



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 12:05 PM EDT

PDB ID : 1N36 / pdb\_00001n36  
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit in the presence of crystallographically disordered codon and near-cognate transfer RNA anticodon stem-loop mismatched at the second codon position  
Authors : Ogle, J.M.; Murphy IV, F.V.; Tarry, M.J.; Ramakrishnan, V.  
Deposited on : 2002-10-25  
Resolution : 3.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | NOT EXECUTED                                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

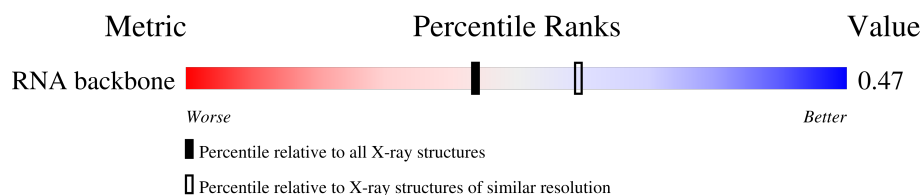
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 Å.

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.



| <b>Metric</b> | <b>Whole archive<br/>(#Entries)</b> | <b>Similar resolution<br/>(#Entries, resolution range(Å))</b> |
|---------------|-------------------------------------|---------------------------------------------------------------|
| RNA backbone  | 3983                                | 1027 (4.26-3.06)                                              |

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

## 2 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

| Property                                                 | Value                                                       | Source    |
|----------------------------------------------------------|-------------------------------------------------------------|-----------|
| Space group                                              | P 41 21 2                                                   | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 402.84Å 402.84Å 174.28Å<br>90.00° 90.00° 90.00°             | Depositor |
| Resolution (Å)                                           | 141.42 – 3.65                                               | Depositor |
| % Data completeness<br>(in resolution range)             | 92.6 (141.42-3.65)                                          | Depositor |
| $R_{merge}$                                              | (Not available)                                             | Depositor |
| $R_{sym}$                                                | 0.14                                                        | Depositor |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>               | 2.44 (at 3.67Å)                                             | Xtriage   |
| Refinement program                                       | CNS                                                         | Depositor |
| R, $R_{free}$                                            | 0.260 , 0.324                                               | Depositor |
| Wilson B-factor (Å <sup>2</sup> )                        | 107.1                                                       | Xtriage   |
| Anisotropy                                               | 0.426                                                       | Xtriage   |
| L-test for twinning <sup>2</sup>                         | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage   |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtriage   |
| Total number of atoms                                    | 51680                                                       | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 93.0                                                        | wwPDB-VP  |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 3 Model quality

### 3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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 root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.52         | 0/36387        | 0.77        | 61/56789 (0.1%)  |
| 2   | B     | 0.60         | 0/1935         | 1.22        | 27/2609 (1.0%)   |
| 3   | C     | 0.57         | 0/1636         | 1.17        | 13/2205 (0.6%)   |
| 4   | D     | 0.56         | 0/1733         | 1.03        | 13/2318 (0.6%)   |
| 5   | E     | 0.81         | 1/1162 (0.1%)  | 1.23        | 11/1564 (0.7%)   |
| 6   | F     | 0.51         | 0/856          | 1.06        | 8/1154 (0.7%)    |
| 7   | G     | 0.52         | 0/1276         | 1.22        | 17/1709 (1.0%)   |
| 8   | H     | 0.86         | 1/1136 (0.1%)  | 1.32        | 15/1527 (1.0%)   |
| 9   | I     | 0.55         | 0/1029         | 1.17        | 11/1378 (0.8%)   |
| 10  | J     | 0.59         | 0/805          | 1.32        | 14/1082 (1.3%)   |
| 11  | K     | 0.64         | 0/900          | 1.21        | 11/1213 (0.9%)   |
| 12  | L     | 0.64         | 0/986          | 1.24        | 9/1320 (0.7%)    |
| 13  | M     | 0.51         | 0/947          | 1.24        | 16/1270 (1.3%)   |
| 14  | N     | 0.51         | 0/501          | 1.07        | 5/664 (0.8%)     |
| 15  | O     | 0.67         | 1/745 (0.1%)   | 1.04        | 4/992 (0.4%)     |
| 16  | P     | 0.67         | 0/716          | 1.25        | 9/963 (0.9%)     |
| 17  | Q     | 0.75         | 0/870          | 1.34        | 14/1159 (1.2%)   |
| 18  | R     | 0.58         | 0/603          | 1.06        | 2/799 (0.3%)     |
| 19  | S     | 0.59         | 0/661          | 1.35        | 13/890 (1.5%)    |
| 20  | T     | 0.58         | 0/765          | 1.09        | 5/1007 (0.5%)    |
| 21  | V     | 0.56         | 0/212          | 0.96        | 0/277            |
| All | All   | 0.56         | 3/55861 (0.0%) | 0.93        | 278/82889 (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 outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 1                   | 63                  |
| 8   | H     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| All | All   | 1                   | 64                  |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8   | H     | 109 | ILE  | CA-CB | -5.76 | 1.46        | 1.54     |
| 5   | E     | 101 | ILE  | CA-CB | -5.25 | 1.47        | 1.53     |
| 15  | O     | 29  | VAL  | CA-CB | -5.24 | 1.48        | 1.54     |

All (278) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 7   | G     | 30   | ILE  | N-CA-C      | -13.09 | 99.88       | 112.96   |
| 1   | A     | 1498 | U    | C2'-C3'-O3' | 12.81  | 128.71      | 109.50   |
| 18  | R     | 46   | GLU  | N-CA-C      | -11.68 | 98.28       | 111.71   |
| 12  | L     | 26   | ALA  | N-CA-C      | -11.66 | 99.80       | 113.21   |
| 3   | C     | 122  | GLU  | N-CA-C      | -11.49 | 98.77       | 111.07   |
| 1   | A     | 575  | G    | C2'-C3'-O3' | 11.47  | 126.70      | 109.50   |
| 10  | J     | 80   | LYS  | N-CA-C      | -11.38 | 97.89       | 112.23   |
| 1   | A     | 60   | A    | C2'-C3'-O3' | 11.24  | 126.37      | 109.50   |
| 3   | C     | 88   | ARG  | N-CA-C      | -11.07 | 98.98       | 111.82   |
| 19  | S     | 73   | GLU  | N-CA-C      | -10.93 | 99.76       | 112.87   |
| 3   | C     | 125  | GLU  | N-CA-C      | -10.32 | 100.43      | 113.23   |
| 1   | A     | 266  | G    | C2'-C3'-O3' | 10.19  | 124.79      | 109.50   |
| 19  | S     | 14   | HIS  | N-CA-C      | -9.93  | 100.70      | 113.12   |
| 2   | B     | 13   | ALA  | N-CA-C      | -9.93  | 101.09      | 113.01   |
| 7   | G     | 155  | ARG  | N-CA-C      | 9.71   | 121.81      | 111.03   |
| 7   | G     | 51   | GLN  | N-CA-C      | -9.66  | 97.95       | 112.54   |
| 9   | I     | 20   | ARG  | CA-C-N      | 9.58   | 131.81      | 119.84   |
| 9   | I     | 20   | ARG  | C-N-CA      | 9.58   | 131.81      | 119.84   |
| 11  | K     | 75   | TYR  | N-CA-C      | -9.35  | 101.42      | 112.92   |
| 11  | K     | 74   | ALA  | N-CA-C      | -9.13  | 101.42      | 114.12   |
| 2   | B     | 87   | ARG  | N-CA-C      | -9.11  | 102.28      | 112.57   |
| 1   | A     | 1085 | U    | C2'-C3'-O3' | 8.83   | 122.75      | 109.50   |
| 11  | K     | 17   | GLY  | N-CA-C      | 8.77   | 125.13      | 112.60   |
| 19  | S     | 49   | ILE  | N-CA-C      | 8.54   | 120.13      | 108.17   |
| 12  | L     | 118  | SER  | N-CA-C      | -8.51  | 100.26      | 111.24   |
| 1   | A     | 328  | C    | C2'-C3'-O3' | 8.45   | 122.17      | 109.50   |
| 1   | A     | 1498 | U    | C4'-C3'-O3' | 8.41   | 122.02      | 109.40   |
| 2   | B     | 156  | LYS  | N-CA-C      | -8.30  | 105.16      | 114.62   |
| 13  | M     | 112  | GLY  | CA-C-N      | 8.23   | 128.72      | 119.83   |
| 13  | M     | 112  | GLY  | C-N-CA      | 8.23   | 128.72      | 119.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | H     | 56   | LYS  | CA-C-N      | 8.22  | 130.34      | 120.23   |
| 8   | H     | 56   | LYS  | C-N-CA      | 8.22  | 130.34      | 120.23   |
| 1   | A     | 533  | A    | C2'-C3'-O3' | 8.21  | 121.82      | 109.50   |
| 16  | P     | 53   | VAL  | N-CA-C      | -8.10 | 102.06      | 113.07   |
| 1   | A     | 243  | A    | C2'-C3'-O3' | 8.07  | 121.61      | 109.50   |
| 2   | B     | 114  | ARG  | N-CA-C      | -8.05 | 101.58      | 111.40   |
| 13  | M     | 11   | ARG  | N-CA-C      | 7.99  | 121.54      | 108.52   |
| 2   | B     | 134  | GLU  | N-CA-C      | -7.94 | 104.07      | 114.31   |
| 9   | I     | 112  | LYS  | N-CA-C      | 7.93  | 121.77      | 109.96   |
| 1   | A     | 51   | A    | C2'-C3'-O3' | 7.92  | 121.38      | 109.50   |
| 1   | A     | 372  | C    | C2'-C3'-O3' | 7.90  | 121.35      | 109.50   |
| 19  | S     | 41   | VAL  | CA-C-N      | 7.87  | 129.68      | 119.84   |
| 19  | S     | 41   | VAL  | C-N-CA      | 7.87  | 129.68      | 119.84   |
| 17  | Q     | 56   | VAL  | N-CA-C      | -7.85 | 96.94       | 108.87   |
| 13  | M     | 40   | ASN  | CA-C-N      | 7.82  | 127.11      | 118.97   |
| 13  | M     | 40   | ASN  | C-N-CA      | 7.82  | 127.11      | 118.97   |
| 14  | N     | 42   | ILE  | N-CA-C      | -7.82 | 103.07      | 110.42   |
| 7   | G     | 24   | THR  | N-CA-C      | -7.75 | 101.81      | 111.11   |
| 2   | B     | 148  | TYR  | N-CA-C      | 7.72  | 119.48      | 111.14   |
| 16  | P     | 51   | VAL  | N-CA-C      | 7.71  | 125.37      | 109.34   |
| 2   | B     | 23   | ARG  | N-CA-C      | -7.63 | 102.19      | 112.26   |
| 1   | A     | 366  | C    | C2'-C3'-O3' | 7.59  | 120.89      | 109.50   |
| 1   | A     | 1101 | A    | C2'-C3'-O3' | 7.58  | 120.86      | 109.50   |
| 16  | P     | 60   | LEU  | N-CA-C      | -7.54 | 103.64      | 114.12   |
| 2   | B     | 45   | GLN  | N-CA-C      | -7.52 | 102.24      | 111.33   |
| 13  | M     | 66   | LEU  | N-CA-C      | 7.44  | 120.41      | 109.69   |
| 1   | A     | 993  | G    | C2'-C3'-O3' | 7.44  | 120.66      | 109.50   |
| 3   | C     | 91   | LEU  | N-CA-C      | -7.44 | 103.16      | 112.90   |
| 12  | L     | 98   | TYR  | N-CA-C      | 7.44  | 117.82      | 108.45   |
| 19  | S     | 10   | PHE  | N-CA-C      | 7.39  | 120.46      | 108.41   |
| 1   | A     | 1067 | A    | C2'-C3'-O3' | 7.32  | 120.48      | 109.50   |
| 19  | S     | 70   | LYS  | N-CA-C      | 7.15  | 119.34      | 109.54   |
| 3   | C     | 93   | LYS  | N-CA-C      | -7.14 | 104.56      | 113.20   |
| 12  | L     | 122  | THR  | N-CA-C      | -7.14 | 98.16       | 109.23   |
| 1   | A     | 7    | G    | C2'-C3'-O3' | 7.13  | 120.20      | 109.50   |
| 12  | L     | 43   | VAL  | N-CA-C      | 7.12  | 119.08      | 108.96   |
| 8   | H     | 137  | VAL  | N-CA-C      | 7.11  | 119.36      | 109.55   |
| 9   | I     | 82   | ALA  | N-CA-C      | -7.10 | 104.88      | 113.97   |
| 1   | A     | 748  | C    | C2'-C3'-O3' | 7.10  | 120.15      | 109.50   |
| 9   | I     | 122  | ALA  | CA-C-N      | 7.04  | 128.64      | 119.84   |
| 9   | I     | 122  | ALA  | C-N-CA      | 7.04  | 128.64      | 119.84   |
| 17  | Q     | 73   | VAL  | N-CA-C      | 7.01  | 116.71      | 106.55   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Q     | 62   | SER  | N-CA-C      | 6.96  | 118.77      | 108.60   |
| 1   | A     | 587  | G    | C4'-C3'-O3' | -6.94 | 102.59      | 113.00   |
| 2   | B     | 64   | ARG  | N-CA-C      | -6.93 | 104.08      | 112.54   |
| 16  | P     | 32   | TYR  | N-CA-C      | 6.93  | 119.09      | 108.42   |
| 17  | Q     | 63   | ARG  | N-CA-C      | -6.86 | 101.00      | 109.65   |
| 4   | D     | 196  | LEU  | CA-C-N      | 6.85  | 128.40      | 119.84   |
| 4   | D     | 196  | LEU  | C-N-CA      | 6.85  | 128.40      | 119.84   |
| 17  | Q     | 12   | SER  | N-CA-C      | 6.81  | 119.58      | 108.55   |
| 13  | M     | 73   | GLU  | N-CA-C      | -6.80 | 103.79      | 111.14   |
| 12  | L     | 50   | SER  | N-CA-C      | 6.79  | 120.66      | 110.14   |
| 13  | M     | 104  | ARG  | N-CA-C      | -6.79 | 103.12      | 111.40   |
| 19  | S     | 62   | ILE  | N-CA-C      | 6.76  | 118.79      | 109.80   |
| 17  | Q     | 6    | LEU  | N-CA-C      | 6.75  | 119.39      | 108.32   |
| 8   | H     | 69   | ARG  | N-CA-C      | 6.75  | 119.67      | 109.41   |
| 14  | N     | 31   | ARG  | N-CA-C      | 6.73  | 125.13      | 110.80   |
| 10  | J     | 44   | VAL  | N-CA-C      | 6.70  | 118.58      | 108.80   |
| 1   | A     | 30   | U    | C2'-C3'-O3' | 6.69  | 119.54      | 109.50   |
| 1   | A     | 1049 | U    | C2'-C3'-O3' | 6.68  | 119.52      | 109.50   |
| 8   | H     | 88   | LYS  | CA-C-N      | -6.65 | 111.53      | 119.84   |
| 8   | H     | 88   | LYS  | C-N-CA      | -6.65 | 111.53      | 119.84   |
| 1   | A     | 204  | U    | C2'-C3'-O3' | 6.64  | 119.46      | 109.50   |
| 7   | G     | 145  | ALA  | N-CA-C      | -6.63 | 101.78      | 110.33   |
| 8   | H     | 89   | PRO  | N-CA-C      | -6.62 | 98.83       | 112.47   |
| 9   | I     | 118  | LYS  | N-CA-C      | 6.62  | 117.87      | 108.54   |
| 1   | A     | 115  | G    | C2'-C3'-O3' | 6.59  | 119.38      | 109.50   |
| 16  | P     | 20   | VAL  | N-CA-C      | 6.57  | 123.01      | 109.34   |
| 6   | F     | 60   | PHE  | N-CA-C      | 6.53  | 120.47      | 109.76   |
| 5   | E     | 26   | PHE  | N-CA-C      | 6.52  | 116.89      | 108.34   |
| 4   | D     | 39   | PRO  | CA-C-N      | 6.50  | 127.96      | 119.84   |
| 4   | D     | 39   | PRO  | C-N-CA      | 6.50  | 127.96      | 119.84   |
| 13  | M     | 92   | HIS  | N-CA-C      | -6.46 | 104.65      | 112.54   |
| 7   | G     | 9    | VAL  | N-CA-C      | 6.46  | 118.93      | 109.63   |
| 20  | T     | 75   | ASN  | N-CA-C      | -6.46 | 104.33      | 111.82   |
| 5   | E     | 86   | ALA  | N-CA-C      | -6.46 | 105.22      | 113.23   |
| 1   | A     | 290  | C    | N1-C1'-C2'  | -6.45 | 102.33      | 112.00   |
| 7   | G     | 47   | CYS  | N-CA-C      | -6.43 | 103.32      | 112.13   |
| 2   | B     | 137  | ARG  | N-CA-C      | -6.43 | 104.19      | 111.07   |
| 10  | J     | 22   | LYS  | N-CA-C      | -6.42 | 105.48      | 113.38   |
| 19  | S     | 58   | VAL  | CA-C-N      | 6.40  | 126.36      | 119.76   |
| 19  | S     | 58   | VAL  | C-N-CA      | 6.40  | 126.36      | 119.76   |
| 5   | E     | 95   | ALA  | CA-C-N      | 6.40  | 126.37      | 119.78   |
| 5   | E     | 95   | ALA  | C-N-CA      | 6.40  | 126.37      | 119.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 975  | A    | C2'-C3'-O3' | 6.39  | 119.09      | 109.50   |
| 1   | A     | 1281 | U    | C2'-C3'-O3' | 6.38  | 119.07      | 109.50   |
| 3   | C     | 8    | ILE  | N-CA-C      | -6.38 | 104.30      | 110.42   |
| 1   | A     | 792  | A    | C2'-C3'-O3' | 6.35  | 119.03      | 109.50   |
| 16  | P     | 79   | VAL  | N-CA-C      | -6.34 | 102.76      | 111.89   |
| 10  | J     | 26   | ALA  | N-CA-C      | -6.32 | 104.09      | 110.97   |
| 7   | G     | 12   | LEU  | N-CA-C      | 6.30  | 118.13      | 109.18   |
| 8   | H     | 114  | THR  | N-CA-C      | 6.27  | 119.19      | 109.60   |
| 4   | D     | 21   | LEU  | N-CA-C      | -6.26 | 105.36      | 112.87   |
| 10  | J     | 13   | HIS  | N-CA-C      | 6.26  | 117.90      | 111.14   |
| 11  | K     | 50   | TYR  | N-CA-C      | 6.25  | 124.11      | 110.80   |
| 8   | H     | 112  | LEU  | N-CA-C      | -6.18 | 102.81      | 110.41   |
| 4   | D     | 112  | VAL  | N-CA-C      | 6.18  | 118.19      | 111.77   |
| 11  | K     | 39   | PRO  | N-CA-C      | 6.17  | 120.34      | 110.40   |
| 5   | E     | 14   | ARG  | N-CA-C      | 6.17  | 118.56      | 109.24   |
| 6   | F     | 98   | LEU  | N-CA-C      | 6.16  | 119.52      | 109.24   |
| 8   | H     | 52   | ASP  | N-CA-C      | 6.11  | 118.33      | 109.71   |
| 10  | J     | 4    | ILE  | N-CA-C      | 6.10  | 115.13      | 106.53   |
| 1   | A     | 119  | A    | C2'-C3'-O3' | 6.09  | 118.64      | 109.50   |
| 7   | G     | 49   | ILE  | N-CA-C      | -6.08 | 96.68       | 109.34   |
| 2   | B     | 16   | HIS  | CB-CA-C     | -6.01 | 107.93      | 116.34   |
| 1   | A     | 250  | A    | C2'-C3'-O3' | 5.99  | 118.49      | 109.50   |
| 16  | P     | 77   | ALA  | N-CA-C      | -5.99 | 106.06      | 113.19   |
| 6   | F     | 67   | MET  | CA-C-N      | 5.99  | 125.96      | 120.21   |
| 6   | F     | 67   | MET  | C-N-CA      | 5.99  | 125.96      | 120.21   |
| 19  | S     | 58   | VAL  | N-CA-C      | 5.99  | 121.82      | 108.88   |
| 11  | K     | 25   | TYR  | N-CA-C      | -5.98 | 105.84      | 113.02   |
| 2   | B     | 185  | ILE  | N-CA-C      | -5.98 | 99.02       | 107.75   |
| 17  | Q     | 68   | ARG  | N-CA-C      | -5.96 | 103.02      | 111.24   |
| 17  | Q     | 83   | ASP  | N-CA-C      | -5.93 | 104.89      | 111.71   |
| 4   | D     | 208  | SER  | N-CA-C      | -5.91 | 105.66      | 114.64   |
| 20  | T     | 16   | HIS  | N-CA-C      | -5.88 | 103.85      | 111.02   |
| 7   | G     | 109  | ASN  | N-CA-C      | -5.87 | 105.88      | 113.16   |
| 2   | B     | 96   | ARG  | N-CA-C      | 5.83  | 123.22      | 110.80   |
| 2   | B     | 189  | ASP  | N-CA-C      | 5.82  | 115.53      | 107.73   |
| 3   | C     | 96   | GLY  | N-CA-C      | -5.81 | 105.68      | 115.62   |
| 4   | D     | 188  | LEU  | CA-C-N      | 5.81  | 127.10      | 119.84   |
| 4   | D     | 188  | LEU  | C-N-CA      | 5.81  | 127.10      | 119.84   |
| 1   | A     | 992  | U    | C2'-C3'-O3' | 5.80  | 118.21      | 109.50   |
| 2   | B     | 111  | ARG  | N-CA-C      | -5.80 | 103.76      | 111.24   |
| 11  | K     | 116  | HIS  | N-CA-C      | -5.78 | 105.34      | 113.20   |
| 15  | O     | 64   | ARG  | N-CA-C      | -5.76 | 105.35      | 112.38   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | G     | 70   | LYS  | CA-C-N      | 5.75  | 127.03      | 119.84   |
| 7   | G     | 70   | LYS  | C-N-CA      | 5.75  | 127.03      | 119.84   |
| 1   | A     | 438  | G    | C4'-C3'-O3' | 5.75  | 118.03      | 109.40   |
| 1   | A     | 1443 | G    | N9-C1'-C2'  | 5.75  | 120.62      | 112.00   |
| 1   | A     | 573  | A    | N9-C1'-C2'  | 5.74  | 120.61      | 112.00   |
| 1   | A     | 839  | U    | N1-C1'-C2'  | 5.74  | 120.61      | 112.00   |
| 3   | C     | 203  | PHE  | N-CA-C      | -5.73 | 103.08      | 110.19   |
| 1   | A     | 1529 | G    | N9-C1'-C2'  | 5.73  | 122.59      | 114.00   |
| 5   | E     | 69   | VAL  | CB-CA-C     | -5.72 | 104.25      | 110.37   |
| 13  | M     | 102  | ARG  | N-CA-C      | -5.71 | 103.39      | 110.41   |
| 2   | B     | 32   | ILE  | N-CA-C      | 5.70  | 116.09      | 108.11   |
| 16  | P     | 76   | GLN  | N-CA-C      | -5.70 | 104.75      | 110.97   |
| 18  | R     | 81   | PHE  | N-CA-C      | -5.70 | 105.58      | 112.54   |
| 5   | E     | 105  | VAL  | CA-C-N      | -5.69 | 112.72      | 119.84   |
| 5   | E     | 105  | VAL  | C-N-CA      | -5.69 | 112.72      | 119.84   |
| 8   | H     | 56   | LYS  | N-CA-C      | -5.69 | 102.61      | 109.72   |
| 12  | L     | 11   | VAL  | N-CA-C      | -5.68 | 104.39      | 110.36   |
| 9   | I     | 70   | LYS  | N-CA-C      | 5.67  | 118.24      | 111.71   |
| 19  | S     | 36   | ARG  | N-CA-C      | -5.67 | 104.95      | 112.94   |
| 13  | M     | 116  | THR  | N-CA-C      | 5.62  | 117.79      | 110.43   |
| 3   | C     | 124  | ILE  | N-CA-C      | -5.62 | 108.37      | 113.71   |
| 20  | T     | 57   | ARG  | N-CA-C      | -5.62 | 104.80      | 111.03   |
| 1   | A     | 1201 | A    | C2'-C3'-O3' | 5.60  | 117.90      | 109.50   |
| 10  | J     | 28   | ARG  | N-CA-C      | -5.60 | 106.30      | 113.02   |
| 11  | K     | 67   | ASP  | N-CA-C      | -5.59 | 104.83      | 111.03   |
| 20  | T     | 73   | HIS  | CB-CA-C     | -5.58 | 108.53      | 116.34   |
| 1   | A     | 351  | G    | C2'-C3'-O3' | 5.56  | 117.84      | 109.50   |
| 2   | B     | 109  | SER  | N-CA-C      | -5.55 | 105.38      | 111.82   |
| 1   | A     | 819  | A    | C3'-C2'-O2' | -5.53 | 106.30      | 114.60   |
| 16  | P     | 61   | SER  | N-CA-C      | -5.53 | 106.61      | 113.19   |
| 8   | H     | 3    | THR  | N-CA-C      | -5.49 | 105.94      | 113.30   |
| 19  | S     | 65   | ASN  | N-CA-C      | -5.49 | 105.37      | 111.36   |
| 11  | K     | 71   | LYS  | N-CA-C      | -5.49 | 105.21      | 111.14   |
| 17  | Q     | 33   | GLY  | N-CA-C      | 5.48  | 126.17      | 113.18   |
| 1   | A     | 560  | U    | C2'-C3'-O3' | 5.47  | 117.70      | 109.50   |
| 2   | B     | 17   | PHE  | N-CA-C      | 5.46  | 122.44      | 110.80   |
| 4   | D     | 205  | GLU  | N-CA-C      | 5.46  | 117.09      | 111.03   |
| 6   | F     | 26   | ILE  | N-CA-C      | -5.46 | 105.01      | 110.30   |
| 8   | H     | 19   | VAL  | N-CA-C      | -5.45 | 106.10      | 111.88   |
| 1   | A     | 7    | G    | C4'-C3'-O3' | 5.45  | 117.58      | 109.40   |
| 7   | G     | 62   | PHE  | N-CA-C      | -5.43 | 102.46      | 111.37   |
| 20  | T     | 64   | ASP  | N-CA-C      | -5.43 | 105.47      | 111.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | O     | 53   | HIS  | N-CA-C      | -5.43 | 105.01      | 111.03   |
| 1   | A     | 484  | G    | C2'-C3'-O3' | 5.42  | 117.64      | 109.50   |
| 8   | H     | 2    | LEU  | N-CA-C      | -5.42 | 103.23      | 110.55   |
| 12  | L     | 119  | LYS  | N-CA-C      | -5.42 | 103.38      | 110.53   |
| 3   | C     | 159  | GLY  | N-CA-C      | -5.41 | 107.31      | 115.32   |
| 10  | J     | 49   | VAL  | N-CA-C      | 5.40  | 117.42      | 108.99   |
| 14  | N     | 5    | ALA  | N-CA-C      | -5.40 | 106.28      | 112.92   |
| 9   | I     | 117  | HIS  | N-CA-C      | -5.39 | 104.90      | 112.12   |
| 1   | A     | 1196 | U    | C4'-C3'-O3' | 5.39  | 117.48      | 109.40   |
| 1   | A     | 1454 | G    | N9-C1'-C2'  | -5.38 | 103.92      | 112.00   |
| 10  | J     | 90   | LEU  | CA-C-N      | 5.38  | 125.68      | 119.92   |
| 10  | J     | 90   | LEU  | C-N-CA      | 5.38  | 125.68      | 119.92   |
| 1   | A     | 1037 | C    | N1-C1'-C2'  | 5.38  | 120.06      | 112.00   |
| 2   | B     | 222  | ILE  | N-CA-C      | -5.37 | 105.09      | 110.30   |
| 4   | D     | 140  | VAL  | CB-CA-C     | -5.35 | 104.46      | 111.25   |
| 1   | A     | 563  | A    | N9-C1'-C2'  | 5.34  | 120.01      | 112.00   |
| 17  | Q     | 39   | SER  | N-CA-C      | 5.34  | 117.30      | 109.24   |
| 13  | M     | 57   | ARG  | N-CA-C      | -5.32 | 104.53      | 111.02   |
| 1   | A     | 1138 | G    | N9-C1'-C2'  | 5.32  | 119.98      | 112.00   |
| 1   | A     | 563  | A    | C4'-C3'-O3' | -5.31 | 105.04      | 113.00   |
| 14  | N     | 10   | ALA  | N-CA-C      | -5.31 | 105.44      | 112.34   |
| 5   | E     | 25   | ARG  | N-CA-C      | -5.31 | 102.61      | 110.46   |
| 10  | J     | 91   | PRO  | N-CA-C      | 5.30  | 119.56      | 111.34   |
| 1   | A     | 1224 | G    | C2'-C3'-O3' | 5.30  | 117.44      | 109.50   |
| 1   | A     | 812  | C    | N1-C1'-C2'  | 5.29  | 121.93      | 114.00   |
| 9   | I     | 91   | ASP  | N-CA-C      | -5.27 | 106.90      | 113.55   |
| 12  | L     | 43   | VAL  | CB-CA-C     | -5.27 | 103.97      | 111.19   |
| 15  | O     | 65   | ARG  | N-CA-C      | -5.27 | 105.18      | 111.03   |
| 3   | C     | 34   | LEU  | N-CA-C      | -5.26 | 104.54      | 111.96   |
| 10  | J     | 10   | GLY  | N-CA-C      | 5.25  | 118.80      | 111.19   |
| 13  | M     | 56   | LEU  | N-CA-C      | -5.24 | 105.57      | 111.28   |
| 1   | A     | 150  | C    | C4'-C3'-O3' | -5.23 | 105.15      | 113.00   |
| 1   | A     | 1200 | C    | N1-C1'-C2'  | 5.23  | 119.84      | 112.00   |
| 2   | B     | 201  | ILE  | N-CA-C      | -5.23 | 97.59       | 108.88   |
| 2   | B     | 90   | MET  | CA-C-N      | 5.23  | 125.13      | 119.85   |
| 2   | B     | 90   | MET  | C-N-CA      | 5.23  | 125.13      | 119.85   |
| 17  | Q     | 9    | VAL  | N-CA-C      | 5.22  | 117.14      | 108.99   |
| 17  | Q     | 75   | ARG  | N-CA-C      | 5.22  | 116.14      | 107.73   |
| 5   | E     | 17   | ALA  | N-CA-C      | 5.22  | 114.72      | 107.73   |
| 2   | B     | 200  | ILE  | N-CA-C      | 5.22  | 115.37      | 107.80   |
| 1   | A     | 1212 | U    | N1-C1'-C2'  | 5.21  | 119.82      | 112.00   |
| 1   | A     | 1337 | G    | N9-C1'-C2'  | 5.21  | 119.81      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Q     | 29   | HIS  | N-CA-C      | -5.19 | 102.00      | 109.48   |
| 7   | G     | 114  | ARG  | N-CA-C      | 5.19  | 121.86      | 110.80   |
| 7   | G     | 31   | MET  | N-CA-C      | -5.19 | 102.62      | 110.24   |
| 17  | Q     | 7    | THR  | N-CA-C      | -5.19 | 101.24      | 109.96   |
| 13  | M     | 37   | THR  | N-CA-C      | -5.18 | 107.50      | 113.88   |
| 13  | M     | 99   | ARG  | N-CA-C      | 5.18  | 119.66      | 113.23   |
| 7   | G     | 68   | ASN  | N-CA-C      | -5.18 | 105.25      | 112.45   |
| 3   | C     | 133  | ALA  | N-CA-C      | -5.17 | 105.53      | 111.07   |
| 8   | H     | 109  | ILE  | CB-CA-C     | -5.17 | 102.81      | 111.29   |
| 10  | J     | 9    | ARG  | N-CA-C      | -5.17 | 104.05      | 110.41   |
| 3   | C     | 59   | ARG  | N-CA-C      | 5.16  | 115.15      | 107.88   |
| 11  | K     | 38   | ASN  | CA-C-N      | 5.16  | 126.50      | 120.98   |
| 11  | K     | 38   | ASN  | C-N-CA      | 5.16  | 126.50      | 120.98   |
| 1   | A     | 1278 | U    | N1-C1'-C2'  | 5.15  | 119.72      | 112.00   |
| 2   | B     | 123  | ALA  | N-CA-C      | -5.14 | 105.37      | 110.97   |
| 5   | E     | 7    | GLU  | N-CA-C      | -5.14 | 102.15      | 110.32   |
| 10  | J     | 15   | THR  | N-CA-C      | -5.13 | 99.86       | 110.80   |
| 1   | A     | 616  | G    | C5'-C4'-C3' | 5.12  | 123.67      | 116.00   |
| 15  | O     | 58   | MET  | N-CA-C      | -5.10 | 105.63      | 111.14   |
| 13  | M     | 50   | GLU  | N-CA-C      | 5.10  | 117.96      | 111.69   |
| 1   | A     | 1517 | G    | N9-C1'-C2'  | -5.09 | 104.36      | 112.00   |
| 1   | A     | 687  | A    | C2'-C3'-O3' | 5.09  | 117.13      | 109.50   |
| 4   | D     | 155  | LEU  | N-CA-C      | 5.08  | 116.87      | 108.13   |
| 1   | A     | 128  | G    | C3'-C2'-O2' | 5.08  | 118.32      | 110.70   |
| 14  | N     | 22   | THR  | N-CA-C      | 5.06  | 121.57      | 110.80   |
| 6   | F     | 77   | ARG  | N-CA-C      | -5.05 | 106.96      | 113.23   |
| 2   | B     | 233  | SER  | CA-C-N      | 5.05  | 126.15      | 119.84   |
| 2   | B     | 233  | SER  | C-N-CA      | 5.05  | 126.15      | 119.84   |
| 6   | F     | 11   | ASN  | CA-C-N      | 5.05  | 124.22      | 118.97   |
| 6   | F     | 11   | ASN  | C-N-CA      | 5.05  | 124.22      | 118.97   |
| 1   | A     | 454  | C    | N1-C1'-C2'  | 5.04  | 119.57      | 112.00   |
| 9   | I     | 21   | PRO  | N-CA-C      | 5.04  | 122.85      | 112.47   |
| 1   | A     | 1374 | A    | C4'-C3'-O3' | -5.04 | 105.44      | 113.00   |
| 4   | D     | 116  | GLN  | N-CA-C      | -5.03 | 107.14      | 113.28   |
| 2   | B     | 112  | VAL  | N-CA-C      | -5.02 | 98.89       | 109.34   |
| 1   | A     | 389  | A    | C5'-C4'-C3' | 5.02  | 123.53      | 116.00   |
| 7   | G     | 69   | VAL  | N-CA-C      | -5.01 | 106.39      | 112.76   |
| 1   | A     | 1213 | A    | N9-C1'-C2'  | 5.01  | 119.51      | 112.00   |

All (1) chirality outliers are listed below:

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
|-----|-------|-----|------|------|

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | A     | 1498 | U    | C3'  |

All (64) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1066 | C    | Sidechain |
| 1   | A     | 1067 | A    | Sidechain |
| 1   | A     | 1094 | G    | Sidechain |
| 1   | A     | 1196 | U    | Sidechain |
| 1   | A     | 1213 | A    | Sidechain |
| 1   | A     | 1231 | G    | Sidechain |
| 1   | A     | 127  | G    | Sidechain |
| 1   | A     | 1281 | U    | Sidechain |
| 1   | A     | 129  | U    | Sidechain |
| 1   | A     | 1301 | U    | Sidechain |
| 1   | A     | 1370 | G    | Sidechain |
| 1   | A     | 1381 | U    | Sidechain |
| 1   | A     | 1401 | G    | Sidechain |
| 1   | A     | 1454 | G    | Sidechain |
| 1   | A     | 1455 | G    | Sidechain |
| 1   | A     | 1502 | A    | Sidechain |
| 1   | A     | 1531 | A    | Sidechain |
| 1   | A     | 156  | G    | Sidechain |
| 1   | A     | 183  | G    | Sidechain |
| 1   | A     | 239  | U    | Sidechain |
| 1   | A     | 250  | A    | Sidechain |
| 1   | A     | 263  | A    | Sidechain |
| 1   | A     | 265  | G    | Sidechain |
| 1   | A     | 296  | U    | Sidechain |
| 1   | A     | 303  | A    | Sidechain |
| 1   | A     | 305  | G    | Sidechain |
| 1   | A     | 317  | G    | Sidechain |
| 1   | A     | 332  | G    | Sidechain |
| 1   | A     | 352  | C    | Sidechain |
| 1   | A     | 396  | G    | Sidechain |
| 1   | A     | 397  | A    | Sidechain |
| 1   | A     | 434  | U    | Sidechain |
| 1   | A     | 444  | C    | Sidechain |
| 1   | A     | 490  | G    | Sidechain |
| 1   | A     | 498  | U    | Sidechain |
| 1   | A     | 533  | A    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 551 | U    | Sidechain |
| 1   | A     | 560 | U    | Sidechain |
| 1   | A     | 572 | A    | Sidechain |
| 1   | A     | 573 | A    | Sidechain |
| 1   | A     | 574 | A    | Sidechain |
| 1   | A     | 576 | G    | Sidechain |
| 1   | A     | 634 | C    | Sidechain |
| 1   | A     | 666 | G    | Sidechain |
| 1   | A     | 682 | G    | Sidechain |
| 1   | A     | 686 | U    | Sidechain |
| 1   | A     | 691 | G    | Sidechain |
| 1   | A     | 694 | A    | Sidechain |
| 1   | A     | 740 | U    | Sidechain |
| 1   | A     | 756 | C    | Sidechain |
| 1   | A     | 767 | A    | Sidechain |
| 1   | A     | 77  | G    | Sidechain |
| 1   | A     | 777 | A    | Sidechain |
| 1   | A     | 801 | U    | Sidechain |
| 1   | A     | 811 | C    | Sidechain |
| 1   | A     | 819 | A    | Sidechain |
| 1   | A     | 829 | G    | Sidechain |
| 1   | A     | 835 | U    | Sidechain |
| 1   | A     | 870 | U    | Sidechain |
| 1   | A     | 882 | C    | Sidechain |
| 1   | A     | 887 | G    | Sidechain |
| 1   | A     | 898 | G    | Sidechain |
| 1   | A     | 913 | A    | Sidechain |
| 8   | H     | 48  | TYR  | Sidechain |

## 3.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 3.3 Torsion angles ⓘ

### 3.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

### 3.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 3.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1511/1522 (99%) | 253 (16%)         | 0               |

All (253) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 8      | A    |
| 1   | A     | 9      | G    |
| 1   | A     | 31     | G    |
| 1   | A     | 32     | A    |
| 1   | A     | 39     | G    |
| 1   | A     | 41     | G    |
| 1   | A     | 42     | G    |
| 1   | A     | 47     | C    |
| 1   | A     | 48     | C    |
| 1   | A     | 49     | U    |
| 1   | A     | 50     | A    |
| 1   | A     | 51     | A    |
| 1   | A     | 52     | G    |
| 1   | A     | 61     | G    |
| 1   | A     | 64     | G    |
| 1   | A     | 65     | U    |
| 1   | A     | 73     | C    |
| 1   | A     | 81     | U    |
| 1   | A     | 82     | U    |
| 1   | A     | 89     | C    |
| 1   | A     | 91     | C    |
| 1   | A     | 116    | A    |
| 1   | A     | 120    | A    |
| 1   | A     | 121    | C    |
| 1   | A     | 129(A) | G    |
| 1   | A     | 130    | A    |
| 1   | A     | 131    | C    |
| 1   | A     | 163    | C    |
| 1   | A     | 182    | U    |
| 1   | A     | 183    | G    |
| 1   | A     | 190(E) | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 190(F) | G    |
| 1   | A     | 190(G) | G    |
| 1   | A     | 195    | A    |
| 1   | A     | 197    | A    |
| 1   | A     | 199    | G    |
| 1   | A     | 201    | C    |
| 1   | A     | 202    | U    |
| 1   | A     | 216    | G    |
| 1   | A     | 217    | C    |
| 1   | A     | 244    | U    |
| 1   | A     | 247    | G    |
| 1   | A     | 251    | G    |
| 1   | A     | 252    | U    |
| 1   | A     | 266    | G    |
| 1   | A     | 267    | C    |
| 1   | A     | 280    | C    |
| 1   | A     | 282    | A    |
| 1   | A     | 283    | C    |
| 1   | A     | 289    | G    |
| 1   | A     | 326    | G    |
| 1   | A     | 328    | C    |
| 1   | A     | 329    | A    |
| 1   | A     | 330    | C    |
| 1   | A     | 345    | C    |
| 1   | A     | 352    | C    |
| 1   | A     | 353    | A    |
| 1   | A     | 354    | G    |
| 1   | A     | 366    | C    |
| 1   | A     | 367    | U    |
| 1   | A     | 372    | C    |
| 1   | A     | 373    | A    |
| 1   | A     | 384    | G    |
| 1   | A     | 392    | G    |
| 1   | A     | 397    | A    |
| 1   | A     | 398    | C    |
| 1   | A     | 412    | A    |
| 1   | A     | 413    | G    |
| 1   | A     | 414    | A    |
| 1   | A     | 421    | U    |
| 1   | A     | 423    | G    |
| 1   | A     | 424    | G    |
| 1   | A     | 428    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 429 | U    |
| 1   | A     | 430 | A    |
| 1   | A     | 436 | C    |
| 1   | A     | 439 | A    |
| 1   | A     | 452 | A    |
| 1   | A     | 453 | A    |
| 1   | A     | 460 | A    |
| 1   | A     | 461 | C    |
| 1   | A     | 481 | G    |
| 1   | A     | 482 | A    |
| 1   | A     | 484 | G    |
| 1   | A     | 485 | G    |
| 1   | A     | 497 | A    |
| 1   | A     | 498 | U    |
| 1   | A     | 500 | G    |
| 1   | A     | 509 | A    |
| 1   | A     | 510 | A    |
| 1   | A     | 511 | C    |
| 1   | A     | 512 | U    |
| 1   | A     | 517 | G    |
| 1   | A     | 518 | C    |
| 1   | A     | 519 | C    |
| 1   | A     | 527 | G    |
| 1   | A     | 531 | U    |
| 1   | A     | 533 | A    |
| 1   | A     | 534 | U    |
| 1   | A     | 545 | C    |
| 1   | A     | 547 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 560 | U    |
| 1   | A     | 561 | U    |
| 1   | A     | 562 | C    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 575 | G    |
| 1   | A     | 576 | G    |
| 1   | A     | 577 | G    |
| 1   | A     | 596 | C    |
| 1   | A     | 598 | U    |
| 1   | A     | 632 | A    |
| 1   | A     | 653 | A    |
| 1   | A     | 665 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 687 | A    |
| 1   | A     | 688 | G    |
| 1   | A     | 695 | A    |
| 1   | A     | 702 | A    |
| 1   | A     | 703 | G    |
| 1   | A     | 718 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 724 | G    |
| 1   | A     | 731 | G    |
| 1   | A     | 734 | G    |
| 1   | A     | 749 | C    |
| 1   | A     | 755 | G    |
| 1   | A     | 777 | A    |
| 1   | A     | 792 | A    |
| 1   | A     | 793 | U    |
| 1   | A     | 794 | A    |
| 1   | A     | 817 | C    |
| 1   | A     | 820 | U    |
| 1   | A     | 828 | A    |
| 1   | A     | 839 | U    |
| 1   | A     | 840 | C    |
| 1   | A     | 841 | U    |
| 1   | A     | 848 | C    |
| 1   | A     | 859 | A    |
| 1   | A     | 867 | G    |
| 1   | A     | 902 | G    |
| 1   | A     | 913 | A    |
| 1   | A     | 914 | A    |
| 1   | A     | 926 | G    |
| 1   | A     | 927 | G    |
| 1   | A     | 934 | C    |
| 1   | A     | 935 | A    |
| 1   | A     | 945 | G    |
| 1   | A     | 960 | U    |
| 1   | A     | 961 | U    |
| 1   | A     | 966 | G    |
| 1   | A     | 968 | A    |
| 1   | A     | 969 | A    |
| 1   | A     | 971 | G    |
| 1   | A     | 974 | A    |
| 1   | A     | 975 | A    |
| 1   | A     | 976 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 977  | A    |
| 1   | A     | 983  | A    |
| 1   | A     | 984  | C    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 994  | A    |
| 1   | A     | 1000 | U    |
| 1   | A     | 1024 | G    |
| 1   | A     | 1026 | G    |
| 1   | A     | 1027 | C    |
| 1   | A     | 1029 | C    |
| 1   | A     | 1031 | G    |
| 1   | A     | 1038 | C    |
| 1   | A     | 1048 | G    |
| 1   | A     | 1050 | G    |
| 1   | A     | 1054 | C    |
| 1   | A     | 1066 | C    |
| 1   | A     | 1068 | G    |
| 1   | A     | 1086 | U    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1102 | A    |
| 1   | A     | 1104 | G    |
| 1   | A     | 1108 | G    |
| 1   | A     | 1116 | C    |
| 1   | A     | 1117 | G    |
| 1   | A     | 1125 | U    |
| 1   | A     | 1126 | U    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1131 | G    |
| 1   | A     | 1136 | U    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1138 | G    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1142 | G    |
| 1   | A     | 1146 | A    |
| 1   | A     | 1150 | U    |
| 1   | A     | 1152 | A    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1183 | A    |
| 1   | A     | 1184 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1196 | U    |
| 1   | A     | 1197 | G    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1202 | G    |
| 1   | A     | 1211 | U    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1215 | G    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1226 | C    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1241 | G    |
| 1   | A     | 1250 | A    |
| 1   | A     | 1256 | A    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1258 | G    |
| 1   | A     | 1279 | A    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1282 | C    |
| 1   | A     | 1285 | A    |
| 1   | A     | 1286 | A    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1297 | C    |
| 1   | A     | 1299 | A    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1303 | C    |
| 1   | A     | 1305 | G    |
| 1   | A     | 1306 | A    |
| 1   | A     | 1323 | G    |
| 1   | A     | 1331 | G    |
| 1   | A     | 1338 | G    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1348 | U    |
| 1   | A     | 1359 | C    |
| 1   | A     | 1362 | C    |
| 1   | A     | 1363 | A    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1427 | U    |
| 1   | A     | 1428 | A    |
| 1   | A     | 1442 | G    |
| 1   | A     | 1446 | A    |
| 1   | A     | 1452 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1476 | G    |
| 1   | A     | 1492 | A    |
| 1   | A     | 1493 | A    |
| 1   | A     | 1499 | A    |
| 1   | A     | 1504 | G    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1517 | G    |
| 1   | A     | 1518 | A    |
| 1   | A     | 1520 | G    |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |
| 1   | A     | 1533 | C    |

There are no RNA pucker outliers to report.

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

Mogul was not executed - this section is therefore empty.

### 3.5 Carbohydrates [i](#)

Mogul was not executed - this section is therefore empty.

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

Mogul was not executed - this section is therefore empty.

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

Mogul was not executed - this section is therefore empty.

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

There are no chain breaks in this entry.

## 4 Fit of model and data ⓘ

### 4.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 4.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 4.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 4.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 4.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.