



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:18 PM GMT

PDB ID : 1JGP
Title : The Path of Messenger RNA Through the Ribosome. THIS FILE, 1JGP, CONTAINS THE 30S RIBOSOME SUBUNIT, THREE TRNA, AND MRNA MOLECULES. 50S RIBOSOME SUBUNIT IS IN THE FILE 1GIY
Authors : Yusupova, G.Z.; Yusupov, M.M.; Cate, J.H.D.; Noller, H.F.
Deposited on : 2001-06-26
Resolution : 7.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

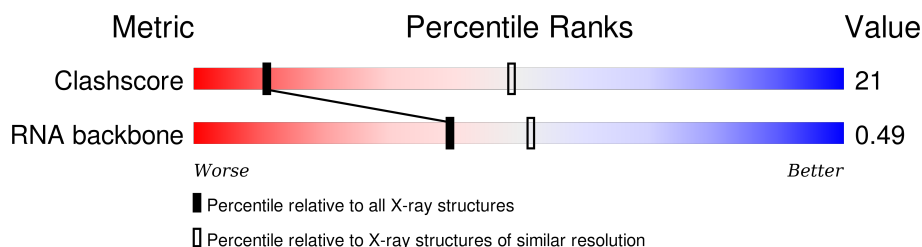
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 Å.

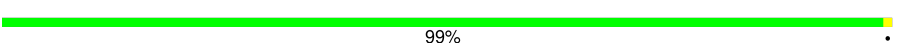


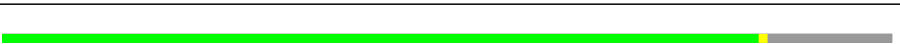

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|--------------|-----------------------------|---|
| Clashscore | 102246 | 1063 (10.00-3.70) |
| RNA backbone | 2183 | 1105 (10.00-2.80) |


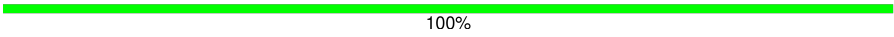
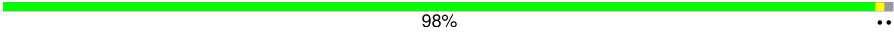
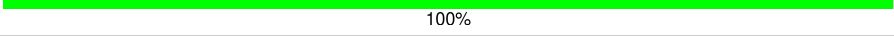
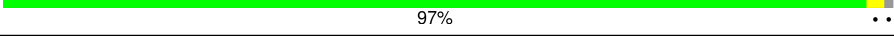



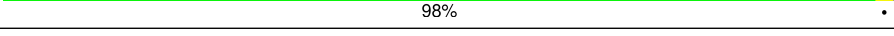
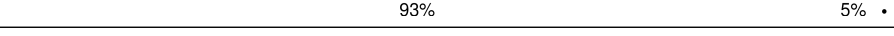
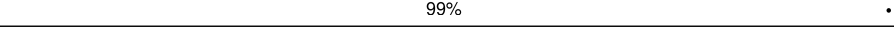
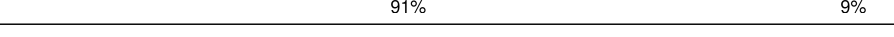
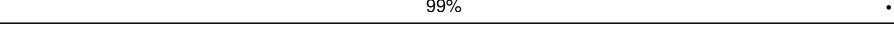
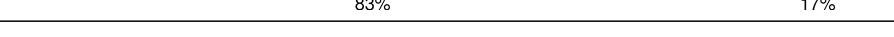

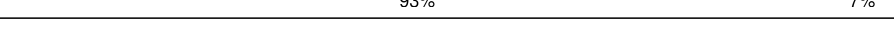
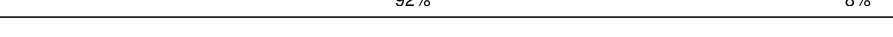
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 1522 |  99% . |
| 2 | B | 76 |  41% 45% 12% . |
| 2 | C | 76 |  38% 43% 14% . |
| 3 | D | 74 |  5% 31% 42% 22% |
| 4 | 1 | 36 |  69% 6% 11% . 11% |
| 5 | E | 256 |  91% 9% |
| 6 | F | 239 |  85% . 14% |
| 7 | G | 209 |  99% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | H | 162 |  |
| 9 | I | 101 |  |
| 10 | J | 156 |  |
| 11 | K | 138 |  |
| 12 | L | 128 |  |
| 13 | M | 105 |  |
| 14 | N | 129 |  |
| 15 | O | 135 |  |
| 16 | P | 126 |  |
| 17 | Q | 61 |  |
| 18 | R | 89 |  |
| 19 | S | 91 |  |
| 20 | T | 105 |  |
| 21 | U | 88 |  |
| 22 | V | 93 |  |
| 23 | W | 106 |  |
| 24 | X | 26 |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2 | M2G | B | 26 | - | - | X | - |
| 3 | 5MC | D | 49 | - | - | X | - |
| 3 | 4SU | D | 8 | - | - | X | - |

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 8935 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 30S 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|---------|---------|-------|
| 1 | A | 1519 | Total | P | 0 | 0 | 1519 |
| | | | 1519 | 1519 | | | |

- Molecule 2 is a RNA chain called tRNA(Phe).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2 | B | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1652 | 746 | 294 | 536 | 76 | | | |
| 2 | C | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1652 | 746 | 294 | 536 | 76 | | | |

There are 28 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------------|-----------|
| B | 10 | 2MG | G | TRNA MODIFICATION | GB 176479 |
| B | 16 | H2U | U | TRNA MODIFICATION | GB 176479 |
| B | 17 | H2U | U | TRNA MODIFICATION | GB 176479 |
| B | 26 | M2G | G | TRNA MODIFICATION | GB 176479 |
| B | 32 | OMC | C | TRNA MODIFICATION | GB 176479 |
| B | 34 | OMG | G | TRNA MODIFICATION | GB 176479 |
| B | 37 | YG | G | TRNA MODIFICATION | GB 176479 |
| B | 39 | PSU | U | TRNA MODIFICATION | GB 176479 |
| B | 40 | 5MC | C | TRNA MODIFICATION | GB 176479 |
| B | 46 | 7MG | G | TRNA MODIFICATION | GB 176479 |
| B | 49 | 5MC | C | TRNA MODIFICATION | GB 176479 |
| B | 54 | 5MU | U | TRNA MODIFICATION | GB 176479 |
| B | 55 | PSU | U | TRNA MODIFICATION | GB 176479 |
| B | 58 | 1MA | A | TRNA MODIFICATION | GB 176479 |
| C | 10 | 2MG | G | TRNA MODIFICATION | GB 176479 |
| C | 16 | H2U | U | TRNA MODIFICATION | GB 176479 |
| C | 17 | H2U | U | TRNA MODIFICATION | GB 176479 |
| C | 26 | M2G | G | TRNA MODIFICATION | GB 176479 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------------|-----------|
| C | 32 | OMC | C | TRNA MODIFICATION | GB 176479 |
| C | 34 | OMG | G | TRNA MODIFICATION | GB 176479 |
| C | 37 | YG | G | TRNA MODIFICATION | GB 176479 |
| C | 39 | PSU | U | TRNA MODIFICATION | GB 176479 |
| C | 40 | 5MC | C | TRNA MODIFICATION | GB 176479 |
| C | 46 | 7MG | G | TRNA MODIFICATION | GB 176479 |
| C | 49 | 5MC | C | TRNA MODIFICATION | GB 176479 |
| C | 54 | 5MU | U | TRNA MODIFICATION | GB 176479 |
| C | 55 | PSU | U | TRNA MODIFICATION | GB 176479 |
| C | 58 | 1MA | A | TRNA MODIFICATION | GB 176479 |

- Molecule 3 is a RNA chain called tRNA(Phe).

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 3 | D | 74 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1570 | 702 | 269 | 524 | 74 | 1 | | | |

- Molecule 4 is a RNA chain called MESSENGER RNA MV36.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|--|---------|---------|-------|
| 4 | 1 | 32 | Total | C | N | O | P | | 0 | 0 | 26 |
| | | | 146 | 54 | 12 | 48 | 32 | | | | |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 5 | E | 234 | Total | C | 0 | 0 | 234 |
| | | | 234 | 234 | | | |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 6 | F | 206 | Total | C | 0 | 0 | 206 |
| | | | 206 | 206 | | | |

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 7 | G | 208 | Total | C | 0 | 0 | 208 |
| | | | 208 | 208 | | | |

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 8 | H | 150 | Total | C | 0 | 0 | 150 |
| | | | 150 | 150 | | | |

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 9 | I | 101 | Total | C | 0 | 0 | 101 |
| | | | 101 | 101 | | | |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 10 | J | 155 | Total | C | 0 | 0 | 155 |
| | | | 155 | 155 | | | |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 11 | K | 138 | Total | C | 0 | 0 | 138 |
| | | | 138 | 138 | | | |

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 12 | L | 127 | Total | C | 0 | 0 | 127 |
| | | | 127 | 127 | | | |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---------|---------|-------|
| 13 | M | 98 | Total | C | 0 | 0 | 98 |
| | | | 98 | 98 | | | |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 14 | N | 119 | Total | C | 0 | 0 | 119 |
| | | | 119 | 119 | | | |

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 15 | O | 124 | Total | C | 0 | 0 | 124 |
| | | | 124 | 124 | | | |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 16 | P | 125 | Total | C | 0 | 0 | 125 |
| | | | 125 | 125 | | | |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S14.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---------|---------|-------|
| 17 | Q | 60 | Total | C | 0 | 0 | 60 |
| | | | 60 | 60 | | | |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---------|---------|-------|
| 18 | R | 88 | Total | C | 0 | 0 | 88 |
| | | | 88 | 88 | | | |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---------|---------|-------|
| 19 | S | 83 | Total | C | 0 | 0 | 83 |
| | | | 83 | 83 | | | |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 20 | T | 104 | Total | C | 0 | 0 | 104 |
| | | | 104 | 104 | | | |

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---------|---------|-------|
| 21 | U | 73 | Total | C | 0 | 0 | 73 |
| | | | 73 | 73 | | | |

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|------------------|---------|---------|-------|
| 22 | V | 80 | Total C 80 80 | 0 | 0 | 80 |

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|------------------|---------|---------|-------|
| 23 | W | 99 | Total C 99 99 | 0 | 0 | 99 |

- Molecule 24 is a protein called 30S RIBOSOMAL PROTEIN THX.

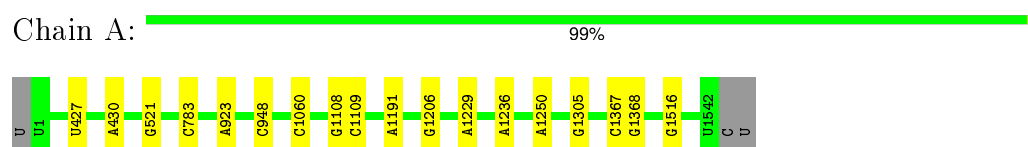
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf | Trace |
|-----|-------|----------|------------------|---------|---------|-------|
| 24 | X | 24 | Total C 24 24 | 0 | 0 | 24 |

3 Residue-property plots

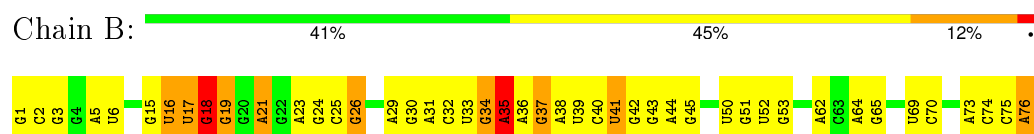
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

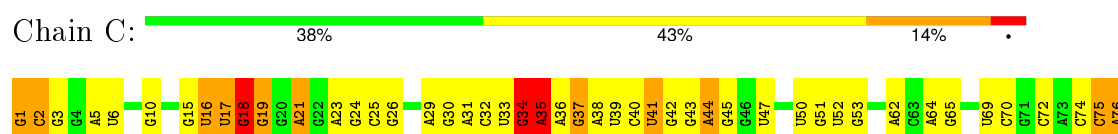
- Molecule 1: 30S 16S ribosomal RNA



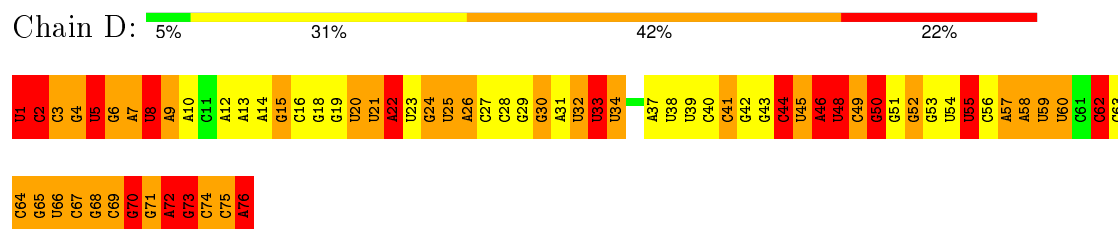
- Molecule 2: tRNA(Phe)



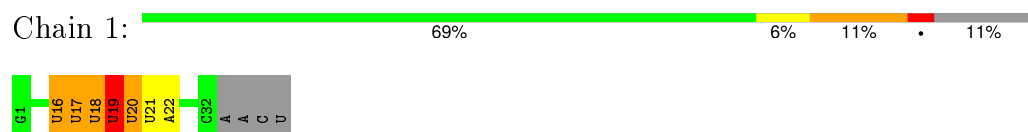
- Molecule 2: tRNA(Phe)



- Molecule 3: tRNA(Phe)

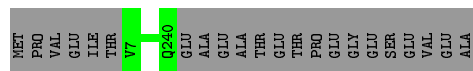


- Molecule 4: MESSENGER RNA MV36




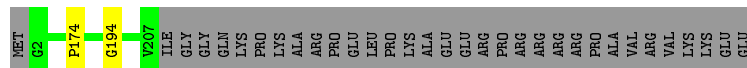
- Molecule 5: 30S RIBOSOMAL PROTEIN S2

Chain E:  91% 9%



- Molecule 6: 30S RIBOSOMAL PROTEIN S3

Chain F:  85% 14%



- Molecule 7: 30S RIBOSOMAL PROTEIN S4

Chain G:  99%



- Molecule 8: 30S RIBOSOMAL PROTEIN S5

Chain H:  92% 7%



- Molecule 9: 30S RIBOSOMAL PROTEIN S6

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: 30S RIBOSOMAL PROTEIN S7

Chain J:  98%



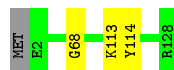
- Molecule 11: 30S RIBOSOMAL PROTEIN S8

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: 30S RIBOSOMAL PROTEIN S9

Chain L:  97%



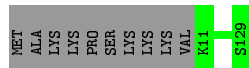
- Molecule 13: 30S RIBOSOMAL PROTEIN S10

Chain M:  90% 7%



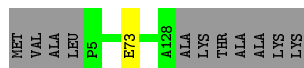
- Molecule 14: 30S RIBOSOMAL PROTEIN S11

Chain N:  92% 8%



- Molecule 15: 30S RIBOSOMAL PROTEIN S12

Chain O:  91% 8%



- Molecule 16: 30S RIBOSOMAL PROTEIN S13

Chain P:  98% ..



- Molecule 17: 30S RIBOSOMAL PROTEIN S14

Chain Q:  93% 5%




- Molecule 18: 30S RIBOSOMAL PROTEIN S15

Chain R:  99%



- Molecule 19: 30S RIBOSOMAL PROTEIN S16

Chain S:  91% 9%



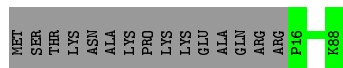
- Molecule 20: 30S RIBOSOMAL PROTEIN S17

Chain T:  99%



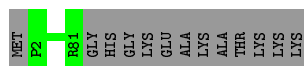
- Molecule 21: 30S RIBOSOMAL PROTEIN S18

Chain U: 83% 17%



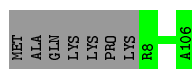
- Molecule 22: 30S RIBOSOMAL PROTEIN S19

Chain V: 86% 14%



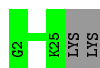
- Molecule 23: 30S RIBOSOMAL PROTEIN S20

Chain W: 93% 7%



- Molecule 24: 30S RIBOSOMAL PROTEIN THX

Chain X: 92% 8%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | I 4 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 507.20Å 507.20Å 803.66Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 250.00 – 7.00 | Depositor |
| % Data completeness (in resolution range) | 89.5 (250.00-7.00) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.09 | Depositor |
| Refinement program | O | Depositor |
| R, R_{free} | (Not available) , (Not available) | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 8935 | wwPDB-VP |
| Average B, all atoms (Å ²) | 0.0 | wwPDB-VP |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, M2G, OMG, H2U, YG, 2MG, 5MC, 1MA, 4SU, 7MG, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 2 | B | 1.21 | 4/1486 (0.3%) | 1.43 | 13/2311 (0.6%) |
| 2 | C | 1.44 | 7/1487 (0.5%) | 1.47 | 22/2315 (1.0%) |
| 3 | D | 1.95 | 17/1616 (1.1%) | 2.85 | 154/2512 (6.1%) |
| 4 | 1 | 2.35 | 5/131 (3.8%) | 2.46 | 3/200 (1.5%) |
| All | All | 1.60 | 33/4720 (0.7%) | 2.07 | 192/7338 (2.6%) |

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 |
|-----|-------|---------------------|---------------------|
| 2 | B | 0 | 3 |
| 2 | C | 0 | 3 |
| All | All | 0 | 6 |

The worst 5 of 33 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3 | D | 33 | U | O3'-P | 31.20 | 1.98 | 1.61 |
| 2 | C | 74 | C | O3'-P | -27.00 | 1.28 | 1.61 |
| 2 | B | 75 | C | O3'-P | -26.77 | 1.29 | 1.61 |
| 2 | C | 75 | C | O3'-P | -25.61 | 1.30 | 1.61 |
| 3 | D | 15 | G | O3'-P | 24.09 | 1.90 | 1.61 |

The worst 5 of 192 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | B | 35 | A | P-O3'-C3' | 41.11 | 169.03 | 119.70 |
| 3 | D | 25 | U | P-O3'-C3' | 31.41 | 157.40 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 3 | D | 75 | C | P-O3'-C3' | -29.51 | 84.29 | 119.70 |
| 4 | 1 | 18 | U | P-O3'-C3' | 27.61 | 152.83 | 119.70 |
| 3 | D | 8 | 4SU | O3'-P-O5' | -27.11 | 52.48 | 104.00 |

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | B | 18 | G | Sidechain |
| 2 | B | 19 | G | Sidechain |
| 2 | B | 62 | A | Sidechain |
| 2 | C | 18 | G | Sidechain |
| 2 | C | 19 | G | Sidechain |

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1519 | 0 | 0 | 15 | 0 |
| 2 | B | 1652 | 0 | 862 | 56 | 0 |
| 2 | C | 1652 | 0 | 862 | 53 | 0 |
| 3 | D | 1570 | 0 | 801 | 105 | 0 |
| 4 | 1 | 146 | 0 | 61 | 6 | 0 |
| 5 | E | 234 | 0 | 0 | 0 | 0 |
| 6 | F | 206 | 0 | 0 | 2 | 0 |
| 7 | G | 208 | 0 | 0 | 2 | 0 |
| 8 | H | 150 | 0 | 0 | 1 | 0 |
| 9 | I | 101 | 0 | 0 | 0 | 0 |
| 10 | J | 155 | 0 | 0 | 4 | 0 |
| 11 | K | 138 | 0 | 0 | 0 | 0 |
| 12 | L | 127 | 0 | 0 | 3 | 0 |
| 13 | M | 98 | 0 | 0 | 5 | 0 |
| 14 | N | 119 | 0 | 0 | 0 | 0 |
| 15 | O | 124 | 0 | 0 | 1 | 0 |
| 16 | P | 125 | 0 | 0 | 2 | 0 |
| 17 | Q | 60 | 0 | 0 | 4 | 0 |
| 18 | R | 88 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | S | 83 | 0 | 0 | 0 | 0 |
| 20 | T | 104 | 0 | 0 | 0 | 0 |
| 21 | U | 73 | 0 | 0 | 0 | 0 |
| 22 | V | 80 | 0 | 0 | 0 | 0 |
| 23 | W | 99 | 0 | 0 | 0 | 0 |
| 24 | X | 24 | 0 | 0 | 0 | 0 |
| All | All | 8935 | 0 | 2586 | 237 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 237 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------|--------------|--------------------------|-------------------|
| 2:C:1:G:N2 | 2:C:2:C:H41 | 1.22 | 1.34 |
| 1:A:430:A:P | 7:G:7:PRO:CA | 2.16 | 1.32 |
| 3:D:75:C:C2' | 3:D:76:A:H5' | 1.59 | 1.30 |
| 2:C:1:G:N2 | 2:C:2:C:N4 | 1.77 | 1.29 |
| 3:D:75:C:H2' | 3:D:76:A:C5' | 1.62 | 1.27 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 1 | A | 0/1522 | - | - |
| 2 | B | 74/76 (97%) | 13 (17%) | 3 (4%) |
| 2 | C | 75/76 (98%) | 13 (17%) | 3 (4%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|----------------|-------------------|-----------------|
| 3 | D | 73/74 (98%) | 26 (35%) | 2 (2%) |
| 4 | 1 | 5/36 (13%) | 1 (20%) | 0 |
| All | All | 227/1784 (12%) | 53 (23%) | 8 (3%) |

5 of 53 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 2 | C |
| 2 | B | 3 | G |
| 2 | B | 17 | H2U |
| 2 | B | 18 | G |
| 2 | B | 19 | G |

5 of 8 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 16 | H2U |
| 3 | D | 33 | U |
| 2 | C | 35 | A |
| 2 | B | 35 | A |
| 2 | C | 18 | G |

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

34 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).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 2 | 2MG | B | 10 | 2 | 17,26,27 | 1.05 | 1 (5%) | 21,38,41 | 2.65 | 5 (23%) |
| 2 | H2U | B | 16 | 2 | 17,21,22 | 0.79 | 1 (5%) | 23,30,33 | 1.14 | 3 (13%) |
| 2 | H2U | B | 17 | 2 | 17,21,22 | 0.73 | 0 | 23,30,33 | 1.05 | 2 (8%) |
| 2 | M2G | B | 26 | 2 | 17,27,28 | 1.24 | 3 (17%) | 22,40,43 | 2.16 | 2 (9%) |
| 2 | OMC | B | 32 | 2 | 13,22,23 | 0.74 | 0 | 20,31,34 | 0.91 | 1 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | OMG | B | 34 | 2,4 | 17,26,27 | 1.28 | 2 (11%) | 21,38,41 | 2.64 | 3 (14%) |
| 2 | YG | B | 37 | 2 | 27,42,43 | 1.02 | 1 (3%) | 29,62,65 | 2.22 | 8 (27%) |
| 2 | PSU | B | 39 | 2 | 13,21,22 | 1.30 | 2 (15%) | 18,30,33 | 6.15 | 4 (22%) |
| 2 | 5MC | B | 40 | 2 | 13,22,23 | 0.91 | 1 (7%) | 15,32,35 | 0.84 | 1 (6%) |
| 2 | 7MG | B | 46 | 2 | 19,26,27 | 1.12 | 2 (10%) | 24,39,42 | 2.17 | 3 (12%) |
| 2 | 5MC | B | 49 | 2 | 13,22,23 | 1.01 | 1 (7%) | 15,32,35 | 0.90 | 1 (6%) |
| 2 | 5MU | B | 54 | 2 | 12,22,23 | 1.32 | 2 (16%) | 14,32,35 | 4.62 | 2 (14%) |
| 2 | PSU | B | 55 | 2 | 13,21,22 | 1.53 | 2 (15%) | 18,30,33 | 6.05 | 6 (33%) |
| 2 | 1MA | B | 58 | 2 | 14,25,26 | 3.19 | 3 (21%) | 15,37,40 | 2.35 | 2 (13%) |
| 2 | 2MG | C | 10 | 2 | 17,26,27 | 1.05 | 1 (5%) | 21,38,41 | 2.65 | 5 (23%) |
| 2 | H2U | C | 16 | 2 | 17,21,22 | 0.79 | 1 (5%) | 23,30,33 | 1.14 | 3 (13%) |
| 2 | H2U | C | 17 | 2 | 17,21,22 | 0.76 | 0 | 23,30,33 | 1.07 | 2 (8%) |
| 2 | M2G | C | 26 | 2 | 17,27,28 | 1.24 | 3 (17%) | 22,40,43 | 2.16 | 2 (9%) |
| 2 | OMC | C | 32 | 2 | 13,22,23 | 0.75 | 0 | 20,31,34 | 0.91 | 1 (5%) |
| 2 | OMG | C | 34 | 2,4 | 17,26,27 | 1.27 | 2 (11%) | 21,38,41 | 2.64 | 3 (14%) |
| 2 | YG | C | 37 | 2 | 27,42,43 | 1.03 | 1 (3%) | 29,62,65 | 2.22 | 8 (27%) |
| 2 | PSU | C | 39 | 2 | 13,21,22 | 1.30 | 2 (15%) | 18,30,33 | 6.15 | 4 (22%) |
| 2 | 5MC | C | 40 | 2 | 13,22,23 | 0.90 | 1 (7%) | 15,32,35 | 0.84 | 1 (6%) |
| 2 | 7MG | C | 46 | 2 | 19,26,27 | 1.12 | 2 (10%) | 24,39,42 | 2.16 | 3 (12%) |
| 2 | 5MC | C | 49 | 2 | 13,22,23 | 1.00 | 1 (7%) | 15,32,35 | 0.90 | 1 (6%) |
| 2 | 5MU | C | 54 | 2 | 12,22,23 | 1.31 | 2 (16%) | 14,32,35 | 4.62 | 2 (14%) |
| 2 | PSU | C | 55 | 2 | 13,21,22 | 1.52 | 2 (15%) | 18,30,33 | 6.03 | 6 (33%) |
| 2 | 1MA | C | 58 | 2 | 14,25,26 | 3.21 | 3 (21%) | 15,37,40 | 2.34 | 2 (13%) |
| 3 | H2U | D | 20 | 3 | 17,21,22 | 0.38 | 0 | 23,30,33 | 0.75 | 1 (4%) |
| 3 | H2U | D | 21 | 3 | 17,21,22 | 0.58 | 0 | 23,30,33 | 0.68 | 0 |
| 3 | 5MC | D | 49 | 3 | 13,22,23 | 0.93 | 1 (7%) | 15,32,35 | 1.14 | 1 (6%) |
| 3 | 5MU | D | 54 | 3 | 12,22,23 | 1.00 | 1 (8%) | 14,32,35 | 3.18 | 2 (14%) |
| 3 | PSU | D | 55 | 3 | 13,21,22 | 1.62 | 3 (23%) | 18,30,33 | 6.44 | 5 (27%) |
| 3 | 4SU | D | 8 | 3 | 11,21,22 | 1.50 | 1 (9%) | 13,30,33 | 2.53 | 1 (7%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | 2MG | B | 10 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | H2U | B | 16 | 2 | - | 0/7/38/39 | 0/2/2/2 |
| 2 | H2U | B | 17 | 2 | - | 0/7/38/39 | 0/2/2/2 |
| 2 | M2G | B | 26 | 2 | - | 0/7/29/30 | 0/3/3/3 |
| 2 | OMC | B | 32 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | OMG | B | 34 | 2,4 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | YG | B | 37 | 2 | - | 0/20/42/43 | 0/4/4/4 |
| 2 | PSU | B | 39 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 5MC | B | 40 | 2 | - | 0/3/25/26 | 0/2/2/2 |
| 2 | 7MG | B | 46 | 2 | - | 0/7/37/38 | 0/3/3/3 |
| 2 | 5MC | B | 49 | 2 | - | 0/3/25/26 | 0/2/2/2 |
| 2 | 5MU | B | 54 | 2 | - | 0/3/25/26 | 0/2/2/2 |
| 2 | PSU | B | 55 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 1MA | B | 58 | 2 | - | 0/3/25/26 | 0/3/3/3 |
| 2 | 2MG | C | 10 | 2 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | H2U | C | 16 | 2 | - | 0/7/38/39 | 0/2/2/2 |
| 2 | H2U | C | 17 | 2 | - | 0/7/38/39 | 0/2/2/2 |
| 2 | M2G | C | 26 | 2 | - | 0/7/29/30 | 0/3/3/3 |
| 2 | OMC | C | 32 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | OMG | C | 34 | 2,4 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | YG | C | 37 | 2 | - | 0/20/42/43 | 0/4/4/4 |
| 2 | PSU | C | 39 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 5MC | C | 40 | 2 | - | 0/3/25/26 | 0/2/2/2 |
| 2 | 7MG | C | 46 | 2 | - | 0/7/37/38 | 0/3/3/3 |
| 2 | 5MC | C | 49 | 2 | - | 0/3/25/26 | 0/2/2/2 |
| 2 | 5MU | C | 54 | 2 | - | 0/3/25/26 | 0/2/2/2 |
| 2 | PSU | C | 55 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 1MA | C | 58 | 2 | - | 0/3/25/26 | 0/3/3/3 |
| 3 | H2U | D | 20 | 3 | - | 0/7/38/39 | 0/2/2/2 |
| 3 | H2U | D | 21 | 3 | - | 0/7/38/39 | 0/2/2/2 |
| 3 | 5MC | D | 49 | 3 | - | 0/3/25/26 | 0/2/2/2 |
| 3 | 5MU | D | 54 | 3 | - | 0/3/25/26 | 0/2/2/2 |
| 3 | PSU | D | 55 | 3 | - | 0/7/25/26 | 0/2/2/2 |
| 3 | 4SU | D | 8 | 3 | - | 0/3/25/26 | 0/2/2/2 |

The worst 5 of 48 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | B | 39 | PSU | C6-C5 | -3.29 | 1.33 | 1.38 |
| 2 | C | 39 | PSU | C6-C5 | -3.26 | 1.33 | 1.38 |
| 2 | B | 55 | PSU | C6-C5 | -2.92 | 1.34 | 1.38 |
| 3 | D | 55 | PSU | C6-C5 | -2.92 | 1.34 | 1.38 |
| 2 | C | 55 | PSU | C6-C5 | -2.87 | 1.34 | 1.38 |

The worst 5 of 96 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 3 | D | 55 | PSU | N1-C2-N3 | -22.54 | 113.95 | 128.33 |
| 2 | B | 39 | PSU | N1-C2-N3 | -22.05 | 114.26 | 128.33 |
| 2 | C | 39 | PSU | N1-C2-N3 | -22.01 | 114.29 | 128.33 |
| 2 | B | 55 | PSU | N1-C2-N3 | -21.88 | 114.37 | 128.33 |
| 2 | C | 55 | PSU | N1-C2-N3 | -21.80 | 114.43 | 128.33 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 73 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | B | 16 | H2U | 5 | 0 |
| 2 | B | 17 | H2U | 4 | 0 |
| 2 | B | 26 | M2G | 14 | 0 |
| 2 | B | 32 | OMC | 1 | 0 |
| 2 | B | 34 | OMG | 2 | 0 |
| 2 | B | 37 | YG | 7 | 0 |
| 2 | B | 39 | PSU | 1 | 0 |
| 2 | B | 40 | 5MC | 3 | 0 |
| 2 | C | 10 | 2MG | 3 | 0 |
| 2 | C | 16 | H2U | 4 | 0 |
| 2 | C | 17 | H2U | 4 | 0 |
| 2 | C | 26 | M2G | 6 | 0 |
| 2 | C | 32 | OMC | 1 | 0 |
| 2 | C | 34 | OMG | 3 | 0 |
| 2 | C | 37 | YG | 7 | 0 |
| 2 | C | 39 | PSU | 1 | 0 |
| 2 | C | 40 | 5MC | 3 | 0 |
| 3 | D | 20 | H2U | 2 | 0 |
| 3 | D | 49 | 5MC | 8 | 0 |
| 3 | D | 54 | 5MU | 2 | 0 |
| 3 | D | 55 | PSU | 3 | 0 |
| 3 | D | 8 | 4SU | 9 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.