

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 10:28 AM EDT

| PDB ID | : | 6MKN |
|--------------|---|--|
| Title | : | Structure of the Thermus thermophilus 30S ribosomal subunit complexed with |
| | | an inosine (I34) modified anticodon stem loop (ASL) of Escherichia coli transfer |
| | | RNA Arginine 2 (TRNAARG2) bound to an mRNA with an CGU-codon in |
| | | the A-site and paromomycin |
| Authors | : | Cantara, W.A.; DeMirci, H.; Agris, P.F. |
| Deposited on | : | 2018-09-25 |
| Resolution | : | 3.46 Å(reported) |
| | | |

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp 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:

| MolProbity | : | FAILED |
|--------------------------------|---|--|
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | FAILED |
| buster-report | : | 1.1.7(2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35.1 |

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 3.46 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



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2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 52043 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 | | I | Atoms | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|----------------|------------|-----------|------------|-----------|---------|-------|---|
| 1 | А | 1507 | Total 32380 | C 14414 | N 5990 | O 10470 | Р 1506 | 0 | 0 | 0 |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|-------------|
| А | ? | - | G | deletion | GB 55771382 |
| А | ? | - | G | deletion | GB 55771382 |
| А | ? | - | С | deletion | GB 55771382 |
| А | ? | - | G | deletion | GB 55771382 |
| А | ? | - | А | deletion | GB 55771382 |
| А | ? | - | С | deletion | GB 55771382 |
| А | 1540 | U | - | insertion | GB 55771382 |
| А | 1541 | U | - | insertion | GB 55771382 |
| А | 1542 | U | - | insertion | GB 55771382 |
| А | 1543 | С | - | insertion | GB 55771382 |
| А | 1544 | U | - | insertion | GB 55771382 |

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

| Mol | Chain | Residues | | Ate | oms | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|---------------|-----------|----------|----------|------------|---------|-------|---|
| 2 | В | 234 | Total 1900 | C 1213 | N 341 | 0 341 | ${f S}{5}$ | 0 | 0 | 0 |

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

| Mol | Chain | Residues | | At | oms | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|---|
| 3 | С | 206 | Total 1612 | C 1016 | N 314 | O 281 | S 1 | 0 | 0 | 0 |

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



| Mol | Chain | Residues | | At | oms | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|---|
| 4 | D | 208 | Total 1703 | C 1066 | N 339 | 0 291 | S 7 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | | At | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------------|---------|---------|-------|
| 5 | Е | 150 | Total 1146 | С 724 | N 217 | 0 201 | ${S \over 4}$ | 0 | 0 | 0 |

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

| Mol | Chain | Residues | | At | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|---------|-------|
| 6 | F | 101 | Total 843 | C 531 | N 155 | 0 154 | ${ m S} { m 3}$ | 0 | 0 | 0 |

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

| Mol | Chain | Residues | | At | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| 7 | G | 155 | Total 1257 | C 781 | N 252 | 0 218 | S 6 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | | At | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|-----------------|---------|---------|-------|
| 8 | Н | 138 | Total 1116 | C 705 | N 215 | O 193 | ${ m S} { m 3}$ | 0 | 0 | 0 |

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

| Mol | Chain | Residues | | Ato | \mathbf{ms} | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|---------------|----------|---------|---------|-------|
| 9 | Ι | 127 | Total 1011 | C 639 | N 198 | 0 174 | 0 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| Ι | 58 | ARG | HIS | conflict | UNP P80374 |

• Molecule 10 is a protein called 30S ribosomal protein S10.



| Mol | Chain | Residues | | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 10 | J | 98 | Total 792 | C 498 | N 156 | O 137 | S 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---|---------|-------|
| 11 | K | 119 | Total 885 | C 549 | N 168 | 0 165 | ${ m S} { m 3}$ | 0 | 0 | 0 |

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

| Mol | Chain | Residues | | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 12 | L | 124 | Total 970 | C 611 | N 195 | O 163 | S 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---|---------|-------|
| 13 | М | 125 | Total 997 | C 617 | N 207 | 0 171 | ${S \over 2}$ | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|---------------|---------|---------|-------|
| 14 | Ν | 60 | Total 492 | C 312 | N 104 | 0 72 | $\frac{S}{4}$ | 0 | 0 | 0 |

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

| Mol | Chain | Residues | | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|---------|-------|
| 15 | Ο | 88 | Total 734 | C 459 | N 147 | O 126 | ${ m S} { m 2}$ | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 16 | Р | 83 | Total 700 | C 443 | N 139 | 0 117 | S 1 | 0 | 0 | 0 |

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



| Mol | Chain | Residues | | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---|---|---------|-------|
| 17 | Q | 104 | Total 857 | C 547 | N 161 | 0 147 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| Q | 96 | GLN | GLU | conflict | UNP P0DOY7 |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|---------|---------|-------|
| 18 | R | 73 | Total 597 | C 380 | N 118 | O 99 | 0 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| R | 60 | GLY | ALA | conflict | UNP Q5SLQ0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---|---------|---------|-------|
| 19 | S | 80 | Total 647 | C 414 | N 119 | 0 112 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|---------|-------|
| 20 | Т | 99 | Total 762 | C 469 | N 162 | 0 129 | ${ m S} { m 2}$ | 0 | 0 | 0 |

• Molecule 21 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|---|
| 21 | V | 24 | Total 208 | C 128 | N 50 | O 30 | 0 | 0 | 0 |

• Molecule 22 is a RNA chain called tRNA ASL Escherichia coli Arg2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|---------|---------|-------|
| 22 | Х | 11 | Total 232 | C 105 | N 43 | 0 74 | Р 10 | 0 | 0 | 0 |



• Molecule 23 is a RNA chain called mRNA A-site fragment.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|------|-------|----------|-------|---------|----|--------|---|---------|---------|-------|
| 23 W | 4 | Total | C | N 15 | 0 | P 2 | 0 | 0 | 0 | |
| | | | 82 | 38 | 15 | 20 | 3 | | | |

• Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 24 | А | 1 | Total | С | Ν | Ο | 0 | 0 |
| 24 | Π | T | 42 | 23 | 5 | 14 | 0 | |

• Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-------------------|---------|---------|
| 25 | А | 76 | Total Mg 76 76 | 0 | 0 |
| 25 | Е | 1 | Total Mg 1 1 | 0 | 0 |
| 25 | J | 1 | Total Mg 1 1 | 0 | 0 |

MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

| Property | Value | Source |
|--|-----------------------------|-----------|
| Space group | P 41 21 2 | Depositor |
| Cell constants | 403.73Å 403.73Å 177.42Å | Depositor |
| a, b, c, α , β , γ | 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.80 - 3.46 | Depositor |
| % Data completeness | 87 2 (49 80-3 46) | Depositor |
| (in resolution range) | 01.2 (45.00-5.40) | Depositor |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $< I/\sigma(I) > 1$ | $1.42 (at 3.48 \text{\AA})$ | Xtriage |
| Refinement program | PHENIX 1.8.4_1496 | Depositor |
| R, R_{free} | 0.203 , 0.234 | Depositor |
| Wilson B-factor ($Å^2$) | 136.3 | Xtriage |
| Anisotropy | 0.186 | Xtriage |
| L-test for twinning ² | $ < L >=0.43, < L^2>=0.26$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 52043 | wwPDB-VP |
| Average B, all atoms $(Å^2)$ | 141.0 | wwPDB-VP |

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 79 ligands modelled in this entry, 78 are monoatomic - leaving 1 for Mogul analysis.

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).

| Mol | Type | Chain | Res | Link | Bo | ond leng | \mathbf{ths} | Bond angles | | |
|-----|------|-------|------|------|----------|----------|----------------|-------------|------|----------|
| | Type | | | | Counts | RMSZ | # Z >2 | Counts | RMSZ | # Z >2 |
| 24 | PAR | А | 1601 | - | 45,45,45 | 1.27 | 6 (13%) | 64,67,67 | 1.67 | 13 (20%) |

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 | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 24 | PAR | А | 1601 | - | - | 6/18/94/94 | 0/4/4/4 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | $\mathrm{Ideal}(\mathrm{\AA})$ |
|-----|-------|------|------|---------|------|-------------|--------------------------------|
| 24 | А | 1601 | PAR | C64-C54 | 3.80 | 1.57 | 1.52 |
| 24 | А | 1601 | PAR | C13-C23 | 2.78 | 1.56 | 1.52 |
| 24 | А | 1601 | PAR | O54-C14 | 2.48 | 1.48 | 1.41 |
| 24 | А | 1601 | PAR | C52-C42 | 2.42 | 1.57 | 1.52 |
| 24 | А | 1601 | PAR | O43-C13 | 2.11 | 1.45 | 1.41 |
| 24 | A | 1601 | PAR | O33-C14 | 2.02 | 1.47 | 1.41 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|-------|------------------|---------------|
| 24 | А | 1601 | PAR | O33-C14-C24 | 6.71 | 119.77 | 108.22 |
| 24 | А | 1601 | PAR | C34-C24-N24 | -3.46 | 103.97 | 111.05 |
| 24 | А | 1601 | PAR | O52-C13-C23 | 3.22 | 114.62 | 107.96 |
| 24 | А | 1601 | PAR | C14-O33-C33 | -2.96 | 110.64 | 117.96 |
| 24 | А | 1601 | PAR | O34-C34-C44 | -2.83 | 103.81 | 110.35 |
| 24 | А | 1601 | PAR | O11-C11-O51 | 2.78 | 118.45 | 110.67 |
| 24 | А | 1601 | PAR | O52-C13-O43 | -2.77 | 108.43 | 111.43 |
| 24 | А | 1601 | PAR | C11-O51-C51 | 2.46 | 118.51 | 113.69 |
| 24 | А | 1601 | PAR | O54-C54-C44 | 2.44 | 114.12 | 109.69 |
| 24 | А | 1601 | PAR | O51-C51-C61 | 2.28 | 112.10 | 106.44 |
| 24 | А | 1601 | PAR | C13-O52-C52 | -2.27 | 112.35 | 117.96 |
| 24 | А | 1601 | PAR | C13-C23-C33 | 2.25 | 104.81 | 102.10 |
| 24 | А | 1601 | PAR | O34-C34-C24 | -2.02 | 106.59 | 110.22 |

There are no chirality outliers.



| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 24 | А | 1601 | PAR | O54-C54-C64-N64 |
| 24 | А | 1601 | PAR | C52-C42-O11-C11 |
| 24 | А | 1601 | PAR | O43-C13-O52-C52 |
| 24 | А | 1601 | PAR | C23-C13-O52-C52 |
| 24 | А | 1601 | PAR | C23-C33-O33-C14 |
| 24 | А | 1601 | PAR | C44-C54-C64-N64 |

All (6) torsion outliers are listed below:

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

