



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Oct 17, 2018 – 04:37 PM EDT

PDB ID : 6GXO
EMDB ID: : EMD-0082
Title : Cryo-EM structure of a rotated E. coli 70S ribosome in complex with RF3-GDPCP, RF1(GAQ) and P/E-tRNA (State IV)
Authors : Graf, M.; Huter, P.; Maracci, C.; Peterek, M.; Rodnina, M.V.; Wilson, D.N.
Deposited on : 2018-06-27
Resolution : 3.90 Å(reported)

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

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

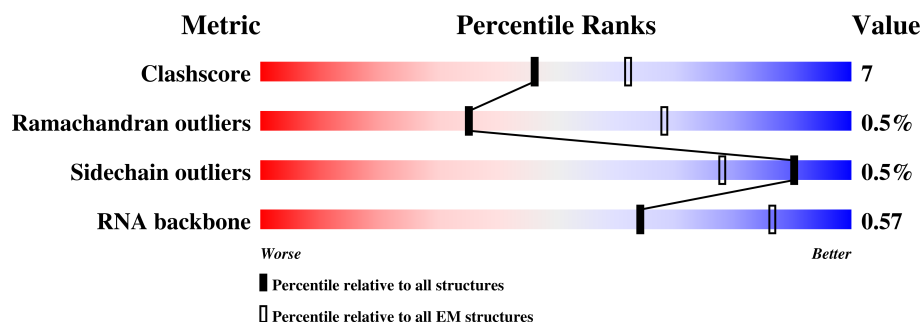
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.
















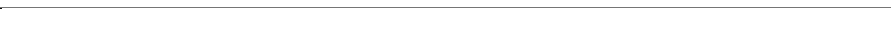

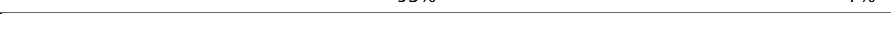
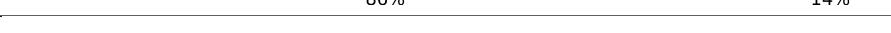
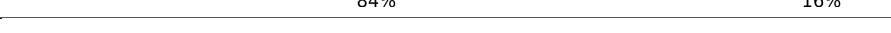







| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 136327 | 1886 |
| Ramachandran outliers | 132723 | 1663 |
| Sidechain outliers | 132532 | 1531 |
| RNA backbone | 3747 | 458 |

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 | 2903 | 62% 32% 5% . |
| 2 | B | 120 | 58% 37% 5% |
| 3 | C | 271 | 83% 17% |
| 4 | D | 209 | 85% 15% |
| 5 | E | 201 | 86% 14% |
| 6 | F | 177 | 84% 16% |
| 7 | G | 176 | 93% 6% . |
| 8 | H | 149 | 83% 17% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 9 | I | 141 |  87% 13% |
| 10 | J | 142 |  87% 13% |
| 11 | K | 122 |  80% 20% |
| 12 | L | 143 |  85% 15% |
| 13 | M | 136 |  86% 13% . |
| 14 | N | 120 |  83% 16% . |
| 15 | O | 116 |  89% 11% |
| 16 | P | 114 |  85% 15% |
| 17 | Q | 117 |  87% 13% |
| 18 | R | 103 |  85% 15% |
| 19 | S | 110 |  88% 12% |
| 20 | T | 93 |  77% 23% |
| 21 | U | 102 |  87% 13% |
| 22 | V | 94 |  88% 12% |
| 23 | W | 75 |  93% 7% |
| 24 | X | 77 |  86% 14% |
| 25 | Y | 63 |  84% 16% |
| 26 | Z | 58 |  84% 16% |
| 27 | 0 | 56 |  82% 18% |
| 28 | 1 | 50 |  90% 10% |
| 29 | 2 | 46 |  80% 20% |
| 30 | 3 | 64 |  84% 13% . . |
| 31 | 4 | 38 |  87% 13% |
| 32 | 5 | 131 |  80% 20% |
| 33 | 7 | 7 |  14% 71% 14% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 34 | a | 1539 | 84% 15% . |
| 35 | b | 218 | 97% . |
| 36 | c | 206 | 100% |
| 37 | d | 205 | 98% . |
| 38 | e | 157 | 98% .. |
| 39 | f | 100 | 96% . |
| 40 | g | 151 | 100% |
| 41 | h | 129 | 100% |
| 42 | i | 127 | 98% .. |
| 43 | j | 98 | 100% |
| 44 | k | 116 | 99% . |
| 45 | l | 123 | 98% . |
| 46 | m | 114 | 98% . |
| 47 | n | 101 | 100% |
| 48 | o | 88 | 100% |
| 49 | p | 82 | 99% . |
| 50 | q | 80 | 95% . . |
| 51 | r | 65 | 100% |
| 52 | s | 79 | 100% |
| 53 | t | 85 | 100% |
| 54 | u | 65 | 97% . |
| 55 | v | 248 | 95% 5% |
| 56 | w | 529 | 92% . 6% |
| 57 | x | 77 | 45% 47% 8% |
| 58 | z | 14 | 93% 7% |

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 151479 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 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1 | A | 2900 | Total | C | N | O | P | 0 | 0 |
| | | | 62262 | 27774 | 11460 | 20128 | 2900 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|---------------|
| A | 747 | C | U | conflict | GB 1036415628 |
| A | 1847 | G | A | conflict | GB 1036415628 |

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 2 | B | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2572 | 1145 | 471 | 836 | 120 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|---------------|
| B | 120 | A | - | expression tag | GB 1373146531 |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3 | C | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | D | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | E | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | F | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | G | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | H | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | |

- Molecule 9 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | I | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | |

- Molecule 10 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | J | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 11 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | K | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | |

- Molecule 12 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | L | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | |

- Molecule 13 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | M | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | |

- Molecule 14 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | N | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | |

- Molecule 15 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 15 | O | 116 | Total | C | N | O | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | |

- Molecule 16 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | P | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 17 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 17 | Q | 117 | Total | C | N | O | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | |

- Molecule 18 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | R | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 19 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | S | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 20 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | T | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | |

- Molecule 21 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 21 | U | 102 | Total | C | N | O | | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | V | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 23 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | W | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 575 | 356 | 116 | 102 | 1 | | |

- Molecule 24 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | X | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

- Molecule 25 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25 | Y | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | |

- Molecule 26 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26 | Z | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27 | 0 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28 | 1 | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29 | 2 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 30 | 3 | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 31 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31 | 4 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

- Molecule 32 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | 5 | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 988 | 625 | 175 | 183 | 5 | | |

- Molecule 33 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 33 | 7 | 7 | Total | C | N | O | P | 0 | 0 |
| | | | 151 | 68 | 29 | 47 | 7 | | |

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 34 | a | 1539 | Total | C | N | O | P | 0 | 0 |
| | | | 33016 | 14725 | 6052 | 10700 | 1539 | | |

- Molecule 35 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35 | b | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | |

- Molecule 36 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36 | c | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | |

- Molecule 37 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37 | d | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | |

- Molecule 38 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | e | 157 | Total | C | N | O | S | 0 | 0 |
| | | | 1141 | 709 | 218 | 208 | 6 | | |

- Molecule 39 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | f | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | |

- Molecule 40 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | g | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1181 | 735 | 227 | 215 | 4 | | |

- Molecule 41 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | h | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | |

- Molecule 42 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | i | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | |

- Molecule 43 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | j | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | |

- Molecule 44 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | k | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 869 | 535 | 173 | 158 | 3 | | |

- Molecule 45 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | l | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | |

- Molecule 46 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | m | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 883 | 546 | 178 | 156 | 3 | | |

- Molecule 47 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47 | n | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 799 | 498 | 165 | 133 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| n | 35 | ALA | - | insertion | UNP P0AG59 |

- Molecule 48 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | o | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | |

- Molecule 49 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49 | p | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | |

- Molecule 50 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50 | q | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | |

- Molecule 51 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 51 | r | 65 | Total | C | N | O | 0 | 0 |
| | | | 504 | 317 | 96 | 91 | | |

- Molecule 52 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52 | s | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 637 | 408 | 120 | 107 | 2 | | |

- Molecule 53 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | t | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | |

- Molecule 54 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 54 | u | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 495 | 307 | 100 | 87 | 1 | | |

- Molecule 55 is a protein called Peptide chain release factor RF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55 | v | 248 | Total | C | N | O | S | 0 | 0 |
| | | | 1932 | 1180 | 368 | 375 | 9 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| v | 167 | CYS | SER | conflict | UNP P0A7I0 |
| v | 234 | ALA | GLY | conflict | UNP P0A7I0 |

- Molecule 56 is a protein called Peptide chain release factor RF3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56 | w | 498 | Total | C | N | O | S | 0 | 0 |
| | | | 3938 | 2495 | 679 | 744 | 20 | | |

- Molecule 57 is a RNA chain called fMet-tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 57 | x | 77 | Total | C | N | O | P | 0 | 0 |
| | | | 1639 | 732 | 297 | 534 | 76 | | |

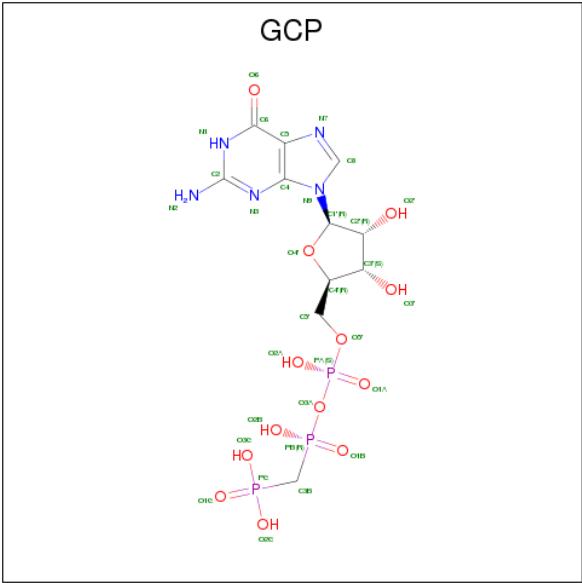
- Molecule 58 is a protein called Apidaecin.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 58 | z | 14 | Total | C | N | O | 0 | 0 |
| | | | 120 | 80 | 25 | 15 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| z | 10 | ARG | GLN | conflict | UNP Q8WSY8 |

- Molecule 59 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



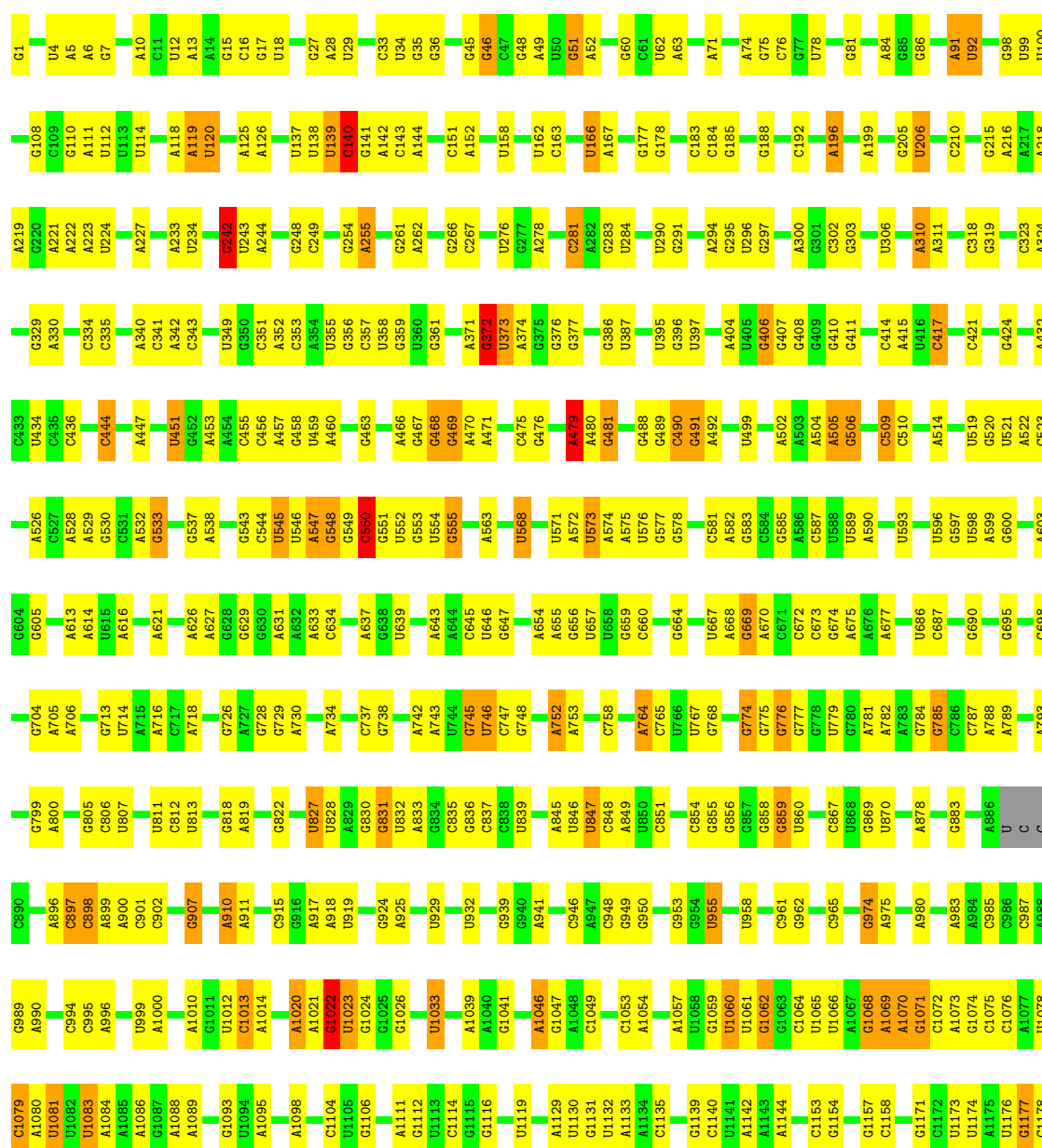
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 59 | w | 1 | 32 | 11 | 5 | 13 | 3 | 0 |

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: 23S ribosomal RNA

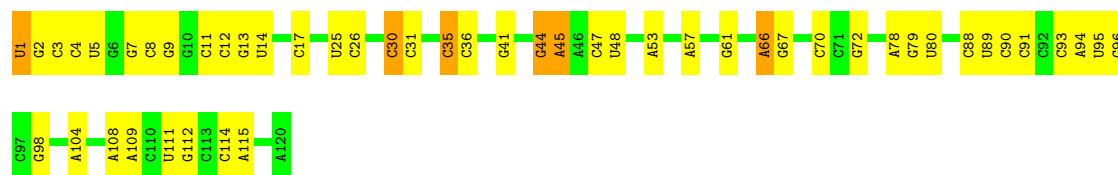
Chain A: 




| | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A2821 | G2719 | U2511 | G2293 | U2195 | A2088 | A1998 | A1900 | G1797 | G1674 | C1536 | C1417 | A1301 | G1179 |
| G2822 | U2720 | C2512 | G2294 | A2198 | G2093 | C1999 | A1901 | U1798 | C1675 | G1537 | G1418 | C1306 | U1180 |
| A2823 | A2721 | A2513 | C2295 | A2199 | A2094 | G2002 | C1905 | G1799 | C1676 | A1544 | A1419 | G1309 | G1182 |
| G2824 | G2722 | C2514 | U2296 | G2204 | A2095 | A2003 | A1906 | A1801 | G1682 | G1555 | G1420 | G1310 | U1188 |
| G2825 | A2726 | C2516 | A2297 | A2211 | C2096 | G2004 | A1912 | A1802 | G1687 | U1559 | C1421 | G1313 | A1189 |
| U2832 | G2731 | G2517 | U2298 | A2212 | C2006 | A2006 | A1913 | C1806 | G1692 | U1560 | C1428 | U1314 | G1190 |
| U2833 | G2732 | U2518 | C2300 | G2213 | U2007 | G2007 | A1914 | G1807 | C1694 | G1569 | G1429 | C1315 | G1191 |
| G2834 | A2733 | C2520 | U2305 | C2214 | G2110 | C2008 | U1917 | A1809 | G1695 | C1565 | G1430 | A1204 | A1205 |
| U2835 | G2734 | G2521 | C2306 | C2215 | U2111 | A2009 | A1918 | A1810 | G1699 | A1569 | G1431 | A1321 | G1206 |
| G2836 | U2739 | C2522 | A2309 | G2216 | G2112 | G2010 | A1919 | G1811 | A1700 | U1578 | G1432 | G1322 | U1209 |
| U2846 | U2743 | G2523 | A2309 | U2220 | U2113 | A2020 | C1920 | U1812 | A1701 | A1579 | G1433 | G1323 | U1210 |
| G2847 | G2744 | G2524 | A2426 | U2221 | U2114 | C2021 | G1921 | G1816 | G1707 | C1585 | G1434 | A1327 | G1212 |
| G2848 | G2745 | G2525 | C2427 | G2223 | A2119 | U2022 | G1922 | G1817 | U1708 | G1592 | G1435 | U1328 | G1215 |
| U2849 | A2746 | G2526 | G2428 | G2224 | G2120 | C2023 | G1923 | U1818 | G1710 | A1593 | G1436 | U1329 | C1221 |
| A2850 | G2747 | G2527 | G2429 | C2225 | G2121 | G2024 | G1924 | G1819 | U1711 | A1597 | C1437 | G1333 | U1222 |
| G2851 | A2748 | G2528 | U2430 | G2226 | G2121 | G2025 | C1925 | U1820 | G1712 | A1598 | G1438 | G1334 | U1223 |
| G2852 | U2749 | G2529 | U2431 | C2227 | U2127 | U2026 | U1926 | G1821 | G1713 | U1602 | C1447 | G1341 | G1225 |
| U2861 | A2750 | C2530 | A2435 | U2229 | G2127 | U2028 | A1928 | G1822 | G1715 | A1603 | G1450 | C1341 | U1242 |
| G2862 | G2751 | G2531 | G2325 | G2230 | U2131 | A2030 | G1929 | U1826 | U1716 | C1604 | C1451 | C1345 | C1221 |
| G2863 | C2752 | A2547 | C2326 | G2231 | U2132 | A2031 | G1930 | U1827 | A1717 | C1604 | G1452 | G1345 | U1222 |
| U2867 | C2755 | U2552 | A2442 | G2232 | G2133 | G2032 | U1931 | G1828 | G1724 | A1598 | C1453 | G1344 | U1223 |
| A2868 | G2762 | G2553 | G2443 | U2233 | G2136 | U2033 | A1932 | G1829 | G1725 | U1602 | C1454 | G1341 | G1225 |
| A2872 | G2763 | U2554 | G2444 | G2234 | G2137 | U2034 | A1933 | C1830 | U1729 | A1603 | C1461 | C1341 | U1226 |
| A2873 | A2764 | G2555 | G2445 | G2235 | G2138 | G2035 | A1934 | G1831 | C1730 | C1604 | C1462 | C1345 | G1227 |
| C2880 | A2765 | C2556 | U2446 | U2236 | G2139 | A2037 | U1935 | G1832 | G1731 | C1604 | C1463 | C1345 | U1228 |
| U2881 | G2766 | C2557 | U2447 | A2241 | G2140 | G2038 | U1936 | U1833 | G1732 | C1604 | C1464 | C1345 | U1229 |
| A2883 | U2768 | A2560 | U2448 | A2242 | G2141 | A2039 | U1937 | G1834 | G1733 | C1604 | C1465 | C1345 | U1230 |
| U2884 | G2769 | G2561 | U2449 | U2243 | G2142 | G2040 | U1938 | U1835 | G1734 | C1604 | C1466 | C1345 | U1231 |
| A2893 | U2770 | A2562 | U2450 | U2244 | G2143 | G2041 | U1939 | G1836 | G1735 | C1604 | C1467 | C1345 | U1232 |
| G2894 | A2771 | G2563 | G2451 | U2245 | C2146 | C2042 | C1941 | G1837 | G1736 | A1610 | G1475 | U1242 | U1242 |
| U2898 | U2772 | C2564 | C2350 | U2246 | A2147 | G2043 | U1942 | U1838 | G1737 | C1611 | U1476 | G1355 | A1247 |
| A2899 | G2773 | A2565 | G2351 | U2247 | G2148 | G2044 | U1943 | U1839 | G1738 | G1612 | G1482 | G1356 | A1248 |
| A2900 | G2774 | G2566 | G2352 | U2248 | G2149 | C2045 | A1953 | G1841 | G1739 | G1613 | G1483 | A1365 | U1249 |
| G2901 | C2782 | C2567 | G2353 | U2249 | G2150 | A2051 | G1954 | G1842 | A1744 | A1634 | A1490 | G1368 | G1250 |
| C2902 | U2788 | G2568 | G2354 | U2250 | G2151 | A2052 | U1955 | G1843 | A1745 | A1635 | A1491 | G1369 | G1251 |
| U2903 | G2791 | U2569 | G2355 | U2251 | G2152 | G2053 | U1956 | G1844 | A1746 | U1636 | G1492 | G1370 | G1252 |
| U2904 | C2795 | G2570 | G2356 | U2252 | G2153 | C2055 | U1957 | U1845 | G1753 | A1637 | C1493 | G1371 | A1253 |
| U2905 | U2796 | C2571 | G2357 | U2253 | G2154 | G2056 | U1958 | G1846 | A1754 | C1638 | G1500 | U1372 | A1254 |
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| A2908 | C2799 | G2574 | G2360 | U2256 | G2157 | A2060 | C1962 | G1849 | G1757 | U1646 | A1505 | G1375 | G1266 |
| G2909 | U2800 | U2575 | G2361 | U2257 | G2158 | G2061 | U1963 | U1850 | U1758 | U1647 | A1506 | A1376 | G1267 |
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| U2911 | U2802 | C2577 | G2363 | U2259 | G2160 | G2063 | U1965 | G1852 | G1760 | G1649 | A1508 | U1294 | U1294 |
| U2912 | G2803 | G2578 | G2364 | U2260 | G2161 | C2064 | U1966 | U1853 | G1761 | A1650 | G1510 | A1395 | U1295 |
| U2913 | U2804 | C2579 | G2365 | U2261 | G2162 | U2065 | C1967 | G1854 | G1762 | G1651 | A1511 | G1386 | C1297 |
| G2914 | G2805 | U2580 | G2366 | U2262 | G2163 | G2066 | U1968 | U1855 | G1763 | A1652 | G1512 | C1387 | G1298 |
| U2915 | U2806 | G2581 | G2367 | U2263 | G2164 | U2067 | U1969 | G1856 | A1764 | G1653 | G1513 | G1388 | C1299 |
| U2916 | C2807 | C2582 | G2368 | U2264 | G2165 | A2068 | A1970 | G1857 | G1765 | C1654 | A1514 | C1389 | U1299 |
| G2917 | U2808 | G2583 | G2369 | U2265 | G2166 | G2069 | U1971 | U1858 | A1766 | G1655 | G1515 | C1390 | G1300 |
| A2918 | G2809 | U2584 | G2370 | U2266 | G2167 | A2070 | U1972 | U1859 | C1774 | G1660 | G1516 | C1391 | U1301 |
| U2919 | U2810 | C2585 | G2371 | U2267 | G2168 | G2071 | C1973 | G1860 | G1775 | U1661 | A1517 | G1416 | G1302 |
| G2920 | C2811 | G2586 | G2372 | U2268 | G2169 | A2072 | C1974 | U1861 | U1779 | G1662 | A1518 | U1303 | U1303 |
| U2921 | U2812 | U2587 | G2373 | U2269 | G2170 | U2073 | C1975 | G1862 | A1780 | A1664 | U1522 | U1304 | U1304 |
| U2922 | G2813 | C2588 | G2374 | U2270 | G2171 | G2074 | U1976 | G1863 | U1781 | A1665 | G1523 | A1396 | U1305 |
| U2923 | U2814 | G2589 | G2375 | U2271 | G2172 | U2075 | C1977 | U1864 | U1782 | A1666 | G1524 | U1397 | U1306 |
| U2924 | G2815 | U2590 | G2376 | U2272 | G2173 | A2076 | U1978 | G1865 | G1783 | G1667 | A1532 | C1398 | C1297 |
| U2925 | U2816 | G2591 | G2377 | U2273 | G2174 | U2077 | U1979 | G1866 | A1784 | A1668 | U1533 | C1399 | U1298 |
| U2926 | C2817 | C2592 | G2378 | U2274 | G2175 | A2078 | U1980 | U1867 | U1785 | U1669 | U1534 | C1400 | G1300 |
| U2927 | U2818 | U2593 | G2379 | U2275 | G2176 | G2079 | U1981 | G1868 | G1786 | C1670 | A1535 | U1401 | U1301 |
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| U2929 | U2820 | C2595 | G2381 | U2277 | G2178 | A2081 | U1983 | U1870 | U1788 | U1672 | U1537 | C1403 | U1303 |
| U2930 | C2821 | G2596 | G2382 | U2278 | G2179 | U2082 | U1984 | G1871 | G1789 | U1673 | U1538 | C1404 | U1304 |
| U2931 | U2822 | U2597 | G2383 | U2279 | G2180 | A2083 | U1985 | U1872 | U1790 | U1674 | U1539 | C1405 | U1305 |
| U2932 | G2823 | C2598 | G2384 | U2280 | G2181 | U2084 | U1986 | G1873 | U1791 | U1675 | U1540 | C1406 | U1306 |
| U2933 | U2824 | U2599 | G2385 | U2281 | G2182 | A2085 | U1987 | U1874 | U1792 | U1676 | U1541 | C1407 | U1307 |
| U2934 | G2825 | G2600 | G2386 | U2282 | G2183 | U2086 | U1988 | G1875 | U1793 | U1677 | U1542 | C1408 | U1308 |
| U2935 | U2826 | C2601 | G2387 | U2283 | G2184 | U2087 | U1989 | U1876 | U1794 | U1678 | U1543 | C1409 | U1309 |
| U2936 | G2827 | U2602 | G2388 | U2284 | G2185 | A2088 | U1990 | G1877 | U1795 | U1679 | U1544 | C1410 | U1310 |
| U2937 | U2828 | C2603 | G2389 | U2285 | G2186 | U2089 | U1991 | U1878 | U1796 | U1680 | U1545 | C1411 | U1311 |
| U2938 | G2829 | U2604 | G2390 | U2286 | G2187 | A2090 | U1992 | G1879 | U1797 | U1681 | U1546 | C1412 | U1312 |
| U2939 | U2830 | C2605 | G2391 | U2287 | G2188 | U2091 | U1993 | U1880 | U1798 | U1682 | U1547 | C1413 | U1313 |
| U2940 | G2831 | U2606 | G2392 | U2288 | G2189 | A2092 | U1994 | U1881 | U1799 | U1683 | U1548 | C1414 | U1314 |
| U2941 | U2832 | C2607 | G2393 | U2289 | G2190 | U2093 | U1995 | G1882 | U1800 | U1684 | U1549 | C1415 | U1315 |
| U2942 | G2833 | U2608 | G2394 | U2290 | G2191 | A2094 | U1996 | U1883 | U1801 | U1685 | U1550 | C1416 | U1316 |
| U2943 | U2834 | C2609 | G2395 | U2291 | G2192 | U2095 | U1997 | G1884 | U1802 | U1686 | U1551 | C1417 | U1317 |
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| U2945 | U2836 | C2611 | G2397 | U2293 | G2194 | U2097 | U1999 | G1886 | U1804 | U1688 | U1553 | C1419 | U1319 |
| U2946 | G2837 | U2612 | G2398 | U2294 | G2195 | A2098 | U2000 | U1887 | U1805 | U1689 | U1554 | C1420 | U1320 |
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| U2949 | U2840 | C2615 | G2401 | U2297 | G2198 | U2101 | U2003 | U1890 | U1808 | U1692 | U1557 | C1423 | U1323 |
| U2950 | G2841 | U2616 | G2402 | U2298 | G2199 | A2102 | U2004 | G1891 | U1809 | U1693 | U1558 | C1424 | U1324 |
| U2951 | U2842 | C2617 | G2403 | U2299 | G2200 | U2103 | U2005 | U1892 | U1810 | U1694 | U1559 | C1425 | U1325 |
| U2952 | G2843 | U2618 | G2404 | U2300 | G2201 | A2104 | U2006 | G1893 | U1811 | U1695 | U1560 | C1426 | U1326 |
| U2953 | U2844 | C2619 | G2405 | U2301 | G2202 | U2105 | U2007 | U1894 | U1812 | U1696 | U1561 | C1427 | U1327 |
| U2954 | G2845 | U2620 | G2406 | U2302 | G2203 | A2106 | U2008 | G1895 | U1813 | U1697 | U1562 | C1428 | U1328 |
| U2955 | U2846 | C2621 | G2407 | U2303 | G2204 | U2107 | U2009 | U1896 | U1814 | U1698 | U1563 | C1429 | U1329 |
| U2956 | G2847 | U2622 | G2408 | U2304 | G2205 | A2108 | U2010 | G1897 | U1815 | U1699 | U1564 | C1430 | U1330 |
| U2957 | U2848 | C2623 | G2409 | U2305 | G2206 | U2109 | U2011 | U1898 | U1816 | U1700 | U1565 | C1431 | U1331 |
| U2958 | G2849 | U2624 | G2410 | U2306 | | | | | | | | | |

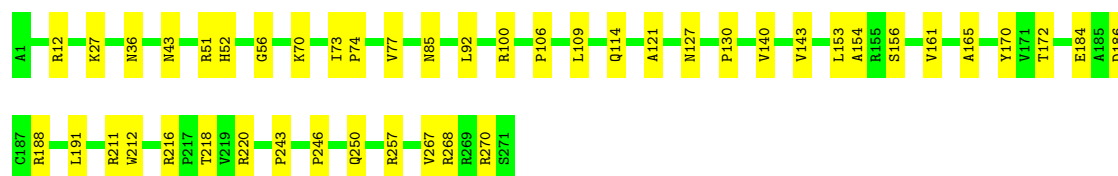
- Molecule 2: 5S ribosomal RNA

Chain B: 




- Molecule 3: 50S ribosomal protein L2

Chain C: 




- Molecule 4: 50S ribosomal protein L3

Chain D: 




- Molecule 5: 50S ribosomal protein L4

Chain E: 



- Molecule 6: 50S ribosomal protein L5

Chain F: 




- Molecule 7: 50S ribosomal protein L6

Chain G: 



- Molecule 8: 50S ribosomal protein L9

Chain H: 



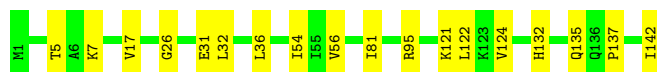
- Molecule 9: 50S ribosomal protein L11

Chain I: 87% 13%



- Molecule 10: 50S ribosomal protein L13

Chain J: 87% 13%



- Molecule 11: 50S ribosomal protein L14

Chain K: 80% 20%



- Molecule 12: 50S ribosomal protein L15

Chain L: 85% 15%



- Molecule 13: 50S ribosomal protein L16

Chain M: 86% 13%



- Molecule 14: 50S ribosomal protein L17

Chain N: 83% 16%

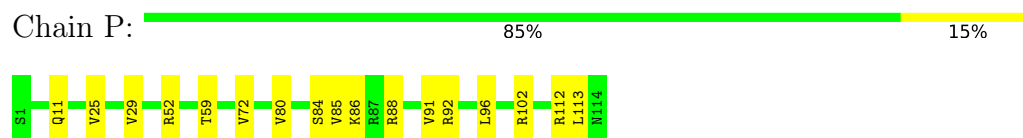


- Molecule 15: 50S ribosomal protein L18

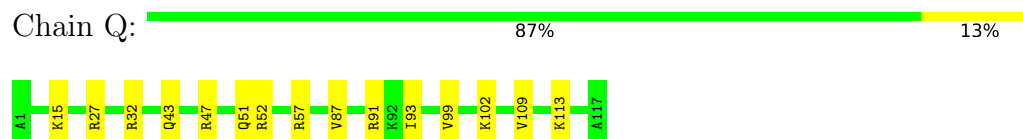
Chain O: 89% 11%



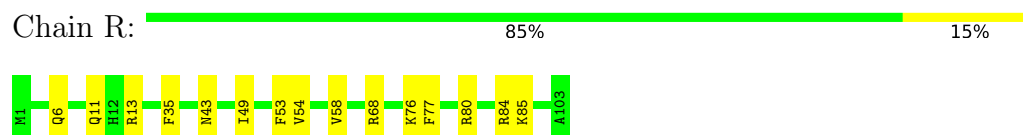
- Molecule 16: 50S ribosomal protein L19



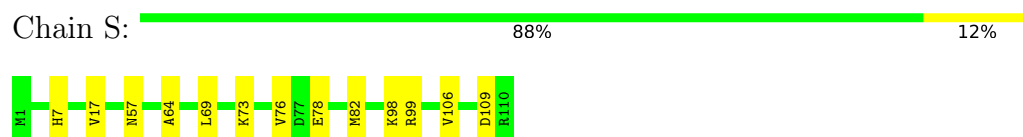
- Molecule 17: 50S ribosomal protein L20



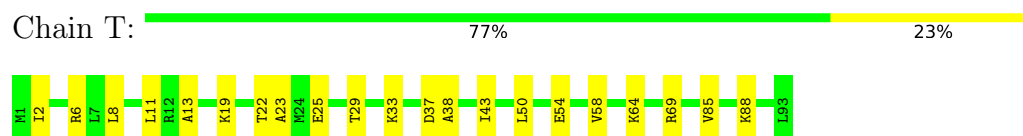
- Molecule 18: 50S ribosomal protein L21



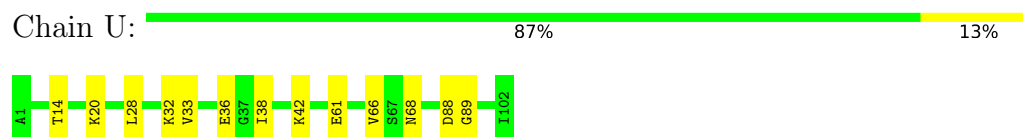
- Molecule 19: 50S ribosomal protein L22



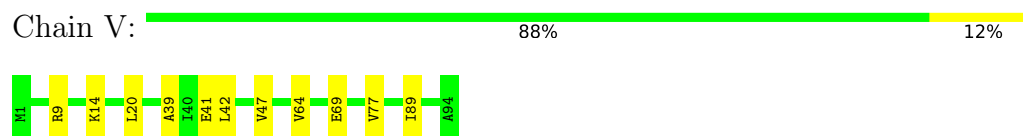
- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25




- Molecule 23: 50S ribosomal protein L27

Chain W:  93% 7%




- Molecule 24: 50S ribosomal protein L28

Chain X:  86% 14%




- Molecule 25: 50S ribosomal protein L29

Chain Y:  84% 16%




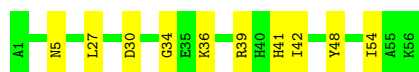
- Molecule 26: 50S ribosomal protein L30

Chain Z:  84% 16%




- Molecule 27: 50S ribosomal protein L32

Chain 0:  82% 18%




- Molecule 28: 50S ribosomal protein L33

Chain 1:  90% 10%




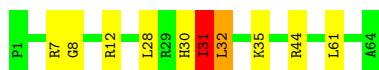
- Molecule 29: 50S ribosomal protein L34

Chain 2:  80% 20%



- Molecule 30: 50S ribosomal protein L35

Chain 3:  84% 13% ..



- Molecule 31: 50S ribosomal protein L36

Chain 4: 87% 13%



- Molecule 32: 50S ribosomal protein L10

Chain 5: 80% 20%



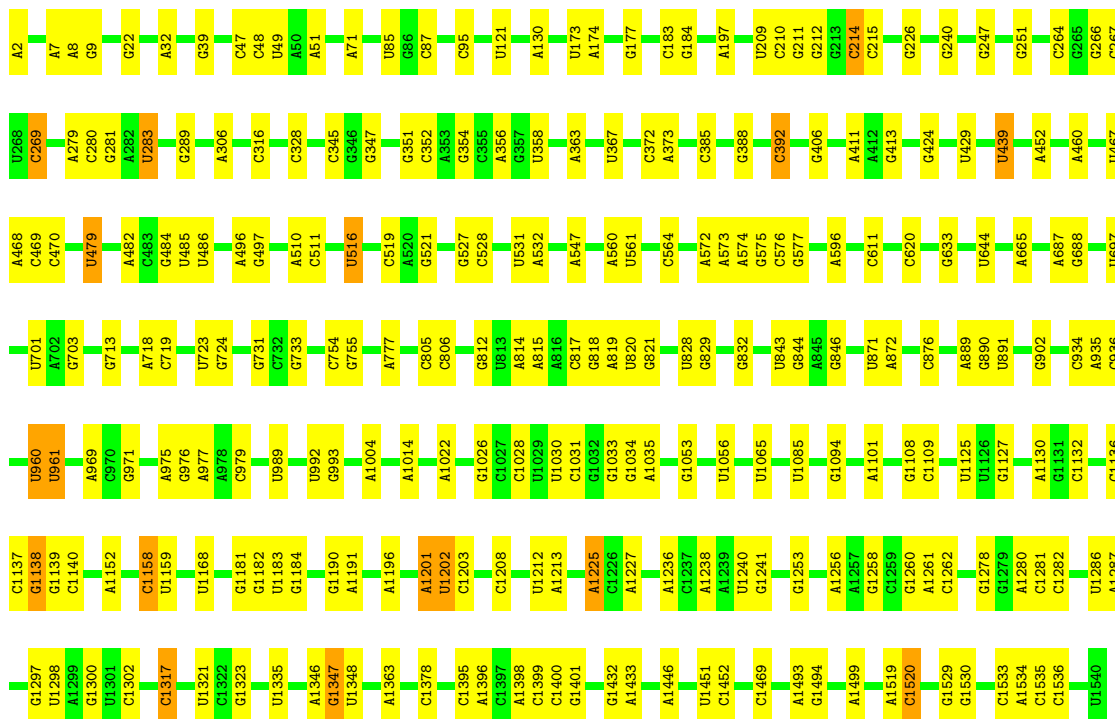
- Molecule 33: mRNA

Chain 7: 14% 71% 14%



- Molecule 34: 16S ribosomal RNA

Chain a: 84% 15%



- Molecule 35: 30S ribosomal protein S2

Chain b:  97% .



- Molecule 36: 30S ribosomal protein S3

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: 30S ribosomal protein S4

Chain d:  98% .



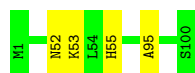
- Molecule 38: 30S ribosomal protein S5

Chain e:  98% ..



- Molecule 39: 30S ribosomal protein S6

Chain f:  96% .



- Molecule 40: 30S ribosomal protein S7

Chain g:  100%

There are no outlier residues recorded for this chain.

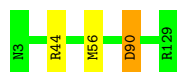
- Molecule 41: 30S ribosomal protein S8

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: 30S ribosomal protein S9

Chain i:  98% ..



- Molecule 43: 30S ribosomal protein S10

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 30S ribosomal protein S11

Chain k:  99%



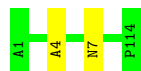
- Molecule 45: 30S ribosomal protein S12

Chain l:  98%



- Molecule 46: 30S ribosomal protein S13

Chain m:  98%



- Molecule 47: 30S ribosomal protein S14

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S15

Chain o:  100%

There are no outlier residues recorded for this chain.

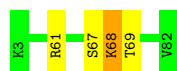
- Molecule 49: 30S ribosomal protein S16

Chain p:  99%



- Molecule 50: 30S ribosomal protein S17

Chain q:  95%



- Molecule 51: 30S ribosomal protein S18

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: 30S ribosomal protein S19

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 53: 30S ribosomal protein S20

Chain t:  100%

There are no outlier residues recorded for this chain.

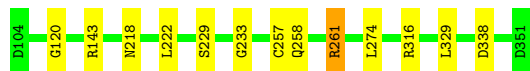
- Molecule 54: 30S ribosomal protein S21

Chain u:  97%



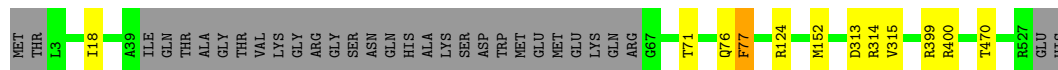
- Molecule 55: Peptide chain release factor RF1

Chain v:  95%



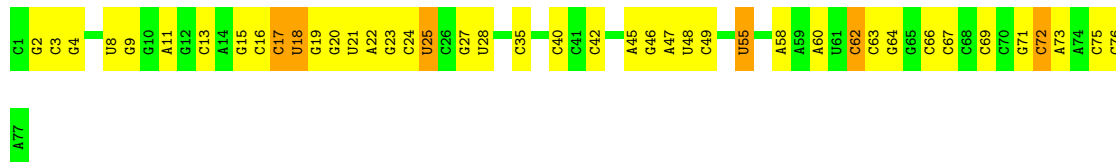
- Molecule 56: Peptide chain release factor RF3

Chain w:  92%



- Molecule 57: fMet-tRNA

Chain x:  45%



- Molecule 58: Apidaecin

Chain z:  93%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 46814 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 45.9 | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 0.29 | 1/69729 (0.0%) | 1.00 | 228/108768 (0.2%) |
| 10 | J | 0.25 | 0/1152 | 0.46 | 0/1551 |
| 11 | K | 0.27 | 0/947 | 0.52 | 0/1268 |
| 12 | L | 0.27 | 0/1054 | 0.54 | 0/1403 |
| 13 | M | 0.27 | 0/1093 | 0.57 | 1/1460 (0.1%) |
| 14 | N | 0.27 | 0/973 | 0.52 | 0/1301 |
| 15 | O | 0.25 | 0/902 | 0.47 | 0/1209 |
| 16 | P | 0.25 | 0/929 | 0.51 | 1/1242 (0.1%) |
| 17 | Q | 0.26 | 0/960 | 0.45 | 0/1278 |
| 18 | R | 0.26 | 0/829 | 0.50 | 0/1107 |
| 19 | S | 0.24 | 0/864 | 0.50 | 0/1156 |
| 2 | B | 0.39 | 1/2876 (0.0%) | 1.16 | 32/4483 (0.7%) |
| 20 | T | 0.25 | 0/744 | 0.51 | 0/994 |
| 21 | U | 0.29 | 0/787 | 0.55 | 0/1051 |
| 22 | V | 0.25 | 0/766 | 0.49 | 0/1025 |
| 23 | W | 0.26 | 0/582 | 0.41 | 0/769 |
| 24 | X | 0.24 | 0/635 | 0.46 | 0/848 |
| 25 | Y | 0.23 | 0/510 | 0.47 | 0/677 |
| 26 | Z | 0.24 | 0/453 | 0.47 | 0/605 |
| 27 | 0 | 0.24 | 0/450 | 0.46 | 0/599 |
| 28 | 1 | 0.26 | 0/416 | 0.50 | 0/554 |
| 29 | 2 | 0.24 | 0/380 | 0.45 | 0/498 |
| 3 | C | 0.26 | 0/2121 | 0.51 | 0/2852 |
| 30 | 3 | 0.26 | 0/513 | 0.64 | 2/676 (0.3%) |
| 31 | 4 | 0.28 | 0/303 | 0.52 | 0/397 |
| 32 | 5 | 0.30 | 0/1001 | 0.64 | 0/1350 |
| 33 | 7 | 0.33 | 0/169 | 0.84 | 0/261 |
| 34 | a | 0.29 | 1/36967 (0.0%) | 0.98 | 80/57666 (0.1%) |
| 35 | b | 0.28 | 0/1735 | 0.55 | 0/2338 |
| 36 | c | 0.25 | 0/1651 | 0.47 | 0/2225 |
| 37 | d | 0.26 | 0/1665 | 0.55 | 2/2227 (0.1%) |
| 38 | e | 0.28 | 0/1154 | 0.58 | 0/1554 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 39 | f | 0.30 | 0/835 | 0.62 | 0/1128 |
| 4 | D | 0.26 | 0/1586 | 0.51 | 0/2134 |
| 40 | g | 0.27 | 0/1195 | 0.52 | 0/1602 |
| 41 | h | 0.26 | 0/989 | 0.55 | 0/1326 |
| 42 | i | 0.27 | 0/1034 | 0.56 | 0/1375 |
| 43 | j | 0.27 | 0/796 | 0.60 | 0/1077 |
| 44 | k | 0.26 | 0/885 | 0.51 | 0/1195 |
| 45 | l | 0.28 | 0/969 | 0.59 | 0/1300 |
| 46 | m | 0.26 | 0/892 | 0.56 | 0/1193 |
| 47 | n | 0.24 | 0/811 | 0.51 | 0/1081 |
| 48 | o | 0.24 | 0/722 | 0.52 | 0/964 |
| 49 | p | 0.26 | 0/659 | 0.51 | 0/884 |
| 5 | E | 0.25 | 0/1571 | 0.47 | 0/2113 |
| 50 | q | 0.28 | 0/657 | 0.60 | 1/881 (0.1%) |
| 51 | r | 0.23 | 0/511 | 0.48 | 0/689 |
| 52 | s | 0.26 | 0/652 | 0.50 | 0/877 |
| 53 | t | 0.29 | 0/671 | 0.49 | 0/888 |
| 54 | u | 0.32 | 0/500 | 0.66 | 0/668 |
| 55 | v | 0.46 | 1/1962 (0.1%) | 0.89 | 6/2643 (0.2%) |
| 56 | w | 0.27 | 0/4011 | 0.61 | 5/5421 (0.1%) |
| 57 | x | 0.38 | 0/1831 | 1.42 | 44/2853 (1.5%) |
| 58 | z | 1.04 | 1/127 (0.8%) | 1.45 | 3/175 (1.7%) |
| 6 | F | 0.28 | 0/1434 | 0.54 | 0/1926 |
| 7 | G | 0.26 | 0/1343 | 0.52 | 1/1816 (0.1%) |
| 8 | H | 0.26 | 0/1122 | 0.47 | 0/1515 |
| 9 | I | 0.29 | 0/1046 | 0.55 | 0/1410 |
| All | All | 0.29 | 5/164121 (0.0%) | 0.90 | 406/244526 (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 |
|-----|-------|---------------------|---------------------|
| 13 | M | 0 | 1 |
| 18 | R | 0 | 1 |
| 21 | U | 0 | 1 |
| 30 | 3 | 0 | 1 |
| 32 | 5 | 0 | 1 |
| 35 | b | 0 | 2 |
| 38 | e | 0 | 1 |
| 39 | f | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 42 | i | 0 | 2 |
| 45 | l | 0 | 1 |
| 46 | m | 0 | 1 |
| 49 | p | 0 | 1 |
| 5 | E | 0 | 1 |
| 50 | q | 0 | 2 |
| 54 | u | 0 | 1 |
| 56 | w | 0 | 1 |
| 6 | F | 0 | 2 |
| 7 | G | 0 | 3 |
| All | All | 0 | 25 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 55 | v | 257 | CYS | C-N | 15.26 | 1.69 | 1.34 |
| 58 | z | 5 | PRO | C-N | 11.35 | 1.60 | 1.34 |
| 1 | A | 1 | G | OP3-P | -10.60 | 1.48 | 1.61 |
| 2 | B | 1 | U | OP3-P | -10.56 | 1.48 | 1.61 |
| 34 | a | 2 | A | OP3-P | -10.53 | 1.48 | 1.61 |

The worst 5 of 406 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 55 | v | 257 | CYS | O-C-N | -28.49 | 77.11 | 122.70 |
| 58 | z | 5 | PRO | O-C-N | 11.62 | 141.28 | 122.70 |
| 57 | x | 62 | C | N1-C2-O2 | 10.90 | 125.44 | 118.90 |
| 1 | A | 2604 | U | C2-N1-C1' | 10.62 | 130.45 | 117.70 |
| 58 | z | 5 | PRO | CA-C-N | -10.55 | 93.99 | 117.20 |

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 5 | E | 82 | GLY | Peptide |
| 6 | F | 173 | ASP | Peptide |
| 6 | F | 174 | PHE | Peptide |
| 7 | G | 45 | ALA | Peptide |
| 7 | G | 46 | ASP | Peptide |

5.2 Too-close contacts ⓘ

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 | 62262 | 0 | 31318 | 464 | 0 |
| 2 | B | 2572 | 0 | 1302 | 19 | 0 |
| 3 | C | 2082 | 0 | 2157 | 29 | 0 |
| 4 | D | 1565 | 0 | 1616 | 19 | 0 |
| 5 | E | 1552 | 0 | 1619 | 18 | 0 |
| 6 | F | 1410 | 0 | 1447 | 18 | 0 |
| 7 | G | 1323 | 0 | 1374 | 5 | 0 |
| 8 | H | 1111 | 0 | 1148 | 15 | 0 |
| 9 | I | 1032 | 0 | 1088 | 11 | 0 |
| 10 | J | 1129 | 0 | 1162 | 13 | 0 |
| 11 | K | 938 | 0 | 1012 | 15 | 0 |
| 12 | L | 1045 | 0 | 1117 | 14 | 0 |
| 13 | M | 1074 | 0 | 1157 | 11 | 0 |
| 14 | N | 960 | 0 | 1000 | 15 | 0 |
| 15 | O | 892 | 0 | 923 | 10 | 0 |
| 16 | P | 917 | 0 | 965 | 11 | 0 |
| 17 | Q | 947 | 0 | 1022 | 12 | 0 |
| 18 | R | 816 | 0 | 839 | 10 | 0 |
| 19 | S | 857 | 0 | 922 | 7 | 0 |
| 20 | T | 738 | 0 | 807 | 15 | 0 |
| 21 | U | 779 | 0 | 834 | 6 | 0 |
| 22 | V | 753 | 0 | 780 | 6 | 0 |
| 23 | W | 575 | 0 | 592 | 3 | 0 |
| 24 | X | 625 | 0 | 655 | 9 | 0 |
| 25 | Y | 509 | 0 | 543 | 8 | 0 |
| 26 | Z | 449 | 0 | 491 | 6 | 0 |
| 27 | 0 | 444 | 0 | 461 | 7 | 0 |
| 28 | 1 | 409 | 0 | 440 | 3 | 0 |
| 29 | 2 | 377 | 0 | 418 | 7 | 0 |
| 30 | 3 | 504 | 0 | 574 | 6 | 0 |
| 31 | 4 | 302 | 0 | 343 | 3 | 0 |
| 32 | 5 | 988 | 0 | 1025 | 14 | 0 |
| 33 | 7 | 151 | 0 | 76 | 5 | 0 |
| 34 | a | 33016 | 0 | 16615 | 0 | 0 |
| 35 | b | 1704 | 0 | 1732 | 0 | 0 |
| 36 | c | 1624 | 0 | 1699 | 0 | 0 |
| 37 | d | 1643 | 0 | 1710 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38 | e | 1141 | 0 | 1170 | 0 | 0 |
| 39 | f | 817 | 0 | 808 | 0 | 0 |
| 40 | g | 1181 | 0 | 1240 | 0 | 0 |
| 41 | h | 979 | 0 | 1034 | 0 | 0 |
| 42 | i | 1022 | 0 | 1070 | 0 | 0 |
| 43 | j | 786 | 0 | 828 | 0 | 0 |
| 44 | k | 869 | 0 | 878 | 0 | 0 |
| 45 | l | 955 | 0 | 1019 | 0 | 0 |
| 46 | m | 883 | 0 | 944 | 0 | 0 |
| 47 | n | 799 | 0 | 841 | 0 | 0 |
| 48 | o | 714 | 0 | 737 | 0 | 0 |
| 49 | p | 649 | 0 | 666 | 0 | 0 |
| 50 | q | 648 | 0 | 691 | 0 | 0 |
| 51 | r | 504 | 0 | 502 | 0 | 0 |
| 52 | s | 637 | 0 | 665 | 0 | 0 |
| 53 | t | 665 | 0 | 714 | 0 | 0 |
| 54 | u | 495 | 0 | 486 | 0 | 0 |
| 55 | v | 1932 | 0 | 1881 | 0 | 0 |
| 56 | w | 3938 | 0 | 3929 | 0 | 0 |
| 57 | x | 1639 | 0 | 837 | 0 | 0 |
| 58 | z | 120 | 0 | 128 | 0 | 0 |
| 59 | w | 32 | 0 | 13 | 0 | 0 |
| All | All | 151479 | 0 | 104064 | 695 | 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 7.

The worst 5 of 695 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) |
|---------------|----------------|--------------------------|-------------------|
| 1:A:1517:G:N1 | 1:A:1920:C:H5' | 103.03 | 1.10 |
| 1:A:306:U:H3 | 1:A:310:A:H62 | 1.06 | 0.99 |
| 1:A:593:U:H3 | 1:A:664:G:H1 | 1.14 | 0.94 |
| 1:A:1476:U:H3 | 1:A:1515:A:H62 | 0.99 | 0.92 |
| 1:A:1517:G:H1 | 1:A:1920:C:H5' | 103.44 | 0.91 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 | C | 269/271 (99%) | 260 (97%) | 9 (3%) | 0 | 100 | 100 |
| 4 | D | 207/209 (99%) | 194 (94%) | 13 (6%) | 0 | 100 | 100 |
| 5 | E | 199/201 (99%) | 187 (94%) | 12 (6%) | 0 | 100 | 100 |
| 6 | F | 175/177 (99%) | 160 (91%) | 15 (9%) | 0 | 100 | 100 |
| 7 | G | 174/176 (99%) | 161 (92%) | 11 (6%) | 2 (1%) | 16 | 56 |
| 8 | H | 147/149 (99%) | 138 (94%) | 9 (6%) | 0 | 100 | 100 |
| 9 | I | 139/141 (99%) | 121 (87%) | 18 (13%) | 0 | 100 | 100 |
| 10 | J | 140/142 (99%) | 137 (98%) | 3 (2%) | 0 | 100 | 100 |
| 11 | K | 120/122 (98%) | 108 (90%) | 12 (10%) | 0 | 100 | 100 |
| 12 | L | 141/143 (99%) | 124 (88%) | 15 (11%) | 2 (1%) | 12 | 51 |
| 13 | M | 134/136 (98%) | 124 (92%) | 9 (7%) | 1 (1%) | 24 | 64 |
| 14 | N | 118/120 (98%) | 109 (92%) | 9 (8%) | 0 | 100 | 100 |
| 15 | O | 114/116 (98%) | 109 (96%) | 5 (4%) | 0 | 100 | 100 |
| 16 | P | 112/114 (98%) | 108 (96%) | 4 (4%) | 0 | 100 | 100 |
| 17 | Q | 115/117 (98%) | 113 (98%) | 2 (2%) | 0 | 100 | 100 |
| 18 | R | 101/103 (98%) | 93 (92%) | 7 (7%) | 1 (1%) | 17 | 57 |
| 19 | S | 108/110 (98%) | 100 (93%) | 7 (6%) | 1 (1%) | 19 | 59 |
| 20 | T | 91/93 (98%) | 81 (89%) | 10 (11%) | 0 | 100 | 100 |
| 21 | U | 100/102 (98%) | 88 (88%) | 11 (11%) | 1 (1%) | 17 | 57 |
| 22 | V | 92/94 (98%) | 90 (98%) | 2 (2%) | 0 | 100 | 100 |
| 23 | W | 73/75 (97%) | 70 (96%) | 3 (4%) | 0 | 100 | 100 |
| 24 | X | 75/77 (97%) | 73 (97%) | 2 (3%) | 0 | 100 | 100 |
| 25 | Y | 61/63 (97%) | 59 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | Z | 56/58 (97%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 27 | 0 | 54/56 (96%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 28 | 1 | 48/50 (96%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 29 | 2 | 44/46 (96%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 30 | 3 | 62/64 (97%) | 55 (89%) | 5 (8%) | 2 (3%) | 4 | 36 |
| 31 | 4 | 36/38 (95%) | 32 (89%) | 4 (11%) | 0 | 100 | 100 |
| 32 | 5 | 129/131 (98%) | 104 (81%) | 25 (19%) | 0 | 100 | 100 |
| 35 | b | 216/218 (99%) | 195 (90%) | 20 (9%) | 1 (0%) | 31 | 71 |
| 36 | c | 204/206 (99%) | 199 (98%) | 5 (2%) | 0 | 100 | 100 |
| 37 | d | 203/205 (99%) | 181 (89%) | 22 (11%) | 0 | 100 | 100 |
| 38 | e | 155/157 (99%) | 138 (89%) | 15 (10%) | 2 (1%) | 13 | 53 |
| 39 | f | 98/100 (98%) | 81 (83%) | 15 (15%) | 2 (2%) | 8 | 45 |
| 40 | g | 149/151 (99%) | 136 (91%) | 13 (9%) | 0 | 100 | 100 |
| 41 | h | 127/129 (98%) | 122 (96%) | 5 (4%) | 0 | 100 | 100 |
| 42 | i | 125/127 (98%) | 108 (86%) | 16 (13%) | 1 (1%) | 21 | 62 |
| 43 | j | 96/98 (98%) | 81 (84%) | 15 (16%) | 0 | 100 | 100 |
| 44 | k | 114/116 (98%) | 99 (87%) | 15 (13%) | 0 | 100 | 100 |
| 45 | l | 121/123 (98%) | 99 (82%) | 21 (17%) | 1 (1%) | 21 | 62 |
| 46 | m | 112/114 (98%) | 100 (89%) | 12 (11%) | 0 | 100 | 100 |
| 47 | n | 99/101 (98%) | 91 (92%) | 8 (8%) | 0 | 100 | 100 |
| 48 | o | 86/88 (98%) | 76 (88%) | 10 (12%) | 0 | 100 | 100 |
| 49 | p | 80/82 (98%) | 71 (89%) | 9 (11%) | 0 | 100 | 100 |
| 50 | q | 78/80 (98%) | 67 (86%) | 10 (13%) | 1 (1%) | 13 | 53 |
| 51 | r | 63/65 (97%) | 58 (92%) | 5 (8%) | 0 | 100 | 100 |
| 52 | s | 77/79 (98%) | 75 (97%) | 2 (3%) | 0 | 100 | 100 |
| 53 | t | 83/85 (98%) | 78 (94%) | 5 (6%) | 0 | 100 | 100 |
| 54 | u | 63/65 (97%) | 49 (78%) | 13 (21%) | 1 (2%) | 11 | 49 |
| 55 | v | 244/248 (98%) | 221 (91%) | 16 (7%) | 7 (3%) | 5 | 38 |
| 56 | w | 494/529 (93%) | 435 (88%) | 55 (11%) | 4 (1%) | 21 | 62 |
| 58 | z | 12/14 (86%) | 11 (92%) | 1 (8%) | 0 | 100 | 100 |
| All | All | 6533/6674 (98%) | 5966 (91%) | 537 (8%) | 30 (0%) | 35 | 71 |

5 of 30 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 46 | ASP |
| 13 | M | 58 | LYS |
| 30 | 3 | 31 | ILE |
| 50 | q | 69 | THR |
| 55 | v | 143 | ARG |

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 | C | 216/216 (100%) | 214 (99%) | 2 (1%) | 81 | 90 |
| 4 | D | 164/164 (100%) | 163 (99%) | 1 (1%) | 87 | 94 |
| 5 | E | 165/165 (100%) | 164 (99%) | 1 (1%) | 87 | 94 |
| 6 | F | 148/148 (100%) | 148 (100%) | 0 | 100 | 100 |
| 7 | G | 137/137 (100%) | 137 (100%) | 0 | 100 | 100 |
| 8 | H | 114/114 (100%) | 114 (100%) | 0 | 100 | 100 |
| 9 | I | 109/109 (100%) | 109 (100%) | 0 | 100 | 100 |
| 10 | J | 116/116 (100%) | 116 (100%) | 0 | 100 | 100 |
| 11 | K | 103/103 (100%) | 103 (100%) | 0 | 100 | 100 |
| 12 | L | 102/102 (100%) | 102 (100%) | 0 | 100 | 100 |
| 13 | M | 109/109 (100%) | 109 (100%) | 0 | 100 | 100 |
| 14 | N | 100/100 (100%) | 99 (99%) | 1 (1%) | 78 | 89 |
| 15 | O | 86/86 (100%) | 86 (100%) | 0 | 100 | 100 |
| 16 | P | 99/99 (100%) | 99 (100%) | 0 | 100 | 100 |
| 17 | Q | 89/89 (100%) | 89 (100%) | 0 | 100 | 100 |
| 18 | R | 84/84 (100%) | 83 (99%) | 1 (1%) | 74 | 87 |
| 19 | S | 93/93 (100%) | 92 (99%) | 1 (1%) | 76 | 88 |
| 20 | T | 80/80 (100%) | 80 (100%) | 0 | 100 | 100 |
| 21 | U | 83/83 (100%) | 83 (100%) | 0 | 100 | 100 |
| 22 | V | 78/78 (100%) | 78 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 23 | W | 57/57 (100%) | 56 (98%) | 1 (2%) | 62 | 83 |
| 24 | X | 67/67 (100%) | 66 (98%) | 1 (2%) | 67 | 85 |
| 25 | Y | 55/55 (100%) | 55 (100%) | 0 | 100 | 100 |
| 26 | Z | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |
| 27 | 0 | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 28 | 1 | 45/45 (100%) | 45 (100%) | 0 | 100 | 100 |
| 29 | 2 | 38/38 (100%) | 38 (100%) | 0 | 100 | 100 |
| 30 | 3 | 51/51 (100%) | 51 (100%) | 0 | 100 | 100 |
| 31 | 4 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 32 | 5 | 100/100 (100%) | 100 (100%) | 0 | 100 | 100 |
| 35 | b | 180/180 (100%) | 177 (98%) | 3 (2%) | 63 | 83 |
| 36 | c | 170/170 (100%) | 170 (100%) | 0 | 100 | 100 |
| 37 | d | 172/172 (100%) | 170 (99%) | 2 (1%) | 74 | 87 |
| 38 | e | 114/119 (96%) | 113 (99%) | 1 (1%) | 81 | 90 |
| 39 | f | 87/87 (100%) | 87 (100%) | 0 | 100 | 100 |
| 40 | g | 124/124 (100%) | 124 (100%) | 0 | 100 | 100 |
| 41 | h | 104/104 (100%) | 104 (100%) | 0 | 100 | 100 |
| 42 | i | 105/105 (100%) | 104 (99%) | 1 (1%) | 78 | 89 |
| 43 | j | 86/86 (100%) | 86 (100%) | 0 | 100 | 100 |
| 44 | k | 89/89 (100%) | 88 (99%) | 1 (1%) | 76 | 88 |
| 45 | l | 103/103 (100%) | 103 (100%) | 0 | 100 | 100 |
| 46 | m | 92/92 (100%) | 91 (99%) | 1 (1%) | 76 | 88 |
| 47 | n | 79/83 (95%) | 79 (100%) | 0 | 100 | 100 |
| 48 | o | 76/76 (100%) | 76 (100%) | 0 | 100 | 100 |
| 49 | p | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 50 | q | 74/74 (100%) | 73 (99%) | 1 (1%) | 69 | 86 |
| 51 | r | 48/56 (86%) | 48 (100%) | 0 | 100 | 100 |
| 52 | s | 70/70 (100%) | 70 (100%) | 0 | 100 | 100 |
| 53 | t | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 54 | u | 44/55 (80%) | 44 (100%) | 0 | 100 | 100 |
| 55 | v | 201/201 (100%) | 198 (98%) | 3 (2%) | 67 | 85 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 56 | w | 427/453 (94%) | 423 (99%) | 4 (1%) | 81 | 90 |
| 58 | z | 14/14 (100%) | 14 (100%) | 0 | 100 | 100 |
| All | All | 5406/5460 (99%) | 5380 (100%) | 26 (0%) | 90 | 95 |

5 of 26 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | b | 202 | ASN |
| 38 | e | 69 | ASN |
| 56 | w | 124 | ARG |
| 37 | d | 80 | ARG |
| 37 | d | 177 | MET |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | b | 23 | ASN |
| 38 | e | 134 | ASN |
| 56 | w | 409 | GLN |
| 35 | b | 35 | ASN |
| 38 | e | 69 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 2893/2903 (99%) | 540 (18%) | 34 (1%) |
| 2 | B | 119/120 (99%) | 14 (11%) | 2 (1%) |
| 33 | 7 | 6/7 (85%) | 5 (83%) | 1 (16%) |
| 34 | a | 1538/1539 (99%) | 223 (14%) | 0 |
| 57 | x | 76/77 (98%) | 35 (46%) | 0 |
| All | All | 4632/4646 (99%) | 817 (17%) | 37 (0%) |

5 of 817 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 10 | A |
| 1 | A | 12 | U |
| 1 | A | 27 | G |
| 1 | A | 34 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 35 | G |

5 of 37 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1070 | A |
| 1 | A | 1378 | A |
| 2 | B | 66 | A |
| 1 | A | 1130 | U |
| 1 | A | 1182 | G |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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 | $\# Z > 2$ |
| 59 | GCP | w | 601 | 56 | 25,34,34 | 2.48 | 8 (32%) | 31,54,54 | 1.75 | 4 (12%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 59 | GCP | w | 601 | 56 | - | 0/18/38/38 | 0/3/3/3 |

The worst 5 of 8 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 59 | w | 601 | GCP | C4-N9 | -7.34 | 1.38 | 1.47 |
| 59 | w | 601 | GCP | C5-C6 | -4.58 | 1.44 | 1.52 |
| 59 | w | 601 | GCP | C8-N9 | -3.19 | 1.37 | 1.46 |
| 59 | w | 601 | GCP | C5-C4 | -2.29 | 1.38 | 1.52 |
| 59 | w | 601 | GCP | PB-O2B | -2.15 | 1.51 | 1.56 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 59 | w | 601 | GCP | C5-C6-N1 | -5.28 | 111.97 | 118.27 |
| 59 | w | 601 | GCP | PA-O3A-PB | -2.38 | 124.69 | 132.42 |
| 59 | w | 601 | GCP | O6-C6-C5 | 3.69 | 127.44 | 119.82 |
| 59 | w | 601 | GCP | C4-C5-N7 | 6.08 | 110.52 | 102.46 |

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 |
|-----|-------|------------------|
| 1 | A | 5 |
| 55 | v | 2 |

The worst 5 of 7 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 891:G | O3' | 892:A | P | 9.09 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 884:U | O3' | 885:C | P | 7.63 |
| 1 | A | 1905:C | O3' | 1906:G | P | 3.75 |
| 1 | A | 2107:G | O3' | 2108:A | P | 3.38 |
| 1 | A | 2094:A | O3' | 2095:A | P | 3.36 |