



Full wwPDB NMR Structure Validation Report ⓘ

May 7, 2024 – 02:34 pm BST

PDB ID : 1DZ5
Title : The NMR structure of the 38KDa U1A protein-PIE RNA complex reveals the basis of cooperativity in regulation of polyadenylation by human U1A protein
Authors : Varani, L.; Gunderson, S.I.; Mattaj, I.W.; Kay, L.E.; Neuhaus, D.; Varani, G.
Deposited on : 2000-02-16

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

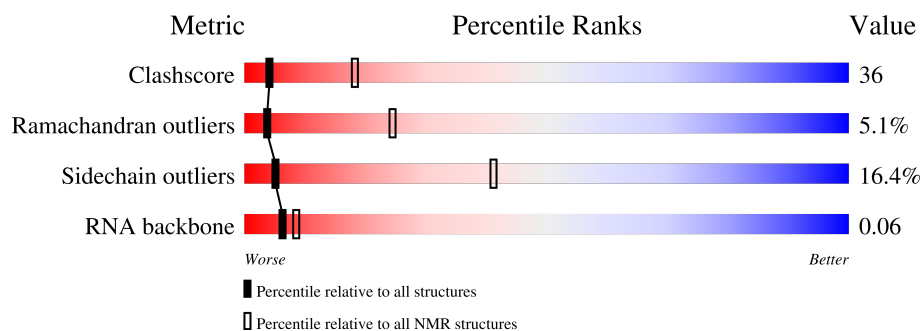
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 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 ≥ 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 | 101 | |
| 1 | B | 101 | |
| 2 | C | 22 | |
| 2 | D | 22 | |

2 Ensemble composition and analysis ⓘ

This entry contains 13 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 1 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|----------------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:6-A:101, B:6-B:101 (192) | 1.36 | 1 |

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4742 atoms, of which 2182 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | A | 101 | Total | C | H | N | O | S | 0 |
| | | | 1666 | 524 | 851 | 143 | 144 | 4 | |
| 1 | B | 101 | Total | C | H | N | O | S | 0 |
| | | | 1666 | 524 | 851 | 143 | 144 | 4 | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 30 | HIS | TYR | engineered mutation | UNP P09012 |
| A | 35 | ARG | GLN | engineered mutation | UNP P09012 |
| B | 30 | HIS | TYR | engineered mutation | UNP P09012 |
| B | 35 | ARG | GLN | engineered mutation | UNP P09012 |

- Molecule 2 is a RNA chain called PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP*CP*GP*GP*AP*GP*UP*CP*UP*C)-3').

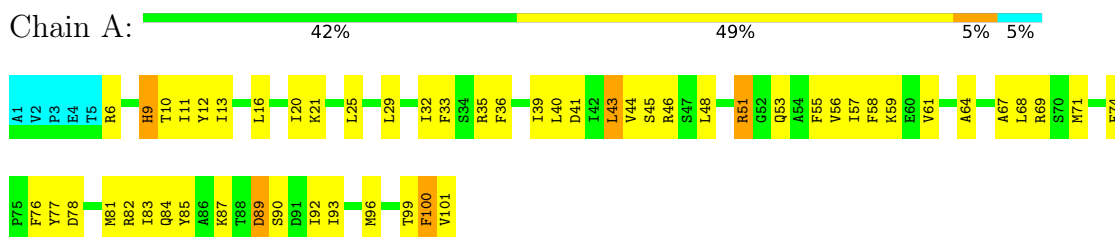
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|----|-------|
| 2 | C | 22 | Total | C | H | N | O | P | 0 |
| | | | 705 | 209 | 240 | 84 | 151 | 21 | |
| 2 | D | 22 | Total | C | H | N | O | P | 0 |
| | | | 705 | 209 | 240 | 84 | 151 | 21 | |

4 Residue-property plots [i](#)

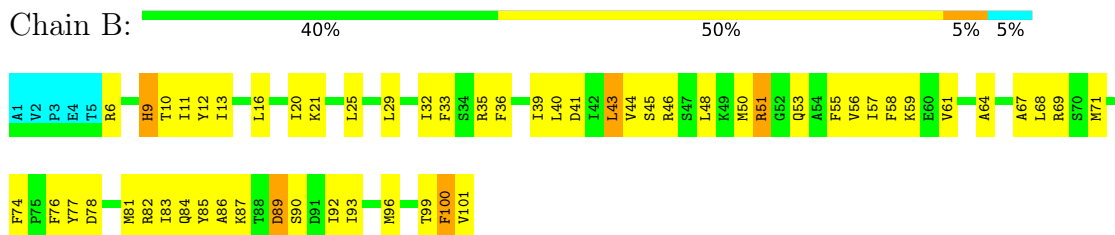
4.1 Average score per residue in the NMR ensemble

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

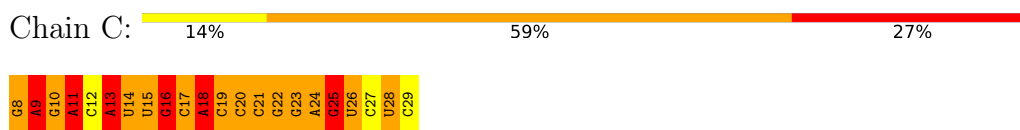
• Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



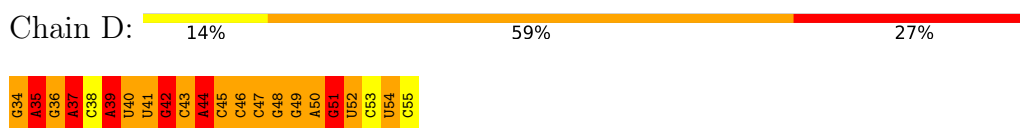
• Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



• Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')



• Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

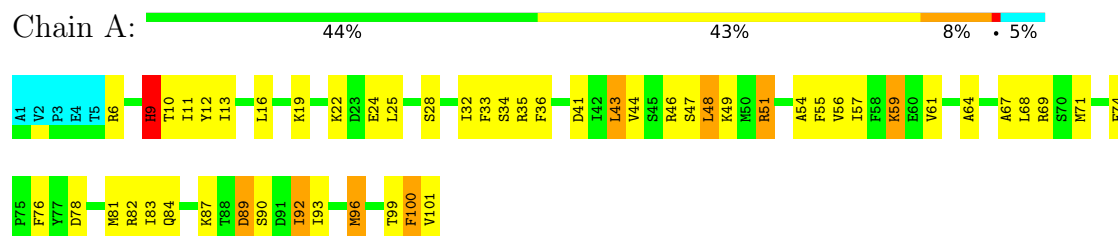


4.2 Scores per residue for each member of the ensemble

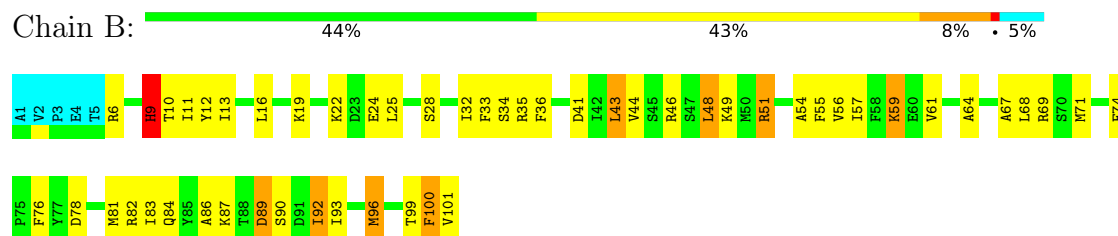
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')



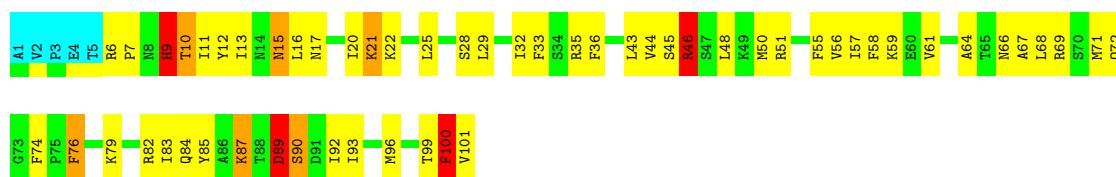
- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')



4.2.2 Score per residue for model 2

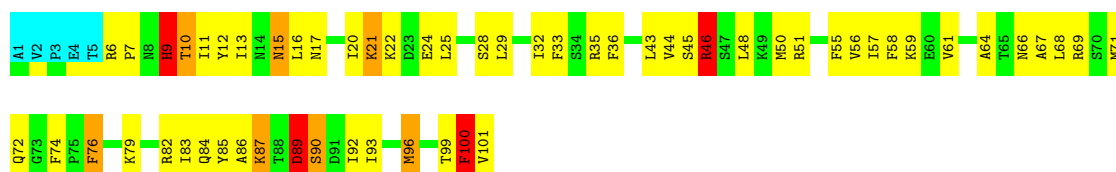
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A





- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain B: 38% 47% 7% 5%



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

Chain C: 18% 36% 45%



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

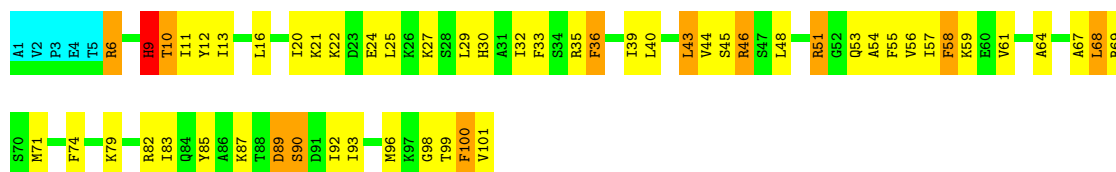
Chain D: 18% 36% 45%



4.2.3 Score per residue for model 3

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain A: 41% 43% 11% 5%



- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain B: 42% 42% 11% 5%





- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')



4.2.4 Score per residue for model 4

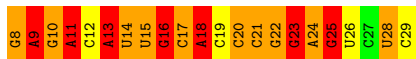
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

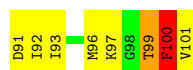
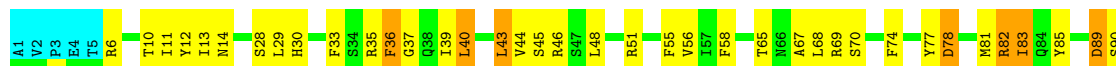
Chain D:  5% 18% 45% 32%



4.2.5 Score per residue for model 5

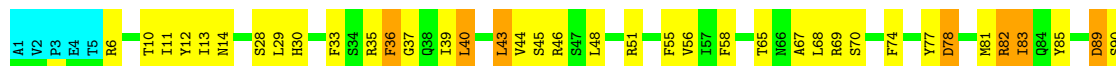
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain A:  50% 37% 8% • 5%



- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain B:  50% 37% 8% • 5%




- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

Chain C:  27% 32% 41%



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

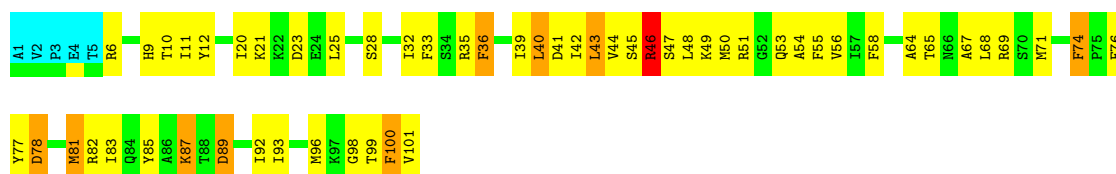
Chain D:  27% 32% 41%



4.2.6 Score per residue for model 6

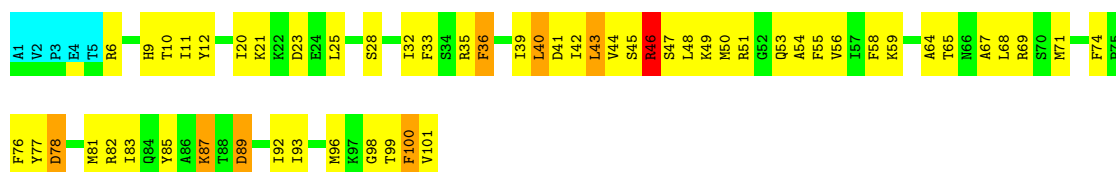
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain A:  41% 45% 9% • 5%



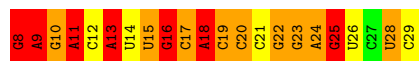
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain B: 40% 48% 7% 5%



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

Chain C: 5% 23% 41% 32%



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

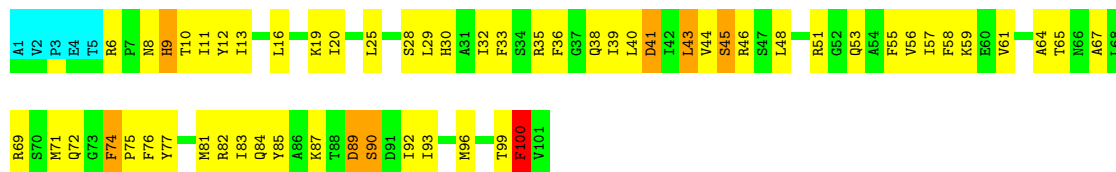
Chain D: 5% 23% 41% 32%



4.2.7 Score per residue for model 7

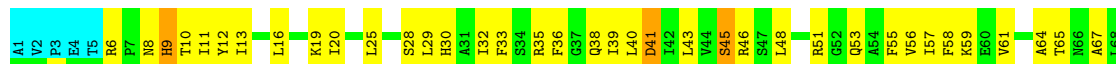
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

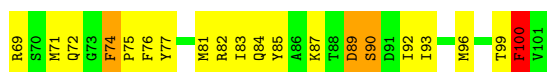
Chain A: 38% 50% 7% 5%



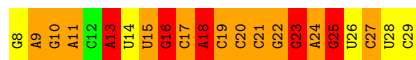
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain B: 39% 50% 6% 5%





- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

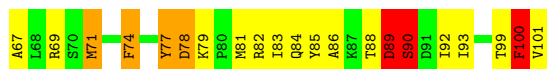


- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')



4.2.8 Score per residue for model 8

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

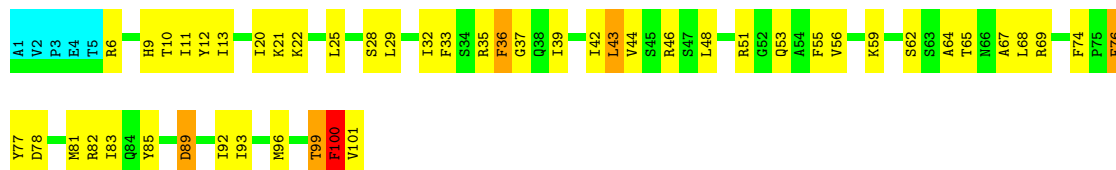
Chain D: 



4.2.9 Score per residue for model 9

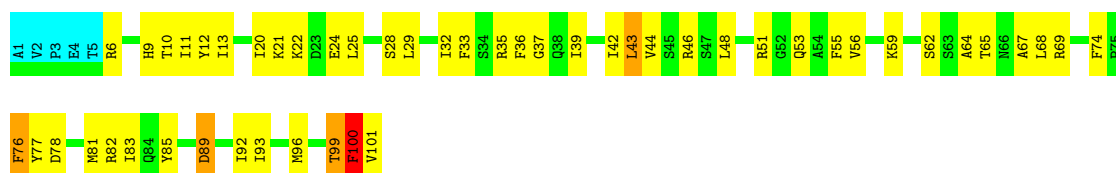
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain A: 




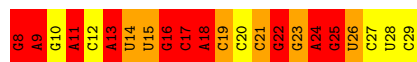
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain B: 



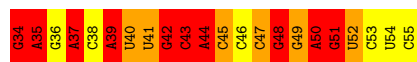
- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

Chain C: 



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

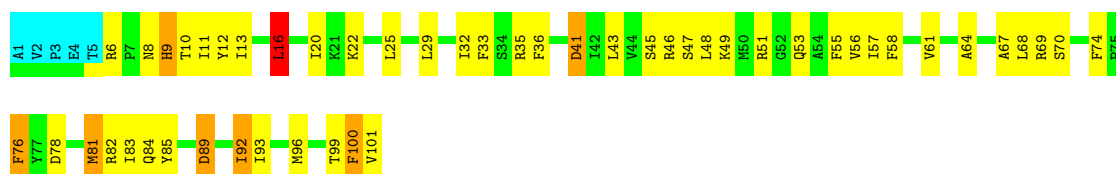
Chain D: 



4.2.10 Score per residue for model 10

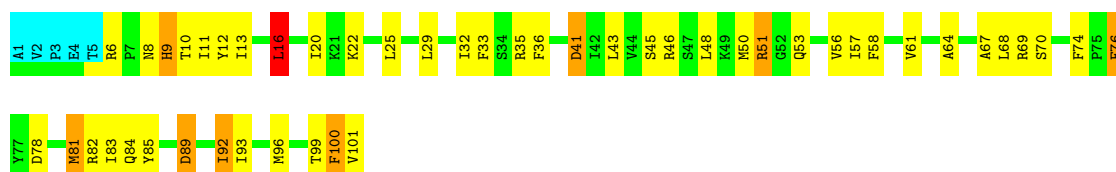
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain A: 



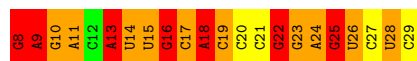
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain B: 48% 39% 8% 5%



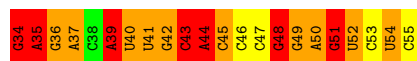
- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

Chain C: 5% 18% 45% 32%



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

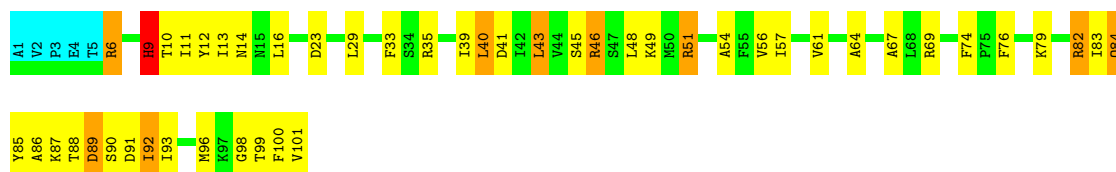
Chain D: 5% 18% 45% 32%



4.2.11 Score per residue for model 11

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain A: 48% 38% 9% 5%



- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain B: 46% 40% 9% 5%





- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

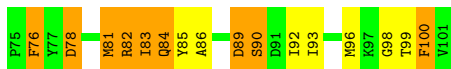
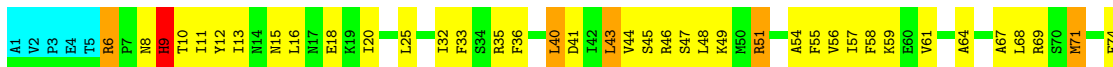


- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

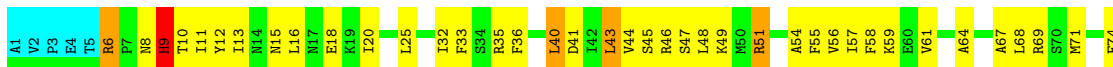


4.2.12 Score per residue for model 12

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

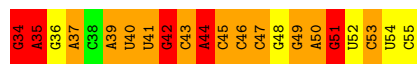


- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

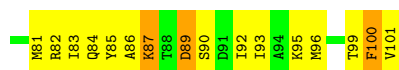
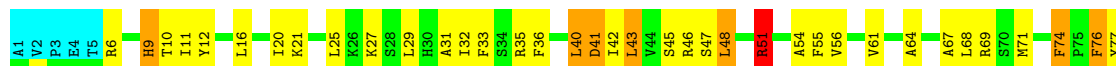
Chain D:  5% 23% 50% 23%



4.2.13 Score per residue for model 13

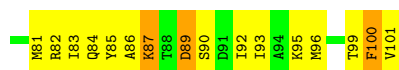
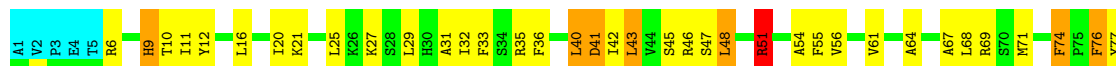
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain A:  43% 42% 10% 5%



- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain B:  43% 42% 10% 5%



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

Chain C:  5% 18% 45% 32%



- Molecule 2: PIE, RNA (5'-R(*GP*AP*GP*AP*CP*AP*UP*UP*GP*CP*AP*CP*CP* CP*G P*GP*AP*GP*UP*CP*UP*C)-3')

Chain D:  5% 18% 45% 32%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *RESTRAINED MOLECULAR DYNAMICS*.

Of the 50 calculated structures, 13 were deposited, based on the following criterion: *AGREEMENT WITH EXPERIMENTAL DATA*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| X-PLOR | refinement | 3.8.1 |
| X-PLOR | structure solution | 3.8.1 |

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------------|-------------|-----------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.97±0.00 | 0±0/794 (0.0± 0.0%) | 0.79±0.00 | 0±0/1061 (0.0± 0.0%) |
| 1 | B | 0.97±0.00 | 0±0/794 (0.0± 0.0%) | 0.79±0.00 | 0±0/1061 (0.0± 0.0%) |
| 2 | C | 1.13±0.01 | 0±0/519 (0.0± 0.0%) | 1.94±0.01 | 27±1/807 (3.4± 0.1%) |
| 2 | D | 1.13±0.00 | 0±0/519 (0.0± 0.0%) | 1.94±0.01 | 27±1/807 (3.3± 0.2%) |
| All | All | 1.04 | 0/34138 (0.0%) | 1.41 | 701/48568 (1.4%) |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1 | A | 0.0±0.0 | 6.0±0.0 |
| 1 | B | 0.0±0.0 | 6.0±0.0 |
| All | All | 0 | 156 |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|----------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 10 | G | N7-C8-N9 | 9.28 | 117.74 | 113.10 | 7 | 13 |
| 2 | C | 16 | G | N7-C8-N9 | 9.28 | 117.74 | 113.10 | 11 | 13 |
| 2 | D | 42 | G | N7-C8-N9 | 9.27 | 117.73 | 113.10 | 5 | 13 |
| 2 | C | 25 | G | N7-C8-N9 | 9.26 | 117.73 | 113.10 | 10 | 13 |
| 2 | D | 48 | G | N7-C8-N9 | 9.23 | 117.72 | 113.10 | 13 | 13 |
| 2 | D | 51 | G | N7-C8-N9 | 9.22 | 117.71 | 113.10 | 13 | 13 |
| 2 | C | 22 | G | N7-C8-N9 | 9.21 | 117.70 | 113.10 | 9 | 13 |
| 2 | C | 8 | G | N7-C8-N9 | 9.18 | 117.69 | 113.10 | 10 | 13 |
| 2 | C | 23 | G | N7-C8-N9 | 9.18 | 117.69 | 113.10 | 10 | 13 |
| 2 | D | 34 | G | N7-C8-N9 | 9.16 | 117.68 | 113.10 | 3 | 13 |
| 2 | D | 49 | G | N7-C8-N9 | 9.16 | 117.68 | 113.10 | 3 | 13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | D | 36 | G | N7-C8-N9 | 9.16 | 117.68 | 113.10 | 5 | 13 |
| 2 | D | 44 | A | N7-C8-N9 | 7.96 | 117.78 | 113.80 | 11 | 13 |
| 2 | C | 18 | A | N7-C8-N9 | 7.81 | 117.70 | 113.80 | 11 | 13 |
| 2 | C | 9 | A | N7-C8-N9 | 7.61 | 117.61 | 113.80 | 7 | 13 |
| 2 | D | 39 | A | N7-C8-N9 | 7.56 | 117.58 | 113.80 | 13 | 13 |
| 2 | D | 50 | A | N7-C8-N9 | 7.53 | 117.56 | 113.80 | 9 | 13 |
| 2 | D | 37 | A | N7-C8-N9 | 7.53 | 117.56 | 113.80 | 6 | 13 |
| 2 | D | 35 | A | N7-C8-N9 | 7.52 | 117.56 | 113.80 | 8 | 13 |
| 2 | C | 13 | A | N7-C8-N9 | 7.52 | 117.56 | 113.80 | 4 | 13 |
| 2 | C | 24 | A | N7-C8-N9 | 7.51 | 117.56 | 113.80 | 11 | 13 |
| 2 | C | 11 | A | N7-C8-N9 | 7.51 | 117.55 | 113.80 | 4 | 13 |
| 2 | C | 10 | G | C8-N9-C4 | -6.93 | 103.63 | 106.40 | 7 | 13 |
| 2 | D | 42 | G | C8-N9-C4 | -6.87 | 103.65 | 106.40 | 5 | 13 |
| 2 | C | 8 | G | C8-N9-C4 | -6.81 | 103.68 | 106.40 | 7 | 13 |
| 2 | C | 22 | G | C8-N9-C4 | -6.81 | 103.68 | 106.40 | 10 | 13 |
| 2 | C | 25 | G | C8-N9-C4 | -6.80 | 103.68 | 106.40 | 10 | 13 |
| 2 | D | 51 | G | C8-N9-C4 | -6.79 | 103.69 | 106.40 | 8 | 13 |
| 2 | C | 16 | G | C8-N9-C4 | -6.76 | 103.69 | 106.40 | 1 | 13 |
| 2 | D | 48 | G | C8-N9-C4 | -6.72 | 103.71 | 106.40 | 13 | 13 |
| 2 | C | 23 | G | C8-N9-C4 | -6.71 | 103.72 | 106.40 | 7 | 13 |
| 2 | D | 36 | G | C8-N9-C4 | -6.71 | 103.72 | 106.40 | 12 | 13 |
| 2 | D | 34 | G | C8-N9-C4 | -6.70 | 103.72 | 106.40 | 11 | 13 |
| 2 | D | 49 | G | C8-N9-C4 | -6.70 | 103.72 | 106.40 | 8 | 13 |
| 2 | D | 43 | C | O4'-C1'-N1 | 6.00 | 113.00 | 108.20 | 8 | 4 |
| 2 | C | 17 | C | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 | 8 | 3 |
| 2 | D | 44 | A | C8-N9-C4 | -5.80 | 103.48 | 105.80 | 11 | 13 |
| 2 | C | 18 | A | C8-N9-C4 | -5.77 | 103.49 | 105.80 | 7 | 13 |
| 2 | C | 13 | A | C8-N9-C4 | -5.69 | 103.52 | 105.80 | 5 | 13 |
| 2 | D | 37 | A | C8-N9-C4 | -5.66 | 103.54 | 105.80 | 12 | 13 |
| 2 | D | 50 | A | C8-N9-C4 | -5.63 | 103.55 | 105.80 | 9 | 13 |
| 2 | D | 39 | A | C8-N9-C4 | -5.63 | 103.55 | 105.80 | 13 | 13 |
| 2 | C | 11 | A | C8-N9-C4 | -5.62 | 103.55 | 105.80 | 6 | 13 |
| 2 | C | 9 | A | C8-N9-C4 | -5.57 | 103.57 | 105.80 | 6 | 13 |
| 2 | C | 24 | A | C8-N9-C4 | -5.55 | 103.58 | 105.80 | 1 | 13 |
| 2 | D | 35 | A | C8-N9-C4 | -5.49 | 103.61 | 105.80 | 1 | 13 |
| 2 | C | 25 | G | C5-N7-C8 | -5.28 | 101.66 | 104.30 | 2 | 12 |
| 2 | D | 51 | G | C5-N7-C8 | -5.21 | 101.69 | 104.30 | 2 | 12 |
| 2 | D | 49 | G | C5-N7-C8 | -5.21 | 101.70 | 104.30 | 3 | 8 |
| 2 | D | 36 | G | C5-N7-C8 | -5.20 | 101.70 | 104.30 | 3 | 7 |
| 2 | D | 48 | G | C5-N7-C8 | -5.19 | 101.70 | 104.30 | 13 | 11 |
| 2 | C | 22 | G | C5-N7-C8 | -5.19 | 101.70 | 104.30 | 9 | 13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | D | 42 | G | C5-N7-C8 | -5.19 | 101.71 | 104.30 | 5 | 10 |
| 2 | C | 8 | G | C5-N7-C8 | -5.18 | 101.71 | 104.30 | 1 | 10 |
| 2 | D | 34 | G | C5-N7-C8 | -5.18 | 101.71 | 104.30 | 9 | 10 |
| 2 | C | 16 | G | C5-N7-C8 | -5.17 | 101.71 | 104.30 | 11 | 9 |
| 2 | C | 10 | G | C5-N7-C8 | -5.17 | 101.72 | 104.30 | 7 | 9 |
| 2 | C | 23 | G | C5-N7-C8 | -5.14 | 101.73 | 104.30 | 11 | 11 |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 6 | ARG | Sidechain | 13 |
| 1 | A | 35 | ARG | Sidechain | 13 |
| 1 | A | 46 | ARG | Sidechain | 13 |
| 1 | A | 51 | ARG | Sidechain | 13 |
| 1 | A | 69 | ARG | Sidechain | 13 |
| 1 | A | 82 | ARG | Sidechain | 13 |
| 1 | B | 6 | ARG | Sidechain | 13 |
| 1 | B | 35 | ARG | Sidechain | 13 |
| 1 | B | 46 | ARG | Sidechain | 13 |
| 1 | B | 51 | ARG | Sidechain | 13 |
| 1 | B | 69 | ARG | Sidechain | 13 |
| 1 | B | 82 | ARG | Sidechain | 13 |

6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 780 | 815 | 815 | 59±11 |
| 1 | B | 780 | 815 | 815 | 59±12 |
| 2 | C | 465 | 240 | 240 | 42±7 |
| 2 | D | 465 | 240 | 240 | 41±7 |
| All | All | 32370 | 27430 | 27430 | 2175 |

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 36.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:99:THR:HG21 | 1:B:99:THR:HG21 | 1.04 | 1.20 | 9 | 2 |
| 1:A:101:VAL:HG11 | 1:B:101:VAL:HG11 | 1.03 | 1.30 | 8 | 1 |
| 1:A:101:VAL:HG13 | 1:B:101:VAL:HG13 | 0.98 | 1.29 | 2 | 5 |
| 1:A:11:ILE:HD12 | 1:A:83:ILE:HG21 | 0.97 | 1.37 | 8 | 6 |
| 1:B:11:ILE:HD12 | 1:B:83:ILE:HG21 | 0.93 | 1.39 | 4 | 6 |
| 1:B:11:ILE:HG23 | 1:B:64:ALA:HB1 | 0.89 | 1.43 | 3 | 9 |
| 1:A:11:ILE:HG23 | 1:A:64:ALA:HB1 | 0.89 | 1.43 | 3 | 9 |
| 1:B:43:LEU:HD22 | 2:C:18:A:N3 | 0.86 | 1.85 | 13 | 9 |
| 1:A:13:ILE:HD13 | 1:A:29:LEU:HD22 | 0.86 | 1.48 | 11 | 4 |
| 1:A:43:LEU:HD22 | 2:D:44:A:N3 | 0.85 | 1.85 | 13 | 9 |
| 1:B:9:HIS:CE1 | 1:B:93:ILE:HG21 | 0.85 | 2.07 | 3 | 12 |
| 1:A:9:HIS:CE1 | 1:A:93:ILE:HG21 | 0.84 | 2.07 | 3 | 12 |
| 1:A:92:ILE:HD13 | 1:A:93:ILE:N | 0.83 | 1.88 | 1 | 3 |
| 1:A:92:ILE:HD12 | 1:A:93:ILE:N | 0.83 | 1.88 | 7 | 9 |
| 1:B:92:ILE:HD13 | 1:B:93:ILE:N | 0.83 | 1.88 | 1 | 3 |
| 1:B:92:ILE:HD12 | 1:B:93:ILE:N | 0.83 | 1.88 | 7 | 9 |
| 1:B:13:ILE:HD13 | 1:B:29:LEU:HD22 | 0.82 | 1.48 | 11 | 4 |
| 1:B:11:ILE:HD12 | 1:B:83:ILE:HG23 | 0.80 | 1.54 | 7 | 3 |
| 1:A:11:ILE:HD12 | 1:A:83:ILE:HG23 | 0.80 | 1.54 | 7 | 3 |
| 1:B:11:ILE:HD12 | 1:B:83:ILE:CG2 | 0.80 | 2.06 | 1 | 9 |
| 2:D:51:G:H3' | 2:D:51:G:OP1 | 0.79 | 1.78 | 1 | 5 |
| 1:B:48:LEU:HD12 | 2:D:51:G:O4' | 0.79 | 1.77 | 12 | 5 |
| 1:A:48:LEU:HD12 | 2:C:25:G:O4' | 0.79 | 1.77 | 12 | 5 |
| 1:B:16:LEU:HD13 | 1:B:25:LEU:HD21 | 0.79 | 1.54 | 1 | 3 |
| 1:A:99:THR:CG2 | 1:B:99:THR:HG21 | 0.79 | 2.06 | 9 | 2 |
| 1:A:11:ILE:HD12 | 1:A:83:ILE:CG2 | 0.79 | 2.06 | 1 | 9 |
| 1:A:11:ILE:HD13 | 1:A:83:ILE:HG23 | 0.79 | 1.55 | 3 | 2 |
| 2:C:25:G:H3' | 2:C:25:G:OP1 | 0.79 | 1.77 | 1 | 5 |
| 1:B:11:ILE:HD13 | 1:B:83:ILE:HG23 | 0.78 | 1.55 | 3 | 2 |
| 1:A:99:THR:HG21 | 1:B:99:THR:CG2 | 0.78 | 2.06 | 9 | 2 |
| 1:A:16:LEU:HD13 | 1:A:25:LEU:HD21 | 0.78 | 1.54 | 1 | 3 |
| 2:C:8:G:O2' | 2:C:9:A:H5' | 0.78 | 1.78 | 2 | 9 |
| 1:A:32:ILE:HD12 | 1:A:76:PHE:CZ | 0.78 | 2.14 | 10 | 2 |
| 1:A:33:PHE:CG | 1:A:56:VAL:HG21 | 0.78 | 2.14 | 4 | 1 |
| 1:B:33:PHE:CG | 1:B:56:VAL:HG21 | 0.78 | 2.14 | 4 | 1 |
| 1:A:11:ILE:HG21 | 1:A:67:ALA:HB3 | 0.77 | 1.56 | 12 | 1 |
| 1:B:32:ILE:HD12 | 1:B:76:PHE:CZ | 0.77 | 2.14 | 10 | 3 |
| 1:B:9:HIS:NE2 | 1:B:93:ILE:HG21 | 0.77 | 1.94 | 4 | 3 |
| 1:A:9:HIS:NE2 | 1:A:93:ILE:HG21 | 0.77 | 1.94 | 4 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:D:34:G:O2' | 2:D:35:A:H5' | 0.77 | 1.79 | 2 | 9 |
| 1:A:101:VAL:CG1 | 1:B:101:VAL:HG11 | 0.77 | 2.08 | 8 | 1 |
| 1:A:32:ILE:HD11 | 1:A:76:PHE:CZ | 0.76 | 2.16 | 2 | 1 |
| 1:B:32:ILE:HD11 | 1:B:76:PHE:CZ | 0.76 | 2.16 | 2 | 1 |
| 1:A:65:THR:HG23 | 1:A:85:TYR:OH | 0.76 | 1.81 | 4 | 4 |
| 1:B:65:THR:HG23 | 1:B:85:TYR:OH | 0.75 | 1.81 | 4 | 4 |
| 1:A:101:VAL:HG11 | 1:B:101:VAL:CG1 | 0.75 | 2.08 | 8 | 1 |
| 2:C:16:G:H3' | 2:C:17:C:O2 | 0.75 | 1.81 | 8 | 1 |
| 1:B:11:ILE:HG21 | 1:B:67:ALA:HB3 | 0.75 | 1.56 | 12 | 1 |
| 1:B:13:ILE:HG12 | 1:B:83:ILE:HD12 | 0.75 | 1.59 | 12 | 1 |
| 2:C:23:G:O2' | 2:C:24:A:H5' | 0.75 | 1.82 | 12 | 10 |
| 2:D:42:G:H3' | 2:D:43:C:O2 | 0.75 | 1.81 | 8 | 1 |
| 1:A:13:ILE:HG12 | 1:A:83:ILE:HD12 | 0.74 | 1.59 | 12 | 1 |
| 2:D:49:G:O2' | 2:D:50:A:H5' | 0.74 | 1.82 | 12 | 10 |
| 1:A:10:THR:HG21 | 2:D:44:A:H61 | 0.74 | 1.43 | 6 | 2 |
| 1:B:43:LEU:HD21 | 2:C:19:C:O4' | 0.73 | 1.83 | 13 | 4 |
| 2:C:26:U:O2' | 2:C:27:C:H5' | 0.73 | 1.83 | 1 | 4 |
| 1:A:101:VAL:HG21 | 1:B:101:VAL:HG21 | 0.73 | 1.59 | 13 | 1 |
| 1:A:11:ILE:CD1 | 1:A:83:ILE:HG21 | 0.73 | 2.11 | 8 | 4 |
| 2:C:15:U:H4' | 2:C:16:G:O5' | 0.73 | 1.83 | 9 | 1 |
| 1:B:11:ILE:CD1 | 1:B:83:ILE:HG21 | 0.73 | 2.12 | 8 | 4 |
| 2:D:41:U:H4' | 2:D:42:G:O5' | 0.73 | 1.83 | 9 | 1 |
| 1:A:43:LEU:HD21 | 2:D:45:C:O4' | 0.73 | 1.83 | 13 | 4 |
| 1:B:10:THR:HG21 | 2:C:18:A:H61 | 0.72 | 1.44 | 6 | 2 |
| 1:B:10:THR:CG2 | 1:B:86:ALA:HB3 | 0.72 | 2.15 | 12 | 1 |
| 1:A:92:ILE:HD12 | 1:A:93:ILE:HD13 | 0.72 | 1.62 | 9 | 3 |
| 1:B:92:ILE:HD12 | 1:B:93:ILE:HD13 | 0.72 | 1.62 | 9 | 3 |
| 2:D:52:U:O2' | 2:D:53:C:H5' | 0.72 | 1.83 | 1 | 4 |
| 1:A:13:ILE:HD11 | 1:A:33:PHE:CE2 | 0.72 | 2.20 | 1 | 5 |
| 1:B:68:LEU:HD13 | 1:B:85:TYR:CE2 | 0.72 | 2.20 | 13 | 3 |
| 1:B:13:ILE:HD11 | 1:B:33:PHE:CE2 | 0.71 | 2.20 | 1 | 5 |
| 1:A:20:ILE:HD13 | 1:A:25:LEU:HD21 | 0.71 | 1.63 | 2 | 1 |
| 1:A:10:THR:CG2 | 1:A:86:ALA:HB3 | 0.71 | 2.15 | 12 | 1 |
| 1:A:20:ILE:HD13 | 1:A:25:LEU:HD11 | 0.71 | 1.61 | 6 | 2 |
| 1:A:68:LEU:HD13 | 1:A:85:TYR:CE2 | 0.71 | 2.20 | 13 | 3 |
| 2:D:46:C:H2' | 2:D:47:C:O4' | 0.71 | 1.86 | 3 | 9 |
| 1:B:20:ILE:HD13 | 1:B:25:LEU:HD11 | 0.71 | 1.61 | 6 | 2 |
| 2:C:20:C:H2' | 2:C:21:C:O4' | 0.70 | 1.87 | 3 | 8 |
| 2:C:18:A:O2' | 2:C:19:C:H5' | 0.70 | 1.86 | 4 | 2 |
| 1:B:10:THR:HG22 | 1:B:89:ASP:HB2 | 0.70 | 1.62 | 5 | 4 |
| 1:A:40:LEU:HD11 | 1:B:98:GLY:O | 0.70 | 1.86 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:68:LEU:HD13 | 1:A:85:TYR:CD2 | 0.70 | 2.22 | 13 | 2 |
| 1:A:10:THR:HG22 | 1:A:89:ASP:HB2 | 0.70 | 1.62 | 5 | 4 |
| 2:D:44:A:O2' | 2:D:45:C:H5' | 0.69 | 1.86 | 4 | 2 |
| 1:B:10:THR:HG21 | 1:B:57:ILE:HD13 | 0.69 | 1.65 | 2 | 3 |
| 1:B:68:LEU:HD13 | 1:B:85:TYR:CD2 | 0.69 | 2.21 | 13 | 2 |
| 1:B:99:THR:CG2 | 1:B:101:VAL:HG13 | 0.69 | 2.17 | 10 | 1 |
| 1:B:8:ASN:C | 1:B:61:VAL:HG22 | 0.69 | 2.08 | 10 | 3 |
| 1:A:10:THR:HG21 | 1:A:57:ILE:HD13 | 0.69 | 1.65 | 2 | 3 |
| 1:A:48:LEU:HD23 | 1:A:48:LEU:O | 0.69 | 1.88 | 12 | 4 |
| 1:A:13:ILE:HG23 | 1:A:82:ARG:O | 0.69 | 1.88 | 12 | 1 |
| 1:B:13:ILE:CD1 | 1:B:29:LEU:HD22 | 0.68 | 2.18 | 5 | 6 |
| 1:A:99:THR:CG2 | 1:A:101:VAL:HG13 | 0.68 | 2.17 | 10 | 1 |
| 1:B:13:ILE:CG1 | 1:B:83:ILE:HD12 | 0.68 | 2.19 | 12 | 1 |
| 1:B:20:ILE:HD13 | 1:B:25:LEU:HD21 | 0.68 | 1.63 | 2 | 1 |
| 1:B:13:ILE:HG23 | 1:B:82:ARG:O | 0.68 | 1.88 | 12 | 1 |
| 1:A:11:ILE:HG23 | 1:A:64:ALA:CB | 0.68 | 2.18 | 2 | 1 |
| 1:A:8:ASN:C | 1:A:61:VAL:HG22 | 0.68 | 2.08 | 10 | 3 |
| 1:A:13:ILE:CG1 | 1:A:83:ILE:HD12 | 0.68 | 2.19 | 12 | 1 |
| 1:B:48:LEU:O | 1:B:48:LEU:HD23 | 0.68 | 1.88 | 12 | 4 |
| 1:B:20:ILE:HD13 | 1:B:25:LEU:CD1 | 0.68 | 2.19 | 6 | 2 |
| 1:A:11:ILE:HD11 | 1:A:33:PHE:CE1 | 0.68 | 2.23 | 10 | 8 |
| 1:B:11:ILE:HD11 | 1:B:33:PHE:CE1 | 0.67 | 2.23 | 10 | 8 |
| 1:A:13:ILE:CD1 | 1:A:29:LEU:HD22 | 0.67 | 2.18 | 5 | 6 |
| 1:B:11:ILE:HG23 | 1:B:64:ALA:CB | 0.67 | 2.18 | 2 | 1 |
| 1:A:98:GLY:O | 1:B:40:LEU:HD11 | 0.67 | 1.89 | 6 | 1 |
| 1:A:20:ILE:HD13 | 1:A:25:LEU:CD1 | 0.67 | 2.19 | 6 | 2 |
| 1:A:86:ALA:HB1 | 2:D:44:A:N6 | 0.67 | 2.04 | 12 | 1 |
| 1:A:11:ILE:HD11 | 1:A:33:PHE:CE2 | 0.67 | 2.24 | 8 | 2 |
| 1:B:11:ILE:HD11 | 1:B:33:PHE:CE2 | 0.67 | 2.24 | 8 | 2 |
| 1:B:42:ILE:CD1 | 1:B:56:VAL:HG13 | 0.67 | 2.19 | 9 | 1 |
| 1:A:33:PHE:CE2 | 1:A:83:ILE:HD11 | 0.67 | 2.25 | 12 | 1 |
| 1:B:33:PHE:CE2 | 1:B:67:ALA:HB1 | 0.66 | 2.24 | 12 | 3 |
| 1:A:10:THR:HG22 | 1:A:89:ASP:CB | 0.66 | 2.20 | 5 | 4 |
| 1:B:10:THR:HG22 | 1:B:89:ASP:CB | 0.66 | 2.20 | 5 | 4 |
| 1:A:33:PHE:CE2 | 1:A:67:ALA:HB1 | 0.66 | 2.24 | 12 | 3 |
| 1:A:99:THR:OG1 | 1:B:40:LEU:HD21 | 0.66 | 1.90 | 13 | 1 |
| 1:B:90:SER:CB | 1:B:93:ILE:HD12 | 0.66 | 2.21 | 8 | 2 |
| 2:D:38:C:H2' | 2:D:39:A:O4' | 0.66 | 1.91 | 2 | 1 |
| 1:A:42:ILE:CD1 | 1:A:56:VAL:HG13 | 0.66 | 2.19 | 9 | 1 |
| 2:C:12:C:H2' | 2:C:13:A:O4' | 0.66 | 1.90 | 2 | 1 |
| 1:B:20:ILE:HG21 | 1:B:25:LEU:HD12 | 0.66 | 1.68 | 10 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:33:PHE:CE2 | 1:B:83:ILE:HD11 | 0.66 | 2.25 | 12 | 1 |
| 1:A:90:SER:CB | 1:A:93:ILE:HD12 | 0.65 | 2.21 | 8 | 2 |
| 1:B:86:ALA:HB1 | 2:C:18:A:N6 | 0.65 | 2.05 | 12 | 1 |
| 1:A:20:ILE:HB | 1:A:25:LEU:HD13 | 0.65 | 1.68 | 3 | 2 |
| 1:A:100:PHE:CD1 | 1:B:99:THR:HG23 | 0.65 | 2.27 | 13 | 1 |
| 1:B:48:LEU:HD23 | 2:D:51:G:C8 | 0.65 | 2.27 | 13 | 4 |
| 1:A:11:ILE:HD12 | 1:A:12:TYR:N | 0.65 | 2.07 | 3 | 1 |
| 1:A:47:SER:OG | 2:C:24:A:H2' | 0.65 | 1.91 | 6 | 5 |
| 1:B:11:ILE:HD13 | 1:B:83:ILE:CG2 | 0.65 | 2.22 | 3 | 3 |
| 1:B:41:ASP:CB | 1:B:57:ILE:HD12 | 0.65 | 2.22 | 7 | 2 |
| 1:A:32:ILE:HD11 | 1:A:76:PHE:CE2 | 0.65 | 2.26 | 2 | 1 |
| 1:B:20:ILE:HB | 1:B:25:LEU:HD13 | 0.65 | 1.68 | 3 | 2 |
| 1:B:92:ILE:CD1 | 1:B:93:ILE:HD13 | 0.64 | 2.22 | 9 | 6 |
| 1:A:68:LEU:HD22 | 1:A:85:TYR:OH | 0.64 | 1.92 | 12 | 1 |
| 2:C:20:C:H6 | 2:C:20:C:O5' | 0.64 | 1.75 | 6 | 7 |
| 1:A:11:ILE:HD13 | 1:A:83:ILE:CG2 | 0.64 | 2.22 | 3 | 3 |
| 1:A:8:ASN:O | 1:A:61:VAL:HG13 | 0.64 | 1.93 | 7 | 1 |
| 1:B:11:ILE:HD12 | 1:B:12:TYR:N | 0.64 | 2.07 | 3 | 1 |
| 1:A:41:ASP:CB | 1:A:57:ILE:HD12 | 0.64 | 2.22 | 7 | 2 |
| 1:B:68:LEU:HD22 | 1:B:85:TYR:OH | 0.64 | 1.92 | 12 | 1 |
| 1:B:32:ILE:HD11 | 1:B:76:PHE:CE2 | 0.64 | 2.26 | 2 | 1 |
| 2:D:49:G:H2' | 2:D:50:A:O4' | 0.64 | 1.93 | 5 | 1 |
| 1:A:92:ILE:CD1 | 1:A:93:ILE:HD13 | 0.64 | 2.22 | 9 | 6 |
| 2:D:46:C:H6 | 2:D:46:C:O5' | 0.64 | 1.76 | 1 | 7 |
| 1:A:48:LEU:HD23 | 2:C:25:G:C8 | 0.64 | 2.27 | 13 | 4 |
| 2:D:37:A:O2' | 2:D:38:C:H5' | 0.64 | 1.93 | 4 | 2 |
| 1:B:8:ASN:O | 1:B:61:VAL:HG13 | 0.64 | 1.93 | 7 | 1 |
| 1:A:16:LEU:HD13 | 1:A:25:LEU:CD2 | 0.64 | 2.22 | 1 | 2 |
| 1:A:40:LEU:HD21 | 1:B:99:THR:OG1 | 0.64 | 1.92 | 13 | 1 |
| 1:B:16:LEU:HD13 | 1:B:25:LEU:CD2 | 0.63 | 2.22 | 1 | 3 |
| 2:C:11:A:O2' | 2:C:12:C:H5' | 0.63 | 1.93 | 4 | 2 |
| 1:B:48:LEU:HD13 | 1:B:48:LEU:O | 0.63 | 1.93 | 13 | 4 |
| 1:A:20:ILE:HG21 | 1:A:25:LEU:HD12 | 0.63 | 1.67 | 10 | 2 |
| 1:A:48:LEU:HD13 | 1:A:48:LEU:O | 0.63 | 1.93 | 13 | 2 |
| 1:B:33:PHE:CD2 | 1:B:67:ALA:HB1 | 0.63 | 2.29 | 9 | 2 |
| 1:A:99:THR:HG23 | 1:B:100:PHE:CD1 | 0.63 | 2.28 | 13 | 1 |
| 1:B:47:SER:OG | 2:D:50:A:H2' | 0.63 | 1.94 | 6 | 4 |
| 1:A:33:PHE:CD2 | 1:A:67:ALA:HB1 | 0.63 | 2.29 | 9 | 2 |
| 2:C:23:G:H2' | 2:C:24:A:O4' | 0.63 | 1.93 | 5 | 1 |
| 1:B:90:SER:HB3 | 1:B:93:ILE:HD12 | 0.62 | 1.72 | 8 | 3 |
| 1:A:43:LEU:HD22 | 2:D:44:A:C2 | 0.62 | 2.30 | 5 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:D:47:C:H6 | 2:D:47:C:O5' | 0.62 | 1.78 | 9 | 12 |
| 1:A:33:PHE:CB | 1:A:56:VAL:HG11 | 0.62 | 2.25 | 12 | 3 |
| 1:B:53:GLN:OE1 | 2:C:16:G:H2' | 0.62 | 1.95 | 6 | 2 |
| 2:C:29:C:H6 | 2:C:29:C:O5' | 0.61 | 1.78 | 6 | 13 |
| 2:D:55:C:H6 | 2:D:55:C:O5' | 0.61 | 1.78 | 3 | 13 |
| 1:A:53:GLN:OE1 | 2:D:42:G:H2' | 0.61 | 1.95 | 6 | 2 |
| 1:B:41:ASP:O | 1:B:57:ILE:HD12 | 0.61 | 1.95 | 10 | 1 |
| 2:D:40:U:H6 | 2:D:40:U:O5' | 0.61 | 1.79 | 13 | 2 |
| 1:B:43:LEU:HD22 | 2:C:18:A:C2 | 0.61 | 2.30 | 5 | 2 |
| 1:A:33:PHE:CB | 1:A:39:ILE:HD11 | 0.61 | 2.26 | 4 | 4 |
| 1:A:16:LEU:HD21 | 1:A:29:LEU:HD21 | 0.61 | 1.73 | 11 | 3 |
| 1:A:33:PHE:CE1 | 1:A:67:ALA:HB1 | 0.61 | 2.31 | 6 | 8 |
| 1:B:33:PHE:CB | 1:B:56:VAL:HG11 | 0.61 | 2.25 | 12 | 3 |
| 1:A:41:ASP:O | 1:A:57:ILE:HD12 | 0.61 | 1.95 | 10 | 1 |
| 2:C:21:C:H6 | 2:C:21:C:O5' | 0.61 | 1.79 | 8 | 12 |
| 1:A:90:SER:HB3 | 1:A:93:ILE:HD12 | 0.61 | 1.72 | 8 | 3 |
| 1:A:68:LEU:HD13 | 1:A:85:TYR:CZ | 0.61 | 2.31 | 12 | 4 |
| 2:C:14:U:H6 | 2:C:14:U:O5' | 0.60 | 1.79 | 13 | 5 |
| 2:D:40:U:H4' | 2:D:41:U:OP1 | 0.60 | 1.96 | 4 | 1 |
| 2:C:22:G:O2' | 2:C:23:G:H5' | 0.60 | 1.96 | 5 | 1 |
| 1:B:100:PHE:CG | 1:B:100:PHE:O | 0.60 | 2.55 | 10 | 3 |
| 1:B:33:PHE:CE1 | 1:B:67:ALA:HB1 | 0.60 | 2.30 | 11 | 8 |
| 1:A:68:LEU:HD22 | 1:A:83:ILE:CG2 | 0.60 | 2.26 | 3 | 1 |
| 1:A:33:PHE:CD1 | 1:A:67:ALA:HB1 | 0.60 | 2.32 | 10 | 8 |
| 1:B:68:LEU:HD13 | 1:B:85:TYR:CZ | 0.60 | 2.31 | 12 | 4 |
| 1:B:68:LEU:HD22 | 1:B:83:ILE:CG2 | 0.60 | 2.26 | 3 | 1 |
| 1:B:33:PHE:CB | 1:B:39:ILE:HD11 | 0.60 | 2.26 | 4 | 4 |
| 1:B:33:PHE:CD1 | 1:B:67:ALA:HB1 | 0.60 | 2.31 | 10 | 8 |
| 1:B:10:THR:HG23 | 1:B:11:ILE:N | 0.60 | 2.12 | 2 | 8 |
| 2:C:26:U:H6 | 2:C:26:U:O5' | 0.60 | 1.79 | 3 | 4 |
| 1:A:100:PHE:CG | 1:A:100:PHE:O | 0.60 | 2.55 | 10 | 2 |
| 1:B:16:LEU:HD21 | 1:B:29:LEU:HD21 | 0.59 | 1.73 | 11 | 3 |
| 1:A:99:THR:HG22 | 1:B:96:MET:HE1 | 0.59 | 1.74 | 13 | 1 |
| 2:D:52:U:H6 | 2:D:52:U:O5' | 0.59 | 1.79 | 3 | 3 |
| 2:C:14:U:H4' | 2:C:15:U:OP1 | 0.59 | 1.96 | 4 | 1 |
| 1:A:10:THR:HG21 | 2:D:44:A:N6 | 0.59 | 2.12 | 6 | 2 |
| 1:A:11:ILE:HD11 | 1:A:33:PHE:CZ | 0.59 | 2.33 | 13 | 3 |
| 1:B:33:PHE:CG | 1:B:56:VAL:HG11 | 0.59 | 2.32 | 2 | 3 |
| 1:B:48:LEU:HD12 | 2:D:51:G:C1' | 0.59 | 2.28 | 2 | 1 |
| 1:A:10:THR:HA | 1:A:64:ALA:HB2 | 0.59 | 1.74 | 13 | 5 |
| 2:D:48:G:O2' | 2:D:49:G:H5' | 0.59 | 1.97 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:11:ILE:HD11 | 1:B:33:PHE:CZ | 0.59 | 2.33 | 13 | 3 |
| 1:A:33:PHE:CG | 1:A:56:VAL:HG11 | 0.59 | 2.32 | 2 | 3 |
| 1:A:101:VAL:HG11 | 1:B:101:VAL:HG21 | 0.58 | 1.74 | 13 | 1 |
| 2:C:15:U:H1' | 2:C:16:G:OP2 | 0.58 | 1.99 | 9 | 2 |
| 1:B:39:ILE:HD11 | 1:B:56:VAL:HB | 0.58 | 1.75 | 7 | 1 |
| 1:A:16:LEU:HD12 | 1:A:53:GLN:C | 0.58 | 2.19 | 3 | 1 |
| 2:D:43:C:H4' | 2:D:44:A:O4' | 0.58 | 1.99 | 8 | 1 |
| 1:A:68:LEU:HA | 1:A:83:ILE:HG21 | 0.58 | 1.76 | 9 | 2 |
| 2:D:41:U:H1' | 2:D:42:G:OP1 | 0.58 | 1.98 | 11 | 2 |
| 1:A:48:LEU:HD12 | 2:C:25:G:C1' | 0.58 | 2.29 | 2 | 1 |
| 1:A:71:MET:HB2 | 1:A:83:ILE:HD11 | 0.58 | 1.76 | 3 | 2 |
| 2:C:17:C:O3' | 2:C:18:A:H8 | 0.58 | 1.82 | 4 | 5 |
| 1:B:49:LYS:O | 2:C:16:G:H2' | 0.58 | 1.99 | 11 | 2 |
| 2:C:28:U:O2' | 2:C:29:C:H5' | 0.58 | 1.98 | 11 | 11 |
| 2:D:54:U:O2' | 2:D:55:C:H5' | 0.58 | 1.98 | 11 | 11 |
| 1:A:10:THR:HG23 | 1:A:11:ILE:N | 0.57 | 2.12 | 2 | 8 |
| 1:A:101:VAL:HG21 | 1:B:101:VAL:HG11 | 0.57 | 1.74 | 13 | 1 |
| 1:A:11:ILE:HD13 | 1:A:83:ILE:HG21 | 0.57 | 1.77 | 2 | 1 |
| 1:B:10:THR:HA | 1:B:64:ALA:HB2 | 0.57 | 1.74 | 13 | 4 |
| 1:B:16:LEU:HD12 | 1:B:53:GLN:C | 0.57 | 2.19 | 3 | 1 |
| 1:A:33:PHE:HB3 | 1:A:39:ILE:HD12 | 0.57 | 1.76 | 7 | 1 |
| 2:C:17:C:H4' | 2:C:18:A:O4' | 0.57 | 2.00 | 8 | 1 |
| 2:C:17:C:OP2 | 2:C:17:C:H6 | 0.57 | 1.83 | 4 | 1 |
| 2:C:17:C:H4' | 2:C:18:A:O5' | 0.57 | 2.00 | 10 | 1 |
| 2:D:43:C:H4' | 2:D:44:A:O5' | 0.57 | 1.99 | 10 | 1 |
| 2:C:15:U:H1' | 2:C:16:G:OP1 | 0.57 | 1.98 | 11 | 2 |
| 2:D:41:U:H1' | 2:D:42:G:OP2 | 0.57 | 1.99 | 9 | 2 |
| 1:A:48:LEU:O | 1:A:48:LEU:HD13 | 0.57 | 2.00 | 1 | 2 |
| 1:B:68:LEU:HA | 1:B:83:ILE:HG21 | 0.57 | 1.76 | 9 | 2 |
| 2:D:43:C:O3' | 2:D:44:A:H8 | 0.57 | 1.82 | 4 | 5 |
| 2:D:43:C:H6 | 2:D:43:C:OP2 | 0.56 | 1.82 | 4 | 1 |
| 1:A:49:LYS:O | 2:D:42:G:H2' | 0.56 | 2.00 | 11 | 2 |
| 1:B:11:ILE:HD13 | 1:B:83:ILE:HG21 | 0.56 | 1.77 | 2 | 1 |
| 1:A:68:LEU:CD2 | 1:A:83:ILE:HG22 | 0.56 | 2.30 | 3 | 1 |
| 1:B:71:MET:HB2 | 1:B:83:ILE:HD11 | 0.56 | 1.76 | 3 | 2 |
| 1:A:39:ILE:HD11 | 1:A:56:VAL:HB | 0.56 | 1.76 | 7 | 1 |
| 1:A:96:MET:HE2 | 1:B:99:THR:OG1 | 0.56 | 1.99 | 12 | 2 |
| 1:B:33:PHE:HB3 | 1:B:39:ILE:HD12 | 0.56 | 1.76 | 7 | 1 |
| 1:A:99:THR:O | 1:A:99:THR:HG22 | 0.56 | 1.99 | 12 | 1 |
| 1:A:41:ASP:O | 1:A:42:ILE:HD13 | 0.56 | 1.99 | 13 | 1 |
| 2:D:49:G:O5' | 2:D:49:G:H8 | 0.56 | 1.84 | 11 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:68:LEU:CD2 | 1:B:83:ILE:HG22 | 0.56 | 2.30 | 3 | 1 |
| 1:A:99:THR:HG21 | 1:A:101:VAL:HG13 | 0.56 | 1.76 | 10 | 1 |
| 1:A:32:ILE:HD12 | 1:A:76:PHE:CE1 | 0.56 | 2.36 | 9 | 1 |
| 1:B:99:THR:HG22 | 1:B:99:THR:O | 0.56 | 2.00 | 12 | 2 |
| 2:C:23:G:H8 | 2:C:23:G:O5' | 0.56 | 1.84 | 11 | 8 |
| 1:B:99:THR:HG21 | 1:B:101:VAL:HG13 | 0.56 | 1.76 | 10 | 1 |
| 1:B:41:ASP:O | 1:B:42:ILE:HD13 | 0.56 | 1.99 | 13 | 1 |
| 1:B:32:ILE:HG21 | 1:B:71:MET:SD | 0.56 | 2.41 | 1 | 1 |
| 1:B:56:VAL:O | 1:B:56:VAL:HG13 | 0.56 | 2.01 | 4 | 3 |
| 1:B:9:HIS:H | 1:B:61:VAL:HG22 | 0.55 | 1.61 | 13 | 6 |
| 1:B:33:PHE:HB2 | 1:B:39:ILE:HD11 | 0.55 | 1.78 | 6 | 3 |
| 1:A:33:PHE:HB2 | 1:A:39:ILE:HD11 | 0.55 | 1.78 | 6 | 3 |
| 1:B:33:PHE:CD1 | 1:B:56:VAL:HG21 | 0.55 | 2.37 | 4 | 1 |
| 1:B:10:THR:HG21 | 2:C:18:A:N6 | 0.55 | 2.13 | 6 | 2 |
| 1:A:32:ILE:HG21 | 1:A:71:MET:SD | 0.55 | 2.41 | 1 | 1 |
| 1:A:44:VAL:HG12 | 1:A:44:VAL:O | 0.55 | 2.02 | 3 | 1 |
| 1:A:98:GLY:HA3 | 1:B:40:LEU:HD11 | 0.55 | 1.77 | 11 | 2 |
| 1:A:42:ILE:CD1 | 1:A:56:VAL:HG23 | 0.55 | 2.32 | 13 | 1 |
| 1:A:33:PHE:CD1 | 1:A:56:VAL:HG21 | 0.55 | 2.37 | 4 | 1 |
| 1:A:96:MET:HB3 | 1:B:99:THR:HG23 | 0.55 | 1.77 | 1 | 1 |
| 2:C:18:A:O2' | 2:C:19:C:H5'' | 0.55 | 2.01 | 2 | 1 |
| 1:B:8:ASN:O | 1:B:61:VAL:HG22 | 0.55 | 2.01 | 10 | 3 |
| 1:A:43:LEU:HD11 | 2:D:45:C:H1' | 0.55 | 1.79 | 13 | 1 |
| 1:B:42:ILE:CD1 | 1:B:56:VAL:HG23 | 0.55 | 2.32 | 13 | 1 |
| 2:D:44:A:O2' | 2:D:45:C:H5'' | 0.55 | 2.01 | 2 | 1 |
| 1:A:8:ASN:O | 1:A:61:VAL:HG22 | 0.55 | 2.01 | 10 | 3 |
| 1:A:101:VAL:HG21 | 1:B:101:VAL:CG2 | 0.55 | 2.31 | 13 | 1 |
| 1:B:48:LEU:HD23 | 2:D:51:G:C1' | 0.55 | 2.32 | 7 | 3 |
| 1:B:32:ILE:HD12 | 1:B:76:PHE:CE1 | 0.55 | 2.36 | 9 | 1 |
| 1:B:68:LEU:HD22 | 1:B:85:TYR:CE2 | 0.55 | 2.37 | 13 | 1 |
| 1:A:68:LEU:HD22 | 1:A:85:TYR:CE2 | 0.54 | 2.37 | 13 | 1 |
| 1:A:40:LEU:HD11 | 1:B:98:GLY:HA3 | 0.54 | 1.77 | 11 | 2 |
| 1:B:10:THR:HG23 | 1:B:86:ALA:HB3 | 0.54 | 1.80 | 12 | 1 |
| 1:A:9:HIS:H | 1:A:61:VAL:HG22 | 0.54 | 1.63 | 1 | 6 |
| 1:A:56:VAL:O | 1:A:56:VAL:HG13 | 0.54 | 2.03 | 5 | 3 |
| 2:C:24:A:N1 | 2:D:46:C:N3 | 0.54 | 2.56 | 10 | 2 |
| 1:A:55:PHE:CD2 | 2:D:44:A:C5 | 0.54 | 2.96 | 7 | 6 |
| 1:A:96:MET:HE1 | 1:B:99:THR:HG22 | 0.54 | 1.77 | 13 | 1 |
| 1:A:101:VAL:CG2 | 1:B:101:VAL:HG21 | 0.54 | 2.31 | 13 | 1 |
| 1:A:48:LEU:HD23 | 2:C:25:G:C1' | 0.54 | 2.33 | 7 | 3 |
| 1:A:68:LEU:O | 1:A:68:LEU:HD13 | 0.54 | 2.03 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:33:PHE:HE2 | 1:A:83:ILE:HD11 | 0.54 | 1.60 | 12 | 1 |
| 2:D:44:A:C2 | 2:D:45:C:N3 | 0.54 | 2.76 | 12 | 2 |
| 2:C:23:G:N2 | 2:C:24:A:C2 | 0.54 | 2.76 | 11 | 2 |
| 1:B:11:ILE:CG2 | 1:B:64:ALA:HB1 | 0.53 | 2.27 | 2 | 2 |
| 1:B:44:VAL:O | 1:B:44:VAL:HG12 | 0.53 | 2.02 | 3 | 1 |
| 2:C:18:A:C2 | 2:C:19:C:N3 | 0.53 | 2.76 | 12 | 2 |
| 2:C:20:C:N3 | 2:D:50:A:N1 | 0.53 | 2.56 | 10 | 2 |
| 1:A:99:THR:HG23 | 1:B:96:MET:HB3 | 0.53 | 1.79 | 1 | 1 |
| 1:B:55:PHE:CD2 | 2:C:18:A:C5 | 0.53 | 2.96 | 7 | 6 |
| 2:D:49:G:N2 | 2:D:50:A:C2 | 0.53 | 2.77 | 11 | 2 |
| 2:D:40:U:O5' | 2:D:40:U:H6 | 0.53 | 1.85 | 9 | 3 |
| 1:B:68:LEU:HD13 | 1:B:68:LEU:O | 0.53 | 2.03 | 3 | 1 |
| 1:A:11:ILE:HG21 | 1:A:68:LEU:HB2 | 0.53 | 1.80 | 6 | 1 |
| 1:B:96:MET:O | 1:B:99:THR:HG22 | 0.53 | 2.04 | 6 | 4 |
| 1:A:98:GLY:HA3 | 1:B:40:LEU:HD21 | 0.53 | 1.81 | 12 | 1 |
| 2:D:41:U:H4' | 2:D:42:G:OP1 | 0.53 | 2.04 | 13 | 1 |
| 2:C:24:A:C2 | 2:D:46:C:N3 | 0.53 | 2.76 | 6 | 1 |
| 1:B:33:PHE:HE2 | 1:B:83:ILE:HD11 | 0.53 | 1.61 | 12 | 1 |
| 2:C:9:A:H8 | 2:C:9:A:O5' | 0.53 | 1.87 | 8 | 6 |
| 1:A:96:MET:HE1 | 1:B:96:MET:HE1 | 0.53 | 1.81 | 13 | 1 |
| 1:B:20:ILE:HG21 | 1:B:25:LEU:CD1 | 0.53 | 2.34 | 10 | 3 |
| 2:C:15:U:H4' | 2:C:16:G:OP1 | 0.53 | 2.04 | 13 | 1 |
| 1:B:13:ILE:HD12 | 1:B:29:LEU:HD21 | 0.53 | 1.81 | 2 | 1 |
| 2:D:44:A:C2 | 2:D:45:C:C2 | 0.53 | 2.97 | 6 | 5 |
| 1:B:68:LEU:HD22 | 1:B:83:ILE:HG22 | 0.52 | 1.81 | 3 | 1 |
| 1:A:96:MET:O | 1:A:99:THR:HG22 | 0.52 | 2.03 | 6 | 4 |
| 2:C:20:C:N3 | 2:D:50:A:C2 | 0.52 | 2.76 | 6 | 1 |
| 2:C:18:A:C6 | 2:C:19:C:C5 | 0.52 | 2.97 | 10 | 1 |
| 1:B:68:LEU:HD12 | 1:B:83:ILE:O | 0.52 | 2.04 | 12 | 1 |
| 1:B:48:LEU:HD13 | 1:B:48:LEU:C | 0.52 | 2.25 | 8 | 7 |
| 1:A:10:THR:HG23 | 1:A:86:ALA:HB3 | 0.52 | 1.80 | 12 | 1 |
| 1:B:43:LEU:HD11 | 2:C:19:C:H1' | 0.52 | 1.79 | 13 | 1 |
| 1:A:13:ILE:HD12 | 1:A:29:LEU:HD21 | 0.52 | 1.81 | 2 | 1 |
| 1:A:68:LEU:HD22 | 1:A:83:ILE:HG22 | 0.52 | 1.81 | 3 | 1 |
| 2:C:11:A:C2 | 2:C:12:C:C2 | 0.52 | 2.98 | 4 | 4 |
| 2:C:25:G:C6 | 2:D:39:A:N1 | 0.52 | 2.78 | 4 | 3 |
| 2:C:25:G:C6 | 2:D:39:A:C2 | 0.52 | 2.98 | 8 | 2 |
| 1:B:11:ILE:HG21 | 1:B:68:LEU:HB2 | 0.52 | 1.80 | 6 | 1 |
| 1:A:68:LEU:HD21 | 1:A:72:GLN:OE1 | 0.52 | 2.04 | 2 | 1 |
| 2:D:44:A:C6 | 2:D:45:C:C5 | 0.52 | 2.97 | 10 | 1 |
| 1:B:55:PHE:CD2 | 2:C:18:A:C6 | 0.52 | 2.98 | 13 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:55:PHE:CE2 | 2:D:44:A:C8 | 0.52 | 2.97 | 6 | 1 |
| 1:A:20:ILE:HG21 | 1:A:25:LEU:CD1 | 0.52 | 2.34 | 10 | 3 |
| 1:B:12:TYR:CE1 | 2:C:17:C:C5 | 0.52 | 2.98 | 4 | 5 |
| 2:C:25:G:N2 | 2:C:26:U:C2 | 0.52 | 2.78 | 12 | 7 |
| 2:C:18:A:C2 | 2:C:19:C:C2 | 0.52 | 2.98 | 6 | 5 |
| 2:D:51:G:N2 | 2:D:52:U:C2 | 0.52 | 2.78 | 1 | 7 |
| 1:B:28:SER:O | 1:B:32:ILE:HD12 | 0.52 | 2.05 | 2 | 3 |
| 1:A:12:TYR:CE1 | 2:D:43:C:N3 | 0.52 | 2.78 | 5 | 2 |
| 1:B:55:PHE:CD1 | 2:C:18:A:C6 | 0.52 | 2.98 | 8 | 1 |
| 1:B:101:VAL:O | 1:B:101:VAL:HG23 | 0.52 | 2.05 | 8 | 1 |
| 1:B:68:LEU:HD21 | 1:B:72:GLN:OE1 | 0.52 | 2.04 | 2 | 1 |
| 2:C:13:A:C2 | 2:D:51:G:C6 | 0.52 | 2.98 | 8 | 2 |
| 2:C:13:A:C2 | 2:D:51:G:C4 | 0.52 | 2.98 | 6 | 2 |
| 1:A:40:LEU:HD21 | 1:B:98:GLY:HA3 | 0.52 | 1.82 | 12 | 1 |
| 1:A:11:ILE:HD11 | 1:A:33:PHE:HE1 | 0.52 | 1.65 | 5 | 3 |
| 1:A:12:TYR:CE1 | 2:D:43:C:C5 | 0.52 | 2.97 | 4 | 5 |
| 2:C:20:C:N3 | 2:C:21:C:C2 | 0.52 | 2.78 | 3 | 2 |
| 2:C:26:U:C4 | 2:C:27:C:N4 | 0.52 | 2.78 | 5 | 10 |
| 1:A:28:SER:O | 1:A:32:ILE:HD12 | 0.52 | 2.05 | 2 | 3 |
| 1:B:12:TYR:CE1 | 2:C:17:C:N3 | 0.52 | 2.78 | 5 | 2 |
| 1:B:55:PHE:CE2 | 2:C:18:A:C8 | 0.52 | 2.98 | 6 | 1 |
| 1:A:55:PHE:CD1 | 2:D:44:A:C6 | 0.52 | 2.98 | 8 | 1 |
| 1:B:12:TYR:CE1 | 1:B:55:PHE:CZ | 0.52 | 2.98 | 12 | 1 |
| 2:D:35:A:H8 | 2:D:35:A:O5' | 0.52 | 1.87 | 8 | 6 |
| 2:D:46:C:N3 | 2:D:47:C:C2 | 0.52 | 2.78 | 3 | 2 |
| 1:A:33:PHE:CE1 | 1:A:56:VAL:HG11 | 0.52 | 2.40 | 4 | 1 |
| 2:C:13:A:N1 | 2:D:51:G:C6 | 0.52 | 2.78 | 4 | 3 |
| 2:D:37:A:C2 | 2:D:38:C:C2 | 0.52 | 2.98 | 4 | 3 |
| 1:B:33:PHE:CE1 | 1:B:56:VAL:HG11 | 0.51 | 2.41 | 4 | 1 |
| 2:C:21:C:N4 | 2:D:47:C:N4 | 0.51 | 2.59 | 13 | 2 |
| 2:D:45:C:C5' | 2:D:46:C:C6 | 0.51 | 2.93 | 9 | 1 |
| 2:D:34:G:N2 | 2:D:35:A:C4 | 0.51 | 2.79 | 11 | 1 |
| 1:A:55:PHE:CD2 | 2:D:44:A:C6 | 0.51 | 2.98 | 3 | 4 |
| 1:B:92:ILE:HD13 | 1:B:92:ILE:C | 0.51 | 2.26 | 1 | 2 |
| 2:C:13:A:C2 | 2:D:51:G:C5 | 0.51 | 2.99 | 2 | 2 |
| 2:C:25:G:C5 | 2:D:39:A:C2 | 0.51 | 2.98 | 2 | 2 |
| 1:A:48:LEU:C | 1:A:48:LEU:HD13 | 0.51 | 2.25 | 8 | 5 |
| 2:D:39:A:C2 | 2:D:40:U:C2 | 0.51 | 2.98 | 4 | 2 |
| 1:A:20:ILE:HG12 | 1:A:25:LEU:HD13 | 0.51 | 1.83 | 7 | 1 |
| 1:A:91:ASP:N | 2:D:45:C:N3 | 0.51 | 2.58 | 11 | 1 |
| 2:D:43:C:H6 | 2:D:43:C:OP1 | 0.51 | 1.87 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:D:52:U:C4 | 2:D:53:C:N4 | 0.51 | 2.78 | 2 | 10 |
| 1:B:50:MET:HA | 1:B:50:MET:HE2 | 0.51 | 1.83 | 4 | 4 |
| 2:D:36:G:C6 | 2:D:37:A:N6 | 0.51 | 2.79 | 2 | 1 |
| 1:A:101:VAL:O | 1:A:101:VAL:HG23 | 0.51 | 2.05 | 8 | 1 |
| 1:A:101:VAL:CG2 | 1:B:101:VAL:HG11 | 0.51 | 2.35 | 13 | 1 |
| 1:A:92:ILE:HD13 | 1:A:92:ILE:C | 0.51 | 2.26 | 1 | 2 |
| 1:A:12:TYR:CE1 | 1:A:55:PHE:CZ | 0.51 | 2.98 | 12 | 1 |
| 1:A:68:LEU:HD12 | 1:A:83:ILE:O | 0.51 | 2.04 | 12 | 1 |
| 1:A:101:VAL:HG11 | 1:B:101:VAL:CG2 | 0.51 | 2.35 | 13 | 1 |
| 1:A:44:VAL:HG22 | 1:A:54:ALA:CB | 0.51 | 2.36 | 3 | 1 |
| 1:A:55:PHE:CE2 | 2:D:44:A:C5 | 0.51 | 2.99 | 12 | 2 |
| 1:B:55:PHE:CE2 | 2:C:18:A:C5 | 0.51 | 2.99 | 12 | 2 |
| 2:C:10:G:C6 | 2:C:11:A:N6 | 0.51 | 2.79 | 2 | 1 |
| 1:B:11:ILE:HD11 | 1:B:33:PHE:HE1 | 0.51 | 1.66 | 4 | 3 |
| 1:B:13:ILE:HD12 | 1:B:29:LEU:CD2 | 0.51 | 2.36 | 2 | 1 |
| 2:C:14:U:O2' | 2:C:15:U:H5'' | 0.51 | 2.06 | 4 | 1 |
| 1:B:91:ASP:N | 2:C:19:C:N3 | 0.51 | 2.59 | 11 | 1 |
| 1:A:12:TYR:CD2 | 2:D:43:C:C2 | 0.51 | 2.99 | 12 | 1 |
| 1:B:44:VAL:HG22 | 1:B:54:ALA:CB | 0.51 | 2.36 | 3 | 1 |
| 2:C:13:A:C2 | 2:C:14:U:C2 | 0.51 | 2.98 | 4 | 2 |
| 2:C:19:C:C5' | 2:C:20:C:C6 | 0.51 | 2.93 | 9 | 1 |
| 2:D:39:A:C5 | 2:D:40:U:C4 | 0.51 | 2.99 | 4 | 1 |
| 1:B:12:TYR:CD2 | 2:C:17:C:C2 | 0.50 | 2.99 | 12 | 1 |
| 2:D:47:C:O5' | 2:D:47:C:H6 | 0.50 | 1.89 | 13 | 1 |
| 2:C:8:G:N2 | 2:C:9:A:C4 | 0.50 | 2.78 | 11 | 1 |
| 1:B:25:LEU:O | 1:B:29:LEU:HD12 | 0.50 | 2.06 | 13 | 1 |
| 2:C:21:C:O5' | 2:C:21:C:H6 | 0.50 | 1.90 | 13 | 1 |
| 2:C:23:G:C6 | 2:C:24:A:C6 | 0.50 | 3.00 | 9 | 10 |
| 2:D:49:G:C6 | 2:D:50:A:C6 | 0.50 | 3.00 | 4 | 10 |
| 1:A:9:HIS:HE1 | 1:A:93:ILE:HG21 | 0.50 | 1.64 | 11 | 1 |
| 1:A:11:ILE:CG1 | 1:A:56:VAL:HG22 | 0.50 | 2.36 | 7 | 2 |
| 1:A:27:LYS:O | 1:A:31:ALA:HB3 | 0.50 | 2.07 | 13 | 2 |
| 1:A:55:PHE:CE1 | 2:D:44:A:C6 | 0.50 | 2.99 | 8 | 1 |
| 2:D:44:A:C6 | 2:D:45:C:C4 | 0.50 | 3.00 | 11 | 1 |
| 1:A:13:ILE:HD12 | 1:A:29:LEU:CD2 | 0.50 | 2.36 | 2 | 1 |
| 2:C:20:C:C4 | 2:C:21:C:C4 | 0.50 | 3.00 | 2 | 6 |
| 2:D:40:U:C2 | 2:D:42:G:N2 | 0.50 | 2.80 | 3 | 2 |
| 1:A:11:ILE:HG13 | 1:A:56:VAL:HG22 | 0.50 | 1.82 | 7 | 2 |
| 2:C:22:G:C2 | 2:D:48:G:C2 | 0.50 | 2.99 | 10 | 1 |
| 2:C:17:C:H6 | 2:C:17:C:OP1 | 0.50 | 1.89 | 13 | 1 |
| 2:C:26:U:C4 | 2:C:27:C:C4 | 0.50 | 3.00 | 11 | 7 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:D:46:C:C4 | 2:D:47:C:C4 | 0.50 | 3.00 | 5 | 6 |
| 1:A:92:ILE:HD12 | 1:A:93:ILE:H | 0.50 | 1.66 | 5 | 3 |
| 1:B:92:ILE:HD12 | 1:B:93:ILE:H | 0.50 | 1.66 | 5 | 2 |
| 1:B:55:PHE:CE1 | 2:C:18:A:C6 | 0.50 | 2.99 | 8 | 1 |
| 1:A:25:LEU:O | 1:A:29:LEU:HD12 | 0.50 | 2.06 | 13 | 1 |
| 2:D:52:U:C4 | 2:D:53:C:C4 | 0.50 | 3.00 | 11 | 6 |
| 2:C:13:A:C5 | 2:C:14:U:C4 | 0.50 | 3.00 | 4 | 1 |
| 1:A:76:PHE:CE1 | 1:A:77:TYR:CD1 | 0.50 | 3.00 | 7 | 1 |
| 1:B:11:ILE:HG13 | 1:B:56:VAL:HG22 | 0.50 | 1.82 | 7 | 2 |
| 1:B:76:PHE:CE1 | 1:B:77:TYR:CD1 | 0.50 | 3.00 | 7 | 1 |
| 1:A:39:ILE:HG23 | 1:A:56:VAL:HG23 | 0.50 | 1.83 | 11 | 1 |
| 2:C:14:U:C2 | 2:C:16:G:N2 | 0.50 | 2.80 | 3 | 2 |
| 2:D:40:U:O2' | 2:D:41:U:H5'' | 0.50 | 2.06 | 4 | 1 |
| 2:C:18:A:C6 | 2:C:19:C:C4 | 0.50 | 3.00 | 11 | 1 |
| 1:A:30:HIS:HA | 1:A:39:ILE:HD13 | 0.49 | 1.84 | 3 | 1 |
| 1:B:55:PHE:CE1 | 2:C:18:A:C5 | 0.49 | 2.99 | 8 | 1 |
| 1:B:39:ILE:HG23 | 1:B:56:VAL:HG23 | 0.49 | 1.83 | 11 | 1 |
| 1:B:11:ILE:CG1 | 1:B:56:VAL:HG22 | 0.49 | 2.36 | 7 | 2 |
| 2:C:18:A:N1 | 2:C:19:C:C4 | 0.49 | 2.80 | 11 | 1 |
| 1:A:40:LEU:HD23 | 1:A:59:LYS:HB2 | 0.49 | 1.83 | 12 | 1 |
| 1:B:92:ILE:HD13 | 1:B:96:MET:HE3 | 0.49 | 1.84 | 13 | 1 |
| 1:A:40:LEU:HD13 | 1:A:58:PHE:O | 0.49 | 2.07 | 5 | 1 |
| 1:A:55:PHE:CE1 | 2:D:44:A:C5 | 0.49 | 3.00 | 8 | 1 |
| 1:B:40:LEU:HD23 | 1:B:59:LYS:HB2 | 0.49 | 1.83 | 12 | 1 |
| 2:C:19:C:P | 2:C:20:C:C5 | 0.49 | 3.06 | 6 | 1 |
| 1:B:90:SER:N | 2:C:18:A:N6 | 0.49 | 2.61 | 8 | 1 |
| 1:A:96:MET:O | 1:A:100:PHE:N | 0.49 | 2.46 | 13 | 1 |
| 1:A:99:THR:CB | 1:B:99:THR:HG21 | 0.49 | 2.38 | 3 | 1 |
| 1:B:13:ILE:HD13 | 1:B:29:LEU:CD2 | 0.49 | 2.32 | 11 | 3 |
| 1:B:33:PHE:HD1 | 1:B:67:ALA:HB1 | 0.49 | 1.67 | 10 | 1 |
| 1:A:48:LEU:HD23 | 2:C:25:G:O4' | 0.49 | 2.08 | 6 | 1 |
| 1:B:48:LEU:HD23 | 2:D:51:G:O4' | 0.49 | 2.08 | 6 | 2 |
| 1:A:33:PHE:HB3 | 1:A:56:VAL:HG11 | 0.49 | 1.83 | 12 | 2 |
| 1:B:40:LEU:HD13 | 1:B:58:PHE:O | 0.49 | 2.07 | 5 | 1 |
| 1:B:20:ILE:HG12 | 1:B:25:LEU:HD13 | 0.49 | 1.83 | 7 | 1 |
| 1:B:27:LYS:O | 1:B:31:ALA:HB3 | 0.49 | 2.07 | 13 | 2 |
| 1:B:99:THR:HG23 | 1:B:101:VAL:HG13 | 0.49 | 1.84 | 10 | 1 |
| 2:C:23:G:C2 | 2:C:24:A:C2 | 0.49 | 3.01 | 11 | 1 |
| 1:A:90:SER:N | 2:D:44:A:N6 | 0.49 | 2.61 | 8 | 1 |
| 2:D:44:A:N1 | 2:D:45:C:C4 | 0.49 | 2.81 | 11 | 1 |
| 1:B:11:ILE:HD12 | 1:B:11:ILE:O | 0.49 | 2.08 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:D:45:C:P | 2:D:46:C:C5 | 0.48 | 3.05 | 6 | 1 |
| 1:B:71:MET:CB | 1:B:83:ILE:HD11 | 0.48 | 2.38 | 7 | 1 |
| 1:B:33:PHE:HB3 | 1:B:56:VAL:HG11 | 0.48 | 1.84 | 12 | 2 |
| 2:D:49:G:C2 | 2:D:50:A:C4 | 0.48 | 3.01 | 10 | 1 |
| 1:A:83:ILE:O | 1:A:83:ILE:HG23 | 0.48 | 2.07 | 12 | 1 |
| 1:A:96:MET:HB2 | 1:B:96:MET:HE2 | 0.48 | 1.85 | 10 | 1 |
| 1:A:11:ILE:CG2 | 1:A:64:ALA:HB1 | 0.48 | 2.27 | 2 | 3 |
| 2:C:23:G:C2 | 2:C:24:A:C4 | 0.48 | 3.01 | 10 | 1 |
| 1:A:98:GLY:HA3 | 1:B:40:LEU:HD13 | 0.48 | 1.86 | 3 | 1 |
| 1:B:30:HIS:HA | 1:B:39:ILE:HD13 | 0.48 | 1.84 | 3 | 1 |
| 2:C:10:G:O5' | 2:C:10:G:H8 | 0.48 | 1.91 | 3 | 2 |
| 1:A:30:HIS:O | 1:A:39:ILE:HD12 | 0.48 | 2.09 | 8 | 2 |
| 1:A:99:THR:HG22 | 1:A:101:VAL:HG22 | 0.48 | 1.86 | 6 | 1 |
| 1:A:13:ILE:HG13 | 1:A:29:LEU:HD22 | 0.48 | 1.85 | 10 | 1 |
| 2:C:18:A:C5 | 2:C:19:C:N4 | 0.48 | 2.81 | 13 | 1 |
| 1:A:101:VAL:HG13 | 1:B:101:VAL:CG1 | 0.48 | 2.21 | 2 | 1 |
| 1:A:99:THR:HG21 | 1:B:99:THR:CB | 0.48 | 2.38 | 3 | 1 |
| 1:A:96:MET:HE2 | 1:B:96:MET:HB2 | 0.48 | 1.85 | 10 | 1 |
| 1:B:13:ILE:HG13 | 1:B:29:LEU:HD22 | 0.48 | 1.85 | 10 | 1 |
| 1:A:99:THR:OG1 | 1:B:96:MET:HE2 | 0.48 | 2.07 | 12 | 1 |
| 1:A:40:LEU:HD13 | 1:B:98:GLY:HA3 | 0.48 | 1.86 | 3 | 1 |
| 1:A:85:TYR:O | 2:D:43:C:H5 | 0.48 | 1.92 | 8 | 1 |
| 1:B:83:ILE:O | 1:B:83:ILE:HG23 | 0.48 | 2.07 | 12 | 1 |
| 2:D:44:A:C5 | 2:D:45:C:N4 | 0.48 | 2.81 | 13 | 1 |
| 1:B:57:ILE:HD11 | 2:C:18:A:N1 | 0.48 | 2.24 | 2 | 1 |
| 1:B:90:SER:OG | 1:B:92:ILE:HD11 | 0.48 | 2.09 | 4 | 1 |
| 1:A:99:THR:HG23 | 1:A:101:VAL:HG13 | 0.48 | 1.83 | 10 | 1 |
| 1:B:11:ILE:HG22 | 1:B:85:TYR:CD1 | 0.48 | 2.44 | 11 | 1 |
| 1:B:96:MET:O | 1:B:100:PHE:N | 0.48 | 2.46 | 13 | 1 |
| 2:C:18:A:P | 2:C:18:A:C8 | 0.48 | 3.07 | 10 | 1 |
| 2:D:41:U:C1' | 2:D:42:G:P | 0.48 | 3.02 | 11 | 2 |
| 1:A:87:LYS:HG2 | 2:D:43:C:N3 | 0.48 | 2.24 | 11 | 5 |
| 2:C:22:G:C6 | 2:D:48:G:C6 | 0.48 | 3.02 | 2 | 1 |
| 1:A:96:MET:HE2 | 1:B:99:THR:CB | 0.48 | 2.38 | 5 | 2 |
| 2:D:44:A:P | 2:D:44:A:C8 | 0.48 | 3.07 | 10 | 1 |
| 1:A:92:ILE:HD12 | 1:A:92:ILE:C | 0.47 | 2.30 | 3 | 5 |
| 1:B:30:HIS:O | 1:B:39:ILE:HD12 | 0.47 | 2.09 | 8 | 2 |
| 1:A:55:PHE:CZ | 2:D:44:A:N7 | 0.47 | 2.82 | 8 | 1 |
| 2:C:18:A:O5' | 2:C:18:A:C8 | 0.47 | 2.67 | 11 | 3 |
| 2:D:44:A:O5' | 2:D:44:A:C8 | 0.47 | 2.67 | 11 | 3 |
| 1:A:11:ILE:HG22 | 1:A:85:TYR:CD1 | 0.47 | 2.44 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:100:PHE:O | 1:A:101:VAL:HG22 | 0.47 | 2.08 | 13 | 1 |
| 1:B:100:PHE:O | 1:B:101:VAL:HG22 | 0.47 | 2.08 | 13 | 1 |
| 1:B:89:ASP:CA | 2:C:18:A:N6 | 0.47 | 2.78 | 3 | 4 |
| 1:A:87:LYS:CD | 2:D:43:C:N3 | 0.47 | 2.77 | 13 | 2 |
| 1:B:92:ILE:HD12 | 1:B:92:ILE:C | 0.47 | 2.30 | 3 | 5 |
| 1:A:13:ILE:HG21 | 1:A:16:LEU:HD21 | 0.47 | 1.86 | 7 | 1 |
| 2:D:51:G:HO2' | 2:D:52:U:H6 | 0.47 | 1.51 | 10 | 1 |
| 2:D:49:G:C2 | 2:D:50:A:C2 | 0.47 | 3.02 | 11 | 1 |
| 1:A:11:ILE:C | 1:A:11:ILE:HD12 | 0.47 | 2.30 | 12 | 1 |
| 1:A:43:LEU:HD21 | 2:D:45:C:C1' | 0.47 | 2.38 | 11 | 1 |
| 1:A:11:ILE:HD12 | 1:A:11:ILE:O | 0.47 | 2.08 | 12 | 1 |
| 1:A:89:ASP:CA | 2:D:44:A:N6 | 0.47 | 2.78 | 3 | 4 |
| 1:B:87:LYS:HG2 | 2:C:17:C:N3 | 0.47 | 2.24 | 11 | 3 |
| 2:C:12:C:C5 | 2:C:13:A:N7 | 0.47 | 2.83 | 4 | 1 |
| 1:B:11:ILE:HD12 | 1:B:11:ILE:C | 0.47 | 2.30 | 3 | 2 |
| 2:D:36:G:H8 | 2:D:36:G:O5' | 0.47 | 1.91 | 3 | 2 |
| 1:A:90:SER:OG | 1:A:92:ILE:HD11 | 0.47 | 2.09 | 4 | 1 |
| 2:D:44:A:N3 | 2:D:44:A:H2' | 0.47 | 2.24 | 5 | 1 |
| 1:A:71:MET:CB | 1:A:83:ILE:HD11 | 0.47 | 2.38 | 7 | 1 |
| 1:B:55:PHE:CZ | 2:C:18:A:N7 | 0.47 | 2.82 | 8 | 1 |
| 1:B:10:THR:CG2 | 2:C:18:A:N6 | 0.47 | 2.78 | 9 | 1 |
| 1:A:68:LEU:HD12 | 1:A:83:ILE:HG23 | 0.47 | 1.87 | 12 | 1 |
| 2:C:25:G:C4 | 2:D:39:A:C2 | 0.47 | 3.01 | 6 | 1 |
| 1:A:71:MET:HB3 | 1:A:83:ILE:HD11 | 0.47 | 1.87 | 7 | 1 |
| 1:B:9:HIS:ND1 | 1:B:89:ASP:O | 0.47 | 2.48 | 9 | 1 |
| 2:C:19:C:O5' | 2:C:20:C:C5 | 0.47 | 2.68 | 11 | 2 |
| 1:B:43:LEU:HD21 | 2:C:19:C:C1' | 0.47 | 2.39 | 11 | 1 |
| 1:B:96:MET:HB3 | 1:B:100:PHE:HB2 | 0.47 | 1.86 | 13 | 1 |
| 2:D:36:G:C6 | 2:D:37:A:C6 | 0.47 | 3.03 | 2 | 3 |
| 2:D:38:C:C5 | 2:D:39:A:N7 | 0.47 | 2.83 | 4 | 1 |
| 1:A:10:THR:CG2 | 2:D:44:A:N6 | 0.47 | 2.78 | 9 | 1 |
| 1:A:33:PHE:HD1 | 1:A:67:ALA:HB1 | 0.47 | 1.67 | 10 | 1 |
| 1:B:68:LEU:HD12 | 1:B:83:ILE:HG23 | 0.47 | 1.87 | 12 | 1 |
| 1:A:96:MET:HE1 | 1:B:96:MET:CE | 0.47 | 2.39 | 13 | 1 |
| 1:A:96:MET:CE | 1:B:96:MET:CE | 0.47 | 2.92 | 13 | 1 |
| 1:A:10:THR:OG1 | 1:A:56:VAL:O | 0.47 | 2.26 | 13 | 3 |
| 2:C:15:U:C1' | 2:C:16:G:P | 0.47 | 3.02 | 11 | 2 |
| 2:C:23:G:O5' | 2:C:23:G:H8 | 0.47 | 1.92 | 13 | 1 |
| 1:A:13:ILE:HD13 | 1:A:29:LEU:CD2 | 0.47 | 2.39 | 4 | 3 |
| 1:B:91:ASP:CB | 2:C:19:C:N3 | 0.47 | 2.78 | 5 | 1 |
| 1:B:100:PHE:CD1 | 1:B:101:VAL:N | 0.47 | 2.83 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:100:PHE:CD1 | 1:A:101:VAL:N | 0.47 | 2.83 | 9 | 1 |
| 1:B:68:LEU:HD22 | 1:B:85:TYR:CZ | 0.47 | 2.46 | 12 | 2 |
| 1:A:91:ASP:CB | 2:D:45:C:N3 | 0.46 | 2.78 | 5 | 1 |
| 1:B:58:PHE:CD1 | 1:B:58:PHE:N | 0.46 | 2.83 | 5 | 2 |
| 2:C:18:A:N3 | 2:C:18:A:H2' | 0.46 | 2.24 | 5 | 1 |
| 1:A:96:MET:HB3 | 1:A:100:PHE:HB2 | 0.46 | 1.86 | 13 | 1 |
| 1:B:68:LEU:HD13 | 1:B:85:TYR:CG | 0.46 | 2.45 | 13 | 1 |
| 1:A:100:PHE:CB | 1:B:101:VAL:HG11 | 0.46 | 2.40 | 2 | 1 |
| 1:B:87:LYS:CD | 2:C:17:C:N3 | 0.46 | 2.78 | 13 | 2 |
| 2:D:45:C:O5' | 2:D:46:C:C5 | 0.46 | 2.68 | 11 | 2 |
| 1:A:68:LEU:HD22 | 1:A:85:TYR:CZ | 0.46 | 2.46 | 12 | 2 |
| 1:A:12:TYR:CE1 | 1:A:84:GLN:CB | 0.46 | 2.99 | 2 | 2 |
| 1:B:99:THR:HG22 | 1:B:101:VAL:HG22 | 0.46 | 1.86 | 6 | 1 |
| 2:D:43:C:P | 2:D:43:C:O4' | 0.46 | 2.74 | 12 | 1 |
| 1:B:55:PHE:CE2 | 2:C:18:A:N7 | 0.46 | 2.84 | 5 | 1 |
| 1:B:58:PHE:CZ | 1:B:67:ALA:CB | 0.46 | 2.99 | 6 | 3 |
| 1:B:71:MET:HB3 | 1:B:83:ILE:HD11 | 0.46 | 1.87 | 7 | 1 |
| 1:A:48:LEU:HD13 | 1:A:48:LEU:C | 0.46 | 2.30 | 6 | 2 |
| 1:A:57:ILE:HD11 | 2:D:44:A:N1 | 0.46 | 2.25 | 2 | 1 |
| 2:C:19:C:O5' | 2:C:20:C:C6 | 0.46 | 2.69 | 3 | 6 |
| 1:B:99:THR:HG23 | 1:B:100:PHE:N | 0.46 | 2.26 | 6 | 3 |
| 2:D:39:A:O2' | 2:D:40:U:P | 0.46 | 2.74 | 4 | 1 |
| 1:A:58:PHE:CZ | 1:A:67:ALA:CB | 0.46 | 2.99 | 6 | 3 |
| 2:C:17:C:O3' | 2:C:18:A:C8 | 0.46 | 2.69 | 11 | 3 |
| 2:D:43:C:O3' | 2:D:44:A:C8 | 0.46 | 2.69 | 11 | 3 |
| 2:C:13:A:C6 | 2:D:51:G:C6 | 0.46 | 3.03 | 7 | 1 |
| 1:A:11:ILE:HD11 | 1:A:33:PHE:HE2 | 0.46 | 1.70 | 8 | 1 |
| 1:B:89:ASP:N | 2:C:18:A:N6 | 0.46 | 2.63 | 10 | 2 |
| 1:A:43:LEU:HD21 | 2:D:45:C:H1' | 0.46 | 1.88 | 11 | 1 |
| 2:C:23:G:N1 | 2:C:24:A:C6 | 0.46 | 2.84 | 2 | 5 |
| 1:A:89:ASP:N | 2:D:44:A:N6 | 0.46 | 2.62 | 10 | 2 |
| 2:D:49:G:N1 | 2:D:50:A:C6 | 0.46 | 2.84 | 2 | 5 |
| 1:B:11:ILE:CG2 | 1:B:68:LEU:HD23 | 0.46 | 2.41 | 3 | 1 |
| 1:A:9:HIS:ND1 | 1:A:89:ASP:O | 0.46 | 2.48 | 9 | 1 |
| 1:B:68:LEU:HD12 | 1:B:83:ILE:HG22 | 0.46 | 1.88 | 6 | 2 |
| 2:C:19:C:OP1 | 2:C:20:C:C6 | 0.46 | 2.69 | 1 | 1 |
| 1:B:42:ILE:HG23 | 1:B:55:PHE:O | 0.46 | 2.11 | 6 | 1 |
| 1:A:89:ASP:O | 2:D:45:C:N4 | 0.46 | 2.49 | 11 | 2 |
| 1:A:50:MET:HE2 | 1:A:50:MET:HA | 0.46 | 1.87 | 4 | 2 |
| 1:A:55:PHE:CE2 | 2:D:44:A:N7 | 0.46 | 2.83 | 5 | 1 |
| 1:A:42:ILE:HG23 | 1:A:55:PHE:O | 0.46 | 2.11 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:85:TYR:O | 2:C:17:C:H5 | 0.46 | 1.93 | 8 | 1 |
| 1:B:89:ASP:O | 2:C:19:C:N4 | 0.46 | 2.50 | 11 | 5 |
| 2:D:45:C:O5' | 2:D:46:C:C6 | 0.46 | 2.69 | 3 | 6 |
| 1:A:58:PHE:CZ | 1:A:67:ALA:HB2 | 0.46 | 2.46 | 4 | 2 |
| 2:C:13:A:O2' | 2:C:14:U:P | 0.46 | 2.74 | 4 | 1 |
| 1:A:12:TYR:CE2 | 1:A:84:GLN:CB | 0.46 | 2.99 | 10 | 4 |
| 1:B:13:ILE:CG2 | 1:B:16:LEU:HD11 | 0.46 | 2.41 | 8 | 1 |
| 1:A:10:THR:CG2 | 1:A:56:VAL:O | 0.45 | 2.64 | 13 | 6 |
| 2:D:45:C:OP1 | 2:D:46:C:N1 | 0.45 | 2.50 | 4 | 3 |
| 1:B:12:TYR:CB | 1:B:55:PHE:CD2 | 0.45 | 2.99 | 9 | 4 |
| 1:A:99:THR:CB | 1:B:96:MET:HE2 | 0.45 | 2.41 | 5 | 1 |
| 1:A:76:PHE:CE1 | 1:A:81:MET:CE | 0.45 | 2.99 | 12 | 2 |
| 1:A:99:THR:CB | 1:B:96:MET:CE | 0.45 | 2.94 | 11 | 1 |
| 1:A:100:PHE:O | 1:A:100:PHE:CG | 0.45 | 2.68 | 11 | 1 |
| 2:D:40:U:H2' | 2:D:42:G:N2 | 0.45 | 2.26 | 11 | 1 |
| 1:A:68:LEU:HD12 | 1:A:83:ILE:HG22 | 0.45 | 1.88 | 6 | 2 |
| 2:C:10:G:C6 | 2:C:11:A:C6 | 0.45 | 3.03 | 2 | 3 |
| 1:A:71:MET:CE | 1:A:74:PHE:CD2 | 0.45 | 3.00 | 8 | 4 |
| 1:A:61:VAL:HG12 | 1:A:65:THR:HG1 | 0.45 | 1.72 | 7 | 1 |
| 1:B:13:ILE:HG21 | 1:B:16:LEU:HD21 | 0.45 | 1.86 | 7 | 1 |
| 1:A:68:LEU:HD13 | 1:A:85:TYR:CG | 0.45 | 2.45 | 13 | 1 |
| 1:A:96:MET:CE | 1:B:99:THR:HG22 | 0.45 | 2.42 | 13 | 1 |
| 1:B:12:TYR:CE1 | 1:B:84:GLN:CB | 0.45 | 2.99 | 2 | 2 |
| 1:A:58:PHE:N | 1:A:58:PHE:CD1 | 0.45 | 2.83 | 5 | 1 |
| 2:D:43:C:O2 | 2:D:43:C:O4' | 0.45 | 2.35 | 10 | 4 |
| 2:C:25:G:C6 | 2:D:39:A:C6 | 0.45 | 3.04 | 7 | 1 |
| 2:D:48:G:H8 | 2:D:48:G:O5' | 0.45 | 1.94 | 9 | 1 |
| 1:A:96:MET:CE | 1:B:99:THR:CB | 0.45 | 2.94 | 11 | 1 |
| 1:A:20:ILE:CD1 | 1:A:77:TYR:CD1 | 0.45 | 2.99 | 13 | 1 |
| 2:D:45:C:OP1 | 2:D:46:C:C6 | 0.45 | 2.69 | 1 | 1 |
| 1:A:99:THR:HG22 | 1:B:101:VAL:HG21 | 0.45 | 1.88 | 2 | 1 |
| 2:C:24:A:O2' | 2:C:25:G:H5'' | 0.45 | 2.11 | 2 | 1 |
| 1:B:10:THR:HG1 | 1:B:56:VAL:C | 0.45 | 2.15 | 4 | 1 |
| 1:B:12:TYR:CE2 | 1:B:84:GLN:CB | 0.45 | 3.00 | 11 | 4 |
| 1:B:20:ILE:CD1 | 1:B:77:TYR:CE2 | 0.45 | 3.00 | 8 | 1 |
| 2:D:49:G:N2 | 2:D:50:A:N3 | 0.45 | 2.64 | 10 | 1 |
| 1:B:9:HIS:HE1 | 1:B:93:ILE:HG21 | 0.45 | 1.63 | 11 | 1 |
| 1:B:89:ASP:O | 2:C:18:A:N6 | 0.45 | 2.46 | 11 | 1 |
| 1:A:58:PHE:CE2 | 1:A:67:ALA:CB | 0.45 | 3.00 | 8 | 2 |
| 2:C:26:U:N3 | 2:C:27:C:C4 | 0.45 | 2.85 | 11 | 6 |
| 1:A:20:ILE:CD1 | 1:A:25:LEU:HD21 | 0.45 | 2.39 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:11:ILE:HD12 | 1:A:11:ILE:C | 0.45 | 2.30 | 3 | 1 |
| 1:B:71:MET:CE | 1:B:74:PHE:CD2 | 0.45 | 3.00 | 13 | 4 |
| 2:C:19:C:C5 | 2:C:19:C:OP2 | 0.45 | 2.70 | 5 | 1 |
| 1:A:89:ASP:O | 2:D:44:A:N6 | 0.45 | 2.46 | 11 | 1 |
| 1:B:20:ILE:CD1 | 1:B:77:TYR:CD1 | 0.45 | 2.99 | 13 | 1 |
| 2:D:52:U:N3 | 2:D:53:C:C4 | 0.45 | 2.85 | 13 | 6 |
| 1:A:12:TYR:CB | 1:A:55:PHE:CD2 | 0.45 | 2.99 | 9 | 4 |
| 2:C:19:C:OP2 | 2:C:20:C:C6 | 0.45 | 2.70 | 6 | 1 |
| 1:A:13:ILE:CG2 | 1:A:16:LEU:HD11 | 0.45 | 2.41 | 8 | 1 |
| 1:B:10:THR:CG2 | 1:B:56:VAL:O | 0.45 | 2.64 | 13 | 6 |
| 1:A:101:VAL:HG11 | 1:B:100:PHE:CB | 0.45 | 2.41 | 2 | 1 |
| 1:A:11:ILE:CG2 | 1:A:68:LEU:HD23 | 0.45 | 2.41 | 3 | 1 |
| 1:B:25:LEU:HD23 | 1:B:44:VAL:HG11 | 0.45 | 1.88 | 3 | 1 |
| 1:A:99:THR:HG23 | 1:A:100:PHE:N | 0.45 | 2.26 | 6 | 3 |
| 2:C:19:C:O3' | 2:C:20:C:C5 | 0.45 | 2.70 | 4 | 2 |
| 1:B:36:PHE:N | 1:B:36:PHE:CD1 | 0.45 | 2.84 | 6 | 1 |
| 1:A:55:PHE:CB | 2:D:44:A:C2 | 0.45 | 3.00 | 7 | 1 |
| 1:A:20:ILE:CD1 | 1:A:77:TYR:CE2 | 0.45 | 3.00 | 8 | 1 |
| 2:C:22:G:H8 | 2:C:22:G:O5' | 0.45 | 1.94 | 9 | 1 |
| 1:B:16:LEU:CD2 | 1:B:76:PHE:CE1 | 0.45 | 3.00 | 11 | 1 |
| 2:C:14:U:H2' | 2:C:16:G:N2 | 0.45 | 2.26 | 11 | 1 |
| 2:C:17:C:O4' | 2:C:17:C:P | 0.45 | 2.74 | 12 | 1 |
| 1:B:55:PHE:CD1 | 1:B:55:PHE:N | 0.45 | 2.85 | 4 | 2 |
| 1:B:58:PHE:CZ | 1:B:67:ALA:HB2 | 0.45 | 2.46 | 4 | 2 |
| 1:B:97:LYS:O | 1:B:101:VAL:HG23 | 0.45 | 2.12 | 5 | 1 |
| 2:D:37:A:H8 | 2:D:37:A:O5' | 0.45 | 1.95 | 5 | 1 |
| 1:B:58:PHE:CE2 | 1:B:67:ALA:CB | 0.45 | 3.00 | 8 | 2 |
| 2:C:19:C:OP1 | 2:D:50:A:N1 | 0.45 | 2.50 | 11 | 4 |
| 2:C:19:C:O3' | 2:C:20:C:C6 | 0.45 | 2.70 | 9 | 2 |
| 2:D:45:C:OP2 | 2:D:46:C:C6 | 0.45 | 2.70 | 6 | 1 |
| 2:C:19:C:OP2 | 2:D:50:A:C2 | 0.45 | 2.70 | 9 | 1 |
| 1:B:76:PHE:CE1 | 1:B:81:MET:CE | 0.45 | 2.99 | 10 | 2 |
| 2:D:40:U:O2' | 2:D:41:U:P | 0.44 | 2.75 | 4 | 1 |
| 1:A:85:TYR:O | 2:D:43:C:C5 | 0.44 | 2.70 | 10 | 4 |
| 1:A:97:LYS:O | 1:A:101:VAL:HG23 | 0.44 | 2.12 | 5 | 1 |
| 1:B:41:ASP:HB3 | 1:B:57:ILE:HD12 | 0.44 | 1.89 | 11 | 2 |
| 1:A:101:VAL:HG11 | 1:B:101:VAL:CB | 0.44 | 2.42 | 8 | 1 |
| 2:C:24:A:C2 | 2:D:45:C:OP2 | 0.44 | 2.70 | 9 | 1 |
| 2:C:19:C:OP1 | 2:C:20:C:N1 | 0.44 | 2.49 | 4 | 3 |
| 2:C:19:C:O5' | 2:C:19:C:H6 | 0.44 | 1.95 | 4 | 2 |
| 1:B:87:LYS:CD | 2:C:17:C:C4 | 0.44 | 3.00 | 2 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:D:42:G:O5' | 2:D:42:G:C8 | 0.44 | 2.71 | 4 | 2 |
| 1:B:11:ILE:CD1 | 1:B:33:PHE:CE2 | 0.44 | 2.99 | 9 | 1 |
| 1:A:99:THR:OG1 | 1:B:96:MET:CE | 0.44 | 2.66 | 12 | 3 |
| 2:D:35:A:O5' | 2:D:35:A:C8 | 0.44 | 2.70 | 3 | 3 |
| 2:D:40:U:O5' | 2:D:40:U:C6 | 0.44 | 2.70 | 1 | 2 |
| 2:D:45:C:O3' | 2:D:46:C:C6 | 0.44 | 2.70 | 9 | 2 |
| 1:A:11:ILE:CD1 | 1:A:33:PHE:CE2 | 0.44 | 2.99 | 9 | 1 |
| 2:D:47:C:O5' | 2:D:47:C:C6 | 0.44 | 2.71 | 10 | 2 |
| 1:B:90:SER:OG | 1:B:92:ILE:HD12 | 0.44 | 2.13 | 11 | 1 |
| 1:A:44:VAL:O | 1:A:44:VAL:HG23 | 0.44 | 2.13 | 8 | 5 |
| 1:A:9:HIS:CB | 1:A:89:ASP:CB | 0.44 | 2.96 | 7 | 3 |
| 1:A:87:LYS:CD | 2:D:43:C:C4 | 0.44 | 3.00 | 2 | 2 |
| 2:D:49:G:C6 | 2:D:50:A:N6 | 0.44 | 2.86 | 2 | 2 |
| 2:D:50:A:O2' | 2:D:51:G:H5'' | 0.44 | 2.12 | 2 | 1 |
| 1:A:55:PHE:CD1 | 1:A:55:PHE:N | 0.44 | 2.85 | 4 | 2 |
| 2:D:45:C:O3' | 2:D:46:C:C5 | 0.44 | 2.70 | 4 | 2 |
| 2:C:11:A:H8 | 2:C:11:A:O5' | 0.44 | 1.95 | 5 | 2 |
| 1:A:11:ILE:CG1 | 1:A:56:VAL:CG2 | 0.44 | 2.96 | 7 | 2 |
| 1:A:30:HIS:CD2 | 1:A:39:ILE:CG2 | 0.44 | 3.01 | 7 | 1 |
| 1:B:30:HIS:CD2 | 1:B:39:ILE:CG2 | 0.44 | 3.01 | 7 | 1 |
| 1:A:101:VAL:CB | 1:B:101:VAL:HG11 | 0.44 | 2.43 | 8 | 1 |
| 2:C:19:C:OP2 | 2:D:50:A:N1 | 0.44 | 2.51 | 9 | 1 |
| 1:B:44:VAL:HG23 | 1:B:44:VAL:O | 0.44 | 2.13 | 8 | 5 |
| 1:A:7:PRO:HB2 | 1:A:61:VAL:HG12 | 0.44 | 1.89 | 2 | 1 |
| 1:B:7:PRO:HB2 | 1:B:61:VAL:HG12 | 0.44 | 1.89 | 2 | 1 |
| 2:D:51:G:OP1 | 2:D:51:G:C8 | 0.44 | 2.70 | 2 | 1 |
| 1:B:44:VAL:HG22 | 1:B:54:ALA:HB1 | 0.44 | 1.90 | 3 | 1 |
| 2:C:13:A:O2' | 2:C:14:U:C6 | 0.44 | 2.70 | 4 | 1 |
| 2:C:17:C:O2 | 2:C:17:C:O4' | 0.44 | 2.35 | 5 | 4 |
| 1:B:43:LEU:HD21 | 2:C:19:C:H1' | 0.44 | 1.89 | 11 | 1 |
| 1:A:92:ILE:HD13 | 1:A:96:MET:HE3 | 0.44 | 1.88 | 13 | 1 |
| 1:A:100:PHE:O | 1:A:101:VAL:CG2 | 0.44 | 2.65 | 13 | 1 |
| 1:A:101:VAL:HG21 | 1:B:101:VAL:CG1 | 0.44 | 2.42 | 13 | 1 |
| 1:A:96:MET:CE | 1:B:99:THR:OG1 | 0.44 | 2.66 | 12 | 3 |
| 2:D:45:C:H6 | 2:D:45:C:O5' | 0.44 | 1.95 | 1 | 2 |
| 1:A:20:ILE:HG22 | 1:A:21:LYS:N | 0.44 | 2.28 | 2 | 5 |
| 1:A:99:THR:CG2 | 1:B:101:VAL:HG21 | 0.44 | 2.43 | 2 | 1 |
| 1:A:101:VAL:HG21 | 1:B:99:THR:HG22 | 0.44 | 1.88 | 2 | 1 |
| 1:B:16:LEU:HD22 | 1:B:25:LEU:HD22 | 0.44 | 1.88 | 2 | 1 |
| 2:C:23:G:C6 | 2:C:24:A:N6 | 0.44 | 2.86 | 2 | 2 |
| 2:C:24:A:N1 | 2:D:45:C:OP1 | 0.44 | 2.50 | 11 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:44:VAL:HG22 | 1:A:54:ALA:HB1 | 0.44 | 1.90 | 3 | 1 |
| 1:B:57:ILE:HD12 | 1:B:90:SER:OG | 0.44 | 2.13 | 3 | 1 |
| 2:D:44:A:C5 | 2:D:45:C:C4 | 0.44 | 3.06 | 3 | 1 |
| 1:A:36:PHE:CD1 | 1:A:36:PHE:N | 0.44 | 2.84 | 6 | 1 |
| 1:A:41:ASP:HB3 | 1:A:57:ILE:HD12 | 0.44 | 1.89 | 7 | 2 |
| 1:B:11:ILE:CG1 | 1:B:56:VAL:CG2 | 0.44 | 2.96 | 7 | 2 |
| 2:C:24:A:N1 | 2:D:45:C:OP2 | 0.44 | 2.51 | 9 | 1 |
| 1:B:13:ILE:HD11 | 1:B:33:PHE:HE2 | 0.44 | 1.72 | 10 | 1 |
| 2:C:23:G:N2 | 2:C:24:A:N3 | 0.44 | 2.65 | 10 | 1 |
| 1:B:100:PHE:O | 1:B:101:VAL:CG2 | 0.44 | 2.65 | 13 | 1 |
| 1:A:101:VAL:HG21 | 1:B:99:THR:CG2 | 0.44 | 2.43 | 2 | 1 |
| 2:D:39:A:O2' | 2:D:40:U:C6 | 0.44 | 2.70 | 4 | 1 |
| 2:D:43:C:OP2 | 2:D:43:C:C6 | 0.44 | 2.69 | 4 | 1 |
| 2:C:21:C:O5' | 2:C:21:C:C6 | 0.44 | 2.71 | 10 | 3 |
| 1:A:16:LEU:CD2 | 1:A:76:PHE:CE1 | 0.44 | 3.00 | 11 | 1 |
| 1:A:89:ASP:N | 2:D:44:A:H61 | 0.44 | 2.11 | 11 | 1 |
| 1:A:25:LEU:HD23 | 1:A:54:ALA:HB2 | 0.44 | 1.89 | 13 | 1 |
| 1:A:12:TYR:O | 1:A:12:TYR:CG | 0.44 | 2.71 | 11 | 10 |
| 1:A:16:LEU:HD22 | 1:A:25:LEU:HD22 | 0.44 | 1.88 | 2 | 1 |
| 2:D:45:C:C5 | 2:D:45:C:OP2 | 0.44 | 2.70 | 5 | 1 |
| 2:D:49:G:O5' | 2:D:49:G:C8 | 0.44 | 2.70 | 10 | 1 |
| 1:A:99:THR:HG22 | 1:B:96:MET:CE | 0.44 | 2.41 | 13 | 1 |
| 1:B:89:ASP:CA | 2:C:18:A:H61 | 0.44 | 2.26 | 7 | 3 |
| 1:B:9:HIS:CB | 1:B:89:ASP:CB | 0.44 | 2.96 | 7 | 3 |
| 2:C:15:U:C6 | 2:C:15:U:OP2 | 0.44 | 2.71 | 10 | 2 |
| 1:B:10:THR:OG1 | 1:B:56:VAL:O | 0.44 | 2.26 | 13 | 2 |
| 2:C:18:A:N6 | 2:C:19:C:N4 | 0.44 | 2.66 | 11 | 1 |
| 1:A:99:THR:HG22 | 1:A:99:THR:O | 0.44 | 2.13 | 13 | 1 |
| 1:A:101:VAL:HG11 | 1:B:100:PHE:HB3 | 0.43 | 1.89 | 5 | 2 |
| 2:C:25:G:OP1 | 2:C:25:G:C8 | 0.43 | 2.70 | 2 | 1 |
| 1:A:89:ASP:HA | 2:D:44:A:N6 | 0.43 | 2.28 | 3 | 4 |
| 1:A:92:ILE:CD1 | 1:A:93:ILE:CD1 | 0.43 | 2.96 | 5 | 2 |
| 1:B:55:PHE:CB | 2:C:18:A:C2 | 0.43 | 3.01 | 7 | 1 |
| 2:C:25:G:O5' | 2:C:25:G:C8 | 0.43 | 2.71 | 8 | 1 |
| 2:D:51:G:O5' | 2:D:51:G:C8 | 0.43 | 2.71 | 8 | 1 |
| 1:B:10:THR:CG2 | 2:C:18:A:H61 | 0.43 | 2.26 | 9 | 1 |
| 1:A:90:SER:OG | 1:A:92:ILE:HD12 | 0.43 | 2.13 | 11 | 1 |
| 2:C:14:U:O5' | 2:C:14:U:C6 | 0.43 | 2.70 | 1 | 2 |
| 2:C:14:U:O2' | 2:C:15:U:P | 0.43 | 2.75 | 4 | 1 |
| 2:D:45:C:OP1 | 2:D:46:C:C2 | 0.43 | 2.71 | 8 | 2 |
| 1:B:25:LEU:HD23 | 1:B:54:ALA:HB2 | 0.43 | 1.89 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:68:LEU:CD1 | 1:B:83:ILE:HG22 | 0.43 | 2.43 | 6 | 2 |
| 2:C:18:A:C5 | 2:C:19:C:C4 | 0.43 | 3.06 | 3 | 1 |
| 1:B:85:TYR:O | 2:C:17:C:C5 | 0.43 | 2.71 | 5 | 4 |
| 1:B:12:TYR:O | 1:B:12:TYR:CG | 0.43 | 2.71 | 11 | 9 |
| 2:C:16:G:O5' | 2:C:16:G:C8 | 0.43 | 2.71 | 4 | 2 |
| 2:C:19:C:OP1 | 2:C:20:C:C4 | 0.43 | 2.72 | 6 | 2 |
| 1:A:96:MET:HE2 | 1:B:99:THR:HB | 0.43 | 1.91 | 9 | 1 |
| 1:B:11:ILE:HG22 | 1:B:85:TYR:HA | 0.43 | 1.91 | 11 | 1 |
| 2:D:44:A:N6 | 2:D:45:C:N4 | 0.43 | 2.66 | 11 | 1 |
| 1:A:68:LEU:CD1 | 1:A:83:ILE:HG22 | 0.43 | 2.43 | 6 | 2 |
| 1:B:12:TYR:HB3 | 1:B:55:PHE:CD2 | 0.43 | 2.48 | 7 | 6 |
| 1:A:99:THR:O | 1:A:100:PHE:CD2 | 0.43 | 2.71 | 2 | 2 |
| 1:B:20:ILE:HG22 | 1:B:21:LYS:N | 0.43 | 2.28 | 4 | 5 |
| 1:B:99:THR:O | 1:B:100:PHE:CD2 | 0.43 | 2.71 | 2 | 2 |
| 1:A:25:LEU:HD23 | 1:A:44:VAL:HG11 | 0.43 | 1.88 | 3 | 1 |
| 1:A:12:TYR:HB3 | 1:A:55:PHE:CD2 | 0.43 | 2.48 | 7 | 6 |
| 1:A:87:LYS:CG | 2:D:43:C:C2 | 0.43 | 3.01 | 11 | 3 |
| 1:A:16:LEU:HD12 | 1:A:53:GLN:CA | 0.43 | 2.43 | 4 | 1 |
| 1:B:87:LYS:CG | 2:C:17:C:C2 | 0.43 | 3.01 | 6 | 3 |
| 2:C:9:A:O5' | 2:C:9:A:C8 | 0.43 | 2.71 | 3 | 3 |
| 1:A:100:PHE:HB3 | 1:B:101:VAL:HG11 | 0.43 | 1.90 | 5 | 2 |
| 1:B:10:THR:CG2 | 1:B:11:ILE:N | 0.43 | 2.82 | 2 | 2 |
| 1:B:20:ILE:CD1 | 1:B:25:LEU:HD21 | 0.43 | 2.39 | 2 | 1 |
| 1:B:32:ILE:CD1 | 1:B:76:PHE:CZ | 0.43 | 2.98 | 2 | 2 |
| 1:B:85:TYR:O | 2:C:17:C:N4 | 0.43 | 2.52 | 7 | 3 |
| 2:C:19:C:OP1 | 2:C:20:C:C2 | 0.43 | 2.71 | 8 | 2 |
| 1:A:99:THR:CG2 | 1:A:101:VAL:CG2 | 0.43 | 2.96 | 11 | 1 |
| 1:A:32:ILE:HD13 | 1:A:71:MET:HE2 | 0.43 | 1.90 | 12 | 1 |
| 1:A:100:PHE:C | 1:A:101:VAL:HG22 | 0.43 | 2.34 | 13 | 1 |
| 1:A:57:ILE:HD12 | 1:A:90:SER:OG | 0.43 | 2.13 | 3 | 1 |
| 2:D:45:C:OP1 | 2:D:46:C:C4 | 0.43 | 2.72 | 6 | 2 |
| 2:D:41:U:O4' | 2:D:42:G:C6 | 0.43 | 2.72 | 8 | 2 |
| 2:C:25:G:HO2' | 2:C:26:U:H6 | 0.43 | 1.57 | 10 | 1 |
| 1:A:96:MET:CE | 1:B:96:MET:HE1 | 0.43 | 2.43 | 13 | 1 |
| 1:A:89:ASP:CA | 2:D:44:A:H61 | 0.43 | 2.25 | 1 | 3 |
| 1:B:17:ASN:HB2 | 1:B:20:ILE:HD11 | 0.43 | 1.91 | 2 | 1 |
| 1:B:89:ASP:HA | 2:C:18:A:H61 | 0.43 | 1.74 | 7 | 3 |
| 2:D:51:G:H2' | 2:D:52:U:C6 | 0.43 | 2.49 | 11 | 1 |
| 1:A:96:MET:O | 1:A:99:THR:N | 0.43 | 2.52 | 13 | 1 |
| 1:B:100:PHE:C | 1:B:101:VAL:HG22 | 0.43 | 2.34 | 13 | 1 |
| 1:A:44:VAL:HG12 | 1:A:54:ALA:CB | 0.43 | 2.44 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:44:VAL:HG12 | 1:B:54:ALA:CB | 0.43 | 2.44 | 1 | 1 |
| 2:D:54:U:H2' | 2:D:55:C:C6 | 0.43 | 2.49 | 11 | 5 |
| 1:B:89:ASP:HA | 2:C:18:A:N6 | 0.43 | 2.28 | 3 | 4 |
| 2:D:42:G:OP2 | 2:D:42:G:C4 | 0.43 | 2.72 | 12 | 2 |
| 2:C:18:A:O5' | 2:C:18:A:H8 | 0.43 | 1.97 | 10 | 2 |
| 1:B:99:THR:CG2 | 1:B:101:VAL:CG2 | 0.43 | 2.96 | 11 | 1 |
| 2:C:16:G:C4 | 2:C:16:G:OP2 | 0.43 | 2.72 | 12 | 1 |
| 2:D:41:U:O4' | 2:D:42:G:C2 | 0.42 | 2.73 | 13 | 4 |
| 1:A:85:TYR:O | 2:D:43:C:N4 | 0.42 | 2.52 | 12 | 3 |
| 2:C:11:A:C2 | 2:C:12:C:O2 | 0.42 | 2.72 | 6 | 2 |
| 2:C:15:U:C4' | 2:C:16:G:OP2 | 0.42 | 2.67 | 6 | 1 |
| 1:B:14:ASN:OD1 | 2:C:16:G:C8 | 0.42 | 2.72 | 11 | 1 |
| 1:A:12:TYR:CD2 | 2:D:43:C:N3 | 0.42 | 2.87 | 12 | 1 |
| 1:B:92:ILE:O | 1:B:96:MET:HG3 | 0.42 | 2.14 | 13 | 1 |
| 2:C:15:U:O4' | 2:C:16:G:C2 | 0.42 | 2.72 | 13 | 4 |
| 2:C:12:C:O2' | 2:C:13:A:H5' | 0.42 | 2.15 | 5 | 1 |
| 1:A:89:ASP:HA | 2:D:44:A:H61 | 0.42 | 1.74 | 7 | 2 |
| 1:B:45:SER:OG | 2:D:50:A:N6 | 0.42 | 2.53 | 7 | 3 |
| 2:C:15:U:O4' | 2:C:16:G:C6 | 0.42 | 2.72 | 8 | 2 |
| 2:D:41:U:C6 | 2:D:41:U:OP2 | 0.42 | 2.72 | 10 | 2 |
| 1:B:12:TYR:CE1 | 2:C:17:C:C2 | 0.42 | 3.06 | 9 | 1 |
| 1:A:14:ASN:OD1 | 2:D:42:G:C8 | 0.42 | 2.72 | 11 | 1 |
| 1:A:92:ILE:O | 1:A:96:MET:HG3 | 0.42 | 2.14 | 13 | 1 |
| 1:B:33:PHE:O | 1:B:58:PHE:CE1 | 0.42 | 2.72 | 2 | 1 |
| 1:B:85:TYR:O | 2:C:17:C:C4 | 0.42 | 2.73 | 11 | 3 |
| 1:B:99:THR:CG2 | 1:B:100:PHE:N | 0.42 | 2.82 | 4 | 3 |
| 1:B:56:VAL:O | 1:B:58:PHE:CE1 | 0.42 | 2.73 | 5 | 2 |
| 2:C:16:G:OP2 | 2:C:16:G:C4 | 0.42 | 2.72 | 6 | 1 |
| 2:C:24:A:C2 | 2:D:46:C:O2 | 0.42 | 2.72 | 10 | 1 |
| 2:D:44:A:O5' | 2:D:44:A:H8 | 0.42 | 1.97 | 12 | 2 |
| 1:A:11:ILE:HG22 | 1:A:85:TYR:HA | 0.42 | 1.90 | 11 | 1 |
| 1:B:89:ASP:N | 2:C:18:A:H61 | 0.42 | 2.12 | 11 | 1 |
| 2:D:48:G:C2 | 2:D:49:G:C5 | 0.42 | 3.08 | 11 | 1 |
| 2:D:43:C:OP1 | 2:D:43:C:C6 | 0.42 | 2.71 | 13 | 1 |
| 1:A:99:THR:CG2 | 1:A:100:PHE:N | 0.42 | 2.82 | 4 | 3 |
| 1:B:61:VAL:HG12 | 1:B:65:THR:OG1 | 0.42 | 2.15 | 7 | 1 |
| 1:B:51:ARG:O | 2:C:16:G:N2 | 0.42 | 2.53 | 8 | 1 |
| 1:A:10:THR:CG2 | 2:D:44:A:H61 | 0.42 | 2.27 | 9 | 1 |
| 1:A:100:PHE:O | 1:A:100:PHE:CD2 | 0.42 | 2.72 | 11 | 2 |
| 2:C:23:G:O6 | 2:C:24:A:N6 | 0.42 | 2.53 | 12 | 1 |
| 1:B:11:ILE:CG1 | 1:B:56:VAL:CG1 | 0.42 | 2.97 | 8 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:C:21:C:O2 | 2:D:49:G:N2 | 0.42 | 2.53 | 2 | 7 |
| 2:D:44:A:H2' | 2:D:45:C:C5 | 0.42 | 2.50 | 2 | 1 |
| 1:B:92:ILE:CD1 | 1:B:93:ILE:CD1 | 0.42 | 2.96 | 5 | 3 |
| 1:B:20:ILE:HB | 1:B:25:LEU:HD21 | 0.42 | 1.91 | 8 | 1 |
| 1:B:100:PHE:O | 1:B:100:PHE:CD2 | 0.42 | 2.72 | 11 | 2 |
| 2:C:20:C:O2 | 2:D:50:A:C2 | 0.42 | 2.73 | 10 | 1 |
| 2:D:49:G:O6 | 2:D:50:A:N6 | 0.42 | 2.53 | 12 | 1 |
| 2:C:23:G:N2 | 2:D:47:C:O2 | 0.42 | 2.53 | 1 | 7 |
| 2:D:40:U:O2 | 2:D:42:G:N2 | 0.42 | 2.53 | 1 | 2 |
| 1:A:17:ASN:HB2 | 1:A:20:ILE:HD11 | 0.42 | 1.91 | 2 | 1 |
| 1:A:85:TYR:O | 2:D:43:C:C4 | 0.42 | 2.72 | 11 | 3 |
| 1:B:44:VAL:HG12 | 1:B:45:SER:N | 0.42 | 2.30 | 2 | 2 |
| 2:C:27:C:O2 | 2:D:37:A:C2 | 0.42 | 2.72 | 3 | 1 |
| 1:B:16:LEU:HD12 | 1:B:53:GLN:CA | 0.42 | 2.43 | 4 | 1 |
| 1:A:58:PHE:CD1 | 1:A:58:PHE:N | 0.42 | 2.88 | 6 | 1 |
| 2:C:22:G:C2 | 2:C:23:G:C5 | 0.42 | 3.08 | 11 | 1 |
| 2:C:25:G:H2' | 2:C:26:U:C6 | 0.42 | 2.49 | 11 | 1 |
| 1:A:11:ILE:CG1 | 1:A:56:VAL:CG1 | 0.42 | 2.98 | 13 | 5 |
| 2:C:28:U:H2' | 2:C:29:C:C6 | 0.42 | 2.49 | 11 | 5 |
| 2:D:38:C:O2' | 2:D:39:A:H5' | 0.42 | 2.14 | 5 | 1 |
| 2:D:41:U:C1' | 2:D:42:G:OP2 | 0.42 | 2.68 | 9 | 2 |
| 1:A:61:VAL:HG12 | 1:A:65:THR:OG1 | 0.42 | 2.15 | 7 | 1 |
| 1:A:20:ILE:CD1 | 1:A:77:TYR:CD2 | 0.42 | 3.02 | 9 | 1 |
| 2:C:19:C:H5' | 2:C:20:C:C6 | 0.42 | 2.50 | 9 | 1 |
| 2:D:45:C:H5' | 2:D:46:C:C6 | 0.42 | 2.50 | 9 | 1 |
| 1:A:101:VAL:CG1 | 1:B:101:VAL:HG21 | 0.42 | 2.42 | 13 | 1 |
| 2:C:17:C:OP1 | 2:C:17:C:C6 | 0.42 | 2.72 | 13 | 1 |
| 1:A:33:PHE:O | 1:A:58:PHE:CZ | 0.42 | 2.72 | 2 | 1 |
| 1:B:33:PHE:O | 1:B:58:PHE:CZ | 0.42 | 2.72 | 2 | 1 |
| 2:C:18:A:H2' | 2:C:18:A:OP2 | 0.42 | 2.15 | 2 | 1 |
| 1:B:57:ILE:HG22 | 1:B:58:PHE:N | 0.42 | 2.30 | 4 | 2 |
| 2:D:41:U:C4' | 2:D:42:G:OP2 | 0.42 | 2.67 | 6 | 1 |
| 1:B:12:TYR:CD2 | 2:C:17:C:N3 | 0.42 | 2.87 | 12 | 1 |
| 1:A:20:ILE:CG2 | 1:A:24:GLU:CB | 0.42 | 2.98 | 8 | 3 |
| 2:D:37:A:C2 | 2:D:38:C:O2 | 0.42 | 2.73 | 3 | 1 |
| 1:A:56:VAL:O | 1:A:58:PHE:CE1 | 0.42 | 2.73 | 5 | 2 |
| 2:D:52:U:O5' | 2:D:52:U:C6 | 0.42 | 2.70 | 5 | 1 |
| 1:B:53:GLN:OE1 | 2:C:16:G:C8 | 0.42 | 2.73 | 6 | 3 |
| 2:C:26:U:O4 | 2:C:27:C:N4 | 0.42 | 2.53 | 10 | 2 |
| 1:A:13:ILE:HA | 1:A:83:ILE:HG23 | 0.42 | 1.92 | 11 | 1 |
| 1:A:58:PHE:CD2 | 1:A:64:ALA:HA | 0.42 | 2.50 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:96:MET:O | 1:B:99:THR:N | 0.42 | 2.52 | 13 | 1 |
| 1:A:44:VAL:HG12 | 1:A:45:SER:N | 0.42 | 2.30 | 2 | 2 |
| 1:B:13:ILE:CD1 | 1:B:29:LEU:CD2 | 0.42 | 2.98 | 2 | 1 |
| 2:C:20:C:OP2 | 2:C:21:C:C5 | 0.42 | 2.73 | 2 | 1 |
| 1:B:99:THR:CG2 | 1:B:101:VAL:HG22 | 0.42 | 2.45 | 6 | 2 |
| 1:A:45:SER:OG | 2:C:24:A:N6 | 0.42 | 2.52 | 7 | 2 |
| 1:B:13:ILE:HA | 1:B:83:ILE:HG23 | 0.42 | 1.92 | 11 | 1 |
| 2:C:18:A:C6 | 2:C:19:C:N4 | 0.42 | 2.88 | 11 | 2 |
| 1:B:55:PHE:CZ | 2:C:18:A:C8 | 0.41 | 3.08 | 5 | 1 |
| 1:B:76:PHE:O | 1:B:77:TYR:CB | 0.41 | 2.68 | 6 | 1 |
| 1:B:89:ASP:C | 2:C:18:A:N6 | 0.41 | 2.73 | 8 | 1 |
| 1:B:20:ILE:CD1 | 1:B:77:TYR:CD2 | 0.41 | 3.02 | 9 | 1 |
| 2:D:52:U:O4 | 2:D:53:C:N4 | 0.41 | 2.53 | 10 | 2 |
| 1:A:86:ALA:HA | 2:D:43:C:N3 | 0.41 | 2.30 | 11 | 2 |
| 1:B:12:TYR:O | 1:B:12:TYR:CD1 | 0.41 | 2.73 | 11 | 1 |
| 2:C:15:U:C2 | 2:C:16:G:C6 | 0.41 | 3.08 | 13 | 1 |
| 1:B:86:ALA:HA | 2:C:17:C:N3 | 0.41 | 2.30 | 13 | 3 |
| 2:C:14:U:O2 | 2:C:16:G:N2 | 0.41 | 2.53 | 1 | 2 |
| 1:A:33:PHE:O | 1:A:58:PHE:CE1 | 0.41 | 2.72 | 2 | 1 |
| 1:A:48:LEU:HD23 | 1:A:48:LEU:C | 0.41 | 2.35 | 2 | 1 |
| 1:A:87:LYS:HG3 | 2:D:43:C:C2 | 0.41 | 2.50 | 6 | 2 |
| 1:A:51:ARG:O | 2:D:42:G:N2 | 0.41 | 2.53 | 8 | 1 |
| 1:B:12:TYR:CD1 | 1:B:55:PHE:CE2 | 0.41 | 3.08 | 12 | 1 |
| 2:C:10:G:O6 | 2:C:11:A:N6 | 0.41 | 2.53 | 2 | 1 |
| 2:D:44:A:H2' | 2:D:44:A:OP2 | 0.41 | 2.15 | 2 | 1 |
| 1:A:96:MET:CE | 1:B:96:MET:O | 0.41 | 2.68 | 4 | 1 |
| 1:A:99:THR:CG2 | 1:A:101:VAL:HG22 | 0.41 | 2.45 | 6 | 2 |
| 1:A:13:ILE:HG22 | 1:A:16:LEU:HD11 | 0.41 | 1.92 | 8 | 1 |
| 1:A:89:ASP:C | 2:D:44:A:N6 | 0.41 | 2.73 | 8 | 1 |
| 2:C:23:G:C2 | 2:D:47:C:O2 | 0.41 | 2.73 | 10 | 1 |
| 1:A:12:TYR:O | 1:A:12:TYR:CD1 | 0.41 | 2.74 | 11 | 1 |
| 1:B:12:TYR:N | 1:B:84:GLN:O | 0.41 | 2.47 | 12 | 1 |
| 1:B:87:LYS:HD2 | 2:C:17:C:C4 | 0.41 | 2.51 | 2 | 2 |
| 2:C:21:C:O2' | 2:C:22:G:H5' | 0.41 | 2.15 | 2 | 1 |
| 1:A:55:PHE:CZ | 2:D:44:A:C8 | 0.41 | 3.08 | 5 | 1 |
| 1:A:76:PHE:O | 1:A:77:TYR:CB | 0.41 | 2.68 | 6 | 1 |
| 1:A:96:MET:O | 1:A:99:THR:CG2 | 0.41 | 2.69 | 6 | 1 |
| 1:A:20:ILE:HB | 1:A:25:LEU:HD21 | 0.41 | 1.91 | 8 | 1 |
| 1:B:13:ILE:HG22 | 1:B:16:LEU:HD11 | 0.41 | 1.92 | 8 | 1 |
| 2:D:44:A:C6 | 2:D:45:C:N4 | 0.41 | 2.89 | 11 | 2 |
| 1:B:58:PHE:CD2 | 1:B:64:ALA:HA | 0.41 | 2.50 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:43:LEU:HD11 | 2:C:19:C:C1' | 0.41 | 2.46 | 13 | 1 |
| 1:B:55:PHE:CE1 | 1:B:86:ALA:HB2 | 0.41 | 2.50 | 8 | 1 |
| 1:B:20:ILE:CG2 | 1:B:24:GLU:CB | 0.41 | 2.99 | 4 | 5 |
| 1:A:12:TYR:CE2 | 1:A:14:ASN:OD1 | 0.41 | 2.74 | 5 | 2 |
| 2:C:9:A:C6 | 2:C:10:G:C6 | 0.41 | 3.08 | 5 | 1 |
| 1:B:9:HIS:CE1 | 1:B:93:ILE:CG2 | 0.41 | 2.99 | 7 | 2 |
| 1:A:55:PHE:CE1 | 1:A:86:ALA:HB2 | 0.41 | 2.50 | 8 | 1 |
| 1:B:11:ILE:HD11 | 1:B:33:PHE:HE2 | 0.41 | 1.70 | 8 | 1 |
| 2:C:15:U:OP2 | 2:C:15:U:C5 | 0.41 | 2.74 | 10 | 1 |
| 1:A:12:TYR:CD1 | 1:A:55:PHE:CE2 | 0.41 | 3.08 | 12 | 1 |
| 2:D:41:U:C2 | 2:D:42:G:C6 | 0.41 | 3.08 | 13 | 1 |
| 1:B:48:LEU:HD23 | 1:B:48:LEU:C | 0.41 | 2.35 | 2 | 1 |
| 2:C:18:A:H2' | 2:C:19:C:C5 | 0.41 | 2.50 | 2 | 1 |
| 1:A:86:ALA:HA | 2:D:43:C:C2 | 0.41 | 2.51 | 4 | 1 |
| 1:A:96:MET:O | 1:B:96:MET:CE | 0.41 | 2.68 | 4 | 1 |
| 2:D:39:A:C4' | 2:D:40:U:OP1 | 0.41 | 2.69 | 4 | 1 |
| 1:B:12:TYR:CZ | 2:C:17:C:C2 | 0.41 | 3.09 | 5 | 1 |
| 1:A:12:TYR:CE1 | 2:D:43:C:C2 | 0.41 | 3.08 | 9 | 1 |
| 1:B:9:HIS:N | 1:B:61:VAL:HG22 | 0.41 | 2.31 | 11 | 1 |
| 2:D:37:A:O5' | 2:D:37:A:H8 | 0.41 | 1.99 | 11 | 1 |
| 1:A:12:TYR:CE1 | 1:A:55:PHE:CE2 | 0.41 | 3.08 | 12 | 1 |
| 1:B:32:ILE:O | 1:B:36:PHE:CE2 | 0.41 | 2.74 | 12 | 1 |
| 1:A:32:ILE:O | 1:A:36:PHE:CZ | 0.41 | 2.74 | 3 | 3 |
| 1:B:68:LEU:HD13 | 1:B:85:TYR:CE1 | 0.41 | 2.51 | 2 | 1 |
| 2:D:36:G:O6 | 2:D:37:A:N6 | 0.41 | 2.53 | 2 | 1 |
| 1:B:33:PHE:O | 1:B:36:PHE:CE2 | 0.41 | 2.74 | 5 | 1 |
| 2:D:35:A:C6 | 2:D:36:G:C6 | 0.41 | 3.08 | 5 | 1 |
| 1:A:11:ILE:HG12 | 1:A:56:VAL:CG2 | 0.41 | 2.46 | 7 | 1 |
| 2:C:21:C:O2 | 2:D:49:G:C2 | 0.41 | 2.73 | 10 | 1 |
| 1:A:92:ILE:HD13 | 1:A:93:ILE:HG13 | 0.41 | 1.93 | 1 | 1 |
| 1:B:12:TYR:CE1 | 1:B:84:GLN:HB2 | 0.41 | 2.51 | 1 | 2 |
| 1:A:10:THR:CG2 | 1:A:11:ILE:N | 0.41 | 2.83 | 3 | 2 |
| 1:A:13:ILE:CD1 | 1:A:29:LEU:CD2 | 0.41 | 2.98 | 2 | 1 |
| 1:B:32:ILE:O | 1:B:36:PHE:CZ | 0.41 | 2.74 | 3 | 3 |
| 2:C:12:C:C4 | 2:C:13:A:N7 | 0.41 | 2.88 | 2 | 1 |
| 2:D:38:C:C4 | 2:D:39:A:N7 | 0.41 | 2.89 | 2 | 1 |
| 2:D:47:C:O2' | 2:D:48:G:H5' | 0.41 | 2.15 | 2 | 1 |
| 1:B:10:THR:OG1 | 1:B:58:PHE:N | 0.41 | 2.54 | 3 | 1 |
| 2:C:11:A:C2 | 2:D:53:C:O2 | 0.41 | 2.74 | 3 | 1 |
| 2:C:23:G:HO2' | 2:C:24:A:H5' | 0.41 | 1.74 | 3 | 1 |
| 1:A:51:ARG:O | 2:D:42:G:C2 | 0.41 | 2.74 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:57:ILE:HG22 | 1:A:58:PHE:N | 0.41 | 2.30 | 4 | 2 |
| 2:C:19:C:OP1 | 2:C:20:C:C1' | 0.41 | 2.69 | 5 | 2 |
| 2:C:19:C:C2' | 2:C:20:C:OP1 | 0.41 | 2.69 | 4 | 2 |
| 1:A:33:PHE:O | 1:A:36:PHE:CE2 | 0.41 | 2.74 | 9 | 2 |
| 2:C:15:U:C1' | 2:C:16:G:C6 | 0.41 | 3.04 | 8 | 1 |
| 2:D:45:C:C2' | 2:D:46:C:OP1 | 0.41 | 2.69 | 8 | 1 |
| 1:A:51:ARG:O | 2:D:42:G:C5 | 0.41 | 2.74 | 11 | 2 |
| 1:A:32:ILE:O | 1:A:36:PHE:CE2 | 0.41 | 2.74 | 12 | 1 |
| 1:A:57:ILE:HD12 | 1:A:90:SER:H | 0.41 | 1.76 | 12 | 1 |
| 1:B:12:TYR:CE1 | 1:B:55:PHE:CE2 | 0.41 | 3.08 | 12 | 1 |
| 1:B:57:ILE:HD12 | 1:B:90:SER:H | 0.41 | 1.76 | 12 | 1 |
| 1:B:99:THR:O | 1:B:99:THR:CG2 | 0.41 | 2.69 | 12 | 1 |
| 1:A:12:TYR:CE1 | 1:A:84:GLN:HB2 | 0.41 | 2.51 | 8 | 2 |
| 1:A:87:LYS:HD2 | 2:D:43:C:C4 | 0.41 | 2.51 | 13 | 2 |
| 1:B:90:SER:CB | 1:B:93:ILE:CD1 | 0.41 | 2.99 | 2 | 1 |
| 1:A:12:TYR:CZ | 2:D:43:C:C2 | 0.41 | 3.09 | 5 | 1 |
| 1:A:10:THR:CG2 | 1:A:89:ASP:HA | 0.41 | 2.46 | 6 | 1 |
| 1:A:58:PHE:CD1 | 1:A:64:ALA:HA | 0.41 | 2.51 | 6 | 1 |
| 2:C:15:U:O4' | 2:C:16:G:C5 | 0.41 | 2.74 | 7 | 1 |
| 1:A:29:LEU:HD23 | 1:A:76:PHE:CE2 | 0.41 | 2.51 | 9 | 1 |
| 1:B:51:ARG:O | 2:C:16:G:C6 | 0.41 | 2.74 | 10 | 1 |
| 1:B:51:ARG:O | 2:C:16:G:C5 | 0.41 | 2.73 | 11 | 2 |
| 1:A:84:GLN:HB3 | 2:D:43:C:N4 | 0.41 | 2.31 | 12 | 1 |
| 1:B:86:ALA:HA | 2:C:17:C:C2 | 0.40 | 2.50 | 4 | 2 |
| 1:B:9:HIS:HB3 | 1:B:89:ASP:CB | 0.40 | 2.46 | 10 | 2 |
| 2:C:13:A:C4' | 2:C:14:U:OP1 | 0.40 | 2.69 | 4 | 1 |
| 2:D:45:C:OP1 | 2:D:46:C:C1' | 0.40 | 2.69 | 5 | 2 |
| 1:A:33:PHE:O | 1:A:36:PHE:CD2 | 0.40 | 2.74 | 5 | 1 |
| 1:B:58:PHE:CD1 | 1:B:64:ALA:HA | 0.40 | 2.51 | 6 | 1 |
| 1:B:87:LYS:HG3 | 2:C:17:C:C2 | 0.40 | 2.51 | 6 | 2 |
| 1:A:53:GLN:OE1 | 2:D:42:G:C8 | 0.40 | 2.73 | 7 | 2 |
| 1:B:11:ILE:HG12 | 1:B:56:VAL:CG2 | 0.40 | 2.46 | 7 | 1 |
| 2:D:41:U:C1' | 2:D:42:G:C6 | 0.40 | 3.04 | 8 | 1 |
| 1:B:29:LEU:HD23 | 1:B:76:PHE:CE2 | 0.40 | 2.51 | 9 | 1 |
| 1:A:47:SER:O | 1:A:49:LYS:N | 0.40 | 2.54 | 10 | 1 |
| 1:A:96:MET:CE | 1:B:99:THR:HB | 0.40 | 2.47 | 11 | 1 |
| 1:A:99:THR:CG2 | 1:B:101:VAL:CG2 | 0.40 | 3.00 | 2 | 1 |
| 1:A:99:THR:N | 1:B:96:MET:CE | 0.40 | 2.84 | 2 | 1 |
| 1:A:101:VAL:CG2 | 1:B:99:THR:HG21 | 0.40 | 2.46 | 2 | 1 |
| 2:D:46:C:OP2 | 2:D:47:C:C5 | 0.40 | 2.74 | 2 | 1 |
| 2:D:40:U:C4' | 2:D:41:U:OP1 | 0.40 | 2.69 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:12:TYR:CE2 | 1:B:14:ASN:OD1 | 0.40 | 2.74 | 5 | 1 |
| 1:B:58:PHE:O | 1:B:59:LYS:CG | 0.40 | 2.69 | 6 | 1 |
| 1:A:43:LEU:HD13 | 1:A:44:VAL:H | 0.40 | 1.77 | 7 | 1 |
| 1:B:14:ASN:ND2 | 2:C:16:G:N7 | 0.40 | 2.69 | 8 | 1 |
| 1:B:39:ILE:HG21 | 1:B:42:ILE:HD11 | 0.40 | 1.94 | 9 | 1 |
| 2:C:23:G:O5' | 2:C:23:G:C8 | 0.40 | 2.71 | 10 | 1 |
| 1:A:99:THR:HB | 1:B:96:MET:CE | 0.40 | 2.47 | 11 | 1 |
| 1:A:99:THR:O | 1:A:99:THR:CG2 | 0.40 | 2.69 | 12 | 1 |
| 1:B:43:LEU:HD13 | 2:C:18:A:C2 | 0.40 | 2.52 | 1 | 1 |
| 2:C:13:A:C6 | 2:D:51:G:O6 | 0.40 | 2.75 | 2 | 1 |
| 1:A:74:PHE:O | 1:A:81:MET:N | 0.40 | 2.55 | 6 | 1 |
| 1:A:74:PHE:CG | 1:A:75:PRO:HD2 | 0.40 | 2.52 | 7 | 1 |
| 1:B:74:PHE:CG | 1:B:75:PRO:HD2 | 0.40 | 2.52 | 7 | 1 |
| 1:A:20:ILE:CB | 1:A:25:LEU:HD21 | 0.40 | 2.47 | 8 | 1 |
| 1:A:39:ILE:HG21 | 1:A:42:ILE:HD11 | 0.40 | 1.94 | 9 | 1 |
| 1:A:32:ILE:CD1 | 1:A:76:PHE:CZ | 0.40 | 3.04 | 13 | 1 |
| 1:A:100:PHE:CD1 | 1:A:100:PHE:O | 0.40 | 2.74 | 13 | 1 |
| 1:B:100:PHE:CD1 | 1:B:100:PHE:O | 0.40 | 2.74 | 13 | 1 |
| 1:A:10:THR:OG1 | 1:A:58:PHE:N | 0.40 | 2.54 | 3 | 1 |
| 1:B:43:LEU:HD23 | 2:C:18:A:O2' | 0.40 | 2.16 | 3 | 1 |
| 2:C:15:U:C2 | 2:C:16:G:O6 | 0.40 | 2.75 | 3 | 1 |
| 2:D:46:C:C4 | 2:D:47:C:N3 | 0.40 | 2.89 | 3 | 1 |
| 1:A:87:LYS:HG2 | 2:D:43:C:C2 | 0.40 | 2.51 | 4 | 1 |
| 2:C:15:U:C1' | 2:C:16:G:OP2 | 0.40 | 2.69 | 6 | 1 |
| 1:B:36:PHE:CE1 | 1:B:67:ALA:HB2 | 0.40 | 2.51 | 11 | 1 |
| 1:A:101:VAL:CG2 | 1:B:101:VAL:CG2 | 0.40 | 2.97 | 13 | 1 |
| 1:A:43:LEU:HD13 | 2:D:44:A:C2 | 0.40 | 2.52 | 1 | 1 |
| 1:B:51:ARG:O | 2:C:16:G:C2 | 0.40 | 2.74 | 4 | 1 |
| 1:B:33:PHE:O | 1:B:36:PHE:CD2 | 0.40 | 2.74 | 5 | 1 |
| 1:B:61:VAL:HG12 | 1:B:65:THR:HG1 | 0.40 | 1.77 | 7 | 1 |
| 2:D:41:U:O4' | 2:D:42:G:C5 | 0.40 | 2.74 | 7 | 1 |
| 1:A:16:LEU:HD21 | 1:A:29:LEU:CD2 | 0.40 | 2.46 | 8 | 1 |
| 1:A:9:HIS:HB3 | 1:A:89:ASP:CB | 0.40 | 2.46 | 10 | 1 |
| 1:A:9:HIS:N | 1:A:61:VAL:HG22 | 0.40 | 2.31 | 11 | 1 |
| 1:B:9:HIS:CD2 | 1:B:59:LYS:O | 0.40 | 2.75 | 12 | 1 |

6.3 Torsion angles

6.3.1 Protein backbone

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|--------------|------------|-------------|----|
| 1 | A | 95/101 (94%) | 74±3 (78±3%) | 16±4 (17±4%) | 5±1 (5±2%) | 4 | 24 |
| 1 | B | 95/101 (94%) | 74±3 (78±3%) | 16±4 (17±4%) | 5±1 (5±2%) | 4 | 24 |
| All | All | 2470/2626 (94%) | 1918 (78%) | 426 (17%) | 126 (5%) | 4 | 24 |

All 40 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 89 | ASP | 12 |
| 1 | B | 89 | ASP | 12 |
| 1 | A | 100 | PHE | 10 |
| 1 | B | 100 | PHE | 10 |
| 1 | A | 59 | LYS | 7 |
| 1 | A | 78 | ASP | 7 |
| 1 | B | 59 | LYS | 7 |
| 1 | B | 78 | ASP | 7 |
| 1 | A | 9 | HIS | 6 |
| 1 | B | 9 | HIS | 6 |
| 1 | A | 54 | ALA | 3 |
| 1 | B | 54 | ALA | 3 |
| 1 | A | 46 | ARG | 2 |
| 1 | A | 71 | MET | 2 |
| 1 | B | 46 | ARG | 2 |
| 1 | B | 71 | MET | 2 |
| 1 | A | 79 | LYS | 2 |
| 1 | B | 79 | LYS | 2 |
| 1 | A | 37 | GLY | 2 |
| 1 | B | 37 | GLY | 2 |
| 1 | A | 15 | ASN | 1 |
| 1 | B | 15 | ASN | 1 |
| 1 | A | 45 | SER | 1 |
| 1 | B | 45 | SER | 1 |
| 1 | A | 19 | LYS | 1 |
| 1 | A | 38 | GLN | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | B | 19 | LYS | 1 |
| 1 | B | 38 | GLN | 1 |
| 1 | A | 90 | SER | 1 |
| 1 | B | 90 | SER | 1 |
| 1 | A | 62 | SER | 1 |
| 1 | B | 62 | SER | 1 |
| 1 | A | 16 | LEU | 1 |
| 1 | B | 16 | LEU | 1 |
| 1 | A | 6 | ARG | 1 |
| 1 | B | 6 | ARG | 1 |
| 1 | A | 83 | ILE | 1 |
| 1 | A | 84 | GLN | 1 |
| 1 | B | 83 | ILE | 1 |
| 1 | B | 84 | GLN | 1 |

6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1 | A | 86/90 (96%) | 72±3 (84±4%) | 14±3 (16±4%) | 5 | 41 |
| 1 | B | 86/90 (96%) | 72±3 (84±4%) | 14±3 (16±4%) | 5 | 41 |
| All | All | 2236/2340 (96%) | 1870 (84%) | 366 (16%) | 5 | 41 |

All 104 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 43 | LEU | 13 |
| 1 | A | 74 | PHE | 13 |
| 1 | B | 43 | LEU | 13 |
| 1 | B | 74 | PHE | 13 |
| 1 | A | 36 | PHE | 10 |
| 1 | A | 100 | PHE | 10 |
| 1 | B | 36 | PHE | 10 |
| 1 | B | 100 | PHE | 10 |
| 1 | A | 9 | HIS | 9 |
| 1 | A | 81 | MET | 9 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | B | 9 | HIS | 9 |
| 1 | B | 81 | MET | 9 |
| 1 | A | 90 | SER | 8 |
| 1 | B | 90 | SER | 8 |
| 1 | A | 41 | ASP | 7 |
| 1 | B | 41 | ASP | 7 |
| 1 | A | 76 | PHE | 6 |
| 1 | B | 76 | PHE | 6 |
| 1 | A | 40 | LEU | 6 |
| 1 | A | 45 | SER | 6 |
| 1 | B | 40 | LEU | 6 |
| 1 | B | 45 | SER | 6 |
| 1 | A | 22 | LYS | 5 |
| 1 | B | 22 | LYS | 5 |
| 1 | A | 87 | LYS | 5 |
| 1 | B | 87 | LYS | 5 |
| 1 | A | 51 | ARG | 4 |
| 1 | B | 51 | ARG | 4 |
| 1 | A | 46 | ARG | 4 |
| 1 | B | 46 | ARG | 4 |
| 1 | A | 78 | ASP | 4 |
| 1 | B | 78 | ASP | 4 |
| 1 | A | 28 | SER | 3 |
| 1 | A | 92 | ILE | 3 |
| 1 | A | 96 | MET | 3 |
| 1 | B | 28 | SER | 3 |
| 1 | B | 92 | ILE | 3 |
| 1 | B | 96 | MET | 3 |
| 1 | A | 89 | ASP | 3 |
| 1 | B | 89 | ASP | 3 |
| 1 | A | 50 | MET | 3 |
| 1 | A | 53 | GLN | 3 |
| 1 | B | 50 | MET | 3 |
| 1 | B | 53 | GLN | 3 |
| 1 | A | 48 | LEU | 2 |
| 1 | A | 49 | LYS | 2 |
| 1 | B | 48 | LEU | 2 |
| 1 | B | 49 | LYS | 2 |
| 1 | A | 10 | THR | 2 |
| 1 | A | 15 | ASN | 2 |
| 1 | A | 21 | LYS | 2 |
| 1 | A | 79 | LYS | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | B | 10 | THR | 2 |
| 1 | B | 15 | ASN | 2 |
| 1 | B | 21 | LYS | 2 |
| 1 | B | 79 | LYS | 2 |
| 1 | A | 6 | ARG | 2 |
| 1 | A | 27 | LYS | 2 |
| 1 | B | 6 | ARG | 2 |
| 1 | B | 27 | LYS | 2 |
| 1 | A | 71 | MET | 2 |
| 1 | B | 71 | MET | 2 |
| 1 | A | 70 | SER | 2 |
| 1 | A | 77 | TYR | 2 |
| 1 | A | 82 | ARG | 2 |
| 1 | A | 99 | THR | 2 |
| 1 | B | 70 | SER | 2 |
| 1 | B | 77 | TYR | 2 |
| 1 | B | 82 | ARG | 2 |
| 1 | B | 99 | THR | 2 |
| 1 | A | 23 | ASP | 2 |
| 1 | B | 23 | ASP | 2 |
| 1 | A | 18 | GLU | 2 |
| 1 | A | 88 | THR | 2 |
| 1 | B | 18 | GLU | 2 |
| 1 | B | 88 | THR | 2 |
| 1 | A | 19 | LYS | 1 |
| 1 | A | 24 | GLU | 1 |
| 1 | A | 34 | SER | 1 |
| 1 | A | 59 | LYS | 1 |
| 1 | B | 19 | LYS | 1 |
| 1 | B | 24 | GLU | 1 |
| 1 | B | 34 | SER | 1 |
| 1 | B | 59 | LYS | 1 |
| 1 | A | 66 | ASN | 1 |
| 1 | B | 66 | ASN | 1 |
| 1 | A | 58 | PHE | 1 |
| 1 | A | 68 | LEU | 1 |
| 1 | B | 58 | PHE | 1 |
| 1 | B | 68 | LEU | 1 |
| 1 | A | 91 | ASP | 1 |
| 1 | B | 91 | ASP | 1 |
| 1 | A | 83 | ILE | 1 |
| 1 | B | 83 | ILE | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 72 | GLN | 1 |
| 1 | B | 72 | GLN | 1 |
| 1 | A | 55 | PHE | 1 |
| 1 | B | 55 | PHE | 1 |
| 1 | A | 16 | LEU | 1 |
| 1 | B | 16 | LEU | 1 |
| 1 | A | 84 | GLN | 1 |
| 1 | B | 84 | GLN | 1 |
| 1 | A | 95 | LYS | 1 |
| 1 | B | 95 | LYS | 1 |

6.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers | Suiteness |
|-----|-------|---------------|-------------------|-----------------|-----------|
| 2 | C | 21/22 (95%) | 14±1 (67±6%) | 4±1 (19±5%) | 0.06±0.02 |
| 2 | D | 21/22 (95%) | 14±1 (67±6%) | 4±1 (19±5%) | 0.06±0.02 |
| All | All | 566/572 (99%) | 368 (65%) | 104 (18%) | 0.06 |

The overall RNA backbone suiteness is 0.06.

All unique RNA backbone outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | C | 11 | A | 13 |
| 2 | C | 16 | G | 13 |
| 2 | C | 17 | C | 13 |
| 2 | C | 18 | A | 13 |
| 2 | D | 37 | A | 13 |
| 2 | D | 42 | G | 13 |
| 2 | D | 43 | C | 13 |
| 2 | D | 44 | A | 13 |
| 2 | C | 14 | U | 12 |
| 2 | C | 25 | G | 12 |
| 2 | D | 40 | U | 12 |
| 2 | D | 51 | G | 12 |
| 2 | C | 10 | G | 11 |
| 2 | C | 20 | C | 11 |
| 2 | D | 36 | G | 11 |
| 2 | D | 46 | C | 11 |
| 2 | C | 19 | C | 11 |
| 2 | D | 45 | C | 11 |
| 2 | C | 13 | A | 10 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | C | 21 | C | 10 |
| 2 | D | 39 | A | 10 |
| 2 | D | 47 | C | 10 |
| 2 | C | 22 | G | 9 |
| 2 | D | 48 | G | 9 |
| 2 | C | 9 | A | 9 |
| 2 | D | 35 | A | 9 |
| 2 | C | 26 | U | 8 |
| 2 | C | 28 | U | 8 |
| 2 | D | 52 | U | 8 |
| 2 | D | 54 | U | 8 |
| 2 | C | 15 | U | 8 |
| 2 | D | 41 | U | 8 |
| 2 | C | 23 | G | 5 |
| 2 | D | 49 | G | 5 |
| 2 | C | 24 | A | 4 |
| 2 | D | 50 | A | 4 |
| 2 | C | 27 | C | 4 |
| 2 | D | 53 | C | 4 |

All unique RNA pucker outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | C | 17 | C | 13 |
| 2 | D | 43 | C | 13 |
| 2 | C | 16 | G | 11 |
| 2 | D | 42 | G | 11 |
| 2 | C | 8 | G | 10 |
| 2 | D | 34 | G | 10 |
| 2 | C | 18 | A | 5 |
| 2 | D | 44 | A | 5 |
| 2 | C | 13 | A | 4 |
| 2 | D | 39 | A | 4 |
| 2 | C | 14 | U | 4 |
| 2 | D | 40 | U | 4 |
| 2 | C | 15 | U | 4 |
| 2 | D | 41 | U | 4 |
| 2 | C | 25 | G | 1 |
| 2 | D | 51 | G | 1 |

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided