



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 12:09 am GMT

PDB ID : 2LKR
Title : Yeast U2/U6 complex
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Deposited on : 2011-10-19

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

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

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | trunk28760 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | recalc28949 |

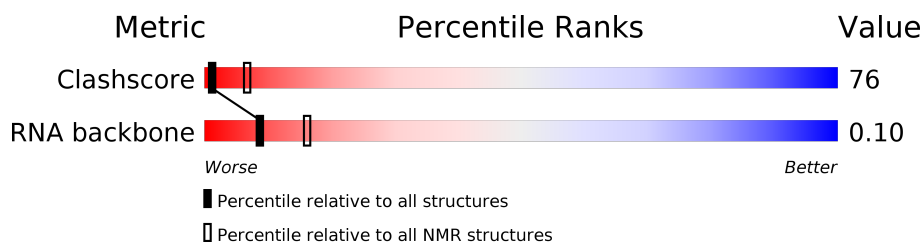
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 3%.

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 | 125131 | 11601 |
| RNA backbone | 3398 | 623 |

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 | 111 | |

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3536 atoms, of which 1186 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (111-MER).

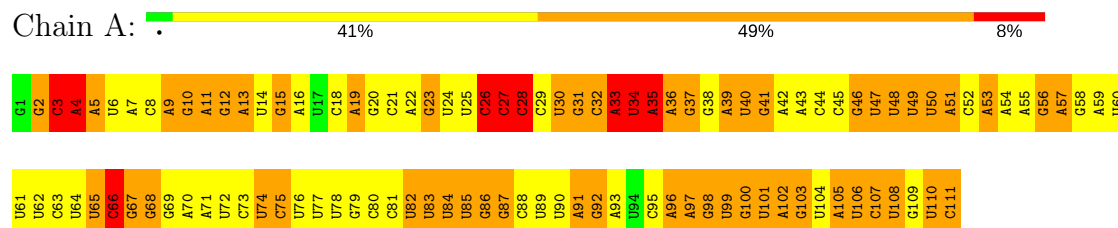
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|------|------|-----|-----|-----|-------|
| 1 | A | 111 | Total | C | H | N | O | P | 0 |
| | | | 3536 | 1053 | 1186 | 406 | 781 | 110 | |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: RNA (111-MER)

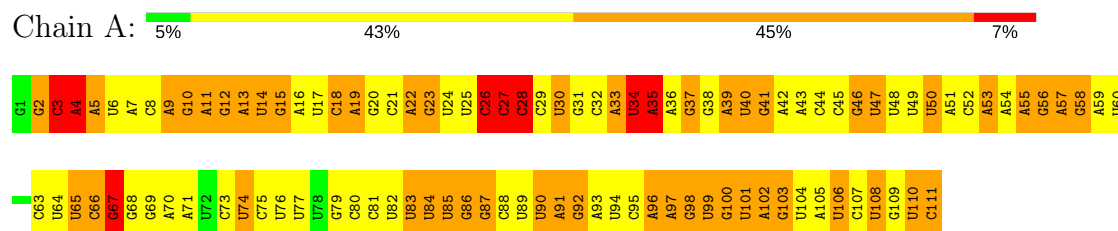


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

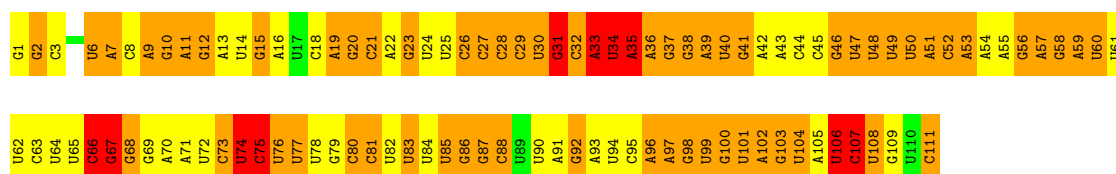
- Molecule 1: RNA (111-MER)



4.2.2 Score per residue for model 2

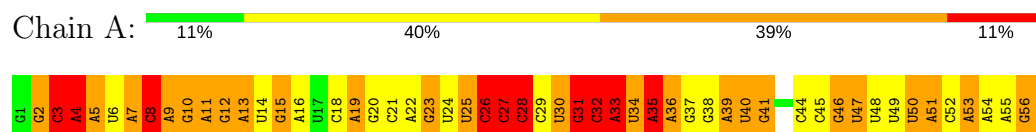
- Molecule 1: RNA (111-MER)





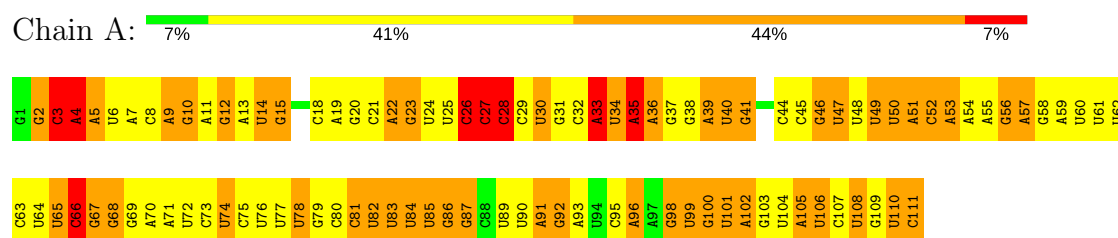
4.2.3 Score per residue for model 3

- Molecule 1: RNA (111-MER)



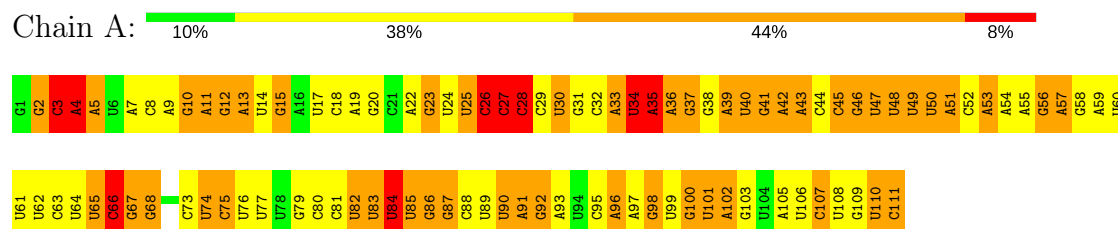
4.2.4 Score per residue for model 4

- Molecule 1: RNA (111-MER)



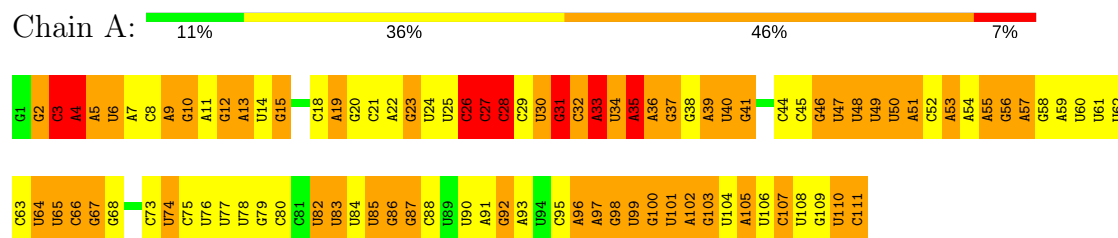
4.2.5 Score per residue for model 5

- Molecule 1: RNA (111-MER)



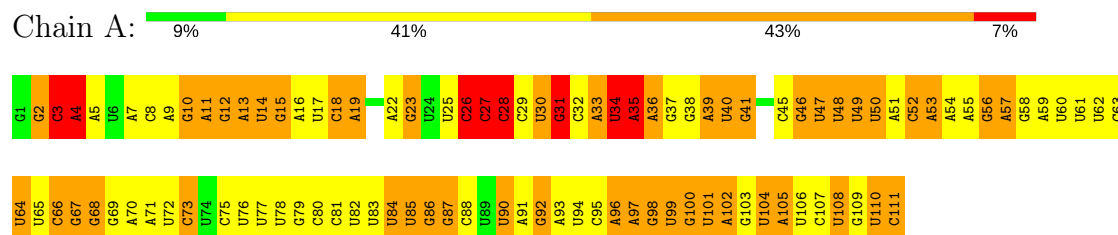
4.2.6 Score per residue for model 6

- Molecule 1: RNA (111-MER)



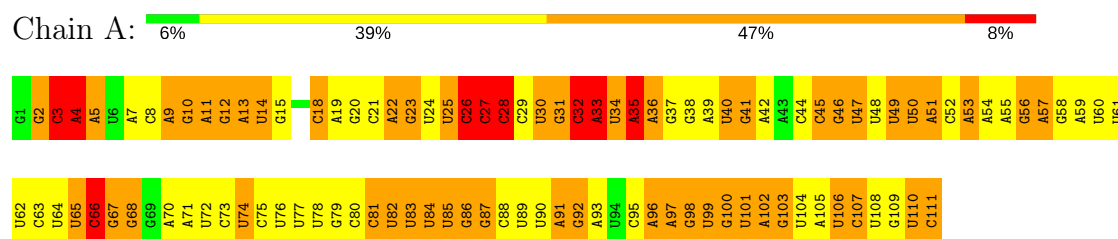
4.2.7 Score per residue for model 7

- Molecule 1: RNA (111-MER)



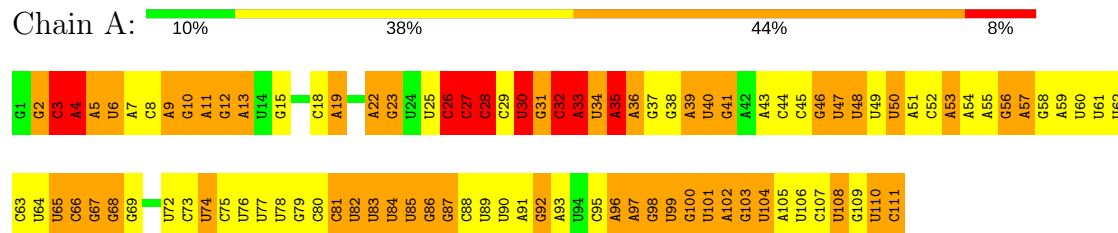
4.2.8 Score per residue for model 8

- Molecule 1: RNA (111-MER)



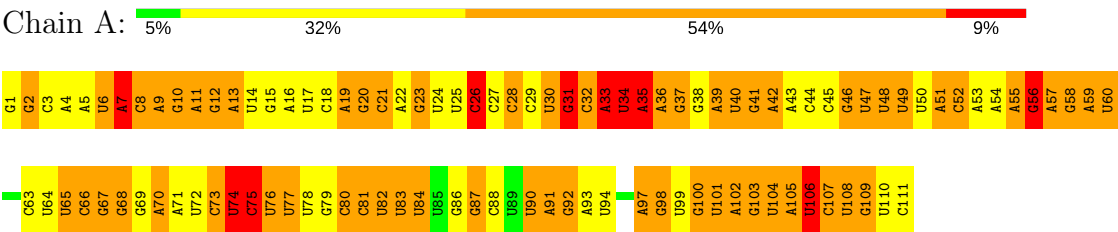
4.2.9 Score per residue for model 9

- Molecule 1: RNA (111-MER)



4.2.10 Score per residue for model 10

● Molecule 1: RNA (111-MER)



5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| X-PLOR NIH | refinement | 2.21 |
| MC-SYM | structure solution | 4.2.2 |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| | |
|--|-------------|
| Chemical shift file(s) | 2lkr_cs.str |
| Number of chemical shift lists | 2 |
| Total number of shifts | 95 |
| Number of shifts mapped to atoms | 95 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 3% |

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

6 Model quality i

6.1 Standard geometry i

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------------|-------------|----------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 1.16±0.04 | 6±3/2625 (0.2±0.1%) | 1.37±0.02 | 12±2/4086 (0.3±0.0%) |
| All | All | 1.16 | 59/26250 (0.2%) | 1.37 | 124/40860 (0.3%) |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1 | A | 0.0±0.0 | 3.4±1.3 |
| All | All | 0 | 34 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 33 | A | N9-C8 | -12.84 | 1.27 | 1.37 | 8 | 7 |
| 1 | A | 33 | A | N3-C4 | -11.88 | 1.27 | 1.34 | 8 | 3 |
| 1 | A | 35 | A | N9-C4 | -8.89 | 1.32 | 1.37 | 8 | 3 |
| 1 | A | 3 | C | N1-C6 | -8.60 | 1.31 | 1.37 | 7 | 3 |
| 1 | A | 31 | G | N9-C8 | -8.32 | 1.32 | 1.37 | 8 | 7 |
| 1 | A | 33 | A | C5-C4 | -8.15 | 1.33 | 1.38 | 9 | 3 |
| 1 | A | 35 | A | C5-C6 | -7.74 | 1.34 | 1.41 | 8 | 3 |
| 1 | A | 34 | U | N1-C6 | -7.23 | 1.31 | 1.38 | 2 | 2 |
| 1 | A | 28 | C | N1-C6 | -7.05 | 1.32 | 1.37 | 9 | 8 |
| 1 | A | 33 | A | N9-C4 | -6.63 | 1.33 | 1.37 | 10 | 3 |
| 1 | A | 33 | A | C2'-C1' | -6.58 | 1.46 | 1.53 | 2 | 3 |
| 1 | A | 33 | A | C2-N3 | -5.84 | 1.28 | 1.33 | 8 | 2 |
| 1 | A | 35 | A | C6-N1 | -5.78 | 1.31 | 1.35 | 4 | 3 |
| 1 | A | 34 | U | C5-C6 | -5.77 | 1.28 | 1.34 | 2 | 1 |
| 1 | A | 75 | C | P-O5' | 5.42 | 1.65 | 1.59 | 2 | 2 |
| 1 | A | 56 | G | C6-N1 | -5.40 | 1.35 | 1.39 | 10 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 8 | C | N1-C6 | -5.33 | 1.33 | 1.37 | 3 | 1 |
| 1 | A | 35 | A | C6-N6 | -5.33 | 1.29 | 1.33 | 3 | 2 |
| 1 | A | 33 | A | C5-C6 | -5.11 | 1.36 | 1.41 | 10 | 1 |
| 1 | A | 34 | U | C2'-C1' | -5.04 | 1.47 | 1.53 | 5 | 1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 3 | C | P-O3'-C3' | 11.93 | 134.02 | 119.70 | 3 | 8 |
| 1 | A | 74 | U | O4'-C1'-N1 | 11.20 | 117.16 | 108.20 | 10 | 2 |
| 1 | A | 35 | A | C1'-O4'-C4' | -10.71 | 101.33 | 109.90 | 1 | 6 |
| 1 | A | 26 | C | P-O3'-C3' | 9.71 | 131.35 | 119.70 | 6 | 8 |
| 1 | A | 3 | C | O4'-C1'-N1 | 8.69 | 115.15 | 108.20 | 3 | 7 |
| 1 | A | 34 | U | O4'-C1'-N1 | 8.11 | 114.69 | 108.20 | 5 | 2 |
| 1 | A | 75 | C | P-O5'-C5' | 7.97 | 133.65 | 120.90 | 2 | 2 |
| 1 | A | 34 | U | C1'-O4'-C4' | -7.53 | 103.87 | 109.90 | 1 | 2 |
| 1 | A | 35 | A | C5'-C4'-O4' | 7.45 | 118.03 | 109.10 | 1 | 3 |
| 1 | A | 4 | A | C8-N9-C4 | -7.33 | 102.87 | 105.80 | 5 | 8 |
| 1 | A | 27 | C | P-O5'-C5' | 7.01 | 132.12 | 120.90 | 3 | 8 |
| 1 | A | 33 | A | C2-N3-C4 | 6.74 | 113.97 | 110.60 | 9 | 3 |
| 1 | A | 35 | A | O4'-C1'-N9 | -6.74 | 102.81 | 108.20 | 9 | 3 |
| 1 | A | 4 | A | O4'-C1'-N9 | 6.73 | 113.59 | 108.20 | 9 | 8 |
| 1 | A | 74 | U | P-O3'-C3' | 6.68 | 127.72 | 119.70 | 10 | 2 |
| 1 | A | 28 | C | C3'-C2'-C1' | 6.57 | 106.75 | 101.50 | 8 | 8 |
| 1 | A | 75 | C | O4'-C1'-N1 | 6.37 | 113.29 | 108.20 | 2 | 1 |
| 1 | A | 34 | U | P-O3'-C3' | 6.32 | 127.29 | 119.70 | 10 | 1 |
| 1 | A | 31 | G | C3'-C2'-C1' | 6.18 | 106.44 | 101.50 | 10 | 3 |
| 1 | A | 106 | U | C1'-O4'-C4' | -6.09 | 105.03 | 109.90 | 10 | 1 |
| 1 | A | 33 | A | N9-C4-C5 | 6.06 | 108.22 | 105.80 | 8 | 3 |
| 1 | A | 106 | U | P-O3'-C3' | 6.05 | 126.96 | 119.70 | 10 | 2 |
| 1 | A | 3 | C | C1'-O4'-C4' | -5.90 | 105.18 | 109.90 | 3 | 1 |
| 1 | A | 35 | A | C5-N7-C8 | -5.75 | 101.02 | 103.90 | 6 | 2 |
| 1 | A | 32 | C | C3'-C2'-C1' | 5.75 | 106.10 | 101.50 | 9 | 2 |
| 1 | A | 84 | U | C1'-O4'-C4' | -5.69 | 105.35 | 109.90 | 5 | 1 |
| 1 | A | 25 | U | C3'-C2'-C1' | 5.66 | 106.03 | 101.50 | 8 | 3 |
| 1 | A | 27 | C | C4'-C3'-C2' | 5.54 | 108.14 | 102.60 | 6 | 1 |
| 1 | A | 67 | G | C1'-O4'-C4' | -5.52 | 105.48 | 109.90 | 3 | 3 |
| 1 | A | 35 | A | C6-N1-C2 | 5.50 | 121.90 | 118.60 | 6 | 2 |
| 1 | A | 26 | C | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 | 7 | 2 |
| 1 | A | 4 | A | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 | 10 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 30 | U | C3'-C2'-C1' | 5.38 | 105.81 | 101.50 | 9 | 1 |
| 1 | A | 35 | A | C3'-C2'-C1' | 5.33 | 105.77 | 101.50 | 8 | 4 |
| 1 | A | 26 | C | C3'-C2'-C1' | 5.26 | 105.71 | 101.50 | 10 | 1 |
| 1 | A | 34 | U | C4'-C3'-C2' | -5.25 | 97.35 | 102.60 | 2 | 1 |
| 1 | A | 34 | U | C6-N1-C1' | -5.25 | 113.85 | 121.20 | 2 | 1 |
| 1 | A | 105 | A | O4'-C1'-N9 | 5.25 | 112.40 | 108.20 | 10 | 1 |
| 1 | A | 74 | U | C2'-C3'-O3' | -5.24 | 97.97 | 109.50 | 2 | 1 |
| 1 | A | 24 | U | C3'-C2'-C1' | 5.15 | 105.62 | 101.50 | 5 | 1 |
| 1 | A | 5 | A | C1'-O4'-C4' | -5.12 | 105.80 | 109.90 | 10 | 1 |
| 1 | A | 107 | C | O3'-P-O5' | -5.11 | 94.30 | 104.00 | 2 | 1 |
| 1 | A | 27 | C | P-O3'-C3' | 5.08 | 125.79 | 119.70 | 3 | 1 |
| 1 | A | 32 | C | C4'-C3'-C2' | -5.02 | 97.58 | 102.60 | 3 | 1 |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 35 | A | Sidechain | 10 |
| 1 | A | 3 | C | Sidechain | 8 |
| 1 | A | 66 | C | Sidechain | 5 |
| 1 | A | 27 | C | Sidechain | 4 |
| 1 | A | 34 | U | Sidechain | 2 |
| 1 | A | 28 | C | Sidechain | 1 |
| 1 | A | 7 | A | Sidechain | 1 |
| 1 | A | 75 | C | Sidechain | 1 |
| 1 | A | 8 | C | Sidechain | 1 |
| 1 | A | 31 | G | Sidechain | 1 |

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 | 2350 | 1186 | 1188 | 270±19 |
| All | All | 23500 | 11860 | 11880 | 2705 |

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 76.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|----------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:33:A:N3 | 1:A:35:A:N1 | 1.32 | 1.76 | 6 | 3 |
| 1:A:32:C:H2' | 1:A:33:A:N7 | 1.21 | 1.51 | 9 | 5 |
| 1:A:31:G:O2' | 1:A:33:A:N1 | 1.11 | 1.81 | 7 | 3 |
| 1:A:33:A:N3 | 1:A:35:A:C6 | 1.06 | 2.23 | 9 | 5 |
| 1:A:33:A:N3 | 1:A:35:A:N6 | 1.03 | 2.07 | 9 | 5 |
| 1:A:33:A:O2' | 1:A:34:U:C6 | 1.01 | 2.12 | 2 | 5 |
| 1:A:33:A:H1' | 1:A:34:U:OP2 | 1.00 | 1.57 | 5 | 1 |
| 1:A:80:C:O2' | 1:A:81:C:H5' | 0.96 | 1.60 | 8 | 5 |
| 1:A:33:A:C6 | 1:A:35:A:N1 | 0.94 | 2.36 | 2 | 3 |
| 1:A:51:A:HO2' | 1:A:52:C:H6 | 0.94 | 1.05 | 3 | 1 |
| 1:A:64:U:O2' | 1:A:66:C:C5 | 0.93 | 2.22 | 8 | 6 |
| 1:A:33:A:C2 | 1:A:35:A:C6 | 0.93 | 2.57 | 7 | 6 |
| 1:A:84:U:H4' | 1:A:86:G:O6 | 0.91 | 1.65 | 4 | 2 |
| 1:A:101:U:HO2' | 1:A:102:A:H8 | 0.90 | 0.92 | 8 | 1 |
| 1:A:37:G:O2' | 1:A:38:G:H5' | 0.90 | 1.66 | 5 | 10 |
| 1:A:34:U:O2' | 1:A:35:A:O5' | 0.89 | 1.89 | 2 | 3 |
| 1:A:9:A:H4' | 1:A:10:G:OP1 | 0.89 | 1.66 | 2 | 3 |
| 1:A:40:U:O2' | 1:A:41:G:H5' | 0.89 | 1.67 | 2 | 4 |
| 1:A:31:G:O2' | 1:A:33:A:C2 | 0.88 | 2.26 | 7 | 3 |
| 1:A:42:A:HO2' | 1:A:43:A:H8 | 0.88 | 1.07 | 5 | 1 |
| 1:A:32:C:C2' | 1:A:33:A:N7 | 0.88 | 2.35 | 9 | 5 |
| 1:A:34:U:OP2 | 1:A:34:U:O4' | 0.88 | 1.91 | 5 | 1 |
| 1:A:11:A:H4' | 1:A:12:G:OP1 | 0.88 | 1.68 | 4 | 4 |
| 1:A:8:C:O2' | 1:A:9:A:H2' | 0.88 | 1.69 | 3 | 3 |
| 1:A:101:U:H4' | 1:A:102:A:OP1 | 0.87 | 1.69 | 10 | 2 |
| 1:A:3:C:O2' | 1:A:4:A:C8 | 0.86 | 2.26 | 7 | 8 |
| 1:A:12:G:OP2 | 1:A:12:G:H2' | 0.86 | 1.71 | 6 | 1 |
| 1:A:73:C:H2' | 1:A:74:U:O4' | 0.85 | 1.71 | 8 | 7 |
| 1:A:107:C:H4' | 1:A:108:U:O5' | 0.85 | 1.70 | 2 | 2 |
| 1:A:33:A:C2 | 1:A:35:A:N6 | 0.85 | 2.45 | 7 | 6 |
| 1:A:31:G:O2' | 1:A:33:A:C4 | 0.85 | 2.30 | 9 | 3 |
| 1:A:103:G:H2' | 1:A:104:U:O4' | 0.85 | 1.70 | 10 | 1 |
| 1:A:33:A:C2 | 1:A:35:A:N1 | 0.84 | 2.45 | 6 | 3 |
| 1:A:33:A:N1 | 1:A:35:A:C6 | 0.83 | 2.47 | 10 | 3 |
| 1:A:56:G:N7 | 1:A:57:A:C5 | 0.82 | 2.48 | 10 | 2 |
| 1:A:34:U:H4' | 1:A:35:A:OP1 | 0.82 | 1.75 | 5 | 2 |
| 1:A:46:G:H4' | 1:A:48:U:O4 | 0.81 | 1.74 | 7 | 2 |
| 1:A:96:A:C2 | 1:A:97:A:N7 | 0.81 | 2.49 | 9 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:33:A:C1' | 1:A:34:U:OP2 | 0.81 | 2.29 | 5 | 1 |
| 1:A:34:U:C5 | 1:A:35:A:C5 | 0.80 | 2.70 | 5 | 2 |
| 1:A:85:U:H5' | 1:A:86:G:OP1 | 0.80 | 1.76 | 9 | 7 |
| 1:A:30:U:H2' | 1:A:31:G:O4' | 0.80 | 1.74 | 10 | 6 |
| 1:A:39:A:H4' | 1:A:40:U:OP1 | 0.80 | 1.74 | 10 | 1 |
| 1:A:56:G:O6 | 1:A:57:A:C2 | 0.80 | 2.34 | 10 | 2 |
| 1:A:49:U:H4' | 1:A:50:U:OP2 | 0.80 | 1.76 | 6 | 1 |
| 1:A:31:G:H21 | 1:A:35:A:H62 | 0.79 | 1.21 | 6 | 3 |
| 1:A:66:C:C2 | 1:A:67:G:C5 | 0.79 | 2.71 | 3 | 6 |
| 1:A:32:C:H3' | 1:A:33:A:C8 | 0.79 | 2.11 | 4 | 3 |
| 1:A:102:A:H2' | 1:A:103:G:O4' | 0.79 | 1.78 | 10 | 2 |
| 1:A:7:A:C2 | 1:A:8:C:C4 | 0.79 | 2.70 | 10 | 1 |
| 1:A:66:C:C2 | 1:A:67:G:N7 | 0.79 | 2.51 | 8 | 6 |
| 1:A:26:C:O2' | 1:A:27:C:C6 | 0.78 | 2.36 | 9 | 8 |
| 1:A:50:U:O2' | 1:A:51:A:H5' | 0.78 | 1.78 | 9 | 4 |
| 1:A:46:G:O3' | 1:A:47:U:H4' | 0.78 | 1.77 | 8 | 4 |
| 1:A:67:G:H2' | 1:A:68:G:O4' | 0.78 | 1.78 | 8 | 1 |
| 1:A:9:A:O2' | 1:A:10:G:N2 | 0.77 | 2.17 | 6 | 2 |
| 1:A:84:U:H5' | 1:A:85:U:OP1 | 0.77 | 1.79 | 5 | 5 |
| 1:A:31:G:O2' | 1:A:33:A:C6 | 0.77 | 2.36 | 10 | 3 |
| 1:A:76:U:O2' | 1:A:77:U:H5' | 0.77 | 1.79 | 10 | 10 |
| 1:A:31:G:N2 | 1:A:35:A:H62 | 0.76 | 1.78 | 6 | 3 |
| 1:A:32:C:H3' | 1:A:33:A:N7 | 0.76 | 1.95 | 4 | 2 |
| 1:A:64:U:O2' | 1:A:66:C:N4 | 0.76 | 2.19 | 5 | 5 |
| 1:A:13:A:H2' | 1:A:13:A:N3 | 0.76 | 1.96 | 3 | 1 |
| 1:A:102:A:N3 | 1:A:102:A:H5' | 0.76 | 1.95 | 10 | 2 |
| 1:A:82:U:H4' | 1:A:83:U:OP1 | 0.75 | 1.80 | 3 | 5 |
| 1:A:101:U:H2' | 1:A:101:U:O2 | 0.75 | 1.79 | 1 | 2 |
| 1:A:7:A:O2' | 1:A:8:C:H5' | 0.75 | 1.82 | 6 | 8 |
| 1:A:105:A:N7 | 1:A:106:U:C5 | 0.75 | 2.55 | 10 | 1 |
| 1:A:33:A:O2' | 1:A:34:U:C2 | 0.75 | 2.39 | 1 | 6 |
| 1:A:34:U:H4' | 1:A:35:A:O5' | 0.74 | 1.81 | 2 | 1 |
| 1:A:98:G:O2' | 1:A:99:U:H5' | 0.74 | 1.82 | 4 | 3 |
| 1:A:9:A:H4' | 1:A:10:G:O5' | 0.74 | 1.80 | 7 | 1 |
| 1:A:65:U:O2' | 1:A:66:C:OP1 | 0.74 | 2.06 | 9 | 6 |
| 1:A:37:G:O2' | 1:A:38:G:O5' | 0.74 | 2.06 | 2 | 1 |
| 1:A:103:G:C6 | 1:A:104:U:C2 | 0.74 | 2.75 | 10 | 1 |
| 1:A:38:G:N3 | 1:A:39:A:N7 | 0.74 | 2.35 | 2 | 1 |
| 1:A:33:A:O2' | 1:A:34:U:O4' | 0.73 | 2.05 | 3 | 6 |
| 1:A:83:U:O2 | 1:A:83:U:H2' | 0.73 | 1.82 | 7 | 1 |
| 1:A:46:G:H1' | 1:A:48:U:O4 | 0.73 | 1.84 | 5 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|----------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:66:C:O2 | 1:A:67:G:N7 | 0.73 | 2.22 | 9 | 4 |
| 1:A:37:G:O2' | 1:A:38:G:C5' | 0.73 | 2.36 | 2 | 6 |
| 1:A:100:G:H2' | 1:A:100:G:OP2 | 0.73 | 1.83 | 1 | 1 |
| 1:A:28:C:O2' | 1:A:29:C:H5' | 0.73 | 1.82 | 1 | 9 |
| 1:A:10:G:H2' | 1:A:11:A:O4' | 0.72 | 1.84 | 2 | 1 |
| 1:A:101:U:O2' | 1:A:102:A:H8 | 0.72 | 1.67 | 8 | 2 |
| 1:A:33:A:C4 | 1:A:35:A:N1 | 0.72 | 2.56 | 9 | 3 |
| 1:A:38:G:O2' | 1:A:39:A:C8 | 0.71 | 2.43 | 1 | 9 |
| 1:A:76:U:H6 | 1:A:76:U:O5' | 0.71 | 1.68 | 2 | 1 |
| 1:A:57:A:C2 | 1:A:75:C:N4 | 0.71 | 2.59 | 2 | 2 |
| 1:A:33:A:N1 | 1:A:35:A:N6 | 0.71 | 2.38 | 7 | 3 |
| 1:A:98:G:N3 | 1:A:98:G:H2' | 0.71 | 1.98 | 5 | 3 |
| 1:A:13:A:O2' | 1:A:14:U:H5' | 0.71 | 1.85 | 2 | 5 |
| 1:A:35:A:H2' | 1:A:36:A:O4' | 0.71 | 1.84 | 9 | 5 |
| 1:A:67:G:N3 | 1:A:67:G:H2' | 0.71 | 2.00 | 3 | 5 |
| 1:A:102:A:H5' | 1:A:102:A:N3 | 0.71 | 2.01 | 4 | 2 |
| 1:A:100:G:H5'' | 1:A:100:G:N3 | 0.71 | 2.01 | 10 | 2 |
| 1:A:49:U:O3' | 1:A:50:U:H4' | 0.70 | 1.86 | 8 | 2 |
| 1:A:13:A:C2 | 1:A:14:U:C2 | 0.70 | 2.80 | 7 | 2 |
| 1:A:102:A:O2' | 1:A:103:G:H5' | 0.70 | 1.87 | 10 | 2 |
| 1:A:97:A:H5'' | 1:A:98:G:OP2 | 0.70 | 1.86 | 9 | 1 |
| 1:A:34:U:O2' | 1:A:35:A:P | 0.70 | 2.49 | 10 | 1 |
| 1:A:65:U:H1' | 1:A:66:C:OP1 | 0.70 | 1.86 | 7 | 3 |
| 1:A:10:G:O2' | 1:A:11:A:H5' | 0.70 | 1.86 | 4 | 5 |
| 1:A:50:U:H1' | 1:A:84:U:O2 | 0.70 | 1.86 | 3 | 1 |
| 1:A:44:C:H4' | 1:A:49:U:O4 | 0.70 | 1.87 | 4 | 1 |
| 1:A:26:C:O2' | 1:A:27:C:H6 | 0.70 | 1.69 | 9 | 8 |
| 1:A:8:C:O2' | 1:A:9:A:C2' | 0.70 | 2.39 | 3 | 3 |
| 1:A:67:G:O2' | 1:A:68:G:H5' | 0.69 | 1.87 | 1 | 9 |
| 1:A:107:C:O2 | 1:A:108:U:H5 | 0.69 | 1.71 | 2 | 1 |
| 1:A:103:G:C5 | 1:A:104:U:C2 | 0.69 | 2.80 | 10 | 1 |
| 1:A:9:A:O2' | 1:A:11:A:N6 | 0.69 | 2.25 | 6 | 1 |
| 1:A:33:A:O2' | 1:A:34:U:N1 | 0.68 | 2.25 | 8 | 4 |
| 1:A:32:C:H2' | 1:A:33:A:C8 | 0.68 | 2.24 | 6 | 2 |
| 1:A:23:G:H8 | 1:A:23:G:OP2 | 0.68 | 1.72 | 9 | 2 |
| 1:A:102:A:H4' | 1:A:103:G:OP1 | 0.68 | 1.87 | 1 | 1 |
| 1:A:33:A:H3' | 1:A:33:A:OP2 | 0.68 | 1.88 | 5 | 1 |
| 1:A:34:U:HO2' | 1:A:35:A:P | 0.68 | 2.10 | 2 | 1 |
| 1:A:74:U:O2' | 1:A:75:C:C5 | 0.68 | 2.46 | 10 | 2 |
| 1:A:33:A:O5' | 1:A:33:A:C8 | 0.68 | 2.46 | 9 | 4 |
| 1:A:76:U:H2' | 1:A:77:U:O4' | 0.68 | 1.89 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:47:U:H4' | 1:A:48:U:OP2 | 0.68 | 1.89 | 6 | 1 |
| 1:A:31:G:O2' | 1:A:33:A:N6 | 0.68 | 2.27 | 2 | 2 |
| 1:A:13:A:N3 | 1:A:13:A:H2' | 0.68 | 2.02 | 9 | 1 |
| 1:A:102:A:N3 | 1:A:102:A:H3' | 0.68 | 2.03 | 10 | 1 |
| 1:A:31:G:O2' | 1:A:33:A:C5 | 0.67 | 2.45 | 9 | 3 |
| 1:A:52:C:C2 | 1:A:53:A:C8 | 0.67 | 2.82 | 9 | 8 |
| 1:A:47:U:O2' | 1:A:48:U:P | 0.67 | 2.52 | 6 | 3 |
| 1:A:31:G:HO2' | 1:A:33:A:N6 | 0.67 | 1.87 | 2 | 1 |
| 1:A:50:U:H2' | 1:A:51:A:O4' | 0.67 | 1.89 | 10 | 2 |
| 1:A:12:G:C2 | 1:A:102:A:C2 | 0.67 | 2.83 | 3 | 1 |
| 1:A:29:C:C2 | 1:A:38:G:N2 | 0.67 | 2.63 | 4 | 4 |
| 1:A:33:A:O2' | 1:A:34:U:C5 | 0.67 | 2.48 | 7 | 3 |
| 1:A:42:A:N3 | 1:A:43:A:N7 | 0.67 | 2.43 | 5 | 1 |
| 1:A:10:G:H5'' | 1:A:10:G:N3 | 0.67 | 2.03 | 7 | 1 |
| 1:A:33:A:C6 | 1:A:35:A:C2 | 0.67 | 2.82 | 10 | 4 |
| 1:A:23:G:N2 | 1:A:24:U:C2 | 0.67 | 2.63 | 3 | 3 |
| 1:A:55:A:C6 | 1:A:56:G:N7 | 0.67 | 2.62 | 2 | 1 |
| 1:A:65:U:O2' | 1:A:66:C:P | 0.67 | 2.52 | 8 | 3 |
| 1:A:108:U:C5 | 1:A:109:G:N7 | 0.67 | 2.63 | 7 | 8 |
| 1:A:47:U:O2 | 1:A:49:U:H1' | 0.67 | 1.90 | 2 | 1 |
| 1:A:9:A:O3' | 1:A:11:A:N6 | 0.67 | 2.28 | 3 | 1 |
| 1:A:3:C:O3' | 1:A:4:A:H8 | 0.66 | 1.72 | 7 | 6 |
| 1:A:12:G:N1 | 1:A:100:G:N2 | 0.66 | 2.43 | 8 | 2 |
| 1:A:10:G:C2 | 1:A:102:A:C8 | 0.66 | 2.82 | 10 | 1 |
| 1:A:79:G:C6 | 1:A:80:C:N4 | 0.66 | 2.63 | 6 | 8 |
| 1:A:63:C:C4 | 1:A:64:U:C4 | 0.66 | 2.83 | 2 | 10 |
| 1:A:33:A:O5' | 1:A:33:A:H8 | 0.66 | 1.72 | 8 | 5 |
| 1:A:12:G:C2 | 1:A:100:G:N2 | 0.66 | 2.64 | 5 | 4 |
| 1:A:15:G:C6 | 1:A:95:C:N4 | 0.66 | 2.64 | 2 | 1 |
| 1:A:57:A:N3 | 1:A:75:C:N4 | 0.66 | 2.44 | 2 | 1 |
| 1:A:92:G:O2' | 1:A:93:A:H5' | 0.66 | 1.91 | 5 | 10 |
| 1:A:31:G:N2 | 1:A:36:A:C6 | 0.66 | 2.64 | 4 | 5 |
| 1:A:10:G:N2 | 1:A:102:A:C5 | 0.66 | 2.63 | 10 | 1 |
| 1:A:66:C:O2 | 1:A:67:G:C2 | 0.66 | 2.48 | 1 | 4 |
| 1:A:52:C:N3 | 1:A:53:A:C5 | 0.66 | 2.64 | 3 | 6 |
| 1:A:55:A:N7 | 1:A:57:A:N6 | 0.66 | 2.43 | 2 | 1 |
| 1:A:10:G:O2' | 1:A:11:A:C8 | 0.66 | 2.49 | 10 | 1 |
| 1:A:52:C:O2' | 1:A:53:A:P | 0.66 | 2.54 | 3 | 8 |
| 1:A:46:G:O2' | 1:A:47:U:H4' | 0.65 | 1.91 | 1 | 4 |
| 1:A:51:A:H4' | 1:A:51:A:OP1 | 0.65 | 1.90 | 2 | 1 |
| 1:A:59:A:C6 | 1:A:60:U:C4 | 0.65 | 2.84 | 1 | 10 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:12:G:N2 | 1:A:100:G:N2 | 0.65 | 2.45 | 10 | 3 |
| 1:A:56:G:C6 | 1:A:76:U:C4 | 0.65 | 2.84 | 10 | 1 |
| 1:A:98:G:N2 | 1:A:99:U:C2 | 0.65 | 2.65 | 6 | 3 |
| 1:A:8:C:C4 | 1:A:9:A:N1 | 0.65 | 2.64 | 9 | 2 |
| 1:A:22:A:N6 | 1:A:87:G:N3 | 0.65 | 2.44 | 1 | 3 |
| 1:A:52:C:O2' | 1:A:53:A:H5'' | 0.65 | 1.91 | 7 | 7 |
| 1:A:74:U:O2' | 1:A:75:C:C6 | 0.65 | 2.50 | 10 | 2 |
| 1:A:96:A:N3 | 1:A:97:A:N7 | 0.65 | 2.45 | 9 | 1 |
| 1:A:58:G:N3 | 1:A:59:A:C8 | 0.65 | 2.65 | 2 | 7 |
| 1:A:32:C:H2' | 1:A:32:C:O5' | 0.65 | 1.91 | 3 | 1 |
| 1:A:84:U:H2' | 1:A:84:U:O2 | 0.65 | 1.92 | 3 | 2 |
| 1:A:11:A:H3' | 1:A:12:G:O4' | 0.65 | 1.90 | 10 | 2 |
| 1:A:55:A:C2 | 1:A:77:U:C2 | 0.65 | 2.85 | 10 | 4 |
| 1:A:7:A:N1 | 1:A:103:G:O6 | 0.65 | 2.30 | 10 | 1 |
| 1:A:9:A:H5'' | 1:A:10:G:OP1 | 0.65 | 1.92 | 9 | 4 |
| 1:A:2:G:OP2 | 1:A:2:G:H8 | 0.65 | 1.75 | 4 | 4 |
| 1:A:58:G:O2' | 1:A:59:A:P | 0.65 | 2.54 | 2 | 9 |
| 1:A:102:A:N6 | 1:A:103:G:C6 | 0.65 | 2.65 | 10 | 1 |
| 1:A:8:C:C4 | 1:A:9:A:N6 | 0.65 | 2.65 | 1 | 2 |
| 1:A:99:U:O3' | 1:A:100:G:H4' | 0.65 | 1.91 | 2 | 2 |
| 1:A:87:G:N2 | 1:A:88:C:C2 | 0.64 | 2.65 | 10 | 2 |
| 1:A:2:G:H8 | 1:A:2:G:OP2 | 0.64 | 1.75 | 8 | 4 |
| 1:A:30:U:C2' | 1:A:31:G:O4' | 0.64 | 2.45 | 9 | 4 |
| 1:A:30:U:O2' | 1:A:31:G:H5' | 0.64 | 1.92 | 7 | 3 |
| 1:A:46:G:C2 | 1:A:47:U:C2 | 0.64 | 2.85 | 2 | 2 |
| 1:A:97:A:C8 | 1:A:98:G:N7 | 0.64 | 2.65 | 8 | 1 |
| 1:A:103:G:C5 | 1:A:104:U:C4 | 0.64 | 2.86 | 2 | 1 |
| 1:A:100:G:N3 | 1:A:102:A:N6 | 0.64 | 2.46 | 4 | 1 |
| 1:A:34:U:C2' | 1:A:34:U:O2 | 0.64 | 2.45 | 5 | 1 |
| 1:A:108:U:C4 | 1:A:109:G:C5 | 0.64 | 2.85 | 6 | 8 |
| 1:A:104:U:C4 | 1:A:105:A:N7 | 0.64 | 2.65 | 2 | 2 |
| 1:A:53:A:C2 | 1:A:79:G:C6 | 0.64 | 2.86 | 3 | 6 |
| 1:A:13:A:C5 | 1:A:98:G:N2 | 0.64 | 2.65 | 3 | 2 |
| 1:A:64:U:O2' | 1:A:66:C:H5 | 0.64 | 1.68 | 8 | 6 |
| 1:A:32:C:HO2' | 1:A:33:A:C5' | 0.64 | 2.05 | 6 | 3 |
| 1:A:4:A:N6 | 1:A:109:G:C2 | 0.64 | 2.66 | 1 | 8 |
| 1:A:32:C:O2' | 1:A:33:A:C8 | 0.64 | 2.51 | 1 | 3 |
| 1:A:100:G:N3 | 1:A:100:G:C5' | 0.64 | 2.61 | 2 | 2 |
| 1:A:100:G:C4 | 1:A:102:A:N6 | 0.64 | 2.66 | 6 | 1 |
| 1:A:26:C:HO2' | 1:A:27:C:H6 | 0.64 | 1.28 | 6 | 1 |
| 1:A:49:U:H6 | 1:A:49:U:OP2 | 0.64 | 1.76 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:32:C:C2' | 1:A:33:A:C8 | 0.64 | 2.81 | 6 | 4 |
| 1:A:84:U:O2 | 1:A:84:U:H2' | 0.64 | 1.93 | 7 | 4 |
| 1:A:33:A:O2' | 1:A:34:U:H6 | 0.64 | 1.71 | 2 | 1 |
| 1:A:69:G:N3 | 1:A:70:A:C8 | 0.64 | 2.66 | 1 | 1 |
| 1:A:53:A:C2 | 1:A:79:G:N1 | 0.64 | 2.66 | 4 | 8 |
| 1:A:79:G:C2 | 1:A:80:C:N3 | 0.64 | 2.66 | 1 | 7 |
| 1:A:12:G:N2 | 1:A:100:G:N3 | 0.64 | 2.47 | 1 | 1 |
| 1:A:13:A:N6 | 1:A:99:U:C6 | 0.64 | 2.66 | 3 | 1 |
| 1:A:13:A:C6 | 1:A:98:G:C2 | 0.63 | 2.86 | 9 | 2 |
| 1:A:101:U:H2' | 1:A:102:A:N7 | 0.63 | 2.08 | 5 | 1 |
| 1:A:30:U:C5 | 1:A:31:G:C6 | 0.63 | 2.85 | 3 | 4 |
| 1:A:91:A:O2' | 1:A:92:G:C8 | 0.63 | 2.51 | 1 | 3 |
| 1:A:108:U:OP2 | 1:A:108:U:H4' | 0.63 | 1.94 | 8 | 3 |
| 1:A:19:A:N1 | 1:A:20:G:C5 | 0.63 | 2.67 | 2 | 3 |
| 1:A:38:G:C2 | 1:A:39:A:N7 | 0.63 | 2.66 | 2 | 1 |
| 1:A:33:A:O2' | 1:A:34:U:P | 0.63 | 2.55 | 5 | 1 |
| 1:A:38:G:C2 | 1:A:39:A:N6 | 0.63 | 2.67 | 10 | 1 |
| 1:A:80:C:O2' | 1:A:81:C:N3 | 0.63 | 2.31 | 10 | 1 |
| 1:A:8:C:C4 | 1:A:9:A:C6 | 0.63 | 2.87 | 7 | 4 |
| 1:A:100:G:O2' | 1:A:101:U:O4' | 0.63 | 2.16 | 9 | 5 |
| 1:A:31:G:O3' | 1:A:33:A:C6 | 0.63 | 2.51 | 8 | 3 |
| 1:A:33:A:C2 | 1:A:35:A:C5 | 0.63 | 2.86 | 10 | 1 |
| 1:A:66:C:C2 | 1:A:67:G:C2 | 0.63 | 2.87 | 10 | 4 |
| 1:A:39:A:O2' | 1:A:40:U:H5' | 0.63 | 1.93 | 3 | 2 |
| 1:A:84:U:H4' | 1:A:85:U:O5' | 0.63 | 1.92 | 3 | 2 |
| 1:A:33:A:O4' | 1:A:35:A:N3 | 0.63 | 2.32 | 3 | 2 |
| 1:A:11:A:C8 | 1:A:11:A:O5' | 0.63 | 2.51 | 3 | 1 |
| 1:A:18:C:C5 | 1:A:19:A:N7 | 0.63 | 2.67 | 9 | 9 |
| 1:A:63:C:C5 | 1:A:64:U:C4 | 0.63 | 2.87 | 2 | 8 |
| 1:A:34:U:C5 | 1:A:35:A:C4 | 0.63 | 2.86 | 1 | 2 |
| 1:A:8:C:O2' | 1:A:10:G:N2 | 0.63 | 2.32 | 9 | 1 |
| 1:A:67:G:N2 | 1:A:68:G:C5 | 0.63 | 2.67 | 1 | 7 |
| 1:A:38:G:N2 | 1:A:39:A:N7 | 0.63 | 2.47 | 2 | 1 |
| 1:A:39:A:C2 | 1:A:40:U:N3 | 0.63 | 2.67 | 2 | 1 |
| 1:A:70:A:C2 | 1:A:71:A:C4 | 0.63 | 2.87 | 1 | 1 |
| 1:A:101:U:O2' | 1:A:102:A:C8 | 0.63 | 2.46 | 8 | 3 |
| 1:A:51:A:C5 | 1:A:52:C:N4 | 0.62 | 2.67 | 9 | 2 |
| 1:A:53:A:N1 | 1:A:54:A:C5 | 0.62 | 2.67 | 6 | 7 |
| 1:A:8:C:N3 | 1:A:9:A:C8 | 0.62 | 2.67 | 2 | 1 |
| 1:A:102:A:O2' | 1:A:103:G:C4 | 0.62 | 2.52 | 1 | 2 |
| 1:A:83:U:O2' | 1:A:84:U:C6 | 0.62 | 2.51 | 4 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:64:U:O2' | 1:A:66:C:C4 | 0.62 | 2.51 | 5 | 5 |
| 1:A:110:U:O5' | 1:A:110:U:H6 | 0.62 | 1.76 | 5 | 5 |
| 1:A:108:U:C5 | 1:A:109:G:C5 | 0.62 | 2.88 | 7 | 4 |
| 1:A:39:A:C2 | 1:A:40:U:C2 | 0.62 | 2.88 | 2 | 5 |
| 1:A:58:G:O2' | 1:A:59:A:O5' | 0.62 | 2.18 | 2 | 10 |
| 1:A:100:G:O2' | 1:A:101:U:C6 | 0.62 | 2.52 | 1 | 1 |
| 1:A:49:U:H4' | 1:A:50:U:OP1 | 0.62 | 1.93 | 4 | 1 |
| 1:A:101:U:O2' | 1:A:102:A:N7 | 0.62 | 2.30 | 7 | 3 |
| 1:A:12:G:C2 | 1:A:100:G:C2 | 0.62 | 2.88 | 9 | 3 |
| 1:A:53:A:C2 | 1:A:79:G:C2 | 0.62 | 2.88 | 6 | 7 |
| 1:A:56:G:N2 | 1:A:76:U:C2 | 0.62 | 2.68 | 5 | 6 |
| 1:A:46:G:N2 | 1:A:47:U:C2 | 0.62 | 2.67 | 2 | 1 |
| 1:A:33:A:C5 | 1:A:35:A:C2 | 0.62 | 2.87 | 10 | 5 |
| 1:A:10:G:N2 | 1:A:11:A:C2 | 0.62 | 2.68 | 5 | 2 |
| 1:A:13:A:N6 | 1:A:97:A:C6 | 0.62 | 2.67 | 8 | 1 |
| 1:A:31:G:H1' | 1:A:33:A:C2 | 0.62 | 2.30 | 8 | 3 |
| 1:A:39:A:C2 | 1:A:40:U:O2 | 0.62 | 2.52 | 3 | 8 |
| 1:A:103:G:H8 | 1:A:103:G:O5' | 0.62 | 1.77 | 2 | 1 |
| 1:A:66:C:N3 | 1:A:67:G:C5 | 0.62 | 2.67 | 2 | 2 |
| 1:A:31:G:N2 | 1:A:36:A:N6 | 0.62 | 2.47 | 8 | 4 |
| 1:A:31:G:HO2' | 1:A:32:C:H6 | 0.62 | 1.37 | 1 | 1 |
| 1:A:13:A:N7 | 1:A:98:G:N2 | 0.62 | 2.47 | 9 | 2 |
| 1:A:37:G:C2 | 1:A:38:G:C4 | 0.62 | 2.88 | 2 | 3 |
| 1:A:13:A:N1 | 1:A:97:A:N1 | 0.62 | 2.46 | 8 | 1 |
| 1:A:44:C:N4 | 1:A:45:C:N4 | 0.62 | 2.48 | 8 | 3 |
| 1:A:102:A:N1 | 1:A:103:G:C6 | 0.62 | 2.68 | 2 | 1 |
| 1:A:47:U:O2' | 1:A:48:U:C2 | 0.62 | 2.53 | 2 | 1 |
| 1:A:8:C:C4 | 1:A:9:A:N7 | 0.62 | 2.68 | 2 | 1 |
| 1:A:31:G:O2' | 1:A:32:C:H6 | 0.62 | 1.76 | 1 | 1 |
| 1:A:22:A:N7 | 1:A:45:C:H1' | 0.62 | 2.10 | 5 | 2 |
| 1:A:51:A:C2 | 1:A:52:C:N4 | 0.62 | 2.67 | 4 | 2 |
| 1:A:101:U:O3' | 1:A:102:A:N7 | 0.62 | 2.33 | 3 | 1 |
| 1:A:31:G:N2 | 1:A:36:A:C2 | 0.62 | 2.68 | 5 | 1 |
| 1:A:79:G:N1 | 1:A:80:C:N4 | 0.62 | 2.48 | 8 | 5 |
| 1:A:32:C:C6 | 1:A:33:A:N6 | 0.62 | 2.68 | 2 | 4 |
| 1:A:26:C:C2' | 1:A:27:C:H5'' | 0.62 | 2.25 | 7 | 7 |
| 1:A:70:A:N6 | 1:A:71:A:N6 | 0.62 | 2.47 | 10 | 3 |
| 1:A:69:G:C2 | 1:A:70:A:C8 | 0.62 | 2.88 | 1 | 1 |
| 1:A:33:A:O4' | 1:A:35:A:C2 | 0.62 | 2.52 | 4 | 2 |
| 1:A:54:A:N1 | 1:A:55:A:C5 | 0.62 | 2.68 | 4 | 5 |
| 1:A:38:G:C2 | 1:A:39:A:C6 | 0.62 | 2.88 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:22:A:N1 | 1:A:87:G:N3 | 0.61 | 2.48 | 9 | 4 |
| 1:A:67:G:O2' | 1:A:68:G:C5' | 0.61 | 2.48 | 3 | 10 |
| 1:A:20:G:C2 | 1:A:21:C:C2 | 0.61 | 2.88 | 1 | 3 |
| 1:A:10:G:H2' | 1:A:10:G:N3 | 0.61 | 2.10 | 3 | 3 |
| 1:A:31:G:H1' | 1:A:35:A:N6 | 0.61 | 2.10 | 5 | 2 |
| 1:A:31:G:O2' | 1:A:35:A:N1 | 0.61 | 2.33 | 3 | 2 |
| 1:A:48:U:O5' | 1:A:48:U:H6 | 0.61 | 1.78 | 5 | 2 |
| 1:A:89:U:O2' | 1:A:90:U:C6 | 0.61 | 2.53 | 5 | 1 |
| 1:A:53:A:C6 | 1:A:54:A:C5 | 0.61 | 2.88 | 5 | 7 |
| 1:A:92:G:C4' | 1:A:92:G:OP1 | 0.61 | 2.48 | 7 | 4 |
| 1:A:77:U:C4 | 1:A:78:U:C5 | 0.61 | 2.88 | 6 | 3 |
| 1:A:103:G:C6 | 1:A:104:U:C4 | 0.61 | 2.89 | 2 | 1 |
| 1:A:22:A:N1 | 1:A:87:G:C4 | 0.61 | 2.67 | 4 | 1 |
| 1:A:53:A:N3 | 1:A:79:G:C2 | 0.61 | 2.69 | 6 | 7 |
| 1:A:78:U:C4 | 1:A:79:G:N7 | 0.61 | 2.68 | 10 | 1 |
| 1:A:27:C:OP1 | 1:A:27:C:C6 | 0.61 | 2.53 | 6 | 3 |
| 1:A:97:A:O2' | 1:A:98:G:C8 | 0.61 | 2.52 | 7 | 4 |
| 1:A:108:U:H2' | 1:A:109:G:O4' | 0.61 | 1.95 | 6 | 4 |
| 1:A:1:G:C6 | 1:A:111:C:N3 | 0.61 | 2.68 | 2 | 1 |
| 1:A:54:A:C4 | 1:A:55:A:C8 | 0.61 | 2.88 | 6 | 4 |
| 1:A:82:U:O2' | 1:A:83:U:P | 0.61 | 2.58 | 5 | 4 |
| 1:A:91:A:O2' | 1:A:92:G:N9 | 0.61 | 2.34 | 2 | 3 |
| 1:A:20:G:N2 | 1:A:21:C:C2 | 0.61 | 2.68 | 1 | 6 |
| 1:A:13:A:C5 | 1:A:98:G:C2 | 0.61 | 2.89 | 9 | 1 |
| 1:A:63:C:C5 | 1:A:64:U:C5 | 0.61 | 2.88 | 9 | 10 |
| 1:A:72:U:O2' | 1:A:73:C:O5' | 0.61 | 2.19 | 10 | 7 |
| 1:A:97:A:N7 | 1:A:98:G:C6 | 0.61 | 2.68 | 5 | 2 |
| 1:A:110:U:H6 | 1:A:110:U:O5' | 0.61 | 1.79 | 8 | 3 |
| 1:A:13:A:N6 | 1:A:98:G:C4 | 0.61 | 2.68 | 9 | 1 |
| 1:A:54:A:C6 | 1:A:55:A:C5 | 0.61 | 2.89 | 1 | 6 |
| 1:A:33:A:N6 | 1:A:35:A:N1 | 0.61 | 2.48 | 2 | 1 |
| 1:A:94:U:C4 | 1:A:95:C:N4 | 0.61 | 2.68 | 7 | 2 |
| 1:A:33:A:N3 | 1:A:34:U:C6 | 0.61 | 2.69 | 3 | 3 |
| 1:A:1:G:N2 | 1:A:2:G:C5 | 0.61 | 2.69 | 2 | 2 |
| 1:A:102:A:C6 | 1:A:103:G:C6 | 0.61 | 2.89 | 10 | 1 |
| 1:A:48:U:H1' | 1:A:49:U:OP1 | 0.61 | 1.95 | 10 | 1 |
| 1:A:102:A:O2' | 1:A:103:G:C5 | 0.61 | 2.53 | 1 | 1 |
| 1:A:66:C:O2 | 1:A:67:G:C8 | 0.61 | 2.54 | 2 | 2 |
| 1:A:15:G:C6 | 1:A:96:A:N6 | 0.61 | 2.69 | 6 | 5 |
| 1:A:53:A:C2 | 1:A:54:A:C4 | 0.61 | 2.89 | 7 | 5 |
| 1:A:44:C:C4 | 1:A:45:C:N4 | 0.60 | 2.69 | 9 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:1:G:N1 | 1:A:111:C:C2 | 0.60 | 2.69 | 2 | 1 |
| 1:A:84:U:O2' | 1:A:85:U:C6 | 0.60 | 2.53 | 6 | 3 |
| 1:A:11:A:H2' | 1:A:11:A:N3 | 0.60 | 2.11 | 2 | 1 |
| 1:A:69:G:C2 | 1:A:70:A:N7 | 0.60 | 2.70 | 1 | 1 |
| 1:A:66:C:C4 | 1:A:67:G:O6 | 0.60 | 2.55 | 9 | 6 |
| 1:A:101:U:O2' | 1:A:102:A:C2 | 0.60 | 2.54 | 2 | 2 |
| 1:A:12:G:N7 | 1:A:13:A:N7 | 0.60 | 2.49 | 10 | 1 |
| 1:A:46:G:H4' | 1:A:46:G:OP1 | 0.60 | 1.95 | 5 | 1 |
| 1:A:87:G:O2' | 1:A:88:C:C4' | 0.60 | 2.49 | 8 | 2 |
| 1:A:92:G:H4' | 1:A:92:G:OP1 | 0.60 | 1.94 | 5 | 8 |
| 1:A:33:A:C6 | 1:A:35:A:N3 | 0.60 | 2.70 | 5 | 2 |
| 1:A:42:A:C2 | 1:A:43:A:N7 | 0.60 | 2.69 | 5 | 1 |
| 1:A:66:C:O4' | 1:A:66:C:O2 | 0.60 | 2.18 | 3 | 6 |
| 1:A:103:G:O6 | 1:A:104:U:N3 | 0.60 | 2.34 | 10 | 1 |
| 1:A:15:G:N1 | 1:A:95:C:N4 | 0.60 | 2.49 | 2 | 1 |
| 1:A:10:G:C6 | 1:A:102:A:C8 | 0.60 | 2.89 | 2 | 1 |
| 1:A:13:A:H61 | 1:A:97:A:N6 | 0.60 | 1.95 | 2 | 2 |
| 1:A:49:U:O3' | 1:A:50:U:C4' | 0.60 | 2.50 | 4 | 2 |
| 1:A:10:G:H3' | 1:A:11:A:N7 | 0.60 | 2.12 | 3 | 1 |
| 1:A:11:A:N1 | 1:A:103:G:N2 | 0.60 | 2.50 | 9 | 1 |
| 1:A:28:C:H5' | 1:A:28:C:C6 | 0.60 | 2.31 | 7 | 6 |
| 1:A:83:U:O2' | 1:A:84:U:C2 | 0.60 | 2.54 | 3 | 3 |
| 1:A:32:C:O2' | 1:A:33:A:P | 0.60 | 2.60 | 4 | 2 |
| 1:A:80:C:H4' | 1:A:81:C:OP1 | 0.60 | 1.94 | 10 | 1 |
| 1:A:8:C:O2' | 1:A:9:A:C8 | 0.60 | 2.51 | 3 | 1 |
| 1:A:42:A:H8 | 1:A:42:A:O5' | 0.60 | 1.79 | 8 | 1 |
| 1:A:40:U:O2' | 1:A:41:G:C8 | 0.60 | 2.55 | 5 | 8 |
| 1:A:25:U:O2' | 1:A:26:C:O5' | 0.60 | 2.19 | 7 | 9 |
| 1:A:101:U:C4' | 1:A:102:A:OP1 | 0.60 | 2.50 | 2 | 1 |
| 1:A:32:C:O2' | 1:A:33:A:H8 | 0.59 | 1.79 | 1 | 1 |
| 1:A:23:G:OP2 | 1:A:23:G:H8 | 0.59 | 1.80 | 8 | 4 |
| 1:A:34:U:OP2 | 1:A:34:U:C1' | 0.59 | 2.50 | 5 | 1 |
| 1:A:84:U:O2' | 1:A:85:U:C2 | 0.59 | 2.55 | 7 | 1 |
| 1:A:32:C:C5 | 1:A:33:A:N6 | 0.59 | 2.70 | 9 | 2 |
| 1:A:53:A:N6 | 1:A:54:A:N6 | 0.59 | 2.50 | 9 | 7 |
| 1:A:64:U:HO2' | 1:A:66:C:H5 | 0.59 | 1.39 | 2 | 3 |
| 1:A:103:G:C6 | 1:A:104:U:N3 | 0.59 | 2.70 | 10 | 2 |
| 1:A:18:C:C4 | 1:A:19:A:N7 | 0.59 | 2.70 | 10 | 1 |
| 1:A:67:G:H2' | 1:A:67:G:N3 | 0.59 | 2.12 | 7 | 4 |
| 1:A:9:A:H2' | 1:A:9:A:N3 | 0.59 | 2.11 | 2 | 1 |
| 1:A:110:U:O2' | 1:A:111:C:H4' | 0.59 | 1.97 | 5 | 8 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:7:A:O2' | 1:A:8:C:O5' | 0.59 | 2.20 | 10 | 2 |
| 1:A:31:G:N2 | 1:A:36:A:H61 | 0.59 | 1.95 | 10 | 1 |
| 1:A:54:A:C6 | 1:A:55:A:N7 | 0.59 | 2.71 | 6 | 3 |
| 1:A:50:U:OP1 | 1:A:50:U:H4' | 0.59 | 1.98 | 6 | 1 |
| 1:A:92:G:OP1 | 1:A:92:G:C4' | 0.59 | 2.50 | 3 | 4 |
| 1:A:33:A:C8 | 1:A:33:A:O5' | 0.59 | 2.55 | 3 | 1 |
| 1:A:34:U:C5 | 1:A:35:A:C6 | 0.59 | 2.91 | 5 | 1 |
| 1:A:10:G:C2 | 1:A:11:A:N6 | 0.59 | 2.71 | 9 | 1 |
| 1:A:44:C:OP1 | 1:A:49:U:H1' | 0.59 | 1.97 | 3 | 2 |
| 1:A:66:C:N3 | 1:A:67:G:N7 | 0.59 | 2.50 | 2 | 1 |
| 1:A:1:G:N2 | 1:A:2:G:C4 | 0.59 | 2.71 | 10 | 1 |
| 1:A:13:A:C6 | 1:A:98:G:N1 | 0.59 | 2.71 | 3 | 1 |
| 1:A:83:U:O2' | 1:A:84:U:N1 | 0.59 | 2.35 | 5 | 3 |
| 1:A:78:U:O2' | 1:A:79:G:H5' | 0.59 | 1.98 | 2 | 1 |
| 1:A:47:U:O2 | 1:A:49:U:H4' | 0.59 | 1.98 | 10 | 1 |
| 1:A:12:G:C6 | 1:A:102:A:N3 | 0.59 | 2.71 | 3 | 1 |
| 1:A:99:U:O3' | 1:A:100:G:C4' | 0.58 | 2.50 | 2 | 1 |
| 1:A:56:G:N7 | 1:A:57:A:N7 | 0.58 | 2.50 | 2 | 1 |
| 1:A:97:A:H4' | 1:A:98:G:OP1 | 0.58 | 1.96 | 10 | 2 |
| 1:A:50:U:HO2' | 1:A:51:A:H5' | 0.58 | 1.58 | 9 | 1 |
| 1:A:7:A:O2' | 1:A:8:C:C5' | 0.58 | 2.50 | 3 | 9 |
| 1:A:70:A:C6 | 1:A:71:A:C5 | 0.58 | 2.92 | 10 | 1 |
| 1:A:76:U:C6 | 1:A:76:U:O5' | 0.58 | 2.56 | 10 | 1 |
| 1:A:96:A:O2' | 1:A:97:A:O4' | 0.58 | 2.19 | 8 | 1 |
| 1:A:40:U:O2' | 1:A:41:G:H8 | 0.58 | 1.79 | 1 | 6 |
| 1:A:3:C:N4 | 1:A:106:U:O4 | 0.58 | 2.36 | 5 | 2 |
| 1:A:7:A:C6 | 1:A:8:C:C4 | 0.58 | 2.91 | 2 | 1 |
| 1:A:104:U:O2' | 1:A:105:A:H5' | 0.58 | 1.98 | 10 | 2 |
| 1:A:66:C:O2' | 1:A:67:G:OP2 | 0.58 | 2.20 | 2 | 8 |
| 1:A:38:G:H2' | 1:A:40:U:O4 | 0.58 | 1.99 | 3 | 7 |
| 1:A:5:A:H8 | 1:A:5:A:O5' | 0.58 | 1.82 | 8 | 2 |
| 1:A:3:C:O3' | 1:A:4:A:C8 | 0.58 | 2.56 | 7 | 5 |
| 1:A:13:A:C2' | 1:A:13:A:N3 | 0.58 | 2.66 | 3 | 1 |
| 1:A:6:U:O2 | 1:A:105:A:C2 | 0.58 | 2.57 | 10 | 2 |
| 1:A:10:G:H22 | 1:A:11:A:H62 | 0.58 | 1.41 | 4 | 1 |
| 1:A:19:A:C2 | 1:A:20:G:C4 | 0.58 | 2.92 | 2 | 3 |
| 1:A:52:C:O2' | 1:A:53:A:C5' | 0.58 | 2.52 | 6 | 8 |
| 1:A:84:U:O2 | 1:A:84:U:C2' | 0.58 | 2.51 | 4 | 4 |
| 1:A:13:A:N6 | 1:A:97:A:N6 | 0.58 | 2.51 | 10 | 2 |
| 1:A:35:A:C6 | 1:A:36:A:C2 | 0.58 | 2.92 | 6 | 1 |
| 1:A:9:A:O2' | 1:A:11:A:C8 | 0.57 | 2.56 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:102:A:N3 | 1:A:102:A:C3' | 0.57 | 2.67 | 10 | 2 |
| 1:A:7:A:C2 | 1:A:8:C:C5 | 0.57 | 2.91 | 10 | 1 |
| 1:A:8:C:N4 | 1:A:104:U:O2 | 0.57 | 2.36 | 10 | 1 |
| 1:A:99:U:OP2 | 1:A:99:U:H6 | 0.57 | 1.81 | 7 | 1 |
| 1:A:55:A:N1 | 1:A:56:G:N7 | 0.57 | 2.51 | 2 | 1 |
| 1:A:90:U:O2' | 1:A:91:A:N7 | 0.57 | 2.28 | 1 | 1 |
| 1:A:12:G:C6 | 1:A:100:G:N2 | 0.57 | 2.72 | 8 | 2 |
| 1:A:56:G:C2 | 1:A:76:U:C2 | 0.57 | 2.91 | 5 | 3 |
| 1:A:79:G:O2' | 1:A:80:C:H5' | 0.57 | 1.99 | 7 | 7 |
| 1:A:89:U:O2 | 1:A:91:A:N6 | 0.57 | 2.38 | 1 | 6 |
| 1:A:28:C:O2' | 1:A:29:C:C5' | 0.57 | 2.52 | 10 | 6 |
| 1:A:87:G:N2 | 1:A:88:C:O2 | 0.57 | 2.37 | 8 | 4 |
| 1:A:33:A:H2' | 1:A:33:A:OP2 | 0.57 | 1.99 | 7 | 2 |
| 1:A:5:A:N6 | 1:A:106:U:C4 | 0.57 | 2.72 | 3 | 2 |
| 1:A:55:A:C6 | 1:A:56:G:C5 | 0.57 | 2.93 | 7 | 6 |
| 1:A:66:C:O4' | 1:A:67:G:C5 | 0.57 | 2.57 | 10 | 3 |
| 1:A:9:A:O4' | 1:A:10:G:N2 | 0.57 | 2.38 | 9 | 4 |
| 1:A:55:A:C6 | 1:A:56:G:C6 | 0.57 | 2.92 | 7 | 7 |
| 1:A:65:U:O2' | 1:A:66:C:O5' | 0.57 | 2.20 | 1 | 3 |
| 1:A:44:C:C5' | 1:A:48:U:O2 | 0.57 | 2.53 | 4 | 1 |
| 1:A:65:U:C2' | 1:A:66:C:C4 | 0.57 | 2.88 | 3 | 5 |
| 1:A:106:U:O2' | 1:A:107:C:H5'' | 0.57 | 1.99 | 2 | 2 |
| 1:A:28:C:H1' | 1:A:40:U:O4 | 0.57 | 1.98 | 2 | 1 |
| 1:A:64:U:C2 | 1:A:66:C:N4 | 0.57 | 2.73 | 10 | 2 |
| 1:A:58:G:HO2' | 1:A:59:A:P | 0.57 | 2.22 | 3 | 4 |
| 1:A:8:C:N3 | 1:A:9:A:N1 | 0.57 | 2.53 | 1 | 2 |
| 1:A:29:C:H1' | 1:A:39:A:N1 | 0.57 | 2.15 | 8 | 4 |
| 1:A:39:A:O2' | 1:A:40:U:O5' | 0.57 | 2.22 | 5 | 6 |
| 1:A:33:A:N1 | 1:A:35:A:N1 | 0.57 | 2.51 | 10 | 2 |
| 1:A:63:C:N4 | 1:A:64:U:C4 | 0.57 | 2.73 | 10 | 1 |
| 1:A:13:A:N6 | 1:A:98:G:N3 | 0.57 | 2.53 | 9 | 1 |
| 1:A:55:A:N6 | 1:A:56:G:O6 | 0.57 | 2.38 | 7 | 7 |
| 1:A:72:U:HO2' | 1:A:73:C:P | 0.57 | 2.22 | 2 | 3 |
| 1:A:83:U:H5' | 1:A:84:U:OP2 | 0.57 | 2.00 | 10 | 2 |
| 1:A:22:A:C6 | 1:A:87:G:N3 | 0.57 | 2.73 | 1 | 2 |
| 1:A:31:G:O2' | 1:A:32:C:C6 | 0.57 | 2.57 | 1 | 1 |
| 1:A:33:A:O2' | 1:A:34:U:N3 | 0.57 | 2.38 | 5 | 1 |
| 1:A:65:U:C6 | 1:A:65:U:OP1 | 0.56 | 2.58 | 9 | 2 |
| 1:A:38:G:O2' | 1:A:39:A:O5' | 0.56 | 2.23 | 2 | 1 |
| 1:A:55:A:C2 | 1:A:56:G:C8 | 0.56 | 2.93 | 2 | 1 |
| 1:A:10:G:N2 | 1:A:11:A:N7 | 0.56 | 2.53 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:84:U:H1' | 1:A:85:U:O4' | 0.56 | 2.00 | 5 | 1 |
| 1:A:103:G:N7 | 1:A:104:U:C4 | 0.56 | 2.73 | 10 | 1 |
| 1:A:47:U:O2' | 1:A:48:U:OP2 | 0.56 | 2.23 | 8 | 4 |
| 1:A:66:C:C4 | 1:A:67:G:C6 | 0.56 | 2.93 | 2 | 2 |
| 1:A:65:U:OP1 | 1:A:65:U:C6 | 0.56 | 2.58 | 5 | 4 |
| 1:A:102:A:O2' | 1:A:103:G:C5' | 0.56 | 2.54 | 10 | 2 |
| 1:A:40:U:O5' | 1:A:40:U:C6 | 0.56 | 2.58 | 1 | 4 |
| 1:A:51:A:H1' | 1:A:83:U:O4 | 0.56 | 2.01 | 1 | 2 |
| 1:A:50:U:O2' | 1:A:51:A:C5' | 0.56 | 2.52 | 5 | 1 |
| 1:A:31:G:H1' | 1:A:33:A:N1 | 0.56 | 2.14 | 7 | 2 |
| 1:A:84:U:H4' | 1:A:84:U:OP1 | 0.56 | 1.99 | 7 | 1 |
| 1:A:10:G:N1 | 1:A:11:A:N6 | 0.56 | 2.53 | 9 | 1 |
| 1:A:56:G:C6 | 1:A:57:A:C6 | 0.56 | 2.93 | 5 | 6 |
| 1:A:79:G:C2 | 1:A:80:C:C4 | 0.56 | 2.94 | 8 | 4 |
| 1:A:82:U:O2' | 1:A:83:U:H5' | 0.56 | 2.01 | 6 | 1 |
| 1:A:39:A:O4' | 1:A:40:U:C6 | 0.56 | 2.59 | 10 | 1 |
| 1:A:82:U:O2' | 1:A:83:U:OP1 | 0.56 | 2.23 | 6 | 3 |
| 1:A:100:G:C3' | 1:A:101:U:O4' | 0.56 | 2.53 | 5 | 1 |
| 1:A:102:A:O2' | 1:A:103:G:C8 | 0.56 | 2.59 | 1 | 1 |
| 1:A:56:G:C6 | 1:A:57:A:C5 | 0.56 | 2.93 | 5 | 1 |
| 1:A:55:A:N6 | 1:A:56:G:C6 | 0.56 | 2.74 | 7 | 1 |
| 1:A:43:A:N6 | 1:A:44:C:N4 | 0.56 | 2.54 | 1 | 2 |
| 1:A:40:U:C6 | 1:A:40:U:O5' | 0.56 | 2.59 | 8 | 4 |
| 1:A:54:A:C2 | 1:A:55:A:C4 | 0.56 | 2.94 | 4 | 7 |
| 1:A:29:C:N3 | 1:A:38:G:C2 | 0.56 | 2.74 | 3 | 4 |
| 1:A:102:A:O5' | 1:A:102:A:H8 | 0.56 | 1.83 | 6 | 1 |
| 1:A:65:U:H2' | 1:A:66:C:C4 | 0.56 | 2.35 | 5 | 6 |
| 1:A:20:G:HO2' | 1:A:21:C:P | 0.56 | 2.24 | 2 | 1 |
| 1:A:103:G:N7 | 1:A:104:U:C5 | 0.56 | 2.74 | 10 | 1 |
| 1:A:22:A:N1 | 1:A:87:G:H1' | 0.56 | 2.16 | 10 | 1 |
| 1:A:80:C:O2' | 1:A:81:C:C2 | 0.56 | 2.58 | 10 | 1 |
| 1:A:28:C:C6 | 1:A:28:C:C5' | 0.55 | 2.89 | 9 | 2 |
| 1:A:39:A:C6 | 1:A:40:U:C4 | 0.55 | 2.93 | 2 | 1 |
| 1:A:49:U:OP1 | 1:A:49:U:H4' | 0.55 | 2.01 | 2 | 1 |
| 1:A:95:C:C2 | 1:A:96:A:N7 | 0.55 | 2.74 | 6 | 3 |
| 1:A:59:A:N6 | 1:A:71:A:N6 | 0.55 | 2.53 | 3 | 3 |
| 1:A:51:A:H5' | 1:A:83:U:O2 | 0.55 | 2.01 | 9 | 1 |
| 1:A:1:G:N2 | 1:A:2:G:N7 | 0.55 | 2.54 | 2 | 1 |
| 1:A:38:G:N3 | 1:A:40:U:O4 | 0.55 | 2.40 | 4 | 4 |
| 1:A:34:U:OP1 | 1:A:34:U:C2 | 0.55 | 2.59 | 5 | 1 |
| 1:A:109:G:O2' | 1:A:110:U:O4' | 0.55 | 2.25 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:33:A:H1' | 1:A:34:U:C6 | 0.55 | 2.37 | 1 | 2 |
| 1:A:66:C:C2 | 1:A:66:C:OP1 | 0.55 | 2.59 | 9 | 2 |
| 1:A:96:A:H2 | 1:A:97:A:N7 | 0.55 | 1.94 | 9 | 2 |
| 1:A:38:G:H21 | 1:A:39:A:H62 | 0.55 | 1.43 | 2 | 1 |
| 1:A:91:A:O2' | 1:A:92:G:C4 | 0.55 | 2.60 | 2 | 1 |
| 1:A:31:G:C4 | 1:A:35:A:N6 | 0.55 | 2.74 | 4 | 1 |
| 1:A:11:A:C2 | 1:A:12:G:O6 | 0.55 | 2.60 | 8 | 1 |
| 1:A:32:C:O2' | 1:A:33:A:O5' | 0.55 | 2.23 | 6 | 4 |
| 1:A:65:U:O2' | 1:A:66:C:C4 | 0.55 | 2.60 | 2 | 5 |
| 1:A:55:A:H62 | 1:A:57:A:N6 | 0.55 | 2.00 | 2 | 1 |
| 1:A:55:A:C2 | 1:A:77:U:O2 | 0.55 | 2.59 | 2 | 5 |
| 1:A:12:G:C6 | 1:A:101:U:O4 | 0.55 | 2.59 | 10 | 1 |
| 1:A:101:U:O3' | 1:A:102:A:C8 | 0.55 | 2.60 | 8 | 3 |
| 1:A:13:A:C6 | 1:A:97:A:N6 | 0.55 | 2.74 | 8 | 1 |
| 1:A:4:A:O2' | 1:A:5:A:H5' | 0.55 | 2.00 | 1 | 6 |
| 1:A:80:C:O2' | 1:A:81:C:C5' | 0.55 | 2.54 | 1 | 4 |
| 1:A:39:A:C1' | 1:A:40:U:OP1 | 0.55 | 2.55 | 2 | 1 |
| 1:A:12:G:C8 | 1:A:13:A:N7 | 0.55 | 2.75 | 10 | 1 |
| 1:A:48:U:H2' | 1:A:48:U:O2 | 0.55 | 2.02 | 7 | 1 |
| 1:A:56:G:C8 | 1:A:57:A:C8 | 0.55 | 2.94 | 2 | 1 |
| 1:A:52:C:O2' | 1:A:53:A:OP2 | 0.55 | 2.25 | 1 | 7 |
| 1:A:98:G:N2 | 1:A:99:U:O2 | 0.55 | 2.40 | 8 | 2 |
| 1:A:15:G:N2 | 1:A:95:C:N3 | 0.55 | 2.55 | 2 | 1 |
| 1:A:47:U:O2' | 1:A:48:U:N1 | 0.55 | 2.40 | 2 | 1 |
| 1:A:76:U:O5' | 1:A:76:U:C6 | 0.55 | 2.57 | 2 | 1 |
| 1:A:26:C:O2 | 1:A:42:A:C2 | 0.55 | 2.60 | 1 | 2 |
| 1:A:10:G:C2' | 1:A:10:G:N3 | 0.55 | 2.69 | 3 | 1 |
| 1:A:11:A:C8 | 1:A:11:A:OP2 | 0.55 | 2.60 | 3 | 1 |
| 1:A:65:U:O2' | 1:A:66:C:C5' | 0.55 | 2.54 | 6 | 1 |
| 1:A:7:A:C2 | 1:A:105:A:C5 | 0.54 | 2.95 | 2 | 1 |
| 1:A:37:G:N2 | 1:A:38:G:C4 | 0.54 | 2.76 | 2 | 4 |
| 1:A:25:U:O2' | 1:A:26:C:O4' | 0.54 | 2.26 | 1 | 3 |
| 1:A:65:U:C1' | 1:A:66:C:OP1 | 0.54 | 2.55 | 1 | 4 |
| 1:A:76:U:C4 | 1:A:77:U:C4 | 0.54 | 2.96 | 1 | 3 |
| 1:A:34:U:C4 | 1:A:35:A:C6 | 0.54 | 2.95 | 5 | 2 |
| 1:A:58:G:N2 | 1:A:74:U:O2 | 0.54 | 2.40 | 5 | 6 |
| 1:A:39:A:O2' | 1:A:40:U:C5' | 0.54 | 2.55 | 3 | 7 |
| 1:A:47:U:HO2' | 1:A:48:U:P | 0.54 | 2.25 | 6 | 3 |
| 1:A:30:U:C4 | 1:A:31:G:C2 | 0.54 | 2.95 | 7 | 4 |
| 1:A:104:U:O2' | 1:A:105:A:C5' | 0.54 | 2.55 | 10 | 2 |
| 1:A:10:G:N1 | 1:A:102:A:C8 | 0.54 | 2.75 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:6:U:O2 | 1:A:7:A:C8 | 0.54 | 2.61 | 10 | 1 |
| 1:A:55:A:C6 | 1:A:76:U:O4 | 0.54 | 2.61 | 10 | 1 |
| 1:A:14:U:H6 | 1:A:14:U:O5' | 0.54 | 1.84 | 1 | 2 |
| 1:A:28:C:C5' | 1:A:28:C:C6 | 0.54 | 2.91 | 7 | 4 |
| 1:A:47:U:OP1 | 1:A:48:U:H5 | 0.54 | 1.84 | 7 | 1 |
| 1:A:53:A:C6 | 1:A:54:A:N7 | 0.54 | 2.74 | 8 | 3 |
| 1:A:55:A:N6 | 1:A:57:A:N6 | 0.54 | 2.55 | 2 | 1 |
| 1:A:65:U:N1 | 1:A:65:U:OP1 | 0.54 | 2.41 | 3 | 2 |
| 1:A:48:U:O2' | 1:A:49:U:H5'' | 0.54 | 2.02 | 5 | 2 |
| 1:A:90:U:O5' | 1:A:90:U:H6 | 0.54 | 1.84 | 10 | 1 |
| 1:A:34:U:O4 | 1:A:35:A:C6 | 0.54 | 2.60 | 1 | 2 |
| 1:A:24:U:O2' | 1:A:25:U:H5' | 0.54 | 2.03 | 3 | 4 |
| 1:A:97:A:N7 | 1:A:98:G:N1 | 0.54 | 2.56 | 5 | 1 |
| 1:A:26:C:O2' | 1:A:27:C:C5 | 0.54 | 2.61 | 8 | 6 |
| 1:A:61:U:O2' | 1:A:62:U:H5' | 0.54 | 2.02 | 6 | 7 |
| 1:A:15:G:C2 | 1:A:95:C:N3 | 0.54 | 2.76 | 2 | 1 |
| 1:A:55:A:N6 | 1:A:57:A:C6 | 0.54 | 2.76 | 2 | 1 |
| 1:A:57:A:N1 | 1:A:58:G:C6 | 0.54 | 2.75 | 2 | 1 |
| 1:A:13:A:O2' | 1:A:14:U:C5' | 0.54 | 2.54 | 10 | 5 |
| 1:A:10:G:C2 | 1:A:101:U:O2 | 0.54 | 2.61 | 10 | 1 |
| 1:A:6:U:O2' | 1:A:7:A:O4' | 0.54 | 2.26 | 10 | 1 |
| 1:A:23:G:O6 | 1:A:45:C:N4 | 0.54 | 2.41 | 1 | 1 |
| 1:A:81:C:O2' | 1:A:82:U:H5' | 0.54 | 2.01 | 7 | 4 |
| 1:A:29:C:C2 | 1:A:38:G:C2 | 0.54 | 2.96 | 3 | 4 |
| 1:A:32:C:O2' | 1:A:33:A:N7 | 0.54 | 2.38 | 10 | 1 |
| 1:A:35:A:C5 | 1:A:36:A:C2 | 0.54 | 2.96 | 10 | 1 |
| 1:A:84:U:C4' | 1:A:85:U:OP1 | 0.54 | 2.56 | 4 | 1 |
| 1:A:82:U:O2' | 1:A:83:U:O5' | 0.54 | 2.26 | 8 | 4 |
| 1:A:65:U:O2' | 1:A:66:C:O4' | 0.54 | 2.25 | 1 | 1 |
| 1:A:46:G:O2' | 1:A:47:U:C4' | 0.54 | 2.56 | 5 | 2 |
| 1:A:44:C:C6 | 1:A:45:C:N4 | 0.54 | 2.75 | 5 | 1 |
| 1:A:13:A:C6 | 1:A:97:A:C6 | 0.54 | 2.95 | 8 | 1 |
| 1:A:102:A:N9 | 1:A:102:A:O5' | 0.54 | 2.41 | 9 | 2 |
| 1:A:47:U:O2 | 1:A:49:U:C4' | 0.54 | 2.56 | 10 | 1 |
| 1:A:65:U:H2' | 1:A:67:G:O6 | 0.54 | 2.03 | 7 | 2 |
| 1:A:101:U:OP2 | 1:A:101:U:N1 | 0.54 | 2.41 | 1 | 1 |
| 1:A:84:U:C2' | 1:A:84:U:O2 | 0.54 | 2.54 | 5 | 2 |
| 1:A:5:A:C8 | 1:A:5:A:O5' | 0.54 | 2.61 | 3 | 2 |
| 1:A:50:U:O2' | 1:A:51:A:O5' | 0.54 | 2.24 | 6 | 2 |
| 1:A:97:A:C5 | 1:A:98:G:O6 | 0.54 | 2.61 | 5 | 1 |
| 1:A:13:A:HO2' | 1:A:14:U:H6 | 0.54 | 1.46 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:78:U:O2' | 1:A:79:G:C5' | 0.54 | 2.56 | 2 | 1 |
| 1:A:43:A:C5 | 1:A:44:C:C4 | 0.54 | 2.95 | 1 | 1 |
| 1:A:29:C:O2 | 1:A:38:G:N2 | 0.54 | 2.41 | 8 | 4 |
| 1:A:108:U:H4' | 1:A:108:U:OP2 | 0.54 | 2.01 | 7 | 3 |
| 1:A:11:A:C5 | 1:A:102:A:N1 | 0.54 | 2.76 | 5 | 1 |
| 1:A:45:C:OP1 | 1:A:48:U:N3 | 0.54 | 2.40 | 8 | 1 |
| 1:A:79:G:N7 | 1:A:80:C:C5 | 0.54 | 2.76 | 2 | 1 |
| 1:A:13:A:N6 | 1:A:97:A:H61 | 0.54 | 2.01 | 10 | 2 |
| 1:A:101:U:C2' | 1:A:101:U:O2 | 0.54 | 2.56 | 1 | 1 |
| 1:A:26:C:N4 | 1:A:28:C:H41 | 0.54 | 2.01 | 6 | 7 |
| 1:A:50:U:C6 | 1:A:85:U:O4 | 0.54 | 2.60 | 8 | 2 |
| 1:A:52:C:OP2 | 1:A:52:C:H6 | 0.54 | 1.85 | 7 | 1 |
| 1:A:31:G:O3' | 1:A:33:A:N6 | 0.53 | 2.41 | 9 | 3 |
| 1:A:43:A:C6 | 1:A:44:C:N4 | 0.53 | 2.76 | 1 | 2 |
| 1:A:53:A:HO2' | 1:A:54:A:P | 0.53 | 2.26 | 3 | 8 |
| 1:A:38:G:N2 | 1:A:39:A:N1 | 0.53 | 2.56 | 10 | 1 |
| 1:A:55:A:N1 | 1:A:76:U:C4 | 0.53 | 2.75 | 10 | 1 |
| 1:A:102:A:O5' | 1:A:102:A:C8 | 0.53 | 2.60 | 6 | 1 |
| 1:A:8:C:N4 | 1:A:9:A:N6 | 0.53 | 2.56 | 7 | 1 |
| 1:A:13:A:C8 | 1:A:99:U:O2 | 0.53 | 2.61 | 9 | 1 |
| 1:A:66:C:O2 | 1:A:66:C:H5' | 0.53 | 2.03 | 2 | 1 |
| 1:A:56:G:N7 | 1:A:57:A:C4 | 0.53 | 2.77 | 10 | 1 |
| 1:A:98:G:C2' | 1:A:98:G:N3 | 0.53 | 2.71 | 1 | 3 |
| 1:A:11:A:O2' | 1:A:12:G:H2' | 0.53 | 2.03 | 1 | 3 |
| 1:A:34:U:O4 | 1:A:35:A:N6 | 0.53 | 2.41 | 1 | 2 |
| 1:A:25:U:O2' | 1:A:26:C:C4' | 0.53 | 2.55 | 7 | 2 |
| 1:A:54:A:C5 | 1:A:55:A:N7 | 0.53 | 2.76 | 6 | 2 |
| 1:A:81:C:O2 | 1:A:82:U:C5 | 0.53 | 2.62 | 8 | 1 |
| 1:A:65:U:H2' | 1:A:66:C:N4 | 0.53 | 2.18 | 3 | 4 |
| 1:A:69:G:O2' | 1:A:70:A:C5' | 0.53 | 2.56 | 10 | 1 |
| 1:A:10:G:O2' | 1:A:11:A:C5' | 0.53 | 2.56 | 4 | 4 |
| 1:A:84:U:H4' | 1:A:85:U:OP1 | 0.53 | 2.03 | 4 | 1 |
| 1:A:2:G:C8 | 1:A:2:G:OP2 | 0.53 | 2.61 | 5 | 2 |
| 1:A:65:U:O2' | 1:A:66:C:H5' | 0.53 | 2.04 | 6 | 1 |
| 1:A:13:A:O2' | 1:A:14:U:O5' | 0.53 | 2.26 | 7 | 1 |
| 1:A:5:A:C5 | 1:A:6:U:C5 | 0.53 | 2.96 | 9 | 2 |
| 1:A:75:C:O2' | 1:A:76:U:H5' | 0.53 | 2.03 | 9 | 9 |
| 1:A:102:A:C4 | 1:A:102:A:O5' | 0.53 | 2.61 | 7 | 2 |
| 1:A:5:A:O5' | 1:A:5:A:C8 | 0.53 | 2.61 | 1 | 3 |
| 1:A:79:G:N1 | 1:A:80:C:C4 | 0.53 | 2.76 | 8 | 3 |
| 1:A:43:A:C6 | 1:A:44:C:C4 | 0.53 | 2.96 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:46:G:O2' | 1:A:47:U:O5' | 0.53 | 2.25 | 2 | 1 |
| 1:A:26:C:O2' | 1:A:27:C:H5'' | 0.53 | 2.03 | 5 | 5 |
| 1:A:85:U:C5' | 1:A:86:G:OP1 | 0.53 | 2.56 | 7 | 6 |
| 1:A:35:A:C2' | 1:A:36:A:O4' | 0.53 | 2.56 | 9 | 5 |
| 1:A:12:G:N2 | 1:A:100:G:C2 | 0.53 | 2.76 | 10 | 4 |
| 1:A:102:A:C6 | 1:A:103:G:C5 | 0.53 | 2.96 | 10 | 1 |
| 1:A:12:G:O6 | 1:A:102:A:N7 | 0.53 | 2.41 | 4 | 1 |
| 1:A:98:G:O2' | 1:A:99:U:C5' | 0.53 | 2.56 | 4 | 3 |
| 1:A:66:C:C4' | 1:A:67:G:O5' | 0.53 | 2.57 | 3 | 2 |
| 1:A:57:A:O2' | 1:A:58:G:H5' | 0.53 | 2.03 | 4 | 7 |
| 1:A:38:G:C4 | 1:A:39:A:N6 | 0.53 | 2.77 | 10 | 1 |
| 1:A:87:G:HO2' | 1:A:88:C:C4' | 0.53 | 2.15 | 8 | 2 |
| 1:A:108:U:O4 | 1:A:109:G:C6 | 0.53 | 2.61 | 1 | 8 |
| 1:A:34:U:H4' | 1:A:35:A:C5' | 0.53 | 2.33 | 2 | 1 |
| 1:A:28:C:O2 | 1:A:40:U:O4 | 0.53 | 2.27 | 2 | 1 |
| 1:A:46:G:O2' | 1:A:47:U:P | 0.53 | 2.67 | 10 | 1 |
| 1:A:46:G:O2' | 1:A:47:U:O4' | 0.53 | 2.27 | 5 | 2 |
| 1:A:50:U:C2 | 1:A:84:U:O4 | 0.53 | 2.62 | 8 | 1 |
| 1:A:52:C:N3 | 1:A:53:A:N7 | 0.53 | 2.57 | 9 | 3 |
| 1:A:19:A:C2 | 1:A:20:G:C5 | 0.53 | 2.97 | 2 | 4 |
| 1:A:86:G:C8 | 1:A:86:G:O5' | 0.53 | 2.61 | 4 | 2 |
| 1:A:102:A:N3 | 1:A:102:A:C5' | 0.53 | 2.71 | 10 | 1 |
| 1:A:38:G:C2 | 1:A:39:A:N1 | 0.53 | 2.76 | 10 | 1 |
| 1:A:4:A:H2' | 1:A:5:A:O4' | 0.53 | 2.03 | 5 | 3 |
| 1:A:31:G:H21 | 1:A:35:A:N6 | 0.53 | 2.02 | 8 | 2 |
| 1:A:22:A:C8 | 1:A:45:C:O2 | 0.53 | 2.62 | 8 | 1 |
| 1:A:56:G:C2 | 1:A:76:U:O2 | 0.53 | 2.61 | 5 | 8 |
| 1:A:92:G:O2' | 1:A:93:A:C5' | 0.53 | 2.57 | 5 | 6 |
| 1:A:53:A:N1 | 1:A:79:G:C6 | 0.53 | 2.77 | 6 | 5 |
| 1:A:30:U:C4 | 1:A:31:G:N1 | 0.53 | 2.77 | 7 | 4 |
| 1:A:37:G:N3 | 1:A:38:G:C8 | 0.53 | 2.77 | 2 | 1 |
| 1:A:103:G:O5' | 1:A:103:G:C8 | 0.52 | 2.61 | 2 | 2 |
| 1:A:95:C:O2' | 1:A:96:A:O5' | 0.52 | 2.25 | 2 | 1 |
| 1:A:11:A:OP1 | 1:A:11:A:H4' | 0.52 | 2.04 | 10 | 1 |
| 1:A:13:A:C5 | 1:A:99:U:O2 | 0.52 | 2.62 | 1 | 1 |
| 1:A:20:G:N2 | 1:A:21:C:O2 | 0.52 | 2.43 | 6 | 2 |
| 1:A:58:G:C2 | 1:A:59:A:C8 | 0.52 | 2.97 | 5 | 6 |
| 1:A:1:G:N2 | 1:A:2:G:C2 | 0.52 | 2.78 | 10 | 1 |
| 1:A:35:A:N7 | 1:A:36:A:C2 | 0.52 | 2.78 | 10 | 1 |
| 1:A:64:U:C6 | 1:A:66:C:N4 | 0.52 | 2.77 | 10 | 2 |
| 1:A:20:G:C2 | 1:A:89:U:O2 | 0.52 | 2.63 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:44:C:H4' | 1:A:49:U:O2 | 0.52 | 2.04 | 5 | 1 |
| 1:A:63:C:N4 | 1:A:64:U:O4 | 0.52 | 2.42 | 3 | 9 |
| 1:A:37:G:HO2' | 1:A:38:G:H5' | 0.52 | 1.63 | 5 | 3 |
| 1:A:107:C:C4' | 1:A:108:U:O5' | 0.52 | 2.51 | 2 | 2 |
| 1:A:39:A:H1' | 1:A:40:U:OP1 | 0.52 | 2.04 | 2 | 1 |
| 1:A:85:U:OP1 | 1:A:86:G:N1 | 0.52 | 2.43 | 2 | 1 |
| 1:A:34:U:H4' | 1:A:34:U:OP1 | 0.52 | 2.04 | 10 | 1 |
| 1:A:53:A:O2' | 1:A:54:A:O5' | 0.52 | 2.25 | 4 | 4 |
| 1:A:46:G:O5' | 1:A:87:G:N7 | 0.52 | 2.42 | 5 | 1 |
| 1:A:53:A:N3 | 1:A:79:G:N2 | 0.52 | 2.58 | 7 | 3 |
| 1:A:20:G:O2' | 1:A:21:C:O5' | 0.52 | 2.28 | 2 | 2 |
| 1:A:20:G:O2' | 1:A:21:C:P | 0.52 | 2.68 | 2 | 2 |
| 1:A:49:U:C4 | 1:A:82:U:O4 | 0.52 | 2.62 | 10 | 1 |
| 1:A:11:A:C4' | 1:A:12:G:OP1 | 0.52 | 2.54 | 1 | 2 |
| 1:A:54:A:N6 | 1:A:55:A:N6 | 0.52 | 2.57 | 1 | 2 |
| 1:A:14:U:O2 | 1:A:97:A:N6 | 0.52 | 2.42 | 3 | 2 |
| 1:A:10:G:N2 | 1:A:11:A:C6 | 0.52 | 2.77 | 5 | 1 |
| 1:A:105:A:O2' | 1:A:106:U:O5' | 0.52 | 2.27 | 1 | 6 |
| 1:A:77:U:C4 | 1:A:78:U:C4 | 0.52 | 2.97 | 7 | 3 |
| 1:A:32:C:C2' | 1:A:32:C:O5' | 0.52 | 2.57 | 3 | 1 |
| 1:A:27:C:C6 | 1:A:27:C:P | 0.52 | 3.03 | 6 | 1 |
| 1:A:83:U:C4 | 1:A:84:U:C4 | 0.52 | 2.97 | 6 | 1 |
| 1:A:2:G:OP2 | 1:A:2:G:C8 | 0.52 | 2.62 | 4 | 6 |
| 1:A:59:A:N6 | 1:A:71:A:H61 | 0.52 | 2.03 | 3 | 3 |
| 1:A:57:A:O2' | 1:A:58:G:C5' | 0.52 | 2.58 | 5 | 5 |
| 1:A:65:U:OP1 | 1:A:65:U:N1 | 0.52 | 2.43 | 5 | 4 |
| 1:A:7:A:C6 | 1:A:8:C:N4 | 0.52 | 2.77 | 2 | 1 |
| 1:A:8:C:N4 | 1:A:9:A:N7 | 0.52 | 2.58 | 2 | 1 |
| 1:A:66:C:O2 | 1:A:67:G:N2 | 0.52 | 2.43 | 7 | 1 |
| 1:A:5:A:O5' | 1:A:5:A:H8 | 0.52 | 1.88 | 4 | 3 |
| 1:A:12:G:N1 | 1:A:101:U:O4 | 0.52 | 2.43 | 2 | 1 |
| 1:A:48:U:C1' | 1:A:49:U:OP1 | 0.52 | 2.58 | 10 | 2 |
| 1:A:39:A:O4' | 1:A:40:U:H5'' | 0.52 | 2.04 | 10 | 1 |
| 1:A:56:G:N7 | 1:A:57:A:C6 | 0.52 | 2.77 | 10 | 1 |
| 1:A:63:C:O2' | 1:A:64:U:O5' | 0.52 | 2.27 | 10 | 1 |
| 1:A:31:G:C2 | 1:A:35:A:N6 | 0.52 | 2.78 | 3 | 1 |
| 1:A:30:U:C5 | 1:A:31:G:C5 | 0.52 | 2.98 | 3 | 2 |
| 1:A:1:G:C2 | 1:A:111:C:O2 | 0.52 | 2.63 | 2 | 1 |
| 1:A:47:U:O2' | 1:A:48:U:O4' | 0.52 | 2.28 | 10 | 1 |
| 1:A:4:A:N6 | 1:A:109:G:N2 | 0.52 | 2.58 | 6 | 2 |
| 1:A:27:C:C6 | 1:A:27:C:OP1 | 0.52 | 2.63 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:13:A:O2' | 1:A:14:U:P | 0.52 | 2.68 | 7 | 1 |
| 1:A:33:A:N3 | 1:A:33:A:O2' | 0.52 | 2.43 | 2 | 1 |
| 1:A:55:A:N6 | 1:A:74:U:O4 | 0.52 | 2.43 | 2 | 1 |
| 1:A:98:G:N3 | 1:A:98:G:C2' | 0.52 | 2.73 | 2 | 4 |
| 1:A:14:U:C6 | 1:A:14:U:O5' | 0.52 | 2.63 | 4 | 1 |
| 1:A:103:G:OP2 | 1:A:103:G:C8 | 0.52 | 2.62 | 6 | 1 |
| 1:A:103:G:OP2 | 1:A:103:G:N7 | 0.52 | 2.43 | 6 | 1 |
| 1:A:76:U:O2' | 1:A:77:U:C5' | 0.51 | 2.59 | 7 | 8 |
| 1:A:106:U:O2' | 1:A:107:C:C5' | 0.51 | 2.58 | 2 | 1 |
| 1:A:48:U:O2 | 1:A:49:U:C1' | 0.51 | 2.58 | 2 | 1 |
| 1:A:12:G:H2' | 1:A:12:G:OP2 | 0.51 | 2.04 | 5 | 1 |
| 1:A:56:G:C6 | 1:A:57:A:N6 | 0.51 | 2.78 | 9 | 4 |
| 1:A:16:A:O2' | 1:A:17:U:O4' | 0.51 | 2.28 | 10 | 3 |
| 1:A:91:A:O5' | 1:A:91:A:C8 | 0.51 | 2.63 | 1 | 1 |
| 1:A:31:G:N2 | 1:A:34:U:O2' | 0.51 | 2.44 | 6 | 1 |
| 1:A:107:C:O4' | 1:A:107:C:O2 | 0.51 | 2.29 | 2 | 2 |
| 1:A:10:G:N1 | 1:A:101:U:O2 | 0.51 | 2.43 | 10 | 1 |
| 1:A:23:G:C8 | 1:A:23:G:OP2 | 0.51 | 2.64 | 10 | 2 |
| 1:A:27:C:C5 | 1:A:27:C:OP1 | 0.51 | 2.64 | 8 | 3 |
| 1:A:10:G:P | 1:A:11:A:H62 | 0.51 | 2.28 | 3 | 1 |
| 1:A:85:U:OP1 | 1:A:86:G:C6 | 0.51 | 2.63 | 9 | 1 |
| 1:A:102:A:H3' | 1:A:102:A:N3 | 0.51 | 2.20 | 2 | 1 |
| 1:A:52:C:O2' | 1:A:53:A:O4' | 0.51 | 2.28 | 2 | 1 |
| 1:A:73:C:C4 | 1:A:74:U:C4 | 0.51 | 2.99 | 2 | 1 |
| 1:A:80:C:O2' | 1:A:81:C:O2 | 0.51 | 2.27 | 2 | 2 |
| 1:A:65:U:OP1 | 1:A:65:U:C2 | 0.51 | 2.63 | 10 | 2 |
| 1:A:33:A:O3' | 1:A:34:U:O4' | 0.51 | 2.28 | 7 | 2 |
| 1:A:69:G:C4 | 1:A:70:A:N7 | 0.51 | 2.79 | 1 | 1 |
| 1:A:102:A:C8 | 1:A:102:A:O5' | 0.51 | 2.63 | 3 | 1 |
| 1:A:56:G:N2 | 1:A:76:U:O2 | 0.51 | 2.44 | 7 | 5 |
| 1:A:59:A:H2' | 1:A:59:A:N3 | 0.51 | 2.19 | 2 | 1 |
| 1:A:8:C:C4 | 1:A:9:A:C8 | 0.51 | 2.99 | 2 | 1 |
| 1:A:48:U:O2 | 1:A:49:U:C6 | 0.51 | 2.63 | 10 | 2 |
| 1:A:10:G:O2' | 1:A:11:A:O4' | 0.51 | 2.28 | 10 | 1 |
| 1:A:59:A:N6 | 1:A:60:U:C4 | 0.51 | 2.78 | 10 | 2 |
| 1:A:110:U:O5' | 1:A:110:U:C6 | 0.51 | 2.62 | 5 | 2 |
| 1:A:54:A:HO2' | 1:A:55:A:P | 0.51 | 2.29 | 6 | 3 |
| 1:A:56:G:C6 | 1:A:76:U:O4 | 0.51 | 2.64 | 10 | 1 |
| 1:A:53:A:N1 | 1:A:79:G:O6 | 0.51 | 2.44 | 3 | 1 |
| 1:A:97:A:N6 | 1:A:98:G:O6 | 0.51 | 2.43 | 3 | 1 |
| 1:A:10:G:C2 | 1:A:102:A:N7 | 0.51 | 2.79 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:81:C:O2' | 1:A:82:U:C5' | 0.51 | 2.59 | 7 | 1 |
| 1:A:13:A:N3 | 1:A:13:A:C2' | 0.51 | 2.72 | 9 | 1 |
| 1:A:56:G:N1 | 1:A:57:A:C6 | 0.51 | 2.79 | 9 | 4 |
| 1:A:26:C:O2' | 1:A:27:C:C5' | 0.51 | 2.59 | 2 | 1 |
| 1:A:37:G:C2 | 1:A:38:G:N9 | 0.51 | 2.79 | 2 | 1 |
| 1:A:44:C:OP1 | 1:A:48:U:H1' | 0.51 | 2.05 | 4 | 1 |
| 1:A:29:C:O2 | 1:A:39:A:C6 | 0.51 | 2.64 | 3 | 3 |
| 1:A:33:A:O2' | 1:A:34:U:C4 | 0.51 | 2.64 | 5 | 1 |
| 1:A:83:U:C4 | 1:A:84:U:O4 | 0.51 | 2.63 | 6 | 1 |
| 1:A:92:G:OP1 | 1:A:92:G:H4' | 0.51 | 2.05 | 10 | 2 |
| 1:A:66:C:O2' | 1:A:67:G:P | 0.51 | 2.69 | 8 | 4 |
| 1:A:14:U:O2' | 1:A:15:G:O5' | 0.51 | 2.29 | 1 | 2 |
| 1:A:10:G:N2 | 1:A:11:A:H62 | 0.51 | 2.03 | 4 | 1 |
| 1:A:84:U:C5' | 1:A:85:U:OP1 | 0.51 | 2.55 | 5 | 3 |
| 1:A:87:G:O2' | 1:A:88:C:O4' | 0.51 | 2.26 | 6 | 1 |
| 1:A:40:U:C5 | 1:A:40:U:OP2 | 0.50 | 2.64 | 9 | 2 |
| 1:A:11:A:H62 | 1:A:12:G:H21 | 0.50 | 1.49 | 2 | 1 |
| 1:A:52:C:O2 | 1:A:53:A:N9 | 0.50 | 2.44 | 3 | 2 |
| 1:A:100:G:C2' | 1:A:100:G:N3 | 0.50 | 2.74 | 5 | 1 |
| 1:A:80:C:O2' | 1:A:81:C:C6 | 0.50 | 2.64 | 5 | 1 |
| 1:A:46:G:C4 | 1:A:49:U:O4 | 0.50 | 2.64 | 9 | 1 |
| 1:A:59:A:N1 | 1:A:60:U:C2 | 0.50 | 2.80 | 5 | 4 |
| 1:A:7:A:C4 | 1:A:8:C:C5 | 0.50 | 2.99 | 2 | 1 |
| 1:A:96:A:N1 | 1:A:97:A:N6 | 0.50 | 2.60 | 2 | 1 |
| 1:A:76:U:O5' | 1:A:76:U:H6 | 0.50 | 1.90 | 10 | 1 |
| 1:A:81:C:O2 | 1:A:81:C:C3' | 0.50 | 2.59 | 10 | 1 |
| 1:A:101:U:H1' | 1:A:102:A:N7 | 0.50 | 2.22 | 1 | 1 |
| 1:A:23:G:C2 | 1:A:24:U:C2 | 0.50 | 2.99 | 6 | 1 |
| 1:A:101:U:C6 | 1:A:101:U:OP2 | 0.50 | 2.64 | 1 | 1 |
| 1:A:89:U:O2' | 1:A:90:U:H2' | 0.50 | 2.05 | 1 | 1 |
| 1:A:11:A:O2' | 1:A:12:G:O5' | 0.50 | 2.29 | 4 | 2 |
| 1:A:56:G:N1 | 1:A:57:A:C5 | 0.50 | 2.80 | 4 | 4 |
| 1:A:84:U:C4' | 1:A:84:U:OP1 | 0.50 | 2.60 | 7 | 1 |
| 1:A:28:C:H2' | 1:A:29:C:C6 | 0.50 | 2.42 | 8 | 5 |
| 1:A:67:G:O2' | 1:A:68:G:O5' | 0.50 | 2.28 | 3 | 2 |
| 1:A:90:U:H6 | 1:A:90:U:O5' | 0.50 | 1.90 | 7 | 1 |
| 1:A:40:U:HO2' | 1:A:41:G:H5' | 0.50 | 1.62 | 2 | 1 |
| 1:A:32:C:O5' | 1:A:32:C:C6 | 0.50 | 2.64 | 10 | 1 |
| 1:A:38:G:C4 | 1:A:40:U:O4 | 0.50 | 2.65 | 3 | 3 |
| 1:A:8:C:O2' | 1:A:9:A:C1' | 0.50 | 2.59 | 6 | 1 |
| 1:A:21:C:N4 | 1:A:87:G:C6 | 0.50 | 2.80 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:38:G:C2' | 1:A:40:U:O4 | 0.50 | 2.58 | 7 | 6 |
| 1:A:101:U:O2 | 1:A:101:U:O2' | 0.50 | 2.30 | 3 | 1 |
| 1:A:44:C:C5 | 1:A:45:C:N4 | 0.50 | 2.79 | 5 | 1 |
| 1:A:63:C:O2' | 1:A:64:U:O4' | 0.50 | 2.25 | 7 | 2 |
| 1:A:46:G:OP2 | 1:A:87:G:N7 | 0.50 | 2.45 | 8 | 1 |
| 1:A:29:C:C1' | 1:A:39:A:H61 | 0.50 | 2.19 | 2 | 1 |
| 1:A:19:A:C2 | 1:A:91:A:N1 | 0.50 | 2.80 | 3 | 1 |
| 1:A:97:A:C5 | 1:A:98:G:C6 | 0.50 | 3.00 | 5 | 1 |
| 1:A:1:G:N2 | 1:A:2:G:C6 | 0.49 | 2.80 | 2 | 1 |
| 1:A:25:U:HO2' | 1:A:26:C:P | 0.49 | 2.28 | 8 | 6 |
| 1:A:23:G:O2' | 1:A:24:U:O5' | 0.49 | 2.25 | 2 | 1 |
| 1:A:58:G:O2' | 1:A:59:A:C5' | 0.49 | 2.60 | 2 | 1 |
| 1:A:20:G:C2 | 1:A:89:U:C2 | 0.49 | 3.00 | 1 | 2 |
| 1:A:52:C:O2' | 1:A:53:A:O5' | 0.49 | 2.31 | 3 | 2 |
| 1:A:52:C:O2 | 1:A:53:A:C1' | 0.49 | 2.60 | 3 | 1 |
| 1:A:59:A:C6 | 1:A:60:U:N3 | 0.49 | 2.80 | 5 | 8 |
| 1:A:71:A:O2' | 1:A:72:U:O4' | 0.49 | 2.24 | 10 | 2 |
| 1:A:38:G:O2' | 1:A:39:A:H5' | 0.49 | 2.07 | 10 | 1 |
| 1:A:97:A:C8 | 1:A:98:G:C6 | 0.49 | 3.00 | 5 | 1 |
| 1:A:54:A:O2' | 1:A:55:A:O5' | 0.49 | 2.26 | 6 | 3 |
| 1:A:101:U:O2 | 1:A:101:U:H3' | 0.49 | 2.08 | 7 | 1 |
| 1:A:81:C:HO2' | 1:A:82:U:P | 0.49 | 2.31 | 4 | 2 |
| 1:A:31:G:O2' | 1:A:33:A:N3 | 0.49 | 2.41 | 8 | 2 |
| 1:A:25:U:H6 | 1:A:25:U:O5' | 0.49 | 1.91 | 10 | 2 |
| 1:A:56:G:O6 | 1:A:76:U:O4 | 0.49 | 2.30 | 10 | 1 |
| 1:A:49:U:O4 | 1:A:82:U:C5 | 0.49 | 2.66 | 10 | 1 |
| 1:A:34:U:OP1 | 1:A:34:U:O2 | 0.49 | 2.31 | 5 | 1 |
| 1:A:56:G:O6 | 1:A:57:A:N6 | 0.49 | 2.46 | 6 | 3 |
| 1:A:11:A:N6 | 1:A:100:G:H22 | 0.49 | 2.05 | 2 | 1 |
| 1:A:54:A:C5 | 1:A:55:A:C8 | 0.49 | 3.00 | 10 | 1 |
| 1:A:102:A:C4 | 1:A:102:A:C5' | 0.49 | 2.95 | 7 | 2 |
| 1:A:98:G:N2 | 1:A:99:U:C4 | 0.49 | 2.80 | 5 | 1 |
| 1:A:87:G:O2' | 1:A:88:C:H4' | 0.49 | 2.08 | 7 | 2 |
| 1:A:53:A:C5 | 1:A:54:A:N7 | 0.49 | 2.81 | 8 | 3 |
| 1:A:110:U:C6 | 1:A:110:U:O5' | 0.49 | 2.65 | 8 | 4 |
| 1:A:56:G:O2' | 1:A:57:A:O4' | 0.49 | 2.29 | 8 | 7 |
| 1:A:81:C:C3' | 1:A:81:C:O2 | 0.49 | 2.60 | 2 | 1 |
| 1:A:8:C:N3 | 1:A:9:A:C2 | 0.49 | 2.80 | 9 | 1 |
| 1:A:63:C:C4 | 1:A:64:U:O4 | 0.49 | 2.66 | 3 | 4 |
| 1:A:83:U:O2' | 1:A:84:U:C2' | 0.49 | 2.60 | 3 | 1 |
| 1:A:97:A:C6 | 1:A:98:G:O6 | 0.49 | 2.65 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|----------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:13:A:N6 | 1:A:98:G:C2 | 0.49 | 2.81 | 3 | 1 |
| 1:A:106:U:O2' | 1:A:107:C:C2 | 0.49 | 2.62 | 2 | 1 |
| 1:A:107:C:O2 | 1:A:108:U:C5 | 0.49 | 2.61 | 2 | 1 |
| 1:A:15:G:N1 | 1:A:95:C:C4 | 0.49 | 2.81 | 2 | 1 |
| 1:A:19:A:O2' | 1:A:20:G:O5' | 0.49 | 2.31 | 2 | 2 |
| 1:A:33:A:C6 | 1:A:35:A:C6 | 0.49 | 2.95 | 2 | 1 |
| 1:A:38:G:H21 | 1:A:39:A:N6 | 0.49 | 2.05 | 2 | 1 |
| 1:A:99:U:H6 | 1:A:99:U:O5' | 0.49 | 1.91 | 2 | 2 |
| 1:A:44:C:C5 | 1:A:45:C:C4 | 0.49 | 3.01 | 4 | 1 |
| 1:A:50:U:C1' | 1:A:84:U:O2 | 0.49 | 2.59 | 3 | 1 |
| 1:A:65:U:O2' | 1:A:67:G:N7 | 0.49 | 2.46 | 7 | 1 |
| 1:A:10:G:N2 | 1:A:102:A:N7 | 0.49 | 2.60 | 10 | 1 |
| 1:A:98:G:H2' | 1:A:98:G:N3 | 0.49 | 2.23 | 1 | 2 |
| 1:A:82:U:HO2' | 1:A:83:U:P | 0.49 | 2.29 | 8 | 3 |
| 1:A:47:U:O2' | 1:A:48:U:OP1 | 0.49 | 2.30 | 6 | 1 |
| 1:A:7:A:C5 | 1:A:8:C:C5 | 0.48 | 3.01 | 2 | 1 |
| 1:A:30:U:O2' | 1:A:31:G:O4' | 0.48 | 2.24 | 1 | 2 |
| 1:A:68:G:O2' | 1:A:69:G:O5' | 0.48 | 2.31 | 7 | 2 |
| 1:A:13:A:N1 | 1:A:96:A:H2 | 0.48 | 2.06 | 7 | 1 |
| 1:A:107:C:O2 | 1:A:107:C:O4' | 0.48 | 2.29 | 6 | 3 |
| 1:A:39:A:C4' | 1:A:40:U:OP1 | 0.48 | 2.61 | 2 | 2 |
| 1:A:7:A:C6 | 1:A:105:A:C6 | 0.48 | 3.02 | 2 | 1 |
| 1:A:50:U:O2 | 1:A:50:U:C3' | 0.48 | 2.62 | 4 | 1 |
| 1:A:49:U:H5' | 1:A:50:U:OP2 | 0.48 | 2.08 | 3 | 1 |
| 1:A:75:C:O2' | 1:A:76:U:C5' | 0.48 | 2.62 | 9 | 4 |
| 1:A:56:G:C8 | 1:A:57:A:N7 | 0.48 | 2.81 | 2 | 2 |
| 1:A:83:U:O2' | 1:A:85:U:OP1 | 0.48 | 2.32 | 2 | 1 |
| 1:A:81:C:O2 | 1:A:81:C:H3' | 0.48 | 2.08 | 10 | 1 |
| 1:A:11:A:C5' | 1:A:12:G:OP1 | 0.48 | 2.62 | 7 | 1 |
| 1:A:104:U:O2' | 1:A:105:A:O4' | 0.48 | 2.28 | 7 | 4 |
| 1:A:7:A:N1 | 1:A:105:A:C5 | 0.48 | 2.81 | 2 | 1 |
| 1:A:29:C:C1' | 1:A:39:A:N6 | 0.48 | 2.77 | 2 | 1 |
| 1:A:48:U:H1' | 1:A:49:U:O4' | 0.48 | 2.09 | 2 | 1 |
| 1:A:102:A:C5' | 1:A:102:A:N3 | 0.48 | 2.74 | 4 | 2 |
| 1:A:54:A:C2 | 1:A:55:A:C8 | 0.48 | 3.02 | 4 | 3 |
| 1:A:54:A:C2 | 1:A:78:U:N3 | 0.48 | 2.81 | 4 | 1 |
| 1:A:105:A:HO2' | 1:A:106:U:P | 0.48 | 2.32 | 4 | 5 |
| 1:A:11:A:C3' | 1:A:12:G:O4' | 0.48 | 2.62 | 10 | 1 |
| 1:A:79:G:N2 | 1:A:80:C:N3 | 0.48 | 2.62 | 8 | 2 |
| 1:A:51:A:C1' | 1:A:83:U:O4 | 0.48 | 2.62 | 6 | 1 |
| 1:A:23:G:HO2' | 1:A:24:U:P | 0.48 | 2.30 | 2 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:69:G:O2' | 1:A:70:A:O5' | 0.48 | 2.32 | 10 | 1 |
| 1:A:32:C:HO2' | 1:A:33:A:P | 0.48 | 2.30 | 4 | 1 |
| 1:A:100:G:O3' | 1:A:101:U:H4' | 0.48 | 2.09 | 3 | 2 |
| 1:A:84:U:O2' | 1:A:85:U:O2 | 0.48 | 2.29 | 3 | 2 |
| 1:A:13:A:C5 | 1:A:99:U:O4 | 0.48 | 2.67 | 5 | 1 |
| 1:A:51:A:N1 | 1:A:79:G:O6 | 0.48 | 2.47 | 9 | 1 |
| 1:A:77:U:HO2' | 1:A:78:U:P | 0.48 | 2.32 | 6 | 4 |
| 1:A:79:G:O6 | 1:A:80:C:N4 | 0.48 | 2.46 | 2 | 1 |
| 1:A:95:C:HO2' | 1:A:96:A:P | 0.48 | 2.32 | 2 | 1 |
| 1:A:51:A:O2' | 1:A:52:C:O5' | 0.48 | 2.29 | 10 | 1 |
| 1:A:2:G:O2' | 1:A:3:C:O4' | 0.48 | 2.23 | 6 | 1 |
| 1:A:95:C:O2' | 1:A:96:A:C4' | 0.48 | 2.62 | 9 | 1 |
| 1:A:69:G:O2' | 1:A:70:A:H5' | 0.48 | 2.09 | 10 | 2 |
| 1:A:70:A:C5 | 1:A:71:A:N7 | 0.48 | 2.82 | 10 | 1 |
| 1:A:12:G:C4 | 1:A:100:G:N2 | 0.48 | 2.82 | 4 | 1 |
| 1:A:30:U:C4 | 1:A:31:G:C6 | 0.48 | 3.02 | 3 | 2 |
| 1:A:11:A:N6 | 1:A:12:G:H21 | 0.48 | 2.07 | 2 | 1 |
| 1:A:1:G:C2 | 1:A:2:G:C5 | 0.48 | 3.02 | 10 | 1 |
| 1:A:9:A:C1' | 1:A:11:A:H62 | 0.48 | 2.22 | 5 | 1 |
| 1:A:50:U:HO2' | 1:A:51:A:P | 0.48 | 2.31 | 6 | 1 |
| 1:A:22:A:N7 | 1:A:45:C:O2 | 0.48 | 2.47 | 8 | 1 |
| 1:A:34:U:C5' | 1:A:35:A:OP1 | 0.47 | 2.62 | 7 | 2 |
| 1:A:31:G:O3' | 1:A:33:A:C5 | 0.47 | 2.67 | 6 | 3 |
| 1:A:87:G:O2' | 1:A:88:C:O5' | 0.47 | 2.31 | 2 | 1 |
| 1:A:105:A:C2' | 1:A:106:U:O5' | 0.47 | 2.62 | 10 | 1 |
| 1:A:9:A:H4' | 1:A:10:G:OP2 | 0.47 | 2.08 | 10 | 1 |
| 1:A:38:G:C5 | 1:A:39:A:N6 | 0.47 | 2.82 | 10 | 1 |
| 1:A:101:U:O2 | 1:A:101:U:C3' | 0.47 | 2.62 | 7 | 1 |
| 1:A:74:U:C4 | 1:A:75:C:C4 | 0.47 | 3.02 | 6 | 4 |
| 1:A:87:G:HO2' | 1:A:88:C:P | 0.47 | 2.32 | 2 | 1 |
| 1:A:38:G:C6 | 1:A:39:A:N6 | 0.47 | 2.82 | 10 | 1 |
| 1:A:101:U:O2' | 1:A:102:A:P | 0.47 | 2.72 | 1 | 1 |
| 1:A:66:C:N3 | 1:A:67:G:C6 | 0.47 | 2.82 | 3 | 1 |
| 1:A:100:G:C2' | 1:A:101:U:O4' | 0.47 | 2.61 | 5 | 1 |
| 1:A:34:U:O2' | 1:A:34:U:O2 | 0.47 | 2.30 | 5 | 1 |
| 1:A:90:U:O5' | 1:A:90:U:C6 | 0.47 | 2.66 | 1 | 1 |
| 1:A:20:G:N2 | 1:A:89:U:C2 | 0.47 | 2.81 | 4 | 1 |
| 1:A:91:A:H5'' | 1:A:92:G:OP2 | 0.47 | 2.08 | 4 | 1 |
| 1:A:33:A:C2' | 1:A:34:U:OP2 | 0.47 | 2.63 | 5 | 1 |
| 1:A:47:U:O2 | 1:A:49:U:C1' | 0.47 | 2.62 | 2 | 1 |
| 1:A:9:A:C4 | 1:A:101:U:C4 | 0.47 | 3.03 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:100:G:N3 | 1:A:100:G:C2' | 0.47 | 2.77 | 6 | 1 |
| 1:A:52:C:HO2' | 1:A:53:A:P | 0.47 | 2.31 | 8 | 1 |
| 1:A:108:U:C4' | 1:A:108:U:OP2 | 0.47 | 2.62 | 4 | 3 |
| 1:A:66:C:OP1 | 1:A:66:C:C2 | 0.47 | 2.67 | 5 | 1 |
| 1:A:23:G:OP2 | 1:A:23:G:C8 | 0.47 | 2.65 | 8 | 4 |
| 1:A:33:A:C1' | 1:A:34:U:C6 | 0.47 | 2.98 | 1 | 1 |
| 1:A:33:A:OP2 | 1:A:33:A:C3' | 0.47 | 2.62 | 5 | 1 |
| 1:A:13:A:N6 | 1:A:99:U:O2 | 0.47 | 2.47 | 8 | 1 |
| 1:A:9:A:C5' | 1:A:10:G:OP1 | 0.47 | 2.62 | 9 | 2 |
| 1:A:49:U:OP1 | 1:A:49:U:C4' | 0.47 | 2.63 | 2 | 1 |
| 1:A:40:U:OP2 | 1:A:40:U:C5 | 0.47 | 2.68 | 4 | 3 |
| 1:A:85:U:C4' | 1:A:86:G:OP1 | 0.47 | 2.62 | 3 | 3 |
| 1:A:52:C:OP2 | 1:A:52:C:C6 | 0.47 | 2.67 | 7 | 1 |
| 1:A:52:C:C4 | 1:A:53:A:N7 | 0.47 | 2.83 | 9 | 2 |
| 1:A:30:U:O4 | 1:A:31:G:N1 | 0.47 | 2.48 | 3 | 3 |
| 1:A:44:C:H5' | 1:A:48:U:O2 | 0.47 | 2.09 | 4 | 1 |
| 1:A:99:U:O3' | 1:A:100:G:H2' | 0.47 | 2.10 | 7 | 1 |
| 1:A:57:A:C2 | 1:A:75:C:O2 | 0.47 | 2.67 | 7 | 1 |
| 1:A:56:G:C2 | 1:A:57:A:C4 | 0.47 | 3.03 | 1 | 4 |
| 1:A:91:A:O3' | 1:A:92:G:O4' | 0.47 | 2.33 | 4 | 5 |
| 1:A:103:G:C8 | 1:A:104:U:C5 | 0.47 | 3.03 | 1 | 1 |
| 1:A:49:U:C6 | 1:A:49:U:OP2 | 0.47 | 2.63 | 7 | 1 |
| 1:A:12:G:H22 | 1:A:102:A:N6 | 0.47 | 2.07 | 7 | 2 |
| 1:A:37:G:C2 | 1:A:38:G:C8 | 0.47 | 3.03 | 2 | 1 |
| 1:A:98:G:H21 | 1:A:99:U:C1' | 0.47 | 2.23 | 6 | 3 |
| 1:A:82:U:O2' | 1:A:83:U:C5' | 0.47 | 2.62 | 6 | 1 |
| 1:A:56:G:C2 | 1:A:57:A:C5 | 0.46 | 3.03 | 1 | 3 |
| 1:A:86:G:O5' | 1:A:86:G:C8 | 0.46 | 2.69 | 5 | 1 |
| 1:A:91:A:O2' | 1:A:92:G:OP1 | 0.46 | 2.33 | 6 | 2 |
| 1:A:95:C:O2' | 1:A:96:A:O4' | 0.46 | 2.33 | 8 | 1 |
| 1:A:51:A:C5' | 1:A:83:U:O2 | 0.46 | 2.64 | 9 | 1 |
| 1:A:51:A:N6 | 1:A:80:C:H42 | 0.46 | 2.08 | 2 | 2 |
| 1:A:66:C:O2 | 1:A:66:C:C5' | 0.46 | 2.63 | 2 | 1 |
| 1:A:34:U:O2' | 1:A:35:A:OP2 | 0.46 | 2.33 | 10 | 1 |
| 1:A:56:G:C8 | 1:A:57:A:C5 | 0.46 | 3.03 | 10 | 1 |
| 1:A:9:A:N3 | 1:A:9:A:H2' | 0.46 | 2.24 | 10 | 1 |
| 1:A:77:U:C2 | 1:A:78:U:C5 | 0.46 | 3.03 | 4 | 1 |
| 1:A:10:G:N2 | 1:A:11:A:N1 | 0.46 | 2.63 | 5 | 1 |
| 1:A:46:G:C4' | 1:A:48:U:O4 | 0.46 | 2.63 | 6 | 1 |
| 1:A:65:U:N1 | 1:A:65:U:O5' | 0.46 | 2.48 | 6 | 1 |
| 1:A:56:G:C6 | 1:A:57:A:C2 | 0.46 | 3.03 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|--------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:32:C:OP2 | 1:A:33:A:N6 | 0.46 | 2.47 | 3 | 2 |
| 1:A:55:A:O2' | 1:A:56:G:O5' | 0.46 | 2.29 | 5 | 2 |
| 1:A:64:U:C2 | 1:A:66:C:N3 | 0.46 | 2.84 | 6 | 1 |
| 1:A:66:C:O4' | 1:A:67:G:C8 | 0.46 | 2.69 | 8 | 1 |
| 1:A:70:A:O2' | 1:A:71:A:O5' | 0.46 | 2.29 | 2 | 3 |
| 1:A:31:G:H4' | 1:A:33:A:N6 | 0.46 | 2.25 | 8 | 1 |
| 1:A:68:G:H8 | 1:A:68:G:O5' | 0.46 | 1.93 | 8 | 1 |
| 1:A:45:C:OP1 | 1:A:49:U:O4 | 0.46 | 2.33 | 5 | 4 |
| 1:A:74:U:C2' | 1:A:75:C:H5'' | 0.46 | 2.41 | 10 | 1 |
| 1:A:23:G:N1 | 1:A:24:U:C4 | 0.46 | 2.84 | 1 | 1 |
| 1:A:34:U:C4' | 1:A:34:U:OP1 | 0.46 | 2.64 | 1 | 1 |
| 1:A:47:U:C4' | 1:A:48:U:OP2 | 0.46 | 2.63 | 6 | 1 |
| 1:A:6:U:C2 | 1:A:105:A:N1 | 0.46 | 2.84 | 2 | 2 |
| 1:A:77:U:O5' | 1:A:77:U:H6 | 0.46 | 1.93 | 10 | 1 |
| 1:A:102:A:P | 1:A:102:A:C8 | 0.46 | 3.09 | 3 | 1 |
| 1:A:64:U:N1 | 1:A:66:C:N4 | 0.46 | 2.63 | 10 | 1 |
| 1:A:34:U:P | 1:A:34:U:O4' | 0.46 | 2.74 | 1 | 1 |
| 1:A:9:A:C8 | 1:A:101:U:O4 | 0.46 | 2.69 | 4 | 1 |
| 1:A:34:U:H2' | 1:A:34:U:O2 | 0.46 | 2.10 | 5 | 1 |
| 1:A:45:C:OP1 | 1:A:48:U:C4 | 0.46 | 2.69 | 8 | 1 |
| 1:A:51:A:C8 | 1:A:52:C:C5 | 0.46 | 3.04 | 8 | 1 |
| 1:A:74:U:C4 | 1:A:75:C:N4 | 0.46 | 2.84 | 6 | 4 |
| 1:A:55:A:N1 | 1:A:56:G:C5 | 0.46 | 2.84 | 4 | 3 |
| 1:A:56:G:C5 | 1:A:57:A:C4 | 0.46 | 3.03 | 10 | 1 |
| 1:A:52:C:O2 | 1:A:53:A:O4' | 0.46 | 2.34 | 3 | 1 |
| 1:A:34:U:N1 | 1:A:34:U:OP2 | 0.46 | 2.48 | 5 | 1 |
| 1:A:58:G:N2 | 1:A:74:U:C2 | 0.46 | 2.84 | 5 | 1 |
| 1:A:90:U:O2 | 1:A:90:U:O4' | 0.46 | 2.33 | 5 | 1 |
| 1:A:81:C:H3' | 1:A:81:C:O2 | 0.46 | 2.11 | 2 | 1 |
| 1:A:9:A:O2' | 1:A:10:G:OP1 | 0.46 | 2.31 | 10 | 1 |
| 1:A:50:U:O2 | 1:A:50:U:H3' | 0.46 | 2.11 | 4 | 1 |
| 1:A:15:G:O6 | 1:A:96:A:N6 | 0.46 | 2.48 | 7 | 2 |
| 1:A:12:G:N1 | 1:A:102:A:C2 | 0.46 | 2.84 | 3 | 1 |
| 1:A:50:U:C2' | 1:A:50:U:O2 | 0.46 | 2.64 | 8 | 2 |
| 1:A:85:U:H4' | 1:A:86:G:O5' | 0.46 | 2.11 | 8 | 1 |
| 1:A:33:A:O2' | 1:A:34:U:C1' | 0.45 | 2.64 | 9 | 1 |
| 1:A:58:G:C4 | 1:A:59:A:C8 | 0.45 | 3.04 | 1 | 2 |
| 1:A:55:A:C5 | 1:A:57:A:N6 | 0.45 | 2.84 | 2 | 1 |
| 1:A:98:G:N2 | 1:A:99:U:N3 | 0.45 | 2.65 | 5 | 1 |
| 1:A:22:A:H61 | 1:A:87:G:C1' | 0.45 | 2.24 | 8 | 1 |
| 1:A:39:A:C6 | 1:A:40:U:O4 | 0.45 | 2.69 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:95:C:O2' | 1:A:96:A:C5' | 0.45 | 2.65 | 2 | 1 |
| 1:A:108:U:H2' | 1:A:109:G:C8 | 0.45 | 2.46 | 10 | 1 |
| 1:A:64:U:C2 | 1:A:66:C:C4 | 0.45 | 3.05 | 10 | 2 |
| 1:A:100:G:O2' | 1:A:102:A:N6 | 0.45 | 2.49 | 4 | 1 |
| 1:A:84:U:O2' | 1:A:85:U:N1 | 0.45 | 2.49 | 4 | 3 |
| 1:A:44:C:O5' | 1:A:49:U:O2 | 0.45 | 2.35 | 9 | 4 |
| 1:A:65:U:O2' | 1:A:66:C:N4 | 0.45 | 2.49 | 3 | 2 |
| 1:A:46:G:O2' | 1:A:47:U:OP2 | 0.45 | 2.34 | 10 | 1 |
| 1:A:77:U:O2' | 1:A:78:U:O4' | 0.45 | 2.32 | 4 | 1 |
| 1:A:15:G:O2' | 1:A:16:A:H5' | 0.45 | 2.11 | 7 | 2 |
| 1:A:33:A:C5 | 1:A:35:A:N1 | 0.45 | 2.84 | 7 | 1 |
| 1:A:59:A:C2 | 1:A:60:U:C2 | 0.45 | 3.04 | 2 | 3 |
| 1:A:66:C:C2 | 1:A:67:G:C4 | 0.45 | 3.04 | 2 | 2 |
| 1:A:44:C:C5' | 1:A:49:U:O2 | 0.45 | 2.65 | 1 | 1 |
| 1:A:12:G:O2' | 1:A:100:G:C6 | 0.45 | 2.63 | 7 | 1 |
| 1:A:68:G:N2 | 1:A:69:G:C4 | 0.45 | 2.85 | 9 | 1 |
| 1:A:102:A:C2 | 1:A:103:G:C6 | 0.45 | 3.04 | 2 | 1 |
| 1:A:104:U:C2 | 1:A:105:A:C8 | 0.45 | 3.04 | 10 | 2 |
| 1:A:105:A:C8 | 1:A:106:U:C5 | 0.45 | 3.04 | 10 | 1 |
| 1:A:27:C:OP1 | 1:A:27:C:C5 | 0.45 | 2.70 | 1 | 2 |
| 1:A:46:G:C4' | 1:A:46:G:OP1 | 0.45 | 2.64 | 5 | 1 |
| 1:A:83:U:O2 | 1:A:83:U:C2' | 0.45 | 2.58 | 7 | 1 |
| 1:A:67:G:C2' | 1:A:68:G:O4' | 0.45 | 2.60 | 8 | 1 |
| 1:A:46:G:C2 | 1:A:47:U:N1 | 0.45 | 2.84 | 2 | 1 |
| 1:A:65:U:H2' | 1:A:66:C:C5 | 0.45 | 2.47 | 8 | 2 |
| 1:A:84:U:O3' | 1:A:85:U:O4' | 0.45 | 2.35 | 7 | 3 |
| 1:A:108:U:OP2 | 1:A:108:U:C4' | 0.45 | 2.64 | 1 | 3 |
| 1:A:13:A:N1 | 1:A:97:A:C6 | 0.45 | 2.85 | 8 | 1 |
| 1:A:43:A:O2' | 1:A:44:C:O5' | 0.45 | 2.32 | 10 | 1 |
| 1:A:77:U:N3 | 1:A:78:U:C5 | 0.45 | 2.85 | 4 | 1 |
| 1:A:66:C:H4' | 1:A:67:G:O5' | 0.45 | 2.10 | 3 | 1 |
| 1:A:99:U:O2' | 1:A:100:G:H5' | 0.45 | 2.12 | 3 | 1 |
| 1:A:39:A:HO2' | 1:A:40:U:C5' | 0.45 | 2.25 | 9 | 1 |
| 1:A:84:U:C2 | 1:A:85:U:N3 | 0.45 | 2.85 | 3 | 1 |
| 1:A:66:C:C2 | 1:A:67:G:C8 | 0.44 | 3.04 | 2 | 1 |
| 1:A:46:G:C1' | 1:A:48:U:O4 | 0.44 | 2.63 | 5 | 2 |
| 1:A:102:A:O4' | 1:A:102:A:N3 | 0.44 | 2.50 | 4 | 1 |
| 1:A:9:A:C4' | 1:A:10:G:OP1 | 0.44 | 2.64 | 8 | 3 |
| 1:A:9:A:O2' | 1:A:11:A:N7 | 0.44 | 2.50 | 5 | 1 |
| 1:A:45:C:OP1 | 1:A:49:U:N3 | 0.44 | 2.51 | 6 | 1 |
| 1:A:60:U:C4 | 1:A:61:U:C4 | 0.44 | 3.05 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:53:A:C4 | 1:A:54:A:C8 | 0.44 | 3.05 | 8 | 1 |
| 1:A:11:A:H62 | 1:A:12:G:N2 | 0.44 | 2.10 | 2 | 1 |
| 1:A:33:A:N3 | 1:A:33:A:C2' | 0.44 | 2.81 | 2 | 1 |
| 1:A:103:G:C8 | 1:A:104:U:C6 | 0.44 | 3.06 | 10 | 1 |
| 1:A:41:G:O2' | 1:A:42:A:O5' | 0.44 | 2.35 | 10 | 1 |
| 1:A:54:A:H2' | 1:A:55:A:O4' | 0.44 | 2.12 | 10 | 1 |
| 1:A:49:U:C4' | 1:A:50:U:OP1 | 0.44 | 2.65 | 4 | 1 |
| 1:A:54:A:C2 | 1:A:55:A:N9 | 0.44 | 2.85 | 4 | 2 |
| 1:A:44:C:OP1 | 1:A:49:U:C1' | 0.44 | 2.64 | 3 | 1 |
| 1:A:101:U:O3' | 1:A:102:A:H8 | 0.44 | 1.95 | 5 | 1 |
| 1:A:54:A:C2 | 1:A:78:U:C2 | 0.44 | 3.05 | 6 | 1 |
| 1:A:12:G:H21 | 1:A:100:G:N2 | 0.44 | 2.08 | 2 | 1 |
| 1:A:79:G:O2' | 1:A:80:C:C5' | 0.44 | 2.65 | 9 | 3 |
| 1:A:53:A:C6 | 1:A:54:A:C6 | 0.44 | 3.05 | 6 | 3 |
| 1:A:29:C:C2 | 1:A:39:A:N6 | 0.44 | 2.85 | 2 | 1 |
| 1:A:92:G:O4' | 1:A:92:G:OP1 | 0.44 | 2.35 | 3 | 1 |
| 1:A:2:G:C2 | 1:A:109:G:N2 | 0.44 | 2.86 | 6 | 1 |
| 1:A:77:U:O2' | 1:A:78:U:O5' | 0.44 | 2.30 | 7 | 3 |
| 1:A:48:U:O2' | 1:A:49:U:O5' | 0.44 | 2.28 | 9 | 1 |
| 1:A:63:C:C6 | 1:A:64:U:C5 | 0.44 | 3.06 | 9 | 4 |
| 1:A:102:A:C2 | 1:A:103:G:C5 | 0.44 | 3.05 | 2 | 1 |
| 1:A:38:G:HO2' | 1:A:39:A:P | 0.44 | 2.36 | 2 | 1 |
| 1:A:53:A:N1 | 1:A:54:A:C6 | 0.44 | 2.86 | 6 | 2 |
| 1:A:64:U:O2' | 1:A:67:G:O6 | 0.44 | 2.36 | 10 | 1 |
| 1:A:7:A:N3 | 1:A:8:C:C5 | 0.44 | 2.85 | 10 | 1 |
| 1:A:54:A:N3 | 1:A:55:A:C8 | 0.44 | 2.86 | 6 | 2 |
| 1:A:65:U:C2' | 1:A:66:C:C5 | 0.44 | 3.01 | 8 | 1 |
| 1:A:83:U:O3' | 1:A:84:U:O4' | 0.44 | 2.36 | 3 | 1 |
| 1:A:65:U:O4' | 1:A:65:U:O2 | 0.44 | 2.36 | 6 | 1 |
| 1:A:37:G:C2 | 1:A:38:G:C5 | 0.44 | 3.06 | 7 | 1 |
| 1:A:13:A:N7 | 1:A:99:U:H1' | 0.44 | 2.27 | 9 | 1 |
| 1:A:85:U:C2' | 1:A:86:G:OP2 | 0.44 | 2.66 | 2 | 1 |
| 1:A:101:U:O2' | 1:A:102:A:O5' | 0.44 | 2.35 | 1 | 1 |
| 1:A:87:G:OP2 | 1:A:87:G:H4' | 0.44 | 2.12 | 3 | 1 |
| 1:A:49:U:O2 | 1:A:49:U:C2' | 0.44 | 2.65 | 2 | 1 |
| 1:A:34:U:OP1 | 1:A:34:U:O4' | 0.44 | 2.36 | 1 | 1 |
| 1:A:85:U:OP1 | 1:A:86:G:O6 | 0.44 | 2.35 | 4 | 1 |
| 1:A:12:G:N3 | 1:A:100:G:N2 | 0.44 | 2.66 | 6 | 1 |
| 1:A:31:G:C2' | 1:A:33:A:N1 | 0.43 | 2.81 | 2 | 2 |
| 1:A:38:G:N3 | 1:A:39:A:C6 | 0.43 | 2.86 | 10 | 1 |
| 1:A:39:A:N3 | 1:A:40:U:C5 | 0.43 | 2.85 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|--------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:66:C:O3' | 1:A:67:G:O4' | 0.43 | 2.36 | 7 | 2 |
| 1:A:55:A:C2 | 1:A:77:U:N3 | 0.43 | 2.86 | 4 | 2 |
| 1:A:81:C:O2 | 1:A:81:C:C2' | 0.43 | 2.65 | 5 | 1 |
| 1:A:48:U:N3 | 1:A:49:U:C4 | 0.43 | 2.85 | 8 | 1 |
| 1:A:26:C:O2' | 1:A:27:C:O5' | 0.43 | 2.36 | 2 | 1 |
| 1:A:85:U:P | 1:A:86:G:O6 | 0.43 | 2.76 | 4 | 1 |
| 1:A:11:A:C8 | 1:A:11:A:P | 0.43 | 3.11 | 3 | 1 |
| 1:A:85:U:H4' | 1:A:86:G:OP1 | 0.43 | 2.13 | 3 | 2 |
| 1:A:49:U:O2' | 1:A:50:U:P | 0.43 | 2.76 | 6 | 1 |
| 1:A:101:U:H4' | 1:A:102:A:N7 | 0.43 | 2.28 | 8 | 1 |
| 1:A:55:A:N1 | 1:A:56:G:C6 | 0.43 | 2.86 | 8 | 1 |
| 1:A:7:A:N6 | 1:A:8:C:N4 | 0.43 | 2.66 | 2 | 1 |
| 1:A:94:U:O2 | 1:A:95:C:H5 | 0.43 | 1.96 | 2 | 1 |
| 1:A:17:U:O2' | 1:A:18:C:O4' | 0.43 | 2.35 | 1 | 1 |
| 1:A:59:A:H61 | 1:A:71:A:N6 | 0.43 | 2.09 | 3 | 1 |
| 1:A:97:A:C8 | 1:A:98:G:N1 | 0.43 | 2.87 | 5 | 1 |
| 1:A:45:C:OP1 | 1:A:48:U:O4 | 0.43 | 2.36 | 9 | 1 |
| 1:A:63:C:HO2' | 1:A:64:U:C5' | 0.43 | 2.25 | 10 | 1 |
| 1:A:9:A:C1' | 1:A:10:G:N2 | 0.43 | 2.81 | 1 | 2 |
| 1:A:33:A:N9 | 1:A:34:U:C5 | 0.43 | 2.86 | 5 | 1 |
| 1:A:51:A:C6 | 1:A:52:C:N4 | 0.43 | 2.86 | 9 | 1 |
| 1:A:39:A:H3' | 1:A:39:A:OP2 | 0.43 | 2.14 | 2 | 1 |
| 1:A:10:G:N2 | 1:A:11:A:N6 | 0.43 | 2.66 | 4 | 1 |
| 1:A:32:C:O5' | 1:A:33:A:N7 | 0.43 | 2.52 | 6 | 1 |
| 1:A:50:U:O2 | 1:A:84:U:O4 | 0.43 | 2.36 | 6 | 1 |
| 1:A:98:G:O2' | 1:A:99:U:O5' | 0.43 | 2.31 | 6 | 1 |
| 1:A:52:C:N3 | 1:A:53:A:C8 | 0.43 | 2.87 | 9 | 2 |
| 1:A:59:A:N3 | 1:A:59:A:H2' | 0.43 | 2.28 | 9 | 1 |
| 1:A:65:U:C2' | 1:A:66:C:N4 | 0.43 | 2.82 | 3 | 2 |
| 1:A:48:U:O2 | 1:A:49:U:H6 | 0.43 | 1.96 | 10 | 1 |
| 1:A:7:A:HO2' | 1:A:8:C:H5' | 0.43 | 1.74 | 4 | 1 |
| 1:A:10:G:O2' | 1:A:11:A:O5' | 0.43 | 2.30 | 9 | 1 |
| 1:A:59:A:N6 | 1:A:60:U:O4 | 0.43 | 2.52 | 10 | 1 |
| 1:A:8:C:H2' | 1:A:9:A:O4' | 0.43 | 2.13 | 2 | 1 |
| 1:A:31:G:H2' | 1:A:33:A:N1 | 0.43 | 2.28 | 4 | 1 |
| 1:A:60:U:C4 | 1:A:61:U:C5 | 0.43 | 3.07 | 7 | 1 |
| 1:A:8:C:HO2' | 1:A:10:G:N2 | 0.43 | 2.11 | 9 | 1 |
| 1:A:35:A:N7 | 1:A:36:A:N1 | 0.43 | 2.67 | 10 | 1 |
| 1:A:48:U:C4' | 1:A:49:U:OP1 | 0.43 | 2.66 | 10 | 1 |
| 1:A:6:U:O2 | 1:A:105:A:H2 | 0.43 | 1.97 | 10 | 1 |
| 1:A:100:G:O2' | 1:A:101:U:H6 | 0.43 | 1.94 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:29:C:O2 | 1:A:38:G:C2 | 0.43 | 2.71 | 7 | 4 |
| 1:A:13:A:C2 | 1:A:14:U:O2 | 0.43 | 2.72 | 7 | 1 |
| 1:A:40:U:C6 | 1:A:40:U:OP2 | 0.42 | 2.72 | 9 | 1 |
| 1:A:57:A:H2 | 1:A:75:C:N4 | 0.42 | 2.12 | 10 | 1 |
| 1:A:54:A:C6 | 1:A:55:A:C6 | 0.42 | 3.07 | 1 | 1 |
| 1:A:58:G:C2 | 1:A:74:U:O2 | 0.42 | 2.72 | 8 | 2 |
| 1:A:2:G:N1 | 1:A:109:G:N2 | 0.42 | 2.67 | 6 | 1 |
| 1:A:47:U:OP1 | 1:A:48:U:C5 | 0.42 | 2.70 | 7 | 1 |
| 1:A:7:A:N6 | 1:A:105:A:N6 | 0.42 | 2.66 | 2 | 1 |
| 1:A:109:G:H8 | 1:A:109:G:O5' | 0.42 | 1.96 | 10 | 1 |
| 1:A:32:C:H2' | 1:A:33:A:C5 | 0.42 | 2.49 | 10 | 1 |
| 1:A:34:U:C4 | 1:A:35:A:C5 | 0.42 | 3.06 | 1 | 1 |
| 1:A:8:C:C5 | 1:A:9:A:N6 | 0.42 | 2.87 | 1 | 1 |
| 1:A:9:A:H1' | 1:A:11:A:N7 | 0.42 | 2.29 | 9 | 1 |
| 1:A:11:A:H62 | 1:A:100:G:H22 | 0.42 | 1.55 | 2 | 1 |
| 1:A:102:A:C2' | 1:A:103:G:O4' | 0.42 | 2.68 | 2 | 2 |
| 1:A:44:C:OP1 | 1:A:49:U:O4' | 0.42 | 2.37 | 5 | 1 |
| 1:A:40:U:O2' | 1:A:41:G:O4' | 0.42 | 2.37 | 6 | 2 |
| 1:A:5:A:C6 | 1:A:6:U:C4 | 0.42 | 3.07 | 9 | 1 |
| 1:A:55:A:N3 | 1:A:55:A:H2' | 0.42 | 2.28 | 10 | 1 |
| 1:A:14:U:HO2' | 1:A:15:G:P | 0.42 | 2.38 | 7 | 2 |
| 1:A:12:G:O6 | 1:A:102:A:O4' | 0.42 | 2.37 | 3 | 1 |
| 1:A:45:C:OP1 | 1:A:49:U:C4 | 0.42 | 2.72 | 6 | 1 |
| 1:A:11:A:H1' | 1:A:12:G:N7 | 0.42 | 2.29 | 8 | 1 |
| 1:A:7:A:C6 | 1:A:105:A:N6 | 0.42 | 2.87 | 2 | 1 |
| 1:A:33:A:H4' | 1:A:34:U:OP2 | 0.42 | 2.14 | 1 | 1 |
| 1:A:100:G:O2' | 1:A:101:U:H4' | 0.42 | 2.15 | 4 | 1 |
| 1:A:12:G:C6 | 1:A:102:A:N7 | 0.42 | 2.88 | 4 | 1 |
| 1:A:85:U:O5' | 1:A:86:G:O6 | 0.42 | 2.38 | 4 | 1 |
| 1:A:87:G:C2 | 1:A:88:C:C2 | 0.42 | 3.07 | 6 | 1 |
| 1:A:108:U:O2' | 1:A:109:G:H5' | 0.42 | 2.14 | 7 | 2 |
| 1:A:49:U:O2' | 1:A:50:U:H5' | 0.42 | 2.13 | 10 | 1 |
| 1:A:9:A:C4' | 1:A:10:G:N2 | 0.42 | 2.82 | 4 | 1 |
| 1:A:78:U:O4 | 1:A:79:G:O6 | 0.42 | 2.38 | 10 | 1 |
| 1:A:33:A:N3 | 1:A:34:U:C5 | 0.42 | 2.88 | 3 | 1 |
| 1:A:9:A:O4' | 1:A:11:A:N6 | 0.42 | 2.51 | 5 | 1 |
| 1:A:100:G:N9 | 1:A:102:A:N6 | 0.42 | 2.68 | 6 | 1 |
| 1:A:32:C:C3' | 1:A:33:A:C8 | 0.42 | 3.03 | 8 | 1 |
| 1:A:93:A:O2' | 1:A:94:U:H5' | 0.42 | 2.15 | 10 | 2 |
| 1:A:38:G:O2' | 1:A:39:A:C5' | 0.42 | 2.68 | 10 | 1 |
| 1:A:100:G:O3' | 1:A:101:U:C4' | 0.42 | 2.67 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:97:A:C8 | 1:A:98:G:C5 | 0.42 | 3.08 | 3 | 1 |
| 1:A:82:U:C4' | 1:A:83:U:OP1 | 0.42 | 2.66 | 5 | 1 |
| 1:A:31:G:O2' | 1:A:34:U:H5 | 0.42 | 1.98 | 6 | 1 |
| 1:A:51:A:C2 | 1:A:80:C:N4 | 0.42 | 2.88 | 8 | 1 |
| 1:A:77:U:O4 | 1:A:78:U:O4 | 0.42 | 2.38 | 9 | 2 |
| 1:A:66:C:O4' | 1:A:67:G:N7 | 0.42 | 2.53 | 10 | 1 |
| 1:A:76:U:O4 | 1:A:77:U:O4 | 0.42 | 2.37 | 1 | 1 |
| 1:A:87:G:H2' | 1:A:88:C:O4' | 0.42 | 2.15 | 1 | 1 |
| 1:A:101:U:O2 | 1:A:101:U:C2' | 0.42 | 2.68 | 7 | 1 |
| 1:A:13:A:N6 | 1:A:96:A:C2 | 0.42 | 2.88 | 7 | 1 |
| 1:A:12:G:H22 | 1:A:100:G:N2 | 0.41 | 2.13 | 10 | 1 |
| 1:A:25:U:O2' | 1:A:26:C:P | 0.41 | 2.77 | 3 | 3 |
| 1:A:34:U:OP1 | 1:A:34:U:H2' | 0.41 | 2.15 | 5 | 1 |
| 1:A:74:U:H2' | 1:A:74:U:O2 | 0.41 | 2.15 | 5 | 1 |
| 1:A:13:A:N1 | 1:A:97:A:N7 | 0.41 | 2.67 | 7 | 1 |
| 1:A:1:G:O6 | 1:A:111:C:C4 | 0.41 | 2.73 | 2 | 1 |
| 1:A:48:U:C2 | 1:A:49:U:C6 | 0.41 | 3.08 | 2 | 1 |
| 1:A:97:A:O2' | 1:A:99:U:OP2 | 0.41 | 2.36 | 2 | 1 |
| 1:A:31:G:H22 | 1:A:36:A:N6 | 0.41 | 2.12 | 4 | 1 |
| 1:A:23:G:C2 | 1:A:44:C:O2 | 0.41 | 2.73 | 6 | 1 |
| 1:A:31:G:C1' | 1:A:33:A:N1 | 0.41 | 2.83 | 7 | 1 |
| 1:A:94:U:N3 | 1:A:95:C:N4 | 0.41 | 2.68 | 7 | 1 |
| 1:A:50:U:H2' | 1:A:84:U:O4 | 0.41 | 2.16 | 8 | 1 |
| 1:A:91:A:C2' | 1:A:92:G:C8 | 0.41 | 3.03 | 8 | 1 |
| 1:A:100:G:O4' | 1:A:100:G:N3 | 0.41 | 2.53 | 10 | 1 |
| 1:A:68:G:HO2' | 1:A:69:G:P | 0.41 | 2.37 | 7 | 1 |
| 1:A:108:U:C4 | 1:A:109:G:C6 | 0.41 | 3.09 | 9 | 3 |
| 1:A:66:C:H1' | 1:A:67:G:C4 | 0.41 | 2.50 | 9 | 2 |
| 1:A:47:U:O2 | 1:A:48:U:O2 | 0.41 | 2.38 | 2 | 1 |
| 1:A:38:G:N1 | 1:A:39:A:N6 | 0.41 | 2.68 | 10 | 1 |
| 1:A:58:G:HO2' | 1:A:59:A:C5' | 0.41 | 2.26 | 1 | 1 |
| 1:A:53:A:C2 | 1:A:54:A:C5 | 0.41 | 3.09 | 6 | 1 |
| 1:A:43:A:HO2' | 1:A:44:C:P | 0.41 | 2.38 | 2 | 2 |
| 1:A:75:C:C6 | 1:A:75:C:OP1 | 0.41 | 2.74 | 10 | 1 |
| 1:A:97:A:OP1 | 1:A:97:A:H4' | 0.41 | 2.15 | 1 | 1 |
| 1:A:53:A:N6 | 1:A:54:A:C6 | 0.41 | 2.88 | 4 | 1 |
| 1:A:13:A:N1 | 1:A:96:A:C2 | 0.41 | 2.88 | 7 | 1 |
| 1:A:73:C:N4 | 1:A:74:U:O4 | 0.41 | 2.53 | 2 | 1 |
| 1:A:9:A:H1' | 1:A:10:G:N2 | 0.41 | 2.31 | 6 | 1 |
| 1:A:65:U:OP1 | 1:A:65:U:O4' | 0.41 | 2.38 | 9 | 1 |
| 1:A:31:G:C2 | 1:A:34:U:O2 | 0.41 | 2.74 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:59:A:N1 | 1:A:60:U:N3 | 0.41 | 2.69 | 2 | 1 |
| 1:A:101:U:O2 | 1:A:103:G:N1 | 0.41 | 2.54 | 8 | 1 |
| 1:A:70:A:C6 | 1:A:71:A:C6 | 0.41 | 3.09 | 10 | 1 |
| 1:A:101:U:C2' | 1:A:102:A:OP2 | 0.41 | 2.67 | 1 | 1 |
| 1:A:66:C:N3 | 1:A:67:G:O6 | 0.41 | 2.54 | 9 | 1 |
| 1:A:104:U:N3 | 1:A:105:A:N7 | 0.41 | 2.69 | 2 | 1 |
| 1:A:31:G:N2 | 1:A:34:U:O2 | 0.41 | 2.54 | 2 | 1 |
| 1:A:103:G:C5 | 1:A:104:U:N3 | 0.41 | 2.89 | 10 | 1 |
| 1:A:26:C:O2' | 1:A:27:C:H5' | 0.41 | 2.16 | 10 | 1 |
| 1:A:6:U:C2 | 1:A:7:A:C8 | 0.41 | 3.09 | 10 | 1 |
| 1:A:34:U:O2 | 1:A:34:U:H2' | 0.41 | 2.15 | 1 | 1 |
| 1:A:33:A:N3 | 1:A:34:U:H6 | 0.41 | 2.12 | 4 | 1 |
| 1:A:65:U:O4' | 1:A:65:U:OP1 | 0.41 | 2.39 | 4 | 1 |
| 1:A:39:A:N3 | 1:A:40:U:C2 | 0.41 | 2.89 | 3 | 1 |
| 1:A:24:U:O2' | 1:A:25:U:C5' | 0.41 | 2.69 | 6 | 2 |
| 1:A:46:G:O2' | 1:A:47:U:C5' | 0.41 | 2.69 | 2 | 1 |
| 1:A:84:U:C2 | 1:A:85:U:C4 | 0.41 | 3.09 | 3 | 1 |
| 1:A:100:G:H1' | 1:A:102:A:N6 | 0.41 | 2.30 | 6 | 1 |
| 1:A:17:U:HO2' | 1:A:18:C:H6 | 0.41 | 1.59 | 7 | 1 |
| 1:A:81:C:O2' | 1:A:82:U:O5' | 0.40 | 2.35 | 9 | 1 |
| 1:A:13:A:N7 | 1:A:99:U:O2 | 0.40 | 2.55 | 1 | 1 |
| 1:A:100:G:H3' | 1:A:101:U:O4' | 0.40 | 2.15 | 5 | 1 |
| 1:A:19:A:C2 | 1:A:20:G:C8 | 0.40 | 3.09 | 5 | 1 |
| 1:A:26:C:N4 | 1:A:28:C:N4 | 0.40 | 2.69 | 6 | 1 |
| 1:A:13:A:O2' | 1:A:14:U:H6 | 0.40 | 1.97 | 7 | 1 |
| 1:A:11:A:H5'' | 1:A:12:G:OP1 | 0.40 | 2.16 | 8 | 1 |
| 1:A:32:C:O2' | 1:A:33:A:C5' | 0.40 | 2.70 | 9 | 1 |
| 1:A:21:C:N3 | 1:A:87:G:C2 | 0.40 | 2.90 | 10 | 1 |
| 1:A:40:U:OP2 | 1:A:40:U:C6 | 0.40 | 2.74 | 5 | 1 |
| 1:A:89:U:O2' | 1:A:90:U:C5 | 0.40 | 2.66 | 5 | 1 |
| 1:A:3:C:O2' | 1:A:4:A:N7 | 0.40 | 2.40 | 6 | 1 |
| 1:A:13:A:N6 | 1:A:96:A:N1 | 0.40 | 2.70 | 7 | 1 |
| 1:A:55:A:C2 | 1:A:56:G:N7 | 0.40 | 2.89 | 2 | 1 |
| 1:A:22:A:H61 | 1:A:87:G:H1' | 0.40 | 1.76 | 5 | 1 |
| 1:A:9:A:H1' | 1:A:11:A:N6 | 0.40 | 2.31 | 7 | 1 |
| 1:A:66:C:C2' | 1:A:66:C:O5' | 0.40 | 2.69 | 8 | 1 |
| 1:A:89:U:C2 | 1:A:91:A:N6 | 0.40 | 2.90 | 8 | 1 |
| 1:A:39:A:C5 | 1:A:40:U:C4 | 0.40 | 3.09 | 2 | 1 |
| 1:A:39:A:N1 | 1:A:40:U:N3 | 0.40 | 2.69 | 2 | 1 |
| 1:A:12:G:C5 | 1:A:100:G:N2 | 0.40 | 2.89 | 4 | 1 |
| 1:A:97:A:N7 | 1:A:98:G:O6 | 0.40 | 2.54 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|--------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:58:G:O2' | 1:A:59:A:O4' | 0.40 | 2.40 | 9 | 1 |
| 1:A:19:A:HO2' | 1:A:20:G:P | 0.40 | 2.40 | 2 | 1 |
| 1:A:6:U:O2 | 1:A:105:A:N1 | 0.40 | 2.55 | 10 | 1 |
| 1:A:10:G:H22 | 1:A:11:A:N6 | 0.40 | 2.12 | 4 | 1 |
| 1:A:73:C:C2' | 1:A:74:U:O4' | 0.40 | 2.65 | 6 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

6.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers | Suiteness |
|-----|-------|-----------------|-------------------|-----------------|-----------|
| 1 | A | 110/111 (99%) | 64±6 (59±6%) | 0±0 (0±0%) | 0.10±0.03 |
| All | All | 1100/1110 (99%) | 644 (59%) | 0 (0%) | 0.11 |

The overall RNA backbone suiteness is 0.10.

All unique RNA backbone outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 53 | A | 10 |
| 1 | A | 101 | U | 10 |
| 1 | A | 2 | G | 10 |
| 1 | A | 36 | A | 10 |
| 1 | A | 23 | G | 10 |
| 1 | A | 46 | G | 10 |
| 1 | A | 87 | G | 10 |
| 1 | A | 40 | U | 10 |
| 1 | A | 34 | U | 10 |
| 1 | A | 111 | C | 10 |
| 1 | A | 56 | G | 10 |
| 1 | A | 35 | A | 10 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 41 | G | 10 |
| 1 | A | 86 | G | 10 |
| 1 | A | 107 | C | 10 |
| 1 | A | 98 | G | 10 |
| 1 | A | 102 | A | 10 |
| 1 | A | 67 | G | 10 |
| 1 | A | 30 | U | 10 |
| 1 | A | 12 | G | 10 |
| 1 | A | 90 | U | 10 |
| 1 | A | 15 | G | 10 |
| 1 | A | 92 | G | 10 |
| 1 | A | 47 | U | 10 |
| 1 | A | 100 | G | 10 |
| 1 | A | 3 | C | 10 |
| 1 | A | 57 | A | 10 |
| 1 | A | 10 | G | 10 |
| 1 | A | 66 | C | 10 |
| 1 | A | 26 | C | 10 |
| 1 | A | 28 | C | 10 |
| 1 | A | 85 | U | 9 |
| 1 | A | 83 | U | 9 |
| 1 | A | 33 | A | 9 |
| 1 | A | 27 | C | 9 |
| 1 | A | 74 | U | 9 |
| 1 | A | 39 | A | 9 |
| 1 | A | 84 | U | 9 |
| 1 | A | 13 | A | 9 |
| 1 | A | 50 | U | 9 |
| 1 | A | 103 | G | 9 |
| 1 | A | 96 | A | 9 |
| 1 | A | 110 | U | 8 |
| 1 | A | 68 | G | 8 |
| 1 | A | 11 | A | 8 |
| 1 | A | 5 | A | 8 |
| 1 | A | 97 | A | 8 |
| 1 | A | 4 | A | 8 |
| 1 | A | 9 | A | 8 |
| 1 | A | 48 | U | 7 |
| 1 | A | 65 | U | 7 |
| 1 | A | 6 | U | 7 |
| 1 | A | 99 | U | 7 |
| 1 | A | 104 | U | 7 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 49 | U | 7 |
| 1 | A | 82 | U | 7 |
| 1 | A | 19 | A | 7 |
| 1 | A | 108 | U | 7 |
| 1 | A | 106 | U | 7 |
| 1 | A | 51 | A | 7 |
| 1 | A | 22 | A | 7 |
| 1 | A | 32 | C | 7 |
| 1 | A | 91 | A | 6 |
| 1 | A | 37 | G | 5 |
| 1 | A | 45 | C | 5 |
| 1 | A | 81 | C | 5 |
| 1 | A | 18 | C | 4 |
| 1 | A | 52 | C | 4 |
| 1 | A | 14 | U | 4 |
| 1 | A | 105 | A | 4 |
| 1 | A | 31 | G | 4 |
| 1 | A | 55 | A | 3 |
| 1 | A | 88 | C | 3 |
| 1 | A | 42 | A | 3 |
| 1 | A | 7 | A | 3 |
| 1 | A | 58 | G | 3 |
| 1 | A | 73 | C | 3 |
| 1 | A | 75 | C | 3 |
| 1 | A | 60 | U | 2 |
| 1 | A | 64 | U | 2 |
| 1 | A | 76 | U | 2 |
| 1 | A | 109 | G | 2 |
| 1 | A | 77 | U | 2 |
| 1 | A | 21 | C | 2 |
| 1 | A | 20 | G | 2 |
| 1 | A | 59 | A | 2 |
| 1 | A | 80 | C | 2 |
| 1 | A | 29 | C | 1 |
| 1 | A | 78 | U | 1 |
| 1 | A | 8 | C | 1 |
| 1 | A | 70 | A | 1 |
| 1 | A | 17 | U | 1 |
| 1 | A | 43 | A | 1 |
| 1 | A | 38 | G | 1 |
| 1 | A | 16 | A | 1 |

There are no RNA pucker outliers to report.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: 2lkr_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

| | |
|---|----|
| Total number of shifts | 45 |
| Number of shifts mapped to atoms | 45 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 2%, i.e. 45 atoms were assigned a chemical shift out of a possible 2064. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|--------------|----------------|-----------------|-----------------|
| Backbone | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Sidechain | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Aromatic | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Overall | 45/2064 (2%) | 45/1176 (4%) | 0/752 (0%) | 0/136 (0%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 45 atoms were assigned a chemical shift out of a possible 2064. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|--------------|----------------|-----------------|-----------------|
| Backbone | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Sidechain | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Aromatic | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Overall | 45/2064 (2%) | 45/1176 (4%) | 0/752 (0%) | 0/136 (0%) |

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.

7.2 Chemical shift list 2

File name: 2lkr_cs.str

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping [i](#)

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

| | |
|---|----|
| Total number of shifts | 50 |
| Number of shifts mapped to atoms | 50 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 2%, i.e. 50 atoms were assigned a chemical

shift out of a possible 2064. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹H | ¹³C | ¹⁵N |
|-----------|--------------|----------------------|-----------------------|-----------------------|
| Backbone | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Sidechain | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Aromatic | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Overall | 50/2064 (2%) | 25/1176 (2%) | 0/752 (0%) | 25/136 (18%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 50 atoms were assigned a chemical shift out of a possible 2064. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹H | ¹³C | ¹⁵N |
|-----------|--------------|----------------------|-----------------------|-----------------------|
| Backbone | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Sidechain | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Aromatic | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) | 0/0 (—%) |
| Overall | 50/2064 (2%) | 25/1176 (2%) | 0/752 (0%) | 25/136 (18%) |

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_2). RCI is only applicable to proteins.