



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:37 pm BST

PDB ID : 2KM8  
Title : Interdomain RRM packing contributes to RNA recognition in the rna15, hrp1, anchor RNA 3' processing ternary complex  
Authors : Leeper, T.C.; Varani, G.  
Deposited on : 2009-07-24

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

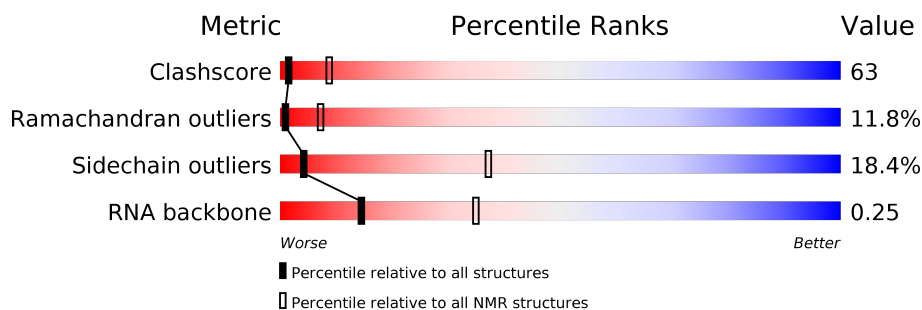
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 25%.

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



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 158937                      | 12864                     |
| Ramachandran outliers | 154571                      | 11451                     |
| Sidechain outliers    | 154315                      | 11428                     |
| RNA backbone          | 4643                        | 676                       |

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

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--------------------|
| 1   | A     | 13     | <br>77% 23%        |
| 2   | B     | 84     | <br>14% 65% 17% •• |
| 3   | C     | 167    | <br>23% 62% 12% •  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues |                                  |                   |              |
|--------------------------------------|----------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)            | Backbone RMSD (Å) | Medoid model |
| 1                                    | B:22-B:103, C:158-C:319<br>(244) | 1.31              | 1            |

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

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

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4375 atoms, of which 2102 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'.

| Mol | Chain | Residues | Atoms |     |     |    |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|-------|
| 1   | A     | 13       | Total | C   | H   | N  | O  | P  | 0     |
|     |       |          | 414   | 124 | 139 | 47 | 91 | 13 |       |

- Molecule 2 is a protein called mRNA 3'-end-processing protein RNA15.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 2   | B     | 84       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1296  | 411 | 640 | 112 | 129 | 4 |       |

- Molecule 3 is a protein called Nuclear polyadenylated RNA-binding protein 4.


| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 3   | C     | 167      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2665  | 849 | 1323 | 232 | 256 | 5 |       |

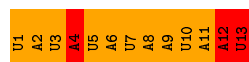
## 4 Residue-property plots

### 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.

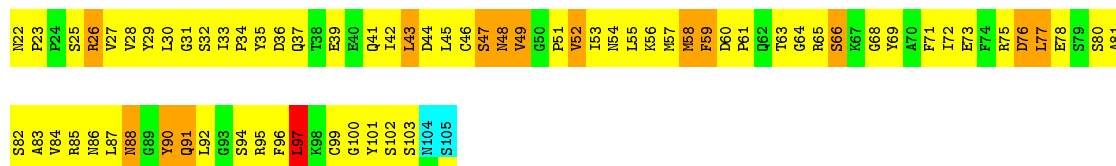
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A: 



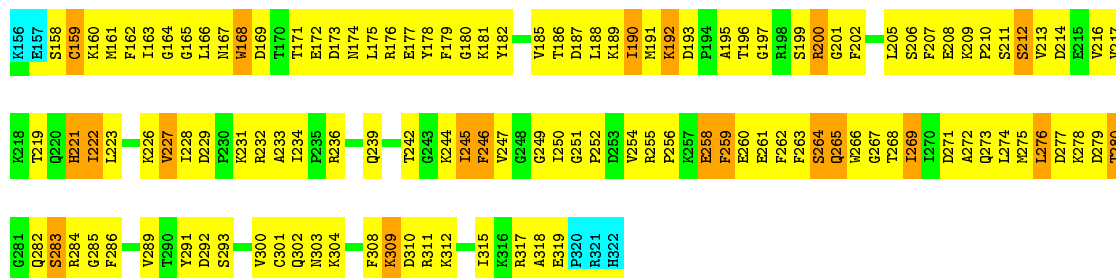
- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B: 



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

Chain C: 



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

Colouring as in section 4.1 above.

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

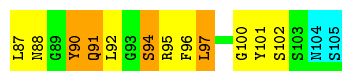
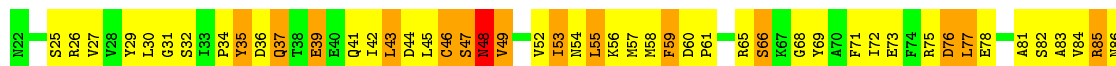
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A:



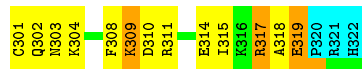
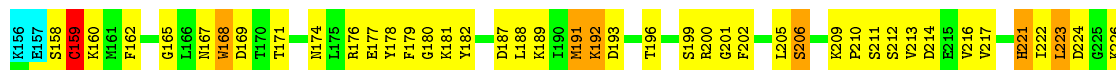
- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B:



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

Chain C:



### 4.2.2 Score per residue for model 2

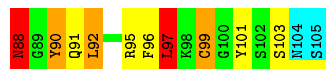
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A:

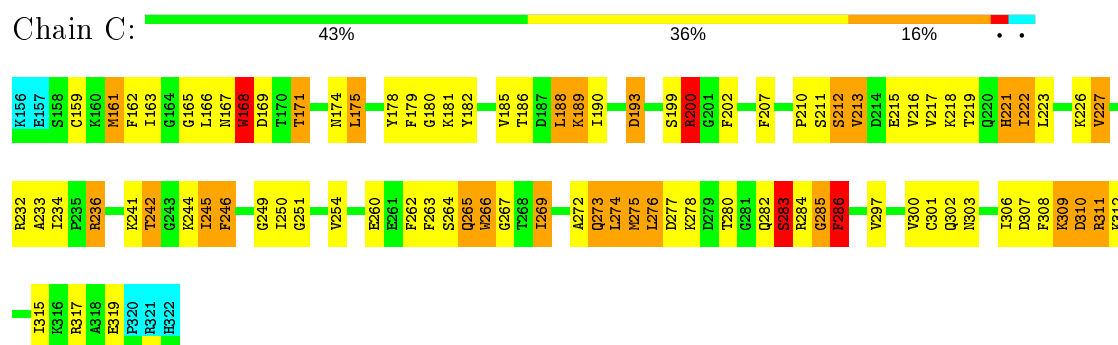


- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B:

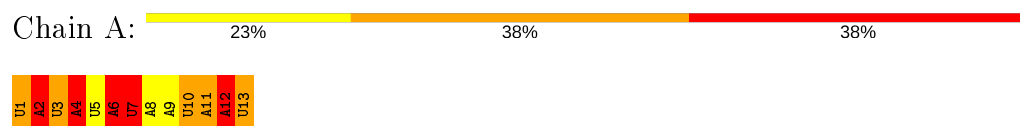


- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

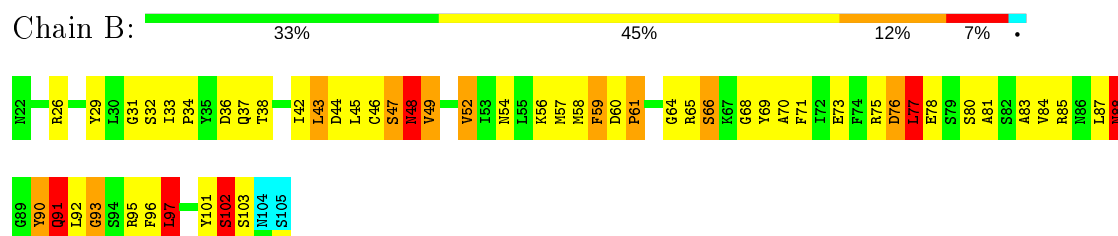


#### 4.2.3 Score per residue for model 3

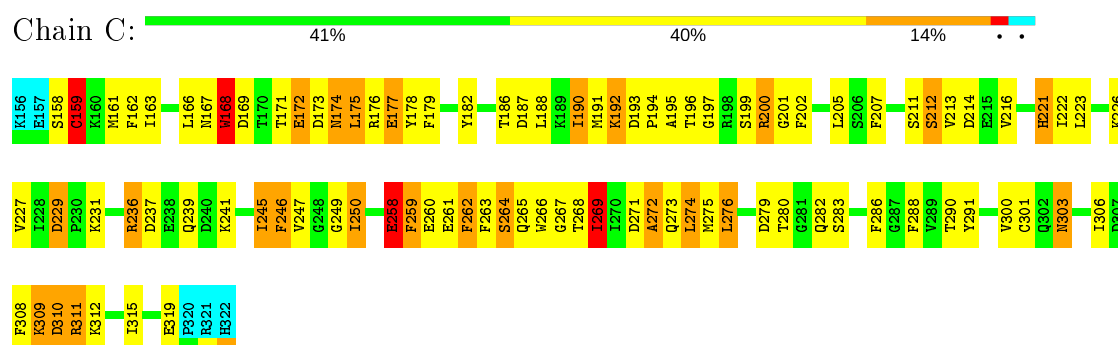
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'



- Molecule 2: mRNA 3'-end-processing protein RNA15




- Molecule 3: Nuclear polyadenylated RNA-binding protein 4



#### 4.2.4 Score per residue for model 4

- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A: 

U1  
A2  
U3  
A4  
U5  
A6  
U7  
A8  
A9  
U10  
A11  
A12  
U13

- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B: 

U22  
R26  
V27  
V28  
Y29  
L30  
G31  
S32  
P34  
P34  
Y35  
D36  
Q37  
T38  
E39  
Q40  
Q41  
T42  
L43  
D44  
L45  
C46  
C46  
S47  
N48  
V49  
G50  
P51  
V52  
I53  
N54  
L55  
K56  
N57  
M58  
F59  
D60  
P61  
Q62  
T63  
S66  
Y69  
A70  
F71  
I72  
E73  
F74  
R75  
D76  
L77  
E78  
A81  
S82  
A83  
V84  
L87

- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

Chain C: 

K156  
E157  
S158  
C159  
K160  
M161  
F162  
I163  
G164  
G165  
L166  
M167  
M168  
T170  
T171  
D172  
D173  
N174  
L175  
R176  
E177  
Y178  
Y179  
G180  
K181  
Y182  
V185  
L188  
K189  
I190  
M191  
K192  
D193  
P194  
A195  
T196  
G197  
R198  
S199  
R200  
G201  
L205  
K209  
P210  
S211  
S212  
D214  
D215  
V216  
H221  
L222  
L223

K226  
V227  
I228  
R232  
A233  
I234  
E238  
Q239  
T242  
I245  
F246  
G249  
I250  
G251  
F252  
V254  
R255  
E258  
F259  
E260  
E261  
F262  
F263  
S264  
Q265  
W266  
G267  
T268  
I269  
I270  
D271  
A272  
Q273  
L276  
D277  
K278  
D279  
T280  
G281  
Q282  
S283  
R284  
G285  
F286  
Y291  
D292  
S293  
V300  
C301  
Q302

N303  
F308  
K309  
D310  
R311  
K312  
I313  
E314  
I315  
E319  
P320  
R321  
H322

#### 4.2.5 Score per residue for model 5

- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A: 

U1  
A2  
U3  
A4  
U5  
A6  
U7  
A8  
A9  
U10  
A11  
A12  
U13

- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B: 

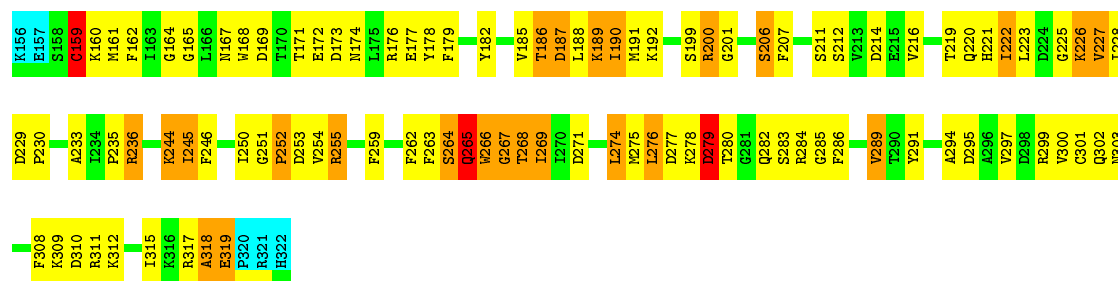
R22  
F23  
P24  
S25  
R26  
V27  
V28  
Y29  
L30  
G31  
S32  
I33  
P34  
P34  
Y35  
D36  
Q37  
T38  
E39  
D44  
L45  
C46  
C46  
S47  
N48  
V49  
G50  
P51  
V52  
I53  
N54  
M57  
M58  
F59  
D60  
P61  
Q62  
T63  
G64  
R65  
S66  
K67  
G68  
Y69  
A70  
F71  
I72  
E73  
F74  
R75  
D76  
L77  
E78  
S79  
S80  
A81  
S82  
A83  
V84  
R85

N86  
L87  
N88  
G89  
Y90  
Q91  
L92  
F96  
L97  
R98  
C99  
G100  
Y101  
S102  
S103  
N104  
S105

- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

Chain C: 

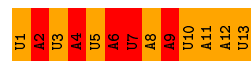




#### 4.2.6 Score per residue for model 6

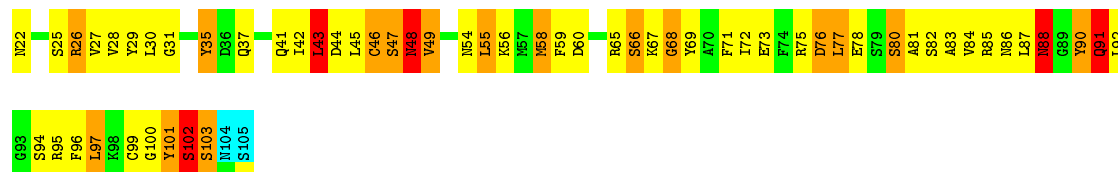
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

Chain A: 62% 38%



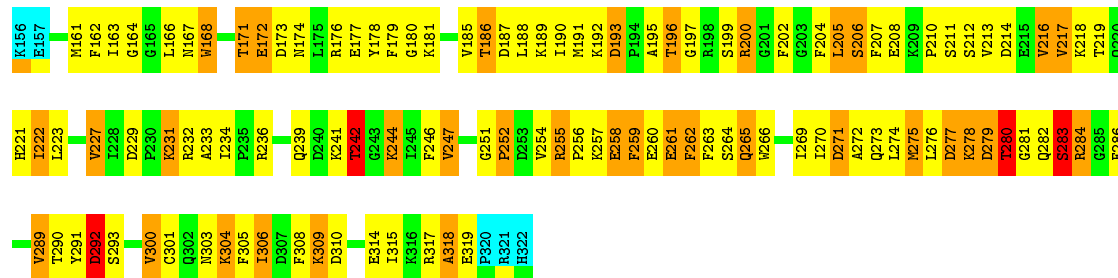
- Molecule 2: mRNA 3'-end-processing protein RNA15

Chain B: 29% 44% 19% 6%



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

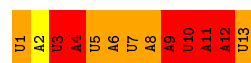
Chain C: 29% 44% 21% 6%



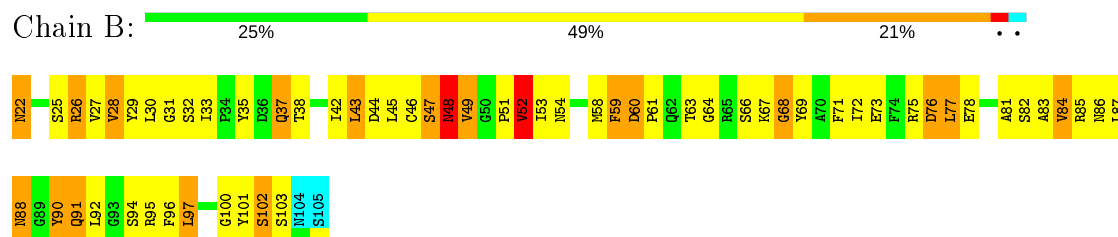
#### 4.2.7 Score per residue for model 7

- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

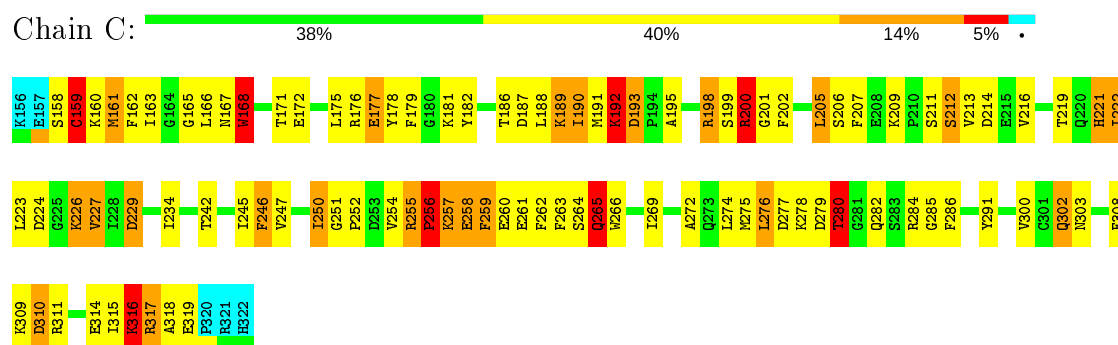
Chain A: 8% 46% 46%



- Molecule 2: mRNA 3'-end-processing protein RNA15



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

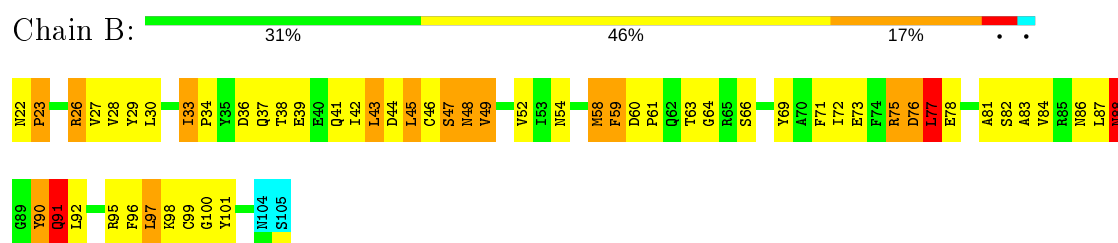


#### 4.2.8 Score per residue for model 8

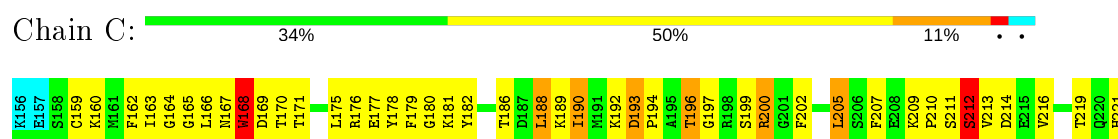
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'

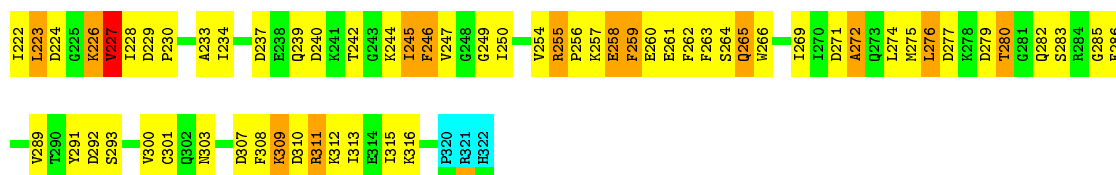


- Molecule 2: mRNA 3'-end-processing protein RNA15



- Molecule 3: Nuclear polyadenylated RNA-binding protein 4





#### 4.2.9 Score per residue for model 9

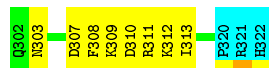
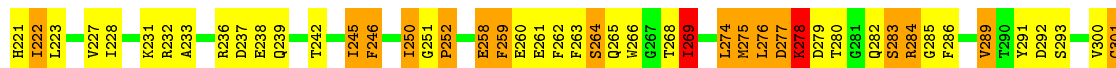
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'



- Molecule 2: mRNA 3'-end-processing protein RNA15

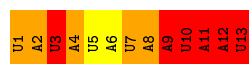


- Molecule 3: Nuclear polyadenylated RNA-binding protein 4

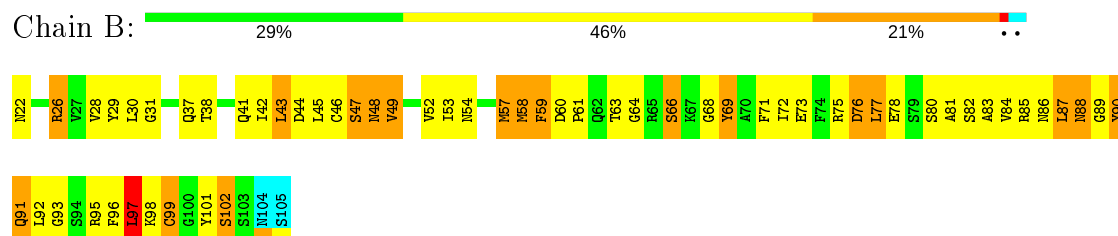


#### 4.2.10 Score per residue for model 10

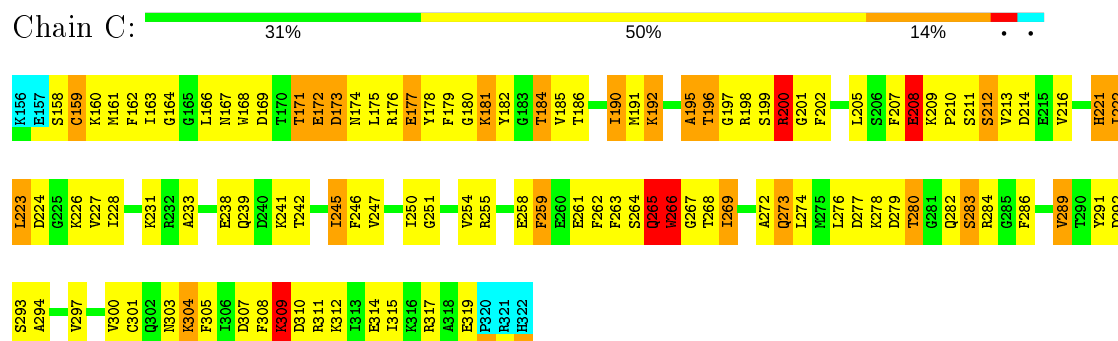
- Molecule 1: 5'-R(P\*UP\*AP\*UP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*AP\*U)-3'



- Molecule 2: mRNA 3'-end-processing protein RNA15



• Molecule 3: Nuclear polyadenylated RNA-binding protein 4



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| X-PLOR NIH    | refinement         |         |
| CYANA         | structure solution |         |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

|  |              |
|--|--------------|
| Chemical shift file(s)                       | input_cs.cif |
| Number of chemical shift lists               | 1            |
| Total number of shifts                       | 922          |
| Number of shifts mapped to atoms             | 922          |
| Number of unparsed shifts                    | 0            |
| Number of shifts with mapping errors         | 0            |
| Number of shifts with mapping warnings       | 0            |
| Assignment completeness (well-defined parts) | 25%          |

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 275   | 139      | 138      | 98±23   |
| 2   | B     | 641   | 629      | 626      | 99±25   |
| 3   | C     | 1295  | 1274     | 1273     | 134±14  |
| All | All   | 22110 | 20420    | 20370    | 2660    |

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 63.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:11:A:H3'     | 2:B:69:TYR:N     | 1.31     | 1.37        | 7      | 1     |
| 1:A:6:A:H4'      | 1:A:7:U:H5'      | 1.13     | 1.17        | 9      | 7     |
| 1:A:12:A:H5'     | 2:B:67:LYS:O     | 1.09     | 1.47        | 7      | 1     |
| 1:A:12:A:C5'     | 2:B:67:LYS:O     | 1.07     | 2.00        | 7      | 1     |
| 1:A:10:U:H5'     | 2:B:71:PHE:CE1   | 1.03     | 1.86        | 5      | 4     |
| 1:A:12:A:P       | 2:B:58:MET:O     | 1.03     | 2.17        | 7      | 1     |
| 1:A:12:A:O5'     | 2:B:68:GLY:HA2   | 1.02     | 1.54        | 7      | 1     |
| 2:B:49:VAL:HG11  | 2:B:83:ALA:HB2   | 0.98     | 1.29        | 5      | 4     |
| 1:A:11:A:H4'     | 2:B:58:MET:C     | 0.97     | 1.79        | 7      | 1     |
| 1:A:3:U:O2'      | 1:A:4:A:H5'      | 0.96     | 1.60        | 2      | 1     |
| 2:B:90:TYR:CE1   | 2:B:97:LEU:HD11  | 0.95     | 1.96        | 5      | 2     |
| 1:A:12:A:HO2'    | 1:A:13:U:H6      | 0.95     | 0.98        | 3      | 4     |
| 3:C:188:LEU:HD12 | 3:C:189:LYS:N    | 0.94     | 1.76        | 8      | 2     |
| 1:A:12:A:P       | 2:B:68:GLY:HA2   | 0.94     | 2.03        | 7      | 1     |
| 1:A:6:A:O4'      | 1:A:7:U:H5''     | 0.94     | 1.62        | 3      | 2     |
| 1:A:6:A:H4'      | 1:A:7:U:C5'      | 0.93     | 1.94        | 5      | 8     |
| 1:A:6:A:C4'      | 1:A:7:U:H5'      | 0.92     | 1.94        | 4      | 7     |
| 2:B:47:SER:O     | 2:B:49:VAL:N     | 0.92     | 2.02        | 9      | 7     |
| 1:A:11:A:H4'     | 2:B:58:MET:O     | 0.92     | 1.63        | 7      | 1     |
| 1:A:11:A:H5'     | 2:B:69:TYR:O     | 0.91     | 1.64        | 7      | 1     |
| 1:A:9:A:H5''     | 2:B:69:TYR:OH    | 0.90     | 1.65        | 6      | 3     |
| 3:C:179:PHE:O    | 3:C:181:LYS:N    | 0.89     | 2.05        | 9      | 5     |
| 1:A:11:A:O2'     | 2:B:68:GLY:N     | 0.89     | 2.05        | 7      | 1     |
| 1:A:11:A:H3'     | 2:B:69:TYR:H     | 0.88     | 1.28        | 7      | 1     |
| 3:C:269:ILE:HG23 | 3:C:291:TYR:CE1  | 0.88     | 2.03        | 3      | 2     |
| 1:A:2:A:HO2'     | 1:A:3:U:H6       | 0.88     | 0.97        | 2      | 3     |
| 1:A:11:A:C3'     | 2:B:69:TYR:N     | 0.87     | 2.32        | 7      | 1     |
| 1:A:9:A:HO2'     | 1:A:10:U:H6      | 0.87     | 1.07        | 2      | 1     |
| 1:A:11:A:HO2'    | 1:A:12:A:H8      | 0.87     | 0.92        | 10     | 4     |
| 3:C:276:LEU:H    | 3:C:276:LEU:HD22 | 0.87     | 1.30        | 7      | 1     |
| 2:B:80:SER:O     | 2:B:84:VAL:HG22  | 0.86     | 1.70        | 10     | 1     |
| 1:A:6:A:C4'      | 1:A:7:U:H5''     | 0.86     | 2.01        | 8      | 2     |
| 2:B:97:LEU:N     | 2:B:97:LEU:HD12  | 0.85     | 1.86        | 5      | 1     |
| 2:B:72:ILE:N     | 2:B:72:ILE:HD12  | 0.85     | 1.86        | 5      | 3     |
| 1:A:9:A:H2'      | 1:A:10:U:C6      | 0.85     | 2.05        | 3      | 1     |
| 3:C:274:LEU:O    | 3:C:274:LEU:HD23 | 0.85     | 1.70        | 5      | 1     |
| 1:A:12:A:C8      | 2:B:68:GLY:N     | 0.85     | 2.44        | 7      | 1     |
| 1:A:1:U:HO2'     | 1:A:2:A:H8       | 0.85     | 0.90        | 8      | 5     |
| 1:A:9:A:H5''     | 2:B:69:TYR:CZ    | 0.85     | 2.06        | 2      | 2     |
| 3:C:245:ILE:HD13 | 3:C:245:ILE:O    | 0.84     | 1.71        | 9      | 1     |
| 1:A:10:U:H5''    | 2:B:69:TYR:CZ    | 0.84     | 2.07        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:8:A:H4'      | 2:B:95:ARG:NH2   | 0.84     | 1.88        | 10     | 2     |
| 1:A:4:A:C6       | 3:C:168:TRP:CD1  | 0.84     | 2.65        | 6      | 1     |
| 1:A:9:A:H4'      | 2:B:69:TYR:CE1   | 0.83     | 2.08        | 8      | 4     |
| 3:C:274:LEU:HD23 | 3:C:274:LEU:O    | 0.83     | 1.73        | 3      | 2     |
| 2:B:72:ILE:HD12  | 2:B:72:ILE:N     | 0.83     | 1.88        | 9      | 3     |
| 1:A:2:A:H4'      | 3:C:286:PHE:CD1  | 0.83     | 2.08        | 10     | 2     |
| 3:C:226:LYS:O    | 3:C:227:VAL:HG13 | 0.83     | 1.74        | 8      | 2     |
| 1:A:10:U:H5'     | 2:B:71:PHE:CZ    | 0.83     | 2.07        | 7      | 6     |
| 1:A:7:U:H4'      | 3:C:202:PHE:CZ   | 0.82     | 2.09        | 8      | 3     |
| 1:A:11:A:C4'     | 2:B:58:MET:O     | 0.82     | 2.28        | 7      | 1     |
| 2:B:97:LEU:HD12  | 2:B:97:LEU:N     | 0.81     | 1.90        | 2      | 3     |
| 1:A:12:A:H5''    | 2:B:35:TYR:OH    | 0.81     | 1.75        | 7      | 1     |
| 3:C:226:LYS:O    | 3:C:227:VAL:HG23 | 0.81     | 1.76        | 5      | 1     |
| 1:A:9:A:H1'      | 2:B:71:PHE:CZ    | 0.81     | 2.11        | 9      | 2     |
| 1:A:9:A:N3       | 2:B:71:PHE:CZ    | 0.80     | 2.50        | 8      | 8     |
| 1:A:10:U:H5'     | 2:B:71:PHE:CE2   | 0.80     | 2.11        | 7      | 1     |
| 3:C:276:LEU:HD12 | 3:C:276:LEU:H    | 0.80     | 1.34        | 3      | 1     |
| 1:A:10:U:H4'     | 2:B:71:PHE:CE2   | 0.80     | 2.12        | 5      | 3     |
| 1:A:9:A:H5''     | 2:B:69:TYR:CE2   | 0.80     | 2.10        | 9      | 1     |
| 3:C:210:PRO:O    | 3:C:213:VAL:HG22 | 0.80     | 1.75        | 6      | 2     |
| 2:B:90:TYR:CD1   | 2:B:97:LEU:HD11  | 0.79     | 2.12        | 5      | 2     |
| 3:C:221:HIS:C    | 3:C:222:ILE:HD13 | 0.79     | 1.98        | 4      | 3     |
| 3:C:276:LEU:HD12 | 3:C:276:LEU:N    | 0.79     | 1.92        | 3      | 1     |
| 3:C:226:LYS:NZ   | 3:C:280:THR:HG23 | 0.79     | 1.91        | 5      | 1     |
| 1:A:6:A:H5'      | 1:A:8:A:OP2      | 0.79     | 1.76        | 3      | 2     |
| 3:C:212:SER:O    | 3:C:216:VAL:HG23 | 0.79     | 1.78        | 3      | 8     |
| 1:A:11:A:O2'     | 1:A:12:A:H8      | 0.78     | 1.62        | 4      | 6     |
| 2:B:77:LEU:O     | 2:B:81:ALA:HB2   | 0.78     | 1.78        | 9      | 10    |
| 1:A:5:U:H1'      | 3:C:201:GLY:O    | 0.78     | 1.77        | 7      | 1     |
| 3:C:222:ILE:N    | 3:C:222:ILE:HD13 | 0.78     | 1.94        | 4      | 1     |
| 3:C:309:LYS:O    | 3:C:311:ARG:N    | 0.78     | 2.16        | 3      | 2     |
| 1:A:9:A:H4'      | 2:B:69:TYR:CE2   | 0.78     | 2.14        | 1      | 2     |
| 1:A:9:A:H2'      | 1:A:10:U:C5      | 0.78     | 2.14        | 3      | 2     |
| 1:A:6:A:H1'      | 1:A:7:U:OP2      | 0.78     | 1.79        | 3      | 3     |
| 1:A:2:A:H4'      | 3:C:286:PHE:CE1  | 0.77     | 2.14        | 5      | 2     |
| 1:A:10:U:H2'     | 1:A:11:A:H8      | 0.77     | 1.39        | 10     | 4     |
| 1:A:10:U:OP2     | 2:B:69:TYR:CG    | 0.77     | 2.37        | 5      | 2     |
| 1:A:1:U:O2'      | 1:A:2:A:H8       | 0.77     | 1.63        | 8      | 5     |
| 3:C:303:ASN:O    | 3:C:303:ASN:ND2  | 0.77     | 2.18        | 3      | 1     |
| 1:A:10:U:H6      | 1:A:10:U:O5'     | 0.77     | 1.62        | 6      | 2     |
| 1:A:9:A:N3       | 2:B:71:PHE:CE1   | 0.76     | 2.53        | 5      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:7:U:N3       | 3:C:202:PHE:CG   | 0.76     | 2.54        | 6      | 1     |
| 3:C:221:HIS:CD2  | 3:C:221:HIS:H    | 0.76     | 1.96        | 10     | 1     |
| 2:B:45:LEU:O     | 2:B:45:LEU:HD12  | 0.76     | 1.81        | 8      | 1     |
| 1:A:5:U:C2       | 3:C:162:PHE:CE2  | 0.75     | 2.74        | 6      | 4     |
| 3:C:163:ILE:HD11 | 3:C:205:LEU:HD12 | 0.75     | 1.58        | 10     | 1     |
| 3:C:276:LEU:N    | 3:C:276:LEU:HD13 | 0.75     | 1.97        | 7      | 1     |
| 1:A:12:A:H8      | 2:B:68:GLY:N     | 0.75     | 1.79        | 7      | 1     |
| 3:C:275:MET:C    | 3:C:276:LEU:HD13 | 0.75     | 2.02        | 7      | 1     |
| 3:C:308:PHE:O    | 3:C:309:LYS:O    | 0.74     | 2.04        | 2      | 2     |
| 3:C:258:GLU:O    | 3:C:261:GLU:N    | 0.74     | 2.20        | 8      | 8     |
| 3:C:163:ILE:HG22 | 3:C:166:LEU:HD21 | 0.74     | 1.58        | 2      | 1     |
| 1:A:6:A:C5       | 3:C:162:PHE:CE2  | 0.74     | 2.75        | 6      | 7     |
| 1:A:10:U:HO2'    | 1:A:11:A:H8      | 0.74     | 1.19        | 8      | 2     |
| 1:A:10:U:H4'     | 2:B:71:PHE:CZ    | 0.74     | 2.17        | 6      | 3     |
| 1:A:9:A:C2       | 2:B:29:TYR:CZ    | 0.74     | 2.76        | 5      | 9     |
| 1:A:10:U:H2'     | 1:A:11:A:C8      | 0.74     | 2.17        | 10     | 7     |
| 1:A:9:A:C4       | 2:B:29:TYR:CE2   | 0.73     | 2.76        | 4      | 1     |
| 1:A:9:A:H4'      | 2:B:69:TYR:CD1   | 0.73     | 2.17        | 2      | 1     |
| 1:A:4:A:C4       | 3:C:168:TRP:CZ2  | 0.73     | 2.77        | 1      | 3     |
| 1:A:9:A:C2       | 2:B:71:PHE:CE2   | 0.73     | 2.76        | 4      | 4     |
| 1:A:9:A:C2       | 2:B:29:TYR:CE1   | 0.72     | 2.77        | 6      | 8     |
| 3:C:276:LEU:N    | 3:C:276:LEU:HD22 | 0.72     | 1.98        | 7      | 1     |
| 1:A:10:U:O2'     | 1:A:11:A:H8      | 0.72     | 1.68        | 8      | 2     |
| 1:A:9:A:N1       | 2:B:29:TYR:CZ    | 0.72     | 2.58        | 10     | 5     |
| 3:C:188:LEU:HD12 | 3:C:188:LEU:O    | 0.72     | 1.84        | 4      | 1     |
| 1:A:12:A:C8      | 2:B:67:LYS:N     | 0.72     | 2.57        | 7      | 1     |
| 1:A:4:A:C6       | 3:C:168:TRP:CZ3  | 0.72     | 2.77        | 4      | 9     |
| 1:A:3:U:H5'      | 3:C:286:PHE:CZ   | 0.72     | 2.20        | 9      | 6     |
| 1:A:6:A:C6       | 3:C:162:PHE:CD2  | 0.72     | 2.78        | 8      | 7     |
| 1:A:2:A:C4       | 3:C:246:PHE:CE2  | 0.72     | 2.77        | 4      | 3     |
| 1:A:11:A:O3'     | 2:B:59:PHE:HA    | 0.72     | 1.85        | 7      | 1     |
| 2:B:43:LEU:HD13  | 2:B:43:LEU:O     | 0.72     | 1.85        | 9      | 1     |
| 1:A:11:A:H1'     | 2:B:66:SER:O     | 0.71     | 1.85        | 7      | 1     |
| 1:A:10:U:H5''    | 2:B:60:ASP:CG    | 0.71     | 2.06        | 4      | 1     |
| 1:A:6:A:C6       | 3:C:162:PHE:CG   | 0.71     | 2.79        | 7      | 5     |
| 1:A:10:U:O5'     | 1:A:10:U:H6      | 0.71     | 1.69        | 2      | 2     |
| 2:B:69:TYR:OH    | 2:B:71:PHE:CZ    | 0.71     | 2.43        | 10     | 1     |
| 1:A:10:U:H1'     | 2:B:58:MET:CE    | 0.71     | 2.15        | 4      | 1     |
| 2:B:87:LEU:O     | 2:B:97:LEU:HD11  | 0.71     | 1.85        | 9      | 1     |
| 1:A:10:U:C5'     | 2:B:71:PHE:CZ    | 0.71     | 2.73        | 7      | 4     |
| 1:A:12:A:O5'     | 2:B:67:LYS:O     | 0.71     | 2.09        | 7      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:6:A:H5''     | 1:A:8:A:C8       | 0.71     | 2.21        | 3      | 1     |
| 1:A:10:U:H5''    | 2:B:69:TYR:OH    | 0.71     | 1.84        | 10     | 1     |
| 3:C:221:HIS:CD2  | 3:C:221:HIS:N    | 0.70     | 2.59        | 1      | 2     |
| 1:A:5:U:N3       | 3:C:162:PHE:CD2  | 0.70     | 2.59        | 6      | 2     |
| 1:A:5:U:C2       | 3:C:162:PHE:CD2  | 0.70     | 2.79        | 2      | 2     |
| 1:A:12:A:O2'     | 1:A:13:U:H6      | 0.70     | 1.68        | 3      | 4     |
| 1:A:5:U:H5'      | 3:C:200:ARG:CD   | 0.70     | 2.16        | 3      | 1     |
| 1:A:4:A:N1       | 3:C:168:TRP:NE1  | 0.70     | 2.38        | 6      | 1     |
| 1:A:12:A:P       | 2:B:67:LYS:O     | 0.70     | 2.49        | 7      | 1     |
| 1:A:2:A:H4'      | 3:C:286:PHE:CG   | 0.70     | 2.21        | 10     | 1     |
| 1:A:6:A:N7       | 3:C:162:PHE:CZ   | 0.70     | 2.60        | 7      | 2     |
| 1:A:10:U:C5      | 2:B:71:PHE:CZ    | 0.70     | 2.80        | 1      | 1     |
| 3:C:188:LEU:HD23 | 3:C:188:LEU:N    | 0.70     | 2.02        | 6      | 2     |
| 1:A:12:A:OP2     | 2:B:69:TYR:N     | 0.70     | 2.25        | 7      | 1     |
| 1:A:12:A:OP1     | 2:B:59:PHE:CD2   | 0.70     | 2.45        | 7      | 1     |
| 1:A:7:U:C2       | 3:C:202:PHE:CE2  | 0.70     | 2.80        | 6      | 1     |
| 3:C:181:LYS:NZ   | 3:C:182:TYR:CZ   | 0.70     | 2.60        | 7      | 1     |
| 3:C:216:VAL:O    | 3:C:221:HIS:NE2  | 0.70     | 2.25        | 8      | 2     |
| 2:B:46:CYS:O     | 2:B:48:ASN:N     | 0.69     | 2.24        | 7      | 10    |
| 3:C:221:HIS:N    | 3:C:221:HIS:CD2  | 0.69     | 2.61        | 3      | 6     |
| 2:B:38:THR:O     | 2:B:42:ILE:HD13  | 0.69     | 1.88        | 10     | 1     |
| 3:C:221:HIS:O    | 3:C:222:ILE:HD13 | 0.69     | 1.87        | 2      | 2     |
| 1:A:9:A:C2       | 2:B:29:TYR:CE2   | 0.69     | 2.80        | 9      | 4     |
| 3:C:161:MET:SD   | 3:C:162:PHE:N    | 0.69     | 2.65        | 7      | 1     |
| 1:A:6:A:C8       | 3:C:162:PHE:CZ   | 0.69     | 2.81        | 1      | 5     |
| 3:C:205:LEU:HD22 | 3:C:207:PHE:CE1  | 0.69     | 2.22        | 6      | 1     |
| 1:A:11:A:H3'     | 2:B:68:GLY:C     | 0.69     | 2.08        | 7      | 1     |
| 2:B:83:ALA:O     | 2:B:87:LEU:N     | 0.69     | 2.26        | 4      | 7     |
| 1:A:2:A:C6       | 3:C:246:PHE:CD2  | 0.69     | 2.81        | 2      | 1     |
| 1:A:5:U:H5'      | 3:C:200:ARG:NE   | 0.69     | 2.01        | 3      | 1     |
| 1:A:5:U:N3       | 3:C:201:GLY:O    | 0.69     | 2.25        | 5      | 2     |
| 3:C:254:VAL:O    | 3:C:255:ARG:O    | 0.69     | 2.11        | 8      | 1     |
| 1:A:6:A:C4       | 3:C:162:PHE:CZ   | 0.69     | 2.80        | 2      | 4     |
| 3:C:226:LYS:NZ   | 3:C:278:LYS:NZ   | 0.69     | 2.40        | 2      | 1     |
| 1:A:5:U:O4       | 3:C:165:GLY:N    | 0.69     | 2.26        | 5      | 5     |
| 3:C:226:LYS:HZ1  | 3:C:279:ASP:N    | 0.69     | 1.85        | 5      | 2     |
| 1:A:12:A:H5''    | 2:B:35:TYR:CE1   | 0.69     | 2.22        | 7      | 1     |
| 3:C:161:MET:SD   | 3:C:163:ILE:N    | 0.69     | 2.65        | 7      | 1     |
| 1:A:10:U:H5''    | 2:B:69:TYR:CE2   | 0.69     | 2.22        | 10     | 1     |
| 3:C:172:GLU:OE1  | 3:C:190:ILE:HG23 | 0.69     | 1.87        | 3      | 1     |
| 2:B:59:PHE:CD1   | 2:B:59:PHE:N     | 0.68     | 2.61        | 5      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:267:GLY:O    | 3:C:269:ILE:N    | 0.68     | 2.24        | 5      | 1     |
| 2:B:59:PHE:N     | 2:B:59:PHE:CD1   | 0.68     | 2.60        | 7      | 2     |
| 1:A:6:A:N7       | 3:C:239:GLN:NE2  | 0.68     | 2.40        | 3      | 3     |
| 3:C:226:LYS:NZ   | 3:C:280:THR:N    | 0.68     | 2.42        | 5      | 1     |
| 1:A:10:U:C5'     | 2:B:71:PHE:CE1   | 0.68     | 2.76        | 7      | 4     |
| 3:C:266:TRP:O    | 3:C:266:TRP:CD1  | 0.68     | 2.47        | 10     | 1     |
| 1:A:5:U:O2'      | 1:A:6:A:H5'      | 0.68     | 1.88        | 7      | 7     |
| 1:A:10:U:C4'     | 2:B:71:PHE:CZ    | 0.68     | 2.77        | 8      | 3     |
| 1:A:7:U:C2       | 3:C:202:PHE:CD2  | 0.68     | 2.82        | 6      | 1     |
| 1:A:7:U:C4       | 3:C:202:PHE:CD1  | 0.68     | 2.81        | 6      | 1     |
| 1:A:2:A:O2'      | 1:A:3:U:H6       | 0.68     | 1.71        | 2      | 6     |
| 1:A:10:U:P       | 2:B:69:TYR:CD1   | 0.67     | 2.88        | 7      | 1     |
| 2:B:45:LEU:HD13  | 2:B:45:LEU:O     | 0.67     | 1.90        | 3      | 6     |
| 1:A:6:A:C2       | 3:C:162:PHE:CD1  | 0.67     | 2.83        | 9      | 3     |
| 3:C:275:MET:N    | 3:C:275:MET:SD   | 0.67     | 2.67        | 6      | 1     |
| 1:A:4:A:OP2      | 3:C:280:THR:HG21 | 0.67     | 1.88        | 10     | 1     |
| 3:C:259:PHE:CE1  | 3:C:274:LEU:HD23 | 0.67     | 2.24        | 8      | 1     |
| 1:A:4:A:C2       | 3:C:168:TRP:CH2  | 0.67     | 2.82        | 9      | 6     |
| 1:A:6:A:C4       | 3:C:162:PHE:CE1  | 0.67     | 2.82        | 2      | 4     |
| 1:A:9:A:C2       | 2:B:29:TYR:CD1   | 0.67     | 2.83        | 4      | 2     |
| 3:C:227:VAL:HG11 | 3:C:279:ASP:O    | 0.67     | 1.90        | 8      | 1     |
| 1:A:12:A:H5''    | 2:B:35:TYR:CZ    | 0.67     | 2.24        | 7      | 1     |
| 1:A:2:A:C2       | 3:C:246:PHE:CD2  | 0.67     | 2.82        | 9      | 5     |
| 1:A:7:U:C2       | 3:C:191:MET:SD   | 0.67     | 2.88        | 3      | 1     |
| 3:C:275:MET:O    | 3:C:276:LEU:HD12 | 0.67     | 1.89        | 8      | 1     |
| 1:A:10:U:C6      | 1:A:10:U:O5'     | 0.67     | 2.48        | 10     | 3     |
| 3:C:275:MET:O    | 3:C:276:LEU:HD22 | 0.67     | 1.91        | 1      | 2     |
| 1:A:6:A:P        | 3:C:236:ARG:NH2  | 0.67     | 2.68        | 5      | 1     |
| 1:A:1:U:H4'      | 3:C:284:ARG:NH1  | 0.67     | 2.05        | 5      | 1     |
| 2:B:76:ASP:O     | 2:B:78:GLU:N     | 0.66     | 2.27        | 6      | 10    |
| 3:C:195:ALA:O    | 3:C:196:THR:HG23 | 0.66     | 1.90        | 6      | 1     |
| 1:A:12:A:C5'     | 2:B:35:TYR:OH    | 0.66     | 2.43        | 7      | 1     |
| 3:C:188:LEU:HD23 | 3:C:188:LEU:C    | 0.66     | 2.10        | 9      | 1     |
| 1:A:4:A:C2       | 3:C:168:TRP:NE1  | 0.66     | 2.64        | 6      | 1     |
| 1:A:1:U:H3       | 3:C:249:GLY:H    | 0.66     | 1.31        | 4      | 1     |
| 3:C:251:GLY:N    | 3:C:252:PRO:CD   | 0.66     | 2.59        | 7      | 4     |
| 3:C:226:LYS:NZ   | 3:C:279:ASP:N    | 0.66     | 2.43        | 7      | 1     |
| 1:A:2:A:N1       | 3:C:246:PHE:CG   | 0.66     | 2.64        | 9      | 2     |
| 3:C:274:LEU:HD13 | 3:C:275:MET:N    | 0.66     | 2.05        | 8      | 1     |
| 1:A:2:A:C5       | 3:C:246:PHE:CE2  | 0.66     | 2.83        | 2      | 3     |
| 2:B:69:TYR:CE2   | 2:B:71:PHE:CE1   | 0.66     | 2.84        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:6:A:C8       | 3:C:239:GLN:NE2  | 0.66     | 2.63        | 1      | 2     |
| 1:A:9:A:N3       | 2:B:29:TYR:CD2   | 0.66     | 2.64        | 5      | 2     |
| 1:A:4:A:C2       | 3:C:168:TRP:CE2  | 0.66     | 2.84        | 6      | 1     |
| 3:C:219:THR:CG2  | 3:C:221:HIS:CE1  | 0.66     | 2.79        | 7      | 1     |
| 3:C:258:GLU:O    | 3:C:259:PHE:C    | 0.66     | 2.34        | 9      | 8     |
| 2:B:90:TYR:CZ    | 2:B:97:LEU:HD21  | 0.66     | 2.25        | 5      | 1     |
| 1:A:8:A:H4'      | 2:B:95:ARG:HH21  | 0.66     | 1.49        | 10     | 1     |
| 2:B:28:VAL:HG23  | 2:B:98:LYS:O     | 0.65     | 1.92        | 4      | 1     |
| 2:B:35:TYR:CD1   | 2:B:35:TYR:N     | 0.65     | 2.59        | 6      | 2     |
| 2:B:90:TYR:OH    | 2:B:97:LEU:HD21  | 0.65     | 1.91        | 5      | 1     |
| 1:A:6:A:C2       | 3:C:162:PHE:CG   | 0.65     | 2.84        | 10     | 4     |
| 2:B:72:ILE:N     | 2:B:72:ILE:CD1   | 0.65     | 2.60        | 5      | 3     |
| 3:C:269:ILE:O    | 3:C:269:ILE:HG22 | 0.65     | 1.90        | 2      | 4     |
| 2:B:45:LEU:C     | 2:B:45:LEU:HD13  | 0.65     | 2.12        | 7      | 3     |
| 3:C:254:VAL:O    | 3:C:254:VAL:HG12 | 0.65     | 1.91        | 8      | 1     |
| 3:C:311:ARG:O    | 3:C:313:ILE:N    | 0.65     | 2.30        | 9      | 1     |
| 3:C:207:PHE:O    | 3:C:208:GLU:O    | 0.65     | 2.13        | 10     | 1     |
| 1:A:3:U:H5'      | 3:C:286:PHE:CE2  | 0.65     | 2.25        | 10     | 4     |
| 3:C:226:LYS:NZ   | 3:C:280:THR:H    | 0.65     | 1.90        | 5      | 1     |
| 1:A:10:U:C5      | 2:B:65:ARG:NH2   | 0.65     | 2.65        | 6      | 1     |
| 1:A:7:U:C4'      | 3:C:202:PHE:CZ   | 0.65     | 2.80        | 8      | 2     |
| 3:C:245:ILE:HD13 | 3:C:245:ILE:C    | 0.65     | 2.12        | 9      | 1     |
| 1:A:2:A:N3       | 1:A:3:U:C6       | 0.65     | 2.64        | 9      | 3     |
| 2:B:97:LEU:H     | 2:B:97:LEU:HD12  | 0.65     | 1.52        | 2      | 2     |
| 1:A:6:A:N7       | 3:C:162:PHE:CE2  | 0.65     | 2.65        | 5      | 6     |
| 1:A:9:A:C4'      | 2:B:69:TYR:CE1   | 0.65     | 2.79        | 6      | 3     |
| 3:C:188:LEU:HD23 | 3:C:188:LEU:H    | 0.65     | 1.51        | 6      | 1     |
| 3:C:179:PHE:C    | 3:C:181:LYS:H    | 0.65     | 1.95        | 8      | 5     |
| 1:A:2:A:C6       | 3:C:246:PHE:CD1  | 0.65     | 2.84        | 9      | 1     |
| 1:A:2:A:C4       | 1:A:3:U:C5       | 0.64     | 2.84        | 10     | 2     |
| 1:A:10:U:H5'     | 2:B:71:PHE:CD2   | 0.64     | 2.27        | 7      | 1     |
| 3:C:305:PHE:CE1  | 3:C:314:GLU:CG   | 0.64     | 2.80        | 10     | 1     |
| 1:A:8:A:N3       | 2:B:29:TYR:CD2   | 0.64     | 2.65        | 9      | 1     |
| 2:B:90:TYR:O     | 2:B:92:LEU:N     | 0.64     | 2.29        | 5      | 10    |
| 3:C:308:PHE:CG   | 3:C:309:LYS:N    | 0.64     | 2.64        | 5      | 8     |
| 3:C:250:ILE:CG2  | 3:C:254:VAL:HG11 | 0.64     | 2.23        | 2      | 1     |
| 3:C:161:MET:SD   | 3:C:216:VAL:HG11 | 0.64     | 2.32        | 3      | 2     |
| 1:A:11:A:H5'     | 2:B:69:TYR:C     | 0.64     | 2.12        | 7      | 1     |
| 1:A:3:U:O2'      | 1:A:4:A:H5''     | 0.64     | 1.93        | 1      | 2     |
| 1:A:8:A:C2       | 2:B:29:TYR:CE2   | 0.64     | 2.85        | 3      | 7     |
| 3:C:276:LEU:CD1  | 3:C:276:LEU:N    | 0.64     | 2.58        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:11:A:C3'     | 2:B:58:MET:O     | 0.64     | 2.46        | 7      | 1     |
| 2:B:84:VAL:O     | 2:B:88:ASN:N     | 0.64     | 2.30        | 9      | 4     |
| 3:C:226:LYS:O    | 3:C:227:VAL:CG2  | 0.64     | 2.46        | 5      | 1     |
| 3:C:245:ILE:HD12 | 3:C:315:ILE:CG2  | 0.64     | 2.23        | 7      | 6     |
| 1:A:10:U:O5'     | 1:A:10:U:C6      | 0.64     | 2.51        | 2      | 3     |
| 3:C:263:PHE:O    | 3:C:265:GLN:N    | 0.64     | 2.31        | 4      | 5     |
| 3:C:286:PHE:N    | 3:C:286:PHE:CD1  | 0.64     | 2.66        | 2      | 2     |
| 1:A:2:A:N1       | 3:C:246:PHE:CD2  | 0.64     | 2.66        | 2      | 1     |
| 1:A:2:A:N3       | 3:C:246:PHE:CD2  | 0.64     | 2.66        | 5      | 4     |
| 1:A:5:U:H3       | 3:C:165:GLY:H    | 0.64     | 1.36        | 7      | 2     |
| 1:A:11:A:C4      | 2:B:66:SER:OG    | 0.63     | 2.51        | 7      | 1     |
| 2:B:45:LEU:HD13  | 2:B:45:LEU:C     | 0.63     | 2.14        | 10     | 4     |
| 1:A:10:U:O2      | 1:A:11:A:C5      | 0.63     | 2.51        | 4      | 1     |
| 3:C:255:ARG:N    | 3:C:255:ARG:CD   | 0.63     | 2.60        | 5      | 2     |
| 3:C:251:GLY:O    | 3:C:254:VAL:HG12 | 0.63     | 1.94        | 2      | 2     |
| 3:C:226:LYS:HZ1  | 3:C:279:ASP:H    | 0.63     | 1.36        | 5      | 1     |
| 3:C:205:LEU:HD13 | 3:C:207:PHE:CZ   | 0.63     | 2.27        | 7      | 1     |
| 3:C:158:SER:O    | 3:C:160:LYS:N    | 0.63     | 2.32        | 9      | 2     |
| 2:B:27:VAL:O     | 2:B:100:GLY:N    | 0.63     | 2.31        | 1      | 4     |
| 1:A:4:A:C4       | 3:C:168:TRP:CH2  | 0.63     | 2.85        | 10     | 4     |
| 1:A:11:A:N7      | 2:B:58:MET:CE    | 0.63     | 2.62        | 9      | 3     |
| 1:A:3:U:O2'      | 1:A:4:A:H4'      | 0.63     | 1.94        | 6      | 1     |
| 1:A:12:A:P       | 2:B:68:GLY:CA    | 0.63     | 2.86        | 7      | 1     |
| 1:A:11:A:C8      | 2:B:58:MET:SD    | 0.63     | 2.91        | 3      | 1     |
| 3:C:274:LEU:C    | 3:C:274:LEU:HD23 | 0.63     | 2.14        | 5      | 2     |
| 1:A:4:A:N1       | 3:C:199:SER:O    | 0.63     | 2.32        | 6      | 1     |
| 3:C:188:LEU:HD23 | 3:C:189:LYS:N    | 0.63     | 2.09        | 7      | 1     |
| 1:A:6:A:C6       | 3:C:234:ILE:O    | 0.63     | 2.52        | 8      | 2     |
| 2:B:35:TYR:N     | 2:B:35:TYR:CD1   | 0.63     | 2.62        | 1      | 1     |
| 1:A:11:A:O3'     | 2:B:67:LYS:O     | 0.63     | 2.16        | 7      | 1     |
| 2:B:42:ILE:O     | 2:B:44:ASP:N     | 0.63     | 2.32        | 7      | 8     |
| 3:C:226:LYS:HZ3  | 3:C:280:THR:HG23 | 0.63     | 1.52        | 5      | 1     |
| 1:A:10:U:C6      | 1:A:11:A:N7      | 0.63     | 2.66        | 7      | 1     |
| 3:C:308:PHE:O    | 3:C:310:ASP:N    | 0.63     | 2.32        | 8      | 3     |
| 2:B:44:ASP:O     | 2:B:48:ASN:ND2   | 0.62     | 2.32        | 8      | 7     |
| 2:B:32:SER:OG    | 2:B:95:ARG:N     | 0.62     | 2.27        | 7      | 3     |
| 1:A:5:U:O2'      | 1:A:7:U:N3       | 0.62     | 2.32        | 6      | 1     |
| 1:A:7:U:H5       | 3:C:204:PHE:CE2  | 0.62     | 2.10        | 6      | 1     |
| 3:C:308:PHE:O    | 3:C:309:LYS:C    | 0.62     | 2.37        | 3      | 8     |
| 2:B:57:MET:SD    | 2:B:70:ALA:HB2   | 0.62     | 2.34        | 2      | 2     |
| 3:C:199:SER:O    | 3:C:201:GLY:N    | 0.62     | 2.33        | 3      | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:12:A:H8     | 2:B:67:LYS:N     | 0.62     | 1.89        | 7      | 1     |
| 1:A:10:U:P      | 1:A:10:U:C6      | 0.62     | 2.92        | 10     | 1     |
| 3:C:178:TYR:CD2 | 3:C:223:LEU:HD12 | 0.62     | 2.29        | 1      | 3     |
| 3:C:188:LEU:C   | 3:C:188:LEU:HD12 | 0.62     | 2.14        | 8      | 2     |
| 1:A:4:A:H8      | 3:C:166:LEU:O    | 0.62     | 1.77        | 9      | 3     |
| 2:B:84:VAL:HG13 | 2:B:99:CYS:CB    | 0.62     | 2.25        | 4      | 1     |
| 2:B:97:LEU:N    | 2:B:97:LEU:CD1   | 0.62     | 2.58        | 5      | 1     |
| 3:C:168:TRP:CZ2 | 3:C:198:ARG:CZ   | 0.62     | 2.83        | 10     | 1     |
| 1:A:2:A:N3      | 1:A:3:U:C5       | 0.62     | 2.68        | 3      | 4     |
| 1:A:9:A:C5'     | 2:B:69:TYR:CE1   | 0.62     | 2.82        | 2      | 2     |
| 1:A:2:A:C5      | 3:C:246:PHE:CZ   | 0.62     | 2.87        | 9      | 2     |
| 3:C:226:LYS:C   | 3:C:227:VAL:HG22 | 0.62     | 2.15        | 8      | 2     |
| 1:A:4:A:C5      | 3:C:168:TRP:CZ3  | 0.62     | 2.87        | 10     | 7     |
| 3:C:301:CYS:SG  | 3:C:317:ARG:NH2  | 0.62     | 2.73        | 6      | 1     |
| 3:C:182:TYR:OH  | 3:C:221:HIS:ND1  | 0.62     | 2.32        | 2      | 5     |
| 3:C:264:SER:O   | 3:C:266:TRP:N    | 0.62     | 2.33        | 8      | 2     |
| 2:B:46:CYS:O    | 2:B:49:VAL:N     | 0.62     | 2.33        | 5      | 2     |
| 1:A:3:U:C5'     | 3:C:286:PHE:CZ   | 0.62     | 2.83        | 3      | 3     |
| 1:A:11:A:C8     | 2:B:58:MET:CE    | 0.62     | 2.83        | 5      | 2     |
| 3:C:188:LEU:O   | 3:C:188:LEU:HD23 | 0.62     | 1.94        | 5      | 2     |
| 2:B:30:LEU:HD13 | 2:B:72:ILE:CD1   | 0.62     | 2.25        | 6      | 1     |
| 3:C:316:LYS:O   | 3:C:317:ARG:O    | 0.62     | 2.18        | 7      | 1     |
| 1:A:5:U:H3'     | 1:A:5:U:O2       | 0.61     | 1.95        | 3      | 1     |
| 1:A:5:U:C5'     | 3:C:200:ARG:NE   | 0.61     | 2.63        | 3      | 1     |
| 1:A:12:A:N6     | 2:B:58:MET:SD    | 0.61     | 2.72        | 8      | 1     |
| 2:B:101:TYR:O   | 2:B:103:SER:N    | 0.61     | 2.33        | 3      | 3     |
| 3:C:236:ARG:N   | 3:C:236:ARG:HE   | 0.61     | 1.92        | 3      | 1     |
| 1:A:7:U:O4      | 3:C:162:PHE:CE1  | 0.61     | 2.53        | 6      | 1     |
| 1:A:12:A:OP1    | 2:B:59:PHE:CG    | 0.61     | 2.53        | 7      | 1     |
| 2:B:52:VAL:HG12 | 2:B:53:ILE:H     | 0.61     | 1.56        | 1      | 1     |
| 1:A:7:U:H4'     | 1:A:8:A:OP2      | 0.61     | 1.93        | 4      | 3     |
| 3:C:166:LEU:N   | 3:C:166:LEU:HD12 | 0.61     | 2.10        | 3      | 1     |
| 3:C:259:PHE:CZ  | 3:C:289:VAL:HG13 | 0.61     | 2.31        | 10     | 1     |
| 3:C:238:GLU:O   | 3:C:242:THR:HG23 | 0.61     | 1.95        | 9      | 4     |
| 1:A:6:A:C5      | 3:C:162:PHE:CZ   | 0.61     | 2.88        | 6      | 3     |
| 3:C:263:PHE:CD2 | 3:C:266:TRP:CH2  | 0.61     | 2.88        | 3      | 9     |
| 3:C:276:LEU:O   | 3:C:282:GLN:N    | 0.61     | 2.34        | 8      | 1     |
| 3:C:301:CYS:SG  | 3:C:317:ARG:CZ   | 0.61     | 2.89        | 6      | 1     |
| 1:A:4:A:N7      | 3:C:167:ASN:O    | 0.61     | 2.33        | 2      | 5     |
| 2:B:90:TYR:CE1  | 2:B:97:LEU:HD21  | 0.61     | 2.31        | 5      | 1     |
| 2:B:85:ARG:O    | 2:B:88:ASN:ND2   | 0.61     | 2.33        | 7      | 2     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:12:A:N3      | 1:A:13:U:C6     | 0.61     | 2.68        | 7      | 1     |
| 3:C:276:LEU:N    | 3:C:280:THR:OG1 | 0.61     | 2.33        | 8      | 3     |
| 1:A:6:A:N6       | 3:C:162:PHE:CD2 | 0.61     | 2.68        | 8      | 2     |
| 3:C:282:GLN:O    | 3:C:284:ARG:N   | 0.61     | 2.31        | 1      | 7     |
| 2:B:35:TYR:OH    | 2:B:59:PHE:CG   | 0.61     | 2.54        | 2      | 2     |
| 3:C:262:PHE:O    | 3:C:265:GLN:NE2 | 0.61     | 2.34        | 5      | 2     |
| 2:B:32:SER:OG    | 2:B:94:SER:N    | 0.61     | 2.34        | 7      | 1     |
| 1:A:1:U:O2'      | 1:A:2:A:H2'     | 0.61     | 1.95        | 9      | 1     |
| 1:A:8:A:H4'      | 2:B:95:ARG:NH1  | 0.60     | 2.11        | 6      | 1     |
| 1:A:6:A:H4'      | 1:A:7:U:H3'     | 0.60     | 1.73        | 3      | 2     |
| 2:B:88:ASN:N     | 2:B:88:ASN:OD1  | 0.60     | 2.34        | 9      | 3     |
| 3:C:317:ARG:CD   | 3:C:317:ARG:H   | 0.60     | 2.08        | 1      | 1     |
| 2:B:84:VAL:O     | 2:B:88:ASN:CB   | 0.60     | 2.49        | 9      | 7     |
| 3:C:266:TRP:CD1  | 3:C:266:TRP:O   | 0.60     | 2.55        | 8      | 1     |
| 2:B:82:SER:O     | 2:B:86:ASN:ND2  | 0.60     | 2.34        | 5      | 7     |
| 3:C:216:VAL:HG12 | 3:C:216:VAL:O   | 0.60     | 1.96        | 6      | 1     |
| 1:A:6:A:C4       | 3:C:162:PHE:CD1 | 0.60     | 2.90        | 7      | 3     |
| 3:C:269:ILE:CG2  | 3:C:269:ILE:O   | 0.60     | 2.49        | 5      | 3     |
| 2:B:48:ASN:O     | 2:B:49:VAL:HG23 | 0.60     | 1.95        | 9      | 2     |
| 1:A:6:A:C5       | 3:C:162:PHE:CD2 | 0.60     | 2.90        | 5      | 6     |
| 3:C:176:ARG:O    | 3:C:178:TYR:N   | 0.60     | 2.35        | 10     | 8     |
| 3:C:227:VAL:HG12 | 3:C:227:VAL:O   | 0.60     | 1.94        | 5      | 1     |
| 1:A:11:A:O3'     | 2:B:67:LYS:C    | 0.60     | 2.40        | 7      | 1     |
| 2:B:58:MET:SD    | 2:B:59:PHE:O    | 0.60     | 2.59        | 2      | 3     |
| 2:B:22:ASN:OD1   | 2:B:22:ASN:N    | 0.60     | 2.34        | 7      | 1     |
| 1:A:10:U:O2'     | 1:A:11:A:H5'    | 0.60     | 1.97        | 5      | 6     |
| 2:B:90:TYR:CE1   | 2:B:91:GLN:O    | 0.60     | 2.55        | 3      | 8     |
| 2:B:53:ILE:HG22  | 2:B:54:ASN:OD1  | 0.60     | 1.97        | 10     | 2     |
| 3:C:266:TRP:CD1  | 3:C:267:GLY:N   | 0.60     | 2.69        | 3      | 1     |
| 3:C:277:ASP:O    | 3:C:280:THR:N   | 0.60     | 2.32        | 4      | 1     |
| 1:A:10:U:OP1     | 2:B:70:ALA:N    | 0.60     | 2.35        | 5      | 1     |
| 3:C:219:THR:O    | 3:C:221:HIS:CD2 | 0.60     | 2.55        | 6      | 3     |
| 2:B:68:GLY:O     | 2:B:69:TYR:CD2  | 0.60     | 2.54        | 7      | 1     |
| 1:A:7:U:C5       | 3:C:204:PHE:CE2 | 0.60     | 2.89        | 6      | 1     |
| 1:A:9:A:N1       | 2:B:29:TYR:CE2  | 0.60     | 2.70        | 10     | 1     |
| 3:C:283:SER:O    | 3:C:285:GLY:N   | 0.59     | 2.31        | 2      | 1     |
| 3:C:246:PHE:CD1  | 3:C:246:PHE:O   | 0.59     | 2.55        | 9      | 3     |
| 3:C:219:THR:O    | 3:C:221:HIS:NE2 | 0.59     | 2.35        | 6      | 4     |
| 3:C:250:ILE:O    | 3:C:286:PHE:N   | 0.59     | 2.35        | 9      | 3     |
| 1:A:11:A:C8      | 2:B:58:MET:HE1  | 0.59     | 2.32        | 8      | 1     |
| 1:A:5:U:O2'      | 1:A:6:A:C5'     | 0.59     | 2.50        | 1      | 7     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:54:ASN:ND2  | 2:B:73:GLU:OE1   | 0.59     | 2.35        | 2      | 9     |
| 1:A:3:U:O2'     | 1:A:4:A:C5'      | 0.59     | 2.51        | 6      | 4     |
| 1:A:6:A:C5'     | 1:A:7:U:H5'      | 0.59     | 2.27        | 2      | 1     |
| 2:B:30:LEU:HD11 | 2:B:97:LEU:HD23  | 0.59     | 1.74        | 2      | 1     |
| 2:B:60:ASP:OD2  | 2:B:66:SER:N     | 0.59     | 2.36        | 8      | 4     |
| 3:C:159:CYS:SG  | 3:C:207:PHE:O    | 0.59     | 2.61        | 3      | 2     |
| 3:C:221:HIS:HB3 | 3:C:228:ILE:HD11 | 0.59     | 1.74        | 5      | 2     |
| 1:A:1:U:N3      | 3:C:314:GLU:OE1  | 0.59     | 2.35        | 10     | 2     |
| 3:C:238:GLU:OE1 | 3:C:238:GLU:N    | 0.59     | 2.36        | 10     | 1     |
| 3:C:167:ASN:O   | 3:C:168:TRP:CG   | 0.59     | 2.56        | 7      | 3     |
| 1:A:8:A:H2      | 2:B:29:TYR:CD2   | 0.59     | 2.16        | 3      | 1     |
| 2:B:29:TYR:CD1  | 2:B:29:TYR:N     | 0.59     | 2.70        | 4      | 2     |
| 2:B:88:ASN:O    | 2:B:97:LEU:HD13  | 0.59     | 1.95        | 5      | 1     |
| 2:B:22:ASN:ND2  | 2:B:102:SER:O    | 0.59     | 2.36        | 6      | 1     |
| 3:C:300:VAL:O   | 3:C:303:ASN:N    | 0.59     | 2.36        | 9      | 9     |
| 2:B:33:ILE:HD12 | 2:B:33:ILE:N     | 0.59     | 2.13        | 8      | 3     |
| 1:A:9:A:C4'     | 2:B:69:TYR:CE2   | 0.59     | 2.85        | 3      | 1     |
| 2:B:22:ASN:OD1  | 2:B:101:TYR:CE2  | 0.59     | 2.56        | 4      | 1     |
| 2:B:58:MET:CG   | 2:B:59:PHE:N     | 0.59     | 2.66        | 7      | 1     |
| 3:C:261:GLU:OE1 | 3:C:261:GLU:N    | 0.59     | 2.35        | 7      | 1     |
| 2:B:22:ASN:N    | 2:B:23:PRO:CD    | 0.59     | 2.65        | 8      | 1     |
| 1:A:10:U:C5     | 1:A:10:U:P       | 0.59     | 2.95        | 10     | 1     |
| 3:C:237:ASP:OD1 | 3:C:238:GLU:N    | 0.59     | 2.36        | 1      | 2     |
| 2:B:82:SER:O    | 2:B:86:ASN:OD1   | 0.59     | 2.20        | 2      | 1     |
| 1:A:6:A:N9      | 3:C:162:PHE:CZ   | 0.59     | 2.71        | 2      | 1     |
| 2:B:35:TYR:OH   | 2:B:59:PHE:CD1   | 0.59     | 2.55        | 9      | 2     |
| 3:C:187:ASP:OD2 | 3:C:189:LYS:NZ   | 0.59     | 2.35        | 5      | 1     |
| 1:A:6:A:N6      | 3:C:234:ILE:H    | 0.59     | 1.96        | 6      | 1     |
| 1:A:5:U:H4'     | 3:C:200:ARG:CB   | 0.59     | 2.28        | 10     | 1     |
| 3:C:199:SER:O   | 3:C:200:ARG:C    | 0.59     | 2.41        | 6      | 8     |
| 1:A:9:A:C6      | 2:B:29:TYR:OH    | 0.59     | 2.56        | 2      | 2     |
| 2:B:101:TYR:N   | 2:B:101:TYR:CD1  | 0.59     | 2.67        | 6      | 2     |
| 3:C:181:LYS:NZ  | 3:C:182:TYR:OH   | 0.59     | 2.36        | 7      | 1     |
| 1:A:1:U:C4      | 1:A:3:U:O4       | 0.59     | 2.56        | 9      | 1     |
| 3:C:211:SER:O   | 3:C:213:VAL:N    | 0.59     | 2.36        | 4      | 8     |
| 1:A:5:U:C5'     | 3:C:200:ARG:HE   | 0.59     | 2.10        | 3      | 1     |
| 3:C:176:ARG:O   | 3:C:179:PHE:N    | 0.59     | 2.35        | 4      | 7     |
| 2:B:45:LEU:C    | 2:B:45:LEU:HD12  | 0.59     | 2.19        | 8      | 1     |
| 3:C:167:ASN:O   | 3:C:169:ASP:N    | 0.58     | 2.35        | 1      | 2     |
| 3:C:160:LYS:NZ  | 3:C:189:LYS:NZ   | 0.58     | 2.51        | 1      | 1     |
| 3:C:282:GLN:O   | 3:C:286:PHE:CZ   | 0.58     | 2.56        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:210:PRO:O    | 3:C:213:VAL:HG12 | 0.58     | 1.97        | 2      | 1     |
| 3:C:269:ILE:HG21 | 3:C:272:ALA:HB2  | 0.58     | 1.75        | 7      | 1     |
| 3:C:279:ASP:OD1  | 3:C:280:THR:N    | 0.58     | 2.35        | 7      | 1     |
| 3:C:302:GLN:NE2  | 3:C:303:ASN:OD1  | 0.58     | 2.36        | 7      | 1     |
| 1:A:1:U:O2       | 1:A:2:A:N7       | 0.58     | 2.36        | 9      | 1     |
| 1:A:6:A:C4       | 3:C:162:PHE:CE2  | 0.58     | 2.91        | 10     | 2     |
| 2:B:69:TYR:OH    | 2:B:71:PHE:CE2   | 0.58     | 2.51        | 10     | 1     |
| 1:A:4:A:P        | 3:C:280:THR:HG21 | 0.58     | 2.38        | 10     | 1     |
| 2:B:84:VAL:O     | 2:B:88:ASN:ND2   | 0.58     | 2.36        | 2      | 3     |
| 2:B:52:VAL:CG1   | 2:B:53:ILE:N     | 0.58     | 2.66        | 4      | 1     |
| 2:B:90:TYR:C     | 2:B:90:TYR:CD1   | 0.58     | 2.76        | 6      | 3     |
| 1:A:5:U:O4       | 3:C:231:LYS:NZ   | 0.58     | 2.37        | 9      | 1     |
| 2:B:60:ASP:O     | 2:B:64:GLY:N     | 0.58     | 2.36        | 10     | 1     |
| 3:C:220:GLN:O    | 3:C:221:HIS:CG   | 0.58     | 2.55        | 5      | 1     |
| 3:C:277:ASP:OD1  | 3:C:278:LYS:N    | 0.58     | 2.36        | 10     | 3     |
| 1:A:11:A:C2      | 2:B:63:THR:OG1   | 0.58     | 2.54        | 7      | 1     |
| 1:A:2:A:N6       | 3:C:319:GLU:O    | 0.58     | 2.36        | 7      | 1     |
| 3:C:170:THR:OG1  | 3:C:192:LYS:NZ   | 0.58     | 2.36        | 9      | 1     |
| 1:A:10:U:H3'     | 2:B:69:TYR:OH    | 0.58     | 1.97        | 10     | 1     |
| 1:A:9:A:C5'      | 2:B:69:TYR:CZ    | 0.58     | 2.84        | 2      | 1     |
| 3:C:249:GLY:O    | 3:C:311:ARG:NH1  | 0.58     | 2.36        | 2      | 1     |
| 2:B:84:VAL:O     | 2:B:88:ASN:CA    | 0.58     | 2.51        | 5      | 6     |
| 1:A:10:U:OP1     | 2:B:69:TYR:CG    | 0.58     | 2.56        | 8      | 2     |
| 1:A:12:A:H2'     | 2:B:68:GLY:HA3   | 0.58     | 1.75        | 7      | 1     |
| 1:A:10:U:C2'     | 1:A:11:A:H8      | 0.58     | 2.11        | 8      | 4     |
| 2:B:87:LEU:O     | 2:B:88:ASN:C     | 0.58     | 2.40        | 9      | 2     |
| 2:B:27:VAL:HG12  | 2:B:102:SER:N    | 0.58     | 2.13        | 6      | 1     |
| 1:A:2:A:C6       | 3:C:246:PHE:CE2  | 0.58     | 2.92        | 2      | 1     |
| 3:C:171:THR:OG1  | 3:C:174:ASN:ND2  | 0.58     | 2.36        | 2      | 2     |
| 1:A:2:A:O4'      | 3:C:286:PHE:CE1  | 0.58     | 2.57        | 2      | 1     |
| 1:A:7:U:O4       | 3:C:162:PHE:CZ   | 0.58     | 2.57        | 6      | 1     |
| 3:C:279:ASP:C    | 3:C:280:THR:HG22 | 0.58     | 2.18        | 7      | 1     |
| 3:C:193:ASP:OD2  | 3:C:197:GLY:N    | 0.58     | 2.37        | 8      | 1     |
| 2:B:97:LEU:CD1   | 2:B:97:LEU:H     | 0.58     | 2.10        | 2      | 1     |
| 1:A:2:A:O2'      | 1:A:3:U:C6       | 0.58     | 2.56        | 10     | 5     |
| 2:B:45:LEU:O     | 2:B:48:ASN:ND2   | 0.58     | 2.36        | 4      | 2     |
| 1:A:12:A:O5'     | 2:B:68:GLY:CA    | 0.58     | 2.45        | 7      | 1     |
| 3:C:250:ILE:N    | 3:C:285:GLY:O    | 0.58     | 2.37        | 8      | 1     |
| 2:B:27:VAL:O     | 2:B:100:GLY:CA   | 0.58     | 2.52        | 6      | 2     |
| 2:B:99:CYS:O     | 2:B:99:CYS:SG    | 0.58     | 2.61        | 10     | 2     |
| 3:C:269:ILE:HD11 | 3:C:289:VAL:HB   | 0.58     | 1.75        | 5      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:174:ASN:OD1  | 3:C:175:LEU:N    | 0.58     | 2.35        | 10     | 1     |
| 2:B:50:GLY:O     | 2:B:52:VAL:N     | 0.58     | 2.37        | 5      | 1     |
| 3:C:249:GLY:O    | 3:C:313:ILE:HG22 | 0.58     | 1.98        | 8      | 1     |
| 2:B:87:LEU:HD12  | 2:B:87:LEU:O     | 0.58     | 1.99        | 1      | 1     |
| 3:C:200:ARG:NE   | 3:C:200:ARG:C    | 0.58     | 2.57        | 2      | 1     |
| 3:C:277:ASP:N    | 3:C:283:SER:OG   | 0.58     | 2.36        | 6      | 1     |
| 1:A:10:U:C5      | 1:A:11:A:N7      | 0.58     | 2.72        | 7      | 1     |
| 2:B:26:ARG:NE    | 2:B:76:ASP:OD1   | 0.58     | 2.37        | 8      | 1     |
| 2:B:90:TYR:CD1   | 2:B:90:TYR:C     | 0.57     | 2.77        | 4      | 5     |
| 3:C:263:PHE:O    | 3:C:264:SER:C    | 0.57     | 2.43        | 9      | 10    |
| 3:C:297:VAL:O    | 3:C:301:CYS:SG   | 0.57     | 2.62        | 10     | 2     |
| 2:B:26:ARG:NH2   | 2:B:76:ASP:OD2   | 0.57     | 2.37        | 8      | 1     |
| 3:C:167:ASN:ND2  | 3:C:224:ASP:OD2  | 0.57     | 2.36        | 1      | 2     |
| 1:A:2:A:C2       | 1:A:3:U:C5       | 0.57     | 2.92        | 2      | 4     |
| 3:C:193:ASP:N    | 3:C:197:GLY:O    | 0.57     | 2.36        | 6      | 1     |
| 3:C:164:GLY:O    | 3:C:166:LEU:N    | 0.57     | 2.37        | 10     | 1     |
| 1:A:9:A:O2'      | 1:A:10:U:C5'     | 0.57     | 2.53        | 2      | 4     |
| 3:C:199:SER:O    | 3:C:200:ARG:O    | 0.57     | 2.23        | 2      | 3     |
| 1:A:10:U:H1'     | 2:B:58:MET:HE3   | 0.57     | 1.75        | 4      | 1     |
| 2:B:99:CYS:SG    | 2:B:99:CYS:O     | 0.57     | 2.62        | 5      | 3     |
| 3:C:303:ASN:OD1  | 3:C:303:ASN:O    | 0.57     | 2.22        | 6      | 1     |
| 2:B:23:PRO:O     | 2:B:101:TYR:CG   | 0.57     | 2.57        | 2      | 1     |
| 3:C:280:THR:OG1  | 3:C:281:GLY:N    | 0.57     | 2.35        | 4      | 1     |
| 3:C:178:TYR:OH   | 3:C:222:ILE:N    | 0.57     | 2.37        | 6      | 3     |
| 3:C:180:GLY:O    | 3:C:182:TYR:N    | 0.57     | 2.36        | 10     | 1     |
| 3:C:244:LYS:O    | 3:C:318:ALA:HB2  | 0.57     | 2.00        | 1      | 1     |
| 1:A:4:A:C8       | 3:C:167:ASN:O    | 0.57     | 2.57        | 7      | 4     |
| 3:C:258:GLU:H    | 3:C:258:GLU:CD   | 0.57     | 2.03        | 3      | 1     |
| 3:C:166:LEU:HA   | 3:C:228:ILE:HG22 | 0.57     | 1.76        | 4      | 2     |
| 1:A:8:A:O2'      | 1:A:9:A:O5'      | 0.57     | 2.23        | 5      | 5     |
| 3:C:211:SER:O    | 3:C:214:ASP:N    | 0.57     | 2.37        | 4      | 9     |
| 1:A:9:A:H2'      | 1:A:10:U:H6      | 0.57     | 1.54        | 3      | 1     |
| 1:A:9:A:C4       | 2:B:29:TYR:CD2   | 0.57     | 2.92        | 4      | 1     |
| 2:B:48:ASN:OD1   | 2:B:49:VAL:N     | 0.57     | 2.32        | 4      | 1     |
| 3:C:190:ILE:HG23 | 3:C:190:ILE:O    | 0.57     | 1.99        | 7      | 1     |
| 1:A:4:A:C8       | 3:C:166:LEU:O    | 0.57     | 2.58        | 7      | 7     |
| 2:B:33:ILE:N     | 2:B:33:ILE:HD12  | 0.57     | 2.15        | 4      | 1     |
| 2:B:26:ARG:N     | 2:B:80:SER:OG    | 0.57     | 2.38        | 10     | 2     |
| 3:C:292:ASP:OD1  | 3:C:293:SER:N    | 0.57     | 2.36        | 10     | 3     |
| 2:B:45:LEU:O     | 2:B:45:LEU:HD13  | 0.57     | 2.00        | 10     | 1     |
| 1:A:11:A:O2'     | 1:A:12:A:O5'     | 0.57     | 2.23        | 4      | 6     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:30:LEU:CD1  | 2:B:97:LEU:HD23  | 0.57     | 2.30        | 2      | 1     |
| 3:C:303:ASN:ND2 | 3:C:306:ILE:CG1  | 0.57     | 2.67        | 3      | 1     |
| 3:C:172:GLU:H   | 3:C:172:GLU:CD   | 0.57     | 2.03        | 10     | 2     |
| 3:C:294:ALA:O   | 3:C:297:VAL:N    | 0.57     | 2.38        | 5      | 1     |
| 3:C:173:ASP:O   | 3:C:176:ARG:N    | 0.57     | 2.38        | 10     | 2     |
| 1:A:8:A:C6      | 2:B:101:TYR:OH   | 0.57     | 2.55        | 6      | 1     |
| 1:A:11:A:O2'    | 2:B:67:LYS:C     | 0.57     | 2.43        | 7      | 1     |
| 2:B:77:LEU:O    | 2:B:81:ALA:CB    | 0.56     | 2.53        | 2      | 10    |
| 1:A:4:A:O2'     | 1:A:5:U:C4       | 0.56     | 2.56        | 4      | 1     |
| 1:A:3:U:H3'     | 3:C:277:ASP:OD2  | 0.56     | 2.00        | 4      | 1     |
| 1:A:2:A:C2      | 3:C:246:PHE:CG   | 0.56     | 2.94        | 9      | 2     |
| 1:A:5:U:O2      | 3:C:163:ILE:O    | 0.56     | 2.23        | 9      | 3     |
| 3:C:263:PHE:CD2 | 3:C:266:TRP:CZ2  | 0.56     | 2.94        | 9      | 3     |
| 3:C:274:LEU:CD1 | 3:C:286:PHE:O    | 0.56     | 2.54        | 7      | 3     |
| 2:B:30:LEU:N    | 2:B:30:LEU:CD2   | 0.56     | 2.68        | 2      | 1     |
| 1:A:4:A:N1      | 3:C:168:TRP:CZ3  | 0.56     | 2.73        | 4      | 2     |
| 1:A:6:A:P       | 3:C:236:ARG:HH22 | 0.56     | 2.24        | 5      | 1     |
| 3:C:190:ILE:O   | 3:C:191:MET:SD   | 0.56     | 2.64        | 5      | 1     |
| 3:C:271:ASP:O   | 3:C:272:ALA:C    | 0.56     | 2.44        | 8      | 2     |
| 2:B:97:LEU:H    | 2:B:97:LEU:CD1   | 0.56     | 2.11        | 5      | 1     |
| 2:B:67:LYS:O    | 2:B:69:TYR:N     | 0.56     | 2.38        | 6      | 1     |
| 3:C:276:LEU:O   | 3:C:278:LYS:N    | 0.56     | 2.33        | 6      | 1     |
| 1:A:10:U:OP1    | 2:B:69:TYR:CD2   | 0.56     | 2.59        | 8      | 3     |
| 1:A:1:U:O2      | 1:A:2:A:N6       | 0.56     | 2.38        | 9      | 1     |
| 1:A:9:A:O2'     | 1:A:10:U:C6      | 0.56     | 2.56        | 2      | 2     |
| 1:A:6:A:O2'     | 3:C:236:ARG:NH1  | 0.56     | 2.38        | 9      | 2     |
| 3:C:268:THR:O   | 3:C:269:ILE:C    | 0.56     | 2.43        | 3      | 4     |
| 1:A:7:U:N3      | 3:C:202:PHE:CD2  | 0.56     | 2.74        | 6      | 1     |
| 2:B:60:ASP:OD2  | 2:B:65:ARG:N     | 0.56     | 2.37        | 1      | 2     |
| 3:C:167:ASN:OD1 | 3:C:168:TRP:N    | 0.56     | 2.36        | 2      | 3     |
| 3:C:282:GLN:O   | 3:C:283:SER:C    | 0.56     | 2.44        | 2      | 1     |
| 1:A:7:U:OP2     | 3:C:236:ARG:NH1  | 0.56     | 2.39        | 3      | 1     |
| 3:C:266:TRP:CG  | 3:C:267:GLY:N    | 0.56     | 2.73        | 3      | 1     |
| 1:A:7:U:O2      | 3:C:191:MET:SD   | 0.56     | 2.63        | 7      | 2     |
| 2:B:58:MET:C    | 2:B:58:MET:SD    | 0.56     | 2.84        | 5      | 1     |
| 3:C:261:GLU:CD  | 3:C:261:GLU:N    | 0.56     | 2.58        | 6      | 1     |
| 1:A:8:A:C4'     | 2:B:95:ARG:NH2   | 0.56     | 2.65        | 10     | 1     |
| 1:A:5:U:OP2     | 1:A:5:U:C5       | 0.56     | 2.59        | 1      | 5     |
| 3:C:200:ARG:O   | 3:C:200:ARG:NE   | 0.56     | 2.38        | 2      | 1     |
| 3:C:166:LEU:C   | 3:C:166:LEU:HD12 | 0.56     | 2.21        | 4      | 1     |
| 3:C:220:GLN:C   | 3:C:221:HIS:CG   | 0.56     | 2.79        | 5      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:11:A:O2'     | 1:A:12:A:N7      | 0.56     | 2.37        | 6      | 1     |
| 1:A:6:A:H4'      | 1:A:7:U:O5'      | 0.56     | 1.99        | 6      | 1     |
| 2:B:42:ILE:O     | 2:B:46:CYS:SG    | 0.56     | 2.64        | 6      | 2     |
| 1:A:8:A:N1       | 2:B:99:CYS:O     | 0.56     | 2.38        | 6      | 1     |
| 1:A:6:A:C1'      | 1:A:7:U:OP2      | 0.56     | 2.54        | 3      | 2     |
| 1:A:6:A:C5       | 3:C:162:PHE:CE1  | 0.56     | 2.94        | 7      | 1     |
| 3:C:275:MET:SD   | 3:C:279:ASP:OD2  | 0.56     | 2.63        | 1      | 1     |
| 2:B:51:PRO:O     | 2:B:52:VAL:O     | 0.56     | 2.24        | 2      | 2     |
| 3:C:246:PHE:C    | 3:C:246:PHE:CD1  | 0.56     | 2.78        | 3      | 2     |
| 1:A:12:A:C2      | 1:A:13:U:C6      | 0.56     | 2.94        | 7      | 1     |
| 3:C:163:ILE:HD12 | 3:C:175:LEU:HD21 | 0.56     | 1.76        | 7      | 1     |
| 1:A:7:U:O4'      | 3:C:202:PHE:CZ   | 0.56     | 2.59        | 9      | 2     |
| 3:C:254:VAL:HG13 | 3:C:309:LYS:HG3  | 0.56     | 1.76        | 8      | 1     |
| 1:A:5:U:O2       | 3:C:201:GLY:O    | 0.56     | 2.24        | 1      | 2     |
| 1:A:2:A:N1       | 3:C:318:ALA:O    | 0.56     | 2.39        | 1      | 1     |
| 1:A:2:A:O2'      | 1:A:3:U:C5       | 0.56     | 2.59        | 4      | 2     |
| 1:A:5:U:C4       | 1:A:5:U:OP2      | 0.56     | 2.59        | 7      | 1     |
| 3:C:191:MET:O    | 3:C:202:PHE:CZ   | 0.56     | 2.59        | 7      | 1     |
| 2:B:43:LEU:C     | 2:B:43:LEU:HD13  | 0.56     | 2.22        | 9      | 1     |
| 1:A:12:A:O2'     | 1:A:13:U:C5'     | 0.55     | 2.54        | 5      | 9     |
| 1:A:4:A:N6       | 3:C:279:ASP:OD2  | 0.55     | 2.39        | 5      | 1     |
| 1:A:10:U:H5'     | 2:B:71:PHE:CD1   | 0.55     | 2.36        | 7      | 1     |
| 1:A:5:U:C6       | 1:A:5:U:O5'      | 0.55     | 2.58        | 4      | 2     |
| 2:B:45:LEU:HD21  | 2:B:90:TYR:CE2   | 0.55     | 2.36        | 5      | 1     |
| 1:A:10:U:O5'     | 2:B:71:PHE:CE1   | 0.55     | 2.60        | 7      | 1     |
| 3:C:191:MET:O    | 3:C:192:LYS:C    | 0.55     | 2.45        | 10     | 3     |
| 2:B:101:TYR:O    | 2:B:102:SER:C    | 0.55     | 2.43        | 6      | 5     |
| 3:C:246:PHE:CD1  | 3:C:246:PHE:C    | 0.55     | 2.80        | 7      | 6     |
| 1:A:10:U:OP1     | 2:B:58:MET:SD    | 0.55     | 2.63        | 2      | 1     |
| 1:A:9:A:C8       | 1:A:10:U:H5      | 0.55     | 2.19        | 3      | 1     |
| 3:C:166:LEU:HD12 | 3:C:167:ASN:O    | 0.55     | 2.00        | 10     | 2     |
| 1:A:11:A:O2'     | 1:A:12:A:C5'     | 0.55     | 2.55        | 2      | 6     |
| 3:C:226:LYS:NZ   | 3:C:278:LYS:HZ2  | 0.55     | 1.99        | 2      | 1     |
| 1:A:9:A:N3       | 2:B:29:TYR:CE2   | 0.55     | 2.75        | 5      | 1     |
| 3:C:316:LYS:O    | 3:C:317:ARG:C    | 0.55     | 2.45        | 7      | 1     |
| 1:A:6:A:C1'      | 1:A:7:U:H5''     | 0.55     | 2.31        | 8      | 2     |
| 3:C:200:ARG:NE   | 3:C:200:ARG:N    | 0.55     | 2.55        | 4      | 1     |
| 2:B:90:TYR:CE1   | 2:B:97:LEU:CD1   | 0.55     | 2.84        | 5      | 1     |
| 1:A:11:A:O3'     | 2:B:58:MET:O     | 0.55     | 2.24        | 7      | 1     |
| 1:A:9:A:N1       | 2:B:29:TYR:OH    | 0.55     | 2.35        | 2      | 5     |
| 3:C:222:ILE:N    | 3:C:222:ILE:CD1  | 0.55     | 2.61        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:10:U:C5      | 1:A:10:U:OP1     | 0.55     | 2.60        | 10     | 1     |
| 2:B:27:VAL:HG13  | 2:B:73:GLU:HA    | 0.55     | 1.78        | 1      | 1     |
| 1:A:10:U:H5'     | 2:B:60:ASP:OD1   | 0.55     | 2.01        | 4      | 1     |
| 3:C:215:GLU:CD   | 3:C:215:GLU:H    | 0.55     | 2.04        | 4      | 1     |
| 1:A:11:A:OP2     | 2:B:58:MET:SD    | 0.55     | 2.65        | 6      | 3     |
| 1:A:11:A:H2'     | 2:B:69:TYR:HB2   | 0.55     | 1.79        | 7      | 1     |
| 1:A:7:U:H4'      | 3:C:202:PHE:CE2  | 0.55     | 2.37        | 8      | 2     |
| 1:A:10:U:O4      | 2:B:65:ARG:CZ    | 0.55     | 2.54        | 9      | 1     |
| 3:C:182:TYR:OH   | 3:C:219:THR:HG21 | 0.55     | 2.02        | 9      | 1     |
| 1:A:6:A:C8       | 3:C:162:PHE:CE2  | 0.55     | 2.95        | 1      | 1     |
| 1:A:10:U:O2'     | 1:A:11:A:C5'     | 0.55     | 2.55        | 5      | 5     |
| 3:C:163:ILE:HG22 | 3:C:166:LEU:HD11 | 0.55     | 1.78        | 3      | 1     |
| 3:C:246:PHE:CD1  | 3:C:247:VAL:N    | 0.55     | 2.75        | 3      | 2     |
| 1:A:10:U:O2      | 1:A:11:A:N7      | 0.55     | 2.39        | 4      | 1     |
| 1:A:2:A:O2'      | 1:A:3:U:H5       | 0.55     | 1.84        | 4      | 2     |
| 3:C:198:ARG:C    | 3:C:198:ARG:NE   | 0.55     | 2.60        | 7      | 1     |
| 1:A:11:A:O2'     | 1:A:12:A:C8      | 0.55     | 2.59        | 2      | 3     |
| 3:C:175:LEU:HD12 | 3:C:190:ILE:CD1  | 0.55     | 2.32        | 2      | 1     |
| 1:A:8:A:H2       | 2:B:29:TYR:CE2   | 0.55     | 2.18        | 3      | 1     |
| 2:B:38:THR:O     | 2:B:42:ILE:CG1   | 0.55     | 2.54        | 7      | 2     |
| 1:A:10:U:OP2     | 2:B:69:TYR:CD2   | 0.55     | 2.59        | 5      | 1     |
| 1:A:12:A:N6      | 2:B:57:MET:O     | 0.55     | 2.40        | 10     | 2     |
| 1:A:12:A:O2'     | 1:A:13:U:O5'     | 0.54     | 2.25        | 8      | 9     |
| 1:A:6:A:N7       | 3:C:239:GLN:CD   | 0.54     | 2.60        | 4      | 2     |
| 1:A:6:A:N6       | 3:C:234:ILE:O    | 0.54     | 2.40        | 7      | 1     |
| 3:C:181:LYS:NZ   | 3:C:181:LYS:CB   | 0.54     | 2.70        | 8      | 1     |
| 1:A:9:A:C2       | 2:B:29:TYR:CD2   | 0.54     | 2.95        | 10     | 1     |
| 3:C:173:ASP:O    | 3:C:174:ASN:C    | 0.54     | 2.43        | 3      | 3     |
| 3:C:292:ASP:CG   | 3:C:293:SER:N    | 0.54     | 2.60        | 4      | 2     |
| 2:B:24:PRO:O     | 2:B:99:CYS:SG    | 0.54     | 2.63        | 5      | 1     |
| 3:C:226:LYS:HZ2  | 3:C:280:THR:N    | 0.54     | 1.99        | 5      | 1     |
| 3:C:307:ASP:OD1  | 3:C:312:LYS:NZ   | 0.54     | 2.37        | 10     | 1     |
| 1:A:5:U:O5'      | 1:A:5:U:C6       | 0.54     | 2.61        | 8      | 3     |
| 3:C:226:LYS:O    | 3:C:227:VAL:CB   | 0.54     | 2.56        | 5      | 2     |
| 1:A:5:U:O2       | 1:A:5:U:C3'      | 0.54     | 2.55        | 3      | 1     |
| 2:B:45:LEU:O     | 2:B:48:ASN:OD1   | 0.54     | 2.25        | 4      | 1     |
| 3:C:300:VAL:O    | 3:C:303:ASN:OD1  | 0.54     | 2.24        | 6      | 1     |
| 1:A:11:A:C5'     | 2:B:69:TYR:CB    | 0.54     | 2.86        | 7      | 1     |
| 1:A:4:A:C5       | 3:C:168:TRP:CH2  | 0.54     | 2.94        | 10     | 3     |
| 2:B:27:VAL:HG21  | 2:B:102:SER:O    | 0.54     | 2.01        | 1      | 2     |
| 2:B:49:VAL:HG11  | 2:B:83:ALA:CB    | 0.54     | 2.19        | 5      | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:88:ASN:O     | 2:B:97:LEU:CB    | 0.54     | 2.55        | 6      | 2     |
| 3:C:188:LEU:CD2  | 3:C:188:LEU:N    | 0.54     | 2.70        | 6      | 2     |
| 1:A:11:A:C5'     | 2:B:69:TYR:O     | 0.54     | 2.50        | 7      | 1     |
| 1:A:4:A:O5'      | 1:A:4:A:N3       | 0.54     | 2.40        | 3      | 1     |
| 2:B:26:ARG:NH1   | 2:B:76:ASP:OD1   | 0.54     | 2.40        | 6      | 1     |
| 3:C:168:TRP:HE1  | 3:C:198:ARG:HH21 | 0.54     | 1.43        | 7      | 1     |
| 1:A:10:U:O4      | 2:B:65:ARG:NH1   | 0.54     | 2.41        | 9      | 1     |
| 2:B:96:PHE:N     | 2:B:96:PHE:CD1   | 0.54     | 2.71        | 9      | 1     |
| 3:C:277:ASP:O    | 3:C:279:ASP:N    | 0.54     | 2.41        | 9      | 1     |
| 3:C:245:ILE:HD11 | 3:C:315:ILE:CG2  | 0.54     | 2.32        | 10     | 2     |
| 3:C:188:LEU:C    | 3:C:188:LEU:HD23 | 0.54     | 2.23        | 5      | 1     |
| 3:C:317:ARG:O    | 3:C:319:GLU:N    | 0.54     | 2.41        | 5      | 2     |
| 3:C:164:GLY:C    | 3:C:166:LEU:N    | 0.54     | 2.60        | 10     | 1     |
| 2:B:87:LEU:HD12  | 2:B:87:LEU:C     | 0.54     | 2.23        | 1      | 1     |
| 2:B:75:ARG:O     | 2:B:76:ASP:CB    | 0.54     | 2.55        | 4      | 9     |
| 2:B:31:GLY:O     | 2:B:68:GLY:O     | 0.54     | 2.26        | 10     | 4     |
| 1:A:9:A:N3       | 2:B:71:PHE:CE2   | 0.54     | 2.76        | 8      | 4     |
| 3:C:309:LYS:O    | 3:C:310:ASP:C    | 0.54     | 2.46        | 3      | 2     |
| 3:C:186:THR:OG1  | 3:C:208:GLU:N    | 0.54     | 2.40        | 6      | 1     |
| 1:A:10:U:H5''    | 1:A:11:A:OP2     | 0.54     | 2.03        | 7      | 1     |
| 3:C:162:PHE:CD2  | 3:C:162:PHE:O    | 0.54     | 2.61        | 7      | 1     |
| 3:C:171:THR:O    | 3:C:174:ASN:OD1  | 0.54     | 2.26        | 10     | 1     |
| 3:C:317:ARG:CD   | 3:C:317:ARG:N    | 0.54     | 2.70        | 1      | 1     |
| 1:A:8:A:C2       | 2:B:29:TYR:CD2   | 0.54     | 2.95        | 10     | 5     |
| 2:B:88:ASN:OD1   | 2:B:99:CYS:SG    | 0.54     | 2.66        | 2      | 1     |
| 3:C:241:LYS:O    | 3:C:242:THR:C    | 0.54     | 2.46        | 6      | 3     |
| 1:A:5:U:O2       | 3:C:162:PHE:CD2  | 0.54     | 2.61        | 2      | 1     |
| 3:C:250:ILE:HG23 | 3:C:254:VAL:HG11 | 0.54     | 1.79        | 2      | 1     |
| 3:C:258:GLU:CD   | 3:C:258:GLU:N    | 0.54     | 2.62        | 3      | 1     |
| 3:C:166:LEU:HD12 | 3:C:167:ASN:N    | 0.54     | 2.17        | 4      | 1     |
| 1:A:2:A:C6       | 3:C:246:PHE:CE1  | 0.54     | 2.96        | 9      | 2     |
| 1:A:9:A:OP2      | 3:C:200:ARG:NE   | 0.54     | 2.40        | 6      | 1     |
| 1:A:13:U:N3      | 2:B:94:SER:OG    | 0.54     | 2.41        | 7      | 1     |
| 3:C:182:TYR:OH   | 3:C:219:THR:CG2  | 0.54     | 2.56        | 9      | 1     |
| 3:C:265:GLN:CG   | 3:C:266:TRP:H    | 0.54     | 2.16        | 5      | 2     |
| 3:C:178:TYR:O    | 3:C:181:LYS:NZ   | 0.54     | 2.41        | 8      | 1     |
| 2:B:66:SER:CB    | 2:B:69:TYR:CD1   | 0.53     | 2.91        | 3      | 1     |
| 2:B:37:GLN:HE22  | 2:B:92:LEU:HD11  | 0.53     | 1.63        | 4      | 1     |
| 3:C:254:VAL:HG22 | 3:C:255:ARG:N    | 0.53     | 2.18        | 4      | 1     |
| 1:A:4:A:C2       | 1:A:4:A:OP1      | 0.53     | 2.61        | 7      | 3     |
| 1:A:11:A:N3      | 2:B:66:SER:O     | 0.53     | 2.41        | 7      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:25:SER:O     | 2:B:77:LEU:CD2   | 0.53     | 2.56        | 1      | 1     |
| 1:A:10:U:C2      | 2:B:58:MET:CE    | 0.53     | 2.91        | 1      | 1     |
| 3:C:176:ARG:O    | 3:C:177:GLU:C    | 0.53     | 2.44        | 4      | 9     |
| 1:A:11:A:C2'     | 1:A:12:A:C8      | 0.53     | 2.91        | 2      | 1     |
| 1:A:9:A:N1       | 2:B:102:SER:CB   | 0.53     | 2.71        | 7      | 1     |
| 2:B:47:SER:OG    | 2:B:52:VAL:HG21  | 0.53     | 2.03        | 10     | 1     |
| 3:C:266:TRP:CG   | 3:C:266:TRP:O    | 0.53     | 2.59        | 10     | 1     |
| 3:C:226:LYS:O    | 3:C:227:VAL:CG1  | 0.53     | 2.53        | 8      | 2     |
| 3:C:216:VAL:CG1  | 3:C:217:VAL:N    | 0.53     | 2.71        | 2      | 1     |
| 2:B:84:VAL:HG12  | 2:B:88:ASN:ND2   | 0.53     | 2.18        | 8      | 2     |
| 3:C:276:LEU:CA   | 3:C:283:SER:OG   | 0.53     | 2.56        | 3      | 1     |
| 3:C:262:PHE:O    | 3:C:265:GLN:HG2  | 0.53     | 2.03        | 4      | 1     |
| 1:A:4:A:OP2      | 3:C:282:GLN:NE2  | 0.53     | 2.41        | 7      | 1     |
| 3:C:158:SER:C    | 3:C:160:LYS:N    | 0.53     | 2.61        | 7      | 1     |
| 2:B:92:LEU:O     | 2:B:95:ARG:O     | 0.53     | 2.26        | 10     | 6     |
| 3:C:258:GLU:O    | 3:C:260:GLU:N    | 0.53     | 2.42        | 8      | 6     |
| 3:C:242:THR:O    | 3:C:291:TYR:O    | 0.53     | 2.27        | 7      | 2     |
| 1:A:9:A:O2'      | 1:A:10:U:O4'     | 0.53     | 2.26        | 5      | 2     |
| 3:C:254:VAL:CG1  | 3:C:310:ASP:OD2  | 0.53     | 2.56        | 6      | 1     |
| 3:C:278:LYS:CD   | 3:C:278:LYS:N    | 0.53     | 2.70        | 9      | 1     |
| 3:C:269:ILE:O    | 3:C:269:ILE:CG2  | 0.53     | 2.57        | 1      | 1     |
| 3:C:158:SER:C    | 3:C:159:CYS:SG   | 0.53     | 2.87        | 10     | 3     |
| 2:B:23:PRO:O     | 2:B:101:TYR:CB   | 0.53     | 2.57        | 2      | 2     |
| 3:C:200:ARG:NH2  | 3:C:202:PHE:CE2  | 0.53     | 2.77        | 2      | 1     |
| 1:A:6:A:O2'      | 1:A:7:U:OP2      | 0.53     | 2.26        | 8      | 2     |
| 1:A:1:U:O4       | 3:C:249:GLY:N    | 0.53     | 2.42        | 4      | 1     |
| 3:C:226:LYS:HZ2  | 3:C:280:THR:HG23 | 0.53     | 1.62        | 5      | 1     |
| 1:A:3:U:HO2'     | 1:A:4:A:C5'      | 0.53     | 2.16        | 6      | 1     |
| 1:A:12:A:O2'     | 1:A:13:U:P       | 0.53     | 2.66        | 7      | 1     |
| 2:B:53:ILE:N     | 2:B:73:GLU:O     | 0.53     | 2.42        | 7      | 1     |
| 3:C:254:VAL:O    | 3:C:274:LEU:CD2  | 0.53     | 2.56        | 7      | 1     |
| 1:A:12:A:H61     | 2:B:57:MET:N     | 0.53     | 2.02        | 10     | 1     |
| 2:B:88:ASN:O     | 2:B:97:LEU:O     | 0.53     | 2.27        | 9      | 9     |
| 1:A:4:A:N3       | 1:A:4:A:O5'      | 0.53     | 2.41        | 9      | 3     |
| 3:C:205:LEU:HD23 | 3:C:207:PHE:CE2  | 0.53     | 2.39        | 8      | 1     |
| 1:A:11:A:N7      | 2:B:58:MET:HE3   | 0.53     | 2.18        | 9      | 1     |
| 1:A:7:U:H4'      | 3:C:202:PHE:CE1  | 0.53     | 2.38        | 9      | 1     |
| 1:A:10:U:O4      | 2:B:71:PHE:CD2   | 0.53     | 2.61        | 1      | 1     |
| 1:A:4:A:N3       | 3:C:168:TRP:CH2  | 0.53     | 2.77        | 1      | 2     |
| 1:A:6:A:C2'      | 3:C:236:ARG:HH22 | 0.53     | 2.16        | 2      | 1     |
| 3:C:226:LYS:HZ3  | 3:C:278:LYS:NZ   | 0.53     | 2.00        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:46:CYS:O     | 2:B:87:LEU:CD1   | 0.53     | 2.56        | 7      | 3     |
| 2:B:90:TYR:CE1   | 2:B:92:LEU:HD13  | 0.53     | 2.38        | 5      | 1     |
| 1:A:8:A:O2'      | 1:A:9:A:P        | 0.53     | 2.67        | 6      | 3     |
| 3:C:166:LEU:CD1  | 3:C:192:LYS:HZ1  | 0.53     | 2.16        | 8      | 1     |
| 3:C:212:SER:O    | 3:C:216:VAL:CG2  | 0.53     | 2.55        | 1      | 3     |
| 3:C:239:GLN:O    | 3:C:242:THR:OG1  | 0.53     | 2.27        | 6      | 5     |
| 3:C:200:ARG:NH1  | 3:C:201:GLY:O    | 0.53     | 2.42        | 3      | 1     |
| 1:A:6:A:N1       | 3:C:162:PHE:CG   | 0.53     | 2.76        | 9      | 3     |
| 1:A:9:A:N3       | 2:B:29:TYR:CG    | 0.53     | 2.77        | 4      | 1     |
| 1:A:10:U:H5'     | 2:B:69:TYR:CG    | 0.53     | 2.39        | 4      | 1     |
| 2:B:34:PRO:O     | 2:B:36:ASP:N     | 0.53     | 2.42        | 5      | 3     |
| 1:A:7:U:C4       | 3:C:202:PHE:CG   | 0.53     | 2.96        | 6      | 1     |
| 2:B:86:ASN:HD22  | 2:B:86:ASN:N     | 0.53     | 2.02        | 9      | 1     |
| 1:A:11:A:O2'     | 2:B:66:SER:C     | 0.53     | 2.47        | 7      | 1     |
| 1:A:6:A:N1       | 3:C:234:ILE:N    | 0.53     | 2.48        | 7      | 1     |
| 2:B:29:TYR:OH    | 2:B:101:TYR:N    | 0.53     | 2.42        | 10     | 1     |
| 1:A:1:U:O2'      | 1:A:2:A:O5'      | 0.53     | 2.27        | 6      | 6     |
| 1:A:2:A:C6       | 3:C:246:PHE:CG   | 0.53     | 2.97        | 9      | 2     |
| 1:A:4:A:C6       | 3:C:168:TRP:CE3  | 0.53     | 2.97        | 4      | 1     |
| 2:B:27:VAL:HG12  | 2:B:102:SER:H    | 0.53     | 1.62        | 6      | 1     |
| 2:B:87:LEU:N     | 2:B:87:LEU:HD22  | 0.53     | 2.18        | 6      | 1     |
| 1:A:12:A:OP2     | 2:B:58:MET:O     | 0.53     | 2.26        | 7      | 1     |
| 2:B:32:SER:C     | 2:B:33:ILE:HD12  | 0.53     | 2.24        | 7      | 1     |
| 3:C:254:VAL:HG11 | 3:C:308:PHE:CE2  | 0.53     | 2.38        | 7      | 2     |
| 1:A:9:A:H1'      | 2:B:71:PHE:CE1   | 0.53     | 2.38        | 9      | 2     |
| 3:C:159:CYS:SG   | 3:C:213:VAL:HG21 | 0.53     | 2.44        | 9      | 1     |
| 3:C:208:GLU:CG   | 3:C:209:LYS:H    | 0.53     | 2.15        | 10     | 1     |
| 1:A:12:A:H8      | 2:B:67:LYS:CA    | 0.52     | 2.17        | 7      | 1     |
| 1:A:9:A:O2'      | 1:A:10:U:O5'     | 0.52     | 2.27        | 10     | 6     |
| 3:C:229:ASP:OD2  | 3:C:231:LYS:NZ   | 0.52     | 2.42        | 3      | 1     |
| 3:C:262:PHE:O    | 3:C:263:PHE:C    | 0.52     | 2.48        | 9      | 5     |
| 3:C:172:GLU:CD   | 3:C:172:GLU:H    | 0.52     | 2.07        | 6      | 1     |
| 2:B:87:LEU:O     | 2:B:97:LEU:CD1   | 0.52     | 2.56        | 9      | 1     |
| 2:B:46:CYS:C     | 2:B:48:ASN:N     | 0.52     | 2.63        | 10     | 9     |
| 2:B:90:TYR:O     | 2:B:91:GLN:C     | 0.52     | 2.48        | 3      | 9     |
| 3:C:226:LYS:HZ2  | 3:C:226:LYS:HB2  | 0.52     | 1.64        | 4      | 1     |
| 3:C:193:ASP:CB   | 3:C:197:GLY:O    | 0.52     | 2.57        | 6      | 1     |
| 1:A:11:A:C5'     | 2:B:69:TYR:HB2   | 0.52     | 2.35        | 7      | 1     |
| 1:A:2:A:O2'      | 1:A:3:U:P        | 0.52     | 2.68        | 5      | 5     |
| 3:C:227:VAL:O    | 3:C:227:VAL:HG22 | 0.52     | 2.03        | 7      | 2     |
| 1:A:11:A:C2'     | 1:A:12:A:H8      | 0.52     | 2.17        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:6:A:N1       | 3:C:162:PHE:CB   | 0.52     | 2.73        | 3      | 1     |
| 1:A:1:U:O2       | 1:A:2:A:C5       | 0.52     | 2.62        | 9      | 1     |
| 3:C:276:LEU:O    | 3:C:277:ASP:O    | 0.52     | 2.27        | 9      | 1     |
| 2:B:97:LEU:CD1   | 2:B:97:LEU:N     | 0.52     | 2.60        | 2      | 1     |
| 3:C:276:LEU:N    | 3:C:280:THR:O    | 0.52     | 2.33        | 2      | 1     |
| 1:A:2:A:C4'      | 3:C:286:PHE:CE1  | 0.52     | 2.93        | 2      | 1     |
| 3:C:269:ILE:HG23 | 3:C:291:TYR:CZ   | 0.52     | 2.39        | 3      | 1     |
| 3:C:274:LEU:HD23 | 3:C:274:LEU:C    | 0.52     | 2.25        | 3      | 1     |
| 3:C:182:TYR:OH   | 3:C:221:HIS:CE1  | 0.52     | 2.63        | 4      | 3     |
| 3:C:270:ILE:HD13 | 3:C:291:TYR:O    | 0.52     | 2.03        | 6      | 1     |
| 3:C:247:VAL:HG21 | 3:C:263:PHE:CZ   | 0.52     | 2.40        | 10     | 1     |
| 3:C:164:GLY:O    | 3:C:229:ASP:N    | 0.52     | 2.34        | 8      | 1     |
| 3:C:207:PHE:O    | 3:C:208:GLU:C    | 0.52     | 2.48        | 10     | 1     |
| 3:C:229:ASP:N    | 3:C:229:ASP:OD1  | 0.52     | 2.43        | 7      | 1     |
| 2:B:36:ASP:CB    | 2:B:37:GLN:NE2   | 0.52     | 2.72        | 2      | 1     |
| 3:C:307:ASP:O    | 3:C:307:ASP:OD1  | 0.52     | 2.28        | 8      | 2     |
| 3:C:166:LEU:N    | 3:C:166:LEU:CD1  | 0.52     | 2.73        | 3      | 1     |
| 1:A:10:U:H1'     | 2:B:58:MET:HE2   | 0.52     | 1.82        | 4      | 1     |
| 1:A:12:A:H8      | 2:B:67:LYS:C     | 0.52     | 2.08        | 7      | 1     |
| 2:B:96:PHE:O     | 2:B:97:LEU:C     | 0.52     | 2.48        | 4      | 9     |
| 3:C:165:GLY:O    | 3:C:227:VAL:O    | 0.52     | 2.28        | 4      | 2     |
| 3:C:227:VAL:HG12 | 3:C:273:GLN:OE1  | 0.52     | 2.05        | 6      | 1     |
| 1:A:10:U:H4'     | 2:B:66:SER:CB    | 0.51     | 2.34        | 1      | 1     |
| 3:C:172:GLU:O    | 3:C:175:LEU:N    | 0.51     | 2.43        | 4      | 1     |
| 1:A:2:A:C4       | 3:C:246:PHE:CD2  | 0.51     | 2.99        | 9      | 3     |
| 3:C:269:ILE:HB   | 3:C:272:ALA:HB2  | 0.51     | 1.81        | 3      | 1     |
| 2:B:60:ASP:OD1   | 2:B:63:THR:CG2   | 0.51     | 2.58        | 4      | 1     |
| 3:C:313:ILE:O    | 3:C:313:ILE:CG1  | 0.51     | 2.57        | 4      | 1     |
| 3:C:264:SER:N    | 3:C:269:ILE:HD11 | 0.51     | 2.19        | 9      | 1     |
| 2:B:34:PRO:C     | 2:B:36:ASP:H     | 0.51     | 2.08        | 5      | 5     |
| 2:B:23:PRO:CB    | 2:B:24:PRO:CD    | 0.51     | 2.89        | 5      | 2     |
| 1:A:10:U:P       | 2:B:30:LEU:O     | 0.51     | 2.68        | 5      | 1     |
| 3:C:266:TRP:HE1  | 3:C:300:VAL:CG1  | 0.51     | 2.17        | 6      | 1     |
| 1:A:10:U:H5'     | 2:B:71:PHE:CG    | 0.51     | 2.40        | 7      | 1     |
| 3:C:167:ASN:N    | 3:C:167:ASN:OD1  | 0.51     | 2.43        | 7      | 2     |
| 3:C:254:VAL:O    | 3:C:255:ARG:C    | 0.51     | 2.48        | 8      | 1     |
| 1:A:10:U:O2      | 2:B:58:MET:SD    | 0.51     | 2.68        | 1      | 1     |
| 3:C:179:PHE:C    | 3:C:181:LYS:N    | 0.51     | 2.60        | 6      | 4     |
| 3:C:172:GLU:CD   | 3:C:172:GLU:N    | 0.51     | 2.64        | 3      | 1     |
| 2:B:60:ASP:CG    | 2:B:60:ASP:O     | 0.51     | 2.48        | 7      | 3     |
| 3:C:308:PHE:CD2  | 3:C:309:LYS:N    | 0.51     | 2.78        | 4      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:47:SER:O     | 2:B:50:GLY:N     | 0.51     | 2.38        | 9      | 1     |
| 3:C:168:TRP:CZ2  | 3:C:198:ARG:NH2  | 0.51     | 2.79        | 10     | 1     |
| 3:C:226:LYS:NZ   | 3:C:278:LYS:O    | 0.51     | 2.36        | 1      | 1     |
| 1:A:10:U:H5''    | 2:B:60:ASP:OD2   | 0.51     | 2.05        | 4      | 1     |
| 3:C:236:ARG:CG   | 3:C:236:ARG:HH11 | 0.51     | 2.18        | 5      | 1     |
| 1:A:4:A:H2'      | 1:A:4:A:N3       | 0.51     | 2.21        | 10     | 1     |
| 3:C:175:LEU:CD2  | 3:C:205:LEU:HD11 | 0.51     | 2.35        | 10     | 1     |
| 2:B:55:LEU:HD23  | 2:B:56:LYS:N     | 0.51     | 2.21        | 1      | 3     |
| 2:B:36:ASP:CB    | 2:B:37:GLN:HE22  | 0.51     | 2.19        | 2      | 1     |
| 1:A:5:U:H3       | 3:C:201:GLY:C    | 0.51     | 2.06        | 4      | 2     |
| 2:B:53:ILE:O     | 2:B:54:ASN:OD1   | 0.51     | 2.29        | 7      | 2     |
| 1:A:12:A:O4'     | 2:B:67:LYS:CB    | 0.51     | 2.59        | 7      | 1     |
| 3:C:185:VAL:HG12 | 3:C:207:PHE:CE1  | 0.51     | 2.41        | 9      | 1     |
| 3:C:276:LEU:N    | 3:C:283:SER:OG   | 0.51     | 2.43        | 3      | 1     |
| 3:C:221:HIS:CD2  | 3:C:230:PRO:CG   | 0.51     | 2.94        | 5      | 1     |
| 1:A:3:U:O2'      | 1:A:4:A:C4'      | 0.51     | 2.59        | 6      | 1     |
| 1:A:12:A:OP1     | 2:B:58:MET:O     | 0.51     | 2.28        | 7      | 1     |
| 1:A:12:A:OP1     | 2:B:59:PHE:CB    | 0.51     | 2.58        | 7      | 1     |
| 1:A:11:A:H5'     | 2:B:69:TYR:CB    | 0.51     | 2.36        | 7      | 1     |
| 2:B:72:ILE:CD1   | 2:B:72:ILE:N     | 0.51     | 2.72        | 10     | 1     |
| 1:A:5:U:C2       | 3:C:201:GLY:O    | 0.51     | 2.64        | 7      | 2     |
| 2:B:60:ASP:CG    | 2:B:66:SER:H     | 0.51     | 2.09        | 2      | 1     |
| 1:A:10:U:OP1     | 2:B:69:TYR:CB    | 0.51     | 2.59        | 8      | 3     |
| 3:C:161:MET:SD   | 3:C:216:VAL:CG1  | 0.51     | 2.99        | 3      | 1     |
| 3:C:250:ILE:HD11 | 3:C:286:PHE:O    | 0.51     | 2.06        | 3      | 1     |
| 1:A:6:A:C8       | 3:C:162:PHE:CE1  | 0.51     | 2.99        | 7      | 1     |
| 3:C:186:THR:O    | 3:C:187:ASP:OD1  | 0.51     | 2.29        | 7      | 2     |
| 3:C:245:ILE:HD12 | 3:C:315:ILE:HG23 | 0.51     | 1.81        | 7      | 1     |
| 1:A:5:U:H4'      | 3:C:200:ARG:HB2  | 0.51     | 1.82        | 10     | 1     |
| 1:A:6:A:H5''     | 1:A:8:A:H8       | 0.51     | 1.64        | 3      | 1     |
| 3:C:166:LEU:HD12 | 3:C:202:PHE:CA   | 0.51     | 2.36        | 6      | 1     |
| 1:A:6:A:C5       | 3:C:162:PHE:CD1  | 0.51     | 2.99        | 7      | 1     |
| 3:C:163:ILE:HD11 | 3:C:205:LEU:HD13 | 0.51     | 1.83        | 8      | 1     |
| 3:C:178:TYR:CD1  | 3:C:178:TYR:C    | 0.51     | 2.84        | 4      | 3     |
| 3:C:193:ASP:O    | 3:C:195:ALA:N    | 0.51     | 2.44        | 3      | 1     |
| 1:A:8:A:C2       | 2:B:29:TYR:CZ    | 0.51     | 2.98        | 4      | 1     |
| 1:A:9:A:C2       | 2:B:71:PHE:CZ    | 0.51     | 2.99        | 5      | 1     |
| 3:C:311:ARG:CG   | 3:C:312:LYS:N    | 0.51     | 2.74        | 5      | 1     |
| 3:C:161:MET:SD   | 3:C:217:VAL:CG2  | 0.51     | 2.99        | 6      | 1     |
| 3:C:175:LEU:HD22 | 3:C:190:ILE:CD1  | 0.51     | 2.36        | 7      | 1     |
| 3:C:308:PHE:C    | 3:C:310:ASP:N    | 0.51     | 2.64        | 10     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:178:TYR:C    | 3:C:178:TYR:CD1  | 0.50     | 2.85        | 3      | 5     |
| 1:A:11:A:N7      | 2:B:58:MET:HE2   | 0.50     | 2.21        | 2      | 1     |
| 1:A:6:A:C8       | 3:C:236:ARG:NH2  | 0.50     | 2.79        | 2      | 1     |
| 2:B:80:SER:O     | 2:B:84:VAL:HG23  | 0.50     | 2.06        | 2      | 1     |
| 2:B:27:VAL:CG2   | 2:B:28:VAL:N     | 0.50     | 2.75        | 6      | 2     |
| 2:B:81:ALA:O     | 2:B:85:ARG:CG    | 0.50     | 2.59        | 10     | 3     |
| 3:C:241:LYS:O    | 3:C:242:THR:O    | 0.50     | 2.29        | 6      | 1     |
| 3:C:262:PHE:O    | 3:C:264:SER:N    | 0.50     | 2.45        | 6      | 1     |
| 1:A:11:A:H3'     | 2:B:69:TYR:CA    | 0.50     | 2.32        | 7      | 1     |
| 3:C:300:VAL:HG23 | 3:C:303:ASN:OD1  | 0.50     | 2.05        | 3      | 1     |
| 1:A:6:A:H4'      | 1:A:7:U:H5''     | 0.50     | 1.78        | 8      | 2     |
| 2:B:60:ASP:CG    | 2:B:63:THR:HG1   | 0.50     | 2.09        | 4      | 1     |
| 2:B:87:LEU:N     | 2:B:87:LEU:CD2   | 0.50     | 2.74        | 6      | 1     |
| 3:C:229:ASP:OD1  | 3:C:271:ASP:OD2  | 0.50     | 2.29        | 6      | 1     |
| 3:C:188:LEU:CD2  | 3:C:188:LEU:C    | 0.50     | 2.78        | 9      | 1     |
| 2:B:46:CYS:O     | 2:B:47:SER:C     | 0.50     | 2.50        | 5      | 10    |
| 3:C:272:ALA:O    | 3:C:273:GLN:CB   | 0.50     | 2.55        | 10     | 3     |
| 2:B:31:GLY:N     | 2:B:33:ILE:CD1   | 0.50     | 2.74        | 2      | 1     |
| 2:B:60:ASP:CB    | 2:B:66:SER:O     | 0.50     | 2.59        | 7      | 3     |
| 2:B:27:VAL:HG11  | 2:B:102:SER:O    | 0.50     | 2.06        | 5      | 1     |
| 2:B:77:LEU:CD2   | 2:B:77:LEU:N     | 0.50     | 2.74        | 5      | 2     |
| 3:C:207:PHE:CZ   | 3:C:216:VAL:HG21 | 0.50     | 2.41        | 6      | 1     |
| 3:C:262:PHE:CD1  | 3:C:262:PHE:C    | 0.50     | 2.82        | 6      | 1     |
| 3:C:259:PHE:CD1  | 3:C:274:LEU:HD23 | 0.50     | 2.41        | 8      | 1     |
| 2:B:32:SER:H     | 2:B:95:ARG:NH1   | 0.50     | 2.04        | 9      | 1     |
| 3:C:180:GLY:C    | 3:C:182:TYR:H    | 0.50     | 2.09        | 10     | 1     |
| 3:C:213:VAL:O    | 3:C:217:VAL:HG12 | 0.50     | 2.07        | 1      | 1     |
| 3:C:200:ARG:CZ   | 3:C:202:PHE:CE2  | 0.50     | 2.94        | 2      | 1     |
| 3:C:215:GLU:OE2  | 3:C:219:THR:OG1  | 0.50     | 2.30        | 2      | 1     |
| 3:C:237:ASP:O    | 3:C:241:LYS:N    | 0.50     | 2.43        | 3      | 1     |
| 2:B:77:LEU:N     | 2:B:77:LEU:CD2   | 0.50     | 2.74        | 2      | 2     |
| 2:B:84:VAL:HG13  | 2:B:99:CYS:SG    | 0.50     | 2.47        | 4      | 1     |
| 3:C:166:LEU:HD12 | 3:C:167:ASN:C    | 0.50     | 2.27        | 4      | 1     |
| 3:C:301:CYS:SG   | 3:C:317:ARG:NH1  | 0.50     | 2.85        | 1      | 1     |
| 3:C:193:ASP:O    | 3:C:193:ASP:OD1  | 0.50     | 2.30        | 4      | 1     |
| 2:B:77:LEU:CD2   | 2:B:77:LEU:H     | 0.50     | 2.20        | 5      | 1     |
| 3:C:257:LYS:O    | 3:C:261:GLU:OE1  | 0.50     | 2.29        | 7      | 1     |
| 1:A:8:A:C2       | 2:B:29:TYR:CG    | 0.50     | 2.99        | 9      | 1     |
| 2:B:97:LEU:HD23  | 2:B:97:LEU:H     | 0.50     | 1.66        | 9      | 1     |
| 2:B:76:ASP:C     | 2:B:78:GLU:N     | 0.50     | 2.64        | 9      | 10    |
| 3:C:163:ILE:CG2  | 3:C:166:LEU:HD21 | 0.50     | 2.34        | 2      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:216:VAL:HG13 | 3:C:217:VAL:N    | 0.50     | 2.22        | 2      | 1     |
| 1:A:2:A:H1'      | 3:C:286:PHE:CE2  | 0.50     | 2.41        | 2      | 1     |
| 3:C:182:TYR:N    | 3:C:182:TYR:CD1  | 0.50     | 2.79        | 5      | 1     |
| 3:C:190:ILE:O    | 3:C:190:ILE:CG2  | 0.50     | 2.59        | 7      | 1     |
| 3:C:166:LEU:CB   | 3:C:192:LYS:HZ1  | 0.50     | 2.20        | 8      | 1     |
| 1:A:11:A:O2'     | 1:A:12:A:H5'     | 0.50     | 2.07        | 2      | 1     |
| 3:C:300:VAL:O    | 3:C:301:CYS:C    | 0.50     | 2.50        | 3      | 8     |
| 2:B:96:PHE:O     | 2:B:97:LEU:O     | 0.50     | 2.30        | 6      | 1     |
| 2:B:27:VAL:O     | 2:B:100:GLY:O    | 0.50     | 2.29        | 8      | 1     |
| 3:C:221:HIS:CB   | 3:C:228:ILE:HD11 | 0.50     | 2.36        | 8      | 2     |
| 2:B:30:LEU:HD12  | 2:B:72:ILE:HD11  | 0.50     | 1.84        | 10     | 1     |
| 3:C:276:LEU:O    | 3:C:280:THR:O    | 0.49     | 2.30        | 2      | 1     |
| 1:A:12:A:OP1     | 2:B:58:MET:C     | 0.49     | 2.49        | 7      | 1     |
| 2:B:68:GLY:O     | 2:B:69:TYR:CG    | 0.49     | 2.65        | 7      | 1     |
| 3:C:188:LEU:HD12 | 3:C:189:LYS:H    | 0.49     | 1.63        | 2      | 1     |
| 1:A:11:A:O4'     | 2:B:58:MET:SD    | 0.49     | 2.70        | 3      | 1     |
| 1:A:10:U:C2      | 1:A:11:A:N7      | 0.49     | 2.80        | 4      | 1     |
| 1:A:3:U:O2'      | 1:A:4:A:O5'      | 0.49     | 2.30        | 4      | 2     |
| 2:B:60:ASP:OD1   | 2:B:63:THR:OG1   | 0.49     | 2.30        | 4      | 1     |
| 1:A:9:A:C6       | 2:B:29:TYR:CE2   | 0.49     | 3.00        | 10     | 1     |
| 3:C:192:LYS:O    | 3:C:199:SER:OG   | 0.49     | 2.29        | 10     | 1     |
| 3:C:168:TRP:O    | 3:C:169:ASP:OD1  | 0.49     | 2.30        | 1      | 1     |
| 3:C:260:GLU:O    | 3:C:264:SER:CB   | 0.49     | 2.61        | 2      | 1     |
| 3:C:282:GLN:O    | 3:C:285:GLY:N    | 0.49     | 2.46        | 2      | 1     |
| 2:B:92:LEU:O     | 2:B:93:GLY:O     | 0.49     | 2.30        | 3      | 1     |
| 3:C:166:LEU:CD2  | 3:C:201:GLY:O    | 0.49     | 2.61        | 4      | 1     |
| 1:A:4:A:C6       | 3:C:168:TRP:NE1  | 0.49     | 2.79        | 6      | 1     |
| 2:B:90:TYR:CD1   | 2:B:91:GLN:N     | 0.49     | 2.80        | 7      | 3     |
| 3:C:162:PHE:O    | 3:C:162:PHE:CG   | 0.49     | 2.65        | 7      | 1     |
| 3:C:176:ARG:C    | 3:C:178:TYR:N    | 0.49     | 2.64        | 10     | 7     |
| 1:A:10:U:OP1     | 2:B:70:ALA:O     | 0.49     | 2.31        | 5      | 1     |
| 3:C:214:ASP:OD1  | 3:C:218:LYS:NZ   | 0.49     | 2.45        | 6      | 1     |
| 3:C:259:PHE:CD1  | 3:C:259:PHE:C    | 0.49     | 2.86        | 6      | 1     |
| 1:A:4:A:OP2      | 1:A:4:A:C2       | 0.49     | 2.65        | 1      | 1     |
| 2:B:76:ASP:O     | 2:B:77:LEU:C     | 0.49     | 2.51        | 6      | 10    |
| 2:B:77:LEU:H     | 2:B:77:LEU:CD2   | 0.49     | 2.20        | 7      | 3     |
| 2:B:84:VAL:O     | 2:B:88:ASN:CG    | 0.49     | 2.51        | 4      | 4     |
| 2:B:60:ASP:OD2   | 2:B:66:SER:O     | 0.49     | 2.29        | 5      | 2     |
| 3:C:226:LYS:HZ1  | 3:C:278:LYS:C    | 0.49     | 2.09        | 7      | 1     |
| 3:C:221:HIS:HB2  | 3:C:228:ILE:HD11 | 0.49     | 1.83        | 9      | 2     |
| 2:B:60:ASP:OD2   | 2:B:66:SER:OG    | 0.49     | 2.31        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:236:ARG:CG   | 3:C:236:ARG:NH1  | 0.49     | 2.72        | 5      | 1     |
| 3:C:208:GLU:CG   | 3:C:209:LYS:N    | 0.49     | 2.75        | 10     | 1     |
| 3:C:232:ARG:O    | 3:C:233:ALA:C    | 0.49     | 2.50        | 6      | 4     |
| 3:C:275:MET:SD   | 3:C:280:THR:O    | 0.49     | 2.70        | 5      | 1     |
| 3:C:231:LYS:HG2  | 3:C:234:ILE:HD11 | 0.49     | 1.85        | 6      | 1     |
| 2:B:60:ASP:CG    | 2:B:66:SER:O     | 0.49     | 2.51        | 5      | 6     |
| 3:C:211:SER:O    | 3:C:212:SER:C    | 0.49     | 2.51        | 9      | 10    |
| 1:A:6:A:H2'      | 3:C:236:ARG:HH22 | 0.49     | 1.67        | 2      | 1     |
| 3:C:260:GLU:O    | 3:C:264:SER:OG   | 0.49     | 2.29        | 2      | 1     |
| 2:B:102:SER:OG   | 2:B:102:SER:O    | 0.49     | 2.29        | 3      | 2     |
| 2:B:77:LEU:N     | 2:B:77:LEU:HD22  | 0.49     | 2.23        | 4      | 2     |
| 1:A:10:U:OP2     | 1:A:10:U:C6      | 0.49     | 2.65        | 7      | 1     |
| 3:C:262:PHE:CD2  | 3:C:308:PHE:CE1  | 0.49     | 3.00        | 9      | 1     |
| 2:B:60:ASP:N     | 2:B:60:ASP:OD1   | 0.49     | 2.42        | 1      | 1     |
| 3:C:158:SER:C    | 3:C:160:LYS:H    | 0.49     | 2.10        | 7      | 2     |
| 3:C:251:GLY:O    | 3:C:252:PRO:O    | 0.49     | 2.30        | 9      | 3     |
| 3:C:274:LEU:C    | 3:C:275:MET:SD   | 0.49     | 2.92        | 6      | 1     |
| 1:A:10:U:O5'     | 2:B:71:PHE:CZ    | 0.49     | 2.66        | 7      | 1     |
| 2:B:88:ASN:O     | 2:B:97:LEU:HG    | 0.49     | 2.08        | 9      | 1     |
| 3:C:164:GLY:C    | 3:C:166:LEU:H    | 0.49     | 2.11        | 10     | 1     |
| 1:A:3:U:O4       | 3:C:319:GLU:OE1  | 0.48     | 2.31        | 1      | 1     |
| 3:C:178:TYR:CG   | 3:C:223:LEU:HD12 | 0.48     | 2.43        | 1      | 2     |
| 3:C:172:GLU:O    | 3:C:173:ASP:C    | 0.48     | 2.50        | 3      | 6     |
| 2:B:30:LEU:HD13  | 2:B:72:ILE:HD13  | 0.48     | 1.85        | 6      | 1     |
| 2:B:48:ASN:O     | 2:B:49:VAL:CB    | 0.48     | 2.61        | 9      | 2     |
| 1:A:6:A:C5       | 3:C:162:PHE:CG   | 0.48     | 3.01        | 1      | 3     |
| 1:A:4:A:OP1      | 1:A:4:A:H3'      | 0.48     | 2.08        | 9      | 1     |
| 1:A:11:A:N7      | 2:B:58:MET:SD    | 0.48     | 2.86        | 9      | 1     |
| 3:C:182:TYR:CD1  | 3:C:182:TYR:N    | 0.48     | 2.82        | 8      | 2     |
| 3:C:166:LEU:CD1  | 3:C:167:ASN:O    | 0.48     | 2.61        | 4      | 1     |
| 2:B:88:ASN:O     | 2:B:97:LEU:C     | 0.48     | 2.52        | 6      | 2     |
| 3:C:255:ARG:HH11 | 3:C:255:ARG:CG   | 0.48     | 2.21        | 6      | 1     |
| 3:C:317:ARG:C    | 3:C:319:GLU:H    | 0.48     | 2.12        | 7      | 2     |
| 2:B:69:TYR:CD1   | 2:B:69:TYR:C     | 0.48     | 2.86        | 10     | 1     |
| 3:C:305:PHE:CZ   | 3:C:314:GLU:OE2  | 0.48     | 2.65        | 10     | 1     |
| 3:C:305:PHE:CE1  | 3:C:314:GLU:OE2  | 0.48     | 2.67        | 10     | 1     |
| 2:B:34:PRO:C     | 2:B:36:ASP:N     | 0.48     | 2.67        | 5      | 5     |
| 2:B:26:ARG:C     | 2:B:80:SER:HG    | 0.48     | 2.12        | 2      | 1     |
| 3:C:262:PHE:O    | 3:C:265:GLN:CD   | 0.48     | 2.51        | 7      | 2     |
| 3:C:256:PRO:O    | 3:C:257:LYS:C    | 0.48     | 2.50        | 7      | 3     |
| 3:C:168:TRP:NE1  | 3:C:198:ARG:NH2  | 0.48     | 2.60        | 7      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:175:LEU:HD13 | 3:C:190:ILE:CD1  | 0.48     | 2.38        | 9      | 1     |
| 3:C:262:PHE:CG   | 3:C:263:PHE:N    | 0.48     | 2.80        | 6      | 1     |
| 3:C:191:MET:O    | 3:C:202:PHE:CE1  | 0.48     | 2.66        | 7      | 1     |
| 3:C:277:ASP:C    | 3:C:279:ASP:N    | 0.48     | 2.66        | 9      | 1     |
| 3:C:242:THR:HG22 | 3:C:292:ASP:HA   | 0.48     | 1.86        | 1      | 1     |
| 3:C:200:ARG:O    | 3:C:202:PHE:CD1  | 0.48     | 2.66        | 9      | 1     |
| 3:C:307:ASP:OD1  | 3:C:307:ASP:O    | 0.48     | 2.31        | 9      | 1     |
| 3:C:195:ALA:O    | 3:C:196:THR:C    | 0.48     | 2.52        | 10     | 1     |
| 2:B:45:LEU:C     | 2:B:45:LEU:CD1   | 0.48     | 2.82        | 8      | 6     |
| 2:B:43:LEU:O     | 2:B:47:SER:OG    | 0.48     | 2.30        | 2      | 1     |
| 3:C:276:LEU:N    | 3:C:276:LEU:CD1  | 0.48     | 2.67        | 7      | 1     |
| 1:A:10:U:OP1     | 2:B:69:TYR:CE2   | 0.48     | 2.67        | 10     | 1     |
| 3:C:227:VAL:O    | 3:C:227:VAL:HG12 | 0.48     | 2.09        | 3      | 1     |
| 1:A:4:A:N6       | 3:C:279:ASP:OD1  | 0.48     | 2.46        | 3      | 1     |
| 2:B:52:VAL:HG13  | 2:B:53:ILE:H     | 0.48     | 1.69        | 4      | 1     |
| 3:C:167:ASN:O    | 3:C:167:ASN:OD1  | 0.48     | 2.31        | 5      | 1     |
| 3:C:163:ILE:HG21 | 3:C:166:LEU:HD21 | 0.48     | 1.84        | 8      | 1     |
| 2:B:88:ASN:O     | 2:B:97:LEU:CG    | 0.48     | 2.61        | 1      | 2     |
| 1:A:6:A:C4'      | 1:A:7:U:C5'      | 0.48     | 2.87        | 3      | 6     |
| 1:A:2:A:N6       | 3:C:246:PHE:CE1  | 0.48     | 2.82        | 2      | 2     |
| 1:A:10:U:OP2     | 2:B:69:TYR:CD1   | 0.48     | 2.67        | 5      | 2     |
| 1:A:8:A:N6       | 2:B:101:TYR:CZ   | 0.48     | 2.81        | 8      | 1     |
| 3:C:170:THR:H    | 3:C:192:LYS:CD   | 0.48     | 2.21        | 8      | 1     |
| 3:C:262:PHE:O    | 3:C:265:GLN:OE1  | 0.48     | 2.32        | 2      | 1     |
| 3:C:178:TYR:CE2  | 3:C:223:LEU:HD23 | 0.48     | 2.44        | 5      | 1     |
| 1:A:12:A:OP1     | 2:B:59:PHE:CA    | 0.48     | 2.62        | 7      | 1     |
| 3:C:248:GLY:O    | 3:C:249:GLY:O    | 0.47     | 2.32        | 1      | 1     |
| 2:B:26:ARG:CA    | 2:B:80:SER:OG    | 0.47     | 2.61        | 2      | 1     |
| 1:A:10:U:C5      | 2:B:71:PHE:CE1   | 0.47     | 3.02        | 1      | 1     |
| 2:B:75:ARG:O     | 2:B:76:ASP:HB2   | 0.47     | 2.09        | 2      | 1     |
| 3:C:211:SER:C    | 3:C:213:VAL:N    | 0.47     | 2.67        | 10     | 7     |
| 1:A:12:A:O2'     | 1:A:13:U:C6      | 0.47     | 2.57        | 3      | 4     |
| 1:A:5:U:C4       | 3:C:165:GLY:N    | 0.47     | 2.82        | 4      | 1     |
| 2:B:28:VAL:HG23  | 2:B:98:LYS:C     | 0.47     | 2.28        | 4      | 1     |
| 2:B:31:GLY:C     | 2:B:33:ILE:HD12  | 0.47     | 2.30        | 7      | 3     |
| 3:C:255:ARG:NH1  | 3:C:255:ARG:CG   | 0.47     | 2.76        | 6      | 1     |
| 3:C:161:MET:HE1  | 3:C:217:VAL:HG22 | 0.47     | 1.85        | 9      | 1     |
| 2:B:87:LEU:O     | 2:B:87:LEU:CD1   | 0.47     | 2.63        | 1      | 1     |
| 3:C:209:LYS:O    | 3:C:211:SER:N    | 0.47     | 2.48        | 1      | 2     |
| 3:C:266:TRP:O    | 3:C:267:GLY:O    | 0.47     | 2.32        | 4      | 2     |
| 1:A:2:A:O4'      | 3:C:286:PHE:CD1  | 0.47     | 2.67        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:193:ASP:CA   | 3:C:197:GLY:O    | 0.47     | 2.62        | 6      | 1     |
| 3:C:306:ILE:HG21 | 3:C:315:ILE:HD11 | 0.47     | 1.86        | 6      | 1     |
| 3:C:193:ASP:OD1  | 3:C:199:SER:OG   | 0.47     | 2.32        | 7      | 1     |
| 3:C:184:THR:OG1  | 3:C:208:GLU:OE2  | 0.47     | 2.31        | 10     | 1     |
| 3:C:160:LYS:NZ   | 3:C:189:LYS:HZ2  | 0.47     | 2.08        | 1      | 1     |
| 2:B:60:ASP:OD1   | 2:B:60:ASP:O     | 0.47     | 2.32        | 3      | 2     |
| 3:C:196:THR:HG23 | 3:C:197:GLY:N    | 0.47     | 2.24        | 3      | 1     |
| 2:B:30:LEU:CD1   | 2:B:72:ILE:HD11  | 0.47     | 2.39        | 10     | 1     |
| 2:B:72:ILE:H     | 2:B:72:ILE:HD12  | 0.47     | 1.68        | 10     | 1     |
| 1:A:4:A:C8       | 3:C:168:TRP:CE2  | 0.47     | 3.02        | 1      | 1     |
| 2:B:97:LEU:H     | 2:B:97:LEU:HD23  | 0.47     | 1.70        | 10     | 2     |
| 1:A:5:U:O2'      | 1:A:6:A:O5'      | 0.47     | 2.31        | 5      | 3     |
| 1:A:4:A:OP1      | 3:C:275:MET:CE   | 0.47     | 2.62        | 3      | 1     |
| 2:B:30:LEU:HB3   | 2:B:33:ILE:HD11  | 0.47     | 1.85        | 4      | 2     |
| 2:B:60:ASP:CG    | 2:B:63:THR:OG1   | 0.47     | 2.52        | 4      | 1     |
| 3:C:277:ASP:O    | 3:C:278:LYS:C    | 0.47     | 2.53        | 4      | 1     |
| 1:A:4:A:OP2      | 3:C:280:THR:O    | 0.47     | 2.32        | 5      | 1     |
| 1:A:10:U:OP1     | 2:B:30:LEU:O     | 0.47     | 2.32        | 5      | 1     |
| 3:C:277:ASP:OD1  | 3:C:281:GLY:N    | 0.47     | 2.37        | 6      | 1     |
| 2:B:38:THR:HG23  | 2:B:39:GLU:N     | 0.47     | 2.24        | 8      | 1     |
| 3:C:193:ASP:OD1  | 3:C:196:THR:OG1  | 0.47     | 2.31        | 8      | 1     |
| 1:A:1:U:C4       | 3:C:314:GLU:OE1  | 0.47     | 2.67        | 10     | 1     |
| 3:C:211:SER:O    | 3:C:215:GLU:OE2  | 0.47     | 2.32        | 4      | 1     |
| 3:C:269:ILE:CG2  | 3:C:272:ALA:HB2  | 0.47     | 2.39        | 6      | 2     |
| 3:C:167:ASN:C    | 3:C:169:ASP:H    | 0.47     | 2.13        | 1      | 2     |
| 3:C:282:GLN:C    | 3:C:284:ARG:H    | 0.47     | 2.11        | 5      | 4     |
| 3:C:221:HIS:H    | 3:C:221:HIS:CD2  | 0.47     | 2.27        | 4      | 3     |
| 3:C:246:PHE:CG   | 3:C:247:VAL:N    | 0.47     | 2.82        | 7      | 4     |
| 3:C:274:LEU:CD2  | 3:C:274:LEU:C    | 0.47     | 2.80        | 5      | 2     |
| 2:B:60:ASP:OD2   | 2:B:69:TYR:CE2   | 0.47     | 2.67        | 4      | 1     |
| 3:C:160:LYS:O    | 3:C:233:ALA:HB2  | 0.47     | 2.08        | 5      | 2     |
| 3:C:176:ARG:CD   | 3:C:185:VAL:HG11 | 0.47     | 2.39        | 6      | 1     |
| 3:C:166:LEU:HD12 | 3:C:202:PHE:HA   | 0.47     | 1.87        | 6      | 1     |
| 3:C:195:ALA:O    | 3:C:196:THR:CG2  | 0.47     | 2.61        | 6      | 1     |
| 1:A:11:A:H5'     | 2:B:69:TYR:CA    | 0.47     | 2.40        | 7      | 1     |
| 1:A:5:U:H3       | 3:C:165:GLY:N    | 0.47     | 2.07        | 7      | 1     |
| 2:B:45:LEU:CD1   | 2:B:45:LEU:C     | 0.47     | 2.82        | 7      | 2     |
| 3:C:249:GLY:O    | 3:C:313:ILE:CG2  | 0.47     | 2.62        | 8      | 1     |
| 3:C:274:LEU:C    | 3:C:274:LEU:HD13 | 0.47     | 2.30        | 8      | 1     |
| 3:C:267:GLY:CA   | 3:C:291:TYR:CE1  | 0.47     | 2.97        | 10     | 1     |
| 3:C:283:SER:O    | 3:C:283:SER:OG   | 0.47     | 2.31        | 1      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:75:ARG:O     | 2:B:76:ASP:CG    | 0.47     | 2.53        | 5      | 9     |
| 2:B:37:GLN:OE1   | 2:B:92:LEU:HD11  | 0.47     | 2.09        | 7      | 2     |
| 1:A:5:U:O4'      | 3:C:200:ARG:CZ   | 0.47     | 2.63        | 3      | 1     |
| 3:C:300:VAL:CG2  | 3:C:303:ASN:HD21 | 0.47     | 2.23        | 3      | 1     |
| 3:C:172:GLU:OE2  | 3:C:192:LYS:NZ   | 0.47     | 2.46        | 5      | 1     |
| 3:C:270:ILE:N    | 3:C:290:THR:O    | 0.47     | 2.47        | 6      | 1     |
| 2:B:85:ARG:O     | 2:B:88:ASN:CG    | 0.47     | 2.54        | 7      | 2     |
| 2:B:28:VAL:HG22  | 2:B:72:ILE:HD13  | 0.47     | 1.87        | 7      | 1     |
| 3:C:200:ARG:O    | 3:C:202:PHE:CD2  | 0.47     | 2.68        | 10     | 3     |
| 2:B:52:VAL:HG13  | 2:B:53:ILE:N     | 0.47     | 2.25        | 4      | 1     |
| 2:B:88:ASN:O     | 2:B:97:LEU:HB2   | 0.47     | 2.09        | 6      | 1     |
| 2:B:60:ASP:OD1   | 2:B:64:GLY:N     | 0.47     | 2.37        | 7      | 1     |
| 3:C:222:ILE:HD13 | 3:C:222:ILE:N    | 0.47     | 2.23        | 7      | 1     |
| 3:C:271:ASP:OD1  | 3:C:271:ASP:O    | 0.47     | 2.33        | 8      | 1     |
| 3:C:273:GLN:CG   | 3:C:274:LEU:N    | 0.47     | 2.78        | 10     | 1     |
| 2:B:42:ILE:C     | 2:B:44:ASP:N     | 0.47     | 2.68        | 3      | 6     |
| 3:C:161:MET:SD   | 3:C:216:VAL:HG21 | 0.47     | 2.49        | 2      | 1     |
| 2:B:60:ASP:OD2   | 2:B:64:GLY:C     | 0.47     | 2.54        | 5      | 3     |
| 1:A:9:A:O2'      | 1:A:10:U:H5'     | 0.46     | 2.10        | 10     | 2     |
| 1:A:5:U:O2       | 3:C:200:ARG:C    | 0.46     | 2.54        | 4      | 2     |
| 2:B:46:CYS:O     | 2:B:48:ASN:OD1   | 0.46     | 2.33        | 4      | 1     |
| 3:C:310:ASP:CG   | 3:C:311:ARG:H    | 0.46     | 2.14        | 10     | 3     |
| 2:B:52:VAL:HG11  | 2:B:72:ILE:CG2   | 0.46     | 2.40        | 7      | 2     |
| 3:C:167:ASN:OD1  | 3:C:170:THR:OG1  | 0.46     | 2.32        | 9      | 1     |
| 3:C:305:PHE:CE1  | 3:C:314:GLU:HG2  | 0.46     | 2.45        | 10     | 1     |
| 3:C:253:ASP:O    | 3:C:254:VAL:O    | 0.46     | 2.33        | 4      | 1     |
| 3:C:278:LYS:O    | 3:C:279:ASP:CG   | 0.46     | 2.53        | 6      | 1     |
| 1:A:13:U:OP2     | 2:B:33:ILE:O     | 0.46     | 2.33        | 7      | 1     |
| 1:A:8:A:OP1      | 3:C:199:SER:OG   | 0.46     | 2.33        | 9      | 1     |
| 3:C:283:SER:C    | 3:C:285:GLY:H    | 0.46     | 2.11        | 2      | 1     |
| 2:B:39:GLU:O     | 2:B:43:LEU:CB    | 0.46     | 2.63        | 8      | 3     |
| 1:A:10:U:OP1     | 2:B:66:SER:OG    | 0.46     | 2.33        | 3      | 1     |
| 3:C:167:ASN:O    | 3:C:168:TRP:C    | 0.46     | 2.53        | 10     | 2     |
| 2:B:51:PRO:O     | 2:B:52:VAL:C     | 0.46     | 2.53        | 5      | 2     |
| 3:C:178:TYR:CD2  | 3:C:223:LEU:HD13 | 0.46     | 2.46        | 6      | 1     |
| 2:B:48:ASN:O     | 2:B:49:VAL:CG2   | 0.46     | 2.62        | 9      | 1     |
| 1:A:10:U:C3'     | 2:B:69:TYR:OH    | 0.46     | 2.63        | 10     | 1     |
| 1:A:7:U:H1'      | 3:C:202:PHE:CZ   | 0.46     | 2.46        | 3      | 1     |
| 2:B:60:ASP:OD2   | 2:B:65:ARG:C     | 0.46     | 2.54        | 5      | 1     |
| 3:C:259:PHE:CE1  | 3:C:263:PHE:CE1  | 0.46     | 3.03        | 5      | 2     |
| 2:B:26:ARG:HE    | 2:B:103:SER:CB   | 0.46     | 2.24        | 7      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:37:GLN:HE21  | 2:B:37:GLN:N     | 0.46     | 2.09        | 7      | 1     |
| 1:A:9:A:HO2'     | 1:A:10:U:P       | 0.46     | 2.33        | 10     | 1     |
| 2:B:69:TYR:CZ    | 2:B:71:PHE:CE1   | 0.46     | 3.04        | 10     | 1     |
| 3:C:175:LEU:HD23 | 3:C:175:LEU:O    | 0.46     | 2.11        | 10     | 1     |
| 3:C:265:GLN:C    | 3:C:267:GLY:H    | 0.46     | 2.14        | 10     | 1     |
| 3:C:175:LEU:HD12 | 3:C:190:ILE:HD13 | 0.46     | 1.86        | 2      | 2     |
| 3:C:283:SER:C    | 3:C:285:GLY:N    | 0.46     | 2.68        | 2      | 1     |
| 3:C:289:VAL:CG2  | 3:C:291:TYR:CE2  | 0.46     | 2.98        | 5      | 1     |
| 3:C:308:PHE:O    | 3:C:310:ASP:O    | 0.46     | 2.33        | 9      | 2     |
| 3:C:182:TYR:HH   | 3:C:221:HIS:CE1  | 0.46     | 2.26        | 1      | 2     |
| 1:A:3:U:OP1      | 3:C:282:GLN:OE1  | 0.46     | 2.34        | 3      | 1     |
| 3:C:277:ASP:C    | 3:C:279:ASP:H    | 0.46     | 2.14        | 9      | 1     |
| 3:C:169:ASP:OD1  | 3:C:192:LYS:CD   | 0.46     | 2.64        | 3      | 1     |
| 3:C:206:SER:O    | 3:C:206:SER:OG   | 0.46     | 2.33        | 5      | 1     |
| 3:C:291:TYR:O    | 3:C:292:ASP:CB   | 0.46     | 2.64        | 6      | 1     |
| 2:B:30:LEU:C     | 2:B:33:ILE:HD11  | 0.46     | 2.31        | 8      | 1     |
| 3:C:275:MET:SD   | 3:C:275:MET:N    | 0.46     | 2.88        | 9      | 1     |
| 1:A:7:U:C2       | 3:C:191:MET:HE1  | 0.46     | 2.45        | 1      | 1     |
| 2:B:82:SER:O     | 2:B:86:ASN:CG    | 0.46     | 2.54        | 9      | 3     |
| 1:A:6:A:O2'      | 3:C:236:ARG:CZ   | 0.46     | 2.64        | 2      | 1     |
| 1:A:4:A:C5       | 3:C:168:TRP:CD1  | 0.46     | 3.02        | 6      | 1     |
| 3:C:223:LEU:N    | 3:C:223:LEU:HD12 | 0.46     | 2.26        | 9      | 1     |
| 3:C:263:PHE:C    | 3:C:265:GLN:N    | 0.46     | 2.66        | 9      | 1     |
| 3:C:275:MET:HB2  | 3:C:286:PHE:CE1  | 0.46     | 2.46        | 1      | 1     |
| 3:C:226:LYS:C    | 3:C:227:VAL:CG2  | 0.46     | 2.85        | 8      | 2     |
| 3:C:163:ILE:HG22 | 3:C:166:LEU:CD2  | 0.46     | 2.36        | 2      | 1     |
| 2:B:32:SER:OG    | 2:B:95:ARG:CG    | 0.46     | 2.63        | 3      | 1     |
| 3:C:226:LYS:HZ1  | 3:C:280:THR:H    | 0.46     | 1.54        | 5      | 1     |
| 2:B:27:VAL:HG22  | 2:B:28:VAL:N     | 0.46     | 2.25        | 6      | 1     |
| 2:B:77:LEU:HD22  | 2:B:77:LEU:N     | 0.46     | 2.25        | 7      | 1     |
| 1:A:3:U:O4'      | 3:C:288:PHE:CZ   | 0.46     | 2.69        | 1      | 1     |
| 1:A:9:A:N6       | 2:B:102:SER:OG   | 0.46     | 2.40        | 1      | 1     |
| 1:A:10:U:O4'     | 2:B:69:TYR:CB    | 0.46     | 2.64        | 1      | 1     |
| 3:C:187:ASP:O    | 3:C:206:SER:CB   | 0.46     | 2.64        | 1      | 2     |
| 2:B:76:ASP:OD2   | 2:B:77:LEU:N     | 0.46     | 2.49        | 2      | 1     |
| 3:C:309:LYS:C    | 3:C:311:ARG:H    | 0.46     | 2.12        | 2      | 1     |
| 3:C:280:THR:OG1  | 3:C:280:THR:O    | 0.46     | 2.31        | 6      | 2     |
| 1:A:10:U:O2'     | 1:A:11:A:C8      | 0.46     | 2.59        | 8      | 1     |
| 3:C:292:ASP:OD1  | 3:C:292:ASP:C    | 0.45     | 2.54        | 1      | 2     |
| 1:A:4:A:C6       | 3:C:168:TRP:CH2  | 0.45     | 3.04        | 2      | 2     |
| 2:B:76:ASP:CG    | 2:B:77:LEU:H     | 0.45     | 2.14        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:277:ASP:C    | 3:C:277:ASP:OD1  | 0.45     | 2.55        | 5      | 2     |
| 2:B:91:GLN:NE2   | 2:B:96:PHE:CZ    | 0.45     | 2.85        | 9      | 1     |
| 3:C:169:ASP:C    | 3:C:169:ASP:OD1  | 0.45     | 2.55        | 8      | 1     |
| 2:B:22:ASN:ND2   | 2:B:101:TYR:CD2  | 0.45     | 2.84        | 10     | 1     |
| 2:B:46:CYS:C     | 2:B:48:ASN:H     | 0.45     | 2.14        | 7      | 4     |
| 3:C:178:TYR:O    | 3:C:178:TYR:CD1  | 0.45     | 2.70        | 8      | 1     |
| 1:A:1:U:C2       | 1:A:2:A:C6       | 0.45     | 3.05        | 9      | 1     |
| 3:C:250:ILE:O    | 3:C:285:GLY:C    | 0.45     | 2.55        | 9      | 1     |
| 1:A:2:A:C2       | 1:A:3:U:C6       | 0.45     | 3.04        | 1      | 1     |
| 2:B:81:ALA:C     | 2:B:85:ARG:HE    | 0.45     | 2.14        | 2      | 1     |
| 2:B:35:TYR:OH    | 2:B:59:PHE:CB    | 0.45     | 2.65        | 5      | 1     |
| 3:C:223:LEU:CD2  | 3:C:223:LEU:N    | 0.45     | 2.78        | 6      | 1     |
| 1:A:1:U:C2       | 1:A:2:A:C5       | 0.45     | 3.04        | 9      | 1     |
| 2:B:43:LEU:HD13  | 2:B:44:ASP:OD1   | 0.45     | 2.11        | 9      | 1     |
| 3:C:226:LYS:HZ1  | 3:C:278:LYS:NZ   | 0.45     | 2.06        | 2      | 1     |
| 1:A:11:A:C4      | 2:B:56:LYS:NZ    | 0.45     | 2.74        | 3      | 1     |
| 1:A:10:U:O2'     | 1:A:11:A:OP2     | 0.45     | 2.33        | 3      | 1     |
| 1:A:6:A:H61      | 3:C:234:ILE:H    | 0.45     | 1.53        | 6      | 1     |
| 3:C:303:ASN:O    | 3:C:304:LYS:C    | 0.45     | 2.55        | 6      | 2     |
| 1:A:12:A:O4'     | 2:B:67:LYS:C     | 0.45     | 2.55        | 7      | 1     |
| 3:C:276:LEU:N    | 3:C:276:LEU:CD2  | 0.45     | 2.68        | 7      | 1     |
| 3:C:161:MET:CE   | 3:C:217:VAL:HG22 | 0.45     | 2.42        | 9      | 1     |
| 1:A:4:A:OP2      | 3:C:277:ASP:OD1  | 0.45     | 2.34        | 4      | 1     |
| 3:C:167:ASN:OD1  | 3:C:167:ASN:C    | 0.45     | 2.54        | 6      | 1     |
| 3:C:250:ILE:O    | 3:C:286:PHE:CA   | 0.45     | 2.65        | 9      | 1     |
| 3:C:161:MET:HE2  | 3:C:163:ILE:HD13 | 0.45     | 1.88        | 10     | 1     |
| 3:C:307:ASP:C    | 3:C:307:ASP:OD1  | 0.45     | 2.55        | 2      | 1     |
| 3:C:310:ASP:C    | 3:C:310:ASP:OD1  | 0.45     | 2.55        | 2      | 1     |
| 3:C:169:ASP:OD1  | 3:C:192:LYS:NZ   | 0.45     | 2.36        | 3      | 1     |
| 3:C:286:PHE:CD1  | 3:C:286:PHE:C    | 0.45     | 2.89        | 8      | 2     |
| 2:B:72:ILE:HD12  | 2:B:72:ILE:H     | 0.45     | 1.66        | 5      | 1     |
| 3:C:191:MET:CB   | 3:C:202:PHE:CZ   | 0.45     | 2.99        | 6      | 1     |
| 1:A:7:U:O2       | 3:C:202:PHE:CE2  | 0.45     | 2.69        | 6      | 1     |
| 1:A:1:U:O2       | 1:A:2:A:C6       | 0.45     | 2.70        | 9      | 1     |
| 1:A:8:A:C2       | 2:B:29:TYR:CD1   | 0.45     | 3.05        | 9      | 1     |
| 3:C:208:GLU:CD   | 3:C:209:LYS:H    | 0.45     | 2.14        | 10     | 1     |
| 1:A:5:U:O2       | 3:C:201:GLY:C    | 0.45     | 2.55        | 1      | 1     |
| 3:C:185:VAL:HG22 | 3:C:207:PHE:CE1  | 0.45     | 2.46        | 10     | 2     |
| 2:B:58:MET:O     | 2:B:69:TYR:O     | 0.45     | 2.35        | 4      | 1     |
| 3:C:200:ARG:HE   | 3:C:200:ARG:N    | 0.45     | 2.10        | 4      | 1     |
| 3:C:244:LYS:N    | 3:C:317:ARG:HH12 | 0.45     | 2.09        | 5      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:262:PHE:C    | 3:C:264:SER:N    | 0.45     | 2.66        | 6      | 1     |
| 3:C:276:LEU:C    | 3:C:282:GLN:O    | 0.45     | 2.55        | 8      | 1     |
| 3:C:165:GLY:O    | 3:C:228:ILE:HG22 | 0.45     | 2.12        | 9      | 1     |
| 3:C:171:THR:O    | 3:C:172:GLU:C    | 0.45     | 2.55        | 4      | 1     |
| 1:A:10:U:OP2     | 2:B:65:ARG:NH2   | 0.45     | 2.49        | 6      | 1     |
| 3:C:178:TYR:CD2  | 3:C:223:LEU:CD2  | 0.45     | 3.00        | 8      | 2     |
| 3:C:174:ASN:C    | 3:C:174:ASN:OD1  | 0.44     | 2.55        | 1      | 1     |
| 1:A:11:A:H2'     | 1:A:12:A:C8      | 0.44     | 2.47        | 2      | 1     |
| 1:A:2:A:N6       | 3:C:246:PHE:CD1  | 0.44     | 2.85        | 2      | 2     |
| 3:C:265:GLN:CG   | 3:C:266:TRP:N    | 0.44     | 2.80        | 5      | 2     |
| 2:B:56:LYS:CG    | 2:B:58:MET:SD    | 0.44     | 3.05        | 4      | 1     |
| 3:C:167:ASN:ND2  | 3:C:169:ASP:O    | 0.44     | 2.50        | 5      | 1     |
| 3:C:173:ASP:OD1  | 3:C:176:ARG:NH2  | 0.44     | 2.50        | 5      | 1     |
| 3:C:255:ARG:H    | 3:C:255:ARG:NE   | 0.44     | 2.10        | 6      | 1     |
| 3:C:262:PHE:CD2  | 3:C:263:PHE:CD1  | 0.44     | 3.05        | 6      | 1     |
| 1:A:11:A:C3'     | 2:B:69:TYR:H     | 0.44     | 2.09        | 7      | 1     |
| 3:C:167:ASN:CG   | 3:C:168:TRP:H    | 0.44     | 2.15        | 7      | 2     |
| 3:C:245:ILE:C    | 3:C:245:ILE:CD1  | 0.44     | 2.78        | 9      | 1     |
| 3:C:291:TYR:C    | 3:C:293:SER:H    | 0.44     | 2.15        | 9      | 1     |
| 3:C:274:LEU:CD1  | 3:C:275:MET:O    | 0.44     | 2.64        | 2      | 1     |
| 3:C:178:TYR:CD1  | 3:C:178:TYR:O    | 0.44     | 2.71        | 4      | 1     |
| 2:B:59:PHE:O     | 2:B:61:PRO:CD    | 0.44     | 2.65        | 1      | 5     |
| 3:C:303:ASN:HD21 | 3:C:306:ILE:HD11 | 0.44     | 1.72        | 3      | 1     |
| 1:A:12:A:O2'     | 1:A:13:U:H5'     | 0.44     | 2.12        | 5      | 2     |
| 2:B:37:GLN:CD    | 2:B:41:GLN:HE21  | 0.44     | 2.15        | 4      | 1     |
| 3:C:294:ALA:O    | 3:C:295:ASP:C    | 0.44     | 2.56        | 5      | 1     |
| 3:C:264:SER:C    | 3:C:266:TRP:N    | 0.44     | 2.69        | 6      | 2     |
| 1:A:11:A:C3'     | 2:B:68:GLY:C     | 0.44     | 2.80        | 7      | 1     |
| 3:C:224:ASP:OD1  | 3:C:224:ASP:O    | 0.44     | 2.36        | 7      | 1     |
| 1:A:9:A:H5''     | 2:B:69:TYR:CD2   | 0.44     | 2.44        | 9      | 1     |
| 2:B:71:PHE:C     | 2:B:72:ILE:HD12  | 0.44     | 2.32        | 9      | 1     |
| 2:B:31:GLY:C     | 2:B:33:ILE:H     | 0.44     | 2.15        | 2      | 1     |
| 2:B:49:VAL:HG12  | 2:B:50:GLY:N     | 0.44     | 2.27        | 4      | 1     |
| 3:C:251:GLY:N    | 3:C:252:PRO:HD2  | 0.44     | 2.26        | 9      | 3     |
| 2:B:60:ASP:C     | 2:B:60:ASP:OD1   | 0.44     | 2.55        | 7      | 1     |
| 3:C:170:THR:CB   | 3:C:192:LYS:NZ   | 0.44     | 2.81        | 9      | 1     |
| 3:C:317:ARG:CB   | 3:C:317:ARG:NH1  | 0.44     | 2.80        | 10     | 1     |
| 3:C:275:MET:C    | 3:C:283:SER:OG   | 0.44     | 2.56        | 3      | 1     |
| 3:C:300:VAL:HG23 | 3:C:303:ASN:HD21 | 0.44     | 1.71        | 3      | 1     |
| 1:A:5:U:C5       | 3:C:164:GLY:HA2  | 0.44     | 2.48        | 4      | 1     |
| 1:A:5:U:N3       | 3:C:162:PHE:CE2  | 0.44     | 2.84        | 6      | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 3:C:261:GLU:O    | 3:C:264:SER:OG  | 0.44     | 2.33        | 9      | 1     |
| 3:C:158:SER:OG   | 3:C:232:ARG:NE  | 0.44     | 2.46        | 1      | 1     |
| 3:C:224:ASP:O    | 3:C:224:ASP:OD1 | 0.44     | 2.35        | 1      | 2     |
| 3:C:292:ASP:C    | 3:C:292:ASP:OD1 | 0.44     | 2.54        | 9      | 2     |
| 1:A:2:A:O2'      | 1:A:3:U:OP2     | 0.44     | 2.35        | 5      | 1     |
| 1:A:9:A:H5''     | 2:B:69:TYR:CE1  | 0.44     | 2.48        | 7      | 1     |
| 1:A:8:A:H2       | 2:B:29:TYR:CD1  | 0.44     | 2.31        | 9      | 1     |
| 2:B:23:PRO:O     | 2:B:101:TYR:CD2 | 0.44     | 2.71        | 9      | 1     |
| 1:A:10:U:O2      | 2:B:58:MET:CE   | 0.44     | 2.66        | 1      | 1     |
| 1:A:9:A:H4'      | 2:B:69:TYR:CZ   | 0.44     | 2.47        | 1      | 1     |
| 3:C:193:ASP:CG   | 3:C:196:THR:OG1 | 0.44     | 2.55        | 1      | 2     |
| 1:A:2:A:N1       | 3:C:319:GLU:O   | 0.44     | 2.50        | 7      | 1     |
| 3:C:289:VAL:HG11 | 3:C:291:TYR:CZ  | 0.44     | 2.47        | 8      | 1     |
| 2:B:29:TYR:N     | 2:B:29:TYR:CD1  | 0.44     | 2.80        | 10     | 1     |
| 2:B:43:LEU:HD23  | 2:B:44:ASP:OD1  | 0.44     | 2.13        | 10     | 1     |
| 3:C:277:ASP:O    | 3:C:281:GLY:N   | 0.44     | 2.50        | 1      | 1     |
| 3:C:301:CYS:C    | 3:C:303:ASN:N   | 0.44     | 2.71        | 5      | 2     |
| 2:B:32:SER:CB    | 2:B:94:SER:H    | 0.44     | 2.25        | 7      | 1     |
| 3:C:279:ASP:C    | 3:C:280:THR:CG2 | 0.44     | 2.86        | 7      | 1     |
| 3:C:254:VAL:HG21 | 3:C:308:PHE:CE2 | 0.44     | 2.48        | 1      | 1     |
| 1:A:6:A:O2'      | 3:C:236:ARG:NH2 | 0.44     | 2.50        | 2      | 1     |
| 1:A:5:U:O4       | 3:C:164:GLY:C   | 0.44     | 2.56        | 5      | 1     |
| 2:B:45:LEU:CD2   | 2:B:90:TYR:OH   | 0.44     | 2.65        | 5      | 1     |
| 3:C:164:GLY:O    | 3:C:165:GLY:C   | 0.44     | 2.56        | 5      | 1     |
| 1:A:11:A:C2      | 2:B:63:THR:CB   | 0.44     | 3.00        | 7      | 1     |
| 3:C:269:ILE:HG23 | 3:C:291:TYR:CE2 | 0.44     | 2.48        | 9      | 1     |
| 2:B:30:LEU:CD2   | 2:B:30:LEU:N    | 0.43     | 2.80        | 1      | 1     |
| 3:C:277:ASP:OD1  | 3:C:277:ASP:C   | 0.43     | 2.56        | 1      | 1     |
| 3:C:176:ARG:CG   | 3:C:177:GLU:N   | 0.43     | 2.81        | 3      | 1     |
| 3:C:246:PHE:CE1  | 3:C:247:VAL:C   | 0.43     | 2.92        | 3      | 1     |
| 3:C:318:ALA:O    | 3:C:319:GLU:C   | 0.43     | 2.56        | 5      | 1     |
| 1:A:11:A:C2'     | 2:B:69:TYR:HB2  | 0.43     | 2.43        | 7      | 1     |
| 1:A:5:U:C1'      | 3:C:201:GLY:O   | 0.43     | 2.59        | 7      | 1     |
| 2:B:29:TYR:OH    | 2:B:101:TYR:O   | 0.43     | 2.35        | 10     | 1     |
| 3:C:253:ASP:O    | 3:C:254:VAL:C   | 0.43     | 2.56        | 4      | 1     |
| 3:C:277:ASP:O    | 3:C:281:GLY:O   | 0.43     | 2.36        | 4      | 1     |
| 2:B:31:GLY:CA    | 2:B:69:TYR:CE1  | 0.43     | 3.01        | 5      | 1     |
| 3:C:270:ILE:CG1  | 3:C:291:TYR:O   | 0.43     | 2.65        | 6      | 1     |
| 3:C:249:GLY:O    | 3:C:310:ASP:OD2 | 0.43     | 2.36        | 8      | 1     |
| 1:A:4:A:C5       | 3:C:168:TRP:CE3 | 0.43     | 3.06        | 1      | 1     |
| 2:B:27:VAL:HG13  | 2:B:73:GLU:CA   | 0.43     | 2.42        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:1:U:O2'      | 1:A:2:A:C8       | 0.43     | 2.57        | 6      | 1     |
| 1:A:11:A:C3'     | 2:B:69:TYR:HB2   | 0.43     | 2.44        | 7      | 1     |
| 1:A:2:A:H5''     | 3:C:284:ARG:HD2  | 0.43     | 1.88        | 9      | 1     |
| 3:C:208:GLU:OE1  | 3:C:208:GLU:C    | 0.43     | 2.56        | 9      | 1     |
| 1:A:6:A:N3       | 3:C:162:PHE:CE1  | 0.43     | 2.86        | 2      | 1     |
| 3:C:232:ARG:O    | 3:C:234:ILE:N    | 0.43     | 2.51        | 4      | 1     |
| 1:A:11:A:H4'     | 2:B:58:MET:HG2   | 0.43     | 1.90        | 7      | 1     |
| 2:B:102:SER:O    | 2:B:102:SER:OG   | 0.43     | 2.31        | 10     | 1     |
| 2:B:38:THR:O     | 2:B:42:ILE:CD1   | 0.43     | 2.64        | 10     | 1     |
| 2:B:26:ARG:C     | 2:B:80:SER:OG    | 0.43     | 2.56        | 2      | 2     |
| 2:B:43:LEU:O     | 2:B:47:SER:CB    | 0.43     | 2.66        | 2      | 1     |
| 1:A:11:A:OP1     | 2:B:61:PRO:CG    | 0.43     | 2.67        | 3      | 1     |
| 3:C:250:ILE:O    | 3:C:251:GLY:C    | 0.43     | 2.56        | 4      | 1     |
| 3:C:187:ASP:H    | 3:C:206:SER:CB   | 0.43     | 2.26        | 5      | 1     |
| 3:C:227:VAL:CG1  | 3:C:227:VAL:O    | 0.43     | 2.65        | 5      | 1     |
| 3:C:227:VAL:CG1  | 3:C:273:GLN:OE1  | 0.43     | 2.66        | 6      | 1     |
| 1:A:10:U:OP2     | 1:A:10:U:C5      | 0.43     | 2.71        | 7      | 1     |
| 2:B:31:GLY:HA2   | 2:B:69:TYR:CD1   | 0.43     | 2.48        | 7      | 1     |
| 3:C:193:ASP:N    | 3:C:194:PRO:CD   | 0.43     | 2.81        | 8      | 1     |
| 1:A:4:A:OP1      | 1:A:4:A:H2       | 0.43     | 1.97        | 10     | 1     |
| 2:B:39:GLU:CD    | 2:B:39:GLU:C     | 0.43     | 2.77        | 1      | 1     |
| 1:A:9:A:C5       | 2:B:29:TYR:CE2   | 0.43     | 3.07        | 4      | 1     |
| 2:B:39:GLU:N     | 2:B:57:MET:SD    | 0.43     | 2.92        | 5      | 1     |
| 3:C:254:VAL:O    | 3:C:254:VAL:HG23 | 0.43     | 2.13        | 6      | 1     |
| 1:A:12:A:P       | 2:B:69:TYR:H     | 0.43     | 2.35        | 7      | 1     |
| 2:B:60:ASP:HB3   | 2:B:66:SER:H     | 0.43     | 1.72        | 8      | 1     |
| 3:C:271:ASP:O    | 3:C:272:ALA:O    | 0.43     | 2.37        | 8      | 1     |
| 3:C:310:ASP:OD1  | 3:C:311:ARG:N    | 0.43     | 2.52        | 1      | 1     |
| 2:B:90:TYR:N     | 2:B:90:TYR:CD1   | 0.43     | 2.85        | 5      | 1     |
| 2:B:48:ASN:O     | 2:B:87:LEU:HD11  | 0.43     | 2.14        | 10     | 1     |
| 2:B:81:ALA:O     | 2:B:85:ARG:CB    | 0.43     | 2.67        | 1      | 2     |
| 2:B:83:ALA:HA    | 2:B:86:ASN:OD1   | 0.43     | 2.14        | 2      | 1     |
| 1:A:9:A:OP1      | 2:B:69:TYR:OH    | 0.43     | 2.34        | 7      | 1     |
| 3:C:254:VAL:O    | 3:C:254:VAL:CG1  | 0.43     | 2.62        | 8      | 1     |
| 1:A:10:U:OP1     | 1:A:10:U:C6      | 0.43     | 2.72        | 10     | 1     |
| 3:C:299:ARG:O    | 3:C:302:GLN:CG   | 0.43     | 2.67        | 1      | 1     |
| 1:A:7:U:C4'      | 1:A:8:A:OP2      | 0.43     | 2.64        | 4      | 2     |
| 3:C:217:VAL:HG13 | 3:C:218:LYS:N    | 0.43     | 2.28        | 2      | 1     |
| 3:C:174:ASN:OD1  | 3:C:174:ASN:C    | 0.43     | 2.58        | 3      | 1     |
| 3:C:276:LEU:HD12 | 3:C:278:LYS:N    | 0.43     | 2.29        | 6      | 1     |
| 1:A:6:A:H5''     | 1:A:7:U:C5'      | 0.43     | 2.43        | 2      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:30:LEU:N     | 2:B:30:LEU:HD22  | 0.43     | 2.29        | 2      | 1     |
| 3:C:197:GLY:O    | 3:C:198:ARG:C    | 0.43     | 2.55        | 4      | 1     |
| 3:C:207:PHE:CG   | 3:C:212:SER:OG   | 0.43     | 2.68        | 10     | 1     |
| 3:C:202:PHE:CD1  | 3:C:202:PHE:C    | 0.42     | 2.92        | 1      | 1     |
| 2:B:49:VAL:HG21  | 2:B:87:LEU:HD11  | 0.42     | 1.90        | 2      | 1     |
| 2:B:48:ASN:OD1   | 2:B:48:ASN:N     | 0.42     | 2.52        | 4      | 1     |
| 3:C:185:VAL:HG11 | 3:C:188:LEU:HD23 | 0.42     | 1.91        | 4      | 1     |
| 1:A:5:U:C2       | 3:C:164:GLY:CA   | 0.42     | 3.02        | 6      | 1     |
| 3:C:186:THR:OG1  | 3:C:208:GLU:CA   | 0.42     | 2.67        | 6      | 1     |
| 3:C:308:PHE:CE2  | 3:C:309:LYS:CG   | 0.42     | 3.02        | 6      | 1     |
| 1:A:9:A:C2       | 2:B:29:TYR:CG    | 0.42     | 3.07        | 10     | 1     |
| 1:A:11:A:H5'     | 2:B:61:PRO:HD2   | 0.42     | 1.90        | 1      | 1     |
| 3:C:158:SER:CB   | 3:C:232:ARG:HE   | 0.42     | 2.27        | 1      | 1     |
| 2:B:76:ASP:CG    | 2:B:77:LEU:N     | 0.42     | 2.72        | 2      | 1     |
| 3:C:200:ARG:CD   | 3:C:200:ARG:N    | 0.42     | 2.82        | 4      | 1     |
| 3:C:254:VAL:CG2  | 3:C:255:ARG:N    | 0.42     | 2.82        | 4      | 1     |
| 3:C:190:ILE:C    | 3:C:191:MET:SD   | 0.42     | 2.98        | 5      | 1     |
| 3:C:283:SER:O    | 3:C:284:ARG:C    | 0.42     | 2.57        | 6      | 1     |
| 1:A:4:A:H2       | 1:A:4:A:OP1      | 0.42     | 1.96        | 7      | 1     |
| 3:C:163:ILE:CD1  | 3:C:175:LEU:HD21 | 0.42     | 2.45        | 7      | 1     |
| 1:A:12:A:C6      | 2:B:58:MET:SD    | 0.42     | 3.12        | 8      | 1     |
| 3:C:275:MET:CB   | 3:C:286:PHE:CE1  | 0.42     | 3.03        | 1      | 1     |
| 2:B:42:ILE:O     | 2:B:43:LEU:C     | 0.42     | 2.58        | 3      | 5     |
| 2:B:71:PHE:N     | 2:B:71:PHE:CD1   | 0.42     | 2.86        | 3      | 1     |
| 1:A:10:U:H5'     | 2:B:69:TYR:CD2   | 0.42     | 2.49        | 4      | 1     |
| 3:C:215:GLU:CD   | 3:C:215:GLU:N    | 0.42     | 2.73        | 4      | 1     |
| 3:C:262:PHE:CD2  | 3:C:308:PHE:CD1  | 0.42     | 3.07        | 9      | 1     |
| 2:B:88:ASN:CG    | 2:B:89:GLY:N     | 0.42     | 2.73        | 10     | 1     |
| 3:C:250:ILE:HG21 | 3:C:274:LEU:HD22 | 0.42     | 1.91        | 10     | 1     |
| 1:A:10:U:H5'     | 2:B:71:PHE:HZ    | 0.42     | 1.74        | 2      | 1     |
| 2:B:48:ASN:O     | 2:B:49:VAL:C     | 0.42     | 2.56        | 2      | 2     |
| 1:A:5:U:O5'      | 1:A:5:U:O2       | 0.42     | 2.37        | 3      | 1     |
| 3:C:168:TRP:O    | 3:C:197:GLY:O    | 0.42     | 2.37        | 3      | 1     |
| 2:B:45:LEU:HD21  | 2:B:92:LEU:HD22  | 0.42     | 1.90        | 8      | 1     |
| 2:B:90:TYR:CZ    | 2:B:92:LEU:HD13  | 0.42     | 2.49        | 2      | 1     |
| 3:C:211:SER:C    | 3:C:215:GLU:OE2  | 0.42     | 2.57        | 4      | 1     |
| 2:B:44:ASP:OD1   | 2:B:44:ASP:O     | 0.42     | 2.38        | 7      | 2     |
| 1:A:7:U:H5       | 3:C:204:PHE:CZ   | 0.42     | 2.32        | 6      | 1     |
| 2:B:84:VAL:CG1   | 2:B:99:CYS:CB    | 0.42     | 2.98        | 6      | 1     |
| 1:A:2:A:C6       | 3:C:319:GLU:O    | 0.42     | 2.72        | 7      | 1     |
| 3:C:317:ARG:C    | 3:C:319:GLU:N    | 0.42     | 2.72        | 7      | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:10:U:C2'     | 1:A:11:A:C8     | 0.42     | 2.95        | 8      | 1     |
| 3:C:222:ILE:CG2  | 3:C:226:LYS:O   | 0.42     | 2.68        | 10     | 1     |
| 1:A:10:U:O4      | 2:B:71:PHE:CE2  | 0.42     | 2.73        | 1      | 1     |
| 3:C:264:SER:O    | 3:C:265:GLN:O   | 0.42     | 2.37        | 4      | 2     |
| 1:A:8:A:H4'      | 2:B:95:ARG:HH22 | 0.42     | 1.75        | 4      | 1     |
| 2:B:47:SER:C     | 2:B:49:VAL:H    | 0.42     | 2.17        | 5      | 1     |
| 2:B:60:ASP:HB3   | 2:B:66:SER:N    | 0.42     | 2.30        | 5      | 1     |
| 3:C:252:PRO:C    | 3:C:254:VAL:H   | 0.42     | 2.18        | 5      | 1     |
| 3:C:269:ILE:HG23 | 3:C:269:ILE:O   | 0.42     | 2.13        | 5      | 1     |
| 2:B:33:ILE:CD1   | 2:B:33:ILE:N    | 0.42     | 2.81        | 8      | 1     |
| 3:C:284:ARG:O    | 3:C:285:GLY:C   | 0.42     | 2.57        | 2      | 1     |
| 2:B:83:ALA:O     | 2:B:84:VAL:C    | 0.42     | 2.56        | 6      | 1     |
| 3:C:205:LEU:HD13 | 3:C:207:PHE:CE2 | 0.42     | 2.49        | 7      | 1     |
| 1:A:10:U:C5      | 2:B:63:THR:HG21 | 0.42     | 2.50        | 8      | 1     |
| 1:A:5:U:O4'      | 3:C:201:GLY:O   | 0.42     | 2.37        | 9      | 1     |
| 1:A:2:A:HO2'     | 1:A:3:U:P       | 0.42     | 2.37        | 1      | 1     |
| 2:B:85:ARG:CD    | 2:B:85:ARG:C    | 0.42     | 2.87        | 1      | 1     |
| 2:B:32:SER:OG    | 2:B:94:SER:CB   | 0.42     | 2.68        | 1      | 1     |
| 2:B:35:TYR:OH    | 2:B:59:PHE:CD2  | 0.42     | 2.71        | 2      | 1     |
| 3:C:222:ILE:CD1  | 3:C:222:ILE:N   | 0.42     | 2.83        | 7      | 1     |
| 3:C:168:TRP:CE2  | 3:C:198:ARG:CZ  | 0.42     | 3.03        | 10     | 1     |
| 3:C:213:VAL:CG2  | 3:C:214:ASP:N   | 0.42     | 2.82        | 10     | 1     |
| 3:C:262:PHE:O    | 3:C:265:GLN:CG  | 0.42     | 2.67        | 1      | 2     |
| 3:C:193:ASP:OD2  | 3:C:199:SER:OG  | 0.42     | 2.29        | 2      | 1     |
| 1:A:5:U:O2       | 3:C:162:PHE:CE2 | 0.42     | 2.72        | 9      | 1     |
| 2:B:38:THR:C     | 2:B:57:MET:SD   | 0.42     | 2.98        | 10     | 1     |
| 3:C:186:THR:CG2  | 3:C:187:ASP:N   | 0.42     | 2.83        | 3      | 1     |
| 3:C:300:VAL:HG23 | 3:C:303:ASN:ND2 | 0.42     | 2.30        | 3      | 1     |
| 3:C:221:HIS:CD2  | 3:C:230:PRO:HG3 | 0.42     | 2.49        | 5      | 2     |
| 3:C:180:GLY:C    | 3:C:182:TYR:N   | 0.42     | 2.72        | 10     | 1     |
| 2:B:80:SER:O     | 2:B:84:VAL:CG2  | 0.41     | 2.67        | 2      | 1     |
| 3:C:162:PHE:O    | 3:C:163:ILE:C   | 0.41     | 2.58        | 8      | 2     |
| 3:C:226:LYS:NZ   | 3:C:279:ASP:CA  | 0.41     | 2.83        | 7      | 1     |
| 1:A:10:U:C2      | 2:B:58:MET:HE2  | 0.41     | 2.50        | 1      | 1     |
| 3:C:282:GLN:C    | 3:C:284:ARG:N   | 0.41     | 2.74        | 5      | 2     |
| 3:C:244:LYS:O    | 3:C:318:ALA:CB  | 0.41     | 2.68        | 6      | 3     |
| 2:B:57:MET:SD    | 2:B:70:ALA:CB   | 0.41     | 3.07        | 2      | 1     |
| 1:A:3:U:O4'      | 3:C:288:PHE:CE1 | 0.41     | 2.73        | 3      | 1     |
| 2:B:27:VAL:CG1   | 2:B:102:SER:N   | 0.41     | 2.83        | 6      | 1     |
| 3:C:255:ARG:O    | 3:C:256:PRO:C   | 0.41     | 2.58        | 7      | 1     |
| 2:B:32:SER:OG    | 2:B:32:SER:O    | 0.41     | 2.37        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:271:ASP:O    | 3:C:290:THR:OG1  | 0.41     | 2.30        | 1      | 1     |
| 3:C:232:ARG:O    | 3:C:234:ILE:CD1  | 0.41     | 2.68        | 2      | 1     |
| 1:A:11:A:H3'     | 1:A:12:A:C8      | 0.41     | 2.51        | 5      | 1     |
| 3:C:186:THR:N    | 3:C:206:SER:O    | 0.41     | 2.50        | 5      | 1     |
| 1:A:11:A:O5'     | 2:B:58:MET:HB3   | 0.41     | 2.14        | 7      | 1     |
| 1:A:11:A:C1'     | 2:B:66:SER:O     | 0.41     | 2.64        | 7      | 1     |
| 1:A:12:A:C8      | 2:B:67:LYS:C     | 0.41     | 2.91        | 7      | 1     |
| 1:A:8:A:C5'      | 2:B:95:ARG:NH2   | 0.41     | 2.84        | 10     | 1     |
| 1:A:10:U:C5'     | 2:B:69:TYR:OH    | 0.41     | 2.62        | 10     | 1     |
| 3:C:175:LEU:HD23 | 3:C:175:LEU:C    | 0.41     | 2.35        | 10     | 1     |
| 1:A:2:A:C4'      | 3:C:286:PHE:CG   | 0.41     | 3.01        | 10     | 1     |
| 2:B:88:ASN:O     | 2:B:97:LEU:HD12  | 0.41     | 2.15        | 1      | 1     |
| 3:C:158:SER:O    | 3:C:159:CYS:CB   | 0.41     | 2.68        | 1      | 2     |
| 3:C:301:CYS:O    | 3:C:302:GLN:C    | 0.41     | 2.58        | 5      | 2     |
| 3:C:186:THR:HG23 | 3:C:187:ASP:N    | 0.41     | 2.30        | 3      | 1     |
| 2:B:54:ASN:HD22  | 2:B:73:GLU:CD    | 0.41     | 2.17        | 5      | 1     |
| 2:B:27:VAL:HG22  | 2:B:73:GLU:HG3   | 0.41     | 1.91        | 7      | 1     |
| 1:A:8:A:O2'      | 1:A:9:A:H5'      | 0.41     | 2.15        | 8      | 1     |
| 1:A:8:A:N3       | 2:B:29:TYR:CG    | 0.41     | 2.89        | 9      | 1     |
| 2:B:62:GLN:O     | 2:B:63:THR:C     | 0.41     | 2.58        | 9      | 1     |
| 1:A:4:A:C2       | 3:C:168:TRP:CZ3  | 0.41     | 3.09        | 9      | 1     |
| 1:A:4:A:N1       | 3:C:279:ASP:O    | 0.41     | 2.52        | 10     | 1     |
| 3:C:161:MET:CE   | 3:C:163:ILE:HD13 | 0.41     | 2.46        | 10     | 1     |
| 2:B:59:PHE:O     | 2:B:61:PRO:HD3   | 0.41     | 2.15        | 5      | 1     |
| 2:B:29:TYR:C     | 2:B:30:LEU:HD12  | 0.41     | 2.35        | 6      | 1     |
| 2:B:65:ARG:NH1   | 3:C:200:ARG:NH2  | 0.41     | 2.68        | 6      | 1     |
| 1:A:8:A:OP1      | 3:C:192:LYS:O    | 0.41     | 2.39        | 7      | 1     |
| 2:B:31:GLY:HA2   | 2:B:69:TYR:CE1   | 0.41     | 2.50        | 7      | 1     |
| 3:C:175:LEU:HD22 | 3:C:190:ILE:HD11 | 0.41     | 1.92        | 8      | 1     |
| 2:B:87:LEU:O     | 2:B:87:LEU:CG    | 0.41     | 2.67        | 1      | 1     |
| 3:C:271:ASP:O    | 3:C:290:THR:CB   | 0.41     | 2.69        | 1      | 1     |
| 3:C:159:CYS:SG   | 3:C:213:VAL:CG2  | 0.41     | 3.08        | 2      | 1     |
| 1:A:9:A:C2'      | 1:A:10:U:H6      | 0.41     | 2.26        | 3      | 1     |
| 3:C:282:GLN:O    | 3:C:286:PHE:CE2  | 0.41     | 2.74        | 3      | 1     |
| 1:A:5:U:C6       | 1:A:5:U:P        | 0.41     | 3.14        | 4      | 1     |
| 3:C:270:ILE:HG22 | 3:C:271:ASP:N    | 0.41     | 2.29        | 4      | 1     |
| 3:C:186:THR:OG1  | 3:C:206:SER:O    | 0.41     | 2.34        | 5      | 1     |
| 3:C:301:CYS:O    | 3:C:303:ASN:N    | 0.41     | 2.53        | 5      | 1     |
| 3:C:289:VAL:CG2  | 3:C:291:TYR:CE1  | 0.41     | 3.03        | 6      | 1     |
| 3:C:167:ASN:O    | 3:C:168:TRP:CD2  | 0.41     | 2.74        | 7      | 1     |
| 3:C:186:THR:HG22 | 3:C:206:SER:O    | 0.41     | 2.16        | 7      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:6:A:C5'      | 1:A:8:A:OP2      | 0.41     | 2.66        | 8      | 1     |
| 3:C:273:GLN:HG3  | 3:C:274:LEU:N    | 0.41     | 2.30        | 10     | 1     |
| 1:A:9:A:H4'      | 2:B:69:TYR:CD2   | 0.41     | 2.51        | 3      | 1     |
| 3:C:200:ARG:O    | 3:C:202:PHE:CE2  | 0.41     | 2.72        | 3      | 1     |
| 3:C:159:CYS:CB   | 3:C:209:LYS:O    | 0.41     | 2.69        | 4      | 1     |
| 3:C:166:LEU:C    | 3:C:166:LEU:CD1  | 0.41     | 2.89        | 4      | 1     |
| 3:C:226:LYS:CB   | 3:C:226:LYS:NZ   | 0.41     | 2.83        | 4      | 1     |
| 1:A:8:A:N6       | 2:B:101:TYR:OH   | 0.41     | 2.54        | 6      | 1     |
| 3:C:264:SER:O    | 3:C:265:GLN:C    | 0.41     | 2.59        | 6      | 1     |
| 3:C:305:PHE:CE2  | 3:C:314:GLU:CG   | 0.41     | 3.04        | 6      | 1     |
| 2:B:28:VAL:HG13  | 2:B:98:LYS:O     | 0.41     | 2.14        | 8      | 1     |
| 3:C:174:ASN:CG   | 3:C:175:LEU:N    | 0.41     | 2.73        | 10     | 1     |
| 3:C:178:TYR:CG   | 3:C:223:LEU:CD1  | 0.41     | 3.04        | 1      | 1     |
| 2:B:52:VAL:O     | 2:B:53:ILE:HG12  | 0.41     | 2.16        | 2      | 1     |
| 1:A:9:A:C6       | 2:B:29:TYR:CZ    | 0.41     | 3.08        | 4      | 2     |
| 1:A:11:A:O2'     | 2:B:67:LYS:N     | 0.41     | 2.54        | 7      | 1     |
| 1:A:2:A:O2'      | 1:A:3:U:O5'      | 0.41     | 2.38        | 1      | 1     |
| 3:C:309:LYS:C    | 3:C:311:ARG:N    | 0.41     | 2.74        | 2      | 1     |
| 2:B:35:TYR:CE1   | 2:B:59:PHE:CD1   | 0.41     | 3.09        | 2      | 1     |
| 3:C:306:ILE:HD12 | 3:C:315:ILE:HD11 | 0.41     | 1.91        | 2      | 1     |
| 3:C:193:ASP:C    | 3:C:195:ALA:H    | 0.41     | 2.19        | 3      | 1     |
| 3:C:251:GLY:O    | 3:C:254:VAL:CG1  | 0.41     | 2.69        | 4      | 1     |
| 2:B:31:GLY:N     | 2:B:33:ILE:HD11  | 0.41     | 2.31        | 4      | 1     |
| 3:C:281:GLY:C    | 3:C:283:SER:N    | 0.41     | 2.71        | 6      | 1     |
| 1:A:6:A:C8       | 3:C:239:GLN:OE1  | 0.41     | 2.74        | 6      | 1     |
| 1:A:11:A:N3      | 2:B:60:ASP:HB2   | 0.41     | 2.31        | 7      | 1     |
| 1:A:12:A:C8      | 2:B:67:LYS:CA    | 0.41     | 3.00        | 7      | 1     |
| 1:A:6:A:N9       | 3:C:162:PHE:CE1  | 0.41     | 2.89        | 7      | 1     |
| 3:C:174:ASN:ND2  | 3:C:175:LEU:N    | 0.41     | 2.69        | 9      | 1     |
| 3:C:289:VAL:CG1  | 3:C:291:TYR:CE1  | 0.41     | 3.02        | 9      | 1     |
| 1:A:6:A:OP1      | 3:C:200:ARG:NH2  | 0.41     | 2.54        | 10     | 1     |
| 1:A:7:U:OP1      | 1:A:8:A:N7       | 0.41     | 2.53        | 10     | 1     |
| 3:C:294:ALA:O    | 3:C:297:VAL:CG1  | 0.41     | 2.69        | 10     | 1     |
| 2:B:27:VAL:CG2   | 2:B:102:SER:O    | 0.41     | 2.69        | 1      | 1     |
| 1:A:3:U:H5'      | 3:C:286:PHE:CE1  | 0.41     | 2.51        | 3      | 1     |
| 3:C:266:TRP:C    | 3:C:266:TRP:CD1  | 0.41     | 2.94        | 3      | 1     |
| 3:C:170:THR:O    | 3:C:190:ILE:CD1  | 0.41     | 2.69        | 4      | 1     |
| 1:A:8:A:C2       | 2:B:99:CYS:O     | 0.41     | 2.73        | 6      | 1     |
| 3:C:270:ILE:CD1  | 3:C:291:TYR:O    | 0.41     | 2.69        | 6      | 1     |
| 1:A:3:U:HO2'     | 1:A:4:A:P        | 0.41     | 2.39        | 7      | 1     |
| 2:B:32:SER:O     | 2:B:32:SER:OG    | 0.41     | 2.35        | 7      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:C:161:MET:SD   | 3:C:162:PHE:C    | 0.41     | 2.99        | 7      | 1     |
| 1:A:2:A:C2       | 1:A:3:U:C4       | 0.40     | 3.09        | 1      | 1     |
| 2:B:30:LEU:CD2   | 2:B:42:ILE:HD12  | 0.40     | 2.47        | 6      | 1     |
| 3:C:216:VAL:CG1  | 3:C:216:VAL:O    | 0.40     | 2.67        | 6      | 1     |
| 3:C:255:ARG:N    | 3:C:255:ARG:NE   | 0.40     | 2.69        | 6      | 1     |
| 3:C:188:LEU:CD1  | 3:C:188:LEU:C    | 0.40     | 2.80        | 8      | 1     |
| 1:A:10:U:OP2     | 2:B:30:LEU:O     | 0.40     | 2.39        | 5      | 1     |
| 3:C:289:VAL:HG21 | 3:C:291:TYR:CZ   | 0.40     | 2.52        | 5      | 1     |
| 2:B:38:THR:O     | 2:B:42:ILE:HG12  | 0.40     | 2.16        | 7      | 1     |
| 3:C:170:THR:H    | 3:C:192:LYS:HD2  | 0.40     | 1.77        | 8      | 1     |
| 2:B:69:TYR:CZ    | 2:B:71:PHE:CZ    | 0.40     | 3.09        | 10     | 1     |
| 1:A:5:U:H6       | 1:A:5:U:H2'      | 0.40     | 1.53        | 1      | 1     |
| 3:C:272:ALA:C    | 3:C:273:GLN:CG   | 0.40     | 2.90        | 2      | 2     |
| 3:C:273:GLN:O    | 3:C:288:PHE:O    | 0.40     | 2.39        | 3      | 1     |
| 3:C:263:PHE:HB3  | 3:C:269:ILE:HD12 | 0.40     | 1.93        | 5      | 1     |
| 3:C:240:ASP:OD1  | 3:C:244:LYS:NZ   | 0.40     | 2.53        | 8      | 1     |
| 2:B:35:TYR:CZ    | 2:B:59:PHE:CD1   | 0.40     | 3.09        | 9      | 1     |
| 3:C:167:ASN:C    | 3:C:169:ASP:N    | 0.40     | 2.74        | 1      | 1     |
| 3:C:200:ARG:NE   | 3:C:202:PHE:CE2  | 0.40     | 2.89        | 2      | 1     |
| 3:C:264:SER:HA   | 3:C:269:ILE:HD13 | 0.40     | 1.92        | 2      | 1     |
| 1:A:11:A:N3      | 2:B:56:LYS:NZ    | 0.40     | 2.60        | 3      | 1     |
| 2:B:84:VAL:CG1   | 2:B:99:CYS:SG    | 0.40     | 3.09        | 4      | 1     |
| 3:C:291:TYR:N    | 3:C:291:TYR:CD1  | 0.40     | 2.90        | 7      | 1     |
| 2:B:39:GLU:C     | 2:B:39:GLU:CD    | 0.40     | 2.80        | 9      | 1     |
| 3:C:275:MET:CG   | 3:C:286:PHE:CE2  | 0.40     | 3.05        | 9      | 1     |
| 3:C:251:GLY:O    | 3:C:254:VAL:N    | 0.40     | 2.49        | 10     | 1     |
| 2:B:31:GLY:O     | 2:B:33:ILE:N     | 0.40     | 2.55        | 2      | 1     |
| 2:B:51:PRO:C     | 2:B:52:VAL:O     | 0.40     | 2.60        | 2      | 1     |
| 3:C:297:VAL:C    | 3:C:299:ARG:N    | 0.40     | 2.75        | 5      | 1     |
| 2:B:60:ASP:CG    | 2:B:66:SER:C     | 0.40     | 2.79        | 8      | 1     |
| 3:C:233:ALA:O    | 3:C:234:ILE:CG1  | 0.40     | 2.70        | 8      | 1     |
| 3:C:250:ILE:CD1  | 3:C:259:PHE:CD1  | 0.40     | 3.04        | 9      | 1     |

## 5.2 Torsion angles ⓘ

### 5.2.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured      | Allowed      | Outliers     | Percentiles |   |
|-----|-------|-----------------|---------------|--------------|--------------|-------------|---|
| 2   | B     | 81/84 (96%)     | 56±2 (69±3%)  | 13±2 (16±3%) | 12±2 (15±2%) | 0           | 4 |
| 3   | C     | 162/167 (97%)   | 119±3 (74±2%) | 26±3 (16±2%) | 17±2 (10±1%) | 1           | 9 |
| All | All   | 2430/2510 (97%) | 1752 (72%)    | 392 (16%)    | 286 (12%)    | 1           | 7 |

All 83 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     | 77  | LEU  | 10             |
| 2   | B     | 26  | ARG  | 10             |
| 2   | B     | 91  | GLN  | 10             |
| 2   | B     | 76  | ASP  | 10             |
| 2   | B     | 47  | SER  | 10             |
| 3   | C     | 200 | ARG  | 8              |
| 2   | B     | 43  | LEU  | 8              |
| 3   | C     | 283 | SER  | 8              |
| 3   | C     | 259 | PHE  | 8              |
| 3   | C     | 265 | GLN  | 8              |
| 3   | C     | 212 | SER  | 7              |
| 3   | C     | 258 | GLU  | 7              |
| 2   | B     | 49  | VAL  | 7              |
| 2   | B     | 48  | ASN  | 7              |
| 3   | C     | 168 | TRP  | 6              |
| 2   | B     | 97  | LEU  | 6              |
| 2   | B     | 88  | ASN  | 6              |
| 2   | B     | 102 | SER  | 5              |
| 3   | C     | 180 | GLY  | 5              |
| 2   | B     | 52  | VAL  | 5              |
| 3   | C     | 159 | CYS  | 5              |
| 3   | C     | 309 | LYS  | 5              |
| 3   | C     | 227 | VAL  | 5              |
| 3   | C     | 192 | LYS  | 4              |
| 3   | C     | 269 | ILE  | 4              |
| 2   | B     | 68  | GLY  | 4              |
| 2   | B     | 61  | PRO  | 4              |
| 3   | C     | 177 | GLU  | 4              |
| 3   | C     | 277 | ASP  | 4              |
| 3   | C     | 267 | GLY  | 4              |
| 3   | C     | 242 | THR  | 3              |
| 3   | C     | 264 | SER  | 3              |
| 3   | C     | 252 | PRO  | 3              |
| 3   | C     | 280 | THR  | 3              |
| 3   | C     | 318 | ALA  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 3   | C     | 310 | ASP  | 3              |
| 3   | C     | 311 | ARG  | 3              |
| 3   | C     | 273 | GLN  | 3              |
| 3   | C     | 285 | GLY  | 3              |
| 3   | C     | 304 | LYS  | 3              |
| 3   | C     | 195 | ALA  | 3              |
| 3   | C     | 262 | PHE  | 3              |
| 2   | B     | 35  | TYR  | 2              |
| 2   | B     | 53  | ILE  | 2              |
| 2   | B     | 103 | SER  | 2              |
| 3   | C     | 197 | GLY  | 2              |
| 2   | B     | 23  | PRO  | 2              |
| 2   | B     | 93  | GLY  | 2              |
| 3   | C     | 312 | LYS  | 2              |
| 2   | B     | 51  | PRO  | 2              |
| 3   | C     | 279 | ASP  | 2              |
| 3   | C     | 196 | THR  | 2              |
| 3   | C     | 210 | PRO  | 2              |
| 3   | C     | 272 | ALA  | 2              |
| 3   | C     | 190 | ILE  | 2              |
| 2   | B     | 44  | ASP  | 2              |
| 3   | C     | 249 | GLY  | 2              |
| 3   | C     | 225 | GLY  | 1              |
| 3   | C     | 268 | THR  | 1              |
| 3   | C     | 276 | LEU  | 1              |
| 3   | C     | 317 | ARG  | 1              |
| 2   | B     | 31  | GLY  | 1              |
| 2   | B     | 32  | SER  | 1              |
| 3   | C     | 278 | LYS  | 1              |
| 3   | C     | 173 | ASP  | 1              |
| 3   | C     | 286 | PHE  | 1              |
| 3   | C     | 222 | ILE  | 1              |
| 3   | C     | 257 | LYS  | 1              |
| 3   | C     | 254 | VAL  | 1              |
| 3   | C     | 216 | VAL  | 1              |
| 3   | C     | 194 | PRO  | 1              |
| 3   | C     | 316 | LYS  | 1              |
| 3   | C     | 217 | VAL  | 1              |
| 3   | C     | 181 | LYS  | 1              |
| 3   | C     | 266 | TRP  | 1              |
| 3   | C     | 255 | ARG  | 1              |
| 3   | C     | 208 | GLU  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 3   | C     | 253 | ASP  | 1              |
| 3   | C     | 256 | PRO  | 1              |
| 3   | C     | 292 | ASP  | 1              |
| 3   | C     | 235 | PRO  | 1              |
| 3   | C     | 233 | ALA  | 1              |
| 3   | C     | 319 | GLU  | 1              |

### 5.2.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric     | Outliers     | Percentiles |    |
|-----|-------|-----------------|---------------|--------------|-------------|----|
| 2   | B     | 72/74 (97%)     | 58±2 (80±3%)  | 14±2 (20±3%) | 4           | 34 |
| 3   | C     | 140/145 (97%)   | 115±3 (82±2%) | 25±3 (18±2%) | 4           | 39 |
| All | All   | 2120/2190 (97%) | 1730 (82%)    | 390 (18%)    | 4           | 37 |

All 129 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     | 90  | TYR  | 10             |
| 3   | C     | 276 | LEU  | 9              |
| 3   | C     | 171 | THR  | 9              |
| 2   | B     | 37  | GLN  | 9              |
| 3   | C     | 222 | ILE  | 9              |
| 2   | B     | 97  | LEU  | 9              |
| 2   | B     | 88  | ASN  | 8              |
| 3   | C     | 280 | THR  | 7              |
| 2   | B     | 66  | SER  | 7              |
| 3   | C     | 245 | ILE  | 7              |
| 3   | C     | 205 | LEU  | 6              |
| 3   | C     | 159 | CYS  | 6              |
| 2   | B     | 52  | VAL  | 6              |
| 3   | C     | 246 | PHE  | 6              |
| 3   | C     | 193 | ASP  | 6              |
| 2   | B     | 48  | ASN  | 6              |
| 3   | C     | 190 | ILE  | 6              |
| 3   | C     | 186 | THR  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 59  | PHE  | 6              |
| 3   | C     | 221 | HIS  | 6              |
| 3   | C     | 189 | LYS  | 5              |
| 3   | C     | 168 | TRP  | 5              |
| 3   | C     | 265 | GLN  | 5              |
| 2   | B     | 58  | MET  | 5              |
| 3   | C     | 226 | LYS  | 5              |
| 3   | C     | 269 | ILE  | 5              |
| 2   | B     | 41  | GLN  | 5              |
| 2   | B     | 91  | GLN  | 5              |
| 2   | B     | 25  | SER  | 5              |
| 3   | C     | 172 | GLU  | 5              |
| 3   | C     | 192 | LYS  | 4              |
| 3   | C     | 229 | ASP  | 4              |
| 3   | C     | 274 | LEU  | 4              |
| 2   | B     | 94  | SER  | 4              |
| 3   | C     | 223 | LEU  | 4              |
| 3   | C     | 283 | SER  | 4              |
| 3   | C     | 227 | VAL  | 4              |
| 3   | C     | 289 | VAL  | 4              |
| 3   | C     | 236 | ARG  | 4              |
| 3   | C     | 200 | ARG  | 4              |
| 3   | C     | 188 | LEU  | 4              |
| 3   | C     | 255 | ARG  | 4              |
| 3   | C     | 275 | MET  | 3              |
| 2   | B     | 80  | SER  | 3              |
| 2   | B     | 84  | VAL  | 3              |
| 2   | B     | 33  | ILE  | 3              |
| 2   | B     | 77  | LEU  | 3              |
| 3   | C     | 244 | LYS  | 3              |
| 2   | B     | 99  | CYS  | 3              |
| 2   | B     | 55  | LEU  | 3              |
| 3   | C     | 311 | ARG  | 3              |
| 2   | B     | 102 | SER  | 3              |
| 2   | B     | 57  | MET  | 3              |
| 3   | C     | 319 | GLU  | 3              |
| 3   | C     | 175 | LEU  | 3              |
| 3   | C     | 206 | SER  | 3              |
| 3   | C     | 250 | ILE  | 3              |
| 3   | C     | 266 | TRP  | 3              |
| 2   | B     | 63  | THR  | 2              |
| 3   | C     | 286 | PHE  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 3   | C     | 196 | THR  | 2              |
| 3   | C     | 309 | LYS  | 2              |
| 2   | B     | 86  | ASN  | 2              |
| 2   | B     | 35  | TYR  | 2              |
| 2   | B     | 28  | VAL  | 2              |
| 2   | B     | 26  | ARG  | 2              |
| 3   | C     | 161 | MET  | 2              |
| 3   | C     | 209 | LYS  | 2              |
| 3   | C     | 231 | LYS  | 2              |
| 2   | B     | 60  | ASP  | 2              |
| 3   | C     | 316 | LYS  | 2              |
| 3   | C     | 278 | LYS  | 2              |
| 3   | C     | 242 | THR  | 2              |
| 3   | C     | 213 | VAL  | 2              |
| 3   | C     | 312 | LYS  | 2              |
| 2   | B     | 45  | LEU  | 2              |
| 3   | C     | 271 | ASP  | 2              |
| 2   | B     | 46  | CYS  | 2              |
| 3   | C     | 284 | ARG  | 2              |
| 3   | C     | 181 | LYS  | 2              |
| 2   | B     | 49  | VAL  | 2              |
| 2   | B     | 103 | SER  | 2              |
| 3   | C     | 264 | SER  | 2              |
| 3   | C     | 174 | ASN  | 2              |
| 2   | B     | 98  | LYS  | 2              |
| 3   | C     | 273 | GLN  | 2              |
| 3   | C     | 292 | ASP  | 2              |
| 3   | C     | 163 | ILE  | 1              |
| 3   | C     | 277 | ASP  | 1              |
| 3   | C     | 314 | GLU  | 1              |
| 2   | B     | 32  | SER  | 1              |
| 3   | C     | 215 | GLU  | 1              |
| 3   | C     | 191 | MET  | 1              |
| 2   | B     | 69  | TYR  | 1              |
| 3   | C     | 185 | VAL  | 1              |
| 2   | B     | 101 | TYR  | 1              |
| 3   | C     | 208 | GLU  | 1              |
| 3   | C     | 167 | ASN  | 1              |
| 3   | C     | 279 | ASP  | 1              |
| 2   | B     | 43  | LEU  | 1              |
| 3   | C     | 247 | VAL  | 1              |
| 2   | B     | 22  | ASN  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 3   | C     | 300 | VAL  | 1              |
| 2   | B     | 85  | ARG  | 1              |
| 3   | C     | 169 | ASP  | 1              |
| 3   | C     | 262 | PHE  | 1              |
| 3   | C     | 212 | SER  | 1              |
| 3   | C     | 258 | GLU  | 1              |
| 3   | C     | 170 | THR  | 1              |
| 3   | C     | 184 | THR  | 1              |
| 3   | C     | 303 | ASN  | 1              |
| 3   | C     | 187 | ASP  | 1              |
| 2   | B     | 29  | TYR  | 1              |
| 2   | B     | 87  | LEU  | 1              |
| 2   | B     | 75  | ARG  | 1              |
| 3   | C     | 317 | ARG  | 1              |
| 2   | B     | 39  | GLU  | 1              |
| 3   | C     | 290 | THR  | 1              |
| 2   | B     | 53  | ILE  | 1              |
| 2   | B     | 92  | LEU  | 1              |
| 3   | C     | 302 | GLN  | 1              |
| 3   | C     | 261 | GLU  | 1              |
| 3   | C     | 160 | LYS  | 1              |
| 3   | C     | 306 | ILE  | 1              |
| 3   | C     | 270 | ILE  | 1              |
| 2   | B     | 95  | ARG  | 1              |
| 3   | C     | 198 | ARG  | 1              |
| 3   | C     | 256 | PRO  | 1              |
| 3   | C     | 301 | CYS  | 1              |

### 5.2.3 RNA ⓘ

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers | Suiteness |
|-----|-------|---------------|-------------------|-----------------|-----------|
| 1   | A     | 12/13 (92%)   | 6±1 (46±11%)      | 1±1 (8±8%)      | 0.25±0.07 |
| All | All   | 120/130 (92%) | 55 (46%)          | 9 (8%)          | 0.25      |

The overall RNA backbone suiteness is 0.25.

All unique RNA backbone outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 3   | U    | 8              |
| 1   | A     | 13  | U    | 7              |
| 1   | A     | 4   | A    | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 10  | U    | 6              |
| 1   | A     | 12  | A    | 6              |
| 1   | A     | 9   | A    | 5              |
| 1   | A     | 6   | A    | 5              |
| 1   | A     | 2   | A    | 5              |
| 1   | A     | 11  | A    | 3              |
| 1   | A     | 7   | U    | 3              |
| 1   | A     | 5   | U    | 1              |

All unique RNA pucker outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 5   | U    | 3              |
| 1   | A     | 6   | A    | 3              |
| 1   | A     | 10  | U    | 3              |

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

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

### 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.5 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.6 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.



## 6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 25% for the well-defined parts and 25% for the entire structure.

### 6.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 6.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

|   |     |
|---|-----|
| Total number of shifts                  | 922 |
| Number of shifts mapped to atoms        | 922 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 1   |

#### 6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 80       | $-0.13 \pm 0.14$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 65       | $0.10 \pm 0.15$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 77       | $-0.38 \pm 0.22$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 78       | $0.60 \pm 0.76$                 | None needed (imprecise)    |

#### 6.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 25%, i.e. 812 atoms were assigned a chemical shift out of a possible 3265. 9 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 387/1198 (32%) | 158/477 (33%) | 153/488 (31%)   | 76/233 (33%)    |
| Sidechain | 392/1583 (25%) | 264/933 (28%) | 119/568 (21%)   | 9/82 (11%)      |

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|          | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 33/249 (13%)   | 33/133 (25%)   | 0/112 (0%)      | 0/4 (0%)        |
| Overall  | 812/3265 (25%) | 455/1674 (27%) | 272/1259 (22%)  | 85/332 (26%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 25%, i.e. 831 atoms were assigned a chemical shift out of a possible 3366. 9 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 397/1231 (32%) | 162/490 (33%)  | 157/502 (31%)   | 78/239 (33%)    |
| Sidechain | 401/1643 (24%) | 270/970 (28%)  | 121/586 (21%)   | 10/87 (11%)     |
| Aromatic  | 33/257 (13%)   | 33/137 (24%)   | 0/114 (0%)      | 0/6 (0%)        |
| Overall   | 831/3366 (25%) | 465/1728 (27%) | 278/1293 (22%)  | 88/345 (26%)    |

#### 6.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| Mol | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|-----|-------|-----|------|------|------------|---------------------|---------|
| 2   | B     | 23  | PRO  | HA   | 1.69       | 6.05 – 2.75         | -8.2    |

#### 6.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:

