| 2:B:63:SER:OG    | 2:B:66:ASP:HB3   | 0.58     | 1.98        | 5      | 6     |
| 2:B:21:LEU:CD2   | 2:B:56:PHE:O     | 0.58     | 2.52        | 7      | 13    |
| 2:B:130:SER:HA   | 2:B:136:LYS:CB   | 0.58     | 2.29        | 10     | 17    |
| 2:B:107:LEU:HD12 | 2:B:138:ILE:CA   | 0.58     | 2.29        | 1      | 2     |
| 1:A:5:G:O2'      | 1:A:6:A:C5'      | 0.58     | 2.52        | 4      | 1     |
| 1:A:21:C:O2'     | 1:A:22:C:OP1     | 0.58     | 2.22        | 14     | 2     |
| 1:A:10:C:N3      | 1:A:11:C:C6      | 0.58     | 2.72        | 11     | 8     |
| 2:B:158:GLY:O    | 2:B:166:VAL:N    | 0.58     | 2.37        | 2      | 12    |
| 2:B:66:ASP:O     | 2:B:70:ALA:HB2   | 0.58     | 1.98        | 1      | 8     |
| 1:A:11:C:H2'     | 1:A:12:C:O5'     | 0.58     | 1.99        | 19     | 8     |
| 2:B:116:LEU:CD2  | 2:B:139:ALA:CB   | 0.58     | 2.82        | 8      | 3     |
| 2:B:21:LEU:CD2   | 2:B:78:VAL:HG21  | 0.58     | 2.28        | 9      | 1     |
| 2:B:54:ARG:N     | 2:B:54:ARG:CD    | 0.58     | 2.65        | 1      | 4     |
| 1:A:6:A:C6       | 1:A:7:A:C5       | 0.58     | 2.92        | 2      | 3     |
| 2:B:78:VAL:HG12  | 2:B:81:ASN:O     | 0.58     | 1.98        | 14     | 3     |
| 1:A:2:G:O2'      | 1:A:3:C:O5'      | 0.57     | 2.21        | 12     | 9     |
| 1:A:15:A:C4'     | 1:A:17:U:OP1     | 0.57     | 2.52        | 8      | 1     |
| 1:A:10:C:H42     | 2:B:94:LYS:CE    | 0.57     | 2.12        | 8      | 2     |
| 2:B:103:LEU:CD1  | 2:B:138:ILE:CG2  | 0.57     | 2.80        | 12     | 3     |
| 1:A:3:C:HO2'     | 1:A:4:C:H5'      | 0.57     | 1.57        | 9      | 1     |
| 2:B:102:LEU:HD22 | 2:B:168:LEU:HD12 | 0.57     | 1.76        | 11     | 2     |
| 2:B:67:LEU:O     | 2:B:67:LEU:HD13  | 0.57     | 1.98        | 17     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:29:GLU:O     | 2:B:79:PHE:CD2   | 0.57     | 2.57        | 17     | 1     |
| 2:B:103:LEU:HB2  | 2:B:140:TYR:CD1  | 0.57     | 2.33        | 5      | 3     |
| 2:B:129:VAL:HB   | 2:B:138:ILE:CB   | 0.57     | 2.29        | 15     | 19    |
| 2:B:74:THR:HG22  | 2:B:74:THR:O     | 0.57     | 1.99        | 7      | 3     |
| 2:B:37:LEU:HD22  | 2:B:76:LEU:HD11  | 0.57     | 1.75        | 9      | 1     |
| 2:B:73:LEU:O     | 2:B:76:LEU:CD2   | 0.57     | 2.50        | 9      | 1     |
| 1:A:13:G:C2'     | 1:A:14:A:O5'     | 0.57     | 2.52        | 2      | 4     |
| 2:B:145:SER:O    | 2:B:148:ASP:OD1  | 0.57     | 2.22        | 19     | 1     |
| 1:A:15:A:O2'     | 1:A:16:G:O5'     | 0.57     | 2.21        | 5      | 3     |
| 1:A:14:A:C2      | 2:B:94:LYS:HG2   | 0.57     | 2.34        | 16     | 5     |
| 2:B:74:THR:O     | 2:B:74:THR:HG22  | 0.57     | 2.00        | 5      | 3     |
| 2:B:74:THR:OG1   | 2:B:85:LEU:HD13  | 0.57     | 1.99        | 10     | 1     |
| 1:A:4:C:C2'      | 1:A:5:G:O5'      | 0.57     | 2.52        | 11     | 10    |
| 1:A:3:C:HO2'     | 1:A:4:C:H6       | 0.57     | 1.40        | 12     | 1     |
| 1:A:12:C:P       | 1:A:12:C:C6      | 0.57     | 2.97        | 2      | 3     |
| 2:B:30:LEU:HD11  | 2:B:54:ARG:HG2   | 0.57     | 1.77        | 16     | 1     |
| 2:B:104:ALA:N    | 2:B:139:ALA:O    | 0.57     | 2.38        | 19     | 12    |
| 2:B:21:LEU:CB    | 2:B:54:ARG:O     | 0.57     | 2.53        | 3      | 11    |
| 2:B:63:SER:O     | 2:B:66:ASP:OD2   | 0.57     | 2.23        | 18     | 3     |
| 2:B:17:PHE:O     | 2:B:18:ILE:HD12  | 0.57     | 1.99        | 12     | 1     |
| 1:A:2:G:C4       | 1:A:3:C:C6       | 0.57     | 2.92        | 9      | 4     |
| 2:B:73:LEU:CD1   | 2:B:76:LEU:CD1   | 0.57     | 2.81        | 7      | 2     |
| 2:B:126:ILE:CD1  | 2:B:141:ILE:HG23 | 0.57     | 2.30        | 18     | 1     |
| 1:A:8:A:C2       | 2:B:95:LYS:HG3   | 0.57     | 2.34        | 13     | 1     |
| 2:B:74:THR:HA    | 2:B:85:LEU:HD12  | 0.57     | 1.76        | 11     | 1     |
| 2:B:103:LEU:N    | 2:B:169:TYR:O    | 0.57     | 2.36        | 3      | 8     |
| 1:A:8:A:H61      | 1:A:14:A:C2'     | 0.57     | 2.12        | 14     | 11    |
| 1:A:12:C:C5      | 1:A:12:C:P       | 0.57     | 2.97        | 7      | 3     |
| 2:B:153:LEU:O    | 2:B:153:LEU:HD23 | 0.57     | 1.99        | 2      | 1     |
| 1:A:16:G:C5      | 2:B:27:VAL:CG2   | 0.57     | 2.88        | 6      | 2     |
| 2:B:143:PHE:CD2  | 2:B:149:ALA:CB   | 0.57     | 2.87        | 18     | 1     |
| 1:A:11:C:C2      | 2:B:127:ARG:NH2  | 0.57     | 2.73        | 13     | 1     |
| 2:B:83:ILE:CD1   | 2:B:83:ILE:O     | 0.57     | 2.52        | 14     | 1     |
| 2:B:127:ARG:HB2  | 2:B:140:TYR:CB   | 0.57     | 2.29        | 8      | 14    |
| 1:A:2:G:C2       | 1:A:22:C:N3      | 0.57     | 2.72        | 10     | 4     |
| 2:B:22:ASN:O     | 2:B:54:ARG:CB    | 0.57     | 2.53        | 19     | 10    |
| 2:B:116:LEU:HD22 | 2:B:139:ALA:HB1  | 0.57     | 1.77        | 8      | 1     |
| 2:B:66:ASP:OD1   | 2:B:67:LEU:N     | 0.57     | 2.37        | 18     | 3     |
| 2:B:16:LEU:CD2   | 2:B:17:PHE:O     | 0.57     | 2.53        | 13     | 4     |
| 1:A:14:A:OP2     | 1:A:14:A:N9      | 0.57     | 2.38        | 16     | 1     |
| 2:B:37:LEU:CD1   | 2:B:76:LEU:HD12  | 0.57     | 2.25        | 9      | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 2:B:145:SER:OG   | 2:B:148:ASP:OD2 | 0.57     | 2.22        | 19     | 1     |
| 2:B:124:LEU:N    | 2:B:142:GLU:O   | 0.57     | 2.38        | 8      | 6     |
| 2:B:28:ALA:O     | 2:B:32:VAL:CG2  | 0.57     | 2.53        | 13     | 13    |
| 2:B:25:LYS:HE3   | 2:B:79:PHE:CE1  | 0.57     | 2.35        | 19     | 1     |
| 1:A:14:A:OP2     | 1:A:14:A:O4'    | 0.57     | 2.23        | 4      | 2     |
| 1:A:11:C:N3      | 2:B:94:LYS:CB   | 0.57     | 2.68        | 18     | 1     |
| 1:A:16:G:C1'     | 1:A:17:U:OP2    | 0.57     | 2.53        | 16     | 1     |
| 1:A:18:A:H4'     | 1:A:19:G:OP1    | 0.56     | 2.00        | 17     | 2     |
| 1:A:16:G:N7      | 2:B:27:VAL:HB   | 0.56     | 2.15        | 18     | 10    |
| 2:B:99:ALA:O     | 2:B:170:TYR:OH  | 0.56     | 2.20        | 3      | 10    |
| 2:B:14:PHE:CE2   | 2:B:63:SER:HA   | 0.56     | 2.35        | 7      | 4     |
| 1:A:9:U:C5       | 2:B:138:ILE:CD1 | 0.56     | 2.87        | 3      | 4     |
| 1:A:14:A:C5      | 2:B:94:LYS:CE   | 0.56     | 2.87        | 7      | 3     |
| 1:A:6:A:C6       | 1:A:18:A:C4     | 0.56     | 2.93        | 13     | 2     |
| 2:B:76:LEU:HD13  | 2:B:83:ILE:HD11 | 0.56     | 1.76        | 13     | 2     |
| 2:B:92:ASP:C     | 2:B:93:SER:OG   | 0.56     | 2.43        | 14     | 1     |
| 1:A:4:C:C4'      | 1:A:5:G:OP1     | 0.56     | 2.50        | 18     | 6     |
| 2:B:105:LYS:O    | 2:B:106:ASN:CB  | 0.56     | 2.54        | 15     | 14    |
| 2:B:127:ARG:O    | 2:B:140:TYR:N   | 0.56     | 2.39        | 15     | 5     |
| 2:B:12:THR:HG23  | 2:B:46:VAL:HG11 | 0.56     | 1.75        | 19     | 3     |
| 1:A:11:C:C2      | 2:B:94:LYS:HD3  | 0.56     | 2.35        | 12     | 1     |
| 2:B:70:ALA:O     | 2:B:85:LEU:CD1  | 0.56     | 2.53        | 18     | 1     |
| 2:B:18:ILE:HG12  | 2:B:85:LEU:HD12 | 0.56     | 1.77        | 6      | 1     |
| 1:A:19:G:C8      | 1:A:19:G:OP2    | 0.56     | 2.58        | 11     | 1     |
| 2:B:98:ALA:O     | 2:B:171:THR:CG2 | 0.56     | 2.53        | 11     | 1     |
| 2:B:31:LYS:HG2   | 2:B:48:VAL:HG12 | 0.56     | 1.75        | 17     | 1     |
| 2:B:37:LEU:O     | 2:B:41:ASN:ND2  | 0.56     | 2.39        | 10     | 8     |
| 2:B:161:ILE:O    | 2:B:164:ARG:N   | 0.56     | 2.38        | 16     | 18    |
| 1:A:10:C:C4      | 2:B:140:TYR:CE1 | 0.56     | 2.93        | 10     | 6     |
| 2:B:102:LEU:CD2  | 2:B:143:PHE:CE1 | 0.56     | 2.88        | 15     | 4     |
| 2:B:27:VAL:HG13  | 2:B:54:ARG:NE   | 0.56     | 2.15        | 9      | 2     |
| 1:A:13:G:N2      | 2:B:91:ARG:HB3  | 0.56     | 2.15        | 9      | 1     |
| 2:B:16:LEU:CD2   | 2:B:17:PHE:N    | 0.56     | 2.68        | 4      | 4     |
| 2:B:17:PHE:CE2   | 2:B:86:GLU:HG3  | 0.56     | 2.35        | 4      | 1     |
| 2:B:38:PHE:CD1   | 2:B:43:LEU:HD13 | 0.56     | 2.35        | 16     | 1     |
| 2:B:102:LEU:HD12 | 2:B:149:ALA:HB1 | 0.56     | 1.76        | 10     | 1     |
| 2:B:47:ASP:O     | 2:B:48:VAL:CG2  | 0.56     | 2.53        | 13     | 7     |
| 1:A:15:A:C1'     | 1:A:17:U:OP1    | 0.56     | 2.53        | 8      | 1     |
| 2:B:94:LYS:NZ    | 2:B:94:LYS:O    | 0.56     | 2.39        | 8      | 1     |
| 1:A:14:A:O4'     | 2:B:95:LYS:CE   | 0.56     | 2.53        | 12     | 1     |
| 2:B:127:ARG:NH1  | 2:B:127:ARG:O   | 0.56     | 2.38        | 18     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:16:LEU:CD1  | 2:B:17:PHE:N     | 0.56     | 2.68        | 6      | 9     |
| 2:B:151:LYS:O   | 2:B:155:GLU:CB   | 0.56     | 2.54        | 11     | 8     |
| 2:B:78:VAL:O    | 2:B:81:ASN:N     | 0.56     | 2.38        | 8      | 10    |
| 2:B:101:THR:OG1 | 2:B:142:GLU:HG3  | 0.56     | 2.01        | 3      | 2     |
| 2:B:21:LEU:O    | 2:B:78:VAL:CG1   | 0.56     | 2.54        | 9      | 8     |
| 2:B:85:LEU:C    | 2:B:85:LEU:CD2   | 0.56     | 2.73        | 12     | 1     |
| 1:A:5:G:OP2     | 1:A:5:G:H3'      | 0.56     | 2.01        | 9      | 1     |
| 2:B:24:ASN:O    | 2:B:25:LYS:CD    | 0.56     | 2.54        | 4      | 1     |
| 2:B:111:ILE:O   | 2:B:112:THR:CG2  | 0.56     | 2.53        | 18     | 13    |
| 1:A:15:A:N7     | 1:A:17:U:C2      | 0.56     | 2.74        | 17     | 7     |
| 2:B:92:ASP:CB   | 2:B:96:VAL:CG2   | 0.56     | 2.83        | 12     | 1     |
| 2:B:21:LEU:HD23 | 2:B:78:VAL:HG21  | 0.56     | 1.77        | 9      | 1     |
| 1:A:10:C:OP1    | 2:B:129:VAL:CG1  | 0.56     | 2.54        | 19     | 1     |
| 2:B:38:PHE:CE2  | 2:B:43:LEU:CD1   | 0.56     | 2.85        | 19     | 1     |
| 2:B:102:LEU:O   | 2:B:141:ILE:N    | 0.56     | 2.39        | 17     | 3     |
| 2:B:94:LYS:NZ   | 2:B:95:LYS:CE    | 0.56     | 2.69        | 11     | 1     |
| 1:A:13:G:N2     | 2:B:90:GLY:HA2   | 0.56     | 2.15        | 3      | 1     |
| 1:A:12:C:C6     | 2:B:17:PHE:CZ    | 0.56     | 2.94        | 1      | 4     |
| 2:B:158:GLY:O   | 2:B:159:ALA:O    | 0.56     | 2.24        | 9      | 13    |
| 2:B:21:LEU:CD1  | 2:B:56:PHE:O     | 0.56     | 2.53        | 10     | 8     |
| 2:B:104:ALA:O   | 2:B:107:LEU:CD1  | 0.56     | 2.53        | 9      | 5     |
| 2:B:44:ALA:HB1  | 2:B:62:GLU:HG3   | 0.56     | 1.76        | 8      | 1     |
| 1:A:1:G:O2'     | 1:A:2:G:OP1      | 0.56     | 2.23        | 2      | 1     |
| 1:A:13:G:O2'    | 1:A:15:A:C3'     | 0.56     | 2.45        | 18     | 1     |
| 1:A:14:A:C5     | 2:B:94:LYS:CD    | 0.56     | 2.89        | 16     | 2     |
| 2:B:38:PHE:CG   | 2:B:45:VAL:CG1   | 0.56     | 2.88        | 5      | 6     |
| 1:A:2:G:C2'     | 1:A:3:C:O5'      | 0.56     | 2.53        | 6      | 6     |
| 2:B:102:LEU:HA  | 2:B:171:THR:OG1  | 0.56     | 2.00        | 7      | 2     |
| 2:B:103:LEU:CD1 | 2:B:129:VAL:HG11 | 0.56     | 2.31        | 15     | 1     |
| 2:B:129:VAL:O   | 2:B:136:LYS:CA   | 0.56     | 2.53        | 15     | 1     |
| 1:A:13:G:C8     | 2:B:58:TYR:HB2   | 0.56     | 2.35        | 18     | 1     |
| 2:B:38:PHE:CE1  | 2:B:43:LEU:HD22  | 0.56     | 2.35        | 16     | 1     |
| 2:B:140:TYR:CE2 | 2:B:171:THR:CG2  | 0.56     | 2.88        | 13     | 2     |
| 2:B:97:ARG:O    | 2:B:101:THR:N    | 0.56     | 2.39        | 7      | 1     |
| 2:B:19:GLY:O    | 2:B:20:ASN:CB    | 0.56     | 2.54        | 17     | 15    |
| 2:B:16:LEU:CD1  | 2:B:17:PHE:O     | 0.56     | 2.54        | 18     | 9     |
| 2:B:66:ASP:O    | 2:B:70:ALA:CB    | 0.56     | 2.54        | 16     | 4     |
| 2:B:63:SER:OG   | 2:B:66:ASP:CG    | 0.56     | 2.45        | 19     | 13    |
| 2:B:129:VAL:O   | 2:B:138:ILE:HG13 | 0.56     | 2.01        | 15     | 1     |
| 2:B:14:PHE:CE2  | 2:B:64:ALA:N     | 0.56     | 2.74        | 9      | 1     |
| 1:A:6:A:C2      | 1:A:7:A:N9       | 0.56     | 2.73        | 17     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:16:G:C5      | 2:B:27:VAL:HG23  | 0.56     | 2.35        | 6      | 1     |
| 2:B:47:ASP:C     | 2:B:48:VAL:HG23  | 0.56     | 2.20        | 17     | 9     |
| 1:A:13:G:OP2     | 2:B:89:LYS:CB    | 0.56     | 2.54        | 7      | 4     |
| 2:B:59:VAL:HG11  | 2:B:61:PHE:CZ    | 0.56     | 2.36        | 6      | 6     |
| 2:B:130:SER:CA   | 2:B:136:LYS:HA   | 0.56     | 2.29        | 15     | 1     |
| 2:B:159:ALA:O    | 2:B:160:GLU:C    | 0.56     | 2.45        | 17     | 4     |
| 1:A:11:C:N4      | 1:A:14:A:N6      | 0.56     | 2.53        | 9      | 2     |
| 1:A:13:G:OP1     | 2:B:93:SER:CB    | 0.56     | 2.54        | 13     | 2     |
| 2:B:101:THR:CG2  | 2:B:141:ILE:O    | 0.56     | 2.53        | 16     | 2     |
| 2:B:102:LEU:N    | 2:B:141:ILE:O    | 0.56     | 2.39        | 14     | 2     |
| 2:B:107:LEU:HD11 | 2:B:128:LEU:HD11 | 0.56     | 1.76        | 11     | 1     |
| 1:A:14:A:N3      | 2:B:94:LYS:CG    | 0.56     | 2.67        | 11     | 1     |
| 2:B:107:LEU:N    | 2:B:107:LEU:CD2  | 0.56     | 2.69        | 7      | 1     |
| 1:A:11:C:C2'     | 1:A:12:C:C5'     | 0.55     | 2.84        | 5      | 4     |
| 2:B:146:GLU:O    | 2:B:150:GLU:CB   | 0.55     | 2.54        | 12     | 12    |
| 1:A:11:C:N4      | 1:A:14:A:H61     | 0.55     | 1.99        | 9      | 3     |
| 2:B:27:VAL:HG12  | 2:B:28:ALA:N     | 0.55     | 2.15        | 2      | 4     |
| 2:B:158:GLY:CA   | 2:B:166:VAL:O    | 0.55     | 2.53        | 8      | 3     |
| 2:B:19:GLY:N     | 2:B:84:LYS:O     | 0.55     | 2.39        | 17     | 5     |
| 1:A:9:U:O4'      | 1:A:10:C:OP1     | 0.55     | 2.24        | 15     | 4     |
| 2:B:48:VAL:HA    | 2:B:58:TYR:O     | 0.55     | 2.01        | 19     | 3     |
| 2:B:69:LYS:O     | 2:B:73:LEU:CD2   | 0.55     | 2.54        | 10     | 9     |
| 2:B:69:LYS:O     | 2:B:73:LEU:N     | 0.55     | 2.39        | 13     | 6     |
| 2:B:38:PHE:CD2   | 2:B:43:LEU:CD1   | 0.55     | 2.88        | 7      | 4     |
| 2:B:30:LEU:CD1   | 2:B:54:ARG:HG3   | 0.55     | 2.30        | 16     | 2     |
| 2:B:38:PHE:CZ    | 2:B:73:LEU:CD1   | 0.55     | 2.86        | 9      | 1     |
| 2:B:81:ASN:O     | 2:B:83:ILE:N     | 0.55     | 2.39        | 16     | 8     |
| 2:B:91:ARG:O     | 2:B:92:ASP:CB    | 0.55     | 2.53        | 13     | 3     |
| 1:A:13:G:C4'     | 1:A:14:A:OP1     | 0.55     | 2.53        | 6      | 2     |
| 1:A:13:G:OP1     | 2:B:89:LYS:CB    | 0.55     | 2.54        | 13     | 1     |
| 1:A:14:A:O4'     | 1:A:14:A:OP2     | 0.55     | 2.23        | 3      | 1     |
| 1:A:14:A:N6      | 2:B:94:LYS:HE2   | 0.55     | 2.17        | 2      | 3     |
| 1:A:2:G:O2'      | 1:A:3:C:OP1      | 0.55     | 2.24        | 10     | 2     |
| 2:B:102:LEU:O    | 2:B:102:LEU:CD2  | 0.55     | 2.53        | 10     | 1     |
| 1:A:1:G:C2'      | 1:A:2:G:O5'      | 0.55     | 2.54        | 16     | 6     |
| 1:A:18:A:C2'     | 1:A:19:G:O5'     | 0.55     | 2.55        | 1      | 3     |
| 2:B:61:PHE:CE1   | 2:B:70:ALA:CB    | 0.55     | 2.89        | 16     | 1     |
| 2:B:103:LEU:CD1  | 2:B:140:TYR:CD1  | 0.55     | 2.87        | 14     | 1     |
| 2:B:46:VAL:CG2   | 2:B:61:PHE:C     | 0.55     | 2.75        | 13     | 10    |
| 2:B:102:LEU:CD1  | 2:B:102:LEU:N    | 0.55     | 2.60        | 10     | 5     |
| 2:B:115:GLU:O    | 2:B:119:VAL:HG23 | 0.55     | 2.01        | 8      | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:21:LEU:O    | 2:B:22:ASN:CB    | 0.55     | 2.55        | 9      | 3     |
| 2:B:119:VAL:O   | 2:B:156:LYS:CE   | 0.55     | 2.55        | 9      | 1     |
| 1:A:11:C:C2     | 2:B:94:LYS:HE3   | 0.55     | 2.36        | 5      | 5     |
| 2:B:141:ILE:CG2 | 2:B:143:PHE:CE1  | 0.55     | 2.89        | 9      | 2     |
| 2:B:102:LEU:N   | 2:B:102:LEU:CD2  | 0.55     | 2.65        | 15     | 3     |
| 1:A:9:U:O4      | 2:B:105:LYS:CE   | 0.55     | 2.54        | 6      | 4     |
| 1:A:11:C:C4     | 2:B:94:LYS:HE3   | 0.55     | 2.36        | 13     | 2     |
| 1:A:13:G:N9     | 2:B:58:TYR:CD1   | 0.55     | 2.74        | 18     | 1     |
| 1:A:14:A:N3     | 2:B:95:LYS:HB2   | 0.55     | 2.16        | 13     | 1     |
| 1:A:11:C:O2     | 2:B:94:LYS:CE    | 0.55     | 2.55        | 14     | 1     |
| 1:A:12:C:OP2    | 2:B:89:LYS:CE    | 0.55     | 2.54        | 5      | 2     |
| 1:A:19:G:O2'    | 1:A:20:G:C4'     | 0.55     | 2.54        | 11     | 3     |
| 1:A:10:C:O2     | 2:B:127:ARG:NE   | 0.55     | 2.40        | 6      | 10    |
| 1:A:4:C:C1'     | 1:A:5:G:O4'      | 0.55     | 2.54        | 13     | 3     |
| 2:B:155:GLU:O   | 2:B:156:LYS:CB   | 0.55     | 2.55        | 16     | 2     |
| 2:B:26:SER:OG   | 2:B:29:GLU:CG    | 0.55     | 2.54        | 12     | 1     |
| 2:B:123:ALA:HB2 | 2:B:143:PHE:CE1  | 0.55     | 2.36        | 18     | 1     |
| 1:A:14:A:C6     | 2:B:94:LYS:HG3   | 0.55     | 2.37        | 6      | 1     |
| 2:B:94:LYS:CE   | 2:B:95:LYS:HE2   | 0.55     | 2.32        | 11     | 1     |
| 2:B:90:GLY:O    | 2:B:92:ASP:N     | 0.55     | 2.40        | 3      | 1     |
| 1:A:11:C:C4     | 2:B:94:LYS:HE2   | 0.55     | 2.36        | 5      | 4     |
| 2:B:70:ALA:O    | 2:B:85:LEU:CD2   | 0.55     | 2.55        | 1      | 2     |
| 2:B:49:ARG:HB3  | 2:B:58:TYR:HB2   | 0.55     | 1.78        | 8      | 1     |
| 2:B:102:LEU:N   | 2:B:102:LEU:HD13 | 0.55     | 2.16        | 16     | 2     |
| 2:B:38:PHE:CD2  | 2:B:43:LEU:HB3   | 0.55     | 2.37        | 19     | 2     |
| 2:B:158:GLY:O   | 2:B:165:SER:CA   | 0.55     | 2.55        | 4      | 4     |
| 1:A:14:A:O2'    | 2:B:52:THR:CG2   | 0.55     | 2.48        | 14     | 3     |
| 1:A:14:A:C6     | 2:B:94:LYS:HE3   | 0.55     | 2.36        | 16     | 1     |
| 2:B:127:ARG:O   | 2:B:127:ARG:CG   | 0.55     | 2.54        | 6      | 1     |
| 1:A:8:A:H5'     | 1:A:9:U:OP2      | 0.55     | 2.01        | 17     | 1     |
| 2:B:143:PHE:CG  | 2:B:149:ALA:HA   | 0.55     | 2.37        | 6      | 18    |
| 1:A:19:G:N2     | 1:A:20:G:C4      | 0.55     | 2.75        | 10     | 3     |
| 1:A:21:C:C2     | 1:A:22:C:C6      | 0.55     | 2.95        | 16     | 3     |
| 1:A:15:A:O4'    | 1:A:17:U:H1'     | 0.55     | 2.02        | 11     | 3     |
| 2:B:51:GLY:CA   | 2:B:56:PHE:O     | 0.55     | 2.55        | 19     | 2     |
| 1:A:1:G:HO2'    | 1:A:2:G:P        | 0.55     | 2.24        | 4      | 1     |
| 2:B:46:VAL:CG2  | 2:B:61:PHE:O     | 0.55     | 2.55        | 16     | 1     |
| 1:A:14:A:N6     | 2:B:94:LYS:HD3   | 0.55     | 2.17        | 13     | 1     |
| 2:B:41:ASN:O    | 2:B:42:ASP:HB2   | 0.55     | 2.00        | 9      | 15    |
| 2:B:16:LEU:N    | 2:B:16:LEU:HD13  | 0.55     | 2.17        | 13     | 3     |
| 2:B:128:LEU:N   | 2:B:128:LEU:HD13 | 0.55     | 2.17        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:107:LEU:CD2  | 2:B:107:LEU:N    | 0.55     | 2.69        | 13     | 1     |
| 2:B:14:PHE:CD2   | 2:B:63:SER:N     | 0.55     | 2.75        | 7      | 2     |
| 2:B:104:ALA:HB2  | 2:B:141:ILE:HD12 | 0.55     | 1.79        | 11     | 1     |
| 2:B:78:VAL:CB    | 2:B:83:ILE:HG23  | 0.55     | 2.30        | 14     | 1     |
| 2:B:15:ASN:OD1   | 2:B:15:ASN:N     | 0.55     | 2.40        | 8      | 3     |
| 1:A:15:A:C1'     | 1:A:17:U:C6      | 0.55     | 2.90        | 1      | 4     |
| 2:B:103:LEU:HD11 | 2:B:140:TYR:HE1  | 0.55     | 1.57        | 2      | 2     |
| 2:B:38:PHE:CD2   | 2:B:43:LEU:HG    | 0.55     | 2.37        | 6      | 5     |
| 2:B:127:ARG:CB   | 2:B:127:ARG:CZ   | 0.55     | 2.85        | 16     | 1     |
| 1:A:20:G:C2'     | 1:A:21:C:O5'     | 0.55     | 2.55        | 13     | 1     |
| 1:A:13:G:C5      | 2:B:58:TYR:CZ    | 0.55     | 2.95        | 1      | 1     |
| 1:A:14:A:OP2     | 2:B:91:ARG:O     | 0.55     | 2.25        | 14     | 1     |
| 2:B:16:LEU:HD13  | 2:B:85:LEU:HD21  | 0.54     | 1.77        | 5      | 1     |
| 2:B:17:PHE:O     | 2:B:85:LEU:HD22  | 0.54     | 2.01        | 5      | 1     |
| 2:B:46:VAL:HG21  | 2:B:61:PHE:C     | 0.54     | 2.22        | 13     | 7     |
| 2:B:92:ASP:CB    | 2:B:96:VAL:HG21  | 0.54     | 2.31        | 12     | 1     |
| 2:B:161:ILE:O    | 2:B:164:ARG:O    | 0.54     | 2.25        | 13     | 5     |
| 2:B:21:LEU:HB3   | 2:B:30:LEU:HD22  | 0.54     | 1.80        | 11     | 2     |
| 2:B:105:LYS:O    | 2:B:166:VAL:CG2  | 0.54     | 2.56        | 16     | 1     |
| 1:A:14:A:N1      | 2:B:94:LYS:HE2   | 0.54     | 2.18        | 13     | 1     |
| 2:B:116:LEU:HD12 | 2:B:141:ILE:CD1  | 0.54     | 2.32        | 17     | 1     |
| 2:B:103:LEU:CD1  | 2:B:129:VAL:HG21 | 0.54     | 2.32        | 17     | 2     |
| 2:B:27:VAL:HG22  | 2:B:31:LYS:CE    | 0.54     | 2.31        | 19     | 1     |
| 2:B:102:LEU:C    | 2:B:171:THR:CG2  | 0.54     | 2.76        | 13     | 1     |
| 1:A:14:A:C5      | 2:B:94:LYS:HE3   | 0.54     | 2.37        | 7      | 1     |
| 2:B:73:LEU:O     | 2:B:83:ILE:CD1   | 0.54     | 2.55        | 14     | 1     |
| 2:B:102:LEU:CD1  | 2:B:149:ALA:O    | 0.54     | 2.54        | 17     | 1     |
| 1:A:14:A:O4'     | 1:A:14:A:OP1     | 0.54     | 2.25        | 10     | 4     |
| 2:B:107:LEU:HD23 | 2:B:111:ILE:HD13 | 0.54     | 1.79        | 8      | 1     |
| 2:B:21:LEU:HD13  | 2:B:30:LEU:HD23  | 0.54     | 1.80        | 9      | 1     |
| 1:A:12:C:H1'     | 2:B:56:PHE:CD2   | 0.54     | 2.37        | 19     | 2     |
| 2:B:73:LEU:O     | 2:B:76:LEU:CD1   | 0.54     | 2.56        | 16     | 1     |
| 2:B:74:THR:O     | 2:B:82:GLU:CG    | 0.54     | 2.56        | 14     | 1     |
| 2:B:93:SER:O     | 2:B:97:ARG:N     | 0.54     | 2.40        | 14     | 1     |
| 2:B:111:ILE:HD11 | 2:B:161:ILE:HD12 | 0.54     | 1.79        | 5      | 1     |
| 2:B:111:ILE:C    | 2:B:112:THR:HG23 | 0.54     | 2.22        | 12     | 6     |
| 1:A:19:G:N3      | 1:A:20:G:C1'     | 0.54     | 2.70        | 4      | 4     |
| 2:B:20:ASN:ND2   | 2:B:82:GLU:O     | 0.54     | 2.40        | 6      | 5     |
| 2:B:112:THR:OG1  | 2:B:115:GLU:OE1  | 0.54     | 2.24        | 15     | 3     |
| 2:B:11:THR:CG2   | 2:B:11:THR:O     | 0.54     | 2.55        | 15     | 1     |
| 1:A:8:A:C6       | 1:A:14:A:N9      | 0.54     | 2.76        | 17     | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:127:ARG:NH1  | 2:B:128:LEU:O    | 0.54     | 2.40        | 18     | 1     |
| 2:B:27:VAL:O     | 2:B:30:LEU:N     | 0.54     | 2.41        | 18     | 3     |
| 2:B:130:SER:O    | 2:B:136:LYS:CE   | 0.54     | 2.55        | 1      | 1     |
| 1:A:13:G:O4'     | 2:B:56:PHE:CZ    | 0.54     | 2.60        | 17     | 1     |
| 2:B:170:TYR:CD1  | 2:B:170:TYR:N    | 0.54     | 2.75        | 17     | 1     |
| 2:B:140:TYR:C    | 2:B:141:ILE:CG1  | 0.54     | 2.76        | 5      | 8     |
| 1:A:12:C:OP2     | 2:B:89:LYS:CD    | 0.54     | 2.55        | 18     | 1     |
| 2:B:34:ILE:CD1   | 2:B:83:ILE:HG21  | 0.54     | 2.33        | 14     | 1     |
| 1:A:7:A:C2'      | 1:A:8:A:O5'      | 0.54     | 2.56        | 10     | 1     |
| 2:B:11:THR:O     | 2:B:11:THR:HG22  | 0.54     | 2.02        | 8      | 1     |
| 2:B:25:LYS:O     | 2:B:54:ARG:NH1   | 0.54     | 2.41        | 12     | 2     |
| 2:B:107:LEU:HB2  | 2:B:137:GLY:O    | 0.54     | 2.03        | 15     | 4     |
| 2:B:15:ASN:N     | 2:B:15:ASN:OD1   | 0.54     | 2.41        | 19     | 6     |
| 1:A:17:U:H6      | 1:A:17:U:OP2     | 0.54     | 1.85        | 16     | 1     |
| 2:B:116:LEU:HD23 | 2:B:139:ALA:HB1  | 0.54     | 1.79        | 14     | 1     |
| 2:B:116:LEU:N    | 2:B:116:LEU:CD1  | 0.54     | 2.70        | 14     | 1     |
| 2:B:94:LYS:CE    | 2:B:94:LYS:O     | 0.54     | 2.55        | 8      | 1     |
| 2:B:124:LEU:CD1  | 2:B:144:LYS:N    | 0.54     | 2.70        | 15     | 4     |
| 1:A:11:C:C4'     | 1:A:12:C:OP1     | 0.54     | 2.56        | 17     | 2     |
| 1:A:13:G:N2      | 2:B:90:GLY:HA3   | 0.54     | 2.16        | 15     | 2     |
| 2:B:162:ASP:OD2  | 2:B:164:ARG:CG   | 0.54     | 2.55        | 9      | 1     |
| 2:B:18:ILE:HD11  | 2:B:85:LEU:HD23  | 0.54     | 1.78        | 19     | 1     |
| 1:A:13:G:OP2     | 2:B:89:LYS:CG    | 0.54     | 2.55        | 19     | 2     |
| 2:B:146:GLU:OE2  | 2:B:170:TYR:OH   | 0.54     | 2.24        | 2      | 1     |
| 2:B:102:LEU:HD22 | 2:B:149:ALA:O    | 0.54     | 2.03        | 1      | 1     |
| 2:B:124:LEU:CD1  | 2:B:143:PHE:O    | 0.54     | 2.56        | 5      | 3     |
| 2:B:16:LEU:C     | 2:B:16:LEU:CD1   | 0.54     | 2.76        | 5      | 1     |
| 2:B:53:ASN:OD1   | 2:B:55:LYS:N     | 0.54     | 2.41        | 18     | 19    |
| 1:A:4:C:OP2      | 1:A:4:C:H3'      | 0.54     | 2.02        | 10     | 1     |
| 2:B:84:LYS:C     | 2:B:85:LEU:HD12  | 0.54     | 2.23        | 10     | 1     |
| 2:B:93:SER:OG    | 2:B:97:ARG:HD2   | 0.54     | 2.02        | 9      | 1     |
| 1:A:15:A:C2      | 1:A:17:U:C5      | 0.54     | 2.96        | 5      | 3     |
| 2:B:103:LEU:HG   | 2:B:103:LEU:O    | 0.54     | 2.03        | 5      | 2     |
| 2:B:14:PHE:O     | 2:B:61:PHE:N     | 0.54     | 2.39        | 2      | 11    |
| 2:B:38:PHE:CD1   | 2:B:43:LEU:HG    | 0.54     | 2.37        | 4      | 2     |
| 1:A:14:A:H5'     | 1:A:15:A:O5'     | 0.54     | 2.02        | 14     | 3     |
| 2:B:11:THR:C     | 2:B:12:THR:OG1   | 0.54     | 2.45        | 3      | 6     |
| 2:B:105:LYS:HG3  | 2:B:138:ILE:HG23 | 0.54     | 1.80        | 4      | 3     |
| 2:B:148:ASP:OD1  | 2:B:149:ALA:N    | 0.54     | 2.41        | 19     | 1     |
| 2:B:89:LYS:CG    | 2:B:89:LYS:O     | 0.54     | 2.56        | 4      | 1     |
| 2:B:92:ASP:CG    | 2:B:96:VAL:HG12  | 0.54     | 2.23        | 4      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:127:ARG:O   | 2:B:127:ARG:HG2 | 0.54     | 2.03        | 6      | 1     |
| 1:A:13:G:C4'    | 1:A:14:A:O5'    | 0.54     | 2.56        | 1      | 1     |
| 2:B:101:THR:CG2 | 2:B:140:TYR:CD2 | 0.54     | 2.91        | 14     | 2     |
| 1:A:17:U:OP1    | 1:A:17:U:O4'    | 0.54     | 2.26        | 8      | 1     |
| 1:A:6:A:C6      | 1:A:7:A:N7      | 0.54     | 2.76        | 2      | 2     |
| 2:B:98:ALA:CB   | 2:B:171:THR:O   | 0.54     | 2.55        | 18     | 2     |
| 2:B:74:THR:HG23 | 2:B:85:LEU:HD12 | 0.54     | 1.78        | 16     | 1     |
| 2:B:38:PHE:HE1  | 2:B:76:LEU:HD11 | 0.54     | 1.63        | 1      | 1     |
| 1:A:12:C:N4     | 2:B:84:LYS:NZ   | 0.53     | 2.56        | 15     | 1     |
| 2:B:29:GLU:OE1  | 2:B:79:PHE:CZ   | 0.53     | 2.61        | 1      | 4     |
| 2:B:16:LEU:HD13 | 2:B:16:LEU:N    | 0.53     | 2.17        | 4      | 1     |
| 1:A:14:A:C8     | 1:A:14:A:P      | 0.53     | 3.01        | 6      | 1     |
| 1:A:15:A:H2'    | 2:B:52:THR:OG1  | 0.53     | 2.02        | 3      | 1     |
| 2:B:159:ALA:O   | 2:B:161:ILE:CG1 | 0.53     | 2.56        | 17     | 1     |
| 1:A:19:G:N3     | 1:A:20:G:C8     | 0.53     | 2.76        | 10     | 5     |
| 1:A:12:C:N3     | 1:A:12:C:OP2    | 0.53     | 2.42        | 2      | 2     |
| 1:A:21:C:O2'    | 1:A:22:C:C6     | 0.53     | 2.49        | 11     | 3     |
| 1:A:12:C:P      | 1:A:12:C:C5     | 0.53     | 3.01        | 3      | 1     |
| 1:A:11:C:N3     | 2:B:94:LYS:HG3  | 0.53     | 2.18        | 7      | 1     |
| 2:B:30:LEU:HD21 | 2:B:54:ARG:HB3  | 0.53     | 1.78        | 9      | 3     |
| 1:A:20:G:H5'    | 1:A:21:C:OP2    | 0.53     | 2.04        | 10     | 1     |
| 2:B:38:PHE:HB3  | 2:B:45:VAL:CG2  | 0.53     | 2.33        | 14     | 3     |
| 2:B:25:LYS:O    | 2:B:54:ARG:NH2  | 0.53     | 2.42        | 14     | 4     |
| 1:A:10:C:O2'    | 2:B:127:ARG:NH1 | 0.53     | 2.42        | 18     | 1     |
| 1:A:10:C:O2     | 2:B:127:ARG:NH2 | 0.53     | 2.36        | 18     | 2     |
| 2:B:47:ASP:CB   | 2:B:60:ASP:OD2  | 0.53     | 2.57        | 1      | 3     |
| 1:A:15:A:C6     | 2:B:52:THR:HG22 | 0.53     | 2.39        | 12     | 3     |
| 2:B:17:PHE:CD1  | 2:B:18:ILE:O    | 0.53     | 2.61        | 14     | 8     |
| 1:A:2:G:N2      | 1:A:3:C:C2      | 0.53     | 2.77        | 12     | 1     |
| 2:B:53:ASN:OD1  | 2:B:53:ASN:C    | 0.53     | 2.46        | 14     | 11    |
| 2:B:18:ILE:CG1  | 2:B:85:LEU:CD1  | 0.53     | 2.86        | 6      | 1     |
| 2:B:47:ASP:O    | 2:B:48:VAL:HG23 | 0.53     | 2.02        | 13     | 2     |
| 2:B:78:VAL:HG12 | 2:B:81:ASN:CB   | 0.53     | 2.34        | 5      | 2     |
| 1:A:7:A:C2      | 1:A:8:A:C4      | 0.53     | 2.97        | 4      | 10    |
| 2:B:108:SER:CB  | 2:B:162:ASP:OD2 | 0.53     | 2.57        | 8      | 3     |
| 1:A:17:U:C2'    | 1:A:18:A:O5'    | 0.53     | 2.57        | 15     | 1     |
| 2:B:27:VAL:HG22 | 2:B:50:THR:HB   | 0.53     | 1.79        | 19     | 1     |
| 2:B:93:SER:HB2  | 2:B:95:LYS:NZ   | 0.53     | 2.18        | 19     | 1     |
| 1:A:14:A:OP1    | 1:A:14:A:O4'    | 0.53     | 2.27        | 14     | 2     |
| 2:B:105:LYS:CE  | 2:B:169:TYR:CD2 | 0.53     | 2.92        | 6      | 2     |
| 2:B:93:SER:O    | 2:B:96:VAL:N    | 0.53     | 2.41        | 18     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:14:A:O4'     | 2:B:94:LYS:CG    | 0.53     | 2.56        | 11     | 1     |
| 1:A:16:G:C8      | 2:B:27:VAL:HG11  | 0.53     | 2.39        | 1      | 1     |
| 2:B:123:ALA:C    | 2:B:124:LEU:HD23 | 0.53     | 2.24        | 14     | 1     |
| 2:B:43:LEU:CD2   | 2:B:66:ASP:OD1   | 0.53     | 2.57        | 5      | 1     |
| 2:B:106:ASN:ND2  | 2:B:165:SER:O    | 0.53     | 2.41        | 10     | 5     |
| 1:A:2:G:O2'      | 1:A:3:C:O4'      | 0.53     | 2.27        | 7      | 4     |
| 1:A:8:A:H61      | 2:B:52:THR:HG21  | 0.53     | 1.62        | 4      | 4     |
| 2:B:35:SER:O     | 2:B:39:ALA:HB2   | 0.53     | 2.02        | 8      | 6     |
| 2:B:111:ILE:C    | 2:B:112:THR:CG2  | 0.53     | 2.77        | 13     | 2     |
| 2:B:92:ASP:O     | 2:B:93:SER:CB    | 0.53     | 2.57        | 7      | 2     |
| 1:A:15:A:O3'     | 1:A:16:G:H4'     | 0.53     | 2.03        | 19     | 2     |
| 1:A:21:C:C4'     | 1:A:21:C:OP1     | 0.53     | 2.56        | 18     | 1     |
| 2:B:127:ARG:CZ   | 2:B:127:ARG:CB   | 0.53     | 2.83        | 18     | 1     |
| 1:A:14:A:C6      | 2:B:94:LYS:HD3   | 0.53     | 2.37        | 13     | 1     |
| 1:A:11:C:N3      | 2:B:94:LYS:HE2   | 0.53     | 2.18        | 10     | 2     |
| 2:B:51:GLY:HA3   | 2:B:56:PHE:C     | 0.53     | 2.24        | 7      | 14    |
| 2:B:113:GLU:O    | 2:B:117:LYS:N    | 0.53     | 2.40        | 1      | 14    |
| 2:B:12:THR:CG2   | 2:B:13:PRO:HD2   | 0.53     | 2.34        | 17     | 5     |
| 2:B:107:LEU:HG   | 2:B:166:VAL:HG22 | 0.53     | 1.81        | 12     | 2     |
| 2:B:38:PHE:CD2   | 2:B:45:VAL:HG22  | 0.53     | 2.38        | 8      | 2     |
| 2:B:66:ASP:OD1   | 2:B:66:ASP:C     | 0.53     | 2.46        | 8      | 2     |
| 2:B:130:SER:O    | 2:B:138:ILE:CD1  | 0.53     | 2.55        | 15     | 1     |
| 2:B:145:SER:N    | 2:B:148:ASP:OD2  | 0.53     | 2.42        | 19     | 1     |
| 2:B:119:VAL:HG11 | 2:B:161:ILE:HD11 | 0.53     | 1.79        | 16     | 1     |
| 2:B:157:GLN:CA   | 2:B:168:LEU:HD12 | 0.53     | 2.34        | 16     | 1     |
| 2:B:38:PHE:CE2   | 2:B:43:LEU:HG    | 0.53     | 2.38        | 6      | 1     |
| 2:B:38:PHE:CE2   | 2:B:61:PHE:CE1   | 0.53     | 2.97        | 14     | 2     |
| 1:A:13:G:N1      | 2:B:92:ASP:O     | 0.53     | 2.42        | 17     | 1     |
| 2:B:53:ASN:OD1   | 2:B:55:LYS:HB2   | 0.53     | 2.04        | 5      | 17    |
| 2:B:16:LEU:O     | 2:B:58:TYR:CD1   | 0.53     | 2.61        | 19     | 4     |
| 2:B:60:ASP:N     | 2:B:60:ASP:OD1   | 0.53     | 2.42        | 19     | 5     |
| 2:B:18:ILE:CA    | 2:B:84:LYS:O     | 0.53     | 2.56        | 13     | 9     |
| 1:A:14:A:P       | 2:B:94:LYS:HD2   | 0.53     | 2.44        | 9      | 1     |
| 2:B:27:VAL:HG13  | 2:B:31:LYS:HE2   | 0.53     | 1.81        | 7      | 1     |
| 2:B:103:LEU:HB3  | 2:B:140:TYR:CE1  | 0.53     | 2.39        | 5      | 2     |
| 2:B:26:SER:O     | 2:B:30:LEU:HD12  | 0.53     | 2.03        | 5      | 1     |
| 2:B:127:ARG:HB2  | 2:B:140:TYR:HB2  | 0.53     | 1.81        | 15     | 6     |
| 1:A:11:C:N3      | 2:B:94:LYS:HD3   | 0.53     | 2.19        | 10     | 1     |
| 1:A:10:C:HO2'    | 2:B:128:LEU:N    | 0.53     | 2.02        | 15     | 1     |
| 2:B:86:GLU:OE2   | 2:B:87:LYS:N     | 0.53     | 2.42        | 9      | 1     |
| 2:B:18:ILE:N     | 2:B:57:GLY:O     | 0.53     | 2.42        | 6      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:13:G:N2      | 2:B:91:ARG:HA    | 0.53     | 2.19        | 13     | 2     |
| 2:B:37:LEU:CD2   | 2:B:76:LEU:HD23  | 0.53     | 2.33        | 3      | 2     |
| 2:B:62:GLU:CG    | 2:B:66:ASP:OD2   | 0.53     | 2.56        | 1      | 2     |
| 1:A:17:U:O2'     | 1:A:18:A:OP1     | 0.53     | 2.27        | 11     | 1     |
| 1:A:14:A:OP2     | 2:B:94:LYS:HG2   | 0.53     | 2.04        | 17     | 1     |
| 2:B:119:VAL:O    | 2:B:156:LYS:NZ   | 0.52     | 2.37        | 15     | 3     |
| 2:B:47:ASP:C     | 2:B:48:VAL:CG2   | 0.52     | 2.77        | 8      | 9     |
| 1:A:4:C:C2       | 1:A:20:G:C2      | 0.52     | 2.97        | 17     | 4     |
| 2:B:27:VAL:HG13  | 2:B:31:LYS:HE3   | 0.52     | 1.80        | 8      | 2     |
| 2:B:78:VAL:O     | 2:B:79:PHE:C     | 0.52     | 2.47        | 8      | 11    |
| 2:B:21:LEU:CG    | 2:B:56:PHE:O     | 0.52     | 2.57        | 13     | 2     |
| 2:B:102:LEU:CD2  | 2:B:102:LEU:N    | 0.52     | 2.65        | 13     | 3     |
| 2:B:155:GLU:O    | 2:B:156:LYS:HB3  | 0.52     | 2.04        | 16     | 2     |
| 1:A:10:C:H1'     | 2:B:129:VAL:HG13 | 0.52     | 1.75        | 15     | 3     |
| 2:B:153:LEU:CD1  | 2:B:168:LEU:O    | 0.52     | 2.58        | 17     | 3     |
| 1:A:14:A:OP1     | 1:A:14:A:N9      | 0.52     | 2.42        | 2      | 1     |
| 2:B:119:VAL:HG13 | 2:B:159:ALA:HB1  | 0.52     | 1.80        | 16     | 1     |
| 1:A:10:C:OP2     | 1:A:11:C:C5      | 0.52     | 2.59        | 13     | 1     |
| 2:B:66:ASP:C     | 2:B:66:ASP:OD1   | 0.52     | 2.48        | 13     | 1     |
| 1:A:12:C:C5'     | 1:A:12:C:C6      | 0.52     | 2.92        | 11     | 1     |
| 2:B:38:PHE:CE1   | 2:B:76:LEU:HD11  | 0.52     | 2.39        | 3      | 2     |
| 2:B:46:VAL:HG22  | 2:B:62:GLU:HB3   | 0.52     | 1.80        | 5      | 6     |
| 1:A:5:G:N2       | 1:A:18:A:H62     | 0.52     | 2.02        | 18     | 6     |
| 2:B:30:LEU:CD2   | 2:B:78:VAL:HG11  | 0.52     | 2.35        | 8      | 3     |
| 2:B:38:PHE:CG    | 2:B:43:LEU:HD13  | 0.52     | 2.39        | 8      | 2     |
| 1:A:15:A:N9      | 1:A:17:U:C6      | 0.52     | 2.77        | 1      | 9     |
| 1:A:14:A:C4'     | 1:A:15:A:OP2     | 0.52     | 2.54        | 4      | 5     |
| 2:B:153:LEU:HD12 | 2:B:168:LEU:O    | 0.52     | 2.03        | 9      | 1     |
| 1:A:18:A:HO2'    | 1:A:19:G:H5'     | 0.52     | 1.63        | 18     | 2     |
| 2:B:51:GLY:HA2   | 2:B:56:PHE:CE2   | 0.52     | 2.40        | 18     | 3     |
| 2:B:103:LEU:HD11 | 2:B:138:ILE:HG22 | 0.52     | 1.80        | 14     | 2     |
| 2:B:52:THR:O     | 2:B:53:ASN:CG    | 0.52     | 2.48        | 12     | 19    |
| 2:B:60:ASP:OD1   | 2:B:60:ASP:N     | 0.52     | 2.42        | 16     | 5     |
| 1:A:14:A:OP1     | 2:B:94:LYS:HB3   | 0.52     | 2.04        | 10     | 2     |
| 2:B:37:LEU:CD2   | 2:B:76:LEU:HD22  | 0.52     | 2.33        | 2      | 3     |
| 2:B:21:LEU:CG    | 2:B:30:LEU:HD22  | 0.52     | 2.33        | 2      | 2     |
| 2:B:102:LEU:CD2  | 2:B:143:PHE:CD1  | 0.52     | 2.93        | 15     | 5     |
| 2:B:103:LEU:HD21 | 2:B:140:TYR:CD1  | 0.52     | 2.40        | 2      | 3     |
| 2:B:58:TYR:CE2   | 2:B:88:PRO:HB3   | 0.52     | 2.40        | 16     | 1     |
| 2:B:38:PHE:CZ    | 2:B:73:LEU:HG    | 0.52     | 2.39        | 17     | 4     |
| 2:B:44:ALA:HB3   | 2:B:66:ASP:OD1   | 0.52     | 2.04        | 14     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:29:GLU:O    | 2:B:79:PHE:CE2   | 0.52     | 2.62        | 17     | 1     |
| 1:A:14:A:N1     | 2:B:94:LYS:HG2   | 0.52     | 2.20        | 5      | 2     |
| 2:B:129:VAL:HB  | 2:B:138:ILE:O    | 0.52     | 2.04        | 11     | 12    |
| 1:A:13:G:C8     | 2:B:49:ARG:HD3   | 0.52     | 2.40        | 19     | 4     |
| 1:A:13:G:O2'    | 1:A:14:A:H5'     | 0.52     | 2.04        | 8      | 2     |
| 2:B:51:GLY:CA   | 2:B:56:PHE:CD1   | 0.52     | 2.92        | 3      | 6     |
| 2:B:71:LEU:C    | 2:B:71:LEU:HD23  | 0.52     | 2.24        | 15     | 1     |
| 2:B:53:ASN:OD1  | 2:B:55:LYS:HB3   | 0.52     | 2.04        | 17     | 2     |
| 2:B:153:LEU:C   | 2:B:153:LEU:HD23 | 0.52     | 2.25        | 17     | 3     |
| 1:A:19:G:H2'    | 1:A:20:G:O5'     | 0.52     | 2.05        | 17     | 3     |
| 1:A:10:C:C1'    | 2:B:129:VAL:CG1  | 0.52     | 2.83        | 16     | 1     |
| 2:B:127:ARG:O   | 2:B:128:LEU:O    | 0.52     | 2.27        | 16     | 2     |
| 1:A:14:A:OP2    | 2:B:93:SER:C     | 0.52     | 2.48        | 3      | 1     |
| 2:B:30:LEU:HD11 | 2:B:54:ARG:CD    | 0.52     | 2.35        | 12     | 2     |
| 2:B:140:TYR:OH  | 2:B:171:THR:HG21 | 0.52     | 2.03        | 15     | 2     |
| 2:B:152:ASN:OD1 | 2:B:156:LYS:CE   | 0.52     | 2.58        | 15     | 1     |
| 2:B:152:ASN:O   | 2:B:156:LYS:N    | 0.52     | 2.41        | 2      | 3     |
| 1:A:7:A:H2'     | 1:A:8:A:O4'      | 0.52     | 2.04        | 19     | 1     |
| 2:B:14:PHE:CZ   | 2:B:64:ALA:CA    | 0.52     | 2.93        | 6      | 2     |
| 2:B:149:ALA:O   | 2:B:153:LEU:CB   | 0.52     | 2.58        | 4      | 1     |
| 2:B:51:GLY:HA2  | 2:B:56:PHE:CZ    | 0.52     | 2.39        | 6      | 2     |
| 1:A:5:G:O2'     | 1:A:6:A:O4'      | 0.52     | 2.28        | 13     | 1     |
| 2:B:103:LEU:CB  | 2:B:140:TYR:CE1  | 0.52     | 2.92        | 5      | 2     |
| 2:B:52:THR:O    | 2:B:53:ASN:OD1   | 0.52     | 2.27        | 5      | 18    |
| 1:A:6:A:C4      | 1:A:7:A:C8       | 0.52     | 2.97        | 17     | 3     |
| 1:A:3:C:O2'     | 1:A:4:C:OP2      | 0.52     | 2.27        | 10     | 1     |
| 2:B:107:LEU:CD1 | 2:B:137:GLY:O    | 0.52     | 2.55        | 15     | 2     |
| 1:A:12:C:N1     | 1:A:12:C:OP2     | 0.52     | 2.42        | 19     | 1     |
| 2:B:111:ILE:CD1 | 2:B:161:ILE:HG21 | 0.52     | 2.34        | 17     | 2     |
| 2:B:76:LEU:O    | 2:B:82:GLU:HA    | 0.52     | 2.04        | 5      | 18    |
| 1:A:8:A:N6      | 1:A:14:A:C4      | 0.52     | 2.78        | 14     | 7     |
| 2:B:147:ALA:O   | 2:B:151:LYS:CB   | 0.52     | 2.58        | 12     | 5     |
| 2:B:116:LEU:CD2 | 2:B:139:ALA:HB1  | 0.52     | 2.35        | 16     | 3     |
| 1:A:9:U:O2'     | 1:A:10:C:O4'     | 0.52     | 2.28        | 15     | 1     |
| 2:B:98:ALA:O    | 2:B:171:THR:O    | 0.52     | 2.27        | 9      | 2     |
| 2:B:93:SER:O    | 2:B:94:LYS:C     | 0.52     | 2.47        | 14     | 3     |
| 2:B:12:THR:OG1  | 2:B:60:ASP:HB3   | 0.52     | 2.05        | 19     | 1     |
| 2:B:85:LEU:CD2  | 2:B:85:LEU:N     | 0.52     | 2.70        | 18     | 1     |
| 2:B:89:LYS:O    | 2:B:90:GLY:O     | 0.52     | 2.28        | 18     | 1     |
| 2:B:102:LEU:CA  | 2:B:171:THR:OG1  | 0.52     | 2.58        | 7      | 1     |
| 1:A:11:C:O2     | 2:B:94:LYS:HE3   | 0.52     | 2.05        | 14     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:14:A:H62     | 2:B:94:LYS:NZ    | 0.52     | 2.01        | 5      | 1     |
| 2:B:49:ARG:HD3   | 2:B:58:TYR:CB    | 0.52     | 2.35        | 17     | 8     |
| 2:B:105:LYS:HG2  | 2:B:138:ILE:HG23 | 0.52     | 1.82        | 15     | 3     |
| 2:B:94:LYS:C     | 2:B:94:LYS:CE    | 0.52     | 2.79        | 12     | 2     |
| 2:B:71:LEU:HD23  | 2:B:71:LEU:O     | 0.52     | 2.04        | 15     | 1     |
| 2:B:47:ASP:CB    | 2:B:60:ASP:OD1   | 0.52     | 2.58        | 2      | 1     |
| 2:B:27:VAL:O     | 2:B:31:LYS:CE    | 0.52     | 2.58        | 4      | 1     |
| 1:A:14:A:C4      | 2:B:94:LYS:HD3   | 0.52     | 2.40        | 18     | 1     |
| 2:B:11:THR:C     | 2:B:12:THR:CG2   | 0.52     | 2.78        | 13     | 1     |
| 2:B:34:ILE:HG22  | 2:B:38:PHE:CE2   | 0.52     | 2.39        | 11     | 1     |
| 1:A:10:C:N4      | 2:B:140:TYR:OH   | 0.52     | 2.43        | 6      | 4     |
| 2:B:69:LYS:O     | 2:B:73:LEU:CD1   | 0.52     | 2.54        | 8      | 2     |
| 2:B:103:LEU:CG   | 2:B:138:ILE:HG22 | 0.52     | 2.34        | 3      | 2     |
| 2:B:29:GLU:HB3   | 2:B:79:PHE:CE1   | 0.52     | 2.41        | 9      | 1     |
| 2:B:67:LEU:C     | 2:B:67:LEU:CD1   | 0.52     | 2.79        | 1      | 1     |
| 2:B:127:ARG:O    | 2:B:128:LEU:C    | 0.51     | 2.48        | 16     | 9     |
| 2:B:99:ALA:O     | 2:B:170:TYR:CZ   | 0.51     | 2.63        | 10     | 5     |
| 2:B:30:LEU:CD1   | 2:B:54:ARG:HD2   | 0.51     | 2.35        | 19     | 8     |
| 2:B:127:ARG:NH2  | 2:B:140:TYR:CE2  | 0.51     | 2.78        | 12     | 3     |
| 2:B:102:LEU:HD11 | 2:B:149:ALA:CB   | 0.51     | 2.34        | 16     | 2     |
| 1:A:7:A:C6       | 1:A:8:A:C6       | 0.51     | 2.98        | 4      | 6     |
| 1:A:13:G:OP2     | 2:B:89:LYS:CD    | 0.51     | 2.58        | 6      | 1     |
| 2:B:30:LEU:CD2   | 2:B:54:ARG:HG3   | 0.51     | 2.35        | 14     | 1     |
| 2:B:103:LEU:HB3  | 2:B:138:ILE:HG22 | 0.51     | 1.81        | 19     | 2     |
| 1:A:16:G:C2      | 2:B:54:ARG:NH2   | 0.51     | 2.78        | 8      | 1     |
| 2:B:120:PHE:HZ   | 2:B:168:LEU:HD21 | 0.51     | 1.63        | 4      | 4     |
| 2:B:143:PHE:CD1  | 2:B:143:PHE:N    | 0.51     | 2.78        | 11     | 5     |
| 2:B:75:GLY:O     | 2:B:76:LEU:C     | 0.51     | 2.48        | 16     | 2     |
| 1:A:6:A:N7       | 1:A:15:A:N6      | 0.51     | 2.58        | 18     | 2     |
| 2:B:18:ILE:CG1   | 2:B:85:LEU:CD2   | 0.51     | 2.89        | 16     | 1     |
| 2:B:140:TYR:CZ   | 2:B:171:THR:HG21 | 0.51     | 2.40        | 13     | 2     |
| 2:B:101:THR:HG23 | 2:B:141:ILE:C    | 0.51     | 2.24        | 7      | 1     |
| 1:A:6:A:C2       | 1:A:7:A:C8       | 0.51     | 2.98        | 17     | 1     |
| 1:A:15:A:O4'     | 1:A:15:A:OP1     | 0.51     | 2.29        | 5      | 2     |
| 2:B:29:GLU:HB3   | 2:B:79:PHE:CE2   | 0.51     | 2.40        | 8      | 5     |
| 2:B:120:PHE:CE2  | 2:B:141:ILE:HD12 | 0.51     | 2.40        | 1      | 5     |
| 2:B:92:ASP:HB3   | 2:B:96:VAL:CG2   | 0.51     | 2.35        | 12     | 1     |
| 2:B:15:ASN:ND2   | 2:B:60:ASP:OD2   | 0.51     | 2.42        | 16     | 8     |
| 2:B:47:ASP:OD2   | 2:B:49:ARG:NH1   | 0.51     | 2.43        | 15     | 2     |
| 2:B:104:ALA:O    | 2:B:139:ALA:N    | 0.51     | 2.43        | 2      | 3     |
| 1:A:5:G:H21      | 1:A:18:A:H62     | 0.51     | 1.49        | 9      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:103:LEU:HD22 | 2:B:140:TYR:CZ   | 0.51     | 2.40        | 18     | 2     |
| 1:A:14:A:C8      | 2:B:94:LYS:HD3   | 0.51     | 2.41        | 18     | 1     |
| 2:B:120:PHE:CD2  | 2:B:141:ILE:CD1  | 0.51     | 2.93        | 1      | 3     |
| 2:B:15:ASN:ND2   | 2:B:60:ASP:CG    | 0.51     | 2.63        | 13     | 1     |
| 1:A:14:A:C1'     | 2:B:94:LYS:HG3   | 0.51     | 2.35        | 11     | 1     |
| 2:B:99:ALA:O     | 2:B:170:TYR:CE2  | 0.51     | 2.63        | 11     | 1     |
| 2:B:53:ASN:C     | 2:B:53:ASN:OD1   | 0.51     | 2.48        | 5      | 8     |
| 1:A:14:A:P       | 2:B:93:SER:HA    | 0.51     | 2.46        | 5      | 1     |
| 2:B:103:LEU:CD2  | 2:B:140:TYR:CD1  | 0.51     | 2.94        | 2      | 3     |
| 2:B:105:LYS:HE3  | 2:B:169:TYR:CD2  | 0.51     | 2.41        | 6      | 1     |
| 2:B:22:ASN:C     | 2:B:54:ARG:CB    | 0.51     | 2.78        | 6      | 1     |
| 2:B:73:LEU:CD2   | 2:B:76:LEU:HD11  | 0.51     | 2.29        | 13     | 1     |
| 1:A:14:A:OP1     | 2:B:93:SER:C     | 0.51     | 2.49        | 10     | 2     |
| 2:B:93:SER:O     | 2:B:94:LYS:HB3   | 0.51     | 2.06        | 17     | 4     |
| 2:B:103:LEU:CD1  | 2:B:171:THR:OG1  | 0.51     | 2.56        | 9      | 1     |
| 2:B:110:ASN:O    | 2:B:111:ILE:O    | 0.51     | 2.28        | 6      | 2     |
| 2:B:12:THR:HB    | 2:B:13:PRO:CD    | 0.51     | 2.36        | 13     | 1     |
| 2:B:22:ASN:N     | 2:B:54:ARG:O     | 0.51     | 2.41        | 2      | 2     |
| 2:B:12:THR:OG1   | 2:B:46:VAL:HG11  | 0.51     | 2.06        | 10     | 1     |
| 2:B:46:VAL:CG2   | 2:B:62:GLU:CG    | 0.51     | 2.88        | 17     | 6     |
| 2:B:103:LEU:CD1  | 2:B:171:THR:HG22 | 0.51     | 2.36        | 8      | 1     |
| 2:B:143:PHE:CD2  | 2:B:149:ALA:HA   | 0.51     | 2.41        | 16     | 2     |
| 2:B:102:LEU:CD1  | 2:B:168:LEU:CD1  | 0.51     | 2.87        | 6      | 1     |
| 2:B:22:ASN:ND2   | 2:B:79:PHE:O     | 0.51     | 2.42        | 5      | 3     |
| 2:B:16:LEU:HD13  | 2:B:85:LEU:CD2   | 0.51     | 2.36        | 5      | 1     |
| 2:B:152:ASN:O    | 2:B:156:LYS:CG   | 0.51     | 2.58        | 19     | 3     |
| 2:B:91:ARG:O     | 2:B:92:ASP:C     | 0.51     | 2.49        | 16     | 3     |
| 1:A:20:G:C2      | 1:A:21:C:N1      | 0.51     | 2.79        | 3      | 4     |
| 2:B:88:PRO:C     | 2:B:89:LYS:CG    | 0.51     | 2.79        | 2      | 1     |
| 2:B:146:GLU:HA   | 2:B:170:TYR:OH   | 0.51     | 2.05        | 18     | 2     |
| 2:B:31:LYS:HG3   | 2:B:48:VAL:CG1   | 0.51     | 2.36        | 16     | 1     |
| 1:A:14:A:C6      | 2:B:94:LYS:HD2   | 0.51     | 2.40        | 7      | 1     |
| 2:B:83:ILE:HD12  | 2:B:83:ILE:N     | 0.51     | 2.20        | 14     | 1     |
| 2:B:85:LEU:CD1   | 2:B:86:GLU:N     | 0.51     | 2.64        | 5      | 1     |
| 2:B:46:VAL:CG2   | 2:B:62:GLU:HB3   | 0.51     | 2.36        | 4      | 11    |
| 2:B:51:GLY:N     | 2:B:57:GLY:HA2   | 0.51     | 2.21        | 9      | 10    |
| 2:B:85:LEU:CD1   | 2:B:85:LEU:N     | 0.51     | 2.73        | 10     | 1     |
| 2:B:17:PHE:CE2   | 2:B:86:GLU:HB3   | 0.51     | 2.41        | 2      | 7     |
| 2:B:105:LYS:HG2  | 2:B:138:ILE:HD13 | 0.51     | 1.81        | 15     | 1     |
| 2:B:91:ARG:O     | 2:B:92:ASP:O     | 0.51     | 2.29        | 9      | 2     |
| 1:A:5:G:O2'      | 1:A:6:A:OP1      | 0.51     | 2.21        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:16:G:C8      | 2:B:27:VAL:CG2   | 0.51     | 2.93        | 6      | 3     |
| 2:B:14:PHE:CE1   | 2:B:64:ALA:HA    | 0.51     | 2.41        | 1      | 3     |
| 2:B:103:LEU:O    | 2:B:169:TYR:N    | 0.51     | 2.40        | 18     | 1     |
| 1:A:13:G:C8      | 2:B:58:TYR:CE1   | 0.51     | 2.99        | 1      | 2     |
| 2:B:93:SER:O     | 2:B:94:LYS:HE2   | 0.51     | 2.06        | 11     | 1     |
| 1:A:11:C:N3      | 2:B:94:LYS:NZ    | 0.51     | 2.59        | 14     | 1     |
| 1:A:2:G:O2'      | 1:A:3:C:C6       | 0.51     | 2.64        | 10     | 2     |
| 2:B:41:ASN:O     | 2:B:42:ASP:CG    | 0.51     | 2.49        | 9      | 4     |
| 1:A:10:C:O2'     | 2:B:127:ARG:HB3  | 0.51     | 2.06        | 15     | 1     |
| 2:B:129:VAL:CA   | 2:B:136:LYS:HE2  | 0.51     | 2.36        | 15     | 1     |
| 2:B:76:LEU:HD23  | 2:B:83:ILE:HD11  | 0.51     | 1.81        | 9      | 1     |
| 1:A:10:C:C4'     | 2:B:129:VAL:HG13 | 0.51     | 2.36        | 16     | 5     |
| 2:B:59:VAL:HG13  | 2:B:61:PHE:CE1   | 0.51     | 2.41        | 11     | 1     |
| 2:B:70:ALA:CA    | 2:B:73:LEU:HD22  | 0.51     | 2.36        | 11     | 1     |
| 2:B:146:GLU:O    | 2:B:150:GLU:N    | 0.51     | 2.43        | 7      | 5     |
| 1:A:12:C:C6      | 1:A:12:C:C5'     | 0.51     | 2.94        | 12     | 1     |
| 2:B:116:LEU:HD21 | 2:B:139:ALA:CB   | 0.51     | 2.36        | 16     | 2     |
| 1:A:11:C:OP1     | 1:A:11:C:O4'     | 0.51     | 2.29        | 2      | 1     |
| 2:B:97:ARG:NH2   | 2:B:142:GLU:OE2  | 0.51     | 2.44        | 18     | 1     |
| 2:B:97:ARG:NH1   | 2:B:142:GLU:OE2  | 0.51     | 2.44        | 16     | 1     |
| 2:B:17:PHE:HB2   | 2:B:58:TYR:CE1   | 0.51     | 2.41        | 3      | 1     |
| 2:B:43:LEU:CD1   | 2:B:66:ASP:HA    | 0.51     | 2.36        | 17     | 1     |
| 2:B:12:THR:CG2   | 2:B:46:VAL:CB    | 0.50     | 2.89        | 19     | 1     |
| 1:A:3:C:O2'      | 1:A:4:C:OP1      | 0.50     | 2.27        | 19     | 3     |
| 2:B:107:LEU:O    | 2:B:107:LEU:HD23 | 0.50     | 2.06        | 11     | 1     |
| 2:B:45:VAL:C     | 2:B:46:VAL:CG2   | 0.50     | 2.78        | 11     | 1     |
| 2:B:25:LYS:HD3   | 2:B:79:PHE:CD1   | 0.50     | 2.42        | 11     | 1     |
| 2:B:105:LYS:HD3  | 2:B:138:ILE:HG23 | 0.50     | 1.82        | 5      | 2     |
| 2:B:143:PHE:CD1  | 2:B:149:ALA:HA   | 0.50     | 2.41        | 19     | 5     |
| 1:A:11:C:O4'     | 2:B:127:ARG:HD2  | 0.50     | 2.06        | 14     | 11    |
| 2:B:22:ASN:C     | 2:B:22:ASN:OD1   | 0.50     | 2.49        | 12     | 1     |
| 2:B:22:ASN:OD1   | 2:B:22:ASN:C     | 0.50     | 2.49        | 9      | 1     |
| 1:A:14:A:P       | 2:B:94:LYS:CD    | 0.50     | 2.99        | 9      | 1     |
| 2:B:76:LEU:HB2   | 2:B:83:ILE:CG1   | 0.50     | 2.36        | 13     | 4     |
| 2:B:97:ARG:O     | 2:B:98:ALA:C     | 0.50     | 2.50        | 7      | 6     |
| 1:A:9:U:H4'      | 1:A:10:C:OP1     | 0.50     | 2.07        | 16     | 4     |
| 1:A:6:A:C6       | 1:A:18:A:N3      | 0.50     | 2.78        | 16     | 2     |
| 2:B:94:LYS:CE    | 2:B:95:LYS:CE    | 0.50     | 2.89        | 11     | 1     |
| 2:B:76:LEU:HD12  | 2:B:77:LYS:N     | 0.50     | 2.20        | 17     | 1     |
| 2:B:143:PHE:CE2  | 2:B:152:ASN:CB   | 0.50     | 2.94        | 6      | 4     |
| 2:B:14:PHE:CD2   | 2:B:63:SER:C     | 0.50     | 2.84        | 16     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:48:VAL:C     | 2:B:49:ARG:CG    | 0.50     | 2.79        | 19     | 1     |
| 2:B:76:LEU:CB    | 2:B:83:ILE:HG12  | 0.50     | 2.36        | 13     | 2     |
| 2:B:161:ILE:O    | 2:B:162:ASP:C    | 0.50     | 2.49        | 15     | 19    |
| 1:A:8:A:C4       | 1:A:14:A:C2      | 0.50     | 2.99        | 18     | 2     |
| 2:B:61:PHE:HB3   | 2:B:66:ASP:CG    | 0.50     | 2.25        | 13     | 4     |
| 2:B:158:GLY:O    | 2:B:165:SER:CB   | 0.50     | 2.60        | 4      | 1     |
| 1:A:16:G:OP1     | 1:A:16:G:O3'     | 0.50     | 2.29        | 18     | 1     |
| 2:B:22:ASN:ND2   | 2:B:25:LYS:HB2   | 0.50     | 2.21        | 3      | 3     |
| 1:A:2:G:HO2'     | 1:A:3:C:P        | 0.50     | 2.30        | 7      | 1     |
| 2:B:110:ASN:CB   | 2:B:162:ASP:OD2  | 0.50     | 2.59        | 7      | 1     |
| 2:B:18:ILE:CG1   | 2:B:85:LEU:HD13  | 0.50     | 2.35        | 1      | 1     |
| 2:B:105:LYS:O    | 2:B:106:ASN:HB3  | 0.50     | 2.07        | 15     | 9     |
| 2:B:102:LEU:HD21 | 2:B:143:PHE:CD1  | 0.50     | 2.40        | 1      | 5     |
| 2:B:74:THR:O     | 2:B:74:THR:CG2   | 0.50     | 2.59        | 7      | 2     |
| 1:A:4:C:C2'      | 1:A:5:G:C8       | 0.50     | 2.95        | 8      | 8     |
| 2:B:129:VAL:CA   | 2:B:136:LYS:CE   | 0.50     | 2.89        | 15     | 1     |
| 2:B:13:PRO:HG2   | 2:B:14:PHE:CD2   | 0.50     | 2.41        | 15     | 3     |
| 2:B:27:VAL:CG2   | 2:B:50:THR:CG2   | 0.50     | 2.89        | 19     | 1     |
| 2:B:92:ASP:O     | 2:B:93:SER:C     | 0.50     | 2.49        | 18     | 1     |
| 2:B:153:LEU:HD12 | 2:B:168:LEU:HB3  | 0.50     | 1.83        | 6      | 1     |
| 2:B:143:PHE:CE2  | 2:B:152:ASN:CG   | 0.50     | 2.84        | 10     | 2     |
| 1:A:14:A:H2'     | 2:B:52:THR:CG2   | 0.50     | 2.37        | 10     | 14    |
| 2:B:130:SER:HA   | 2:B:136:LYS:HB2  | 0.50     | 1.84        | 18     | 9     |
| 2:B:21:LEU:HB2   | 2:B:54:ARG:O     | 0.50     | 2.07        | 19     | 10    |
| 2:B:129:VAL:HB   | 2:B:138:ILE:HD12 | 0.50     | 1.84        | 15     | 1     |
| 2:B:71:LEU:O     | 2:B:74:THR:OG1   | 0.50     | 2.22        | 16     | 2     |
| 1:A:3:C:H1'      | 1:A:4:C:OP1      | 0.50     | 2.07        | 19     | 3     |
| 1:A:4:C:HO2'     | 1:A:5:G:H8       | 0.50     | 1.37        | 4      | 1     |
| 2:B:89:LYS:O     | 2:B:90:GLY:C     | 0.50     | 2.50        | 11     | 3     |
| 2:B:38:PHE:CE1   | 2:B:73:LEU:HG    | 0.50     | 2.41        | 6      | 2     |
| 2:B:71:LEU:C     | 2:B:71:LEU:CD1   | 0.50     | 2.80        | 6      | 1     |
| 1:A:15:A:N9      | 2:B:52:THR:HG23  | 0.50     | 2.22        | 4      | 5     |
| 2:B:18:ILE:CG2   | 2:B:19:GLY:N     | 0.50     | 2.75        | 3      | 9     |
| 1:A:12:C:OP2     | 1:A:12:C:O2      | 0.50     | 2.28        | 6      | 1     |
| 2:B:78:VAL:CG1   | 2:B:79:PHE:N     | 0.50     | 2.75        | 4      | 5     |
| 2:B:129:VAL:HG23 | 2:B:139:ALA:CA   | 0.50     | 2.37        | 16     | 8     |
| 2:B:129:VAL:CG2  | 2:B:138:ILE:HB   | 0.50     | 2.37        | 19     | 6     |
| 1:A:20:G:C6      | 1:A:21:C:N3      | 0.50     | 2.80        | 11     | 2     |
| 2:B:16:LEU:HA    | 2:B:88:PRO:CG    | 0.50     | 2.37        | 4      | 13    |
| 2:B:25:LYS:HG3   | 2:B:79:PHE:CD1   | 0.50     | 2.42        | 12     | 1     |
| 2:B:126:ILE:HG23 | 2:B:141:ILE:HD12 | 0.50     | 1.81        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:13:G:OP2     | 2:B:89:LYS:HG2   | 0.50     | 2.07        | 19     | 1     |
| 2:B:95:LYS:C     | 2:B:95:LYS:CD    | 0.50     | 2.78        | 19     | 1     |
| 1:A:4:C:O2'      | 1:A:5:G:H3'      | 0.50     | 2.06        | 4      | 1     |
| 2:B:157:GLN:O    | 2:B:158:GLY:C    | 0.50     | 2.49        | 16     | 1     |
| 2:B:38:PHE:CD2   | 2:B:43:LEU:CG    | 0.50     | 2.95        | 6      | 1     |
| 2:B:123:ALA:CB   | 2:B:141:ILE:CG2  | 0.50     | 2.90        | 11     | 1     |
| 1:A:9:U:P        | 1:A:9:U:H3'      | 0.50     | 2.47        | 14     | 1     |
| 1:A:11:C:N3      | 1:A:14:A:N6      | 0.50     | 2.59        | 17     | 1     |
| 2:B:146:GLU:HG3  | 2:B:170:TYR:OH   | 0.50     | 2.06        | 7      | 5     |
| 1:A:13:G:C5      | 2:B:58:TYR:CE1   | 0.50     | 2.99        | 12     | 1     |
| 1:A:14:A:O4'     | 2:B:95:LYS:HE3   | 0.50     | 2.07        | 12     | 1     |
| 1:A:2:G:HO2'     | 1:A:3:C:C5'      | 0.50     | 2.20        | 15     | 1     |
| 2:B:105:LYS:O    | 2:B:166:VAL:HG22 | 0.50     | 2.06        | 15     | 1     |
| 2:B:18:ILE:HG13  | 2:B:85:LEU:CD2   | 0.50     | 2.36        | 16     | 1     |
| 2:B:102:LEU:CD1  | 2:B:168:LEU:HD13 | 0.50     | 2.31        | 6      | 1     |
| 2:B:47:ASP:OD1   | 2:B:49:ARG:NH1   | 0.50     | 2.45        | 13     | 1     |
| 1:A:10:C:HO2'    | 1:A:11:C:P       | 0.50     | 2.30        | 11     | 1     |
| 1:A:13:G:N2      | 2:B:90:GLY:C     | 0.50     | 2.65        | 7      | 1     |
| 2:B:33:ALA:HB2   | 2:B:79:PHE:HD2   | 0.50     | 1.63        | 17     | 1     |
| 2:B:58:TYR:O     | 2:B:59:VAL:HG22  | 0.49     | 2.07        | 5      | 4     |
| 2:B:38:PHE:CD2   | 2:B:43:LEU:CD2   | 0.49     | 2.84        | 2      | 2     |
| 1:A:7:A:N1       | 1:A:8:A:C4       | 0.49     | 2.80        | 4      | 5     |
| 1:A:15:A:O2'     | 1:A:16:G:H4'     | 0.49     | 2.07        | 11     | 2     |
| 2:B:21:LEU:HB3   | 2:B:30:LEU:CD2   | 0.49     | 2.37        | 5      | 2     |
| 2:B:53:ASN:O     | 2:B:53:ASN:OD1   | 0.49     | 2.29        | 5      | 3     |
| 2:B:77:LYS:HA    | 2:B:82:GLU:HA    | 0.49     | 1.82        | 3      | 9     |
| 2:B:129:VAL:CB   | 2:B:138:ILE:O    | 0.49     | 2.59        | 11     | 11    |
| 2:B:101:THR:C    | 2:B:171:THR:HG1  | 0.49     | 2.09        | 12     | 1     |
| 2:B:124:LEU:CD1  | 2:B:143:PHE:C    | 0.49     | 2.80        | 15     | 6     |
| 2:B:129:VAL:HA   | 2:B:136:LYS:HE3  | 0.49     | 1.83        | 15     | 1     |
| 2:B:21:LEU:O     | 2:B:78:VAL:HG12  | 0.49     | 2.06        | 15     | 1     |
| 2:B:18:ILE:HG23  | 2:B:84:LYS:O     | 0.49     | 2.07        | 14     | 7     |
| 2:B:107:LEU:HD12 | 2:B:138:ILE:C    | 0.49     | 2.27        | 4      | 2     |
| 2:B:16:LEU:CD2   | 2:B:16:LEU:C     | 0.49     | 2.75        | 17     | 2     |
| 2:B:51:GLY:CA    | 2:B:56:PHE:CD2   | 0.49     | 2.94        | 14     | 2     |
| 2:B:153:LEU:HD13 | 2:B:168:LEU:HB3  | 0.49     | 1.83        | 13     | 1     |
| 1:A:12:C:O2      | 2:B:56:PHE:CB    | 0.49     | 2.60        | 3      | 1     |
| 2:B:17:PHE:CD2   | 2:B:86:GLU:HG3   | 0.49     | 2.42        | 7      | 1     |
| 1:A:14:A:C5      | 2:B:94:LYS:NZ    | 0.49     | 2.81        | 7      | 1     |
| 2:B:45:VAL:HG23  | 2:B:45:VAL:O     | 0.49     | 2.07        | 1      | 5     |
| 2:B:104:ALA:O    | 2:B:138:ILE:HG22 | 0.49     | 2.07        | 1      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:18:ILE:CD1   | 2:B:59:VAL:HG21  | 0.49     | 2.37        | 10     | 2     |
| 2:B:143:PHE:N    | 2:B:143:PHE:CD1  | 0.49     | 2.80        | 8      | 1     |
| 2:B:154:GLU:HG3  | 2:B:155:GLU:N    | 0.49     | 2.23        | 3      | 5     |
| 2:B:11:THR:C     | 2:B:12:THR:HG1   | 0.49     | 2.10        | 3      | 3     |
| 2:B:25:LYS:HG3   | 2:B:79:PHE:CG    | 0.49     | 2.42        | 12     | 1     |
| 2:B:85:LEU:O     | 2:B:86:GLU:HB3   | 0.49     | 2.07        | 1      | 4     |
| 1:A:20:G:C4'     | 1:A:21:C:OP1     | 0.49     | 2.61        | 9      | 1     |
| 1:A:10:C:OP1     | 1:A:10:C:O4'     | 0.49     | 2.29        | 14     | 2     |
| 2:B:128:LEU:HD22 | 2:B:128:LEU:O    | 0.49     | 2.06        | 16     | 1     |
| 2:B:83:ILE:HD12  | 2:B:83:ILE:O     | 0.49     | 2.06        | 14     | 1     |
| 1:A:15:A:C5'     | 1:A:16:G:OP1     | 0.49     | 2.60        | 10     | 3     |
| 2:B:161:ILE:O    | 2:B:162:ASP:OD1  | 0.49     | 2.30        | 9      | 1     |
| 2:B:12:THR:CB    | 2:B:13:PRO:HD2   | 0.49     | 2.38        | 9      | 2     |
| 2:B:30:LEU:CD1   | 2:B:54:ARG:CD    | 0.49     | 2.90        | 19     | 1     |
| 2:B:153:LEU:CD1  | 2:B:168:LEU:HB3  | 0.49     | 2.37        | 13     | 2     |
| 2:B:21:LEU:HD23  | 2:B:30:LEU:CD2   | 0.49     | 2.38        | 5      | 1     |
| 1:A:12:C:N1      | 2:B:17:PHE:CZ    | 0.49     | 2.81        | 15     | 4     |
| 2:B:14:PHE:CZ    | 2:B:64:ALA:N     | 0.49     | 2.81        | 1      | 3     |
| 2:B:17:PHE:CE2   | 2:B:18:ILE:O     | 0.49     | 2.66        | 12     | 1     |
| 2:B:111:ILE:HD11 | 2:B:161:ILE:HG22 | 0.49     | 1.84        | 2      | 1     |
| 2:B:154:GLU:CG   | 2:B:155:GLU:N    | 0.49     | 2.74        | 17     | 4     |
| 2:B:101:THR:C    | 2:B:171:THR:CG2  | 0.49     | 2.81        | 18     | 1     |
| 2:B:85:LEU:CD2   | 2:B:86:GLU:N     | 0.49     | 2.73        | 7      | 1     |
| 2:B:107:LEU:HD13 | 2:B:166:VAL:HG21 | 0.49     | 1.84        | 7      | 1     |
| 2:B:104:ALA:HA   | 2:B:167:SER:O    | 0.49     | 2.07        | 5      | 14    |
| 2:B:11:THR:O     | 2:B:12:THR:HG23  | 0.49     | 2.08        | 4      | 4     |
| 1:A:13:G:OP2     | 2:B:89:LYS:HB2   | 0.49     | 2.07        | 17     | 6     |
| 2:B:48:VAL:HG23  | 2:B:59:VAL:CG2   | 0.49     | 2.38        | 9      | 1     |
| 2:B:73:LEU:O     | 2:B:74:THR:C     | 0.49     | 2.51        | 9      | 4     |
| 2:B:94:LYS:CG    | 2:B:95:LYS:N     | 0.49     | 2.75        | 9      | 1     |
| 2:B:128:LEU:HD13 | 2:B:128:LEU:C    | 0.49     | 2.28        | 2      | 1     |
| 2:B:103:LEU:HD22 | 2:B:140:TYR:CE1  | 0.49     | 2.42        | 18     | 2     |
| 2:B:120:PHE:HE1  | 2:B:168:LEU:HD11 | 0.49     | 1.63        | 16     | 1     |
| 2:B:105:LYS:HB2  | 2:B:167:SER:OG   | 0.49     | 2.07        | 6      | 2     |
| 2:B:44:ALA:O     | 2:B:66:ASP:OD2   | 0.49     | 2.31        | 11     | 1     |
| 2:B:100:ARG:NE   | 2:B:142:GLU:OE1  | 0.49     | 2.45        | 11     | 1     |
| 1:A:12:C:O2      | 2:B:56:PHE:CG    | 0.49     | 2.66        | 3      | 1     |
| 2:B:11:THR:CB    | 2:B:47:ASP:OD2   | 0.49     | 2.61        | 3      | 1     |
| 2:B:101:THR:O    | 2:B:170:TYR:HA   | 0.49     | 2.08        | 17     | 2     |
| 1:A:13:G:O2'     | 2:B:51:GLY:HA2   | 0.49     | 2.08        | 17     | 1     |
| 1:A:15:A:C5      | 1:A:17:U:C2      | 0.49     | 3.01        | 18     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:102:LEU:CD2  | 2:B:168:LEU:CD2  | 0.49     | 2.90        | 10     | 1     |
| 2:B:67:LEU:CD2   | 2:B:67:LEU:C     | 0.49     | 2.80        | 8      | 1     |
| 2:B:128:LEU:HD22 | 2:B:130:SER:OG   | 0.49     | 2.07        | 12     | 1     |
| 2:B:107:LEU:CD1  | 2:B:138:ILE:HA   | 0.49     | 2.38        | 6      | 3     |
| 2:B:107:LEU:CD1  | 2:B:138:ILE:CA   | 0.49     | 2.91        | 6      | 3     |
| 1:A:3:C:C4'      | 1:A:4:C:OP1      | 0.49     | 2.60        | 12     | 5     |
| 2:B:38:PHE:CB    | 2:B:45:VAL:CG1   | 0.49     | 2.91        | 9      | 1     |
| 2:B:59:VAL:O     | 2:B:60:ASP:OD1   | 0.49     | 2.31        | 9      | 2     |
| 2:B:78:VAL:O     | 2:B:81:ASN:OD1   | 0.49     | 2.30        | 9      | 1     |
| 2:B:116:LEU:CD2  | 2:B:116:LEU:N    | 0.49     | 2.75        | 9      | 1     |
| 1:A:3:C:C1'      | 1:A:4:C:OP1      | 0.49     | 2.61        | 19     | 3     |
| 2:B:18:ILE:O     | 2:B:56:PHE:HB2   | 0.49     | 2.07        | 16     | 5     |
| 2:B:93:SER:O     | 2:B:97:ARG:NE    | 0.49     | 2.45        | 7      | 1     |
| 2:B:25:LYS:CD    | 2:B:79:PHE:HB3   | 0.49     | 2.38        | 5      | 1     |
| 2:B:30:LEU:CD1   | 2:B:54:ARG:HD3   | 0.49     | 2.38        | 7      | 2     |
| 1:A:15:A:C8      | 1:A:17:U:N1      | 0.49     | 2.81        | 2      | 5     |
| 1:A:5:G:C3'      | 1:A:5:G:OP2      | 0.49     | 2.53        | 4      | 1     |
| 2:B:92:ASP:CA    | 2:B:96:VAL:CG1   | 0.49     | 2.90        | 16     | 1     |
| 2:B:107:LEU:HD22 | 2:B:166:VAL:HG23 | 0.49     | 1.85        | 13     | 1     |
| 1:A:14:A:H61     | 2:B:94:LYS:HE2   | 0.49     | 1.67        | 13     | 1     |
| 1:A:21:C:H1'     | 1:A:22:C:OP1     | 0.49     | 2.07        | 14     | 1     |
| 1:A:7:A:C2       | 1:A:8:A:N3       | 0.49     | 2.81        | 17     | 7     |
| 2:B:38:PHE:CE2   | 2:B:73:LEU:HD21  | 0.49     | 2.43        | 8      | 1     |
| 2:B:120:PHE:CG   | 2:B:141:ILE:HG21 | 0.49     | 2.42        | 12     | 1     |
| 1:A:13:G:OP2     | 2:B:89:LYS:N     | 0.49     | 2.46        | 9      | 1     |
| 2:B:78:VAL:O     | 2:B:78:VAL:HG12  | 0.49     | 2.06        | 9      | 4     |
| 2:B:14:PHE:CD2   | 2:B:67:LEU:HD22  | 0.49     | 2.42        | 19     | 1     |
| 2:B:161:ILE:N    | 2:B:164:ARG:O    | 0.49     | 2.43        | 2      | 2     |
| 1:A:14:A:OP1     | 1:A:14:A:H8      | 0.49     | 1.91        | 16     | 1     |
| 2:B:14:PHE:O     | 2:B:60:ASP:OD1   | 0.49     | 2.30        | 13     | 1     |
| 2:B:102:LEU:CD1  | 2:B:169:TYR:N    | 0.49     | 2.76        | 14     | 1     |
| 2:B:14:PHE:CD1   | 2:B:67:LEU:HG    | 0.49     | 2.43        | 17     | 1     |
| 1:A:7:A:C6       | 1:A:8:A:C4       | 0.49     | 3.00        | 4      | 3     |
| 1:A:4:C:C4'      | 1:A:5:G:O5'      | 0.49     | 2.61        | 8      | 7     |
| 2:B:35:SER:O     | 2:B:39:ALA:CB    | 0.49     | 2.61        | 8      | 2     |
| 1:A:10:C:N4      | 2:B:94:LYS:NZ    | 0.49     | 2.61        | 12     | 1     |
| 2:B:152:ASN:OD1  | 2:B:156:LYS:HE3  | 0.49     | 2.08        | 15     | 1     |
| 2:B:162:ASP:OD2  | 2:B:162:ASP:O    | 0.49     | 2.31        | 9      | 1     |
| 2:B:16:LEU:HD11  | 2:B:18:ILE:HD12  | 0.49     | 1.85        | 19     | 1     |
| 2:B:100:ARG:CG   | 2:B:142:GLU:OE1  | 0.49     | 2.60        | 4      | 1     |
| 2:B:15:ASN:OD1   | 2:B:60:ASP:OD1   | 0.49     | 2.31        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:159:ALA:HB1  | 2:B:161:ILE:HD11 | 0.49     | 1.83        | 14     | 1     |
| 2:B:18:ILE:CG1   | 2:B:85:LEU:HD23  | 0.48     | 2.37        | 5      | 1     |
| 2:B:53:ASN:CG    | 2:B:53:ASN:O     | 0.48     | 2.51        | 5      | 5     |
| 2:B:76:LEU:O     | 2:B:83:ILE:HG12  | 0.48     | 2.08        | 5      | 4     |
| 2:B:127:ARG:N    | 2:B:140:TYR:O    | 0.48     | 2.43        | 19     | 2     |
| 2:B:94:LYS:C     | 2:B:94:LYS:CD    | 0.48     | 2.79        | 8      | 2     |
| 1:A:16:G:N7      | 2:B:27:VAL:CB    | 0.48     | 2.76        | 4      | 3     |
| 1:A:16:G:O6      | 2:B:54:ARG:NH2   | 0.48     | 2.42        | 12     | 3     |
| 1:A:11:C:O2'     | 2:B:94:LYS:NZ    | 0.48     | 2.43        | 15     | 1     |
| 2:B:27:VAL:CG1   | 2:B:28:ALA:N     | 0.48     | 2.76        | 19     | 3     |
| 2:B:111:ILE:CG1  | 2:B:116:LEU:HD11 | 0.48     | 2.38        | 16     | 1     |
| 2:B:34:ILE:HG21  | 2:B:59:VAL:HG21  | 0.48     | 1.83        | 14     | 1     |
| 2:B:124:LEU:HD12 | 2:B:143:PHE:O    | 0.48     | 2.08        | 8      | 2     |
| 2:B:153:LEU:CD1  | 2:B:153:LEU:C    | 0.48     | 2.76        | 15     | 1     |
| 2:B:103:LEU:CG   | 2:B:140:TYR:CD1  | 0.48     | 2.96        | 4      | 2     |
| 1:A:17:U:O2      | 1:A:17:U:H2'     | 0.48     | 2.08        | 3      | 2     |
| 2:B:107:LEU:O    | 2:B:164:ARG:NH1  | 0.48     | 2.45        | 14     | 1     |
| 1:A:6:A:C8       | 1:A:18:A:N1      | 0.48     | 2.81        | 17     | 1     |
| 1:A:11:C:HO2'    | 1:A:12:C:P       | 0.48     | 2.31        | 12     | 2     |
| 1:A:20:G:N2      | 1:A:21:C:C2      | 0.48     | 2.81        | 6      | 2     |
| 2:B:49:ARG:CG    | 2:B:58:TYR:HB2   | 0.48     | 2.38        | 19     | 1     |
| 1:A:14:A:C2      | 2:B:94:LYS:CG    | 0.48     | 2.97        | 19     | 2     |
| 2:B:14:PHE:CD1   | 2:B:67:LEU:HB2   | 0.48     | 2.43        | 6      | 3     |
| 2:B:105:LYS:HG3  | 2:B:169:TYR:CD2  | 0.48     | 2.43        | 3      | 1     |
| 1:A:15:A:N1      | 1:A:17:U:O4      | 0.48     | 2.46        | 5      | 2     |
| 2:B:19:GLY:O     | 2:B:83:ILE:HA    | 0.48     | 2.08        | 17     | 7     |
| 1:A:4:C:C1'      | 1:A:5:G:O5'      | 0.48     | 2.61        | 11     | 9     |
| 2:B:104:ALA:O    | 2:B:138:ILE:HA   | 0.48     | 2.09        | 12     | 8     |
| 2:B:85:LEU:HD13  | 2:B:85:LEU:H     | 0.48     | 1.68        | 12     | 1     |
| 2:B:85:LEU:O     | 2:B:85:LEU:HD22  | 0.48     | 2.07        | 12     | 1     |
| 1:A:7:A:N6       | 1:A:8:A:C6       | 0.48     | 2.82        | 4      | 1     |
| 2:B:90:GLY:O     | 2:B:92:ASP:OD1   | 0.48     | 2.32        | 18     | 1     |
| 2:B:113:GLU:OE1  | 2:B:126:ILE:O    | 0.48     | 2.31        | 16     | 1     |
| 2:B:102:LEU:HD12 | 2:B:143:PHE:CE1  | 0.48     | 2.44        | 17     | 1     |
| 1:A:12:C:OP2     | 2:B:89:LYS:HE3   | 0.48     | 2.09        | 18     | 2     |
| 2:B:102:LEU:CD2  | 2:B:141:ILE:HB   | 0.48     | 2.39        | 19     | 3     |
| 2:B:108:SER:OG   | 2:B:109:PHE:N    | 0.48     | 2.45        | 12     | 3     |
| 1:A:9:U:C6       | 2:B:138:ILE:CD1  | 0.48     | 2.97        | 13     | 2     |
| 2:B:38:PHE:CD2   | 2:B:45:VAL:HG12  | 0.48     | 2.44        | 3      | 4     |
| 2:B:30:LEU:O     | 2:B:34:ILE:CD1   | 0.48     | 2.61        | 1      | 3     |
| 2:B:157:GLN:CB   | 2:B:168:LEU:HD12 | 0.48     | 2.37        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:9:U:OP2      | 1:A:10:C:OP2     | 0.48     | 2.31        | 13     | 1     |
| 1:A:20:G:N7      | 1:A:21:C:C4      | 0.48     | 2.81        | 11     | 1     |
| 2:B:94:LYS:HE2   | 2:B:94:LYS:CA    | 0.48     | 2.38        | 14     | 1     |
| 2:B:76:LEU:O     | 2:B:83:ILE:N     | 0.48     | 2.46        | 5      | 5     |
| 1:A:14:A:C1'     | 2:B:95:LYS:HE3   | 0.48     | 2.39        | 12     | 1     |
| 2:B:43:LEU:HD11  | 2:B:73:LEU:CD2   | 0.48     | 2.39        | 7      | 2     |
| 1:A:2:G:H2'      | 1:A:3:C:O5'      | 0.48     | 2.08        | 9      | 3     |
| 2:B:16:LEU:HD11  | 2:B:18:ILE:CD1   | 0.48     | 2.39        | 19     | 1     |
| 2:B:124:LEU:HD21 | 2:B:144:LYS:HG2  | 0.48     | 1.85        | 4      | 1     |
| 1:A:13:G:C8      | 2:B:49:ARG:NE    | 0.48     | 2.82        | 6      | 2     |
| 2:B:38:PHE:CE1   | 2:B:73:LEU:CD1   | 0.48     | 2.97        | 16     | 1     |
| 2:B:111:ILE:CG1  | 2:B:116:LEU:CD1  | 0.48     | 2.92        | 16     | 1     |
| 2:B:116:LEU:HD13 | 2:B:141:ILE:HD11 | 0.48     | 1.83        | 11     | 1     |
| 2:B:31:LYS:HG2   | 2:B:48:VAL:HG22  | 0.48     | 1.85        | 11     | 1     |
| 2:B:122:ASP:O    | 2:B:143:PHE:CD2  | 0.48     | 2.66        | 3      | 1     |
| 1:A:13:G:H5"     | 2:B:58:TYR:OH    | 0.48     | 2.09        | 1      | 1     |
| 2:B:50:THR:HA    | 2:B:57:GLY:HA2   | 0.48     | 1.86        | 17     | 1     |
| 2:B:47:ASP:O     | 2:B:59:VAL:HA    | 0.48     | 2.08        | 13     | 4     |
| 2:B:78:VAL:HB    | 2:B:83:ILE:CG2   | 0.48     | 2.38        | 13     | 14    |
| 1:A:4:C:H4'      | 1:A:5:G:O5'      | 0.48     | 2.09        | 16     | 4     |
| 2:B:140:TYR:C    | 2:B:141:ILE:HG12 | 0.48     | 2.28        | 8      | 3     |
| 1:A:14:A:OP1     | 2:B:93:SER:HA    | 0.48     | 2.08        | 15     | 1     |
| 1:A:14:A:OP1     | 2:B:94:LYS:HD3   | 0.48     | 2.08        | 9      | 1     |
| 1:A:10:C:O2'     | 1:A:11:C:OP1     | 0.48     | 2.29        | 11     | 1     |
| 1:A:14:A:N6      | 2:B:94:LYS:HD2   | 0.48     | 2.23        | 7      | 1     |
| 2:B:97:ARG:C     | 2:B:101:THR:OG1  | 0.48     | 2.52        | 7      | 1     |
| 2:B:29:GLU:HB3   | 2:B:79:PHE:CD2   | 0.48     | 2.44        | 8      | 1     |
| 1:A:12:C:N1      | 2:B:17:PHE:CE2   | 0.48     | 2.81        | 12     | 1     |
| 1:A:14:A:OP1     | 2:B:92:ASP:CG    | 0.48     | 2.52        | 12     | 1     |
| 1:A:21:C:HO2'    | 1:A:22:C:P       | 0.48     | 2.31        | 12     | 2     |
| 1:A:1:G:C5       | 1:A:2:G:N7       | 0.48     | 2.82        | 12     | 1     |
| 1:A:12:C:C5      | 2:B:17:PHE:CE2   | 0.48     | 3.01        | 15     | 3     |
| 2:B:28:ALA:O     | 2:B:32:VAL:CB    | 0.48     | 2.62        | 11     | 4     |
| 2:B:14:PHE:CE2   | 2:B:64:ALA:HA    | 0.48     | 2.44        | 19     | 1     |
| 1:A:14:A:P       | 2:B:94:LYS:HB2   | 0.48     | 2.48        | 19     | 1     |
| 2:B:74:THR:HA    | 2:B:85:LEU:HD21  | 0.48     | 1.85        | 18     | 2     |
| 2:B:102:LEU:HD11 | 2:B:141:ILE:HB   | 0.48     | 1.85        | 6      | 1     |
| 1:A:13:G:H21     | 2:B:90:GLY:C     | 0.48     | 2.11        | 7      | 1     |
| 1:A:16:G:N1      | 2:B:54:ARG:NH2   | 0.48     | 2.62        | 7      | 1     |
| 2:B:52:THR:O     | 2:B:53:ASN:HB3   | 0.48     | 2.07        | 19     | 14    |
| 1:A:4:C:H2'      | 1:A:5:G:C8       | 0.48     | 2.44        | 13     | 8     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:10:C:H42     | 2:B:94:LYS:HE2   | 0.48     | 1.68        | 8      | 1     |
| 2:B:19:GLY:O     | 2:B:20:ASN:HB3   | 0.48     | 2.08        | 12     | 7     |
| 2:B:129:VAL:HA   | 2:B:136:LYS:CE   | 0.48     | 2.39        | 15     | 1     |
| 1:A:7:A:H4'      | 1:A:8:A:OP1      | 0.48     | 2.09        | 19     | 1     |
| 2:B:73:LEU:CD1   | 2:B:76:LEU:CD2   | 0.48     | 2.91        | 19     | 1     |
| 1:A:1:G:H1'      | 1:A:2:G:OP1      | 0.48     | 2.09        | 4      | 1     |
| 2:B:108:SER:OG   | 2:B:162:ASP:OD2  | 0.48     | 2.26        | 4      | 1     |
| 2:B:98:ALA:C     | 2:B:171:THR:O    | 0.48     | 2.52        | 18     | 1     |
| 1:A:10:C:O2'     | 2:B:129:VAL:HA   | 0.48     | 2.08        | 16     | 1     |
| 2:B:36:GLU:O     | 2:B:40:LYS:N     | 0.48     | 2.45        | 11     | 1     |
| 2:B:51:GLY:CA    | 2:B:56:PHE:CE1   | 0.48     | 2.97        | 3      | 1     |
| 1:A:21:C:C2'     | 1:A:22:C:O5'     | 0.48     | 2.62        | 5      | 1     |
| 2:B:86:GLU:O     | 2:B:87:LYS:C     | 0.48     | 2.53        | 17     | 15    |
| 2:B:103:LEU:HD11 | 2:B:171:THR:HG22 | 0.48     | 1.85        | 8      | 1     |
| 2:B:157:GLN:OE1  | 2:B:168:LEU:N    | 0.48     | 2.40        | 1      | 2     |
| 2:B:128:LEU:HD22 | 2:B:129:VAL:N    | 0.48     | 2.24        | 4      | 1     |
| 2:B:51:GLY:CA    | 2:B:56:PHE:CE2   | 0.48     | 2.97        | 14     | 2     |
| 2:B:22:ASN:O     | 2:B:54:ARG:HB3   | 0.47     | 2.09        | 5      | 7     |
| 2:B:152:ASN:O    | 2:B:156:LYS:CB   | 0.47     | 2.63        | 10     | 3     |
| 2:B:151:LYS:O    | 2:B:155:GLU:HB2  | 0.47     | 2.09        | 14     | 8     |
| 2:B:120:PHE:CD2  | 2:B:141:ILE:HD12 | 0.47     | 2.44        | 15     | 1     |
| 2:B:18:ILE:CD1   | 2:B:59:VAL:HB    | 0.47     | 2.38        | 16     | 2     |
| 2:B:37:LEU:HD22  | 2:B:76:LEU:CG    | 0.47     | 2.39        | 16     | 1     |
| 1:A:14:A:OP2     | 2:B:91:ARG:HB2   | 0.47     | 2.09        | 7      | 1     |
| 2:B:54:ARG:N     | 2:B:54:ARG:HD3   | 0.47     | 2.24        | 1      | 1     |
| 2:B:126:ILE:HA   | 2:B:140:TYR:O    | 0.47     | 2.09        | 6      | 9     |
| 2:B:105:LYS:O    | 2:B:166:VAL:HA   | 0.47     | 2.09        | 8      | 1     |
| 2:B:54:ARG:HG2   | 2:B:54:ARG:NH1   | 0.47     | 2.24        | 8      | 1     |
| 2:B:90:GLY:O     | 2:B:91:ARG:O     | 0.47     | 2.31        | 8      | 1     |
| 2:B:14:PHE:C     | 2:B:15:ASN:OD1   | 0.47     | 2.52        | 3      | 4     |
| 2:B:78:VAL:HG23  | 2:B:83:ILE:CG2   | 0.47     | 2.39        | 6      | 1     |
| 2:B:85:LEU:N     | 2:B:85:LEU:CD2   | 0.47     | 2.74        | 13     | 1     |
| 2:B:146:GLU:O    | 2:B:150:GLU:HB2  | 0.47     | 2.09        | 15     | 8     |
| 2:B:126:ILE:CG2  | 2:B:140:TYR:O    | 0.47     | 2.58        | 15     | 3     |
| 2:B:89:LYS:O     | 2:B:91:ARG:HG3   | 0.47     | 2.10        | 15     | 1     |
| 1:A:15:A:O4'     | 1:A:17:U:C1'     | 0.47     | 2.61        | 9      | 3     |
| 2:B:124:LEU:HD11 | 2:B:144:LYS:HA   | 0.47     | 1.85        | 14     | 1     |
| 2:B:29:GLU:OE1   | 2:B:79:PHE:CE2   | 0.47     | 2.67        | 16     | 2     |
| 1:A:19:G:N3      | 1:A:20:G:N9      | 0.47     | 2.62        | 10     | 4     |
| 2:B:153:LEU:CD2  | 2:B:168:LEU:O    | 0.47     | 2.63        | 15     | 1     |
| 2:B:22:ASN:ND2   | 2:B:79:PHE:HB3   | 0.47     | 2.25        | 6      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:16:G:C5      | 2:B:27:VAL:HG21  | 0.47     | 2.45        | 4      | 2     |
| 2:B:129:VAL:HB   | 2:B:138:ILE:C    | 0.47     | 2.29        | 16     | 5     |
| 1:A:10:C:N4      | 2:B:140:TYR:HH   | 0.47     | 2.07        | 6      | 1     |
| 2:B:12:THR:HG21  | 2:B:62:GLU:HG2   | 0.47     | 1.87        | 17     | 1     |
| 2:B:37:LEU:HD21  | 2:B:76:LEU:HD13  | 0.47     | 1.84        | 5      | 2     |
| 1:A:4:C:O2'      | 1:A:5:G:C4'      | 0.47     | 2.63        | 18     | 7     |
| 2:B:103:LEU:O    | 2:B:103:LEU:HG   | 0.47     | 2.09        | 1      | 2     |
| 2:B:46:VAL:O     | 2:B:47:ASP:CG    | 0.47     | 2.53        | 1      | 1     |
| 2:B:21:LEU:CG    | 2:B:30:LEU:HD23  | 0.47     | 2.39        | 5      | 1     |
| 2:B:78:VAL:N     | 2:B:81:ASN:O     | 0.47     | 2.47        | 5      | 6     |
| 2:B:16:LEU:CD1   | 2:B:16:LEU:C     | 0.47     | 2.78        | 10     | 3     |
| 2:B:122:ASP:O    | 2:B:123:ALA:C    | 0.47     | 2.50        | 8      | 3     |
| 2:B:130:SER:CA   | 2:B:136:LYS:HD2  | 0.47     | 2.40        | 15     | 1     |
| 2:B:111:ILE:HG23 | 2:B:112:THR:N    | 0.47     | 2.25        | 15     | 5     |
| 2:B:11:THR:HG23  | 2:B:12:THR:OG1   | 0.47     | 2.10        | 1      | 2     |
| 2:B:92:ASP:HA    | 2:B:96:VAL:CG1   | 0.47     | 2.40        | 16     | 2     |
| 2:B:96:VAL:HG12  | 2:B:97:ARG:N     | 0.47     | 2.25        | 18     | 2     |
| 2:B:18:ILE:HB    | 2:B:57:GLY:O     | 0.47     | 2.10        | 17     | 4     |
| 1:A:19:G:O2'     | 1:A:20:G:H4'     | 0.47     | 2.10        | 16     | 1     |
| 2:B:34:ILE:O     | 2:B:38:PHE:CD2   | 0.47     | 2.68        | 16     | 1     |
| 2:B:14:PHE:CZ    | 2:B:64:ALA:HA    | 0.47     | 2.44        | 6      | 1     |
| 1:A:8:A:C2       | 2:B:95:LYS:HD3   | 0.47     | 2.44        | 11     | 1     |
| 2:B:115:GLU:O    | 2:B:119:VAL:CG2  | 0.47     | 2.62        | 11     | 1     |
| 2:B:153:LEU:CD2  | 2:B:153:LEU:C    | 0.47     | 2.79        | 14     | 1     |
| 2:B:16:LEU:HA    | 2:B:88:PRO:CB    | 0.47     | 2.40        | 14     | 1     |
| 1:A:4:C:O2       | 1:A:20:G:C2      | 0.47     | 2.68        | 10     | 2     |
| 2:B:58:TYR:O     | 2:B:59:VAL:CG2   | 0.47     | 2.59        | 9      | 5     |
| 2:B:111:ILE:HD11 | 2:B:161:ILE:HD13 | 0.47     | 1.86        | 8      | 1     |
| 2:B:53:ASN:O     | 2:B:53:ASN:CG    | 0.47     | 2.53        | 15     | 8     |
| 2:B:102:LEU:HB3  | 2:B:153:LEU:HD13 | 0.47     | 1.87        | 12     | 1     |
| 2:B:151:LYS:O    | 2:B:155:GLU:HB3  | 0.47     | 2.09        | 12     | 3     |
| 2:B:146:GLU:O    | 2:B:150:GLU:HB3  | 0.47     | 2.10        | 12     | 2     |
| 2:B:84:LYS:HG2   | 2:B:85:LEU:N     | 0.47     | 2.23        | 16     | 4     |
| 1:A:14:A:OP1     | 2:B:94:LYS:CB    | 0.47     | 2.63        | 19     | 1     |
| 2:B:53:ASN:OD1   | 2:B:53:ASN:O     | 0.47     | 2.33        | 14     | 3     |
| 1:A:20:G:C5      | 1:A:21:C:C6      | 0.47     | 3.00        | 14     | 3     |
| 2:B:158:GLY:O    | 2:B:165:SER:HA   | 0.47     | 2.10        | 6      | 4     |
| 1:A:13:G:N7      | 2:B:58:TYR:CB    | 0.47     | 2.78        | 18     | 1     |
| 2:B:101:THR:O    | 2:B:171:THR:CG2  | 0.47     | 2.62        | 18     | 1     |
| 2:B:80:GLY:O     | 2:B:81:ASN:OD1   | 0.47     | 2.33        | 3      | 2     |
| 2:B:112:THR:O    | 2:B:116:LEU:HD13 | 0.47     | 2.10        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:13:G:H21     | 2:B:90:GLY:HA2   | 0.47     | 1.70        | 3      | 1     |
| 2:B:130:SER:O    | 2:B:136:LYS:HE2  | 0.47     | 2.10        | 1      | 1     |
| 1:A:14:A:H2'     | 2:B:52:THR:HG1   | 0.47     | 1.69        | 14     | 1     |
| 1:A:21:C:C1'     | 1:A:22:C:OP1     | 0.47     | 2.62        | 14     | 2     |
| 1:A:21:C:C2'     | 1:A:22:C:OP1     | 0.47     | 2.62        | 14     | 2     |
| 1:A:2:G:O2'      | 1:A:3:C:H6       | 0.47     | 1.92        | 10     | 2     |
| 2:B:43:LEU:HD11  | 2:B:66:ASP:HA    | 0.47     | 1.87        | 10     | 1     |
| 1:A:12:C:C1'     | 2:B:17:PHE:CE2   | 0.47     | 2.98        | 12     | 1     |
| 1:A:2:G:H4'      | 1:A:3:C:OP1      | 0.47     | 2.08        | 12     | 1     |
| 1:A:9:U:C1'      | 2:B:129:VAL:HG12 | 0.47     | 2.36        | 15     | 1     |
| 2:B:130:SER:N    | 2:B:136:LYS:HD2  | 0.47     | 2.24        | 15     | 1     |
| 2:B:15:ASN:O     | 2:B:16:LEU:HB3   | 0.47     | 2.10        | 18     | 4     |
| 2:B:111:ILE:HD13 | 2:B:162:ASP:OD1  | 0.47     | 2.09        | 13     | 1     |
| 2:B:107:LEU:CD1  | 2:B:128:LEU:HD11 | 0.47     | 2.39        | 11     | 1     |
| 2:B:31:LYS:CG    | 2:B:48:VAL:HG22  | 0.47     | 2.40        | 11     | 1     |
| 2:B:153:LEU:O    | 2:B:157:GLN:HB2  | 0.47     | 2.09        | 10     | 7     |
| 2:B:67:LEU:CD1   | 2:B:67:LEU:C     | 0.47     | 2.78        | 6      | 3     |
| 2:B:103:LEU:HG   | 2:B:138:ILE:HG22 | 0.47     | 1.85        | 3      | 2     |
| 2:B:29:GLU:OE2   | 2:B:79:PHE:CZ    | 0.47     | 2.68        | 15     | 2     |
| 2:B:89:LYS:O     | 2:B:91:ARG:CG    | 0.47     | 2.63        | 15     | 1     |
| 2:B:119:VAL:O    | 2:B:156:LYS:HE2  | 0.47     | 2.09        | 9      | 1     |
| 2:B:38:PHE:HB3   | 2:B:45:VAL:HG13  | 0.47     | 1.86        | 9      | 1     |
| 2:B:80:GLY:C     | 2:B:81:ASN:OD1   | 0.47     | 2.53        | 9      | 1     |
| 1:A:13:G:C5'     | 2:B:90:GLY:O     | 0.47     | 2.51        | 9      | 1     |
| 2:B:82:GLU:O     | 2:B:83:ILE:C     | 0.47     | 2.53        | 14     | 2     |
| 1:A:13:G:H5'     | 1:A:14:A:OP1     | 0.47     | 2.10        | 18     | 1     |
| 1:A:10:C:N4      | 1:A:11:C:C4      | 0.47     | 2.83        | 16     | 1     |
| 2:B:31:LYS:NZ    | 2:B:50:THR:HB    | 0.47     | 2.25        | 14     | 2     |
| 2:B:98:ALA:O     | 2:B:101:THR:N    | 0.47     | 2.42        | 11     | 1     |
| 1:A:13:G:OP2     | 2:B:89:LYS:HB3   | 0.47     | 2.09        | 7      | 1     |
| 2:B:74:THR:HA    | 2:B:85:LEU:CD1   | 0.47     | 2.40        | 16     | 3     |
| 2:B:61:PHE:HB2   | 2:B:66:ASP:OD1   | 0.47     | 2.10        | 18     | 3     |
| 1:A:10:C:H42     | 2:B:94:LYS:NZ    | 0.47     | 2.08        | 6      | 2     |
| 2:B:85:LEU:HD23  | 2:B:85:LEU:N     | 0.47     | 2.24        | 15     | 1     |
| 1:A:20:G:C3'     | 1:A:21:C:O4'     | 0.47     | 2.63        | 16     | 2     |
| 2:B:125:GLU:O    | 2:B:126:ILE:CD1  | 0.47     | 2.54        | 16     | 1     |
| 2:B:102:LEU:N    | 2:B:102:LEU:CD1  | 0.47     | 2.75        | 7      | 2     |
| 1:A:16:G:N1      | 2:B:54:ARG:NH1   | 0.47     | 2.63        | 6      | 1     |
| 2:B:21:LEU:CD1   | 2:B:30:LEU:HB3   | 0.47     | 2.40        | 6      | 2     |
| 1:A:12:C:C2      | 1:A:12:C:P       | 0.47     | 3.08        | 13     | 1     |
| 2:B:73:LEU:HD22  | 2:B:76:LEU:HD21  | 0.47     | 1.85        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:13:G:H21     | 2:B:91:ARG:N     | 0.47     | 2.07        | 7      | 1     |
| 2:B:101:THR:C    | 2:B:102:LEU:CD1  | 0.46     | 2.81        | 10     | 1     |
| 2:B:18:ILE:CG1   | 2:B:85:LEU:HG    | 0.46     | 2.40        | 4      | 5     |
| 2:B:24:ASN:O     | 2:B:25:LYS:HD2   | 0.46     | 2.09        | 4      | 2     |
| 2:B:145:SER:CB   | 2:B:148:ASP:OD2  | 0.46     | 2.63        | 19     | 1     |
| 2:B:38:PHE:CD2   | 2:B:43:LEU:CB    | 0.46     | 2.98        | 6      | 2     |
| 2:B:115:GLU:OE2  | 2:B:161:ILE:HD13 | 0.46     | 2.10        | 6      | 1     |
| 1:A:16:G:C4'     | 1:A:17:U:OP1     | 0.46     | 2.60        | 13     | 1     |
| 2:B:93:SER:N     | 2:B:96:VAL:HB    | 0.46     | 2.24        | 13     | 2     |
| 1:A:20:G:O2'     | 1:A:21:C:H5'     | 0.46     | 2.10        | 1      | 2     |
| 2:B:46:VAL:O     | 2:B:47:ASP:OD1   | 0.46     | 2.33        | 3      | 1     |
| 2:B:38:PHE:CD2   | 2:B:45:VAL:CG2   | 0.46     | 2.98        | 7      | 1     |
| 1:A:10:C:C4      | 1:A:11:C:N3      | 0.46     | 2.82        | 14     | 1     |
| 1:A:10:C:N4      | 2:B:94:LYS:HE2   | 0.46     | 2.24        | 8      | 1     |
| 2:B:66:ASP:O     | 2:B:66:ASP:OD1   | 0.46     | 2.34        | 9      | 1     |
| 2:B:76:LEU:CB    | 2:B:83:ILE:CG1   | 0.46     | 2.93        | 13     | 1     |
| 2:B:119:VAL:HG21 | 2:B:161:ILE:HD12 | 0.46     | 1.88        | 13     | 1     |
| 1:A:15:A:N1      | 1:A:17:U:C4      | 0.46     | 2.83        | 5      | 2     |
| 2:B:16:LEU:CB    | 2:B:88:PRO:HD3   | 0.46     | 2.41        | 17     | 5     |
| 2:B:121:GLU:OE2  | 2:B:122:ASP:OD2  | 0.46     | 2.33        | 5      | 1     |
| 1:A:14:A:O4'     | 2:B:95:LYS:HE2   | 0.46     | 2.10        | 7      | 4     |
| 2:B:47:ASP:C     | 2:B:60:ASP:OD1   | 0.46     | 2.54        | 16     | 2     |
| 1:A:10:C:C6      | 2:B:129:VAL:HG13 | 0.46     | 2.45        | 15     | 1     |
| 2:B:103:LEU:HD12 | 2:B:140:TYR:CD2  | 0.46     | 2.46        | 15     | 1     |
| 1:A:13:G:H2'     | 1:A:14:A:O5'     | 0.46     | 2.09        | 2      | 3     |
| 2:B:49:ARG:HG3   | 2:B:58:TYR:CB    | 0.46     | 2.40        | 19     | 1     |
| 1:A:10:C:C4      | 2:B:140:TYR:OH   | 0.46     | 2.68        | 2      | 2     |
| 2:B:102:LEU:HD22 | 2:B:153:LEU:HB2  | 0.46     | 1.86        | 18     | 1     |
| 2:B:15:ASN:ND2   | 2:B:60:ASP:OD1   | 0.46     | 2.47        | 7      | 3     |
| 2:B:105:LYS:HG3  | 2:B:169:TYR:CD1  | 0.46     | 2.45        | 1      | 2     |
| 2:B:21:LEU:C     | 2:B:30:LEU:HD21  | 0.46     | 2.31        | 7      | 1     |
| 1:A:8:A:C5'      | 1:A:9:U:P        | 0.46     | 3.03        | 12     | 1     |
| 2:B:107:LEU:HD21 | 2:B:116:LEU:HD21 | 0.46     | 1.86        | 15     | 2     |
| 2:B:158:GLY:O    | 2:B:161:ILE:CD1  | 0.46     | 2.63        | 15     | 1     |
| 2:B:28:ALA:O     | 2:B:32:VAL:HB    | 0.46     | 2.10        | 11     | 4     |
| 1:A:13:G:C8      | 2:B:58:TYR:CB    | 0.46     | 2.98        | 18     | 1     |
| 2:B:128:LEU:O    | 2:B:128:LEU:HD13 | 0.46     | 2.10        | 16     | 1     |
| 2:B:56:PHE:CG    | 2:B:57:GLY:N     | 0.46     | 2.83        | 17     | 1     |
| 1:A:15:A:H1'     | 1:A:17:U:C6      | 0.46     | 2.45        | 9      | 6     |
| 2:B:125:GLU:C    | 2:B:126:ILE:CG1  | 0.46     | 2.84        | 12     | 1     |
| 1:A:9:U:OP1      | 1:A:9:U:H2'      | 0.46     | 2.11        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:102:LEU:CD1  | 2:B:102:LEU:C    | 0.46     | 2.78        | 18     | 1     |
| 2:B:127:ARG:HB3  | 2:B:140:TYR:HB2  | 0.46     | 1.86        | 18     | 1     |
| 2:B:101:THR:HG21 | 2:B:142:GLU:OE2  | 0.46     | 2.09        | 16     | 1     |
| 1:A:14:A:OP2     | 2:B:91:ARG:CB    | 0.46     | 2.64        | 7      | 1     |
| 2:B:38:PHE:HB3   | 2:B:45:VAL:HG23  | 0.46     | 1.86        | 14     | 1     |
| 2:B:77:LYS:O     | 2:B:78:VAL:C     | 0.46     | 2.54        | 17     | 3     |
| 2:B:160:GLU:HA   | 2:B:165:SER:CA   | 0.46     | 2.41        | 9      | 1     |
| 2:B:49:ARG:HD3   | 2:B:58:TYR:HB2   | 0.46     | 1.88        | 19     | 1     |
| 2:B:91:ARG:O     | 2:B:92:ASP:HB3   | 0.46     | 2.10        | 18     | 3     |
| 2:B:101:THR:O    | 2:B:171:THR:HG22 | 0.46     | 2.10        | 11     | 2     |
| 2:B:103:LEU:CB   | 2:B:140:TYR:HA   | 0.46     | 2.40        | 1      | 2     |
| 2:B:155:GLU:HG3  | 2:B:156:LYS:CD   | 0.46     | 2.41        | 16     | 1     |
| 1:A:9:U:O4       | 2:B:105:LYS:HD3  | 0.46     | 2.11        | 6      | 1     |
| 2:B:125:GLU:O    | 2:B:142:GLU:N    | 0.46     | 2.45        | 11     | 1     |
| 2:B:114:ASP:O    | 2:B:118:GLU:N    | 0.46     | 2.49        | 14     | 1     |
| 2:B:12:THR:CG2   | 2:B:13:PRO:CD    | 0.46     | 2.93        | 17     | 1     |
| 2:B:98:ALA:CB    | 2:B:171:THR:HB   | 0.46     | 2.40        | 5      | 2     |
| 2:B:41:ASN:O     | 2:B:42:ASP:HB3   | 0.46     | 2.08        | 17     | 7     |
| 2:B:158:GLY:HA2  | 2:B:166:VAL:O    | 0.46     | 2.11        | 8      | 3     |
| 2:B:61:PHE:HB2   | 2:B:66:ASP:CG    | 0.46     | 2.31        | 18     | 3     |
| 2:B:50:THR:OG1   | 2:B:54:ARG:HD3   | 0.46     | 2.11        | 19     | 1     |
| 1:A:7:A:C6       | 1:A:8:A:C5       | 0.46     | 3.04        | 4      | 1     |
| 2:B:105:LYS:O    | 2:B:166:VAL:HG23 | 0.46     | 2.11        | 16     | 1     |
| 1:A:16:G:N3      | 1:A:17:U:H5      | 0.46     | 2.09        | 3      | 1     |
| 1:A:20:G:O2'     | 1:A:21:C:H6      | 0.46     | 1.94        | 7      | 1     |
| 2:B:145:SER:N    | 2:B:148:ASP:CG   | 0.46     | 2.69        | 19     | 1     |
| 2:B:18:ILE:CG2   | 2:B:83:ILE:HB    | 0.46     | 2.41        | 19     | 6     |
| 2:B:97:ARG:HG3   | 2:B:98:ALA:N     | 0.46     | 2.25        | 19     | 3     |
| 2:B:12:THR:O     | 2:B:15:ASN:OD1   | 0.46     | 2.34        | 13     | 1     |
| 2:B:153:LEU:HD13 | 2:B:170:TYR:CD1  | 0.46     | 2.46        | 5      | 1     |
| 2:B:126:ILE:HG23 | 2:B:141:ILE:CG1  | 0.46     | 2.37        | 10     | 1     |
| 2:B:125:GLU:OE2  | 2:B:142:GLU:OE1  | 0.46     | 2.33        | 10     | 1     |
| 2:B:59:VAL:C     | 2:B:60:ASP:OD1   | 0.46     | 2.54        | 4      | 4     |
| 1:A:20:G:H5"     | 1:A:21:C:OP2     | 0.46     | 2.11        | 2      | 1     |
| 1:A:1:G:C4'      | 1:A:2:G:OP1      | 0.46     | 2.64        | 2      | 1     |
| 2:B:100:ARG:HG3  | 2:B:142:GLU:OE1  | 0.46     | 2.10        | 4      | 1     |
| 2:B:10:SER:OG    | 2:B:12:THR:O     | 0.46     | 2.34        | 4      | 1     |
| 2:B:153:LEU:O    | 2:B:157:GLN:CG   | 0.46     | 2.63        | 6      | 1     |
| 2:B:157:GLN:OE1  | 2:B:167:SER:HA   | 0.46     | 2.11        | 6      | 1     |
| 2:B:30:LEU:HD12  | 2:B:31:LYS:CA    | 0.46     | 2.39        | 14     | 1     |
| 1:A:19:G:C4'     | 1:A:20:G:OP1     | 0.46     | 2.64        | 15     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:127:ARG:HB2  | 2:B:140:TYR:HB3  | 0.46     | 1.87        | 8      | 5     |
| 2:B:103:LEU:HD11 | 2:B:129:VAL:HG11 | 0.46     | 1.87        | 15     | 1     |
| 2:B:140:TYR:OH   | 2:B:171:THR:HG23 | 0.46     | 2.10        | 15     | 1     |
| 1:A:13:G:C2'     | 1:A:13:G:N3      | 0.46     | 2.78        | 9      | 1     |
| 2:B:16:LEU:HA    | 2:B:88:PRO:HD3   | 0.46     | 1.89        | 2      | 1     |
| 2:B:111:ILE:CG1  | 2:B:115:GLU:OE1  | 0.46     | 2.64        | 2      | 1     |
| 1:A:13:G:C5'     | 2:B:90:GLY:HA3   | 0.46     | 2.41        | 4      | 1     |
| 2:B:87:LYS:O     | 2:B:89:LYS:HE2   | 0.46     | 2.12        | 18     | 1     |
| 2:B:94:LYS:O     | 2:B:98:ALA:HB2   | 0.46     | 2.11        | 18     | 1     |
| 2:B:101:THR:HB   | 2:B:171:THR:HG21 | 0.46     | 1.88        | 11     | 1     |
| 2:B:101:THR:OG1  | 2:B:142:GLU:HG2  | 0.46     | 2.10        | 3      | 1     |
| 1:A:16:G:OP2     | 2:B:49:ARG:HB3   | 0.46     | 2.11        | 3      | 1     |
| 1:A:14:A:OP1     | 2:B:95:LYS:CD    | 0.46     | 2.63        | 14     | 1     |
| 2:B:21:LEU:HD21  | 2:B:30:LEU:HD13  | 0.46     | 1.86        | 14     | 1     |
| 1:A:14:A:O4'     | 2:B:93:SER:O     | 0.46     | 2.35        | 17     | 1     |
| 2:B:116:LEU:HD11 | 2:B:139:ALA:CB   | 0.45     | 2.42        | 10     | 1     |
| 2:B:140:TYR:OH   | 2:B:171:THR:HG22 | 0.45     | 2.10        | 10     | 1     |
| 2:B:64:ALA:O     | 2:B:68:GLU:OE1   | 0.45     | 2.35        | 10     | 1     |
| 2:B:47:ASP:HB3   | 2:B:60:ASP:OD2   | 0.45     | 2.11        | 18     | 5     |
| 2:B:116:LEU:HD23 | 2:B:141:ILE:CD1  | 0.45     | 2.39        | 18     | 2     |
| 2:B:17:PHE:CE2   | 2:B:86:GLU:HG2   | 0.45     | 2.46        | 19     | 1     |
| 1:A:10:C:O2      | 1:A:11:C:C1'     | 0.45     | 2.64        | 18     | 1     |
| 2:B:143:PHE:CD2  | 2:B:149:ALA:HB2  | 0.45     | 2.45        | 18     | 1     |
| 1:A:12:C:C4'     | 1:A:13:G:OP1     | 0.45     | 2.64        | 5      | 1     |
| 2:B:86:GLU:HG3   | 2:B:87:LYS:N     | 0.45     | 2.26        | 13     | 4     |
| 2:B:90:GLY:O     | 2:B:91:ARG:HB2   | 0.45     | 2.11        | 2      | 2     |
| 2:B:21:LEU:HD13  | 2:B:30:LEU:HD22  | 0.45     | 1.87        | 6      | 1     |
| 2:B:102:LEU:C    | 2:B:102:LEU:CD1  | 0.45     | 2.85        | 11     | 1     |
| 2:B:107:LEU:CD1  | 2:B:111:ILE:HG22 | 0.45     | 2.41        | 11     | 1     |
| 1:A:14:A:O4'     | 2:B:94:LYS:CD    | 0.45     | 2.64        | 11     | 1     |
| 1:A:20:G:C4'     | 1:A:20:G:OP1     | 0.45     | 2.63        | 3      | 1     |
| 2:B:22:ASN:ND2   | 2:B:79:PHE:HB2   | 0.45     | 2.25        | 3      | 2     |
| 2:B:53:ASN:C     | 2:B:54:ARG:HG2   | 0.45     | 2.31        | 18     | 9     |
| 2:B:116:LEU:HD22 | 2:B:139:ALA:CB   | 0.45     | 2.41        | 8      | 1     |
| 2:B:37:LEU:O     | 2:B:41:ASN:HB2   | 0.45     | 2.12        | 11     | 4     |
| 2:B:107:LEU:CB   | 2:B:137:GLY:O    | 0.45     | 2.64        | 15     | 1     |
| 1:A:10:C:N1      | 2:B:140:TYR:CD2  | 0.45     | 2.84        | 15     | 1     |
| 2:B:12:THR:CG2   | 2:B:46:VAL:CG1   | 0.45     | 2.94        | 19     | 1     |
| 2:B:102:LEU:HD23 | 2:B:153:LEU:CD1  | 0.45     | 2.32        | 2      | 1     |
| 2:B:119:VAL:HG13 | 2:B:156:LYS:HE3  | 0.45     | 1.89        | 18     | 1     |
| 2:B:27:VAL:O     | 2:B:28:ALA:C     | 0.45     | 2.54        | 18     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:153:LEU:O    | 2:B:157:GLN:HG2  | 0.45     | 2.11        | 6      | 2     |
| 2:B:14:PHE:CZ    | 2:B:63:SER:O     | 0.45     | 2.69        | 13     | 1     |
| 2:B:110:ASN:HB3  | 2:B:162:ASP:OD2  | 0.45     | 2.11        | 7      | 2     |
| 2:B:51:GLY:O     | 2:B:52:THR:O     | 0.45     | 2.35        | 14     | 1     |
| 1:A:8:A:C2       | 2:B:95:LYS:HG2   | 0.45     | 2.47        | 17     | 1     |
| 2:B:159:ALA:O    | 2:B:161:ILE:HG12 | 0.45     | 2.10        | 17     | 1     |
| 2:B:163:GLY:O    | 2:B:164:ARG:HG2  | 0.45     | 2.12        | 5      | 6     |
| 1:A:10:C:H5"     | 1:A:11:C:OP2     | 0.45     | 2.11        | 10     | 2     |
| 2:B:83:ILE:O     | 2:B:83:ILE:HG13  | 0.45     | 2.12        | 10     | 2     |
| 2:B:21:LEU:HD13  | 2:B:56:PHE:CA    | 0.45     | 2.42        | 3      | 3     |
| 1:A:11:C:C2'     | 2:B:94:LYS:HZ2   | 0.45     | 2.25        | 15     | 1     |
| 2:B:61:PHE:CE2   | 2:B:70:ALA:HB2   | 0.45     | 2.45        | 2      | 2     |
| 2:B:22:ASN:OD1   | 2:B:24:ASN:N     | 0.45     | 2.50        | 9      | 1     |
| 2:B:38:PHE:CE2   | 2:B:73:LEU:CD1   | 0.45     | 2.99        | 9      | 1     |
| 2:B:128:LEU:HD11 | 2:B:130:SER:OG   | 0.45     | 2.12        | 4      | 1     |
| 2:B:37:LEU:HG    | 2:B:76:LEU:CD2   | 0.45     | 2.42        | 6      | 1     |
| 2:B:45:VAL:O     | 2:B:45:VAL:CG2   | 0.45     | 2.65        | 3      | 1     |
| 1:A:13:G:OP2     | 2:B:89:LYS:HG3   | 0.45     | 2.12        | 14     | 2     |
| 2:B:140:TYR:O    | 2:B:141:ILE:HG12 | 0.45     | 2.11        | 4      | 6     |
| 2:B:76:LEU:HB2   | 2:B:83:ILE:CD1   | 0.45     | 2.42        | 12     | 2     |
| 2:B:85:LEU:HD13  | 2:B:85:LEU:N     | 0.45     | 2.27        | 12     | 1     |
| 1:A:10:C:C5      | 2:B:140:TYR:OH   | 0.45     | 2.70        | 9      | 2     |
| 2:B:167:SER:C    | 2:B:168:LEU:HD22 | 0.45     | 2.32        | 18     | 2     |
| 2:B:127:ARG:O    | 2:B:140:TYR:HB2  | 0.45     | 2.12        | 11     | 4     |
| 2:B:151:LYS:O    | 2:B:155:GLU:N    | 0.45     | 2.44        | 16     | 1     |
| 2:B:107:LEU:HD22 | 2:B:107:LEU:N    | 0.45     | 2.25        | 13     | 2     |
| 2:B:15:ASN:CG    | 2:B:60:ASP:OD1   | 0.45     | 2.55        | 13     | 1     |
| 2:B:101:THR:HG23 | 2:B:142:GLU:CA   | 0.45     | 2.42        | 3      | 1     |
| 2:B:16:LEU:HA    | 2:B:88:PRO:HB3   | 0.45     | 1.87        | 14     | 3     |
| 2:B:21:LEU:HD23  | 2:B:54:ARG:HA    | 0.45     | 1.88        | 14     | 1     |
| 2:B:56:PHE:CD1   | 2:B:56:PHE:N     | 0.45     | 2.83        | 1      | 3     |
| 2:B:14:PHE:O     | 2:B:60:ASP:HA    | 0.45     | 2.11        | 3      | 4     |
| 1:A:9:U:C2'      | 1:A:10:C:OP1     | 0.45     | 2.63        | 8      | 2     |
| 2:B:157:GLN:HG3  | 2:B:158:GLY:N    | 0.45     | 2.26        | 8      | 1     |
| 2:B:74:THR:OG1   | 2:B:85:LEU:CD1   | 0.45     | 2.64        | 8      | 1     |
| 2:B:33:ALA:HB2   | 2:B:79:PHE:CE2   | 0.45     | 2.47        | 12     | 2     |
| 1:A:17:U:H2'     | 1:A:18:A:O5'     | 0.45     | 2.12        | 15     | 1     |
| 1:A:3:C:C2'      | 1:A:4:C:OP1      | 0.45     | 2.63        | 19     | 2     |
| 1:A:13:G:O5'     | 2:B:90:GLY:HA3   | 0.45     | 2.12        | 4      | 1     |
| 1:A:8:A:N1       | 1:A:14:A:N9      | 0.45     | 2.65        | 13     | 1     |
| 1:A:17:U:H2'     | 1:A:18:A:OP1     | 0.45     | 2.11        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:107:LEU:HD23 | 2:B:111:ILE:HG21 | 0.45     | 1.88        | 5      | 1     |
| 2:B:18:ILE:HG12  | 2:B:84:LYS:O     | 0.45     | 2.11        | 10     | 3     |
| 2:B:30:LEU:CD1   | 2:B:54:ARG:HB3   | 0.45     | 2.39        | 19     | 1     |
| 2:B:107:LEU:HD22 | 2:B:139:ALA:HB2  | 0.45     | 1.89        | 3      | 2     |
| 1:A:10:C:N4      | 2:B:140:TYR:CE2  | 0.45     | 2.85        | 1      | 1     |
| 2:B:14:PHE:CD2   | 2:B:63:SER:CA    | 0.45     | 3.00        | 1      | 1     |
| 2:B:18:ILE:HG12  | 2:B:85:LEU:HD13  | 0.45     | 1.87        | 1      | 1     |
| 2:B:73:LEU:O     | 2:B:83:ILE:HD13  | 0.45     | 2.12        | 14     | 1     |
| 2:B:94:LYS:HE2   | 2:B:94:LYS:HA    | 0.45     | 1.86        | 14     | 1     |
| 2:B:101:THR:HG22 | 2:B:102:LEU:N    | 0.45     | 2.27        | 5      | 2     |
| 2:B:85:LEU:HD13  | 2:B:86:GLU:H     | 0.45     | 1.67        | 5      | 1     |
| 2:B:61:PHE:HB3   | 2:B:66:ASP:CB    | 0.45     | 2.42        | 11     | 9     |
| 2:B:30:LEU:CD2   | 2:B:78:VAL:CG1   | 0.45     | 2.94        | 15     | 3     |
| 2:B:111:ILE:N    | 2:B:162:ASP:OD2  | 0.45     | 2.50        | 12     | 1     |
| 1:A:16:G:O6      | 2:B:54:ARG:NH1   | 0.45     | 2.49        | 15     | 2     |
| 2:B:143:PHE:HB3  | 2:B:148:ASP:OD1  | 0.45     | 2.12        | 19     | 1     |
| 1:A:11:C:O2      | 2:B:94:LYS:HB3   | 0.45     | 2.12        | 18     | 1     |
| 2:B:27:VAL:HG12  | 2:B:31:LYS:HE3   | 0.45     | 1.89        | 16     | 1     |
| 1:A:20:G:C2      | 1:A:21:C:C2      | 0.45     | 3.05        | 6      | 2     |
| 2:B:14:PHE:C     | 2:B:60:ASP:OD1   | 0.45     | 2.55        | 13     | 1     |
| 1:A:16:G:C6      | 2:B:54:ARG:NH2   | 0.45     | 2.85        | 7      | 1     |
| 2:B:47:ASP:C     | 2:B:60:ASP:OD2   | 0.45     | 2.56        | 1      | 1     |
| 1:A:12:C:O2'     | 1:A:13:G:O5'     | 0.45     | 2.34        | 17     | 1     |
| 2:B:53:ASN:C     | 2:B:54:ARG:HD3   | 0.45     | 2.32        | 5      | 3     |
| 1:A:13:G:OP1     | 2:B:89:LYS:HB3   | 0.45     | 2.12        | 12     | 1     |
| 2:B:94:LYS:HG3   | 2:B:95:LYS:N     | 0.45     | 2.27        | 12     | 1     |
| 2:B:34:ILE:HG23  | 2:B:38:PHE:CE1   | 0.45     | 2.46        | 15     | 1     |
| 1:A:10:C:H2'     | 1:A:11:C:OP1     | 0.45     | 2.12        | 2      | 1     |
| 2:B:124:LEU:HD12 | 2:B:143:PHE:C    | 0.45     | 2.32        | 7      | 2     |
| 2:B:129:VAL:HG23 | 2:B:139:ALA:HA   | 0.45     | 1.89        | 3      | 6     |
| 2:B:143:PHE:CG   | 2:B:149:ALA:CA   | 0.45     | 2.99        | 18     | 6     |
| 2:B:16:LEU:HA    | 2:B:88:PRO:CD    | 0.45     | 2.42        | 14     | 5     |
| 2:B:59:VAL:CG1   | 2:B:60:ASP:N     | 0.45     | 2.80        | 2      | 4     |
| 1:A:1:G:C1'      | 1:A:2:G:OP1      | 0.45     | 2.65        | 4      | 1     |
| 2:B:46:VAL:CG2   | 2:B:62:GLU:HG3   | 0.45     | 2.42        | 13     | 2     |
| 2:B:94:LYS:NZ    | 2:B:95:LYS:HE2   | 0.45     | 2.26        | 11     | 1     |
| 2:B:19:GLY:HA2   | 2:B:56:PHE:CB    | 0.44     | 2.42        | 9      | 3     |
| 2:B:74:THR:N     | 2:B:85:LEU:CD1   | 0.44     | 2.80        | 8      | 1     |
| 1:A:12:C:H1'     | 2:B:17:PHE:CE2   | 0.44     | 2.46        | 12     | 1     |
| 2:B:38:PHE:CE1   | 2:B:43:LEU:HD13  | 0.44     | 2.47        | 19     | 1     |
| 1:A:6:A:N1       | 1:A:7:A:C5       | 0.44     | 2.85        | 17     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:111:ILE:HD13 | 2:B:161:ILE:CG2  | 0.44     | 2.41        | 16     | 1     |
| 1:A:13:G:OP2     | 2:B:89:LYS:HD3   | 0.44     | 2.12        | 6      | 1     |
| 1:A:14:A:C8      | 1:A:14:A:O5'     | 0.44     | 2.69        | 6      | 1     |
| 2:B:12:THR:HB    | 2:B:13:PRO:HD2   | 0.44     | 1.87        | 13     | 1     |
| 2:B:159:ALA:O    | 2:B:160:GLU:O    | 0.44     | 2.35        | 13     | 1     |
| 2:B:21:LEU:HD12  | 2:B:50:THR:OG1   | 0.44     | 2.12        | 17     | 1     |
| 2:B:61:PHE:CZ    | 2:B:70:ALA:HB2   | 0.44     | 2.47        | 5      | 1     |
| 2:B:18:ILE:HG13  | 2:B:85:LEU:HD23  | 0.44     | 1.89        | 5      | 1     |
| 1:A:10:C:C2      | 2:B:140:TYR:CD1  | 0.44     | 3.05        | 10     | 1     |
| 2:B:120:PHE:HB3  | 2:B:123:ALA:HB2  | 0.44     | 1.88        | 10     | 1     |
| 2:B:123:ALA:HA   | 2:B:142:GLU:O    | 0.44     | 2.12        | 8      | 1     |
| 2:B:47:ASP:HB3   | 2:B:60:ASP:OD1   | 0.44     | 2.12        | 17     | 4     |
| 2:B:124:LEU:HD11 | 2:B:144:LYS:CA   | 0.44     | 2.42        | 16     | 2     |
| 2:B:14:PHE:CZ    | 2:B:64:ALA:CB    | 0.44     | 2.99        | 19     | 1     |
| 2:B:88:PRO:O     | 2:B:89:LYS:HB3   | 0.44     | 2.12        | 4      | 1     |
| 1:A:9:U:C5       | 2:B:103:LEU:HD22 | 0.44     | 2.48        | 6      | 1     |
| 2:B:110:ASN:O    | 2:B:111:ILE:C    | 0.44     | 2.54        | 6      | 2     |
| 2:B:125:GLU:HG2  | 2:B:142:GLU:CG   | 0.44     | 2.42        | 6      | 1     |
| 1:A:14:A:N1      | 2:B:94:LYS:CE    | 0.44     | 2.81        | 13     | 1     |
| 2:B:105:LYS:HG3  | 2:B:169:TYR:CG   | 0.44     | 2.47        | 11     | 1     |
| 2:B:58:TYR:C     | 2:B:59:VAL:HG23  | 0.44     | 2.32        | 10     | 3     |
| 2:B:156:LYS:HB2  | 2:B:168:LEU:CD1  | 0.44     | 2.41        | 4      | 2     |
| 2:B:147:ALA:O    | 2:B:151:LYS:N    | 0.44     | 2.46        | 8      | 1     |
| 2:B:125:GLU:O    | 2:B:126:ILE:HG12 | 0.44     | 2.12        | 12     | 1     |
| 2:B:130:SER:HB3  | 2:B:136:LYS:HD2  | 0.44     | 1.89        | 15     | 1     |
| 2:B:51:GLY:HA3   | 2:B:56:PHE:HD1   | 0.44     | 1.73        | 19     | 1     |
| 2:B:25:LYS:O     | 2:B:54:ARG:CZ    | 0.44     | 2.66        | 4      | 1     |
| 2:B:168:LEU:CD2  | 2:B:168:LEU:N    | 0.44     | 2.80        | 6      | 3     |
| 2:B:128:LEU:C    | 2:B:128:LEU:CD2  | 0.44     | 2.72        | 16     | 1     |
| 2:B:140:TYR:O    | 2:B:141:ILE:HG13 | 0.44     | 2.11        | 11     | 1     |
| 1:A:9:U:H5       | 2:B:103:LEU:HD11 | 0.44     | 1.71        | 5      | 2     |
| 2:B:14:PHE:CB    | 2:B:61:PHE:HB2   | 0.44     | 2.42        | 15     | 5     |
| 2:B:116:LEU:O    | 2:B:120:PHE:HB2  | 0.44     | 2.13        | 7      | 9     |
| 2:B:152:ASN:O    | 2:B:156:LYS:HG2  | 0.44     | 2.12        | 10     | 1     |
| 2:B:108:SER:HB3  | 2:B:162:ASP:OD2  | 0.44     | 2.13        | 6      | 3     |
| 2:B:120:PHE:O    | 2:B:121:GLU:C    | 0.44     | 2.54        | 11     | 3     |
| 2:B:92:ASP:O     | 2:B:93:SER:HB2   | 0.44     | 2.12        | 12     | 2     |
| 2:B:128:LEU:CD2  | 2:B:136:LYS:HG3  | 0.44     | 2.43        | 15     | 1     |
| 1:A:2:G:N1       | 1:A:3:C:C2       | 0.44     | 2.85        | 9      | 1     |
| 2:B:120:PHE:CD2  | 2:B:141:ILE:HG21 | 0.44     | 2.48        | 9      | 2     |
| 2:B:128:LEU:C    | 2:B:128:LEU:CD1  | 0.44     | 2.85        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:13:G:C5'     | 1:A:14:A:OP1     | 0.44     | 2.66        | 18     | 1     |
| 2:B:31:LYS:HG3   | 2:B:48:VAL:CG2   | 0.44     | 2.42        | 16     | 1     |
| 2:B:47:ASP:CB    | 2:B:60:ASP:CG    | 0.44     | 2.85        | 16     | 1     |
| 2:B:101:THR:HG21 | 2:B:140:TYR:CD2  | 0.44     | 2.48        | 17     | 3     |
| 1:A:13:G:OP1     | 2:B:94:LYS:HB2   | 0.44     | 2.11        | 14     | 1     |
| 2:B:166:VAL:CG1  | 2:B:167:SER:N    | 0.44     | 2.80        | 14     | 1     |
| 1:A:14:A:O5'     | 2:B:94:LYS:CB    | 0.44     | 2.65        | 17     | 1     |
| 1:A:10:C:H42     | 2:B:94:LYS:CD    | 0.44     | 2.26        | 8      | 1     |
| 1:A:10:C:C2      | 2:B:140:TYR:CE2  | 0.44     | 3.05        | 15     | 1     |
| 2:B:162:ASP:OD2  | 2:B:164:ARG:HG2  | 0.44     | 2.12        | 9      | 1     |
| 1:A:12:C:OP1     | 1:A:12:C:N1      | 0.44     | 2.50        | 6      | 1     |
| 2:B:144:LYS:HG2  | 2:B:148:ASP:CB   | 0.44     | 2.43        | 3      | 1     |
| 1:A:12:C:C2'     | 1:A:13:G:OP2     | 0.44     | 2.66        | 1      | 1     |
| 2:B:78:VAL:HG12  | 2:B:81:ASN:HB2   | 0.44     | 1.89        | 5      | 1     |
| 2:B:112:THR:N    | 2:B:115:GLU:OE1  | 0.44     | 2.51        | 17     | 3     |
| 2:B:25:LYS:HG2   | 2:B:79:PHE:CD2   | 0.44     | 2.48        | 15     | 1     |
| 2:B:107:LEU:CD2  | 2:B:111:ILE:HG21 | 0.44     | 2.43        | 9      | 1     |
| 2:B:62:GLU:HG3   | 2:B:66:ASP:OD2   | 0.44     | 2.13        | 4      | 2     |
| 1:A:20:G:H2'     | 1:A:20:G:N3      | 0.44     | 2.27        | 18     | 1     |
| 1:A:17:U:O2'     | 1:A:18:A:O5'     | 0.44     | 2.32        | 16     | 1     |
| 2:B:27:VAL:HG12  | 2:B:31:LYS:CE    | 0.44     | 2.43        | 16     | 1     |
| 1:A:12:C:N3      | 2:B:17:PHE:HZ    | 0.44     | 2.10        | 6      | 2     |
| 2:B:102:LEU:CD1  | 2:B:141:ILE:HB   | 0.44     | 2.43        | 6      | 1     |
| 2:B:151:LYS:CE   | 2:B:155:GLU:OE1  | 0.44     | 2.66        | 3      | 1     |
| 1:A:14:A:P       | 2:B:91:ARG:HB2   | 0.44     | 2.52        | 7      | 1     |
| 2:B:155:GLU:O    | 2:B:155:GLU:OE2  | 0.44     | 2.36        | 1      | 1     |
| 2:B:78:VAL:HG12  | 2:B:78:VAL:O     | 0.44     | 2.13        | 1      | 1     |
| 2:B:98:ALA:CA    | 2:B:171:THR:HB   | 0.44     | 2.42        | 5      | 1     |
| 1:A:11:C:C2      | 2:B:94:LYS:CE    | 0.44     | 3.01        | 6      | 2     |
| 2:B:151:LYS:O    | 2:B:154:GLU:HG2  | 0.44     | 2.12        | 8      | 1     |
| 2:B:92:ASP:OD1   | 2:B:97:ARG:N     | 0.44     | 2.51        | 8      | 1     |
| 2:B:61:PHE:CB    | 2:B:66:ASP:OD1   | 0.44     | 2.66        | 18     | 2     |
| 2:B:26:SER:OG    | 2:B:29:GLU:HG2   | 0.44     | 2.12        | 12     | 1     |
| 2:B:103:LEU:CD1  | 2:B:138:ILE:HG21 | 0.44     | 2.43        | 15     | 2     |
| 2:B:107:LEU:CD1  | 2:B:138:ILE:C    | 0.44     | 2.86        | 9      | 2     |
| 2:B:21:LEU:HD22  | 2:B:30:LEU:HG    | 0.44     | 1.89        | 9      | 1     |
| 2:B:74:THR:CG2   | 2:B:85:LEU:CD1   | 0.44     | 2.96        | 19     | 1     |
| 1:A:14:A:C2'     | 2:B:52:THR:CG2   | 0.44     | 2.95        | 2      | 1     |
| 2:B:111:ILE:CD1  | 2:B:162:ASP:HB2  | 0.44     | 2.43        | 2      | 2     |
| 2:B:105:LYS:HD2  | 2:B:169:TYR:CE1  | 0.44     | 2.47        | 18     | 1     |
| 2:B:18:ILE:HD13  | 2:B:59:VAL:HB    | 0.44     | 1.89        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:14:A:N6      | 2:B:94:LYS:CD    | 0.44     | 2.80        | 13     | 1     |
| 2:B:61:PHE:HB3   | 2:B:66:ASP:OD2   | 0.44     | 2.13        | 5      | 3     |
| 2:B:44:ALA:CB    | 2:B:62:GLU:HG2   | 0.44     | 2.37        | 5      | 1     |
| 2:B:12:THR:OG1   | 2:B:46:VAL:CG1   | 0.44     | 2.66        | 10     | 1     |
| 1:A:16:G:C5      | 2:B:27:VAL:HB    | 0.44     | 2.48        | 8      | 1     |
| 1:A:1:G:C2       | 1:A:2:G:C8       | 0.44     | 3.06        | 12     | 1     |
| 2:B:111:ILE:HG13 | 2:B:115:GLU:CG   | 0.44     | 2.43        | 9      | 1     |
| 2:B:30:LEU:HD13  | 2:B:50:THR:OG1   | 0.44     | 2.12        | 19     | 1     |
| 1:A:20:G:C5'     | 1:A:21:C:OP2     | 0.44     | 2.66        | 2      | 1     |
| 2:B:105:LYS:HE3  | 2:B:169:TYR:CE2  | 0.44     | 2.47        | 6      | 1     |
| 1:A:13:G:P       | 2:B:89:LYS:HB2   | 0.44     | 2.52        | 13     | 1     |
| 2:B:70:ALA:HA    | 2:B:73:LEU:CD2   | 0.44     | 2.42        | 11     | 1     |
| 2:B:101:THR:O    | 2:B:171:THR:CB   | 0.44     | 2.66        | 7      | 1     |
| 2:B:38:PHE:HB3   | 2:B:43:LEU:HB2   | 0.44     | 1.88        | 7      | 1     |
| 1:A:12:C:N4      | 2:B:86:GLU:OE1   | 0.44     | 2.50        | 17     | 1     |
| 1:A:14:A:C4      | 2:B:94:LYS:HB3   | 0.44     | 2.47        | 5      | 1     |
| 2:B:46:VAL:C     | 2:B:47:ASP:CG    | 0.44     | 2.77        | 5      | 1     |
| 2:B:124:LEU:HB2  | 2:B:142:GLU:CG   | 0.44     | 2.43        | 10     | 1     |
| 2:B:152:ASN:O    | 2:B:156:LYS:HB2  | 0.44     | 2.13        | 10     | 4     |
| 2:B:73:LEU:C     | 2:B:76:LEU:HD22  | 0.44     | 2.33        | 9      | 1     |
| 2:B:19:GLY:HA2   | 2:B:56:PHE:HA    | 0.44     | 1.90        | 9      | 1     |
| 2:B:48:VAL:O     | 2:B:49:ARG:HG2   | 0.44     | 2.13        | 19     | 1     |
| 2:B:22:ASN:C     | 2:B:54:ARG:HB2   | 0.44     | 2.33        | 6      | 3     |
| 2:B:142:GLU:HG3  | 2:B:142:GLU:O    | 0.44     | 2.13        | 6      | 1     |
| 2:B:93:SER:HA    | 2:B:97:ARG:HG3   | 0.44     | 1.89        | 7      | 1     |
| 1:A:13:G:H4'     | 1:A:14:A:O5'     | 0.44     | 2.13        | 1      | 1     |
| 2:B:49:ARG:NH2   | 2:B:60:ASP:OD1   | 0.44     | 2.51        | 1      | 1     |
| 2:B:147:ALA:O    | 2:B:151:LYS:HB3  | 0.44     | 2.12        | 17     | 1     |
| 2:B:43:LEU:HD23  | 2:B:66:ASP:OD1   | 0.43     | 2.13        | 5      | 1     |
| 2:B:162:ASP:O    | 2:B:164:ARG:HG3  | 0.43     | 2.13        | 6      | 6     |
| 2:B:102:LEU:C    | 2:B:102:LEU:CD2  | 0.43     | 2.86        | 10     | 1     |
| 2:B:43:LEU:CD1   | 2:B:66:ASP:OD1   | 0.43     | 2.66        | 10     | 2     |
| 2:B:120:PHE:CD1  | 2:B:141:ILE:HG21 | 0.43     | 2.48        | 12     | 1     |
| 2:B:140:TYR:C    | 2:B:141:ILE:CD1  | 0.43     | 2.83        | 12     | 1     |
| 2:B:163:GLY:O    | 2:B:164:ARG:HB3  | 0.43     | 2.13        | 9      | 4     |
| 2:B:104:ALA:O    | 2:B:107:LEU:HD12 | 0.43     | 2.12        | 9      | 1     |
| 2:B:107:LEU:HD12 | 2:B:111:ILE:HG21 | 0.43     | 1.88        | 19     | 1     |
| 2:B:90:GLY:O     | 2:B:91:ARG:CB    | 0.43     | 2.64        | 2      | 1     |
| 2:B:116:LEU:HB3  | 2:B:126:ILE:HG21 | 0.43     | 1.90        | 13     | 2     |
| 1:A:16:G:C6      | 2:B:54:ARG:CZ    | 0.43     | 3.00        | 6      | 1     |
| 1:A:9:U:O4       | 2:B:105:LYS:HE3  | 0.43     | 2.13        | 11     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:102:LEU:CD1  | 2:B:170:TYR:CE1  | 0.43     | 3.01        | 3      | 1     |
| 2:B:33:ALA:O     | 2:B:37:LEU:HB2   | 0.43     | 2.13        | 7      | 10    |
| 2:B:49:ARG:HB3   | 2:B:58:TYR:CB    | 0.43     | 2.42        | 8      | 1     |
| 2:B:74:THR:OG1   | 2:B:85:LEU:HD12  | 0.43     | 2.13        | 8      | 1     |
| 2:B:147:ALA:O    | 2:B:151:LYS:HB2  | 0.43     | 2.12        | 16     | 5     |
| 2:B:92:ASP:HB3   | 2:B:96:VAL:CB    | 0.43     | 2.43        | 15     | 1     |
| 2:B:158:GLY:HA3  | 2:B:166:VAL:CB   | 0.43     | 2.43        | 9      | 1     |
| 2:B:76:LEU:CB    | 2:B:83:ILE:CD1   | 0.43     | 2.96        | 19     | 1     |
| 2:B:77:LYS:HA    | 2:B:82:GLU:CA    | 0.43     | 2.44        | 3      | 2     |
| 2:B:21:LEU:HB2   | 2:B:54:ARG:C     | 0.43     | 2.34        | 13     | 1     |
| 2:B:38:PHE:N     | 2:B:38:PHE:CD1   | 0.43     | 2.86        | 13     | 2     |
| 2:B:30:LEU:HD11  | 2:B:54:ARG:HD2   | 0.43     | 1.89        | 11     | 1     |
| 1:A:3:C:C2'      | 1:A:4:C:O5'      | 0.43     | 2.66        | 14     | 1     |
| 2:B:69:LYS:O     | 2:B:73:LEU:HB2   | 0.43     | 2.13        | 9      | 3     |
| 2:B:107:LEU:HD22 | 2:B:111:ILE:HG21 | 0.43     | 1.88        | 9      | 1     |
| 2:B:111:ILE:HA   | 2:B:115:GLU:OE1  | 0.43     | 2.12        | 19     | 1     |
| 1:A:14:A:C5      | 2:B:94:LYS:HG3   | 0.43     | 2.47        | 2      | 1     |
| 2:B:21:LEU:CD2   | 2:B:30:LEU:HD23  | 0.43     | 2.43        | 4      | 1     |
| 2:B:37:LEU:O     | 2:B:37:LEU:HD23  | 0.43     | 2.12        | 4      | 1     |
| 2:B:37:LEU:HD13  | 2:B:41:ASN:ND2   | 0.43     | 2.29        | 6      | 1     |
| 2:B:16:LEU:C     | 2:B:16:LEU:CD2   | 0.43     | 2.76        | 13     | 1     |
| 1:A:10:C:O2'     | 1:A:11:C:P       | 0.43     | 2.76        | 11     | 1     |
| 2:B:62:GLU:N     | 2:B:66:ASP:OD2   | 0.43     | 2.48        | 17     | 1     |
| 1:A:1:G:O6       | 1:A:2:G:O6       | 0.43     | 2.36        | 12     | 1     |
| 1:A:10:C:C3'     | 2:B:128:LEU:O    | 0.43     | 2.66        | 15     | 1     |
| 2:B:56:PHE:HZ    | 2:B:58:TYR:CE2   | 0.43     | 2.32        | 19     | 1     |
| 2:B:115:GLU:CD   | 2:B:115:GLU:C    | 0.43     | 2.77        | 2      | 1     |
| 2:B:15:ASN:O     | 2:B:16:LEU:HB2   | 0.43     | 2.14        | 16     | 1     |
| 2:B:120:PHE:CE2  | 2:B:168:LEU:HD11 | 0.43     | 2.49        | 6      | 1     |
| 2:B:94:LYS:HD2   | 2:B:94:LYS:O     | 0.43     | 2.14        | 17     | 2     |
| 1:A:12:C:O2      | 1:A:12:C:OP2     | 0.43     | 2.36        | 13     | 1     |
| 2:B:102:LEU:HD11 | 2:B:143:PHE:CD1  | 0.43     | 2.49        | 2      | 2     |
| 2:B:158:GLY:HA3  | 2:B:166:VAL:HB   | 0.43     | 1.89        | 9      | 1     |
| 2:B:27:VAL:CB    | 2:B:31:LYS:HE3   | 0.43     | 2.43        | 9      | 1     |
| 2:B:49:ARG:CG    | 2:B:58:TYR:CB    | 0.43     | 2.96        | 19     | 1     |
| 2:B:18:ILE:HG13  | 2:B:85:LEU:HG    | 0.43     | 1.89        | 16     | 3     |
| 2:B:37:LEU:HD21  | 2:B:76:LEU:CD2   | 0.43     | 2.37        | 2      | 1     |
| 2:B:17:PHE:CD2   | 2:B:86:GLU:CG    | 0.43     | 3.01        | 1      | 2     |
| 2:B:115:GLU:C    | 2:B:115:GLU:CD   | 0.43     | 2.77        | 18     | 1     |
| 2:B:38:PHE:CB    | 2:B:43:LEU:HB2   | 0.43     | 2.44        | 7      | 1     |
| 2:B:38:PHE:HE2   | 2:B:73:LEU:HD21  | 0.43     | 1.72        | 8      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:1:G:C2'     | 1:A:1:G:N3       | 0.43     | 2.76        | 12     | 1     |
| 2:B:59:VAL:C    | 2:B:60:ASP:CG    | 0.43     | 2.77        | 15     | 2     |
| 2:B:32:VAL:HA   | 2:B:35:SER:OG    | 0.43     | 2.13        | 2      | 1     |
| 2:B:69:LYS:HG2  | 2:B:73:LEU:CD2   | 0.43     | 2.43        | 4      | 1     |
| 2:B:97:ARG:CZ   | 2:B:142:GLU:OE2  | 0.43     | 2.66        | 18     | 1     |
| 1:A:9:U:O3'     | 1:A:10:C:C6      | 0.43     | 2.72        | 1      | 2     |
| 2:B:76:LEU:O    | 2:B:83:ILE:HD12  | 0.43     | 2.13        | 12     | 1     |
| 2:B:17:PHE:CE2  | 2:B:86:GLU:CD    | 0.43     | 2.92        | 4      | 1     |
| 2:B:48:VAL:HG13 | 2:B:59:VAL:HG22  | 0.43     | 1.88        | 18     | 1     |
| 2:B:66:ASP:CG   | 2:B:67:LEU:N     | 0.43     | 2.71        | 18     | 1     |
| 2:B:18:ILE:HD11 | 2:B:85:LEU:CD1   | 0.43     | 2.44        | 6      | 1     |
| 2:B:15:ASN:CG   | 2:B:60:ASP:CG    | 0.43     | 2.77        | 13     | 1     |
| 1:A:17:U:O2'    | 1:A:18:A:P       | 0.43     | 2.77        | 11     | 1     |
| 2:B:25:LYS:CE   | 2:B:79:PHE:CD1   | 0.43     | 3.02        | 8      | 1     |
| 2:B:97:ARG:O    | 2:B:100:ARG:N    | 0.43     | 2.51        | 19     | 3     |
| 2:B:73:LEU:HG   | 2:B:76:LEU:CD1   | 0.43     | 2.44        | 18     | 1     |
| 2:B:59:VAL:HG13 | 2:B:61:PHE:CZ    | 0.43     | 2.48        | 1      | 1     |
| 1:A:8:A:H61     | 1:A:14:A:C1'     | 0.43     | 2.27        | 14     | 1     |
| 1:A:6:A:C8      | 1:A:18:A:C6      | 0.43     | 3.06        | 17     | 1     |
| 1:A:6:A:N1      | 1:A:7:A:C4       | 0.43     | 2.87        | 17     | 1     |
| 2:B:153:LEU:O   | 2:B:153:LEU:HD13 | 0.43     | 2.14        | 15     | 1     |
| 2:B:37:LEU:HD13 | 2:B:76:LEU:CG    | 0.43     | 2.44        | 15     | 1     |
| 2:B:102:LEU:O   | 2:B:140:TYR:HA   | 0.43     | 2.13        | 9      | 1     |
| 2:B:144:LYS:O   | 2:B:145:SER:HB3  | 0.43     | 2.14        | 19     | 1     |
| 1:A:4:C:O2'     | 1:A:5:G:C3'      | 0.43     | 2.66        | 4      | 1     |
| 1:A:5:G:C4'     | 1:A:6:A:OP1      | 0.43     | 2.67        | 4      | 1     |
| 2:B:20:ASN:O    | 2:B:83:ILE:HG22  | 0.43     | 2.13        | 4      | 2     |
| 1:A:10:C:O2     | 2:B:127:ARG:CD   | 0.43     | 2.66        | 6      | 2     |
| 2:B:94:LYS:HE2  | 2:B:127:ARG:NH2  | 0.43     | 2.28        | 6      | 1     |
| 2:B:41:ASN:C    | 2:B:42:ASP:CG    | 0.43     | 2.76        | 13     | 2     |
| 1:A:10:C:C5     | 1:A:11:C:C4      | 0.43     | 3.06        | 14     | 1     |
| 2:B:159:ALA:O   | 2:B:161:ILE:HG13 | 0.43     | 2.14        | 9      | 5     |
| 2:B:38:PHE:CB   | 2:B:45:VAL:HG21  | 0.43     | 2.44        | 8      | 2     |
| 2:B:153:LEU:HA  | 2:B:168:LEU:HD12 | 0.43     | 1.91        | 9      | 1     |
| 2:B:159:ALA:O   | 2:B:165:SER:HA   | 0.43     | 2.13        | 9      | 2     |
| 2:B:59:VAL:HG11 | 2:B:61:PHE:CE1   | 0.43     | 2.48        | 18     | 1     |
| 2:B:119:VAL:CG1 | 2:B:159:ALA:HB1  | 0.43     | 2.43        | 16     | 1     |
| 2:B:101:THR:C   | 2:B:171:THR:OG1  | 0.43     | 2.58        | 6      | 1     |
| 2:B:50:THR:OG1  | 2:B:51:GLY:N     | 0.43     | 2.51        | 6      | 1     |
| 2:B:61:PHE:N    | 2:B:61:PHE:CD1   | 0.43     | 2.86        | 11     | 1     |
| 2:B:94:LYS:HE2  | 2:B:94:LYS:O     | 0.43     | 2.13        | 14     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:66:ASP:OD1   | 2:B:66:ASP:O     | 0.42     | 2.37        | 5      | 1     |
| 2:B:130:SER:C    | 2:B:136:LYS:HB2  | 0.42     | 2.34        | 3      | 3     |
| 1:A:6:A:C2'      | 1:A:7:A:O5'      | 0.42     | 2.66        | 10     | 1     |
| 2:B:94:LYS:O     | 2:B:94:LYS:HE3   | 0.42     | 2.14        | 10     | 1     |
| 2:B:47:ASP:CB    | 2:B:60:ASP:HB2   | 0.42     | 2.44        | 8      | 1     |
| 1:A:10:C:C2'     | 2:B:128:LEU:O    | 0.42     | 2.67        | 15     | 1     |
| 2:B:13:PRO:HG2   | 2:B:14:PHE:CE2   | 0.42     | 2.49        | 13     | 2     |
| 2:B:27:VAL:O     | 2:B:31:LYS:HD2   | 0.42     | 2.13        | 9      | 2     |
| 2:B:51:GLY:N     | 2:B:57:GLY:CA    | 0.42     | 2.82        | 9      | 1     |
| 2:B:95:LYS:HG2   | 2:B:95:LYS:O     | 0.42     | 2.13        | 19     | 1     |
| 2:B:46:VAL:HG23  | 2:B:61:PHE:CA    | 0.42     | 2.44        | 18     | 1     |
| 1:A:8:A:C6       | 1:A:14:A:C5      | 0.42     | 3.07        | 5      | 1     |
| 2:B:56:PHE:N     | 2:B:56:PHE:CD1   | 0.42     | 2.87        | 9      | 2     |
| 2:B:38:PHE:CD1   | 2:B:38:PHE:N     | 0.42     | 2.85        | 8      | 2     |
| 2:B:153:LEU:HD23 | 2:B:168:LEU:HB3  | 0.42     | 1.91        | 15     | 1     |
| 2:B:74:THR:CG2   | 2:B:74:THR:O     | 0.42     | 2.66        | 17     | 2     |
| 2:B:81:ASN:OD1   | 2:B:81:ASN:N     | 0.42     | 2.52        | 9      | 1     |
| 2:B:47:ASP:O     | 2:B:48:VAL:HB    | 0.42     | 2.13        | 19     | 1     |
| 1:A:14:A:OP1     | 1:A:14:A:C8      | 0.42     | 2.72        | 17     | 2     |
| 1:A:19:G:C2      | 1:A:20:G:H1'     | 0.42     | 2.49        | 17     | 2     |
| 2:B:29:GLU:O     | 2:B:33:ALA:CB    | 0.42     | 2.67        | 18     | 1     |
| 2:B:73:LEU:HD22  | 2:B:76:LEU:CG    | 0.42     | 2.43        | 13     | 1     |
| 2:B:118:GLU:OE1  | 2:B:118:GLU:HA   | 0.42     | 2.13        | 7      | 1     |
| 2:B:102:LEU:O    | 2:B:102:LEU:HG   | 0.42     | 2.13        | 1      | 1     |
| 1:A:14:A:O5'     | 2:B:94:LYS:HB2   | 0.42     | 2.15        | 17     | 1     |
| 2:B:22:ASN:HB2   | 2:B:30:LEU:CD2   | 0.42     | 2.44        | 17     | 1     |
| 1:A:20:G:O6      | 1:A:21:C:N4      | 0.42     | 2.52        | 5      | 1     |
| 1:A:10:C:H42     | 2:B:94:LYS:HD3   | 0.42     | 1.73        | 8      | 1     |
| 2:B:101:THR:CA   | 2:B:102:LEU:HD13 | 0.42     | 2.43        | 19     | 1     |
| 2:B:22:ASN:OD1   | 2:B:25:LYS:CD    | 0.42     | 2.67        | 2      | 1     |
| 2:B:130:SER:HA   | 2:B:136:LYS:HB3  | 0.42     | 1.91        | 3      | 2     |
| 2:B:21:LEU:HD23  | 2:B:21:LEU:HA    | 0.42     | 1.70        | 18     | 2     |
| 2:B:97:ARG:O     | 2:B:101:THR:CB   | 0.42     | 2.67        | 7      | 1     |
| 2:B:26:SER:O     | 2:B:30:LEU:HG    | 0.42     | 2.14        | 17     | 1     |
| 2:B:37:LEU:CD2   | 2:B:76:LEU:CD2   | 0.42     | 2.88        | 4      | 2     |
| 2:B:158:GLY:HA2  | 2:B:166:VAL:N    | 0.42     | 2.29        | 16     | 3     |
| 2:B:43:LEU:CD2   | 2:B:69:LYS:HD2   | 0.42     | 2.45        | 4      | 1     |
| 2:B:136:LYS:HD3  | 2:B:138:ILE:CD1  | 0.42     | 2.45        | 18     | 1     |
| 2:B:102:LEU:CD2  | 2:B:141:ILE:O    | 0.42     | 2.64        | 13     | 1     |
| 2:B:65:GLU:O     | 2:B:69:LYS:HD2   | 0.42     | 2.15        | 11     | 2     |
| 2:B:53:ASN:C     | 2:B:54:ARG:CG    | 0.42     | 2.85        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:125:GLU:HG3 | 2:B:142:GLU:CB  | 0.42     | 2.45        | 8      | 1     |
| 1:A:10:C:O2'    | 2:B:127:ARG:CB  | 0.42     | 2.67        | 15     | 1     |
| 2:B:16:LEU:HD12 | 2:B:17:PHE:O    | 0.42     | 2.14        | 18     | 1     |
| 1:A:20:G:N3     | 1:A:20:G:H2'    | 0.42     | 2.30        | 16     | 1     |
| 1:A:9:U:O4      | 2:B:105:LYS:HE2 | 0.42     | 2.15        | 7      | 1     |
| 2:B:51:GLY:O    | 2:B:56:PHE:CE1  | 0.42     | 2.71        | 1      | 1     |
| 2:B:48:VAL:HG22 | 2:B:59:VAL:HG23 | 0.42     | 1.92        | 1      | 1     |
| 1:A:9:U:OP2     | 1:A:9:U:H3'     | 0.42     | 2.15        | 14     | 1     |
| 2:B:31:LYS:HG2  | 2:B:48:VAL:CG1  | 0.42     | 2.45        | 17     | 1     |
| 1:A:11:C:O2     | 2:B:94:LYS:HG2  | 0.42     | 2.14        | 12     | 1     |
| 1:A:15:A:C2     | 1:A:16:G:C2     | 0.42     | 3.08        | 12     | 1     |
| 2:B:128:LEU:HG  | 2:B:136:LYS:HB3 | 0.42     | 1.90        | 15     | 1     |
| 2:B:139:ALA:O   | 2:B:141:ILE:CD1 | 0.42     | 2.68        | 15     | 1     |
| 2:B:98:ALA:CB   | 2:B:171:THR:CG2 | 0.42     | 2.85        | 15     | 1     |
| 1:A:2:G:O6      | 1:A:3:C:C4      | 0.42     | 2.72        | 1      | 2     |
| 2:B:142:GLU:CA  | 2:B:142:GLU:OE1 | 0.42     | 2.68        | 9      | 1     |
| 2:B:93:SER:HB2  | 2:B:95:LYS:HZ2  | 0.42     | 1.75        | 19     | 1     |
| 2:B:24:ASN:O    | 2:B:25:LYS:HD3  | 0.42     | 2.15        | 4      | 1     |
| 2:B:127:ARG:NH1 | 2:B:140:TYR:CD2 | 0.42     | 2.88        | 16     | 1     |
| 2:B:158:GLY:O   | 2:B:159:ALA:CB  | 0.42     | 2.64        | 16     | 1     |
| 2:B:31:LYS:O    | 2:B:35:SER:HB2  | 0.42     | 2.14        | 11     | 1     |
| 2:B:92:ASP:HB3  | 2:B:96:VAL:CG1  | 0.42     | 2.45        | 3      | 3     |
| 1:A:9:U:O2      | 1:A:9:U:O4'     | 0.42     | 2.36        | 15     | 1     |
| 2:B:161:ILE:CD1 | 2:B:166:VAL:HB  | 0.42     | 2.44        | 15     | 1     |
| 2:B:92:ASP:HB3  | 2:B:96:VAL:HG12 | 0.42     | 1.91        | 15     | 1     |
| 2:B:18:ILE:HD12 | 2:B:59:VAL:CB   | 0.42     | 2.44        | 9      | 1     |
| 2:B:49:ARG:CD   | 2:B:58:TYR:HB2  | 0.42     | 2.44        | 19     | 1     |
| 2:B:62:GLU:O    | 2:B:63:SER:HB3  | 0.42     | 2.15        | 19     | 2     |
| 2:B:11:THR:O    | 2:B:11:THR:CG2  | 0.42     | 2.68        | 19     | 2     |
| 2:B:114:ASP:O   | 2:B:118:GLU:HB2 | 0.42     | 2.15        | 19     | 2     |
| 2:B:37:LEU:CD2  | 2:B:76:LEU:HB3  | 0.42     | 2.42        | 2      | 1     |
| 1:A:11:C:C4     | 2:B:94:LYS:CE   | 0.42     | 3.03        | 18     | 1     |
| 2:B:37:LEU:HD22 | 2:B:37:LEU:HA   | 0.42     | 1.72        | 6      | 1     |
| 1:A:11:C:O2     | 2:B:94:LYS:HE2  | 0.42     | 2.14        | 6      | 1     |
| 1:A:20:G:HO2'   | 1:A:21:C:P      | 0.42     | 2.37        | 13     | 1     |
| 1:A:16:G:H5"    | 2:B:50:THR:HG22 | 0.42     | 1.91        | 3      | 1     |
| 2:B:153:LEU:C   | 2:B:153:LEU:CD2 | 0.42     | 2.84        | 1      | 1     |
| 1:A:18:A:H2'    | 1:A:19:G:O5'    | 0.42     | 2.14        | 1      | 1     |
| 1:A:3:C:C4      | 1:A:4:C:C4      | 0.42     | 3.07        | 14     | 1     |
| 2:B:116:LEU:N   | 2:B:116:LEU:CD2 | 0.42     | 2.82        | 17     | 1     |
| 2:B:54:ARG:NH1  | 2:B:54:ARG:CG   | 0.42     | 2.83        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:129:VAL:HG23 | 2:B:138:ILE:HB   | 0.42     | 1.91        | 15     | 1     |
| 1:A:13:G:OP1     | 2:B:90:GLY:HA2   | 0.42     | 2.15        | 19     | 1     |
| 2:B:12:THR:HG23  | 2:B:46:VAL:CG1   | 0.42     | 2.45        | 19     | 1     |
| 2:B:48:VAL:HG23  | 2:B:58:TYR:O     | 0.42     | 2.15        | 19     | 1     |
| 2:B:25:LYS:CE    | 2:B:79:PHE:CE1   | 0.42     | 3.03        | 19     | 1     |
| 2:B:157:GLN:N    | 2:B:168:LEU:HD12 | 0.42     | 2.30        | 4      | 1     |
| 2:B:101:THR:HB   | 2:B:171:THR:CG2  | 0.42     | 2.44        | 18     | 1     |
| 2:B:143:PHE:CD2  | 2:B:149:ALA:CA   | 0.42     | 3.02        | 18     | 1     |
| 2:B:92:ASP:HB3   | 2:B:97:ARG:CG    | 0.42     | 2.44        | 6      | 1     |
| 2:B:73:LEU:O     | 2:B:76:LEU:HG    | 0.42     | 2.15        | 13     | 1     |
| 2:B:103:LEU:HB3  | 2:B:169:TYR:O    | 0.42     | 2.14        | 17     | 2     |
| 2:B:159:ALA:O    | 2:B:161:ILE:CD1  | 0.42     | 2.67        | 13     | 1     |
| 1:A:13:G:O6      | 2:B:49:ARG:NH2   | 0.42     | 2.52        | 3      | 1     |
| 2:B:105:LYS:HG2  | 2:B:138:ILE:CG2  | 0.42     | 2.45        | 1      | 1     |
| 2:B:26:SER:OG    | 2:B:29:GLU:HG3   | 0.42     | 2.15        | 1      | 1     |
| 1:A:13:G:OP2     | 2:B:89:LYS:HD2   | 0.42     | 2.14        | 14     | 1     |
| 2:B:76:LEU:O     | 2:B:83:ILE:HG13  | 0.42     | 2.15        | 14     | 1     |
| 1:A:14:A:O4'     | 2:B:94:LYS:HB3   | 0.42     | 2.15        | 17     | 1     |
| 2:B:101:THR:O    | 2:B:170:TYR:CA   | 0.42     | 2.68        | 17     | 1     |
| 2:B:127:ARG:NH1  | 2:B:142:GLU:CD   | 0.42     | 2.73        | 12     | 1     |
| 2:B:117:LYS:O    | 2:B:121:GLU:N    | 0.42     | 2.51        | 9      | 1     |
| 2:B:149:ALA:O    | 2:B:153:LEU:HB2  | 0.42     | 2.15        | 4      | 2     |
| 1:A:14:A:OP2     | 2:B:94:LYS:HB2   | 0.42     | 2.14        | 4      | 1     |
| 2:B:22:ASN:ND2   | 2:B:25:LYS:CB    | 0.42     | 2.83        | 18     | 1     |
| 1:A:13:G:N9      | 2:B:49:ARG:HD2   | 0.42     | 2.30        | 18     | 1     |
| 1:A:7:A:C6       | 1:A:8:A:N1       | 0.42     | 2.88        | 16     | 2     |
| 2:B:31:LYS:N     | 2:B:31:LYS:HD3   | 0.42     | 2.29        | 16     | 1     |
| 1:A:8:A:C6       | 1:A:14:A:C1'     | 0.42     | 3.03        | 17     | 2     |
| 2:B:92:ASP:HB2   | 2:B:96:VAL:HG11  | 0.42     | 1.91        | 16     | 1     |
| 2:B:66:ASP:O     | 2:B:70:ALA:N     | 0.42     | 2.52        | 13     | 1     |
| 1:A:9:U:C6       | 2:B:138:ILE:HD12 | 0.42     | 2.49        | 14     | 2     |
| 2:B:74:THR:OG1   | 2:B:85:LEU:HB3   | 0.42     | 2.15        | 7      | 1     |
| 2:B:62:GLU:HG2   | 2:B:66:ASP:OD2   | 0.42     | 2.15        | 1      | 1     |
| 1:A:18:A:O2'     | 1:A:19:G:O4'     | 0.42     | 2.38        | 17     | 1     |
| 2:B:38:PHE:CD1   | 2:B:43:LEU:CG    | 0.42     | 3.03        | 10     | 1     |
| 1:A:9:U:C6       | 1:A:9:U:OP1      | 0.42     | 2.73        | 15     | 1     |
| 1:A:21:C:O2'     | 1:A:22:C:O4'     | 0.42     | 2.38        | 4      | 1     |
| 2:B:153:LEU:O    | 2:B:157:GLN:CB   | 0.42     | 2.67        | 18     | 1     |
| 1:A:1:G:H2'      | 1:A:2:G:O5'      | 0.42     | 2.14        | 16     | 1     |
| 2:B:107:LEU:CD1  | 2:B:111:ILE:CG2  | 0.42     | 2.97        | 11     | 1     |
| 1:A:10:C:H1'     | 2:B:129:VAL:CG2  | 0.42     | 2.42        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:38:PHE:CZ    | 2:B:76:LEU:HD11  | 0.42     | 2.50        | 3      | 1     |
| 2:B:77:LYS:O     | 2:B:77:LYS:HG3   | 0.42     | 2.14        | 3      | 1     |
| 2:B:149:ALA:O    | 2:B:153:LEU:HB3  | 0.42     | 2.15        | 7      | 1     |
| 2:B:17:PHE:O     | 2:B:85:LEU:HG    | 0.42     | 2.15        | 7      | 1     |
| 2:B:123:ALA:CA   | 2:B:142:GLU:O    | 0.41     | 2.69        | 8      | 1     |
| 2:B:152:ASN:O    | 2:B:155:GLU:HB3  | 0.41     | 2.15        | 8      | 1     |
| 2:B:116:LEU:HD21 | 2:B:139:ALA:HB1  | 0.41     | 1.91        | 12     | 1     |
| 2:B:103:LEU:HD23 | 2:B:105:LYS:HD2  | 0.41     | 1.92        | 15     | 1     |
| 2:B:105:LYS:HD2  | 2:B:169:TYR:CD1  | 0.41     | 2.50        | 18     | 1     |
| 2:B:18:ILE:HG13  | 2:B:85:LEU:CG    | 0.41     | 2.45        | 16     | 1     |
| 2:B:126:ILE:HD12 | 2:B:141:ILE:HG23 | 0.41     | 1.91        | 13     | 1     |
| 1:A:13:G:C5      | 2:B:58:TYR:CD2   | 0.41     | 3.08        | 7      | 2     |
| 2:B:51:GLY:C     | 2:B:56:PHE:CE1   | 0.41     | 2.94        | 1      | 2     |
| 1:A:10:C:N3      | 1:A:11:C:C2      | 0.41     | 2.88        | 14     | 1     |
| 1:A:6:A:C2'      | 1:A:7:A:OP1      | 0.41     | 2.68        | 14     | 1     |
| 2:B:102:LEU:C    | 2:B:102:LEU:HD22 | 0.41     | 2.35        | 10     | 1     |
| 2:B:18:ILE:N     | 2:B:18:ILE:HD12  | 0.41     | 2.30        | 12     | 1     |
| 2:B:89:LYS:O     | 2:B:91:ARG:N     | 0.41     | 2.53        | 15     | 1     |
| 1:A:13:G:H21     | 2:B:91:ARG:HB2   | 0.41     | 1.74        | 9      | 1     |
| 2:B:162:ASP:OD2  | 2:B:164:ARG:CD   | 0.41     | 2.67        | 9      | 1     |
| 2:B:92:ASP:CG    | 2:B:96:VAL:HG21  | 0.41     | 2.35        | 9      | 1     |
| 2:B:27:VAL:CG2   | 2:B:50:THR:CB    | 0.41     | 2.98        | 19     | 1     |
| 1:A:7:A:C5       | 1:A:8:A:C5       | 0.41     | 3.09        | 4      | 1     |
| 2:B:89:LYS:HG3   | 2:B:89:LYS:O     | 0.41     | 2.15        | 4      | 1     |
| 1:A:13:G:C8      | 2:B:49:ARG:HB3   | 0.41     | 2.50        | 18     | 1     |
| 2:B:18:ILE:CG1   | 2:B:84:LYS:O     | 0.41     | 2.67        | 13     | 1     |
| 2:B:120:PHE:O    | 2:B:122:ASP:N    | 0.41     | 2.53        | 11     | 1     |
| 2:B:153:LEU:HD12 | 2:B:168:LEU:CB   | 0.41     | 2.45        | 11     | 1     |
| 2:B:115:GLU:CG   | 2:B:161:ILE:HD13 | 0.41     | 2.45        | 3      | 1     |
| 2:B:113:GLU:O    | 2:B:117:LYS:HB2  | 0.41     | 2.16        | 17     | 2     |
| 2:B:85:LEU:C     | 2:B:85:LEU:HD13  | 0.41     | 2.31        | 5      | 1     |
| 1:A:2:G:O6       | 1:A:3:C:N4       | 0.41     | 2.53        | 15     | 2     |
| 2:B:77:LYS:C     | 2:B:78:VAL:O     | 0.41     | 2.58        | 4      | 2     |
| 1:A:12:C:C2      | 2:B:17:PHE:HZ    | 0.41     | 2.31        | 10     | 1     |
| 2:B:47:ASP:HB3   | 2:B:60:ASP:CG    | 0.41     | 2.36        | 10     | 2     |
| 2:B:155:GLU:CG   | 2:B:156:LYS:HD3  | 0.41     | 2.46        | 8      | 1     |
| 1:A:1:G:C6       | 1:A:2:G:C6       | 0.41     | 3.08        | 12     | 1     |
| 2:B:119:VAL:CG2  | 2:B:161:ILE:HD11 | 0.41     | 2.45        | 9      | 1     |
| 2:B:73:LEU:O     | 2:B:76:LEU:HD23  | 0.41     | 2.16        | 19     | 1     |
| 1:A:1:G:O2'      | 1:A:2:G:C5'      | 0.41     | 2.68        | 2      | 1     |
| 2:B:54:ARG:HG3   | 2:B:54:ARG:NH1   | 0.41     | 2.30        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:14:A:C8      | 2:B:52:THR:HB    | 0.41     | 2.50        | 13     | 1     |
| 2:B:153:LEU:HD13 | 2:B:168:LEU:O    | 0.41     | 2.14        | 11     | 1     |
| 2:B:93:SER:O     | 2:B:94:LYS:CE    | 0.41     | 2.68        | 11     | 1     |
| 2:B:91:ARG:O     | 2:B:92:ASP:HB2   | 0.41     | 2.15        | 8      | 1     |
| 1:A:13:G:C4      | 2:B:58:TYR:CE1   | 0.41     | 3.08        | 12     | 1     |
| 2:B:121:GLU:HG3  | 2:B:122:ASP:N    | 0.41     | 2.29        | 12     | 1     |
| 2:B:76:LEU:HB2   | 2:B:83:ILE:HD11  | 0.41     | 1.91        | 19     | 1     |
| 2:B:20:ASN:O     | 2:B:81:ASN:HB3   | 0.41     | 2.15        | 2      | 2     |
| 1:A:12:C:H1'     | 2:B:17:PHE:CE1   | 0.41     | 2.50        | 6      | 2     |
| 1:A:13:G:C8      | 2:B:49:ARG:CG    | 0.41     | 3.03        | 18     | 1     |
| 2:B:29:GLU:O     | 2:B:33:ALA:HB2   | 0.41     | 2.15        | 18     | 1     |
| 2:B:128:LEU:HA   | 2:B:139:ALA:HA   | 0.41     | 1.92        | 16     | 1     |
| 2:B:73:LEU:CD2   | 2:B:76:LEU:HD21  | 0.41     | 2.45        | 13     | 1     |
| 2:B:34:ILE:HG23  | 2:B:38:PHE:CE2   | 0.41     | 2.48        | 11     | 1     |
| 2:B:17:PHE:O     | 2:B:18:ILE:HG13  | 0.41     | 2.16        | 3      | 1     |
| 2:B:46:VAL:O     | 2:B:47:ASP:OD2   | 0.41     | 2.38        | 1      | 1     |
| 2:B:145:SER:OG   | 2:B:148:ASP:HB2  | 0.41     | 2.16        | 1      | 1     |
| 2:B:102:LEU:HB2  | 2:B:143:PHE:CD1  | 0.41     | 2.49        | 14     | 1     |
| 2:B:69:LYS:HD3   | 2:B:69:LYS:N     | 0.41     | 2.29        | 17     | 1     |
| 2:B:73:LEU:HA    | 2:B:73:LEU:HD13  | 0.41     | 1.71        | 10     | 1     |
| 2:B:20:ASN:HB3   | 2:B:82:GLU:O     | 0.41     | 2.14        | 8      | 1     |
| 2:B:46:VAL:HG21  | 2:B:62:GLU:HB3   | 0.41     | 1.92        | 8      | 1     |
| 2:B:116:LEU:O    | 2:B:120:PHE:N    | 0.41     | 2.43        | 12     | 1     |
| 1:A:13:G:OP1     | 2:B:90:GLY:C     | 0.41     | 2.59        | 9      | 1     |
| 2:B:38:PHE:CG    | 2:B:45:VAL:HG13  | 0.41     | 2.50        | 9      | 1     |
| 2:B:127:ARG:HB3  | 2:B:140:TYR:CB   | 0.41     | 2.46        | 18     | 1     |
| 2:B:111:ILE:CG2  | 2:B:112:THR:N    | 0.41     | 2.83        | 18     | 1     |
| 2:B:124:LEU:O    | 2:B:125:GLU:HB3  | 0.41     | 2.14        | 6      | 1     |
| 2:B:111:ILE:O    | 2:B:112:THR:HG22 | 0.41     | 2.15        | 13     | 1     |
| 2:B:11:THR:CG2   | 2:B:12:THR:OG1   | 0.41     | 2.68        | 1      | 1     |
| 2:B:47:ASP:O     | 2:B:48:VAL:HG22  | 0.41     | 2.16        | 8      | 1     |
| 2:B:102:LEU:N    | 2:B:102:LEU:HD23 | 0.41     | 2.30        | 9      | 1     |
| 2:B:82:GLU:HG3   | 2:B:82:GLU:O     | 0.41     | 2.14        | 2      | 1     |
| 1:A:14:A:OP2     | 1:A:14:A:C1'     | 0.41     | 2.69        | 4      | 1     |
| 1:A:16:G:O5'     | 1:A:17:U:OP1     | 0.41     | 2.38        | 4      | 1     |
| 2:B:111:ILE:HG12 | 2:B:116:LEU:HD11 | 0.41     | 1.91        | 16     | 1     |
| 2:B:155:GLU:CG   | 2:B:156:LYS:HG2  | 0.41     | 2.45        | 16     | 1     |
| 2:B:115:GLU:OE2  | 2:B:161:ILE:CD1  | 0.41     | 2.67        | 6      | 1     |
| 2:B:20:ASN:N     | 2:B:55:LYS:O     | 0.41     | 2.54        | 17     | 1     |
| 2:B:51:GLY:CA    | 2:B:56:PHE:HD1   | 0.41     | 2.27        | 17     | 1     |
| 1:A:13:G:O3'     | 2:B:93:SER:HB2   | 0.41     | 2.15        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:2:G:O6       | 1:A:22:C:N4      | 0.41     | 2.54        | 12     | 1     |
| 2:B:129:VAL:C    | 2:B:138:ILE:HG13 | 0.41     | 2.36        | 15     | 1     |
| 2:B:98:ALA:CB    | 2:B:171:THR:HG22 | 0.41     | 2.35        | 15     | 1     |
| 2:B:22:ASN:HB3   | 2:B:30:LEU:CD2   | 0.41     | 2.42        | 16     | 1     |
| 2:B:107:LEU:CD2  | 2:B:116:LEU:HD11 | 0.41     | 2.45        | 6      | 1     |
| 2:B:94:LYS:HE3   | 2:B:95:LYS:CE    | 0.41     | 2.46        | 11     | 1     |
| 2:B:97:ARG:O     | 2:B:100:ARG:HG2  | 0.41     | 2.15        | 3      | 1     |
| 1:A:2:G:C2'      | 1:A:3:C:OP2      | 0.41     | 2.68        | 7      | 1     |
| 2:B:108:SER:OG   | 2:B:164:ARG:NH2  | 0.41     | 2.54        | 14     | 1     |
| 2:B:142:GLU:OE1  | 2:B:143:PHE:N    | 0.41     | 2.53        | 9      | 1     |
| 2:B:119:VAL:HG22 | 2:B:159:ALA:CB   | 0.41     | 2.45        | 9      | 1     |
| 1:A:14:A:N7      | 2:B:94:LYS:HE2   | 0.41     | 2.31        | 9      | 1     |
| 2:B:101:THR:CG2  | 2:B:142:GLU:HG3  | 0.41     | 2.46        | 19     | 1     |
| 1:A:20:G:N3      | 1:A:20:G:C2'     | 0.41     | 2.83        | 18     | 1     |
| 2:B:91:ARG:C     | 2:B:92:ASP:CG    | 0.41     | 2.76        | 18     | 2     |
| 2:B:73:LEU:HA    | 2:B:73:LEU:HD23  | 0.41     | 1.73        | 16     | 1     |
| 2:B:21:LEU:HB3   | 2:B:54:ARG:O     | 0.41     | 2.15        | 14     | 1     |
| 2:B:30:LEU:CD2   | 2:B:54:ARG:CG    | 0.41     | 2.98        | 14     | 1     |
| 1:A:14:A:O5'     | 2:B:93:SER:HB3   | 0.41     | 2.16        | 5      | 1     |
| 1:A:14:A:N3      | 2:B:94:LYS:HB3   | 0.41     | 2.30        | 5      | 1     |
| 2:B:163:GLY:C    | 2:B:164:ARG:CG   | 0.41     | 2.89        | 18     | 2     |
| 2:B:107:LEU:HB2  | 2:B:137:GLY:C    | 0.41     | 2.35        | 10     | 1     |
| 2:B:104:ALA:O    | 2:B:138:ILE:CG2  | 0.41     | 2.69        | 15     | 1     |
| 2:B:76:LEU:HD12  | 2:B:76:LEU:N     | 0.41     | 2.30        | 15     | 1     |
| 2:B:98:ALA:O     | 2:B:171:THR:HB   | 0.41     | 2.15        | 15     | 1     |
| 2:B:160:GLU:C    | 2:B:161:ILE:HG13 | 0.41     | 2.36        | 14     | 2     |
| 2:B:95:LYS:C     | 2:B:95:LYS:HD2   | 0.41     | 2.36        | 19     | 1     |
| 2:B:30:LEU:O     | 2:B:34:ILE:HG13  | 0.41     | 2.16        | 2      | 1     |
| 2:B:120:PHE:CE2  | 2:B:141:ILE:HG21 | 0.41     | 2.51        | 2      | 1     |
| 2:B:78:VAL:HG13  | 2:B:79:PHE:H     | 0.41     | 1.75        | 4      | 1     |
| 1:A:14:A:N6      | 2:B:94:LYS:HG2   | 0.41     | 2.30        | 6      | 1     |
| 1:A:17:U:H2'     | 1:A:17:U:O2      | 0.41     | 2.16        | 13     | 1     |
| 2:B:107:LEU:O    | 2:B:137:GLY:HA2  | 0.41     | 2.15        | 11     | 1     |
| 2:B:51:GLY:CA    | 2:B:56:PHE:CG    | 0.41     | 3.00        | 11     | 1     |
| 2:B:163:GLY:C    | 2:B:164:ARG:HG2  | 0.41     | 2.36        | 11     | 1     |
| 2:B:33:ALA:CB    | 2:B:78:VAL:CG1   | 0.41     | 2.97        | 3      | 1     |
| 2:B:48:VAL:HG13  | 2:B:58:TYR:O     | 0.41     | 2.15        | 1      | 1     |
| 2:B:102:LEU:HB2  | 2:B:143:PHE:CE1  | 0.41     | 2.51        | 14     | 1     |
| 2:B:116:LEU:HD23 | 2:B:139:ALA:CB   | 0.41     | 2.46        | 14     | 1     |
| 1:A:6:A:C2       | 1:A:7:A:C4       | 0.41     | 3.08        | 17     | 1     |
| 2:B:76:LEU:C     | 2:B:76:LEU:HD12  | 0.41     | 2.36        | 17     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:6:A:HO2'     | 1:A:7:A:H5'      | 0.41     | 1.76        | 5      | 1     |
| 2:B:143:PHE:HB2  | 2:B:149:ALA:CB   | 0.41     | 2.43        | 5      | 1     |
| 2:B:27:VAL:HG13  | 2:B:31:LYS:CE    | 0.41     | 2.46        | 13     | 2     |
| 1:A:2:G:C6       | 1:A:22:C:C4      | 0.41     | 3.09        | 12     | 1     |
| 2:B:166:VAL:HG13 | 2:B:167:SER:N    | 0.41     | 2.31        | 15     | 1     |
| 2:B:100:ARG:O    | 2:B:100:ARG:HG3  | 0.41     | 2.15        | 2      | 1     |
| 2:B:43:LEU:HD13  | 2:B:73:LEU:HD12  | 0.41     | 1.93        | 16     | 1     |
| 2:B:95:LYS:O     | 2:B:95:LYS:HG2   | 0.41     | 2.12        | 16     | 1     |
| 2:B:140:TYR:CE2  | 2:B:171:THR:CB   | 0.41     | 3.04        | 13     | 1     |
| 2:B:51:GLY:O     | 2:B:56:PHE:CD1   | 0.41     | 2.74        | 1      | 1     |
| 2:B:170:TYR:C    | 2:B:170:TYR:CD1  | 0.41     | 2.94        | 17     | 1     |
| 2:B:83:ILE:HG13  | 2:B:83:ILE:O     | 0.41     | 2.15        | 17     | 1     |
| 2:B:129:VAL:O    | 2:B:136:LYS:HB3  | 0.40     | 2.16        | 10     | 1     |
| 1:A:9:U:C1'      | 1:A:10:C:P       | 0.40     | 3.09        | 9      | 1     |
| 2:B:144:LYS:CB   | 2:B:148:ASP:OD2  | 0.40     | 2.69        | 9      | 1     |
| 2:B:160:GLU:HG3  | 2:B:165:SER:OG   | 0.40     | 2.16        | 9      | 1     |
| 2:B:106:ASN:HB3  | 2:B:165:SER:O    | 0.40     | 2.16        | 2      | 1     |
| 1:A:3:C:O2'      | 1:A:4:C:H5"      | 0.40     | 2.14        | 18     | 1     |
| 2:B:73:LEU:HG    | 2:B:76:LEU:HD12  | 0.40     | 1.92        | 18     | 1     |
| 2:B:143:PHE:CE2  | 2:B:152:ASN:HB2  | 0.40     | 2.51        | 16     | 1     |
| 2:B:125:GLU:OE2  | 2:B:127:ARG:NH1  | 0.40     | 2.54        | 14     | 1     |
| 2:B:164:ARG:HG3  | 2:B:164:ARG:O    | 0.40     | 2.15        | 17     | 1     |
| 2:B:142:GLU:O    | 2:B:142:GLU:HG3  | 0.40     | 2.16        | 5      | 1     |
| 2:B:93:SER:O     | 2:B:93:SER:OG    | 0.40     | 2.38        | 8      | 1     |
| 2:B:83:ILE:HD13  | 2:B:83:ILE:O     | 0.40     | 2.16        | 12     | 1     |
| 2:B:24:ASN:O     | 2:B:25:LYS:CE    | 0.40     | 2.70        | 15     | 1     |
| 2:B:47:ASP:HB2   | 2:B:60:ASP:CG    | 0.40     | 2.36        | 2      | 1     |
| 2:B:127:ARG:CZ   | 2:B:140:TYR:HB2  | 0.40     | 2.46        | 18     | 1     |
| 2:B:53:ASN:O     | 2:B:54:ARG:CB    | 0.40     | 2.67        | 18     | 1     |
| 1:A:17:U:OP2     | 1:A:17:U:C5      | 0.40     | 2.74        | 16     | 1     |
| 2:B:46:VAL:HG21  | 2:B:62:GLU:CG    | 0.40     | 2.47        | 13     | 1     |
| 1:A:10:C:O2      | 2:B:127:ARG:HD2  | 0.40     | 2.16        | 14     | 1     |
| 1:A:14:A:OP1     | 2:B:93:SER:CB    | 0.40     | 2.69        | 8      | 1     |
| 2:B:24:ASN:O     | 2:B:25:LYS:HE3   | 0.40     | 2.17        | 15     | 1     |
| 1:A:12:C:OP2     | 1:A:12:C:C4      | 0.40     | 2.74        | 19     | 1     |
| 1:A:21:C:O2      | 1:A:22:C:C5      | 0.40     | 2.74        | 19     | 1     |
| 1:A:8:A:N6       | 2:B:52:THR:HG21  | 0.40     | 2.31        | 4      | 1     |
| 1:A:16:G:OP2     | 1:A:17:U:OP1     | 0.40     | 2.40        | 18     | 1     |
| 2:B:102:LEU:HD22 | 2:B:153:LEU:HD12 | 0.40     | 1.92        | 18     | 1     |
| 1:A:19:G:C8      | 1:A:19:G:O5'     | 0.40     | 2.67        | 13     | 1     |
| 2:B:17:PHE:CG    | 2:B:18:ILE:N     | 0.40     | 2.89        | 11     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:24:ASN:O    | 2:B:25:LYS:HG2   | 0.40     | 2.17        | 3      | 1     |
| 2:B:16:LEU:HB3  | 2:B:59:VAL:HG12  | 0.40     | 1.92        | 1      | 1     |
| 2:B:108:SER:HB2 | 2:B:164:ARG:CD   | 0.40     | 2.46        | 1      | 1     |
| 1:A:15:A:P      | 1:A:15:A:O4'     | 0.40     | 2.80        | 14     | 1     |
| 2:B:31:LYS:CE   | 2:B:50:THR:HB    | 0.40     | 2.46        | 14     | 1     |
| 2:B:83:ILE:CD1  | 2:B:83:ILE:N     | 0.40     | 2.84        | 14     | 1     |
| 2:B:48:VAL:O    | 2:B:48:VAL:HG13  | 0.40     | 2.16        | 14     | 1     |
| 2:B:99:ALA:C    | 2:B:146:GLU:HG3  | 0.40     | 2.37        | 17     | 1     |
| 2:B:140:TYR:C   | 2:B:141:ILE:HG13 | 0.40     | 2.37        | 5      | 1     |
| 2:B:43:LEU:HD13 | 2:B:43:LEU:HA    | 0.40     | 1.70        | 10     | 1     |
| 1:A:19:G:H2'    | 1:A:20:G:C8      | 0.40     | 2.52        | 12     | 1     |
| 2:B:37:LEU:HD22 | 2:B:76:LEU:HD12  | 0.40     | 1.89        | 9      | 1     |
| 2:B:85:LEU:O    | 2:B:86:GLU:HB2   | 0.40     | 2.16        | 9      | 3     |
| 2:B:105:LYS:HD2 | 2:B:169:TYR:CG   | 0.40     | 2.52        | 2      | 1     |
| 1:A:6:A:N3      | 1:A:18:A:C2      | 0.40     | 2.89        | 13     | 1     |
| 1:A:14:A:O4'    | 2:B:94:LYS:CB    | 0.40     | 2.70        | 11     | 1     |
| 1:A:14:A:C5'    | 1:A:15:A:O5'     | 0.40     | 2.69        | 14     | 1     |
| 2:B:21:LEU:HD12 | 2:B:21:LEU:HA    | 0.40     | 1.81        | 14     | 1     |
| 2:B:56:PHE:HZ   | 2:B:58:TYR:CE1   | 0.40     | 2.34        | 17     | 1     |
| 2:B:41:ASN:O    | 2:B:42:ASP:OD1   | 0.40     | 2.39        | 10     | 1     |
| 2:B:94:LYS:C    | 2:B:94:LYS:HE3   | 0.40     | 2.36        | 8      | 1     |
| 1:A:20:G:N1     | 1:A:21:C:C5      | 0.40     | 2.90        | 9      | 1     |
| 1:A:5:G:HO2'    | 1:A:6:A:P        | 0.40     | 2.30        | 4      | 1     |
| 2:B:98:ALA:O    | 2:B:99:ALA:C     | 0.40     | 2.59        | 11     | 1     |
| 2:B:77:LYS:HA   | 2:B:81:ASN:C     | 0.40     | 2.36        | 3      | 1     |
| 2:B:76:LEU:O    | 2:B:83:ILE:HG23  | 0.40     | 2.16        | 3      | 1     |
| 2:B:68:GLU:C    | 2:B:68:GLU:CD    | 0.40     | 2.79        | 3      | 1     |
| 2:B:38:PHE:CG   | 2:B:43:LEU:HD12  | 0.40     | 2.51        | 7      | 1     |
| 2:B:113:GLU:OE2 | 2:B:126:ILE:O    | 0.40     | 2.40        | 14     | 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 |
|-----|-------|---------------|---------------|--------------|-------------|-------------|
| 2   | B     | 158/175 (90%) | 119±3 (75±2%) | 25±2 (16±2%) | 14±2 (9±1%) | 2   12      |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |
|-----|-------|-----------------|------------|-----------|----------|-------------|
| All | All   | 3002/3325 (90%) | 2252 (75%) | 476 (16%) | 274 (9%) | 2   12      |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 157 | GLN  | 19             |
| 2   | B     | 52  | THR  | 19             |
| 2   | B     | 42  | ASP  | 19             |
| 2   | B     | 79  | PHE  | 18             |
| 2   | B     | 170 | TYR  | 17             |
| 2   | B     | 86  | GLU  | 16             |
| 2   | B     | 53  | ASN  | 16             |
| 2   | B     | 22  | ASN  | 15             |
| 2   | B     | 159 | ALA  | 15             |
| 2   | B     | 94  | LYS  | 12             |
| 2   | B     | 21  | LEU  | 12             |
| 2   | B     | 82  | GLU  | 10             |
| 2   | B     | 78  | VAL  | 9              |
| 2   | B     | 44  | ALA  | 9              |
| 2   | B     | 92  | ASP  | 7              |
| 2   | B     | 10  | SER  | 6              |
| 2   | B     | 160 | GLU  | 6              |
| 2   | B     | 91  | ARG  | 5              |
| 2   | B     | 93  | SER  | 5              |
| 2   | B     | 111 | ILE  | 5              |
| 2   | B     | 43  | LEU  | 4              |
| 2   | B     | 90  | GLY  | 4              |
| 2   | B     | 74  | THR  | 3              |
| 2   | B     | 89  | LYS  | 2              |
| 2   | B     | 156 | LYS  | 2              |
| 2   | B     | 128 | LEU  | 2              |
| 2   | B     | 48  | VAL  | 2              |
| 2   | B     | 59  | VAL  | 2              |
| 2   | B     | 83  | ILE  | 2              |
| 2   | B     | 13  | PRO  | 2              |
| 2   | B     | 76  | LEU  | 2              |
| 2   | B     | 45  | VAL  | 1              |
| 2   | B     | 162 | ASP  | 1              |
| 2   | B     | 20  | ASN  | 1              |
| 2   | B     | 158 | GLY  | 1              |
| 2   | B     | 46  | VAL  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 81  | ASN  | 1              |
| 2   | B     | 107 | LEU  | 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 |
|-----|-------|-----------------|--------------|--------------|-------------|
| 2   | B     | 134/147 (91%)   | 87±6 (65±4%) | 47±6 (35±4%) | 1 10        |
| All | All   | 2546/2793 (91%) | 1662 (65%)   | 884 (35%)    | 1 10        |

All 111 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) |
|-----|-------|-----|------|----------------|
| 2   | B     | 17  | PHE  | 19             |
| 2   | B     | 140 | TYR  | 19             |
| 2   | B     | 138 | ILE  | 19             |
| 2   | B     | 65  | GLU  | 19             |
| 2   | B     | 152 | ASN  | 18             |
| 2   | B     | 12  | THR  | 18             |
| 2   | B     | 54  | ARG  | 18             |
| 2   | B     | 43  | LEU  | 17             |
| 2   | B     | 10  | SER  | 16             |
| 2   | B     | 95  | LYS  | 15             |
| 2   | B     | 31  | LYS  | 15             |
| 2   | B     | 58  | TYR  | 14             |
| 2   | B     | 157 | GLN  | 14             |
| 2   | B     | 59  | VAL  | 13             |
| 2   | B     | 53  | ASN  | 13             |
| 2   | B     | 102 | LEU  | 13             |
| 2   | B     | 37  | LEU  | 13             |
| 2   | B     | 108 | SER  | 13             |
| 2   | B     | 93  | SER  | 12             |
| 2   | B     | 171 | THR  | 12             |
| 2   | B     | 27  | VAL  | 12             |
| 2   | B     | 47  | ASP  | 12             |
| 2   | B     | 26  | SER  | 12             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 72  | GLU  | 11             |
| 2   | B     | 142 | GLU  | 11             |
| 2   | B     | 153 | LEU  | 11             |
| 2   | B     | 18  | ILE  | 11             |
| 2   | B     | 62  | GLU  | 11             |
| 2   | B     | 111 | ILE  | 11             |
| 2   | B     | 128 | LEU  | 11             |
| 2   | B     | 94  | LYS  | 10             |
| 2   | B     | 25  | LYS  | 10             |
| 2   | B     | 85  | LEU  | 10             |
| 2   | B     | 91  | ARG  | 10             |
| 2   | B     | 103 | LEU  | 10             |
| 2   | B     | 67  | LEU  | 10             |
| 2   | B     | 73  | LEU  | 10             |
| 2   | B     | 36  | GLU  | 9              |
| 2   | B     | 55  | LYS  | 9              |
| 2   | B     | 169 | TYR  | 9              |
| 2   | B     | 110 | ASN  | 9              |
| 2   | B     | 89  | LYS  | 9              |
| 2   | B     | 167 | SER  | 9              |
| 2   | B     | 86  | GLU  | 9              |
| 2   | B     | 165 | SER  | 9              |
| 2   | B     | 49  | ARG  | 9              |
| 2   | B     | 130 | SER  | 9              |
| 2   | B     | 151 | LYS  | 8              |
| 2   | B     | 71  | LEU  | 8              |
| 2   | B     | 117 | LYS  | 8              |
| 2   | B     | 156 | LYS  | 8              |
| 2   | B     | 69  | LYS  | 8              |
| 2   | B     | 100 | ARG  | 8              |
| 2   | B     | 52  | THR  | 8              |
| 2   | B     | 78  | VAL  | 8              |
| 2   | B     | 68  | GLU  | 8              |
| 2   | B     | 121 | GLU  | 8              |
| 2   | B     | 87  | LYS  | 8              |
| 2   | B     | 112 | THR  | 7              |
| 2   | B     | 168 | LEU  | 7              |
| 2   | B     | 160 | GLU  | 7              |
| 2   | B     | 114 | ASP  | 7              |
| 2   | B     | 76  | LEU  | 7              |
| 2   | B     | 107 | LEU  | 6              |
| 2   | B     | 50  | THR  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 77  | LYS  | 6              |
| 2   | B     | 164 | ARG  | 6              |
| 2   | B     | 109 | PHE  | 6              |
| 2   | B     | 35  | SER  | 5              |
| 2   | B     | 150 | GLU  | 5              |
| 2   | B     | 81  | ASN  | 5              |
| 2   | B     | 83  | ILE  | 5              |
| 2   | B     | 144 | LYS  | 5              |
| 2   | B     | 60  | ASP  | 5              |
| 2   | B     | 148 | ASP  | 5              |
| 2   | B     | 170 | TYR  | 5              |
| 2   | B     | 162 | ASP  | 5              |
| 2   | B     | 113 | GLU  | 5              |
| 2   | B     | 21  | LEU  | 5              |
| 2   | B     | 82  | GLU  | 4              |
| 2   | B     | 118 | GLU  | 4              |
| 2   | B     | 40  | LYS  | 4              |
| 2   | B     | 16  | LEU  | 4              |
| 2   | B     | 122 | ASP  | 4              |
| 2   | B     | 92  | ASP  | 4              |
| 2   | B     | 84  | LYS  | 4              |
| 2   | B     | 79  | PHE  | 4              |
| 2   | B     | 97  | ARG  | 4              |
| 2   | B     | 106 | ASN  | 4              |
| 2   | B     | 136 | LYS  | 3              |
| 2   | B     | 124 | LEU  | 3              |
| 2   | B     | 66  | ASP  | 3              |
| 2   | B     | 115 | GLU  | 3              |
| 2   | B     | 125 | GLU  | 3              |
| 2   | B     | 146 | GLU  | 3              |
| 2   | B     | 155 | GLU  | 3              |
| 2   | B     | 105 | LYS  | 3              |
| 2   | B     | 11  | THR  | 3              |
| 2   | B     | 46  | VAL  | 3              |
| 2   | B     | 154 | GLU  | 3              |
| 2   | B     | 74  | THR  | 3              |
| 2   | B     | 129 | VAL  | 2              |
| 2   | B     | 116 | LEU  | 2              |
| 2   | B     | 101 | THR  | 2              |
| 2   | B     | 127 | ARG  | 2              |
| 2   | B     | 166 | VAL  | 2              |
| 2   | B     | 141 | ILE  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 56  | PHE  | 2              |
| 2   | B     | 34  | ILE  | 1              |
| 2   | B     | 24  | ASN  | 1              |
| 2   | B     | 15  | ASN  | 1              |

### 6.3.3 RNA [\(i\)](#)

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers | Suiteness |
|-----|-------|---------------|-------------------|-----------------|-----------|
| 1   | A     | 21/22 (95%)   | 18±1 (85±6%)      | 8±1 (38±6%)     | 0.05±0.04 |
| All | All   | 401/418 (96%) | 339 (85%)         | 152 (38%)       | 0.05      |

The overall RNA backbone suiteness is 0.05.

All unique RNA backbone outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 12  | C    | 19             |
| 1   | A     | 13  | G    | 19             |
| 1   | A     | 14  | A    | 19             |
| 1   | A     | 15  | A    | 19             |
| 1   | A     | 5   | G    | 19             |
| 1   | A     | 10  | C    | 19             |
| 1   | A     | 9   | U    | 19             |
| 1   | A     | 16  | G    | 19             |
| 1   | A     | 17  | U    | 18             |
| 1   | A     | 3   | C    | 18             |
| 1   | A     | 6   | A    | 17             |
| 1   | A     | 7   | A    | 17             |
| 1   | A     | 4   | C    | 17             |
| 1   | A     | 11  | C    | 16             |
| 1   | A     | 2   | G    | 15             |
| 1   | A     | 20  | G    | 14             |
| 1   | A     | 21  | C    | 13             |
| 1   | A     | 8   | A    | 12             |
| 1   | A     | 19  | G    | 10             |
| 1   | A     | 22  | C    | 10             |
| 1   | A     | 18  | A    | 10             |

All unique RNA pucker outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 12  | C    | 19             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 13  | G    | 19             |
| 1   | A     | 4   | C    | 19             |
| 1   | A     | 15  | A    | 18             |
| 1   | A     | 9   | U    | 17             |
| 1   | A     | 3   | C    | 9              |
| 1   | A     | 8   | A    | 8              |
| 1   | A     | 11  | C    | 8              |
| 1   | A     | 19  | G    | 7              |
| 1   | A     | 14  | A    | 6              |
| 1   | A     | 16  | G    | 6              |
| 1   | A     | 7   | A    | 4              |
| 1   | A     | 20  | G    | 2              |
| 1   | A     | 1   | G    | 2              |
| 1   | A     | 5   | G    | 2              |
| 1   | A     | 21  | C    | 2              |
| 1   | A     | 2   | G    | 2              |
| 1   | A     | 18  | A    | 2              |

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

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

## 6.5 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

## 6.7 Other polymers [\(i\)](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation i

No chemical shift data were provided