



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 17, 2017 – 08:24 PM EDT

PDB ID : 5A8L
EMDB ID: : EMD-3099
Title : Human eRF1 and the hCMV nascent peptide in the translation termination complex
Authors : Matheisl, S.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : unknown
Resolution : 3.80 Å(reported)
Based on PDB ID : 3E1Y

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

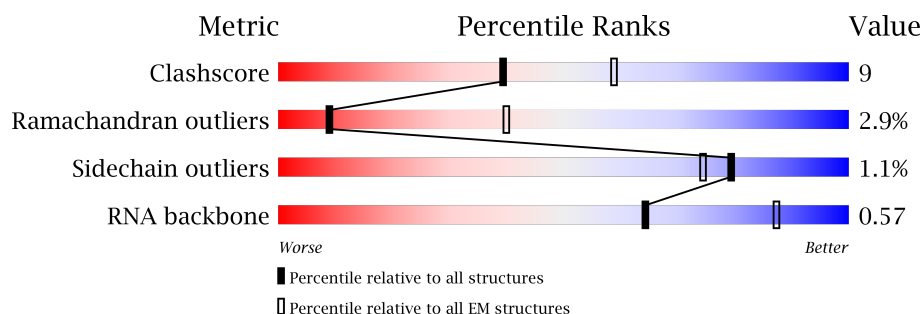
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

i


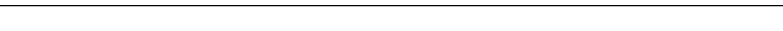
ELECTRON MICROSCOPY

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.



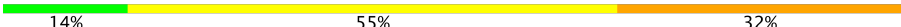
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |
| RNA backbone | 3398 | 335 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 5025 |  |
| 2 | B | 1869 |  |
| 3 | D | 184 |  |
| 4 | G | 165 |  |
| 5 | H | 427 |  |
| 6 | P | 18 |  |
| 7 | Q | 431 |  |
| 8 | R | 9 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 9 | Z | 22 |  14%55%32% |

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12264 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 28S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 1 | A | 253 | Total | C | N | O | P | 0 | 0 |
| | | | 5401 | 2413 | 971 | 1764 | 253 | | |

- Molecule 2 is a RNA chain called HUMAN 18S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2 | B | 67 | Total | C | N | O | P | 0 | 0 |
| | | | 1423 | 636 | 252 | 468 | 67 | | |

- Molecule 3 is a protein called 60S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3 | D | 21 | Total | C | N | O | S | 0 | 0 |
| | | | 179 | 110 | 40 | 27 | 2 | | |

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | G | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1046 | 654 | 196 | 193 | 3 | | |

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 5 | H | 12 | Total | C | N | O | 0 | 0 |
| | | | 88 | 49 | 24 | 15 | | |

- Molecule 6 is a RNA chain called P-SITE TRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 6 | P | 18 | Total | C | N | O | P | 0 | 0 |
| | | | 382 | 172 | 71 | 122 | 17 | | |

- Molecule 7 is a protein called EUKARYOTIC RELEASE FACTOR ERF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7 | Q | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3410 | 2168 | 575 | 655 | 12 | | |

- Molecule 8 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 8 | R | 9 | Total | C | N | O | P | 0 | 0 |
| | | | 190 | 86 | 35 | 60 | 9 | | |

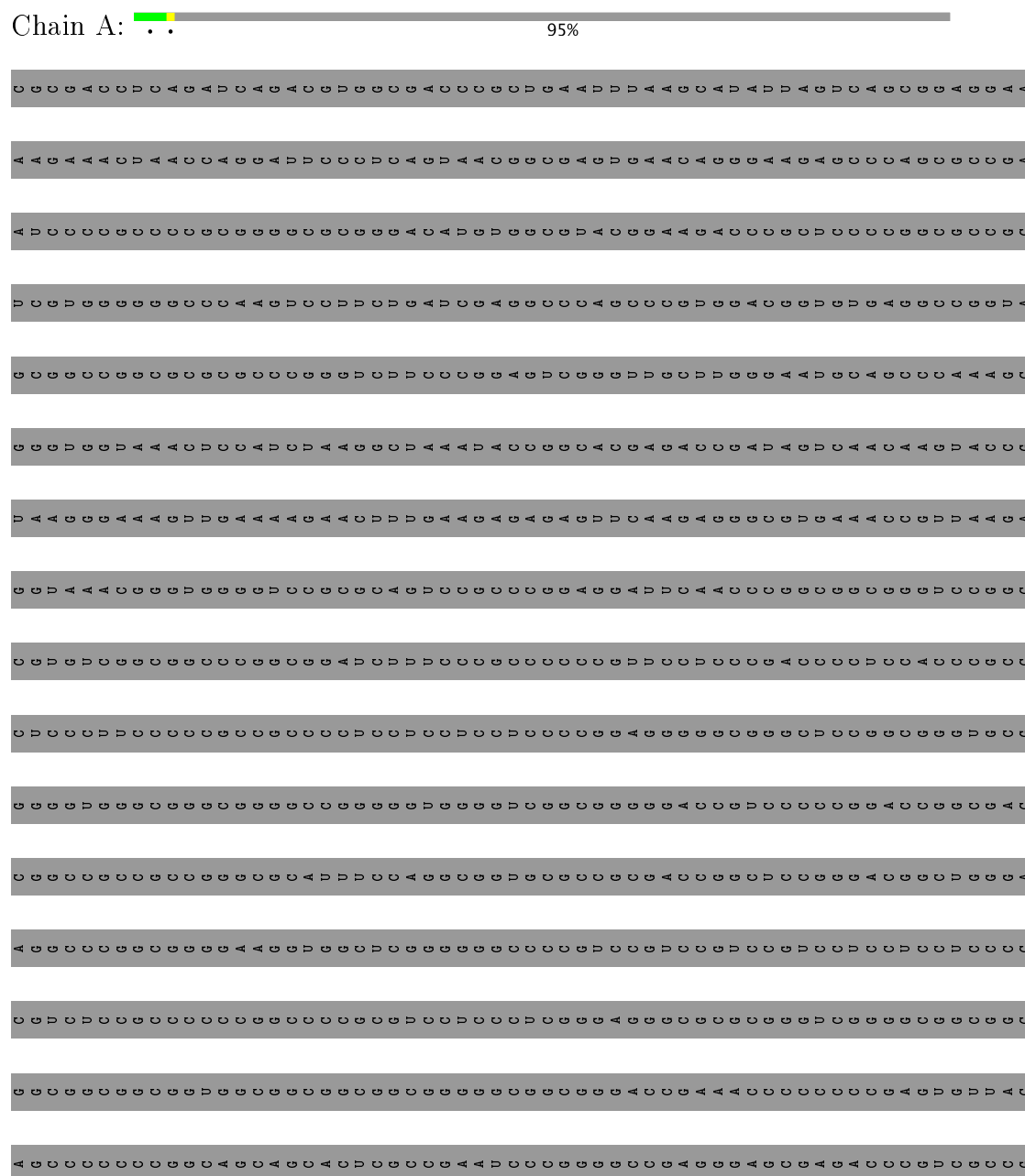
- Molecule 9 is a protein called NASCENT CHAIN.

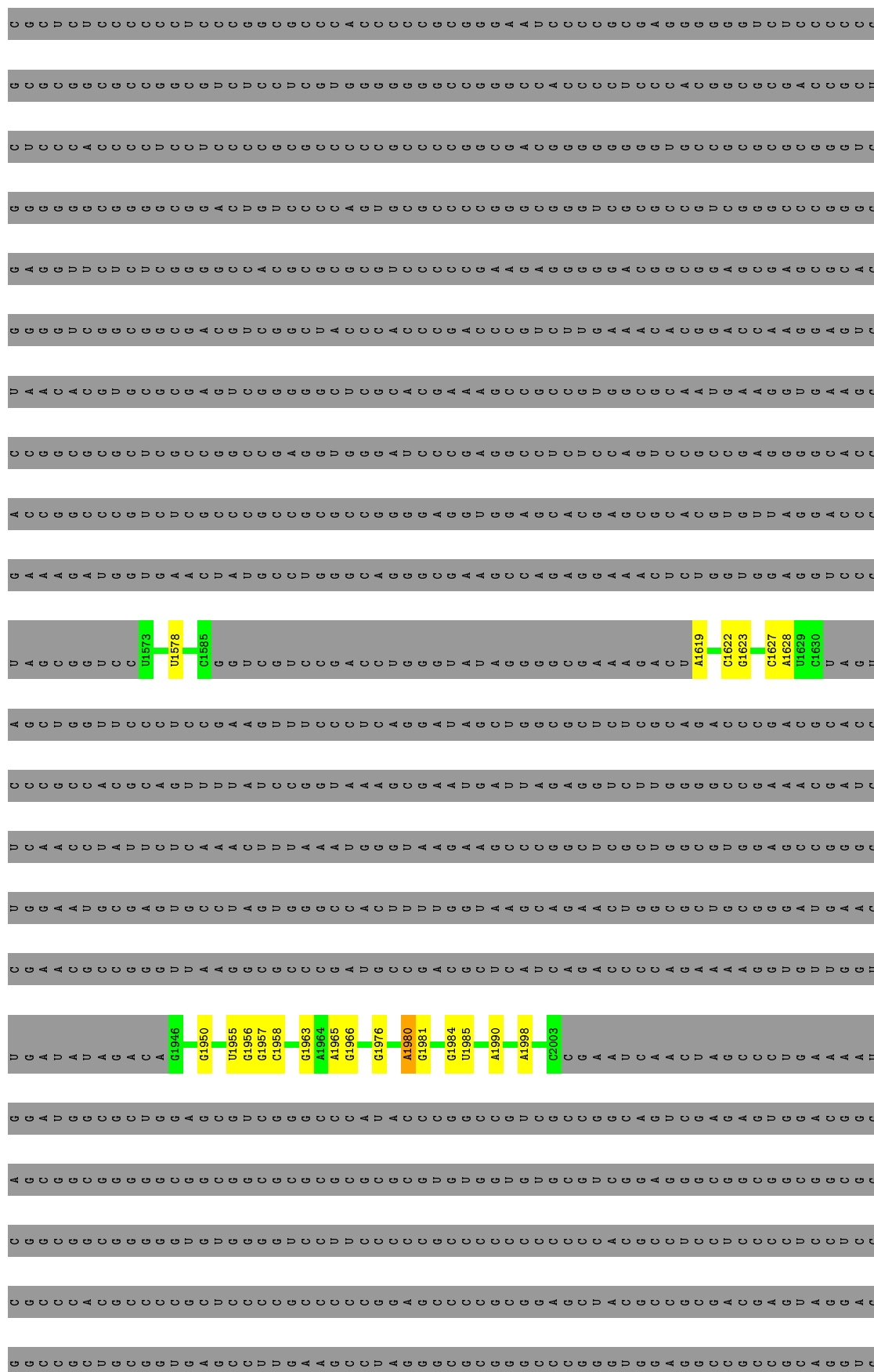
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 9 | Z | 22 | Total | C | N | O | S | 0 | 0 |
| | | | 145 | 92 | 25 | 27 | 1 | | |

3 Residue-property plots

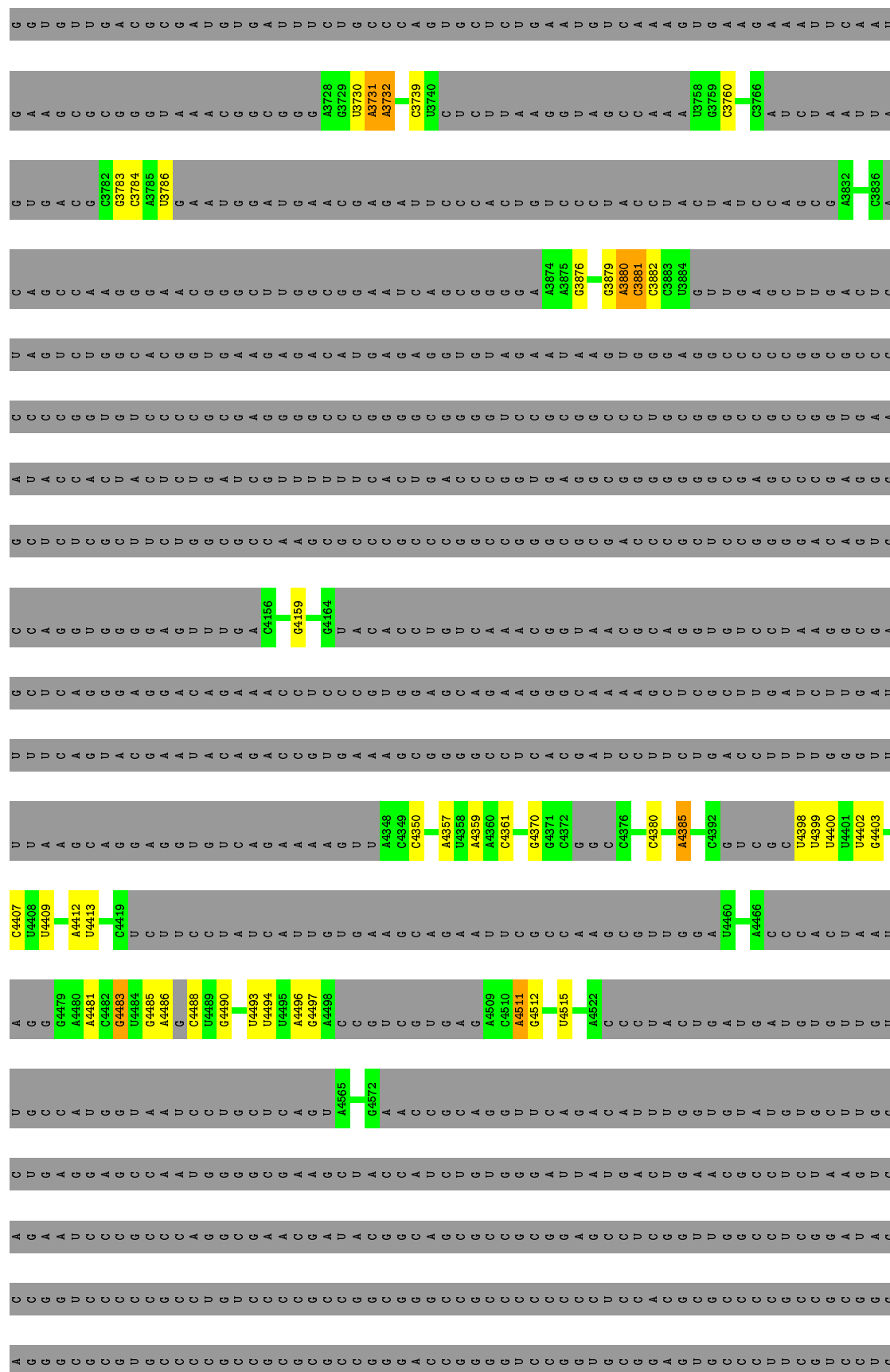
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 28S RIBOSOMAL RNA





3D visualization of a protein structure, likely a viral capsid, showing a hexameric arrangement of subunits. The structure is composed of numerous amino acid residues, each represented by a colored sphere. The residues are color-coded by type: Carbon (C) is light blue, Oxygen (O) is red, Nitrogen (N) is green, and Hydrogen (H) is white. The structure is shown in a perspective view, with a central core and an outer shell. The residues are arranged in a highly ordered, repeating pattern, characteristic of a viral capsid. The structure is labeled with 'A3614' and 'U3617' at the bottom, indicating specific residues or regions of interest.

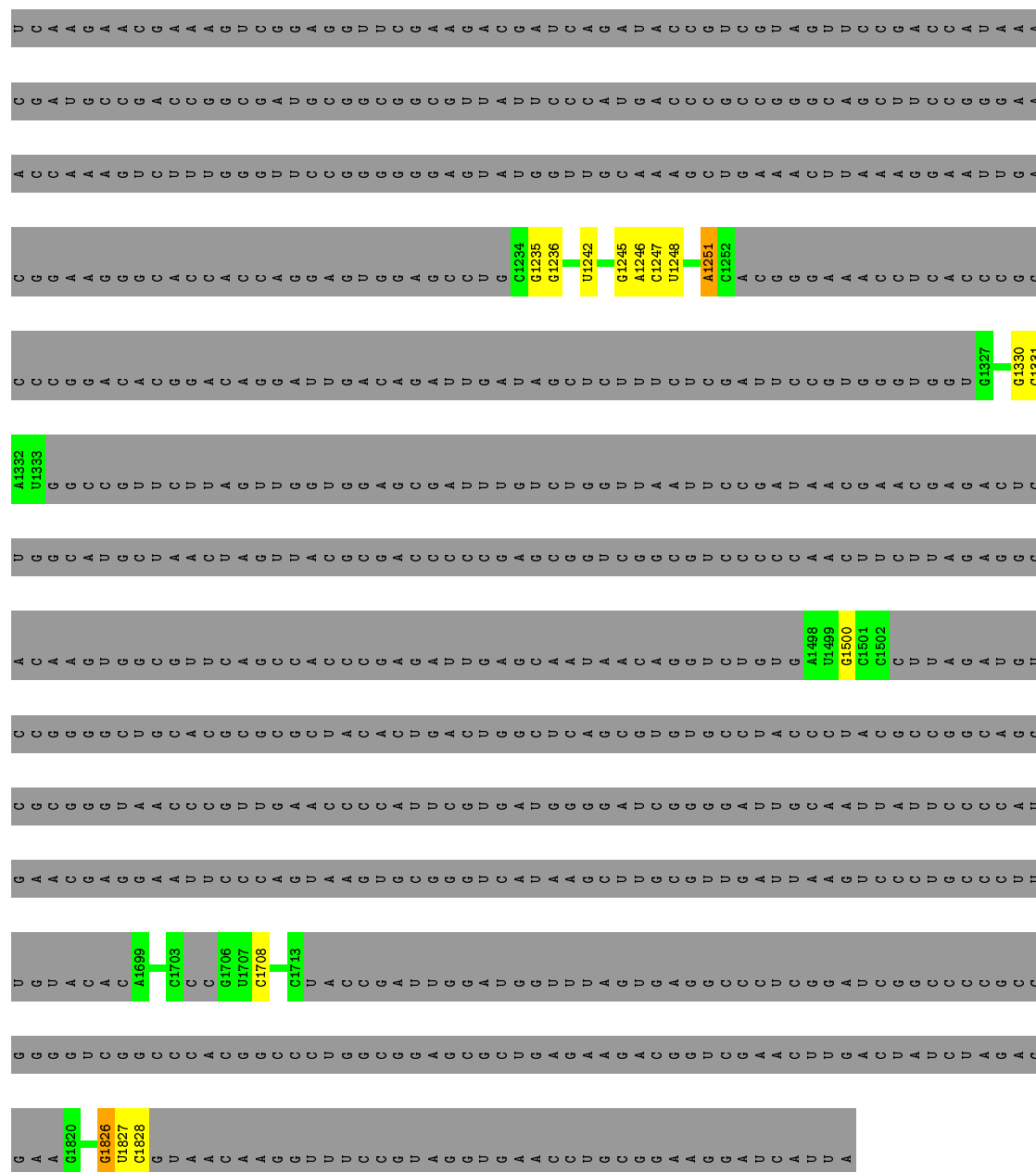


[illegible]

- Molecule 2: HUMAN 18S RIBOSOMAL RNA

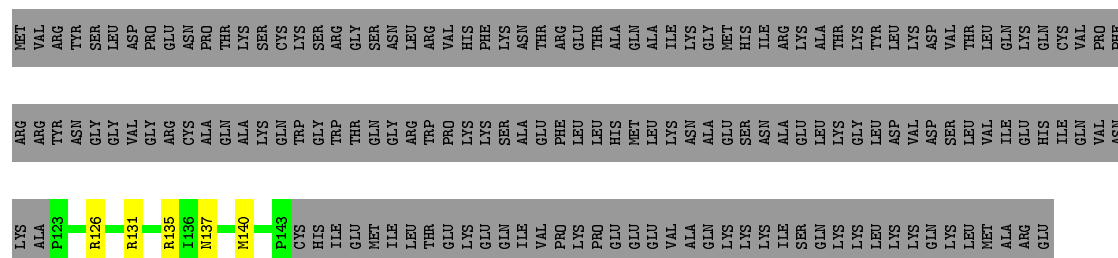
Chain B: 96%

[illegible]

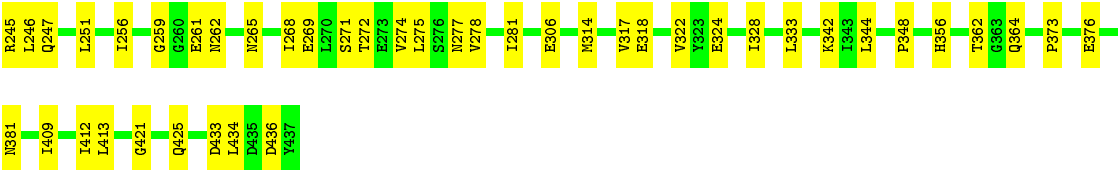


• Molecule 3: 60S RIBOSOMAL PROTEIN L17

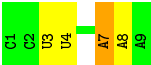
Chain D: 9% . 89%



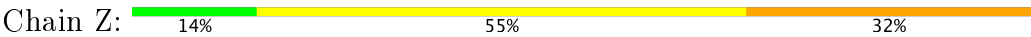
- Molecule 4: 60S RIBOSOMAL PROTEIN L12



• Molecule 8: MRNA



• Molecule 9: NASCENT CHAIN



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 33165 | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | DEFOCUS GROUPS | Depositor |
| Microscope | FEI TECNAI F20 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 2700 | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-------------|
| | | RMSZ | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | A | 0.11 | 0/6024 | 0.66 | 0/9344 |
| 2 | B | 0.11 | 0/1582 | 0.65 | 0/2445 |
| 3 | D | 0.48 | 0/184 | 0.53 | 0/244 |
| 4 | G | 0.36 | 0/1058 | 0.50 | 0/1424 |
| 5 | H | 0.18 | 0/88 | 0.30 | 0/114 |
| 6 | P | 0.10 | 0/426 | 0.63 | 0/660 |
| 7 | Q | 0.27 | 0/3467 | 0.42 | 0/4661 |
| 8 | R | 0.17 | 0/212 | 0.69 | 0/327 |
| 9 | Z | 0.52 | 0/147 | 0.78 | 0/195 |
| All | All | 0.21 | 0/13188 | 0.60 | 0/19414 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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 | 5401 | 0 | 2742 | 46 | 0 |
| 2 | B | 1423 | 0 | 730 | 9 | 0 |
| 3 | D | 179 | 0 | 184 | 4 | 0 |
| 4 | G | 1046 | 0 | 1116 | 18 | 0 |
| 5 | H | 88 | 0 | 86 | 3 | 0 |
| 6 | P | 382 | 0 | 197 | 3 | 0 |
| 7 | Q | 3410 | 0 | 3419 | 84 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8 | R | 190 | 0 | 98 | 3 | 0 |
| 9 | Z | 145 | 0 | 145 | 49 | 0 |
| All | All | 12264 | 0 | 8717 | 179 | 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 9.

The worst 5 of 179 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) |
|----------------|----------------|--------------------------|-------------------|
| 9:Z:15:LEU:CA | 9:Z:18:LYS:HE3 | 1.62 | 1.29 |
| 9:Z:8:ALA:O | 9:Z:12:SER:HB3 | 1.22 | 1.26 |
| 9:Z:15:LEU:O | 9:Z:18:LYS:HD2 | 1.23 | 1.26 |
| 1:A:3880:A:H2' | 9:Z:19:TYR:CE2 | 1.82 | 1.14 |
| 9:Z:9:LYS:HD2 | 9:Z:11:LEU:HB2 | 1.15 | 1.14 |

There are no symmetry-related clashes.

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 | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 3 | D | 19/184 (10%) | 18 (95%) | 1 (5%) | 0 | 100 | 100 |
| 4 | G | 136/165 (82%) | 103 (76%) | 27 (20%) | 6 (4%) | 3 | 32 |
| 5 | H | 10/427 (2%) | 10 (100%) | 0 | 0 | 100 | 100 |
| 7 | Q | 429/431 (100%) | 390 (91%) | 33 (8%) | 6 (1%) | 13 | 54 |
| 9 | Z | 20/22 (91%) | 12 (60%) | 2 (10%) | 6 (30%) | 0 | 0 |
| All | All | 614/1229 (50%) | 533 (87%) | 63 (10%) | 18 (3%) | 9 | 41 |

5 of 18 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | G | 98 | ILE |
| 4 | G | 109 | ILE |
| 7 | Q | 242 | PHE |
| 9 | Z | 3 | PRO |
| 9 | Z | 4 | LEU |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3 | D | 19/163 (12%) | 19 (100%) | 0 | 100 | 100 |
| 4 | G | 114/137 (83%) | 114 (100%) | 0 | 100 | 100 |
| 5 | H | 8/348 (2%) | 8 (100%) | 0 | 100 | 100 |
| 7 | Q | 371/371 (100%) | 371 (100%) | 0 | 100 | 100 |
| 9 | Z | 15/21 (71%) | 9 (60%) | 6 (40%) | 0 | 0 |
| All | All | 527/1040 (51%) | 521 (99%) | 6 (1%) | 79 | 89 |

5 of 6 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | Z | 13 | SER |
| 9 | Z | 19 | TYR |
| 9 | Z | 15 | LEU |
| 9 | Z | 10 | LYS |
| 9 | Z | 18 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | Q | 132 | HIS |
| 7 | Q | 366 | HIS |
| 7 | Q | 265 | ASN |
| 7 | Q | 44 | GLN |
| 7 | Q | 356 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 1 | A | 234/5025 (4%) | 33 (14%) | 1 (0%) |
| 2 | B | 59/1869 (3%) | 11 (18%) | 0 |
| 6 | P | 16/18 (88%) | 2 (12%) | 0 |
| 8 | R | 8/9 (88%) | 3 (37%) | 0 |
| All | All | 317/6921 (4%) | 49 (15%) | 1 (0%) |

5 of 49 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1623 | G |
| 1 | A | 1955 | U |
| 1 | A | 1956 | G |
| 1 | A | 1957 | G |
| 1 | A | 1965 | A |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 3730 | U |

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

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

5.5 Carbohydrates ⓘ

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.