

#### Apr 16, 2024 - 09:52 am BST

| PDB ID                 | : | 6YEF   |
|------------------------|---|--|
| EMDB ID                | : | EMD-10791  |
| Title                  | : | $70\mathrm{S}$ initiation complex with assigned rRNA modifications from Staphylococcus |
|                        |   | aureus   |
| Authors                | : | Fatkhullin, B.; Golubev, A.; Khusainov, I.; Yusupova, G.; Yusupov, M.                  |
| Deposited on           | : | 2020-03-24   |
| Resolution             | : | 3.20 Å(reported)   |
| Based on initial model | : | 5LI0   |

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

| EMDB validation analysis       | : | 0.0.1. dev92   |
|--------------------------------|---|--|
| Mogul                          | : | 1.8.4, CSD as541be (2020)  |
| MolProbity                     | : | 4.02b-467  |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ                           | : | FAILED   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.36   |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 3.20 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.



| Metric                | Whole archive | EM structures |  |  |
|-----------------------|---------------|---------------|--|--|
|                       | (#Entries)    | (#Entries)    |  |  |
| Ramachandran outliers | 154571        | 4023          |  |  |
| Sidechain outliers    | 154315        | 3826          |  |  |
| RNA backbone          | 4643          | 859           |  |  |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

| Mol | Chain | Length | Quality of chain |         |
|-----|-------|--------|------------------|---------|
| 1   | a     | 1556   | 77%              | 21% ••• |
| 2   | b     | 255    | 85%              | • 14%   |
| 3   | с     | 217    | 92%              | 8%      |
| 4   | d     | 200    | 98%              |         |
| 5   | е     | 166    | 93%              | • 5%    |
| 6   | f     | 98     | 96%              |         |
| 7   | g     | 156    | 94%              | 6%      |
| 8   | h     | 132    | 99%              |         |
| 9   | i     | 132    | 95%              |         |



| Conti | nued fron | n previous | page             |              |
|-------|-----------|------------|------------------|--------------|
| Mol   | Chain     | Length     | Quality of chain |              |
| 10    | j         | 102        | 96%              | •            |
| 11    | k         | 129        | 87%              | 12%          |
| 12    | 1         | 137        | 98%              | ••           |
| 13    | m         | 121        | 96%              | ••           |
| 14    | n         | 89         | 67% 33%          |              |
| 15    | О         | 89         | 99%              |              |
| 16    | р         | 91         | 99%              | <del>.</del> |
| 17    | q         | 87         | 97%              |              |
| 18    | r         | 80         | 80% 20           | 1%           |
| 19    | s         | 92         | 85% •            | 11%          |
| 20    | t         | 83         | 96%              | •            |
| 21    | V         | 29         | 45% 24% · 28%    |              |
| 22    | А         | 2923       | 75% 22%          | ••           |
| 23    | В         | 115        | 81% 17           | % •          |
| 24    | D         | 277        | 96%              | •••          |
| 25    | Е         | 220        | 98%              | ·            |
| 26    | F         | 207        | 96%              | ••           |
| 27    | G         | 179        | 85% •            | 14%          |
| 28    | Н         | 178        | 88% •            | 10%          |
| 29    | М         | 145        | 100%             |              |
| 30    | Ν         | 122        | 99%              | •            |
| 31    | О         | 146        | 96%              | •••          |
| 32    | Р         | 144        | 93%              | • 5%         |
| 33    | Q         | 122        | 97%              | ••           |
| 34    | R         | 119        | 99%              | ·            |



| Mol | Chain        | Length | Quality of chain |        |
|-----|--------------|--------|------------------|--------|
| 35  | $\mathbf{S}$ | 116    | 94%              | 6%     |
| 36  | Т            | 118    | 97%              |        |
| 37  | U            | 102    | 98%              |        |
| 38  | V            | 117    | 96%              | •      |
| 39  | W            | 91     | 98%              |        |
| 40  | Х            | 105    | 81%              | • 17%  |
| 41  | Y            | 217    | 43% 57%          |        |
| 42  | Ζ            | 94     | 87%              | 13%    |
| 43  | 0            | 62     | 73%              | 27%    |
| 44  | 1            | 69     | 91%              | • 6%   |
| 45  | 2            | 59     | 93%              | •••    |
| 46  | 3            | 84     | 87%              | •• 11% |
| 47  | 4            | 58     | 84%              | 5% 10% |
| 48  | 5            | 49     | 84%              | 6% 10% |
| 49  | 6            | 45     | 98%              |        |
| 50  | 7            | 66     | 94%              | • •    |
| 51  | 8            | 37     | 100%             |        |
| 52  | х            | 77     | 62% 32%          | 5%     |



# 2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 141837 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues |                | 1          | AltConf   | Trace      |           |   |   |
|-----|-------|----------|----------------|------------|-----------|------------|-----------|---|---|
| 1   | a     | 1545     | Total<br>33097 | C<br>14781 | N<br>6034 | O<br>10737 | Р<br>1545 | 0 | 0 |

• Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|-------|
| 2   | b     | 219      | Total<br>1762 | C<br>1123 | N<br>307 | O<br>325 | ${f S}7$ | 0       | 0     |

• Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms         |          |          |          |               | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------------|---------|-------|
| 3   | с     | 200      | Total<br>1578 | C<br>993 | N<br>296 | 0<br>287 | ${S \over 2}$ | 0       | 0     |

• Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms         |           |          |          |                 | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|-----------------|---------|-------|
| 4   | d     | 197      | Total<br>1600 | C<br>1009 | N<br>300 | O<br>289 | ${ m S} { m 2}$ | 0       | 0     |

• Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms         |          |          |          |   | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---|---------|-------|
| 5   | е     | 157      | Total<br>1169 | C<br>735 | N<br>214 | 0<br>218 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0       | 0     |

• Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms        |          |          |          |                 | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|-------|
| 6   | f     | 96       | Total<br>798 | C<br>503 | N<br>139 | 0<br>153 | ${ m S} { m 3}$ | 0       | 0     |



• Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues |               | At       | oms      |          |               | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------------|---------|-------|
| 7   | g     | 146      | Total<br>1176 | C<br>733 | N<br>225 | 0<br>214 | ${S \atop 4}$ | 0       | 0     |

• Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues |               | At       | oms      |          |               | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------------|---------|-------|
| 8   | h     | 131      | Total<br>1032 | C<br>652 | N<br>183 | O<br>193 | $\frac{S}{4}$ | 0       | 0     |

• Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues |               | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 9   | i     | 127      | Total<br>1008 | C<br>623 | N<br>201 | 0<br>183 | S<br>1 | 0       | 0     |

• Molecule 10 is a protein called ribosomal protein uS10.

| Mol | Chain | Residues |              | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 10  | j     | 98       | Total<br>783 | C<br>494 | N<br>143 | 0<br>145 | S<br>1 | 0       | 0     |

• Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues |              | At       | oms      |          |                 | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|-------|
| 11  | k     | 113      | Total<br>833 | C<br>514 | N<br>156 | 0<br>160 | ${ m S} { m 3}$ | 0       | 0     |

• Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues |               | At       | $\mathbf{oms}$ |          |                 | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------------|----------|-----------------|---------|-------|
| 12  | 1     | 135      | Total<br>1058 | C<br>658 | N<br>214       | 0<br>184 | ${ m S} { m 2}$ | 0       | 0     |

• Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues |              | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 13  | m     | 117      | Total<br>927 | C<br>569 | N<br>184 | 0<br>173 | S<br>1 | 0       | 0     |

• Molecule 14 is a protein called 30S ribosomal protein S14.



| Mol | Chain | Residues |              | Ate      | oms      |         |                 | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|-----------------|---------|-------|
| 14  | n     | 60       | Total<br>481 | C<br>296 | N<br>103 | O<br>80 | ${ m S} { m 2}$ | 0       | 0     |

• Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues |              | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 15  | О     | 88       | Total<br>738 | C<br>454 | N<br>153 | O<br>130 | S<br>1 | 0       | 0     |

• Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace  |   |   |
|-----|-------|----------|--------------|----------|----------|----------|--------|---|---|
| 16  | р     | 90       | Total<br>712 | C<br>448 | N<br>132 | 0<br>131 | S<br>1 | 0 | 0 |

• Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues |              | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 17  | q     | 85       | Total<br>698 | C<br>441 | N<br>125 | 0<br>131 | S<br>1 | 0       | 0     |

• Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues |              | Ato      | $\mathbf{ms}$ |         |                 | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------------|---------|-----------------|---------|-------|
| 18  | r     | 64       | Total<br>527 | C<br>335 | N<br>97       | O<br>92 | ${ m S} { m 3}$ | 0       | 0     |

• Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace           |   |   |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---|---|
| 19  | S     | 82       | Total<br>661 | C<br>426 | N<br>118 | 0<br>115 | ${ m S} { m 2}$ | 0 | 0 |

• Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues |              | At       | oms      |          |               | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---------|-------|
| 20  | t     | 80       | Total<br>606 | C<br>367 | N<br>119 | 0<br>118 | ${S \over 2}$ | 0       | 0     |

• Molecule 21 is a RNA chain called mRNA.



| Mol | Chain | Residues |              | At       | $\mathbf{oms}$ | AltConf  | Trace   |   |   |
|-----|-------|----------|--------------|----------|----------------|----------|---------|---|---|
| 21  | v     | 21       | Total<br>462 | C<br>207 | N<br>96        | O<br>138 | Р<br>21 | 0 | 0 |

• Molecule 22 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues |                |            | Atoms      |            |           | AltConf | Trace |
|-----|-------|----------|----------------|------------|------------|------------|-----------|---------|-------|
| 22  | А     | 2881     | Total<br>61802 | C<br>27593 | N<br>11324 | O<br>20004 | Р<br>2881 | 0       | 0     |

• Molecule 23 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues |               | A         | AltConf  | Trace    |          |   |   |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---|---|
| 23  | В     | 115      | Total<br>2445 | C<br>1094 | N<br>436 | 0<br>801 | Р<br>114 | 0 | 0 |

• Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues |               | At        | AltConf  | Trace    |                |   |   |
|-----|-------|----------|---------------|-----------|----------|----------|----------------|---|---|
| 24  | D     | 274      | Total<br>2094 | C<br>1303 | N<br>415 | 0<br>371 | ${ m S}{ m 5}$ | 0 | 0 |

• Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues |               | At        | AltConf  | Trace    |                |   |   |
|-----|-------|----------|---------------|-----------|----------|----------|----------------|---|---|
| 25  | Е     | 216      | Total<br>1635 | C<br>1023 | N<br>301 | O<br>306 | ${ m S}{ m 5}$ | 0 | 0 |

• Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues |               | At       | oms      |          | AltConf       | Trace |   |
|-----|-------|----------|---------------|----------|----------|----------|---------------|-------|---|
| 26  | F     | 203      | Total<br>1540 | C<br>966 | N<br>284 | 0<br>288 | ${S \over 2}$ | 0     | 0 |

• Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues |               | At       | oms      |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 27  | G     | 154      | Total<br>1191 | C<br>751 | N<br>206 | 0<br>228 | S<br>6 | 0       | 0     |

• Molecule 28 is a protein called 50S ribosomal protein L6.



| Mol | Chain | Residues |               | At       | oms      | AltConf  | Trace           |   |   |
|-----|-------|----------|---------------|----------|----------|----------|-----------------|---|---|
| 28  | Н     | 160      | Total<br>1250 | C<br>781 | N<br>222 | 0<br>244 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 29 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues |               | At       | oms      | AltConf  | Trace           |   |   |
|-----|-------|----------|---------------|----------|----------|----------|-----------------|---|---|
| 29  | М     | 145      | Total<br>1151 | С<br>717 | N<br>211 | O<br>220 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 30 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace         |   |   |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---|---|
| 30  | Ν     | 122      | Total<br>920 | C<br>572 | N<br>174 | 0<br>170 | $\frac{S}{4}$ | 0 | 0 |

• Molecule 31 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues |               | At       | AltConf  | Trace    |        |   |   |
|-----|-------|----------|---------------|----------|----------|----------|--------|---|---|
| 31  | Ο     | 146      | Total<br>1098 | C<br>680 | N<br>215 | O<br>202 | S<br>1 | 0 | 0 |

• Molecule 32 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues |               | At       | AltConf  | Trace    |        |   |   |
|-----|-------|----------|---------------|----------|----------|----------|--------|---|---|
| 32  | Р     | 137      | Total<br>1097 | С<br>704 | N<br>207 | 0<br>182 | S<br>4 | 0 | 0 |

• Molecule 33 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues |              | At   | AltConf  | Trace    |        |   |   |
|-----|-------|----------|--------------|--|----------|----------|--------|---|---|
| 33  | Q     | 119      | Total<br>940 | $\begin{array}{c} \mathrm{C} \\ 575 \end{array}$ | N<br>181 | 0<br>183 | S<br>1 | 0 | 0 |

• Molecule 34 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues |              | Ato      | ms       | AltConf  | Trace |   |
|-----|-------|----------|--------------|----------|----------|----------|-------|---|
| 34  | R     | 118      | Total<br>911 | C<br>568 | N<br>173 | O<br>170 | 0     | 0 |

• Molecule 35 is a protein called 50S ribosomal protein L19.



| Mol | Chain | Residues |              | Ato      | ms       | AltConf  | Trace |   |
|-----|-------|----------|--------------|----------|----------|----------|-------|---|
| 35  | S     | 109      | Total<br>877 | C<br>552 | N<br>176 | O<br>149 | 0     | 0 |

• Molecule 36 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues |              | At       | AltConf  | Trace    |             |   |   |
|-----|-------|----------|--------------|----------|----------|----------|-------------|---|---|
| 36  | Т     | 116      | Total<br>943 | C<br>593 | N<br>189 | 0<br>157 | ${f S}$ $4$ | 0 | 0 |

• Molecule 37 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues |              | At       | AltConf  | Trace    |        |   |   |
|-----|-------|----------|--------------|----------|----------|----------|--------|---|---|
| 37  | U     | 100      | Total<br>784 | C<br>497 | N<br>140 | 0<br>146 | S<br>1 | 0 | 0 |

• Molecule 38 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues |              | At       | AltConf  | Trace    |                 |   |   |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---|---|
| 38  | V     | 112      | Total<br>862 | C<br>537 | N<br>164 | 0<br>158 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 39 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues |              | At       | AltConf  | Trace    |        |   |   |
|-----|-------|----------|--------------|----------|----------|----------|--------|---|---|
| 39  | W     | 89       | Total<br>725 | C<br>457 | N<br>130 | 0<br>134 | S<br>4 | 0 | 0 |

• Molecule 40 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues |              | At       | oms      | AltConf  | Trace  |   |   |
|-----|-------|----------|--------------|----------|----------|----------|--------|---|---|
| 40  | Х     | 87       | Total<br>662 | C<br>420 | N<br>119 | 0<br>122 | S<br>1 | 0 | 0 |

• Molecule 41 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues |              | At       | AltConf  | Trace    |               |   |   |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---|---|
| 41  | Y     | 94       | Total<br>731 | C<br>465 | N<br>131 | 0<br>133 | ${S \over 2}$ | 0 | 0 |

• Molecule 42 is a protein called 50S ribosomal protein L27.



| Mol | Chain | Residues |              | Ato      | $\mathbf{ms}$ | AltConf  | Trace |   |
|-----|-------|----------|--------------|----------|---------------|----------|-------|---|
| 42  | Ζ     | 82       | Total<br>626 | C<br>386 | N<br>122      | 0<br>118 | 0     | 0 |

• Molecule 43 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms        |          |         |         | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 43  | 0     | 45       | Total<br>358 | C<br>222 | N<br>78 | O<br>58 | 0       | 0     |

• Molecule 44 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms        |          |          |          | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|
| 44  | 1     | 65       | Total<br>536 | C<br>330 | N<br>101 | O<br>105 | 0       | 0     |

• Molecule 45 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms        |          |         |         | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 45  | 2     | 57       | Total<br>441 | C<br>274 | N<br>83 | 0<br>84 | 0       | 0     |

• Molecule 46 is a protein called 50S ribosomal protein L31 type B.

| Mol | Chain | Residues | Atoms        |          |          |          |                 | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|-------|
| 46  | 3     | 75       | Total<br>593 | C<br>371 | N<br>106 | 0<br>113 | ${ m S} { m 3}$ | 0       | 0     |

• Molecule 47 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |          |         |                                       | AltConf      | Trace |   |
|-----|-------|----------|-------|----------|---------|---------------------------------------|--------------|-------|---|
| 47  | 4     | 52       | Total | C<br>240 | N<br>85 | $\begin{array}{c} 0\\ 72 \end{array}$ | ${ m S}_{5}$ | 0     | 0 |
|     |       |          | 411   | 249      | 85      | 72                                    | $\mathbf{b}$ |       |   |

• Molecule 48 is a protein called 50S ribosomal protein L33 2.

| Mol | Chain | Residues | Atoms        |          |         |         |               | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------------|---------|-------|
| 48  | 5     | 44       | Total<br>371 | C<br>223 | N<br>76 | O<br>68 | ${S \atop 4}$ | 0       | 0     |

• Molecule 49 is a protein called 50S ribosomal protein L34.



| Mol | Chain | Residues | Atoms        |          |         |         |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 49  | 6     | 44       | Total<br>373 | C<br>228 | N<br>90 | 0<br>54 | S<br>1 | 0       | 0     |

• Molecule 50 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms        |          |          |         |                 | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|-----------------|---------|-------|
| 50  | 7     | 64       | Total<br>521 | C<br>324 | N<br>113 | O<br>82 | ${ m S} { m 2}$ | 0       | 0     |

• Molecule 51 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms        |          |         |         |               | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------------|---------|-------|
| 51  | 8     | 37       | Total<br>296 | C<br>186 | N<br>60 | O<br>46 | $\frac{S}{4}$ | 0       | 0     |

• Molecule 52 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms         |          |          |          |         | AltConf         | Trace |   |
|-----|-------|----------|---------------|----------|----------|----------|---------|-----------------|-------|---|
| 52  | х     | 77       | Total<br>1659 | С<br>741 | N<br>299 | 0<br>541 | Р<br>76 | ${ m S} { m 2}$ | 0     | 0 |

• Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms   | AltConf |
|-----|-------|----------|---|---------|
| 53  | a     | 54       | $\begin{array}{cc} \text{Total} & \text{Mg} \\ 54 & 54 \end{array}$ | 0       |
| 53  | V     | 1        | Total Mg<br>1 1   | 0       |
| 53  | А     | 207      | Total         Mg           207         207                          | 0       |
| 53  | В     | 2        | Total Mg<br>2 2   | 0       |
| 53  | D     | 1        | Total Mg<br>1 1   | 0       |
| 53  | Ο     | 1        | Total Mg<br>1 1   | 0       |
| 53  | Х     | 1        | Total Mg<br>1 1   | 0       |
| 53  | x     | 1        | Total Mg<br>1 1   | 0       |

• Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).



| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 54  | a     | 2        | Total K<br>2 2   | 0       |
| 54  | А     | 18       | Total K<br>18 18 | 0       |



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: 16S rRNA

 $\bullet$  Molecule 2: 30S ribosomal protein S2

Chain b:



| MET<br>VALA<br>VALA<br>VALA<br>VALA<br>VALA<br>VALE<br>SER<br>REA<br>ASP<br>VAL<br>ASP<br>VAL<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>ASP<br>VALA<br>VALA<br>VALA<br>VALA<br>VALA<br>VALA<br>VALA<br>VAL |      |
|---|------|
| • Molecule 3: 30S ribosomal protein S3  |      |
| Chain c: 92%  | 8%   |
| MET<br>146<br>177<br>178<br>178<br>178<br>178<br>178<br>178<br>178<br>178<br>178  |      |
| • Molecule 4: 30S ribosomal protein S4  |      |
| Chain d: 98%  | •    |
| MET 42<br>K24<br>LEU<br>E27<br>R200   |      |
| • Molecule 5: 30S ribosomal protein S5  |      |
| Chain e: 93%  | • 5% |
| MET<br>ALA<br>ARG<br>GLU<br>GLU<br>CLU<br>GLU<br>CLU<br>GLU<br>CLU<br>CLU<br>CLU<br>CLU<br>CLU<br>CLU<br>CLU<br>CLU<br>CLU<br>C   |      |
| • Molecule 6: 30S ribosomal protein S6  |      |
| Chain f: 96%  | • •  |
| M K66 S S S S S S S S S S S S S S S S S S   |      |
| • Molecule 7: 30S ribosomal protein S7  |      |
| Chain g: 94%  | 6%   |
| MRT<br>ARG<br>ARG<br>ARG<br>ARG<br>ARG<br>CI Y<br>CI Y<br>CI Y<br>CI Y<br>CI Y<br>CI Y<br>CI Y  |      |
| • Molecule 8: 30S ribosomal protein S8  |      |
| Chain h: 99%  |      |
|   |      |
| • Molecule 9: 30S ribosomal protein S9  |      |
|   |      |





• Molecule 10: ribosomal protein uS10

Chain j: 96% MET ALA LYS GLN • Molecule 11: 30S ribosomal protein S11 Chain k: 87% 12% MET ALA ARG LYS GLN VAL SER ARG LYS ARG LYS ARG LYS VAL LYS • Molecule 12: 30S ribosomal protein S12 Chain l: 98% • Molecule 13: 30S ribosomal protein S13 Chain m: 96% • Molecule 14: 30S ribosomal protein S14 Chain n: 67% 33% MET LIYS SER LIYS SER LIYS SER LIYS ALA ALA ALA CUU CUU CUU CUU CUU VAR CUU VAR CUU VAR ASN LIYS CUU SU ARC CUU SU ARA ALA ALA ALA SER LIYS SU LIYS SU LIYS SU LIXS SU LIXSU LIXS SU LIXSU LIXU • Molecule 15: 30S ribosomal protein S15 Chain o: 99% MET • Molecule 16: 30S ribosomal protein S16 Chain p: 99%



| MET | A2 | K91 |  |
|-----|----|-----|--|

 $\bullet$  Molecule 17: 30S ribosomal protein S17

| Chain q:  | 97%  | ••   |                              |
|---|--|--|------------------------------|
| MET<br>S2<br>D50<br>I186<br>ILE                             |  |  |                              |
| • Molecule  | 18: 30S ribosomal protein S18  |  |                              |
| Chain r:  | 80%  | 20%  |                              |
| MET<br>ALA<br>GLY<br>GLY<br>PRO<br>PRO<br>ARG<br>GLY<br>GLY | ARG<br>ARG<br>LYS<br>LYS<br>LYS<br>LYS<br>CI6<br>GLN<br>GLN  |  |                              |
| • Molecule  | 19: 30S ribosomal protein S19  |  |                              |
| Chain s:  | 85%  | • 11%  |                              |
| MET<br>ALA<br>ARG<br>84<br>15<br>K7<br>K7<br>K7<br>V51      | V51<br>R55<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP<br>ASP   |  |                              |
| • Molecule :  | 20: 30S ribosomal protein S20  |  |                              |
| Chain t:  | 96%  | •  |                              |
| MET<br>ALA<br>N3<br>N82<br>LYS                              |  |  |                              |
| • Molecule :  | 21: mRNA   |  |                              |
| Chain v:  | 45% 24% ·  | 28%  |                              |
| G<br>G<br>A<br>A12<br>A12<br>A14<br>A14<br>A14              | A14<br>A15<br>A23<br>A24<br>A A<br>A A<br>A A<br>A A   |  |                              |
| • Molecule :  | 22: 23S rRNA   |  |                              |
| Chain A:  | 75%  | 22%  |                              |
| G<br>A<br>U12<br>A13<br>G23<br>G24<br>G24                   | 624<br>034<br>433<br>443<br>443<br>443<br>443<br>443<br>443<br>443<br>44   | A161<br>A161<br>A162<br>A164<br>A164<br>A166<br>U167 | A168<br>G169<br>A173         |
| A176<br>G177<br>A179<br>A179<br>A185<br>A185<br>A209        | A200<br>(2312)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(2313)<br>(231 | C<br>U289<br>U290<br>G294<br>U298<br>U299            | G300<br>U301<br>A302<br>C308 |



| U309<br>C310   | U<br>A         | U                   | : D      | G316           | U321            | A324   | <b>G377</b>    | G328     | A329         | <mark>G338</mark> |       | A354           | A365  | A372              | A373                | U374           | U377   |                      | C380<br>C387   | A388  | C398           |                    | 0401           | 0404                 | U419               |                     | 04.32              | A435           | U451              | G457              | A458           | C463        | C466           |       | 64 / T             | C481<br>U482        | C490                        |
|----------------|----------------|---------------------|----------|----------------|-----------------|--------|----------------|----------|--------------|-------------------|-------|----------------|-------|-------------------|---------------------|----------------|--------|----------------------|----------------|-------|----------------|--------------------|----------------|----------------------|--------------------|---------------------|--------------------|----------------|-------------------|-------------------|----------------|-------------|----------------|-------|--------------------|---------------------|-----------------------------|
| C502           | U510           | 0513<br>0513        |          | A523           | G527            | G539   | ABBO           |          | A553<br>C554 | C555              | U556  | 1.995.V        | G567  | C568              | C572                | CE75           | U576   | A577                 | 8/99           | A583  | C587           |                    | A592<br>U593   | G594                 | G606               | C607                | 2000               | U611           | <mark>G616</mark> | A01 /<br>A618     | 2022           | 1700        | G630           | C644  | 4040<br>A646       | A659                | A660<br>U661                |
| G662           | A666<br>G667   | 0290                |          | A682<br>G683   | IIEGO           |        | 0698<br>11699  | A7 00    | C710         |                   | G714  | A/15<br>C716   | C717  | C724              |                     | U731           | G745   | 02.20                | G774<br>G774   | A775  | C776<br>C777   |                    | C781<br>C782   | G783                 | U792               | <mark>G793</mark>   |                    | G808<br>4809   | A810              | <mark>G813</mark> |                | C821        | G822<br>G823   | A824  | A827               | <u>4828</u><br>U829 | U830                        |
| A834<br>U835   | C836<br>G837   | <u>4838</u><br>4839 |          | A847           | G850<br>C851    | 1000   | C857           | C861     | C862         | U872              | 0873  | C883           |       | <mark>6888</mark> | A891                |                |        | C910                 |                | G919  | A923           |                    | <b>G926</b>    | C929                 | C930<br>C931       | <mark>0932</mark>   | a c                | C935<br>G936   | 6937<br>6937      | 1939<br>1939      | U              | 1 104       | A955<br>A956   | C967  | C959               | C960                | U971<br>A972                |
| <b>A985</b>    | A989           | 0665                | A1001    | G1005          | C1000           |        | A1018          | A1023    | C1026        | A1027             | G1028 | C1029<br>C1030 |       | <b>G1</b> 033     | <mark>C1</mark> 039 | A1040          | U1043  | <b>1</b>             | C1049<br>C1050 |       | A1053<br>A1054 | A1055              | U1056<br>A1057 |                      | 01060<br>G1061     |                     | COULA              | G1069<br>A1070 | A1071             | U1077             | 41000          | 61091       | C1096          |       | 20110              | U1105<br>G1106      | <mark>G1107</mark><br>C1108 |
| U1109<br>U1110 | A1111<br>G1112 | A1113<br>A1114      | G1115    | C1116<br>A1117 | C1100           | A1121  | U1122<br>C1123 | A1124    | 111107       | A1128             | A1129 | A1130<br>G1131 | A1132 | G1133             | G1137               | U1138<br>A1130 | A1140  | 5<br>5<br>5          | G1143<br>C1144 | U1145 | C1146<br>A1147 |                    | G1151<br>U1152 | C1153                | G1154<br>A1155     | G1156               | C1160              | A1171          | A1172             | A11/3<br>U1174    | G1175          | A1177       | C1178<br>C1179 |       | AIIXO              | C1196               | G1201                       |
| G1211          | C1214<br>U1215 | n                   | G1218    | G1219<br>A1220 | C10ED           |        | A1258          | G1276    | C1277        | OUTE              | G1288 | G1294          | C1295 | U1305             | A1306               | 1300           | A1310  | 20<br>20<br>20<br>20 | A1323          | C1326 | A1337          | U1338              | U1339          | U1349                | U1350<br>C1351     |                     | ALGOO              | C1370          | G1375             | 01377<br>U1377    | U1378          | C1382       | C1387          | C1388 | Ulagy              | A1402               | G1405                       |
| U1416          | A1421          | A1432               | C1435    | C1436<br>U1437 | A1 450          | n      | 0 0            | ņ        | U            | n                 | A     | A1459<br>U1460 | C1461 | G1462<br>A1463    | U1464               | G1465          | A1471  | C1472                | 614/3          | A1489 | G1490<br>C1491 | G1492              | 01493<br>G1494 | C1495                | G1496              | 01 <mark>499</mark> | A1502              | U1503<br>U1504 | G1505             |                   | U1510          | C1516       | A1517<br>G1518 | 01519 | U1525              | A1533               | C1536                       |
| A1537          | 01540<br>C1541 | G1550               | U1551    | 01552<br>A1553 | A1554<br>C1555  |        | G1559<br>A1560 | G1561    | G1570        |                   | A1575 | A1576<br>G1577 | Å     | D A               | n                   | n              | 'n     | 5                    | ⊃ U            | U1588 | 01589<br>C1590 | G1591              | A1592          | A1600                | U1601<br>U1602     |                     | A1605<br>C1606     | G1613          | A1614             | A1616             |                | 07010       | A1630<br>G1631 | A1632 | A1633<br>A1634     | A1635<br>U1636      | <mark>G1639</mark>          |
| C1651          | A1652          | C1655               | C1661    | A1662          | U1683           | G1686  | A1690          | G1691    | C1692        | C1696             |       | C1/04          | C1714 | G1718             | C1719               | 111737         | C1738  | G1739                | G1/40          | U1756 | 01757<br>A1758 | G1759              | A1764          |                      | C1768              | G1772               | G1777              | G1785          | 1200              | G1791             | 1101           | 10 <b>1</b> | A1800<br>C1801 | U1802 | 61803              | U1806<br>A1807      | U1808                       |
| A1811<br>A1812 | A1813<br>A1814 | C1815               | G1819    | G1826          | C1827<br>111828 |        | A1837<br>G1838 | G1839    | 111 843      | 01.043<br>G1844   |       |                | A1856 | A1893             | G1894               | C1895          | U1897  | C1898                | 01899<br>G1900 | C1901 | G1902          | <mark>C1909</mark> | C1921          |                      | <mark>G1930</mark> | <mark>G1933</mark>  | <mark>G1937</mark> | U1938<br>A1939 | A1940             | 01941<br>01942    | A1943          | C1947       | G1956          | G1957 | <mark>C1961</mark> | G1962<br>A1963      | A1964<br>A1965              |
| U1966<br>U1967 | G1975          | 111980              |          | C1990<br>G1991 | C1992<br>A1993  | C1994  | A 1997         | A1998    | G1999        | U2009             | 01001 | 02018<br>G2019 | U2020 | C2033             |                     | A2050          |        | A2058                | 62059<br>A2060 |       | C2063          | C2070              | C2071<br>C2072 |                      | C2082<br>G2083     | 2000                | A 2087<br>G 2088   | A2089<br>C2090 |                   | 42094<br>U2095    | G2096<br>G2096 | 16031       | G2114          | G2120 | G2128              | A2132               | U2135                       |
| J2136<br>32137 | J2138<br>A2139 | C2140               | 32142    | 32143<br>A2144 | J2145           | 32147  | 42150          |          | A2153        | J2157             | J2158 | 12159<br>32160 | A2161 | 42162<br>42163    | 32164               | 32165<br>17166 | 32167  | A2168                | 69175          | 22172 | J2173<br>A2174 | 32175              | 22176          | A2179                | 32183              | 32184               | 42185<br>32186     | 32187<br>32188 | 12189             | 12191<br>12191    | 101            | 12195       | 32196<br>32197 | 42198 | 12199<br>12200     | 2201                | 22205                       |
| 2208           | 2211           | 2214 (              | 2216     | 2217           | 2220            | 2255   | 230            | 231      |              | 2241              |       | 2252           |       | 2265              |                     | 2278           | 2295   | 2296                 | 2305           |       | 2309           |                    | 2314           | 2 <mark>321 4</mark> | 1332 (             | 2333                | 2335<br>(1335      |                | 2338              | 347               | 2348           |             | 2352<br>2353   |       | 2361               | 2363                | 2374                        |
| 377 A.         | 383<br>U       | 386 G1              | 404<br>U | 405<br>406     | 010<br>010      | 411 A. | 412            | 418<br>C |              | 430 C3            | -     | 433 A.         | 446   | 450<br>63         | 451                 | 452 G.         | 456 A1 | 457 A1               | 464 A1         |       | 467<br>468     | 469                | 472            | ť                    | 475<br>U           | 483 U.              | 486<br>G           | 492 A          | 493 A.            | 501 A1            | 502 G          | <b>5</b> 05 | 518<br>U       |       | 525 A2             | 528 A.              | 530<br>531                  |
| C2             | C2             | C2                  | A2       | G2.            | 00              | A2     | C2             | G2       | CII          | C2                | 00    | C              | U2    | U2.               | CS                  | A2             | G2,    | A2                   | C2             |       | 8.8            | C2                 | 62.            |                      | A2                 | C2                  | A2                 | CO             | C                 | U21               | C2             | A2          | 02             |       | ڏ                  | 62 C2               | A2<br>U2                    |



# UZ709 02532 UZ16 02533 UZ16 02541 CZ719 UZ549 UZ16 02541 CZ741 02549 UZ16 02566 UZ76 02541 UZ76 02545 UZ76 02546 UZ76 02546 UZ76 02546 UZ76 02546 UZ76 02566 UZ76 02566 UZ76 02566 UZ76 02569 UZ76 02569 UZ76 02666 A2775 0269 UZ76 0264 UZ76 0264 UZ76 0264 UZ76 0264 U260 0264 U260 0264 U260 0264 U263 0264 U263 0264 U263 0264 U263 0264 U263 0264 <

#### C2890 A2893 A2893 C2900 C2900 C2903 C2903 C2903 C2903 C2903 C2903 C2903 C2913 C2913

• Molecule 23: 5S rRNA

| Chain B:  | 81%  | 17% • |
|---|--|-------|
| 11<br>C2<br>M11<br>M11<br>M12<br>M12<br>M12<br>M12<br>M12<br>M12<br>M12<br>M1   | A64<br>A64<br>C87<br>C88<br>C88<br>C87<br>C91<br>C91<br>C92<br>C92<br>C92<br>C92<br>C92<br>C92<br>C92<br>C92<br>C92<br>C92               |       |
| • Molecule 24: 50S rib  | osomal protein L2  |       |
| Chain D:  | 96%  | •••   |
| MET<br>A1<br>126<br>726<br>734<br>734<br>136<br>136<br>136<br>136<br>721<br>7218<br>7274<br>1278<br>1278<br>1278  |  |       |
| • Molecule 25: 50S rib  | osomal protein L3  |       |
| Chain E:  | 98%  |       |
| MET<br>T2<br>H148<br>A 157<br>SER<br>D159<br>C218<br>C218<br>A SN<br>LYS  |  |       |
| • Molecule 26: 50S rib  | osomal protein L4  |       |
| Chain F:  | 96%  | •••   |
| MET<br>ALA<br>NIA<br>NI2<br>1104<br>1104<br>1104<br>1104<br>1104<br>1104<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1100<br>1000000 |  |       |
| • Molecule 27: 50S rib  | osomal protein L5  |       |
| Chain G:  | 85%  | • 14% |
| MET<br>ASN<br>ASN<br>ASN<br>ASN<br>ALA<br>ALA<br>LYS<br>LYS<br>SER<br>LYS<br>SER<br>TLE<br>TLE<br>TLE<br>LEU  | LLE<br>PHE<br>PRE<br>CLU<br>CLU<br>CLU<br>CLU<br>ALA<br>ALA<br>ALA<br>ALA<br>ALA<br>ALA<br>PHE<br>PHE<br>PHE<br>PHE<br>PHE<br>PHE<br>PHE |       |
| • Molecule 28: 50S rib  | osomal protein L6  |       |
| Chain H:  | 88%  | • 10% |
|   |  |       |



••

#### MET SER ARG VAL CLY CLYS LYS LYS TR ARG ARG LYS GLU GLY LYS THR GLY LYS LYS ASF

• Molecule 29: 50S ribosomal protein L13

Chain M: 100% There are no outlier residues recorded for this chain. • Molecule 30: 50S ribosomal protein L14 Chain N: 99% • Molecule 31: 50S ribosomal protein L15 Chain O: 96% • Molecule 32: 50S ribosomal protein L16 Chain P: • 5% 93% GLY GLY GLU GLU ASN ASN GLU SER • Molecule 33: 50S ribosomal protein L17 Chain Q: 97% TY GL • Molecule 34: 50S ribosomal protein L18 Chain R: 99% MET 12 • Molecule 35: 50S ribosomal protein L19 Chain S: 94% 6%





- Molecule 36: 50S ribosomal protein L20 Chain T: 97% • Molecule 37: 50S ribosomal protein L21 Chain U: 98% • Molecule 38: 50S ribosomal protein L22 Chain V: 96% GLU ALA LYS GLU ALA • Molecule 39: 50S ribosomal protein L23 Chain W: 98% ASN • Molecule 40: 50S ribosomal protein L24 Chain X: 81% 17% MET LYS PRO GLN GLN LEU LEU ASN PRO GLU VAI ASF GLY GLY LYS LYS ASN ASN ASN • Molecule 41: 50S ribosomal protein L25 Chain Y: 43% 57% TILE SER ASPN VALLEU VALLEV SER ASPN GUU GUU GUU GUU GUU CGUU VALL THR THR CGUU CGUU VALL THR THR CGUU VALL CUU CGUU VALL VALL VALL VALLEU VAL
- GLU GLU GLU CLYS CLU CLYS GLU GLU
- Molecule 42: 50S ribosomal protein L27

Chain Z:





• Molecule 43: 50S ribosomal protein L28

| Chain 0:  | 73%   | 27% |      |
|---|---|-----|------|
| MET<br>GLY<br>CLNS<br>GLN<br>CYS<br>CYS<br>PHE<br>VAL<br>THR<br>GLY<br>ARG<br>CLY | K55<br>SER<br>CLYS<br>VAL<br>THR<br>ARG<br>VAL                            |     |      |
| • Molecule 44:  | 50S ribosomal protein L29   |     |      |
| Chain 1:  | 91%   |     | • 6% |
| MET<br>K2<br>R7<br>R5<br>R5<br>R66<br>ALA<br>ALA<br>ALA<br>ALA<br>ALA             |   |     |      |
| • Molecule 45:  | 50S ribosomal protein L30   |     |      |
| Chain 2:  | 93%   |     |      |
| MET<br>A2<br>L53<br>V54<br>E58<br>E58<br>LYS                                      |   |     |      |
| • Molecule 46:  | $50\mathrm{S}$ ribosomal protein L<br>31 type B                           |     |      |
| Chain 3:  | 87%   | ••  | 11%  |
| M1<br>H10<br>GLN<br>V12<br>F23<br>LEU<br>SER<br>GLY<br>S27                        | C40<br>LYS<br>CLU<br>PRD<br>PRD<br>PRD<br>PRD<br>PRD<br>PRO<br>N83<br>ASN |     |      |
| • Molecule 47:  | 50S ribosomal protein L32   |     |      |
| Chain 4:  | 84%   | 5%  | 10%  |
| MET<br>A2<br>C30<br>C30<br>C34<br>A2<br>C34<br>A30<br>E36<br>E36<br>R42<br>R42    | VALT<br>ALA<br>ALA<br>LYS<br>LYS  |     |      |
| • Molecule 48:  | 50S ribosomal protein L33 2   |     |      |
| Chain 5:  | 84%   | 6%  | 10%  |
| M2<br>L8<br>CYS<br>CYS<br>CYS<br>D14<br>D14                                       | R38<br>R46<br>THR<br>LVS  |     |      |
| • Molecule 49:  | 50S ribosomal protein L34   |     |      |
| Chain 6:  | 98%   |     |      |



• •



• Molecule 50: 50S ribosomal protein L35

Chain 7:



• Molecule 51: 50S ribosomal protein L36

Chain 8:

100%

94%

There are no outlier residues recorded for this chain.

 $\bullet$  Molecule 52: P-site tRNA

| Cha      | ain | х  | : ' |     |     |     |      |     |     |     |     |     |             | 62  | 2%  | , |     |     |     |     |             |     |            |     |            |     |     |     |     |     |     | 32    | 2% |  | 5% |
|----------|-----|----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-------------|-----|-----|---|-----|-----|-----|-----|-------------|-----|------------|-----|------------|-----|-----|-----|-----|-----|-----|-------|----|--|----|
| C1<br>62 | G5  | U8 | G9  | C13 | 010 | C17 | U17A | G18 | G19 | U20 | 120 | G26 | <b>C3</b> 2 | U33 | C34 |   | C41 | G42 | A43 | 070 | 640<br>11/7 | 041 | 649<br>649 | U54 | 056<br>C56 | A57 | A58 | 100 | 107 | C74 | C75 | 31H76 |    |  |    |



# 4 Experimental information (i)

| Property                           | Value                        | Source    |
|------------------------------------|------------------------------|-----------|
| EM reconstruction method           | SINGLE PARTICLE              | Depositor |
| Imposed symmetry                   | POINT, C1                    | Depositor |
| Number of particles used           | 83000                        | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF            | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE | Depositor |
|                                    | CORRECTION                   |           |
| Microscope                         | FEI TITAN KRIOS              | Depositor |
| Voltage (kV)                       | 300                          | Depositor |
| Electron dose $(e^-/\text{\AA}^2)$ | 1.5                          | Depositor |
| Minimum defocus (nm)               | Not provided                 |           |
| Maximum defocus (nm)               | Not provided                 |           |
| Magnification                      | Not provided                 |           |
| Image detector                     | GATAN K2 SUMMIT (4k x 4k)    | Depositor |



# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 2MA, 4OC, MG, H2U, OMC, K, 31H, 4SU, 7MG, MA6, 2MG, OMG, 5MU

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).

| Mal | Chain | Bo   | ond lengths    | I    | Bond angles       |
|-----|-------|------|----------------|------|-------------------|
|     | Chain | RMSZ | # Z  > 5       | RMSZ | # Z  > 5          |
| 1   | a     | 0.47 | 1/36920~(0.0%) | 0.98 | 103/57570~(0.2%)  |
| 2   | b     | 0.29 | 0/1788         | 0.53 | 0/2397            |
| 3   | с     | 0.27 | 0/1598         | 0.52 | 0/2145            |
| 4   | d     | 0.30 | 0/1629         | 0.54 | 0/2185            |
| 5   | е     | 0.30 | 0/1183         | 0.57 | 1/1595~(0.1%)     |
| 6   | f     | 0.30 | 0/809          | 0.51 | 0/1085            |
| 7   | g     | 0.29 | 0/1192         | 0.50 | 0/1603            |
| 8   | h     | 0.29 | 0/1044         | 0.56 | 0/1401            |
| 9   | i     | 0.30 | 0/1023         | 0.58 | 1/1372~(0.1%)     |
| 10  | j     | 0.28 | 0/795          | 0.55 | 0/1071            |
| 11  | k     | 0.28 | 0/848          | 0.50 | 0/1147            |
| 12  | 1     | 0.30 | 0/1075         | 0.58 | 0/1439            |
| 13  | m     | 0.28 | 0/934          | 0.56 | 0/1253            |
| 14  | n     | 0.26 | 0/490          | 0.49 | 0/650             |
| 15  | 0     | 0.25 | 0/747          | 0.45 | 0/996             |
| 16  | р     | 0.30 | 0/723          | 0.56 | 0/971             |
| 17  | q     | 0.28 | 0/706          | 0.56 | 0/944             |
| 18  | r     | 0.28 | 0/536          | 0.51 | 0/718             |
| 19  | S     | 0.27 | 0/679          | 0.50 | 0/912             |
| 20  | t     | 0.23 | 0/606          | 0.47 | 0/810             |
| 21  | V     | 0.43 | 0/521          | 1.02 | 1/812~(0.1%)      |
| 22  | А     | 0.78 | 4/69062~(0.0%) | 1.06 | 202/107697~(0.2%) |
| 23  | В     | 0.49 | 0/2733         | 1.06 | 21/4257~(0.5%)    |
| 24  | D     | 0.45 | 2/2129~(0.1%)  | 0.64 | 2/2858~(0.1%)     |
| 25  | Е     | 0.40 | 0/1659         | 0.59 | 1/2224~(0.0%)     |
| 26  | F     | 0.39 | 0/1563         | 0.56 | 0/2113            |
| 27  | G     | 0.29 | 0/1201         | 0.53 | 0/1610            |
| 28  | Н     | 0.29 | 0/1267         | 0.53 | 0/1710            |
| 29  | М     | 0.35 | 0/1173         | 0.52 | 0/1578            |
| 30  | N     | 0.39 | 0/927          | 0.58 | 0/1243            |
| 31  | 0     | 0.42 | 1/1112~(0.1%)  | 0.63 | 1/1482~(0.1%)     |
| 32  | Р     | 0.39 | 0/1121         | 0.58 | 1/1504~(0.1%)     |



| Mal   | Chain | Bo   | ond lengths     | I    | Bond angles       |  |  |  |  |
|-------|-------|------|-----------------|------|-------------------|--|--|--|--|
| INIOI | Unam  | RMSZ | # Z  > 5        | RMSZ | # Z  > 5          |  |  |  |  |
| 33    | Q     | 0.34 | 0/943           | 0.57 | 0/1259            |  |  |  |  |
| 34    | R     | 0.29 | 0/920           | 0.53 | 0/1230            |  |  |  |  |
| 35    | S     | 0.37 | 0/889           | 0.61 | 0/1189            |  |  |  |  |
| 36    | Т     | 0.40 | 0/955           | 0.52 | 0/1265            |  |  |  |  |
| 37    | U     | 0.37 | 0/791           | 0.55 | 0/1051            |  |  |  |  |
| 38    | V     | 0.36 | 0/870           | 0.58 | 0/1171            |  |  |  |  |
| 39    | W     | 0.36 | 0/733           | 0.57 | 0/978             |  |  |  |  |
| 40    | Х     | 0.32 | 0/666           | 0.66 | 1/886~(0.1%)      |  |  |  |  |
| 41    | Y     | 0.29 | 0/738           | 0.54 | 0/989             |  |  |  |  |
| 42    | Ζ     | 0.43 | 0/632           | 0.55 | 0/838             |  |  |  |  |
| 43    | 0     | 0.39 | 0/363           | 0.66 | 0/486             |  |  |  |  |
| 44    | 1     | 0.29 | 0/537           | 0.49 | 0/714             |  |  |  |  |
| 45    | 2     | 0.34 | 0/443           | 0.61 | 1/597~(0.2%)      |  |  |  |  |
| 46    | 3     | 0.31 | 0/602           | 0.61 | 1/802~(0.1%)      |  |  |  |  |
| 47    | 4     | 0.52 | 1/416~(0.2%)    | 0.63 | 1/550~(0.2%)      |  |  |  |  |
| 48    | 5     | 0.31 | 0/373           | 0.69 | 1/495~(0.2%)      |  |  |  |  |
| 49    | 6     | 0.41 | 0/377           | 0.56 | 0/491             |  |  |  |  |
| 50    | 7     | 0.37 | 0/526           | 0.56 | 0/690             |  |  |  |  |
| 51    | 8     | 0.36 | 0/299           | 0.53 | 0/392             |  |  |  |  |
| 52    | Х     | 0.46 | 0/1671          | 1.08 | 10/2605~(0.4%)    |  |  |  |  |
| All   | All   | 0.61 | 9/153537~(0.0%) | 0.94 | 349/230030~(0.2%) |  |  |  |  |

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 |
|-----|-------|---------------------|---------------------|
| 3   | с     | 0                   | 1                   |
| 5   | е     | 0                   | 1                   |
| 26  | F     | 0                   | 1                   |
| 30  | N     | 0                   | 1                   |
| 36  | Т     | 0                   | 1                   |
| 44  | 1     | 0                   | 2                   |
| 48  | 5     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms |       | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 22  | А     | 774 | G    | N9-C4 | -6.94 | 1.32        | 1.38     |
| 22  | А     | 774 | G    | C2-N3 | -6.62 | 1.27        | 1.32     |



| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | А     | 774  | G    | N3-C4 | -5.88 | 1.31        | 1.35     |
| 1   | a     | 204  | А    | N9-C4 | 5.49  | 1.41        | 1.37     |
| 31  | 0     | 8    | PRO  | N-CD  | 5.43  | 1.55        | 1.47     |
| 24  | D     | 35   | PRO  | N-CD  | 5.29  | 1.55        | 1.47     |
| 24  | D     | 37   | PRO  | N-CD  | 5.23  | 1.55        | 1.47     |
| 22  | А     | 2457 | А    | N9-C4 | -5.18 | 1.34        | 1.37     |
| 47  | 4     | 31   | PRO  | N-CD  | 5.08  | 1.54        | 1.47     |

All (349) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-----------|--------|------------------|---------------|
| 22  | А     | 774  | G    | N3-C4-N9  | -13.61 | 117.83           | 126.00        |
| 22  | А     | 12   | U    | N1-C2-O2  | 12.05  | 131.24           | 122.80        |
| 22  | А     | 12   | U    | N3-C2-O2  | -11.78 | 113.95           | 122.20        |
| 22  | А     | 12   | U    | C2-N1-C1' | 11.58  | 131.59           | 117.70        |
| 23  | В     | 87   | С    | N1-C2-O2  | 10.47  | 125.19           | 118.90        |
| 1   | a     | 1441 | С    | N1-C2-O2  | 9.87   | 124.82           | 118.90        |
| 22  | А     | 774  | G    | N3-C4-C5  | 9.75   | 133.48           | 128.60        |
| 22  | А     | 1802 | U    | N3-C2-O2  | -9.59  | 115.49           | 122.20        |
| 23  | В     | 87   | С    | C2-N1-C1' | 9.51   | 129.26           | 118.80        |
| 22  | А     | 774  | G    | N3-C2-N2  | -9.38  | 113.33           | 119.90        |
| 1   | a     | 1441 | С    | C2-N1-C1' | 9.28   | 129.00           | 118.80        |
| 23  | В     | 87   | С    | N3-C2-O2  | -9.13  | 115.51           | 121.90        |
| 22  | А     | 774  | G    | C8-N9-C1' | 9.03   | 138.73           | 127.00        |
| 1   | a     | 1441 | С    | N3-C2-O2  | -8.90  | 115.67           | 121.90        |
| 1   | a     | 376  | U    | C2-N1-C1' | 8.87   | 128.35           | 117.70        |
| 1   | a     | 762  | С    | C2-N1-C1' | 8.80   | 128.48           | 118.80        |
| 22  | А     | 272  | С    | N1-C2-O2  | 8.68   | 124.11           | 118.90        |
| 22  | А     | 1350 | U    | C2-N1-C1' | 8.61   | 128.03           | 117.70        |
| 22  | А     | 1802 | U    | N1-C2-O2  | 8.53   | 128.77           | 122.80        |
| 1   | a     | 572  | U    | N3-C2-O2  | -8.39  | 116.33           | 122.20        |
| 22  | А     | 1802 | U    | C2-N1-C1' | 8.31   | 127.67           | 117.70        |
| 22  | А     | 1351 | С    | N1-C2-O2  | 8.30   | 123.88           | 118.90        |
| 22  | А     | 1435 | С    | N1-C2-O2  | 8.22   | 123.83           | 118.90        |
| 22  | А     | 774  | G    | N9-C4-C5  | 8.21   | 108.69           | 105.40        |
| 1   | a     | 851  | U    | N1-C2-O2  | 8.20   | 128.54           | 122.80        |
| 1   | a     | 762  | С    | N1-C2-O2  | 8.20   | 123.82           | 118.90        |
| 22  | А     | 1602 | U    | N3-C2-O2  | -8.18  | 116.47           | 122.20        |
| 22  | А     | 1719 | С    | C6-N1-C2  | -8.18  | 117.03           | 120.30        |
| 1   | a     | 315  | U    | C2-N1-C1' | 8.14   | 127.47           | 117.70        |
| 1   | a     | 376  | U    | N1-C2-O2  | 8.14   | 128.50           | 122.80        |
| 22  | А     | 1350 | U    | N1-C2-O2  | 8.11   | 128.48           | 122.80        |



| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 1   | a     | 572  | U    | C2-N1-C1'  | 8.08  | 127.40           | 117.70        |
| 1   | a     | 641  | U    | C2-N1-C1'  | 7.90  | 127.18           | 117.70        |
| 1   | a     | 572  | U    | N1-C2-O2   | 7.84  | 128.29           | 122.80        |
| 22  | А     | 1602 | U    | N1-C2-O2   | 7.84  | 128.29           | 122.80        |
| 1   | a     | 1391 | U    | N3-C2-O2   | -7.76 | 116.77           | 122.20        |
| 22  | А     | 557  | G    | O4'-C1'-N9 | 7.74  | 114.39           | 108.20        |
| 1   | a     | 1391 | U    | N1-C2-O2   | 7.67  | 128.17           | 122.80        |
| 1   | a     | 195  | С    | N1-C2-O2   | 7.66  | 123.49           | 118.90        |
| 22  | А     | 1602 | U    | C2-N1-C1'  | 7.64  | 126.86           | 117.70        |
| 1   | a     | 945  | С    | N1-C2-O2   | 7.61  | 123.46           | 118.90        |
| 1   | a     | 851  | U    | C2-N1-C1'  | 7.60  | 126.82           | 117.70        |
| 1   | a     | 1458 | С    | N1-C2-O2   | 7.60  | 123.46           | 118.90        |
| 22  | А     | 1350 | U    | N3-C2-O2   | -7.58 | 116.90           | 122.20        |
| 22  | А     | 1801 | С    | C6-N1-C2   | -7.55 | 117.28           | 120.30        |
| 22  | А     | 774  | G    | C2-N3-C4   | -7.50 | 108.15           | 111.90        |
| 22  | А     | 12   | U    | C6-N1-C1'  | -7.45 | 110.77           | 121.20        |
| 22  | А     | 835  | U    | N1-C2-O2   | 7.42  | 128.00           | 122.80        |
| 22  | А     | 2467 | С    | O4'-C1'-N1 | 7.42  | 114.14           | 108.20        |
| 23  | В     | 100  | U    | C2-N1-C1'  | 7.41  | 126.59           | 117.70        |
| 1   | a     | 315  | U    | N1-C2-O2   | 7.41  | 127.99           | 122.80        |
| 1   | a     | 315  | U    | N3-C2-O2   | -7.39 | 117.03           | 122.20        |
| 22  | А     | 2807 | G    | C4-N9-C1'  | 7.35  | 136.06           | 126.50        |
| 22  | А     | 1704 | С    | C6-N1-C2   | -7.32 | 117.37           | 120.30        |
| 22  | А     | 587  | С    | N1-C2-O2   | 7.30  | 123.28           | 118.90        |
| 1   | a     | 851  | U    | N3-C2-O2   | -7.30 | 117.09           | 122.20        |
| 1   | a     | 641  | U    | N3-C2-O2   | -7.26 | 117.12           | 122.20        |
| 22  | А     | 272  | С    | C2-N1-C1'  | 7.20  | 126.72           | 118.80        |
| 22  | А     | 1351 | С    | C6-N1-C2   | -7.14 | 117.44           | 120.30        |
| 22  | А     | 2332 | U    | C2-N1-C1'  | 7.09  | 126.21           | 117.70        |
| 1   | a     | 641  | U    | N1-C2-O2   | 7.08  | 127.75           | 122.80        |
| 22  | А     | 2492 | С    | N1-C2-O2   | 7.00  | 123.10           | 118.90        |
| 1   | a     | 195  | С    | N3-C2-O2   | -6.98 | 117.01           | 121.90        |
| 1   | a     | 376  | U    | N3-C2-O2   | -6.98 | 117.31           | 122.20        |
| 22  | А     | 972  | А    | O5'-P-OP2  | -6.97 | 99.43            | 105.70        |
| 22  | А     | 1435 | С    | N3-C2-O2   | -6.95 | 117.03           | 121.90        |
| 5   | е     | 80   | THR  | C-N-CA     | 6.93  | 139.02           | 121.70        |
| 22  | А     | 272  | С    | N3-C2-O2   | -6.90 | 117.07           | 121.90        |
| 22  | A     | 835  | U    | C2-N1-C1'  | 6.90  | 125.98           | 117.70        |
| 22  | А     | 774  | G    | C8-N9-C4   | -6.89 | 103.64           | 106.40        |
| 1   | a     | 1168 | С    | C2-N1-C1'  | 6.88  | 126.36           | 118.80        |
| 22  | A     | 774  | G    | C4-N9-C1'  | -6.83 | 117.62           | 126.50        |
| 22  | А     | 835  | U    | N3-C2-O2   | -6.72 | 117.49           | 122.20        |

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| Mol             | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----------------|-------|------|------|------------|-------|------------------|---------------|
| 1               | a     | 759  | U    | C2-N1-C1'  | 6.69  | 125.73           | 117.70        |
| 1               | a     | 992  | А    | C2-N3-C4   | 6.64  | 113.92           | 110.60        |
| 22              | А     | 1661 | С    | C6-N1-C2   | -6.64 | 117.64           | 120.30        |
| 23              | В     | 87   | С    | C6-N1-C1'  | -6.64 | 112.83           | 120.80        |
| 22              | А     | 2468 | С    | N1-C2-O2   | 6.63  | 122.88           | 118.90        |
| 1               | a     | 762  | С    | N3-C2-O2   | -6.62 | 117.27           | 121.90        |
| 22              | А     | 2072 | С    | C6-N1-C2   | -6.62 | 117.65           | 120.30        |
| 1               | a     | 1171 | С    | N1-C2-O2   | 6.62  | 122.87           | 118.90        |
| 1               | a     | 55   | С    | N1-C2-O2   | 6.60  | 122.86           | 118.90        |
| 22              | А     | 1351 | С    | C5-C6-N1   | 6.58  | 124.29           | 121.00        |
| 22              | А     | 587  | С    | N3-C2-O2   | -6.57 | 117.30           | 121.90        |
| 22              | А     | 1768 | С    | C6-N1-C2   | -6.57 | 117.67           | 120.30        |
| 22              | А     | 1351 | С    | C2-N1-C1'  | 6.55  | 126.01           | 118.80        |
| 1               | a     | 463  | U    | C2-N1-C1'  | 6.54  | 125.54           | 117.70        |
| 1               | a     | 1168 | С    | N1-C2-O2   | 6.53  | 122.82           | 118.90        |
| 1               | a     | 1441 | С    | C6-N1-C1'  | -6.53 | 112.97           | 120.80        |
| 22              | А     | 2468 | С    | C6-N1-C2   | -6.52 | 117.69           | 120.30        |
| 22              | А     | 935  | С    | C2-N1-C1'  | 6.50  | 125.94           | 118.80        |
| 22              | А     | 272  | С    | C6-N1-C2   | -6.49 | 117.70           | 120.30        |
| 22              | А     | 2468 | С    | N3-C2-O2   | -6.46 | 117.38           | 121.90        |
| 1               | a     | 195  | С    | C2-N1-C1'  | 6.46  | 125.91           | 118.80        |
| 22              | А     | 1351 | С    | N3-C2-O2   | -6.45 | 117.38           | 121.90        |
| 22              | А     | 793  | G    | O4'-C1'-N9 | 6.43  | 113.35           | 108.20        |
| 1               | a     | 1458 | С    | C2-N1-C1'  | 6.38  | 125.82           | 118.80        |
| 1               | a     | 762  | С    | C6-N1-C2   | -6.37 | 117.75           | 120.30        |
| 22              | А     | 2457 | А    | C2-N3-C4   | -6.36 | 107.42           | 110.60        |
| 1               | a     | 491  | С    | C2-N1-C1'  | 6.35  | 125.79           | 118.80        |
| 22              | А     | 883  | С    | N1-C2-O2   | 6.34  | 122.70           | 118.90        |
| 22              | А     | 2807 | G    | C8-N9-C1'  | -6.33 | 118.77           | 127.00        |
| 22              | А     | 935  | С    | N1-C2-O2   | 6.30  | 122.68           | 118.90        |
| 1               | a     | 1391 | U    | C2-N1-C1'  | 6.30  | 125.26           | 117.70        |
| 1               | a     | 1458 | С    | N3-C2-O2   | -6.28 | 117.50           | 121.90        |
| 22              | А     | 666  | А    | O4'-C1'-N9 | 6.28  | 113.22           | 108.20        |
| 22              | А     | 1696 | С    | N1-C2-O2   | 6.27  | 122.66           | 118.90        |
| 22              | А     | 328  | G    | P-O3'-C3'  | 6.23  | 127.18           | 119.70        |
| 22              | А     | 714  | G    | N3-C4-C5   | -6.23 | 125.48           | 128.60        |
| 22              | A     | 1683 | U    | N1-C2-O2   | 6.21  | 127.15           | 122.80        |
| 48              | 5     | 8    | LEU  | CA-CB-CG   | 6.21  | 129.59           | 115.30        |
| $\overline{22}$ | А     | 2429 | U    | C2-N1-C1'  | 6.20  | 125.14           | 117.70        |
| 32              | Р     | 84   | GLY  | N-CA-C     | 6.19  | 128.58           | 113.10        |
| 1               | a     | 888  | С    | C6-N1-C2   | -6.19 | 117.82           | 120.30        |
| 22              | А     | 1049 | С    | N1-C2-O2   | 6.17  | 122.60           | 118.90        |



| Mol | Chain | Res  | Type | Atoms     | Z     | $Observed(^{o})$    | $Ideal(^{o})$ |
|-----|-------|------|------|-----------|-------|---------------------|---------------|
| 22  | А     | 862  | С    | C6-N1-C2  | -6.17 | 117.83              | 120.30        |
| 1   | a     | 1178 | С    | N1-C2-O2  | 6.16  | 122.60              | 118.90        |
| 22  | А     | 714  | G    | N3-C4-N9  | 6.13  | 129.68              | 126.00        |
| 22  | А     | 1683 | U    | N3-C2-O2  | -6.11 | 117.93              | 122.20        |
| 22  | А     | 828  | А    | C2-N3-C4  | 6.09  | 113.64              | 110.60        |
| 1   | a     | 818  | С    | N1-C2-O2  | 6.08  | 122.55              | 118.90        |
| 1   | a     | 1171 | С    | C2-N1-C1' | 6.08  | 125.48              | 118.80        |
| 22  | А     | 2492 | С    | N3-C2-O2  | -6.07 | 117.65              | 121.90        |
| 1   | a     | 204  | А    | C2-N3-C4  | 6.06  | 113.63              | 110.60        |
| 1   | a     | 376  | U    | C6-N1-C1' | -6.03 | 112.76              | 121.20        |
| 22  | А     | 2583 | С    | N1-C2-O2  | 6.01  | 122.50              | 118.90        |
| 1   | a     | 621  | С    | N1-C2-O2  | 6.00  | 122.50              | 118.90        |
| 22  | А     | 644  | С    | C6-N1-C2  | -5.99 | 117.90              | 120.30        |
| 22  | А     | 2095 | U    | C2-N3-C4  | 5.97  | 130.58              | 127.00        |
| 23  | В     | 87   | С    | C6-N1-C2  | -5.97 | 117.91              | 120.30        |
| 22  | А     | 1179 | С    | C5-C6-N1  | 5.96  | 123.98              | 121.00        |
| 22  | А     | 1696 | С    | N3-C2-O2  | -5.94 | 117.74              | 121.90        |
| 22  | А     | 714  | G    | C2-N3-C4  | 5.93  | 114.86              | 111.90        |
| 1   | a     | 1441 | С    | C6-N1-C2  | -5.93 | 117.93              | 120.30        |
| 22  | А     | 2900 | С    | N1-C2-O2  | 5.91  | 122.45              | 118.90        |
| 22  | А     | 1043 | U    | N3-C2-O2  | -5.91 | 118.06              | 122.20        |
| 22  | А     | 1714 | С    | C6-N1-C2  | -5.90 | 117.94              | 120.30        |
| 22  | А     | 2492 | С    | C6-N1-C2  | -5.88 | 117.95              | 120.30        |
| 1   | a     | 762  | С    | C6-N1-C1' | -5.88 | 113.75              | 120.80        |
| 22  | А     | 2332 | U    | N1-C2-O2  | 5.88  | 126.91              | 122.80        |
| 1   | a     | 132  | С    | C6-N1-C2  | -5.85 | 117.96              | 120.30        |
| 22  | А     | 1921 | С    | N1-C2-O2  | 5.85  | 122.41              | 118.90        |
| 52  | X     | 74   | С    | N1-C2-O2  | 5.85  | 122.41              | 118.90        |
| 22  | А     | 2071 | С    | C6-N1-C2  | -5.84 | 117.97              | 120.30        |
| 1   | a     | 477  | U    | C2-N1-C1' | 5.84  | 124.70              | 117.70        |
| 22  | А     | 2501 | U    | N1-C2-O2  | 5.83  | 126.88              | 122.80        |
| 22  | А     | 2793 | G    | C4-N9-C1' | 5.83  | 134.08              | 126.50        |
| 52  | Х     | 34   | С    | C6-N1-C2  | -5.83 | 117.97              | 120.30        |
| 21  | V     | 12   | А    | C2-N3-C4  | 5.82  | 113.51              | 110.60        |
| 22  | А     | 2539 | С    | C6-N1-C2  | -5.82 | 117.97              | 120.30        |
| 22  | А     | 2742 | С    | C6-N1-C2  | -5.82 | 117.97              | 120.30        |
| 1   | a     | 463  | U    | N3-C2-O2  | -5.82 | 118.13              | 122.20        |
| 22  | A     | 1704 | C    | N1-C2-O2  | 5.80  | 122.38              | 118.90        |
| 1   | a     | 491  | C    | N3-C2-O2  | -5.79 | $117.8\overline{5}$ | 121.90        |
| 22  | A     | 12   | U    | C6-N1-C2  | -5.78 | 117.53              | 121.00        |
| 22  | A     | 1043 | U    | N1-C2-O2  | 5.78  | 126.84              | 122.80        |
| 22  | A     | 568  | С    | C6-N1-C2  | -5.77 | 117.99              | 120.30        |



| Mol | Chain | Res               | Type | Atoms     | Z     | $Observed(^{o})$    | $Ideal(^{o})$       |
|-----|-------|-------------------|------|-----------|-------|---------------------|---------------------|
| 22  | А     | 2819              | С    | N1-C2-O2  | 5.77  | 122.36              | 118.90              |
| 22  | А     | 828               | А    | C8-N9-C4  | -5.77 | 103.49              | 105.80              |
| 22  | А     | 2492              | С    | C2-N1-C1' | 5.75  | 125.12              | 118.80              |
| 22  | А     | 861               | С    | C6-N1-C2  | -5.75 | 118.00              | 120.30              |
| 23  | В     | 94                | С    | N1-C2-O2  | 5.74  | 122.35              | 118.90              |
| 22  | А     | 1065              | А    | C2-N3-C4  | 5.72  | 113.46              | 110.60              |
| 1   | a     | 491               | С    | N1-C2-O2  | 5.71  | 122.33              | 118.90              |
| 1   | a     | 945               | С    | N3-C2-O2  | -5.70 | 117.91              | 121.90              |
| 1   | a     | 992               | А    | N3-C4-N9  | 5.70  | 131.96              | 127.40              |
| 52  | Х     | 1                 | С    | N1-C2-O2  | 5.69  | 122.31              | 118.90              |
| 1   | a     | 1458              | С    | C6-N1-C2  | -5.69 | 118.03              | 120.30              |
| 22  | А     | 1196              | С    | C6-N1-C2  | -5.69 | 118.03              | 120.30              |
| 22  | А     | 1382              | С    | N1-C2-O2  | 5.69  | 122.31              | 118.90              |
| 47  | 4     | 30                | CYS  | C-N-CD    | 5.68  | 140.33              | 128.40              |
| 22  | А     | 1009              | С    | N1-C2-O2  | 5.68  | 122.31              | 118.90              |
| 22  | А     | 1843              | U    | N1-C2-O2  | 5.67  | 126.77              | 122.80              |
| 22  | А     | 2900              | С    | C6-N1-C2  | -5.67 | 118.03              | 120.30              |
| 23  | В     | 23                | U    | C5-C6-N1  | 5.67  | 125.53              | 122.70              |
| 1   | a     | 1171              | С    | C6-N1-C2  | -5.67 | 118.03              | 120.30              |
| 1   | а     | 463               | U    | N1-C2-O2  | 5.66  | 126.76              | 122.80              |
| 1   | a     | 886               | С    | C6-N1-C2  | -5.65 | 118.04              | 120.30              |
| 22  | А     | 2673              | С    | C6-N1-C2  | -5.65 | 118.04              | 120.30              |
| 52  | Х     | 1                 | С    | P-O3'-C3' | 5.64  | 126.47              | 119.70              |
| 22  | А     | 2070              | С    | C6-N1-C2  | -5.63 | 118.05              | 120.30              |
| 22  | А     | 2719              | С    | C6-N1-C2  | -5.63 | 118.05              | 120.30              |
| 22  | А     | 1171              | А    | C4-N9-C1' | 5.63  | 136.44              | 126.30              |
| 22  | А     | 1661              | С    | C2-N1-C1' | 5.63  | 124.99              | 118.80              |
| 22  | А     | 957               | С    | N1-C2-O2  | 5.63  | 122.28              | 118.90              |
| 1   | a     | 1289              | А    | C4-N9-C1' | 5.62  | 136.41              | 126.30              |
| 22  | А     | 463               | С    | C6-N1-C2  | -5.61 | 118.06              | 120.30              |
| 1   | a     | 627               | U    | C2-N1-C1' | 5.61  | 124.43              | 117.70              |
| 22  | А     | 12                | U    | C5-C6-N1  | 5.60  | 125.50              | 122.70              |
| 1   | a     | 759               | U    | N1-C2-O2  | 5.60  | 126.72              | 122.80              |
| 22  | А     | 2766              | U    | N3-C2-O2  | -5.60 | 118.28              | 122.20              |
| 22  | А     | 1179              | С    | C6-N1-C2  | -5.59 | 118.06              | 120.30              |
| 1   | a     | 1459              | С    | N1-C2-O2  | 5.58  | 122.25              | 118.90              |
| 52  | Х     | 34                | С    | C5-C6-N1  | 5.58  | 123.79              | 121.00              |
| 22  | A     | 1961              | C    | N1-C2-O2  | 5.57  | 122.24              | 118.90              |
| 22  | A     | 1160              | C    | N1-C2-O2  | 5.57  | $122.2\overline{4}$ | 118.90              |
| 24  | D     | 34                | LYS  | C-N-CD    | 5.56  | 140.07              | 128.40              |
| 22  | A     | $20\overline{20}$ | U    | N3-C2-O2  | -5.56 | 118.31              | $122.\overline{20}$ |
| 1   | a     | 320               | С    | C6-N1-C2  | -5.53 | 118.09              | 120.30              |



| Mol | Chain | Res  | Type | Atoms     |                   | $Observed(^{o})$    | $Ideal(^{o})$ |
|-----|-------|------|------|-----------|-------------------|---------------------|---------------|
| 24  | D     | 36   | LEU  | C-N-CD    | 5.53              | 140.02              | 128.40        |
| 22  | А     | 883  | С    | N3-C2-O2  | -5.53             | 118.03              | 121.90        |
| 22  | А     | 627  | С    | N3-C2-O2  | -5.52             | 118.03              | 121.90        |
| 1   | a     | 20   | С    | N1-C2-O2  | 5.52              | 122.21              | 118.90        |
| 23  | В     | 23   | U    | N3-C2-O2  | -5.51             | 118.34              | 122.20        |
| 1   | a     | 759  | U    | N3-C2-O2  | -5.51             | 118.34              | 122.20        |
| 52  | Х     | 74   | С    | N3-C2-O2  | -5.51             | 118.05              | 121.90        |
| 22  | А     | 2430 | С    | N1-C2-O2  | 5.50              | 122.20              | 118.90        |
| 23  | В     | 92   | С    | C6-N1-C2  | -5.50             | 118.10              | 120.30        |
| 23  | В     | 1    | U    | C2-N1-C1' | 5.50              | 124.30              | 117.70        |
| 22  | А     | 1171 | А    | N7-C8-N9  | 5.48              | 116.54              | 113.80        |
| 22  | А     | 666  | А    | N7-C8-N9  | 5.48              | 116.54              | 113.80        |
| 22  | А     | 2457 | А    | N1-C2-N3  | 5.47              | 132.04              | 129.30        |
| 1   | a     | 1289 | А    | C2-N3-C4  | 5.47              | 113.34              | 110.60        |
| 31  | 0     | 7    | LYS  | C-N-CD    | 5.47              | 139.89              | 128.40        |
| 23  | В     | 94   | С    | N3-C2-O2  | -5.46             | 118.08              | 121.90        |
| 1   | a     | 945  | С    | C2-N1-C1' | 5.45              | 124.80              | 118.80        |
| 22  | А     | 1704 | С    | N3-C2-O2  | -5.45             | 118.08              | 121.90        |
| 1   | a     | 20   | С    | C6-N1-C2  | -5.45             | 118.12              | 120.30        |
| 22  | А     | 1350 | U    | C6-N1-C1' | -5.45             | 113.58              | 121.20        |
| 22  | А     | 1806 | U    | C5-C6-N1  | -5.45             | 119.98              | 122.70        |
| 1   | a     | 546  | U    | C5-C6-N1  | 5.44              | 125.42              | 122.70        |
| 22  | А     | 1655 | С    | C6-N1-C2  | -5.43             | 118.13              | 120.30        |
| 1   | a     | 20   | С    | N3-C2-O2  | -5.43             | 118.10              | 121.90        |
| 22  | А     | 2333 | U    | C2-N1-C1' | 5.42              | 124.20              | 117.70        |
| 22  | А     | 1704 | С    | C5-C6-N1  | 5.42              | 123.71              | 121.00        |
| 22  | А     | 1768 | С    | C5-C6-N1  | 5.42              | 123.71              | 121.00        |
| 22  | А     | 2653 | С    | C6-N1-C2  | -5.42             | 118.13              | 120.30        |
| 22  | А     | 627  | С    | N1-C2-O2  | 5.40              | 122.14              | 118.90        |
| 22  | А     | 587  | С    | C2-N1-C1' | 5.39              | 124.73              | 118.80        |
| 22  | А     | 2265 | G    | N3-C4-C5  | -5.39             | 125.91              | 128.60        |
| 1   | a     | 220  | U    | OP1-P-O3' | 5.38              | 117.04              | 105.20        |
| 22  | А     | 1661 | С    | N3-C2-O2  | -5.38             | 118.13              | 121.90        |
| 1   | a     | 55   | С    | N3-C2-O2  | -5.38             | 118.14              | 121.90        |
| 1   | a     | 821  | U    | N1-C2-O2  | 5.38              | 126.56              | 122.80        |
| 22  | А     | 1370 | С    | N1-C2-O2  | 5.38              | 122.13              | 118.90        |
| 1   | a     | 1407 | С    | N1-C2-O2  | 5.37              | 122.12              | 118.90        |
| 22  | А     | 2020 | U    | N1-C2-O2  | 5.37              | 126.56              | 122.80        |
| 22  | A     | 2386 | C    | N1-C2-O2  | 5.37              | $122.1\overline{2}$ | 118.90        |
| 1   | a     | 621  | C    | C6-N1-C2  | -5.36             | 118.16              | 120.30        |
| 22  | A     | 2606 | C    | N1-C2-O2  | $5.3\overline{6}$ | $122.1\overline{2}$ | 118.90        |
| 22  | A     | 1179 | С    | C2-N1-C1  | 5.36              | 124.69              | 118.80        |



| Mol             | Chain | Res  | Type | Atoms                  | Z     | $Observed(^{o})$    | $Ideal(^{o})$ |
|-----------------|-------|------|------|------------------------|-------|---------------------|---------------|
| 22              | А     | 2429 | U    | N1-C2-O2               | 5.36  | 126.55              | 122.80        |
| 22              | А     | 2890 | С    | C6-N1-C2               | -5.36 | 118.16              | 120.30        |
| 22              | А     | 2644 | С    | C6-N1-C2               | -5.35 | 118.16              | 120.30        |
| 22              | А     | 1050 | С    | C6-N1-C2               | -5.35 | 118.16              | 120.30        |
| 1               | a     | 461  | С    | C6-N1-C2               | -5.34 | 118.16              | 120.30        |
| 22              | А     | 2295 | А    | O4'-C1'-N9             | 5.33  | 112.47              | 108.20        |
| 1               | a     | 227  | С    | C6-N1-C2               | -5.33 | 118.17              | 120.30        |
| 22              | А     | 935  | C    | N3-C2-O2               | -5.33 | 118.17              | 121.90        |
| 1               | a     | 137  | U    | N1-C2-O2               | 5.33  | 126.53              | 122.80        |
| 22              | А     | 2070 | C    | C5-C6-N1               | 5.32  | 123.66              | 121.00        |
| 22              | А     | 1802 | U    | C6-N1-C1'              | -5.32 | 113.75              | 121.20        |
| 1               | a     | 762  | С    | C5-C6-N1               | 5.32  | 123.66              | 121.00        |
| 23              | В     | 23   | U    | N1-C2-O2               | 5.31  | 126.52              | 122.80        |
| 22              | А     | 2090 | С    | C6-N1-C2               | -5.30 | 118.18              | 120.30        |
| 23              | В     | 100  | U    | N3-C2-O2               | -5.30 | 118.49              | 122.20        |
| 23              | В     | 1    | U    | N1-C2-O2               | 5.30  | 126.51              | 122.80        |
| 22              | А     | 2464 | С    | C6-N1-C2               | -5.29 | 118.18              | 120.30        |
| 45              | 2     | 53   | LEU  | CA-CB-CG               | 5.29  | 127.47              | 115.30        |
| 1               | a     | 204  | А    | C4-N9-C1'              | 5.28  | 135.81              | 126.30        |
| 1               | a     | 992  | А    | N3-C4-C5               | -5.28 | 123.10              | 126.80        |
| 1               | a     | 59   | С    | C6-N1-C2               | -5.27 | 118.19              | 120.30        |
| 22              | А     | 1171 | А    | N3-C4-N9               | 5.27  | 131.62              | 127.40        |
| 1               | a     | 1168 | С    | N3-C2-O2               | -5.26 | 118.22              | 121.90        |
| 22              | А     | 1631 | G    | C4-N9-C1'              | 5.25  | 133.33              | 126.50        |
| 1               | a     | 478  | G    | C8-N9-C4               | -5.25 | 104.30              | 106.40        |
| 22              | А     | 2469 | С    | N1-C2-O2               | 5.22  | 122.03              | 118.90        |
| 22              | А     | 2834 | C    | C6-N1-C2               | -5.22 | 118.21              | 120.30        |
| 9               | i     | 23   | LEU  | CA-CB-CG               | 5.22  | 127.31              | 115.30        |
| 1               | a     | 572  | U    | C6-N1-C1'              | -5.22 | 113.89              | 121.20        |
| 22              | А     | 37   | C    | N3-C2-O2               | -5.22 | 118.25              | 121.90        |
| 1               | a     | 1171 | С    | N3-C2-O2               | -5.22 | 118.25              | 121.90        |
| 1               | a     | 1033 | U    | C2-N1-C1'              | 5.21  | 123.96              | 117.70        |
| 22              | А     | 777  | C    | C6-N1-C2               | -5.21 | 118.21              | 120.30        |
| 22              | А     | 608  | C    | C6-N1-C2               | -5.20 | 118.22              | 120.30        |
| 22              | А     | 666  | A    | C5-N7-C8               | -5.19 | 101.31              | 103.90        |
| $\overline{22}$ | A     | 1028 | G    | O4'-C1'-N9             | 5.19  | 112.35              | 108.20        |
| 1               | a     | 1032 | C    | C2-N1-C1'              | 5.19  | $1\overline{24.50}$ | 118.80        |
| 23              | B     | 12   | U    | $C2-N1-\overline{C1'}$ | 5.19  | 123.92              | 117.70        |
| 22              | A     | 1214 |      | N1-C2-O2               | 5.18  | $122.0\overline{1}$ | 118.90        |
| 52              | X     | 13   | C    | C6-N1-C2               | -5.18 | 118.23              | 120.30        |
| 1               | a     | 945  | C    | C6-N1-C2               | -5.18 | 118.23              | 120.30        |
| 22              | А     | 212  | C    | C6-N1-C2               | -5.18 | 118.23              | 120.30        |



| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 22  | А     | 201  | С    | C6-N1-C2   | -5.18 | 118.23           | 120.30        |
| 22  | А     | 960  | С    | N1-C2-O2   | 5.18  | 122.01           | 118.90        |
| 22  | А     | 2051 | С    | C6-N1-C2   | -5.18 | 118.23           | 120.30        |
| 23  | В     | 23   | U    | C6-N1-C2   | -5.18 | 117.89           | 121.00        |
| 22  | А     | 724  | С    | C6-N1-C2   | -5.17 | 118.23           | 120.30        |
| 23  | В     | 94   | С    | C6-N1-C2   | -5.17 | 118.23           | 120.30        |
| 23  | В     | 100  | U    | N1-C2-O2   | 5.17  | 126.42           | 122.80        |
| 22  | А     | 1030 | С    | N1-C2-O2   | 5.17  | 122.00           | 118.90        |
| 22  | А     | 1719 | С    | N3-C2-O2   | -5.17 | 118.28           | 121.90        |
| 40  | Х     | 70   | LEU  | CA-CB-CG   | 5.17  | 127.19           | 115.30        |
| 22  | А     | 1382 | С    | C6-N1-C2   | -5.17 | 118.23           | 120.30        |
| 22  | А     | 2253 | С    | N1-C2-O2   | 5.17  | 122.00           | 118.90        |
| 23  | В     | 100  | U    | C6-N1-C1'  | -5.16 | 113.98           | 121.20        |
| 1   | a     | 1178 | С    | C2-N1-C1'  | 5.16  | 124.47           | 118.80        |
| 1   | a     | 315  | U    | C6-N1-C1'  | -5.15 | 113.98           | 121.20        |
| 22  | А     | 644  | С    | N1-C2-O2   | 5.15  | 121.99           | 118.90        |
| 22  | А     | 710  | С    | C6-N1-C2   | -5.15 | 118.24           | 120.30        |
| 22  | А     | 2796 | С    | N1-C2-O2   | 5.15  | 121.99           | 118.90        |
| 22  | А     | 2483 | С    | C6-N1-C2   | -5.15 | 118.24           | 120.30        |
| 22  | А     | 1305 | U    | N3-C2-O2   | -5.15 | 118.60           | 122.20        |
| 46  | 3     | 49   | ASP  | CB-CG-OD2  | 5.15  | 122.93           | 118.30        |
| 22  | А     | 2070 | С    | N1-C2-O2   | 5.14  | 121.98           | 118.90        |
| 52  | Х     | 34   | С    | N1-C2-O2   | 5.13  | 121.98           | 118.90        |
| 1   | a     | 1504 | А    | C2-N3-C4   | 5.13  | 113.17           | 110.60        |
| 22  | А     | 272  | С    | C5-C6-N1   | 5.13  | 123.56           | 121.00        |
| 22  | А     | 490  | С    | C6-N1-C2   | -5.13 | 118.25           | 120.30        |
| 22  | А     | 2451 | С    | N1-C2-O2   | 5.13  | 121.98           | 118.90        |
| 22  | А     | 2750 | С    | C6-N1-C2   | -5.13 | 118.25           | 120.30        |
| 22  | А     | 419  | U    | N1-C2-O2   | 5.13  | 126.39           | 122.80        |
| 1   | a     | 860  | U    | N3-C2-O2   | -5.12 | 118.61           | 122.20        |
| 22  | А     | 2347 | А    | C2-N3-C4   | 5.12  | 113.16           | 110.60        |
| 22  | А     | 937  | G    | OP1-P-O3'  | 5.12  | 116.46           | 105.20        |
| 22  | А     | 2612 | U    | C2-N1-C1'  | 5.11  | 123.84           | 117.70        |
| 22  | А     | 2429 | U    | N3-C2-O2   | -5.11 | 118.62           | 122.20        |
| 22  | А     | 2583 | С    | C2-N1-C1'  | 5.11  | 124.42           | 118.80        |
| 1   | a     | 10   | G    | O4'-C1'-N9 | 5.11  | 112.28           | 108.20        |
| 22  | А     | 1801 | С    | C5-C6-N1   | 5.10  | 123.55           | 121.00        |
| 1   | a     | 1289 | A    | N7-C8-N9   | 5.10  | 116.35           | 113.80        |
| 1   | a     | 621  | С    | C5-C6-N1   | 5.10  | 123.55           | 121.00        |
| 22  | A     | 555  | С    | N1-C2-O2   | 5.09  | 121.95           | 118.90        |
| 22  | A     | 241  | С    | N1-C2-O2   | 5.09  | 121.95           | 118.90        |
| 52  | Х     | 34   | С    | C2-N1-C1'  | 5.09  | 124.40           | 118.80        |



| Mol | Chain | Res  | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 22  | А     | 1461 | С    | C6-N1-C2   | -5.08 | 118.27           | 120.30        |
| 22  | А     | 2493 | С    | N1-C2-O2   | 5.08  | 121.94           | 118.90        |
| 22  | А     | 2583 | С    | C6-N1-C2   | -5.08 | 118.27           | 120.30        |
| 22  | А     | 2807 | G    | N3-C4-N9   | 5.07  | 129.04           | 126.00        |
| 22  | А     | 2900 | С    | N3-C2-O2   | -5.07 | 118.35           | 121.90        |
| 1   | a     | 137  | U    | N3-C2-O2   | -5.07 | 118.65           | 122.20        |
| 22  | А     | 2383 | С    | C6-N1-C2   | -5.06 | 118.28           | 120.30        |
| 22  | А     | 213  | С    | N1-C2-O2   | 5.05  | 121.93           | 118.90        |
| 23  | В     | 100  | U    | O4'-C1'-N1 | 5.05  | 112.24           | 108.20        |
| 1   | a     | 631  | С    | C6-N1-C2   | -5.05 | 118.28           | 120.30        |
| 22  | А     | 957  | С    | C6-N1-C2   | -5.05 | 118.28           | 120.30        |
| 22  | А     | 256  | С    | C6-N1-C2   | -5.04 | 118.28           | 120.30        |
| 22  | А     | 113  | U    | N1-C2-O2   | 5.04  | 126.33           | 122.80        |
| 1   | a     | 377  | С    | C6-N1-C2   | -5.04 | 118.28           | 120.30        |
| 22  | А     | 717  | С    | C6-N1-C2   | -5.04 | 118.29           | 120.30        |
| 22  | А     | 883  | С    | C6-N1-C2   | -5.04 | 118.28           | 120.30        |
| 1   | a     | 1171 | С    | C5-C6-N1   | 5.03  | 123.51           | 121.00        |
| 22  | А     | 1435 | С    | C6-N1-C2   | -5.03 | 118.29           | 120.30        |
| 22  | А     | 1382 | С    | N3-C2-O2   | -5.02 | 118.38           | 121.90        |
| 22  | А     | 1794 | С    | C6-N1-C2   | -5.02 | 118.29           | 120.30        |
| 22  | А     | 607  | С    | C6-N1-C2   | -5.01 | 118.29           | 120.30        |
| 22  | А     | 1030 | С    | C5-C6-N1   | 5.01  | 123.50           | 121.00        |
| 52  | X     | 41   | С    | N1-C2-O2   | 5.01  | 121.91           | 118.90        |
| 25  | Е     | 148  | HIS  | C-N-CA     | 5.00  | 134.21           | 121.70        |

There are no chirality outliers.

| All ( | (8) | planarity | outliers | are listed | below: |
|-------|-----|-----------|----------|------------|--------|
|-------|-----|-----------|----------|------------|--------|

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 44  | 1     | 58  | ARG  | Sidechain |
| 44  | 1     | 7   | ARG  | Sidechain |
| 48  | 5     | 26  | ASN  | Peptide   |
| 26  | F     | 188 | ASN  | Peptide   |
| 30  | Ν     | 17  | ARG  | Sidechain |
| 36  | Т     | 25  | PHE  | Peptide   |
| 3   | с     | 155 | ARG  | Sidechain |
| 5   | е     | 32  | ARG  | Sidechain |

## 5.2 Too-close contacts (i)

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



#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | b     | 215/255~(84%) | 202 (94%) | 13~(6%) | 0        | 100         | 100 |
| 3   | с     | 194/217~(89%) | 186 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 4   | d     | 193/200~(96%) | 187 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 5   | е     | 155/166~(93%) | 151 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 6   | f     | 94/98~(96%)   | 92 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 7   | g     | 142/156~(91%) | 137 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 8   | h     | 129/132~(98%) | 125 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 9   | i     | 123/132~(93%) | 117 (95%) | 6(5%)   | 0        | 100         | 100 |
| 10  | j     | 96/102~(94%)  | 90 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 11  | k     | 111/129~(86%) | 105 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 12  | 1     | 133/137~(97%) | 126 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 13  | m     | 115/121~(95%) | 113 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 14  | n     | 58/89~(65%)   | 58 (100%) | 0       | 0        | 100         | 100 |
| 15  | О     | 86/89~(97%)   | 84 (98%)  | 2(2%)   | 0        | 100         | 100 |
| 16  | р     | 88/91~(97%)   | 83 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 17  | q     | 83/87~(95%)   | 75~(90%)  | 8 (10%) | 0        | 100         | 100 |
| 18  | r     | 62/80~(78%)   | 60 (97%)  | 2(3%)   | 0        | 100         | 100 |
| 19  | s     | 80/92~(87%)   | 78~(98%)  | 2(2%)   | 0        | 100         | 100 |
| 20  | t     | 78/83~(94%)   | 77 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 24  | D     | 272/277~(98%) | 265 (97%) | 7(3%)   | 0        | 100         | 100 |
| 25  | Ε     | 214/220~(97%) | 205 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 26  | F     | 201/207~(97%) | 192 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 27  | G     | 148/179~(83%) | 139 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 28  | Н     | 156/178~(88%) | 145 (93%) | 11 (7%) | 0        | 100         | 100 |
| 29  | М     | 143/145 (99%) | 138 (96%) | 5 (4%)  | 0        | 100         | 100 |


| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Perce | entiles |
|-----|-------|-----------------|------------|----------|----------|-------|---------|
| 30  | N     | 120/122~(98%)   | 115 (96%)  | 5 (4%)   | 0        | 100   | 100     |
| 31  | Ο     | 144/146~(99%)   | 139 (96%)  | 5 (4%)   | 0        | 100   | 100     |
| 32  | Р     | 135/144 (94%)   | 134 (99%)  | 1 (1%)   | 0        | 100   | 100     |
| 33  | Q     | 117/122~(96%)   | 114 (97%)  | 3 (3%)   | 0        | 100   | 100     |
| 34  | R     | 116/119 (98%)   | 114 (98%)  | 2 (2%)   | 0        | 100   | 100     |
| 35  | S     | 107/116~(92%)   | 101 (94%)  | 6 (6%)   | 0        | 100   | 100     |
| 36  | Т     | 114/118 (97%)   | 110 (96%)  | 4 (4%)   | 0        | 100   | 100     |
| 37  | U     | 94/102~(92%)    | 90 (96%)   | 4 (4%)   | 0        | 100   | 100     |
| 38  | V     | 110/117 (94%)   | 106 (96%)  | 4 (4%)   | 0        | 100   | 100     |
| 39  | W     | 87/91~(96%)     | 84 (97%)   | 3 (3%)   | 0        | 100   | 100     |
| 40  | Х     | 81/105~(77%)    | 75 (93%)   | 6 (7%)   | 0        | 100   | 100     |
| 41  | Y     | 92/217~(42%)    | 90 (98%)   | 2 (2%)   | 0        | 100   | 100     |
| 42  | Z     | 80/94~(85%)     | 76 (95%)   | 4 (5%)   | 0        | 100   | 100     |
| 43  | 0     | 43/62~(69%)     | 38 (88%)   | 5 (12%)  | 0        | 100   | 100     |
| 44  | 1     | 63/69~(91%)     | 62 (98%)   | 1 (2%)   | 0        | 100   | 100     |
| 45  | 2     | 55/59~(93%)     | 51 (93%)   | 4 (7%)   | 0        | 100   | 100     |
| 46  | 3     | 67/84~(80%)     | 62 (92%)   | 5 (8%)   | 0        | 100   | 100     |
| 47  | 4     | 47/58 (81%)     | 45 (96%)   | 2 (4%)   | 0        | 100   | 100     |
| 48  | 5     | 40/49~(82%)     | 36 (90%)   | 4 (10%)  | 0        | 100   | 100     |
| 49  | 6     | 42/45~(93%)     | 40 (95%)   | 2 (5%)   | 0        | 100   | 100     |
| 50  | 7     | 62/66~(94%)     | 56 (90%)   | 6 (10%)  | 0        | 100   | 100     |
| 51  | 8     | 35/37~(95%)     | 35 (100%)  | 0        | 0        | 100   | 100     |
| All | All   | 5220/5804 (90%) | 5003 (96%) | 217 (4%) | 0        | 100   | 100     |

There are no Ramachandran outliers to report.

## 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.



| Mol | Chain | Analysed                     | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------------------|------------|----------|-------------|-----|
| 2   | b     | 189/221~(86%)                | 187~(99%)  | 2(1%)    | 73          | 88  |
| 3   | с     | 162/175~(93%)                | 162 (100%) | 0        | 100         | 100 |
| 4   | d     | 172/175~(98%)                | 172 (100%) | 0        | 100         | 100 |
| 5   | е     | 123/131~(94%)                | 122~(99%)  | 1 (1%)   | 81          | 93  |
| 6   | f     | 84/86~(98%)                  | 82~(98%)   | 2(2%)    | 49          | 77  |
| 7   | g     | 125/132~(95%)                | 125~(100%) | 0        | 100         | 100 |
| 8   | h     | 112/113~(99%)                | 112 (100%) | 0        | 100         | 100 |
| 9   | i     | 105/109~(96%)                | 105 (100%) | 0        | 100         | 100 |
| 10  | j     | 88/91~(97%)                  | 88 (100%)  | 0        | 100         | 100 |
| 11  | k     | 89/104 (86%)                 | 88~(99%)   | 1 (1%)   | 73          | 88  |
| 12  | 1     | 117/119~(98%)                | 116 (99%)  | 1 (1%)   | 78          | 91  |
| 13  | m     | 100/104~(96%)                | 99~(99%)   | 1 (1%)   | 76          | 90  |
| 14  | n     | 50/78~(64%)                  | 50 (100%)  | 0        | 100         | 100 |
| 15  | 0     | 80/81~(99%)                  | 80 (100%)  | 0        | 100         | 100 |
| 16  | р     | 76/77~(99%)                  | 76 (100%)  | 0        | 100         | 100 |
| 17  | q     | 80/82~(98%)                  | 79~(99%)   | 1 (1%)   | 69          | 87  |
| 18  | r     | 57/68~(84%)                  | 57~(100%)  | 0        | 100         | 100 |
| 19  | s     | 71/80~(89%)                  | 67~(94%)   | 4 (6%)   | 21          | 57  |
| 20  | t     | 67/69~(97%)                  | 67~(100%)  | 0        | 100         | 100 |
| 24  | D     | 221/224~(99%)                | 218 (99%)  | 3 (1%)   | 67          | 86  |
| 25  | Е     | 173/177~(98%)                | 173 (100%) | 0        | 100         | 100 |
| 26  | F     | 163/169~(96%)                | 158 (97%)  | 5(3%)    | 40          | 72  |
| 27  | G     | 131/158~(83%)                | 130 (99%)  | 1 (1%)   | 81          | 93  |
| 28  | Н     | 141/155~(91%)                | 137~(97%)  | 4 (3%)   | 43          | 74  |
| 29  | М     | 123/123~(100%)               | 123 (100%) | 0        | 100         | 100 |
| 30  | Ν     | 100/100~(100%)               | 100 (100%) | 0        | 100         | 100 |
| 31  | О     | 112/112~(100%)               | 107~(96%)  | 5 (4%)   | 27          | 63  |
| 32  | Р     | 114/119~(96%)                | 112 (98%)  | 2 (2%)   | 59          | 82  |
| 33  | Q     | 100/102~(98%)                | 99~(99%)   | 1 (1%)   | 76          | 90  |
| 34  | R     | 93/95~(98%)                  | 93 (100%)  | 0        | 100         | 100 |
| 35  | S     | $\overline{95/102} \ (93\%)$ | 95 (100%)  | 0        | 100         | 100 |
| 36  | Т     | 96/98~(98%)                  | 95~(99%)   | 1 (1%)   | 76          | 90  |



| Mol | Chain | Analysed        | Rotameric     | Outliers | Perce | ntiles |
|-----|-------|-----------------|---------------|----------|-------|--------|
| 37  | U     | 84/86~(98%)     | 84 (100%)     | 0        | 100   | 100    |
| 38  | V     | 91/94~(97%)     | 91 (100%)     | 0        | 100   | 100    |
| 39  | W     | 80/82~(98%)     | 80 (100%)     | 0        | 100   | 100    |
| 40  | Х     | 72/90~(80%)     | $71 \ (99\%)$ | 1 (1%)   | 67    | 86     |
| 41  | Y     | 82/190~(43%)    | 81 (99%)      | 1 (1%)   | 71    | 88     |
| 42  | Z     | 64/75~(85%)     | 64 (100%)     | 0        | 100   | 100    |
| 43  | 0     | 37/52~(71%)     | 37 (100%)     | 0        | 100   | 100    |
| 44  | 1     | 59/62~(95%)     | 59 (100%)     | 0        | 100   | 100    |
| 45  | 2     | 51/53~(96%)     | 50 (98%)      | 1 (2%)   | 55    | 80     |
| 46  | 3     | 63/75~(84%)     | 61 (97%)      | 2(3%)    | 39    | 71     |
| 47  | 4     | 46/51~(90%)     | 45 (98%)      | 1 (2%)   | 52    | 79     |
| 48  | 5     | 43/47~(92%)     | 42 (98%)      | 1 (2%)   | 50    | 78     |
| 49  | 6     | 39/40~(98%)     | 39 (100%)     | 0        | 100   | 100    |
| 50  | 7     | 55/57~(96%)     | 53~(96%)      | 2 (4%)   | 35    | 69     |
| 51  | 8     | 34/35~(97%)     | 34 (100%)     | 0        | 100   | 100    |
| All | All   | 4509/4918 (92%) | 4465 (99%)    | 44 (1%)  | 77    | 90     |

All (44) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | b     | 138 | LYS  |
| 2   | b     | 167 | ARG  |
| 5   | е     | 88  | ARG  |
| 6   | f     | 52  | ILE  |
| 6   | f     | 56  | LYS  |
| 11  | k     | 113 | VAL  |
| 12  | l     | 99  | ARG  |
| 13  | m     | 102 | THR  |
| 17  | q     | 50  | ASP  |
| 19  | s     | 6   | LYS  |
| 19  | s     | 7   | LYS  |
| 19  | s     | 51  | VAL  |
| 19  | s     | 55  | ARG  |
| 24  | D     | 26  | THR  |
| 24  | D     | 218 | THR  |
| 24  | D     | 274 | LYS  |
| 26  | F     | 117 | LYS  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | F     | 121 | ASN  |
| 26  | F     | 184 | LEU  |
| 26  | F     | 188 | ASN  |
| 26  | F     | 190 | ASP  |
| 27  | G     | 51  | ASP  |
| 28  | Н     | 43  | PHE  |
| 28  | Н     | 56  | SER  |
| 28  | Н     | 61  | ASP  |
| 28  | Н     | 69  | ARG  |
| 31  | 0     | 7   | LYS  |
| 31  | 0     | 19  | VAL  |
| 31  | 0     | 129 | SER  |
| 31  | 0     | 134 | GLU  |
| 31  | 0     | 139 | LYS  |
| 32  | Р     | 14  | ARG  |
| 32  | Р     | 27  | VAL  |
| 33  | Q     | 11  | ASP  |
| 36  | Т     | 27  | SER  |
| 40  | Х     | 72  | ASP  |
| 41  | Y     | 57  | ARG  |
| 45  | 2     | 54  | VAL  |
| 46  | 3     | 49  | ASP  |
| 46  | 3     | 70  | ARG  |
| 47  | 4     | 42  | ARG  |
| 48  | 5     | 38  | ARG  |
| 50  | 7     | 31  | HIS  |
| 50  | 7     | 32  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | b     | 15  | HIS  |
| 2   | b     | 55  | ASN  |
| 2   | b     | 159 | GLN  |
| 3   | с     | 6   | ASN  |
| 3   | с     | 64  | ASN  |
| 3   | с     | 68  | HIS  |
| 3   | с     | 91  | ASN  |
| 3   | с     | 133 | GLN  |
| 4   | d     | 8   | ASN  |
| 4   | d     | 67  | GLN  |
| 4   | d     | 137 | GLN  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | d     | 192 | GLN  |
| 5   | е     | 145 | GLN  |
| 5   | е     | 166 | ASN  |
| 7   | g     | 28  | ASN  |
| 7   | g     | 122 | ASN  |
| 9   | i     | 33  | ASN  |
| 12  | 1     | 25  | ASN  |
| 12  | 1     | 73  | ASN  |
| 13  | m     | 74  | ASN  |
| 15  | 0     | 37  | ASN  |
| 15  | 0     | 42  | HIS  |
| 15  | 0     | 65  | HIS  |
| 15  | 0     | 68  | ASN  |
| 17  | q     | 49  | HIS  |
| 17  | q     | 52  | ASN  |
| 17  | q     | 64  | GLN  |
| 18  | r     | 57  | GLN  |
| 20  | t     | 67  | HIS  |
| 24  | D     | 225 | ASN  |
| 24  | D     | 229 | HIS  |
| 24  | D     | 231 | HIS  |
| 25  | Е     | 33  | ASN  |
| 25  | Е     | 143 | HIS  |
| 26  | F     | 3   | ASN  |
| 26  | F     | 141 | ASN  |
| 26  | F     | 158 | ASN  |
| 28  | Н     | 48  | ASN  |
| 28  | Н     | 65  | HIS  |
| 29  | М     | 3   | GLN  |
| 29  | М     | 11  | ASN  |
| 29  | М     | 81  | HIS  |
| 31  | 0     | 38  | GLN  |
| 31  | 0     | 78  | ASN  |
| 31  | 0     | 126 | HIS  |
| 32  | Р     | 25  | ASN  |
| 32  | Р     | 35  | GLN  |
| 33  | Q     | 106 | GLN  |
| 34  | R     | 8   | ASN  |
| 35  | S     | 4   | HIS  |
| 35  | S     | 79  | HIS  |
| 37  | U     | 18  | GLN  |
| 39  | W     | 37  | GLN  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | Х     | 69  | GLN  |
| 41  | Y     | 20  | GLN  |
| 42  | Ζ     | 58  | ASN  |
| 43  | 0     | 34  | GLN  |
| 46  | 3     | 55  | HIS  |
| 46  | 3     | 75  | ASN  |
| 46  | 3     | 83  | ASN  |
| 48  | 5     | 22  | ASN  |
| 48  | 5     | 25  | ASN  |
| 48  | 5     | 26  | ASN  |
| 49  | 6     | 7   | GLN  |
| 49  | 6     | 17  | HIS  |
| 50  | 7     | 31  | HIS  |
| 50  | 7     | 40  | GLN  |
| 50  | 7     | 60  | GLN  |

## 5.3.3 RNA (i)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | a     | 1541/1556~(99%) | 310 (20%)         | 0               |
| 21  | V     | 20/29~(68%)     | 8 (40%)           | 0               |
| 22  | А     | 2870/2923~(98%) | 584 (20%)         | 8~(0%)          |
| 23  | В     | 114/115~(99%)   | 17 (14%)          | 1 (0%)          |
| 52  | Х     | 75/77~(97%)     | 21 (28%)          | 0               |
| All | All   | 4620/4700 (98%) | 940 (20%)         | 9~(0%)          |

All (940) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 7   | G    |
| 1   | a     | 8   | G    |
| 1   | a     | 10  | G    |
| 1   | a     | 11  | А    |
| 1   | a     | 31  | U    |
| 1   | a     | 33  | А    |
| 1   | a     | 40  | G    |
| 1   | a     | 45  | G    |
| 1   | a     | 48  | С    |
| 1   | a     | 49  | С    |
| 1   | a     | 50  | U    |
| 1   | a     | 51  | А    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 52  | А    |
| 1   | a     | 55  | С    |
| 1   | a     | 64  | С    |
| 1   | a     | 65  | G    |
| 1   | a     | 78  | А    |
| 1   | a     | 80  | А    |
| 1   | a     | 83  | С    |
| 1   | a     | 84  | U    |
| 1   | a     | 85  | U    |
| 1   | a     | 86  | G    |
| 1   | a     | 88  | U    |
| 1   | a     | 89  | U    |
| 1   | a     | 91  | U    |
| 1   | a     | 93  | U    |
| 1   | a     | 94  | G    |
| 1   | a     | 108 | A    |
| 1   | a     | 115 | А    |
| 1   | a     | 120 | С    |
| 1   | a     | 126 | G    |
| 1   | a     | 128 | U    |
| 1   | a     | 129 | А    |
| 1   | a     | 130 | А    |
| 1   | a     | 132 | С    |
| 1   | a     | 138 | А    |
| 1   | a     | 152 | А    |
| 1   | a     | 156 | С    |
| 1   | a     | 159 | G    |
| 1   | a     | 162 | А    |
| 1   | a     | 173 | U    |
| 1   | a     | 177 | G    |
| 1   | a     | 182 | А    |
| 1   | a     | 183 | U    |
| 1   | a     | 184 | А    |
| 1   | a     | 185 | U    |
| 1   | a     | 192 | С    |
| 1   | a     | 195 | С    |
| 1   | a     | 201 | U    |
| 1   | a     | 203 | А    |
| 1   | a     | 204 | A    |
| 1   | a     | 207 | G    |
| 1   | a     | 211 | А    |
| 1   | a     | 212 | А    |



| Mol | Chain | Res              | Type |
|-----|-------|------------------|------|
| 1   | a     | 213              | G    |
| 1   | a     | 216              | G    |
| 1   | a     | 218              | U    |
| 1   | a     | 220              | U    |
| 1   | a     | 221              | U    |
| 1   | a     | 222              | G    |
| 1   | a     | 249              | G    |
| 1   | a     | 253              | U    |
| 1   | a     | 255              | G    |
| 1   | a     | 258              | А    |
| 1   | a     | 259              | G    |
| 1   | a     | 261              | U    |
| 1   | a     | 274              | G    |
| 1   | a     | 275              | С    |
| 1   | a     | 287              | А    |
| 1   | a     | 297              | G    |
| 1   | a     | 310              | G    |
| 1   | a     | 316              | С    |
| 1   | a     | 329              | А    |
| 1   | a     | 336              | С    |
| 1   | a     | 338              | С    |
| 1   | a     | 353              | С    |
| 1   | a     | 355              | G    |
| 1   | a     | 360              | С    |
| 1   | a     | 362              | G    |
| 1   | a     | 375              | U    |
| 1   | a     | 380              | С    |
| 1   | a     | 382              | A    |
| 1   | a     | 392              | G    |
| 1   | a     | 396              | G    |
| 1   | a     | 405              | A    |
| 1   | a     | 406              | C    |
| 1   | a     | 414              | G    |
| 1   | a     | 419              | A    |
| 1   | a     | 420              | U    |
| 1   | a     | 421              | G    |
| 1   | a     | 429              | U    |
| 1   | a     | 432              | G    |
| 1   | a     | 437              | U    |
| 1   | a     | 451              | U    |
| 1   | a     | $45\overline{4}$ | G    |
| 1   | a     | 456              | A    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 462 | А    |
| 1   | a     | 465 | U    |
| 1   | a     | 466 | G    |
| 1   | a     | 467 | U    |
| 1   | a     | 468 | G    |
| 1   | a     | 469 | U    |
| 1   | a     | 472 | G    |
| 1   | a     | 476 | С    |
| 1   | a     | 477 | U    |
| 1   | a     | 480 | G    |
| 1   | a     | 481 | С    |
| 1   | a     | 482 | А    |
| 1   | a     | 483 | С    |
| 1   | a     | 485 | U    |
| 1   | a     | 486 | С    |
| 1   | a     | 493 | G    |
| 1   | a     | 503 | А    |
| 1   | a     | 505 | А    |
| 1   | a     | 517 | A    |
| 1   | a     | 519 | С    |
| 1   | a     | 526 | С    |
| 1   | a     | 527 | С    |
| 1   | a     | 532 | G    |
| 1   | a     | 535 | 7MG  |
| 1   | a     | 536 | С    |
| 1   | a     | 539 | U    |
| 1   | a     | 540 | А    |
| 1   | a     | 546 | U    |
| 1   | a     | 555 | A    |
| 1   | a     | 557 | С    |
| 1   | a     | 567 | A    |
| 1   | a     | 572 | U    |
| 1   | a     | 580 | A    |
| 1   | a     | 581 | A    |
| 1   | a     | 584 | С    |
| 1   | a     | 585 | G    |
| 1   | a     | 595 | G    |
| 1   | a     | 604 | A    |
| 1   | a     | 609 | G    |
| 1   | a     | 626 | С    |
| 1   | a     | 635 | G    |
| 1   | a     | 641 | U    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 646 | G    |
| 1   | a     | 649 | А    |
| 1   | a     | 650 | А    |
| 1   | a     | 659 | С    |
| 1   | a     | 660 | U    |
| 1   | a     | 661 | U    |
| 1   | a     | 662 | G    |
| 1   | a     | 673 | А    |
| 1   | a     | 681 | G    |
| 1   | a     | 693 | G    |
| 1   | a     | 695 | А    |
| 1   | a     | 711 | G    |
| 1   | a     | 715 | U    |
| 1   | a     | 729 | А    |
| 1   | a     | 741 | G    |
| 1   | a     | 742 | А    |
| 1   | a     | 756 | А    |
| 1   | a     | 763 | G    |
| 1   | a     | 769 | G    |
| 1   | a     | 785 | А    |
| 1   | a     | 795 | А    |
| 1   | a     | 801 | U    |
| 1   | a     | 802 | А    |
| 1   | a     | 803 | С    |
| 1   | a     | 807 | G    |
| 1   | a     | 817 | G    |
| 1   | a     | 820 | G    |
| 1   | a     | 823 | А    |
| 1   | a     | 825 | С    |
| 1   | a     | 829 | G    |
| 1   | a     | 836 | A    |
| 1   | a     | 840 | G    |
| 1   | a     | 851 | U    |
| 1   | a     | 852 | C    |
| 1   | a     | 854 | G    |
| 1   | a     | 855 | C    |
| 1   | a     | 862 | G    |
| 1   | a     | 864 | G    |
| 1   | a     | 881 | A    |
| 1   | a     | 911 | G    |
| 1   | a     | 925 | G    |
| 1   | a     | 931 | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 935  | G    |
| 1   | a     | 943  | С    |
| 1   | a     | 944  | А    |
| 1   | a     | 969  | U    |
| 1   | a     | 974  | А    |
| 1   | a     | 977  | А    |
| 1   | a     | 978  | А    |
| 1   | a     | 980  | G    |
| 1   | a     | 984  | А    |
| 1   | a     | 985  | G    |
| 1   | a     | 992  | А    |
| 1   | a     | 1000 | U    |
| 1   | a     | 1001 | U    |
| 1   | a     | 1002 | G    |
| 1   | a     | 1011 | U    |
| 1   | a     | 1013 | А    |
| 1   | a     | 1015 | А    |
| 1   | a     | 1016 | А    |
| 1   | a     | 1019 | С    |
| 1   | a     | 1024 | G    |
| 1   | a     | 1027 | А    |
| 1   | a     | 1029 | А    |
| 1   | a     | 1034 | U    |
| 1   | a     | 1035 | С    |
| 1   | a     | 1036 | С    |
| 1   | a     | 1038 | С    |
| 1   | a     | 1039 | U    |
| 1   | a     | 1040 | U    |
| 1   | a     | 1042 | G    |
| 1   | a     | 1043 | G    |
| 1   | a     | 1044 | G    |
| 1   | a     | 1046 | G    |
| 1   | a     | 1047 | А    |
| 1   | a     | 1055 | A    |
| 1   | a     | 1056 | С    |
| 1   | a     | 1057 | A    |
| 1   | a     | 1064 | G    |
| 1   | a     | 1075 | G    |
| 1   | a     | 1076 | U    |
| 1   | a     | 1097 | U    |
| 1   | a     | 1105 | G    |
| 1   | a     | 1106 | U    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 1112 | А    |
| 1   | a     | 1119 | G    |
| 1   | a     | 1121 | А    |
| 1   | a     | 1135 | G    |
| 1   | a     | 1136 | U    |
| 1   | a     | 1137 | U    |
| 1   | a     | 1138 | G    |
| 1   | a     | 1141 | А    |
| 1   | a     | 1149 | G    |
| 1   | a     | 1150 | U    |
| 1   | a     | 1151 | U    |
| 1   | a     | 1152 | G    |
| 1   | a     | 1155 | С    |
| 1   | a     | 1161 | A    |
| 1   | a     | 1168 | С    |
| 1   | a     | 1169 | U    |
| 1   | a     | 1170 | G    |
| 1   | a     | 1177 | А    |
| 1   | a     | 1178 | С    |
| 1   | a     | 1181 | А    |
| 1   | a     | 1184 | G    |
| 1   | a     | 1193 | U    |
| 1   | a     | 1194 | G    |
| 1   | a     | 1206 | А    |
| 1   | a     | 1207 | А    |
| 1   | a     | 1211 | А    |
| 1   | a     | 1222 | U    |
| 1   | a     | 1224 | U    |
| 1   | a     | 1237 | А    |
| 1   | a     | 1243 | G    |
| 1   | a     | 1248 | A    |
| 1   | a     | 1266 | С    |
| 1   | a     | 1267 | A    |
| 1   | a     | 1270 | G    |
| 1   | a     | 1284 | A    |
| 1   | a     | 1290 | A    |
| 1   | a     | 1295 | A    |
| 1   | a     | 1297 | A    |
| 1   | a     | 1298 | A    |
| 1   | a     | 1300 | G    |
| 1   | a     | 1309 | A    |
| 1   | a     | 1310 | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 1314 | G    |
| 1   | a     | 1315 | G    |
| 1   | a     | 1330 | С    |
| 1   | a     | 1332 | С    |
| 1   | a     | 1337 | А    |
| 1   | a     | 1341 | G    |
| 1   | a     | 1346 | U    |
| 1   | a     | 1348 | G    |
| 1   | a     | 1350 | А    |
| 1   | a     | 1355 | U    |
| 1   | a     | 1356 | А    |
| 1   | a     | 1363 | G    |
| 1   | a     | 1374 | U    |
| 1   | a     | 1378 | A    |
| 1   | a     | 1380 | G    |
| 1   | a     | 1388 | С    |
| 1   | a     | 1390 | U    |
| 1   | a     | 1391 | U    |
| 1   | a     | 1392 | С    |
| 1   | a     | 1393 | С    |
| 1   | a     | 1404 | А    |
| 1   | a     | 1408 | А    |
| 1   | a     | 1435 | А    |
| 1   | a     | 1436 | А    |
| 1   | a     | 1441 | С    |
| 1   | a     | 1452 | G    |
| 1   | a     | 1456 | А    |
| 1   | a     | 1457 | А    |
| 1   | a     | 1459 | С    |
| 1   | a     | 1460 | U    |
| 1   | a     | 1461 | U    |
| 1   | a     | 1463 | U    |
| 1   | a     | 1464 | A    |
| 1   | a     | 1498 | G    |
| 1   | a     | 1504 | A    |
| 1   | a     | 1505 | G    |
| 1   | a     | 1508 | G    |
| 1   | a     | 1510 | A    |
| 1   | a     | 1513 | A    |
| 1   | a     | 1514 | A    |
| 1   | a     | 1517 | U    |
| 1   | a     | 1528 | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 1540 | G    |
| 1   | a     | 1541 | G    |
| 1   | a     | 1544 | С    |
| 1   | a     | 1545 | А    |
| 21  | V     | 12   | А    |
| 21  | V     | 13   | А    |
| 21  | V     | 14   | А    |
| 21  | V     | 15   | А    |
| 21  | V     | 19   | G    |
| 21  | V     | 23   | А    |
| 21  | V     | 24   | А    |
| 21  | V     | 25   | А    |
| 22  | А     | 13   | А    |
| 22  | А     | 23   | G    |
| 22  | А     | 24   | G    |
| 22  | А     | 34   | U    |
| 22  | А     | 37   | С    |
| 22  | А     | 43   | А    |
| 22  | А     | 64   | А    |
| 22  | А     | 71   | А    |
| 22  | А     | 74   | U    |
| 22  | А     | 75   | G    |
| 22  | А     | 89   | U    |
| 22  | А     | 90   | А    |
| 22  | А     | 95   | А    |
| 22  | А     | 96   | G    |
| 22  | А     | 100  | U    |
| 22  | А     | 101  | G    |
| 22  | А     | 117  | А    |
| 22  | А     | 118  | A    |
| 22  | A     | 119  | U    |
| 22  | A     | 120  | G    |
| 22  | А     | 124  | A    |
| 22  | A     | 129  | С    |
| 22  | А     | 130  | А    |
| 22  | A     | 150  | A    |
| 22  | A     | 154  | A    |
| 22  | A     | 161  | A    |
| 22  | A     | 162  | A    |
| 22  | A     | 164  | A    |
| 22  | A     | 165  | С    |
| 22  | A     | 167  | U    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | А     | 168 | А    |
| 22  | А     | 169 | G    |
| 22  | А     | 173 | А    |
| 22  | А     | 176 | A    |
| 22  | А     | 177 | G    |
| 22  | А     | 185 | A    |
| 22  | А     | 199 | A    |
| 22  | А     | 200 | A    |
| 22  | А     | 202 | A    |
| 22  | А     | 218 | G    |
| 22  | А     | 219 | A    |
| 22  | А     | 225 | А    |
| 22  | А     | 227 | G    |
| 22  | A     | 231 | A    |
| 22  | А     | 233 | U    |
| 22  | А     | 236 | A    |
| 22  | А     | 251 | G    |
| 22  | А     | 255 | G    |
| 22  | А     | 268 | A    |
| 22  | А     | 280 | С    |
| 22  | А     | 282 | А    |
| 22  | А     | 290 | U    |
| 22  | А     | 294 | G    |
| 22  | А     | 298 | U    |
| 22  | А     | 300 | G    |
| 22  | А     | 301 | U    |
| 22  | А     | 302 | A    |
| 22  | А     | 308 | С    |
| 22  | А     | 321 | U    |
| 22  | A     | 324 | A    |
| 22  | A     | 327 | G    |
| 22  | A     | 328 | G    |
| 22  | A     | 329 | A    |
| 22  | A     | 338 | G    |
| 22  | A     | 354 | A    |
| 22  | A     | 365 | A    |
| 22  | A     | 372 | A    |
| 22  | A     | 373 | A    |
| 22  | A     | 374 | U    |
| 22  | A     | 377 | U    |
| 22  | A     | 386 | С    |
| 22  | А     | 388 | А    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | А     | 398 | C    |
| 22  | А     | 401 | U    |
| 22  | А     | 404 | U    |
| 22  | А     | 432 | G    |
| 22  | А     | 435 | А    |
| 22  | А     | 451 | U    |
| 22  | А     | 457 | G    |
| 22  | А     | 458 | А    |
| 22  | А     | 466 | С    |
| 22  | А     | 471 | G    |
| 22  | А     | 481 | С    |
| 22  | А     | 482 | U    |
| 22  | А     | 502 | С    |
| 22  | A     | 510 | U    |
| 22  | А     | 513 | G    |
| 22  | А     | 523 | A    |
| 22  | А     | 527 | G    |
| 22  | А     | 539 | G    |
| 22  | А     | 550 | А    |
| 22  | А     | 553 | A    |
| 22  | А     | 554 | С    |
| 22  | А     | 567 | G    |
| 22  | А     | 572 | С    |
| 22  | А     | 575 | G    |
| 22  | А     | 576 | U    |
| 22  | А     | 577 | A    |
| 22  | А     | 578 | G    |
| 22  | А     | 583 | A    |
| 22  | А     | 592 | A    |
| 22  | A     | 593 | U    |
| 22  | A     | 594 | G    |
| 22  | A     | 606 | G    |
| 22  | А     | 611 | U    |
| 22  | A     | 616 | G    |
| 22  | А     | 618 | A    |
| 22  | A     | 630 | G    |
| 22  | А     | 646 | A    |
| 22  | А     | 659 | A    |
| 22  | A     | 661 | U    |
| 22  | A     | 662 | G    |
| 22  | A     | 666 | A    |
| 22  | A     | 667 | G    |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | А     | 679 | G    |
| 22  | А     | 682 | А    |
| 22  | А     | 683 | G    |
| 22  | А     | 690 | U    |
| 22  | А     | 698 | U    |
| 22  | А     | 699 | U    |
| 22  | А     | 700 | A    |
| 22  | А     | 715 | A    |
| 22  | А     | 731 | U    |
| 22  | А     | 745 | G    |
| 22  | А     | 773 | G    |
| 22  | А     | 774 | G    |
| 22  | А     | 775 | A    |
| 22  | А     | 781 | С    |
| 22  | А     | 783 | G    |
| 22  | А     | 792 | U    |
| 22  | А     | 807 | U    |
| 22  | А     | 809 | A    |
| 22  | А     | 810 | A    |
| 22  | А     | 813 | G    |
| 22  | А     | 820 | G    |
| 22  | А     | 822 | G    |
| 22  | А     | 824 | A    |
| 22  | А     | 827 | A    |
| 22  | А     | 829 | U    |
| 22  | А     | 830 | U    |
| 22  | А     | 834 | A    |
| 22  | А     | 837 | G    |
| 22  | А     | 839 | A    |
| 22  | А     | 847 | A    |
| 22  | А     | 850 | G    |
| 22  | A     | 851 | C    |
| 22  | A     | 857 | С    |
| 22  | A     | 872 | U    |
| 22  | A     | 873 | U    |
| 22  | A     | 888 | G    |
| 22  | A     | 891 | A    |
| 22  | A     | 904 | G    |
| 22  | A     | 910 | C    |
| 22  | A     | 911 | A    |
| 22  | A     | 919 | G    |
| 22  | А     | 923 | A    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | А     | 926  | G    |
| 22  | А     | 929  | С    |
| 22  | А     | 930  | С    |
| 22  | А     | 931  | С    |
| 22  | А     | 932  | U    |
| 22  | А     | 936  | G    |
| 22  | А     | 938  | G    |
| 22  | А     | 955  | А    |
| 22  | А     | 959  | С    |
| 22  | А     | 960  | С    |
| 22  | А     | 971  | U    |
| 22  | А     | 972  | A    |
| 22  | А     | 985  | А    |
| 22  | А     | 989  | A    |
| 22  | А     | 990  | G    |
| 22  | А     | 1001 | А    |
| 22  | А     | 1005 | G    |
| 22  | А     | 1018 | А    |
| 22  | А     | 1023 | А    |
| 22  | А     | 1026 | С    |
| 22  | А     | 1027 | А    |
| 22  | А     | 1033 | G    |
| 22  | А     | 1039 | С    |
| 22  | А     | 1040 | А    |
| 22  | А     | 1053 | А    |
| 22  | А     | 1055 | А    |
| 22  | А     | 1056 | U    |
| 22  | А     | 1057 | А    |
| 22  | А     | 1060 | U    |
| 22  | А     | 1061 | G    |
| 22  | A     | 1069 | G    |
| 22  | А     | 1070 | А    |
| 22  | A     | 1071 | A    |
| 22  | А     | 1077 | U    |
| 22  | A     | 1090 | A    |
| 22  | A     | 1091 | G    |
| 22  | А     | 1096 | С    |
| 22  | A     | 1102 | U    |
| 22  | A     | 1105 | U    |
| 22  | A     | 1106 | G    |
| 22  | А     | 1108 | С    |
| 22  | А     | 1109 | U    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | А     | 1110 | U    |
| 22  | А     | 1111 | А    |
| 22  | А     | 1113 | А    |
| 22  | А     | 1114 | А    |
| 22  | А     | 1115 | G    |
| 22  | А     | 1116 | С    |
| 22  | А     | 1117 | А    |
| 22  | А     | 1120 | С    |
| 22  | А     | 1122 | U    |
| 22  | А     | 1124 | А    |
| 22  | А     | 1127 | U    |
| 22  | А     | 1128 | А    |
| 22  | А     | 1129 | А    |
| 22  | А     | 1131 | G    |
| 22  | А     | 1132 | А    |
| 22  | А     | 1133 | G    |
| 22  | А     | 1137 | G    |
| 22  | А     | 1138 | U    |
| 22  | А     | 1139 | А    |
| 22  | А     | 1140 | А    |
| 22  | А     | 1143 | G    |
| 22  | А     | 1145 | U    |
| 22  | А     | 1146 | С    |
| 22  | А     | 1147 | А    |
| 22  | А     | 1151 | G    |
| 22  | А     | 1152 | U    |
| 22  | А     | 1153 | С    |
| 22  | А     | 1154 | G    |
| 22  | А     | 1155 | А    |
| 22  | А     | 1156 | G    |
| 22  | А     | 1171 | А    |
| 22  | A     | 1172 | A    |
| 22  | А     | 1174 | U    |
| 22  | A     | 1176 | U    |
| 22  | А     | 1177 | А    |
| 22  | A     | 1178 | С    |
| 22  | А     | 1179 | С    |
| 22  | A     | 1186 | A    |
| 22  | А     | 1201 | G    |
| 22  | A     | 1211 | G    |
| 22  | А     | 1215 | U    |
| 22  | А     | 1220 | A    |



| Mol | Chain | Res               | Type |
|-----|-------|-------------------|------|
| 22  | А     | 1250              | G    |
| 22  | А     | 1258              | А    |
| 22  | А     | 1276              | G    |
| 22  | А     | 1278              | G    |
| 22  | А     | 1288              | G    |
| 22  | А     | 1294              | G    |
| 22  | А     | 1295              | С    |
| 22  | А     | 1306              | А    |
| 22  | А     | 1309              | G    |
| 22  | А     | 1310              | А    |
| 22  | А     | 1323              | А    |
| 22  | А     | 1326              | С    |
| 22  | А     | 1337              | А    |
| 22  | А     | 1338              | U    |
| 22  | А     | 1339              | U    |
| 22  | А     | 1349              | U    |
| 22  | А     | 1350              | U    |
| 22  | А     | 1358              | А    |
| 22  | А     | 1375              | G    |
| 22  | А     | 1377              | U    |
| 22  | А     | 1378              | U    |
| 22  | А     | 1387              | С    |
| 22  | А     | 1389              | U    |
| 22  | А     | 1402              | А    |
| 22  | А     | 1405              | G    |
| 22  | А     | 1416              | U    |
| 22  | А     | 1421              | А    |
| 22  | А     | 1432              | А    |
| 22  | А     | 1435              | С    |
| 22  | А     | 1436              | С    |
| 22  | A     | 1437              | U    |
| 22  | А     | 1450              | А    |
| 22  | A     | 1463              | A    |
| 22  | А     | 1464              | U    |
| 22  | A     | 1465              | G    |
| 22  | A     | 1471              | A    |
| 22  | A     | 1472              | С    |
| 22  | A     | $1\overline{473}$ | G    |
| 22  | A     | 1489              | A    |
| 22  | A     | 1490              | G    |
| 22  | A     | 1491              | C    |
| 22  | A     | 1492              | G    |



| Mol | Chain | Res  | Type |  |
|-----|-------|------|------|--|
| 22  | А     | 1494 | G    |  |
| 22  | А     | 1495 | С    |  |
| 22  | А     | 1496 | G    |  |
| 22  | А     | 1499 | U    |  |
| 22  | А     | 1502 | А    |  |
| 22  | А     | 1503 | U    |  |
| 22  | А     | 1504 | U    |  |
| 22  | А     | 1505 | G    |  |
| 22  | А     | 1506 | С    |  |
| 22  | А     | 1510 | U    |  |
| 22  | А     | 1516 | С    |  |
| 22  | А     | 1517 | A    |  |
| 22  | А     | 1519 | U    |  |
| 22  | А     | 1525 | U    |  |
| 22  | А     | 1533 | A    |  |
| 22  | А     | 1536 | С    |  |
| 22  | А     | 1537 | А    |  |
| 22  | А     | 1540 | U    |  |
| 22  | А     | 1541 | С    |  |
| 22  | А     | 1550 | G    |  |
| 22  | А     | 1551 | U    |  |
| 22  | А     | 1552 | U    |  |
| 22  | А     | 1553 | А    |  |
| 22  | А     | 1555 | G    |  |
| 22  | А     | 1559 | G    |  |
| 22  | А     | 1561 | G    |  |
| 22  | А     | 1570 | G    |  |
| 22  | А     | 1575 | A    |  |
| 22  | А     | 1576 | А    |  |
| 22  | А     | 1577 | G    |  |
| 22  | A     | 1590 | С    |  |
| 22  | А     | 1592 | A    |  |
| 22  | A     | 1600 | A    |  |
| 22  | А     | 1601 | U    |  |
| 22  | A     | 1605 | A    |  |
| 22  | A     | 1606 | C    |  |
| 22  | А     | 1613 | G    |  |
| 22  | A     | 1614 | A    |  |
| 22  | А     | 1616 | А    |  |
| 22  | A     | 1625 | U    |  |
| 22  | А     | 1630 | А    |  |
| 22  | А     | 1632 | A    |  |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | А     | 1634 | А    |
| 22  | А     | 1635 | А    |
| 22  | А     | 1636 | U    |
| 22  | А     | 1639 | G    |
| 22  | А     | 1651 | С    |
| 22  | А     | 1652 | А    |
| 22  | А     | 1662 | А    |
| 22  | А     | 1683 | U    |
| 22  | А     | 1686 | G    |
| 22  | А     | 1690 | А    |
| 22  | А     | 1691 | G    |
| 22  | А     | 1692 | С    |
| 22  | А     | 1696 | С    |
| 22  | A     | 1718 | G    |
| 22  | А     | 1719 | С    |
| 22  | А     | 1737 | U    |
| 22  | А     | 1738 | С    |
| 22  | А     | 1740 | G    |
| 22  | А     | 1756 | U    |
| 22  | А     | 1757 | U    |
| 22  | А     | 1759 | G    |
| 22  | А     | 1764 | А    |
| 22  | А     | 1768 | С    |
| 22  | А     | 1772 | G    |
| 22  | А     | 1777 | G    |
| 22  | А     | 1785 | G    |
| 22  | А     | 1790 | G    |
| 22  | А     | 1791 | G    |
| 22  | А     | 1800 | А    |
| 22  | А     | 1803 | G    |
| 22  | A     | 1808 | U    |
| 22  | A     | 1811 | А    |
| 22  | A     | 1813 | А    |
| 22  | A     | 1815 | C    |
| 22  | A     | 1819 | G    |
| 22  | A     | 1826 | G    |
| 22  | A     | 1827 | С    |
| 22  | A     | 1828 | U    |
| 22  | A     | 1837 | A    |
| 22  | A     | 1839 | G    |
| 22  | A     | 1843 | U    |
| 22  | А     | 1844 | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | А     | 1847 | U    |
| 22  | А     | 1856 | A    |
| 22  | А     | 1893 | A    |
| 22  | А     | 1895 | С    |
| 22  | А     | 1896 | U    |
| 22  | А     | 1897 | U    |
| 22  | А     | 1899 | U    |
| 22  | А     | 1900 | G    |
| 22  | А     | 1902 | G    |
| 22  | А     | 1909 | С    |
| 22  | А     | 1930 | G    |
| 22  | А     | 1933 | G    |
| 22  | А     | 1937 | G    |
| 22  | А     | 1939 | A    |
| 22  | А     | 1940 | А    |
| 22  | А     | 1941 | С    |
| 22  | А     | 1943 | А    |
| 22  | А     | 1947 | OMC  |
| 22  | А     | 1956 | G    |
| 22  | А     | 1957 | G    |
| 22  | А     | 1963 | A    |
| 22  | А     | 1964 | A    |
| 22  | А     | 1965 | A    |
| 22  | А     | 1966 | 5MU  |
| 22  | А     | 1967 | U    |
| 22  | А     | 1975 | G    |
| 22  | А     | 1982 | U    |
| 22  | А     | 1990 | С    |
| 22  | A     | 1991 | G    |
| 22  | A     | 1993 | A    |
| 22  | A     | 1994 | C    |
| 22  | A     | 1997 | A    |
| 22  | А     | 1998 | A    |
| 22  | A     | 1999 | G    |
| 22  | A     | 2009 | U    |
| 22  | A     | 2018 | U    |
| 22  | A     | 2020 | U    |
| 22  | A     | 2033 | C    |
| 22  | A     | 2050 | A    |
| 22  | A     | 2058 | A    |
| 22  | A     | 2059 | G    |
| 22  | А     | 2060 | A    |



| Mol | Chain | Res               | Type |
|-----|-------|-------------------|------|
| 22  | А     | 2063              | С    |
| 22  | А     | 2070              | С    |
| 22  | А     | 2082              | С    |
| 22  | А     | 2083              | G    |
| 22  | А     | 2087              | А    |
| 22  | А     | 2088              | G    |
| 22  | А     | 2089              | А    |
| 22  | А     | 2094              | G    |
| 22  | А     | 2096              | G    |
| 22  | А     | 2097              | G    |
| 22  | А     | 2114              | G    |
| 22  | А     | 2120              | G    |
| 22  | А     | 2128              | G    |
| 22  | А     | 2132              | A    |
| 22  | А     | 2135              | U    |
| 22  | А     | 2136              | U    |
| 22  | А     | 2137              | G    |
| 22  | А     | 2138              | U    |
| 22  | А     | 2139              | А    |
| 22  | А     | 2140              | С    |
| 22  | А     | 2142              | G    |
| 22  | А     | 2143              | G    |
| 22  | А     | 2144              | А    |
| 22  | А     | 2145              | U    |
| 22  | А     | 2146              | А    |
| 22  | А     | 2147              | G    |
| 22  | А     | 2150              | А    |
| 22  | А     | 2153              | А    |
| 22  | А     | 2157              | U    |
| 22  | А     | 2158              | U    |
| 22  | А     | 2160              | G    |
| 22  | А     | 2161              | А    |
| 22  | A     | 2162              | A    |
| 22  | А     | 2164              | С    |
| 22  | A     | 2165              | G    |
| 22  | A     | 2166              | U    |
| 22  | A     | 2168              | А    |
| 22  | A     | 2169              | G    |
| 22  | A     | 2172              | С    |
| 22  | A     | $2\overline{173}$ | U    |
| 22  | A     | $2\overline{174}$ | A    |
| 22  | А     | 2175              | G    |



| Mol | Chain | Res               | Type |
|-----|-------|-------------------|------|
| 22  | А     | 2176              | С    |
| 22  | А     | 2179              | А    |
| 22  | А     | 2183              | G    |
| 22  | А     | 2184              | G    |
| 22  | А     | 2185              | А    |
| 22  | А     | 2186              | G    |
| 22  | А     | 2188              | С    |
| 22  | А     | 2190              | С    |
| 22  | А     | 2191              | U    |
| 22  | А     | 2194              | U    |
| 22  | А     | 2195              | G    |
| 22  | А     | 2196              | G    |
| 22  | А     | 2198              | А    |
| 22  | А     | 2200              | A    |
| 22  | А     | 2201              | С    |
| 22  | А     | 2205              | С    |
| 22  | А     | 2208              | А    |
| 22  | А     | 2211              | U    |
| 22  | А     | 2214              | G    |
| 22  | А     | 2215              | U    |
| 22  | А     | 2217              | G    |
| 22  | А     | 2220              | U    |
| 22  | А     | 2225              | А    |
| 22  | А     | 2230              | G    |
| 22  | А     | 2231              | С    |
| 22  | А     | 2240              | U    |
| 22  | А     | 2241              | С    |
| 22  | А     | 2252              | А    |
| 22  | А     | 2253              | С    |
| 22  | А     | 2265              | G    |
| 22  | А     | 2266              | G    |
| 22  | А     | 2296              | А    |
| 22  | A     | 2305              | A    |
| 22  | A     | 2309              | G    |
| 22  | A     | $2\overline{310}$ | С    |
| 22  | A     | 2314              | A    |
| 22  | А     | 2321              | С    |
| 22  | A     | $2\overline{332}$ | U    |
| 22  | A     | 2335              | G    |
| 22  | A     | 2347              | А    |
| 22  | A     | 2349              | A    |
| 22  | А     | 2352              | G    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | А     | 2353 | U    |
| 22  | А     | 2361 | U    |
| 22  | А     | 2362 | А    |
| 22  | А     | 2363 | А    |
| 22  | А     | 2374 | С    |
| 22  | А     | 2377 | С    |
| 22  | А     | 2386 | С    |
| 22  | А     | 2404 | A    |
| 22  | А     | 2406 | G    |
| 22  | А     | 2410 | G    |
| 22  | А     | 2412 | С    |
| 22  | А     | 2418 | G    |
| 22  | А     | 2429 | U    |
| 22  | А     | 2433 | С    |
| 22  | А     | 2446 | U    |
| 22  | А     | 2450 | U    |
| 22  | А     | 2452 | А    |
| 22  | А     | 2456 | G    |
| 22  | А     | 2457 | А    |
| 22  | А     | 2467 | С    |
| 22  | А     | 2468 | С    |
| 22  | А     | 2472 | 2MG  |
| 22  | А     | 2475 | А    |
| 22  | А     | 2486 | А    |
| 22  | А     | 2501 | U    |
| 22  | А     | 2502 | С    |
| 22  | А     | 2505 | А    |
| 22  | А     | 2518 | U    |
| 22  | А     | 2525 | OMC  |
| 22  | А     | 2528 | С    |
| 22  | А     | 2529 | G    |
| 22  | А     | 2531 | U    |
| 22  | А     | 2532 | G    |
| 22  | А     | 2533 | U    |
| 22  | А     | 2541 | U    |
| 22  | А     | 2545 | A    |
| 22  | А     | 2547 | С    |
| 22  | А     | 2556 | G    |
| 22  | А     | 2562 | G    |
| 22  | А     | 2565 | С    |
| 22  | А     | 2569 | A    |
| 22  | А     | 2593 | A    |



| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | А     | 2594 | G    |
| 22  | А     | 2600 | С    |
| 22  | А     | 2609 | G    |
| 22  | А     | 2624 | G    |
| 22  | А     | 2628 | С    |
| 22  | А     | 2629 | А    |
| 22  | А     | 2635 | G    |
| 22  | А     | 2636 | U    |
| 22  | А     | 2637 | С    |
| 22  | А     | 2640 | U    |
| 22  | А     | 2642 | U    |
| 22  | А     | 2663 | U    |
| 22  | А     | 2666 | А    |
| 22  | А     | 2672 | G    |
| 22  | А     | 2673 | С    |
| 22  | А     | 2690 | G    |
| 22  | А     | 2697 | G    |
| 22  | А     | 2709 | U    |
| 22  | А     | 2716 | U    |
| 22  | А     | 2727 | G    |
| 22  | А     | 2740 | А    |
| 22  | А     | 2741 | G    |
| 22  | А     | 2753 | U    |
| 22  | А     | 2754 | G    |
| 22  | А     | 2760 | А    |
| 22  | А     | 2762 | G    |
| 22  | А     | 2769 | G    |
| 22  | А     | 2775 | А    |
| 22  | А     | 2784 | А    |
| 22  | А     | 2792 | A    |
| 22  | А     | 2793 | G    |
| 22  | А     | 2796 | С    |
| 22  | A     | 2805 | A    |
| 22  | А     | 2806 | U    |
| 22  | A     | 2817 | A    |
| 22  | А     | 2820 | U    |
| 22  | А     | 2827 | A    |
| 22  | A     | 2833 | U    |
| 22  | A     | 2840 | A    |
| 22  | A     | 2841 | A    |
| 22  | А     | 2853 | U    |
| 22  | А     | 2863 | G    |



| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 22  | А     | 2887  | G    |
| 22  | А     | 2893  | А    |
| 22  | А     | 2900  | С    |
| 22  | А     | 2903  | А    |
| 22  | А     | 2904  | U    |
| 22  | А     | 2906  | G    |
| 22  | А     | 2911  | А    |
| 22  | А     | 2913  | G    |
| 23  | В     | 2     | С    |
| 23  | В     | 10    | U    |
| 23  | В     | 11    | А    |
| 23  | В     | 23    | U    |
| 23  | В     | 24    | С    |
| 23  | В     | 39    | G    |
| 23  | В     | 41    | С    |
| 23  | В     | 43    | А    |
| 23  | В     | 52    | G    |
| 23  | В     | 64    | А    |
| 23  | В     | 87    | С    |
| 23  | В     | 88    | G    |
| 23  | В     | 90    | U    |
| 23  | В     | 97    | G    |
| 23  | В     | 102   | G    |
| 23  | В     | 106   | G    |
| 23  | В     | 108   | U    |
| 52  | X     | 2     | G    |
| 52  | X     | 5     | G    |
| 52  | X     | 8     | 4SU  |
| 52  | X     | 9     | G    |
| 52  | X     | 16    | С    |
| 52  | X     | 17    | С    |
| 52  | X     | 17(A) | U    |
| 52  | X     | 18    | G    |
| 52  | X     | 19    | G    |
| 52  | X     | 20    | H2U  |
| 52  | x     | 21    | А    |
| 52  | X     | 26    | G    |
| 52  | X     | 43    | A    |
| 52  | X     | 46    | 7MG  |
| 52  | X     | 47    | U    |
| 52  | X     | 49    | G    |
| 52  | x     | 56    | С    |



Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | Х     | 58  | А    |
| 52  | Х     | 61  | С    |
| 52  | Х     | 74  | С    |
| 52  | Х     | 75  | С    |

All (9) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | А     | 179  | А    |
| 22  | А     | 327  | G    |
| 22  | А     | 328  | G    |
| 22  | А     | 971  | U    |
| 22  | А     | 1503 | U    |
| 22  | А     | 1550 | G    |
| 22  | А     | 2216 | U    |
| 22  | А     | 2783 | U    |
| 23  | В     | 23   | U    |

## 5.4 Non-standard residues in protein, DNA, RNA chains (i)

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mal  | Turne | Chain | Dec  | Link     | B        | ond leng | gths     | B        | Bond ang          | gles     |
|------|-------|-------|------|----------|----------|----------|----------|----------|-------------------|----------|
| NIOI | туре  | Chain | nes  | LIIIK    | Counts   | RMSZ     | # Z  > 2 | Counts   | RMSZ              | # Z  > 2 |
| 52   | H2U   | х     | 20   | 52       | 22,22,22 | 0.94     | 2 (9%)   | 28,33,33 | 2.84              | 6 (21%)  |
| 22   | OMG   | А     | 2278 | 22,52    | 18,26,27 | 2.31     | 7 (38%)  | 19,38,41 | 1.51              | 4 (21%)  |
| 1    | 2MG   | a     | 1527 | 1        | 18,26,27 | 2.37     | 7 (38%)  | 16,38,41 | 1.43              | 3 (18%)  |
| 52   | 4SU   | х     | 8    | 52       | 22,22,22 | 1.71     | 4 (18%)  | 33,33,33 | 2.82              | 13 (39%) |
| 1    | MA6   | a     | 1530 | 1        | 18,26,27 | 1.03     | 2 (11%)  | 19,38,41 | <mark>3.52</mark> | 2 (10%)  |
| 52   | 31H   | х     | 76   | 52,53    | 28,34,35 | 4.57     | 13 (46%) | 23,47,50 | 2.80              | 6 (26%)  |
| 22   | 5MU   | А     | 1966 | 22,54    | 19,22,23 | 4.82     | 7 (36%)  | 28,32,35 | <mark>3.83</mark> | 9 (32%)  |
| 22   | 2MA   | А     | 2530 | 22,54,53 | 17,25,26 | 2.41     | 5 (29%)  | 17,37,40 | 1.55              | 4 (23%)  |
| 52   | 5MU   | х     | 54   | 52       | 23,23,23 | 4.53     | 7 (30%)  | 35,35,35 | <mark>3.83</mark> | 15 (42%) |



| Mal   | Turne           | Chain | Bond lengths Bond ang |       |          | Bond lengths |          |          | gles |          |
|-------|-----------------|-------|-----------------------|-------|----------|--------------|----------|----------|------|----------|
| IVIOI | туре            | Chain | nes                   | LIIIK | Counts   | RMSZ         | # Z >2   | Counts   | RMSZ | # Z  > 2 |
| 1     | 7MG             | a     | 535                   | 1     | 22,26,27 | 3.80         | 10 (45%) | 29,39,42 | 2.07 | 9 (31%)  |
| 52    | $7 \mathrm{MG}$ | х     | 46                    | 52    | 26,27,27 | 3.49         | 10 (38%) | 36,42,42 | 2.74 | 15 (41%) |
| 22    | $2 \mathrm{MG}$ | А     | 2472                  | 22    | 18,26,27 | 2.25         | 7 (38%)  | 16,38,41 | 1.66 | 4 (25%)  |
| 52    | OMC             | х     | 32                    | 52    | 23,23,23 | 2.73         | 8 (34%)  | 33,34,34 | 2.28 | 8 (24%)  |
| 22    | OMC             | А     | 1947                  | 22    | 19,22,23 | 2.84         | 8 (42%)  | 26,31,34 | 0.88 | 1 (3%)   |
| 22    | OMC             | А     | 2525                  | 22    | 19,22,23 | 2.75         | 7 (36%)  | 26,31,34 | 0.99 | 1 (3%)   |
| 1     | MA6             | а     | 1529                  | 1     | 18,26,27 | 1.04         | 2 (11%)  | 19,38,41 | 3.12 | 2 (10%)  |
| 1     | 4OC             | a     | 1412                  | 1     | 20,23,24 | 3.07         | 8 (40%)  | 26,32,35 | 1.04 | 2 (7%)   |
| 52    | PSU             | х     | 55                    | 52    | 22,22,22 | 1.25         | 3 (13%)  | 29,33,33 | 2.75 | 11 (37%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type            | Chain | $\mathbf{Res}$ | $\operatorname{Link}$ | Chirals | Torsions    | Rings   |
|-----|-----------------|-------|----------------|-----------------------|---------|-------------|---------|
| 52  | H2U             | х     | 20             | 52                    | -       | 4/10/39/39  | 0/2/2/2 |
| 22  | OMG             | А     | 2278           | 22,52                 | -       | 0/5/27/28   | 0/3/3/3 |
| 1   | 2MG             | a     | 1527           | 1                     | -       | 0/5/27/28   | 0/3/3/3 |
| 52  | 4SU             | Х     | 8              | 52                    | -       | 1/10/26/26  | 0/2/2/2 |
| 1   | MA6             | a     | 1530           | 1                     | -       | 2/7/29/30   | 0/3/3/3 |
| 52  | 31H             | х     | 76             | $52,\!53$             | -       | 14/18/40/41 | 0/3/3/3 |
| 22  | $5 \mathrm{MU}$ | А     | 1966           | $22,\!54$             | -       | 2/7/25/26   | 0/2/2/2 |
| 22  | 2MA             | А     | 2530           | $22,\!54,\!53$        | -       | 2/3/25/26   | 0/3/3/3 |
| 52  | 5MU             | х     | 54             | 52                    | -       | 2/10/26/26  | 0/2/2/2 |
| 1   | $7 \mathrm{MG}$ | a     | 535            | 1                     | -       | 2/7/37/38   | 0/3/3/3 |
| 52  | 7MG             | х     | 46             | 52                    | -       | 5/10/38/38  | 0/3/3/3 |
| 22  | 2MG             | А     | 2472           | 22                    | -       | 2/5/27/28   | 0/3/3/3 |
| 52  | OMC             | х     | 32             | 52                    | -       | 4/12/28/28  | 0/2/2/2 |
| 22  | OMC             | А     | 1947           | 22                    | -       | 2/9/27/28   | 0/2/2/2 |
| 22  | OMC             | А     | 2525           | 22                    | -       | 2/9/27/28   | 0/2/2/2 |
| 1   | MA6             | a     | 1529           | 1                     | -       | 1/7/29/30   | 0/3/3/3 |
| 1   | 4OC             | a     | 1412           | 1                     | -       | 2/9/29/30   | 0/2/2/2 |
| 52  | PSU             | х     | 55             | 52                    | -       | 4/10/26/26  | 0/2/2/2 |

All (117) bond length outliers are listed below:



| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 52  | Х     | 76   | 31H  | C4'-C3' | -13.83 | 1.28        | 1.52     |
| 52  | Х     | 54   | 5MU  | C2-N1   | 11.56  | 1.57        | 1.38     |
| 52  | Х     | 54   | 5MU  | C6-N1   | 11.11  | 1.57        | 1.38     |
| 22  | А     | 1966 | 5MU  | C6-N1   | 10.80  | 1.56        | 1.38     |
| 22  | А     | 1966 | 5MU  | C2-N1   | 10.59  | 1.55        | 1.38     |
| 52  | Х     | 54   | 5MU  | C4-C5   | 9.93   | 1.61        | 1.44     |
| 52  | Х     | 76   | 31H  | O4'-C4' | 9.70   | 1.66        | 1.45     |
| 22  | А     | 1966 | 5MU  | C4-C5   | 9.31   | 1.60        | 1.44     |
| 52  | Х     | 46   | 7MG  | C8-N9   | 9.24   | 1.51        | 1.46     |
| 1   | a     | 535  | 7MG  | C8-N9   | 9.04   | 1.51        | 1.46     |
| 52  | Х     | 76   | 31H  | O4'-C1' | -8.26  | 1.29        | 1.41     |
| 52  | Х     | 76   | 31H  | C3'-N3' | 8.21   | 1.58        | 1.45     |
| 1   | a     | 535  | 7MG  | C5-N7   | 8.12   | 1.45        | 1.35     |
| 52  | Х     | 46   | 7MG  | C5-N7   | 8.09   | 1.44        | 1.35     |
| 22  | А     | 1966 | 5MU  | C4-N3   | -7.82  | 1.24        | 1.38     |
| 52  | Х     | 54   | 5MU  | C4-N3   | -7.43  | 1.25        | 1.38     |
| 22  | А     | 1966 | 5MU  | C6-C5   | 6.68   | 1.45        | 1.34     |
| 22  | А     | 2530 | 2MA  | C2-N3   | 6.56   | 1.45        | 1.31     |
| 52  | Х     | 54   | 5MU  | C6-C5   | 6.41   | 1.45        | 1.34     |
| 52  | Х     | 32   | OMC  | C2-N3   | 6.27   | 1.49        | 1.36     |
| 1   | a     | 1412 | 4OC  | C4-N3   | 6.27   | 1.43        | 1.32     |
| 52  | Х     | 76   | 31H  | C-N3'   | 6.22   | 1.47        | 1.34     |
| 1   | a     | 1412 | 4OC  | C6-C5   | 6.22   | 1.49        | 1.35     |
| 22  | А     | 1947 | OMC  | C2-N3   | 5.98   | 1.48        | 1.36     |
| 22  | А     | 1947 | OMC  | C6-C5   | 5.93   | 1.48        | 1.35     |
| 52  | Х     | 76   | 31H  | CN-N    | 5.91   | 1.53        | 1.33     |
| 52  | Х     | 32   | OMC  | C6-C5   | 5.87   | 1.48        | 1.35     |
| 52  | Х     | 46   | 7MG  | C2-N3   | 5.85   | 1.47        | 1.33     |
| 22  | А     | 2525 | OMC  | C2-N3   | 5.84   | 1.48        | 1.36     |
| 1   | a     | 535  | 7MG  | C4-N9   | 5.82   | 1.44        | 1.37     |
| 1   | a     | 535  | 7MG  | C2-N3   | 5.81   | 1.47        | 1.33     |
| 1   | a     | 1412 | 4OC  | C2-N3   | 5.79   | 1.48        | 1.36     |
| 52  | Х     | 46   | 7MG  | C4-N9   | 5.54   | 1.44        | 1.37     |
| 1   | a     | 535  | 7MG  | C4-N3   | 5.54   | 1.47        | 1.34     |
| 22  | А     | 2525 | OMC  | C6-C5   | 5.46   | 1.47        | 1.35     |
| 52  | Х     | 46   | 7MG  | C4-N3   | 5.41   | 1.47        | 1.34     |
| 1   | a     | 1527 | 2MG  | C2-N2   | 5.16   | 1.44        | 1.33     |
| 22  | А     | 2530 | 2MA  | C4-N3   | 5.04   | 1.49        | 1.37     |
| 52  | Х     | 32   | OMC  | C4-N3   | 5.00   | 1.44        | 1.34     |
| 22  | А     | 2278 | OMG  | C2-N3   | 5.00   | 1.45        | 1.33     |
| 1   | a     | 1412 | 4OC  | C4-N4   | 4.88   | 1.45        | 1.35     |
| 52  | Х     | 46   | 7MG  | C2-N2   | 4.87   | 1.45        | 1.34     |
| 52  | х     | 32   | OMC  | C2-N1   | 4.85   | 1.50        | 1.40     |



| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 52  | Х     | 32   | OMC  | C4-N4   | 4.79  | 1.45        | 1.33     |
| 1   | a     | 535  | 7MG  | C2-N2   | 4.77  | 1.45        | 1.34     |
| 22  | А     | 2472 | 2MG  | C2-N2   | 4.70  | 1.43        | 1.33     |
| 22  | А     | 1947 | OMC  | C4-N4   | 4.70  | 1.45        | 1.33     |
| 1   | a     | 1527 | 2MG  | C4-N3   | 4.61  | 1.48        | 1.37     |
| 52  | Х     | 8    | 4SU  | C4-S4   | -4.61 | 1.59        | 1.68     |
| 22  | А     | 2525 | OMC  | C4-N4   | 4.55  | 1.44        | 1.33     |
| 22  | А     | 2472 | 2MG  | C4-N3   | 4.53  | 1.48        | 1.37     |
| 22  | А     | 2278 | OMG  | C4-N3   | 4.49  | 1.48        | 1.37     |
| 22  | А     | 1947 | OMC  | C4-N3   | 4.47  | 1.43        | 1.34     |
| 1   | a     | 1527 | 2MG  | C2-N1   | 4.40  | 1.43        | 1.36     |
| 52  | Х     | 76   | 31H  | O2'-C2' | -4.39 | 1.32        | 1.43     |
| 22  | А     | 2525 | OMC  | C4-N3   | 4.38  | 1.43        | 1.34     |
| 1   | a     | 1412 | 4OC  | C2-N1   | 4.34  | 1.49        | 1.40     |
| 22  | А     | 2525 | OMC  | C2-N1   | 4.28  | 1.49        | 1.40     |
| 22  | А     | 1947 | OMC  | C2-N1   | 4.21  | 1.49        | 1.40     |
| 52  | Х     | 76   | 31H  | C6-N6   | 3.93  | 1.48        | 1.34     |
| 52  | Х     | 8    | 4SU  | C5-C4   | -3.86 | 1.37        | 1.42     |
| 1   | а     | 535  | 7MG  | C5-C6   | 3.77  | 1.53        | 1.43     |
| 1   | a     | 1412 | 4OC  | C5-C4   | 3.73  | 1.48        | 1.40     |
| 1   | a     | 535  | 7MG  | C2-N1   | 3.61  | 1.46        | 1.37     |
| 52  | Х     | 46   | 7MG  | C5-C6   | 3.61  | 1.52        | 1.43     |
| 22  | А     | 2472 | 2MG  | C2-N1   | 3.60  | 1.42        | 1.36     |
| 52  | Х     | 46   | 7MG  | C2-N1   | 3.59  | 1.46        | 1.37     |
| 22  | А     | 2278 | OMG  | C6-N1   | 3.35  | 1.42        | 1.37     |
| 22  | А     | 2278 | OMG  | C2-N2   | 3.29  | 1.42        | 1.34     |
| 22  | А     | 2530 | 2MA  | C5-C4   | -3.24 | 1.34        | 1.43     |
| 1   | a     | 1412 | 4OC  | C6-N1   | 3.24  | 1.45        | 1.38     |
| 22  | А     | 2472 | 2MG  | C5-C4   | -3.23 | 1.34        | 1.43     |
| 1   | a     | 1527 | 2MG  | C6-N1   | 3.21  | 1.42        | 1.37     |
| 52  | Х     | 76   | 31H  | C2'-C1' | 3.20  | 1.58        | 1.53     |
| 22  | А     | 1966 | 5MU  | O4-C4   | -3.15 | 1.17        | 1.23     |
| 52  | Х     | 8    | 4SU  | C4-N3   | -3.15 | 1.34        | 1.37     |
| 52  | Х     | 32   | OMC  | C6-N1   | 3.14  | 1.45        | 1.38     |
| 52  | Х     | 46   | 7MG  | C6-N1   | 3.08  | 1.44        | 1.38     |
| 1   | a     | 535  | 7MG  | C6-N1   | 3.06  | 1.44        | 1.38     |
| 52  | Х     | 55   | PSU  | C6-C5   | 3.05  | 1.38        | 1.35     |
| 52  | X     | 76   | 31H  | C2'-C3' | 3.01  | 1.59        | 1.53     |
| 22  | A     | 1947 | OMC  | C6-N1   | 3.01  | 1.45        | 1.38     |
| 52  | X     | 54   | 5MU  | O4-C4   | -2.98 | 1.17        | 1.23     |
| 22  | A     | 2278 | OMG  | C5-C4   | -2.98 | 1.35        | 1.43     |
| 1   | a     | 1527 | 2MG  | C5-C6   | 2.96  | 1.53        | 1.47     |



| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | А     | 2530 | 2MA  | C6-N1 | 2.93  | 1.44        | 1.38     |
| 22  | А     | 2278 | OMG  | O6-C6 | -2.92 | 1.17        | 1.23     |
| 1   | a     | 1412 | 4OC  | O2-C2 | -2.89 | 1.18        | 1.23     |
| 22  | А     | 1966 | 5MU  | O2-C2 | -2.88 | 1.17        | 1.23     |
| 22  | А     | 2525 | OMC  | O2-C2 | -2.86 | 1.18        | 1.23     |
| 22  | А     | 2472 | 2MG  | O6-C6 | -2.85 | 1.17        | 1.23     |
| 1   | a     | 1527 | 2MG  | C5-C4 | -2.84 | 1.35        | 1.43     |
| 1   | a     | 1530 | MA6  | C5-C4 | -2.83 | 1.33        | 1.40     |
| 22  | А     | 2525 | OMC  | C6-N1 | 2.82  | 1.44        | 1.38     |
| 1   | a     | 1529 | MA6  | C5-C4 | -2.78 | 1.33        | 1.40     |
| 52  | X     | 55   | PSU  | C4-N3 | -2.78 | 1.33        | 1.38     |
| 22  | А     | 1947 | OMC  | O2-C2 | -2.76 | 1.18        | 1.23     |
| 52  | Х     | 32   | OMC  | O2-C2 | -2.72 | 1.18        | 1.23     |
| 52  | х     | 20   | H2U  | C2-N3 | -2.70 | 1.33        | 1.38     |
| 52  | Х     | 46   | 7MG  | O6-C6 | -2.62 | 1.18        | 1.23     |
| 1   | a     | 535  | 7MG  | O6-C6 | -2.60 | 1.18        | 1.23     |
| 52  | х     | 54   | 5MU  | O2-C2 | -2.55 | 1.18        | 1.23     |
| 22  | А     | 2472 | 2MG  | C6-N1 | 2.52  | 1.41        | 1.37     |
| 22  | А     | 2472 | 2MG  | C5-C6 | 2.50  | 1.52        | 1.47     |
| 22  | А     | 2278 | OMG  | C5-C6 | 2.50  | 1.52        | 1.47     |
| 52  | Х     | 76   | 31H  | CB-CG | 2.48  | 1.61        | 1.51     |
| 52  | х     | 8    | 4SU  | C2-N1 | 2.46  | 1.42        | 1.38     |
| 52  | Х     | 76   | 31H  | O-C   | -2.43 | 1.18        | 1.23     |
| 22  | А     | 2530 | 2MA  | C2-N1 | 2.41  | 1.44        | 1.36     |
| 1   | a     | 1529 | MA6  | C2-N3 | 2.30  | 1.35        | 1.32     |
| 52  | х     | 76   | 31H  | C6-C5 | -2.24 | 1.35        | 1.43     |
| 1   | a     | 1527 | 2MG  | O6-C6 | -2.22 | 1.18        | 1.23     |
| 52  | х     | 32   | OMC  | C5-C4 | 2.21  | 1.48        | 1.42     |
| 52  | х     | 55   | PSU  | C2-N3 | -2.18 | 1.33        | 1.37     |
| 52  | X     | 20   | H2U  | C4-N3 | -2.17 | 1.33        | 1.37     |
| 22  | A     | 1947 | OMC  | C5-C4 | 2.09  | 1.47        | 1.42     |
| 1   | a     | 1530 | MA6  | C2-N3 | 2.05  | 1.35        | 1.32     |

All (115) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | $\mathbf{Observed}(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-----------|--------|---------------------------|---------------|
| 1   | a     | 1530 | MA6  | N1-C6-N6  | -13.63 | 102.72                    | 117.06        |
| 22  | А     | 1966 | 5MU  | C5-C4-N3  | 12.76  | 126.20                    | 115.31        |
| 52  | Х     | 54   | 5MU  | C5-C4-N3  | 12.34  | 125.84                    | 115.31        |
| 1   | a     | 1529 | MA6  | N1-C6-N6  | -12.04 | 104.38                    | 117.06        |
| 22  | А     | 1966 | 5MU  | C5-C6-N1  | -11.02 | 112.00                    | 123.34        |
| 52  | Х     | 20   | H2U  | OP3-P-O5' | -10.38 | 79.11                     | 106.73        |



| Mol | Chain | Res  | Type            | Atoms     | Ζ     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|-----------------|-----------|-------|------------------|---------------|
| 52  | Х     | 54   | 5MU             | C5-C6-N1  | -9.40 | 113.67           | 123.34        |
| 52  | Х     | 20   | H2U             | C4-N3-C2  | -8.06 | 119.10           | 125.79        |
| 52  | Х     | 76   | 31H             | C5-C6-N6  | 7.89  | 132.35           | 120.35        |
| 52  | Х     | 55   | PSU             | OP3-P-O5' | -7.53 | 86.69            | 106.73        |
| 52  | Х     | 8    | 4SU             | OP3-P-O5' | -6.71 | 88.88            | 106.73        |
| 52  | Х     | 32   | OMC             | OP3-P-OP1 | -6.66 | 84.60            | 110.68        |
| 1   | a     | 1530 | MA6             | N3-C2-N1  | -6.27 | 118.88           | 128.68        |
| 52  | Х     | 54   | 5MU             | OP3-P-O5' | -6.12 | 90.44            | 106.73        |
| 52  | Х     | 54   | 5MU             | OP3-P-OP1 | -6.00 | 87.21            | 110.68        |
| 52  | Х     | 76   | 31H             | N3-C2-N1  | -5.96 | 119.36           | 128.68        |
| 52  | Х     | 46   | 7MG             | OP3-P-OP1 | -5.95 | 87.39            | 110.68        |
| 52  | Х     | 46   | 7MG             | OP3-P-OP2 | -5.92 | 85.01            | 107.64        |
| 52  | Х     | 46   | 7MG             | OP3-P-O5' | -5.85 | 91.17            | 106.73        |
| 1   | a     | 1529 | MA6             | N3-C2-N1  | -5.85 | 119.54           | 128.68        |
| 52  | Х     | 55   | PSU             | N1-C2-N3  | 5.67  | 121.55           | 115.13        |
| 22  | А     | 1966 | 5MU             | O4-C4-C5  | -5.65 | 118.36           | 124.90        |
| 52  | Х     | 32   | OMC             | OP3-P-OP2 | -5.50 | 86.61            | 107.64        |
| 22  | А     | 1966 | 5MU             | C4-N3-C2  | -5.48 | 120.26           | 127.35        |
| 52  | Х     | 54   | 5MU             | OP3-P-OP2 | -5.47 | 86.73            | 107.64        |
| 52  | Х     | 76   | 31H             | C1'-N9-C4 | -5.47 | 117.03           | 126.64        |
| 52  | Х     | 8    | 4SU             | C4-N3-C2  | -5.42 | 122.07           | 127.34        |
| 52  | Х     | 8    | 4SU             | C5-C4-N3  | 5.32  | 119.63           | 114.69        |
| 52  | Х     | 8    | 4SU             | C5-C4-S4  | -5.32 | 117.61           | 124.47        |
| 52  | Х     | 54   | 5MU             | O4-C4-C5  | -5.26 | 118.81           | 124.90        |
| 52  | Х     | 32   | OMC             | OP3-P-O5' | -5.23 | 92.80            | 106.73        |
| 52  | Х     | 76   | 31H             | N6-C6-N1  | -5.21 | 107.75           | 118.57        |
| 1   | a     | 535  | 7MG             | C5-C6-N1  | 5.17  | 120.11           | 110.99        |
| 52  | Х     | 46   | $7 \mathrm{MG}$ | C5-C6-N1  | 5.17  | 120.11           | 110.99        |
| 52  | Х     | 46   | 7MG             | OP2-P-OP1 | 5.17  | 130.91           | 110.68        |
| 52  | Х     | 8    | 4SU             | OP2-P-OP1 | 5.10  | 130.63           | 110.68        |
| 22  | А     | 1966 | 5MU             | N3-C2-N1  | 5.02  | 121.56           | 114.89        |
| 52  | Х     | 55   | PSU             | OP2-P-OP1 | 4.85  | 129.66           | 110.68        |
| 52  | Х     | 54   | 5MU             | C4-N3-C2  | -4.79 | 121.15           | 127.35        |
| 52  | Х     | 54   | 5MU             | OP2-P-OP1 | 4.72  | 129.16           | 110.68        |
| 52  | Х     | 32   | OMC             | OP2-P-OP1 | 4.66  | 128.92           | 110.68        |
| 1   | a     | 535  | 7MG             | C2-N3-C4  | 4.63  | 120.55           | 112.30        |
| 52  | Х     | 54   | 5MU             | N3-C2-N1  | 4.54  | 120.92           | 114.89        |
| 52  | х     | 46   | 7MG             | C2-N3-C4  | 4.50  | 120.32           | 112.30        |
| 52  | Х     | 8    | 4SU             | OP3-P-OP1 | -4.48 | 93.13            | 110.68        |
| 1   | a     | 535  | 7MG             | C5-C4-N3  | -4.25 | 120.03           | 128.13        |
| 52  | Х     | 8    | 4SU             | C1'-N1-C2 | 4.17  | 125.12           | 117.57        |
| 52  | x     | 55   | PSU             | OP3-P-OP1 | -4.15 | 94.43            | 110.68        |



| Mol | Chain | Res  | Type | Atoms     | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-----------|-------|------------------|---------------|
| 22  | А     | 2472 | 2MG  | C5-C6-N1  | 4.10  | 121.20           | 113.95        |
| 52  | Х     | 54   | 5MU  | C5M-C5-C4 | 4.10  | 123.28           | 118.77        |
| 52  | Х     | 46   | 7MG  | C5-C4-N3  | -4.03 | 120.46           | 128.13        |
| 52  | Х     | 54   | 5MU  | C5M-C5-C6 | -3.95 | 117.58           | 122.85        |
| 52  | Х     | 55   | PSU  | C4-N3-C2  | -3.83 | 120.82           | 126.34        |
| 22  | А     | 2530 | 2MA  | C5-C6-N1  | 3.78  | 120.55           | 114.02        |
| 52  | Х     | 8    | 4SU  | N3-C2-N1  | 3.67  | 119.77           | 114.89        |
| 22  | А     | 2278 | OMG  | C5-C6-N1  | 3.58  | 120.27           | 113.95        |
| 52  | Х     | 20   | H2U  | OP3-P-OP1 | 3.57  | 124.67           | 110.68        |
| 52  | Х     | 55   | PSU  | OP3-P-OP2 | -3.46 | 94.40            | 107.64        |
| 52  | Х     | 8    | 4SU  | O5'-P-OP1 | 3.44  | 116.14           | 106.47        |
| 1   | a     | 535  | 7MG  | C5-C4-N9  | 3.38  | 110.73           | 106.35        |
| 52  | Х     | 46   | 7MG  | C5-C4-N9  | 3.34  | 110.68           | 106.35        |
| 1   | a     | 1527 | 2MG  | C5-C6-N1  | 3.31  | 119.80           | 113.95        |
| 22  | А     | 2472 | 2MG  | CM2-N2-C2 | -3.26 | 116.65           | 123.86        |
| 52  | Х     | 32   | OMC  | O5'-P-OP1 | 3.24  | 115.56           | 106.47        |
| 22  | А     | 2530 | 2MA  | C8-N7-C5  | 3.22  | 109.13           | 102.99        |
| 22  | А     | 2278 | OMG  | C2-N1-C6  | -3.22 | 119.16           | 125.10        |
| 52  | Х     | 55   | PSU  | OP2-P-O5' | 3.18  | 115.19           | 106.73        |
| 52  | Х     | 54   | 5MU  | O5'-P-OP1 | 3.17  | 115.38           | 106.47        |
| 52  | Х     | 8    | 4SU  | C6-N1-C2  | -3.16 | 116.95           | 120.99        |
| 52  | Х     | 54   | 5MU  | OP2-P-O5' | 3.14  | 115.09           | 106.73        |
| 52  | Х     | 32   | OMC  | OP2-P-O5' | 3.13  | 115.06           | 106.73        |
| 52  | Х     | 20   | H2U  | O5'-P-OP1 | -3.05 | 97.93            | 106.47        |
| 52  | Х     | 8    | 4SU  | OP3-P-OP2 | -3.03 | 96.06            | 107.64        |
| 52  | Х     | 55   | PSU  | O2-C2-N1  | -2.96 | 119.53           | 122.79        |
| 52  | Х     | 46   | 7MG  | OP2-P-O5' | 2.96  | 114.62           | 106.73        |
| 52  | Х     | 55   | PSU  | O5'-P-OP1 | 2.94  | 114.73           | 106.47        |
| 22  | А     | 1966 | 5MU  | O2-C2-N1  | -2.92 | 118.90           | 122.79        |
| 1   | a     | 535  | 7MG  | C2-N1-C6  | -2.87 | 119.87           | 125.10        |
| 52  | Х     | 46   | 7MG  | C4-C5-N7  | 2.86  | 109.49           | 105.53        |
| 52  | Х     | 55   | PSU  | C6-C5-C4  | -2.84 | 116.21           | 118.20        |
| 52  | Х     | 46   | 7MG  | C2-N1-C6  | -2.82 | 119.96           | 125.10        |
| 1   | a     | 535  | 7MG  | C4-C5-N7  | 2.75  | 109.35           | 105.53        |
| 1   | a     | 1412 | 4OC  | O2-C2-N3  | -2.68 | 117.97           | 122.33        |
| 52  | Х     | 32   | OMC  | O2-C2-N3  | -2.68 | 117.98           | 122.33        |
| 52  | Х     | 46   | 7MG  | O5'-P-OP1 | 2.67  | 113.96           | 106.47        |
| 1   | a     | 535  | 7MG  | N9-C8-N7  | 2.67  | 107.19           | 103.38        |
| 1   | a     | 1527 | 2MG  | C8-N7-C5  | 2.66  | 108.06           | 102.99        |
| 1   | a     | 1527 | 2MG  | CM2-N2-C2 | -2.66 | 117.99           | 123.86        |
| 52  | X     | 8    | 4SU  | S4-C4-N3  | 2.59  | 122.76           | 120.21        |
| 22  | А     | 2278 | OMG  | C8-N7-C5  | 2.58  | 107.90           | 102.99        |



| Mol | Chain | Res  | Type | Atoms       | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|-------|------------------|---------------|
| 1   | a     | 535  | 7MG  | N9-C4-N3    | 2.52  | 129.24           | 125.47        |
| 22  | А     | 2472 | 2MG  | C8-N7-C5    | 2.51  | 107.77           | 102.99        |
| 52  | Х     | 76   | 31H  | CE-SD-CG    | 2.49  | 108.95           | 100.40        |
| 22  | А     | 2530 | 2MA  | CM2-C2-N1   | 2.49  | 121.76           | 116.23        |
| 52  | Х     | 54   | 5MU  | O4-C4-N3    | -2.49 | 115.35           | 120.12        |
| 52  | Х     | 46   | 7MG  | N9-C8-N7    | 2.48  | 106.93           | 103.38        |
| 22  | А     | 2530 | 2MA  | N1-C2-N3    | -2.48 | 118.95           | 123.06        |
| 22  | А     | 2525 | OMC  | O2-C2-N3    | -2.46 | 118.33           | 122.33        |
| 52  | х     | 20   | H2U  | C5-C6-N1    | -2.44 | 103.57           | 111.61        |
| 22  | А     | 1966 | 5MU  | O4-C4-N3    | -2.44 | 115.44           | 120.12        |
| 22  | А     | 2472 | 2MG  | O6-C6-C5    | -2.43 | 119.63           | 124.37        |
| 22  | А     | 1966 | 5MU  | C5M-C5-C6   | -2.36 | 119.70           | 122.85        |
| 1   | a     | 1412 | 4OC  | C6-C5-C4    | 2.36  | 119.84           | 116.96        |
| 52  | х     | 46   | 7MG  | O6-C6-C5    | -2.35 | 121.78           | 127.54        |
| 52  | Х     | 32   | OMC  | C1'-N1-C2   | 2.30  | 123.55           | 118.42        |
| 52  | Х     | 46   | 7MG  | N9-C4-N3    | 2.27  | 128.86           | 125.47        |
| 52  | х     | 20   | H2U  | OP2-P-OP1   | 2.23  | 119.43           | 110.68        |
| 52  | Х     | 55   | PSU  | O3'-C3'-C4' | 2.22  | 117.47           | 111.05        |
| 1   | a     | 535  | 7MG  | O6-C6-C5    | -2.20 | 122.15           | 127.54        |
| 22  | А     | 1966 | 5MU  | C6-C5-C4    | 2.17  | 119.85           | 118.03        |
| 52  | Х     | 8    | 4SU  | OP2-P-O5'   | 2.15  | 112.45           | 106.73        |
| 22  | А     | 2278 | OMG  | O6-C6-C5    | -2.15 | 120.17           | 124.37        |
| 52  | X     | 76   | 31H  | O4'-C1'-C2' | -2.15 | 103.79           | 106.93        |
| 22  | А     | 1947 | OMC  | O2-C2-N3    | -2.12 | 118.88           | 122.33        |
| 52  | Х     | 54   | 5MU  | C6-N1-C2    | -2.00 | 119.27           | 121.30        |

There are no chirality outliers.

All (51) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | a     | 1530 | MA6  | O4'-C4'-C5'-O5' |
| 22  | А     | 1947 | OMC  | O4'-C4'-C5'-O5' |
| 52  | Х     | 20   | H2U  | O4'-C4'-C5'-O5' |
| 52  | Х     | 32   | OMC  | C5'-O5'-P-OP1   |
| 52  | Х     | 46   | 7MG  | C5'-O5'-P-OP3   |
| 52  | Х     | 54   | 5MU  | C5'-O5'-P-OP3   |
| 52  | Х     | 55   | PSU  | O4'-C1'-C5-C4   |
| 52  | Х     | 55   | PSU  | O4'-C1'-C5-C6   |
| 52  | Х     | 55   | PSU  | C5'-O5'-P-OP1   |
| 52  | Х     | 55   | PSU  | C5'-O5'-P-OP3   |
| 52  | Х     | 76   | 31H  | C3'-C4'-C5'-O5' |
| 52  | Х     | 76   | 31H  | C-CA-N-CN       |


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| Mol | Chain | Res  | Type | Atoms           |  |
|-----|-------|------|------|-----------------|--|
| 52  | х     | 76   | 31H  | CB-CA-N-CN      |  |
| 52  | X     | 76   | 31H  | C-CA-CB-CG      |  |
| 52  | X     | 76   | 31H  | N-CA-CB-CG      |  |
| 52  | X     | 76   | 31H  | OCN-CN-N-CA     |  |
| 1   | a     | 535  | 7MG  | C3'-C4'-C5'-O5' |  |
| 1   | a     | 1412 | 4OC  | O4'-C4'-C5'-O5' |  |
| 1   | a     | 1530 | MA6  | C3'-C4'-C5'-O5' |  |
| 22  | А     | 1947 | OMC  | C3'-C4'-C5'-O5' |  |
| 22  | А     | 1966 | 5MU  | C3'-C4'-C5'-O5' |  |
| 22  | А     | 1966 | 5MU  | O4'-C4'-C5'-O5' |  |
| 52  | Х     | 76   | 31H  | O4'-C4'-C5'-O5' |  |
| 1   | a     | 535  | 7MG  | O4'-C4'-C5'-O5' |  |
| 1   | a     | 1412 | 4OC  | C3'-C4'-C5'-O5' |  |
| 52  | Х     | 20   | H2U  | C2'-C1'-N1-C2   |  |
| 22  | А     | 2472 | 2MG  | C3'-C4'-C5'-O5' |  |
| 22  | А     | 2525 | OMC  | C3'-C4'-C5'-O5' |  |
| 52  | Х     | 46   | 7MG  | C3'-C4'-C5'-O5' |  |
| 52  | Х     | 76   | 31H  | CB-CG-SD-CE     |  |
| 22  | А     | 2525 | OMC  | O4'-C4'-C5'-O5' |  |
| 52  | Х     | 46   | 7MG  | O4'-C4'-C5'-O5' |  |
| 52  | Х     | 20   | H2U  | C2'-C1'-N1-C6   |  |
| 1   | a     | 1529 | MA6  | C5-C6-N6-C9     |  |
| 52  | Х     | 46   | 7MG  | C5'-O5'-P-OP1   |  |
| 52  | Х     | 76   | 31H  | O-C-CA-N        |  |
| 52  | Х     | 76   | 31H  | N3'-C-CA-N      |  |
| 52  | Х     | 76   | 31H  | C4'-C5'-O5'-P   |  |
| 52  | Х     | 76   | 31H  | O-C-CA-CB       |  |
| 22  | А     | 2472 | 2MG  | O4'-C4'-C5'-O5' |  |
| 52  | х     | 20   | H2U  | C3'-C4'-C5'-O5' |  |
| 52  | Х     | 32   | OMC  | C3'-C4'-C5'-O5' |  |
| 52  | Х     | 76   | 31H  | N3'-C-CA-CB     |  |
| 52  | Х     | 8    | 4SU  | C5'-O5'-P-OP1   |  |
| 52  | Х     | 46   | 7MG  | C4'-C5'-O5'-P   |  |
| 22  | А     | 2530 | 2MA  | O4'-C4'-C5'-O5' |  |
| 52  | х     | 32   | OMC  | O4'-C4'-C5'-O5' |  |
| 52  | х     | 32   | OMC  | C5'-O5'-P-OP3   |  |
| 52  | х     | 54   | 5MU  | C5'-O5'-P-OP1   |  |
| 22  | А     | 2530 | 2MA  | C4'-C5'-O5'-P   |  |
| 52  | х     | 76   | 31H  | C4'-C3'-N3'-C   |  |

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There are no ring outliers.

No monomer is involved in short contacts.



#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 288 ligands modelled in this entry, 288 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 47  | 4     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 4     | 53:GLU    | С      | 57:GLU    | Ν      | 9.89         |



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10791. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections (i)

This section was not generated.

#### 6.2 Central slices (i)

This section was not generated.

#### 6.3 Largest variance slices (i)

This section was not generated.

#### 6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

#### 6.5 Orthogonal surface views (i)

This section was not generated.

#### 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



# 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

# 7.1 Map-value distribution (i)

This section was not generated.

#### 7.2 Volume estimate versus contour level (i)

This section was not generated.

## 7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



# 9 Map-model fit (i)

This section was not generated.

